

# Stochastic approximations for financial risk computations

Florian Bourgey

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# Stochastic approximations for financial risk computations

Thèse de doctorat de l'Institut Polytechnique de Paris préparée à l'École Polytechnique

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Thèse présentée et soutenue à distance, le Vendredi 23 Octobre 2020, par

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Thèse de doctorat









THÈSE présentée pour obtenir LE GRADE DE DOCTEUR EN SCIENCES DE L'ÉCOLE POLYTECHNIQUE Spécialité : Mathématiques par

Florian Bourgey

Stochastic approximations for financial risk computations

Soutenue le 23 octobre 2020 devant un jury composé de :

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"Nel mezzo del cammin di nostra vita mi ritrovai per una selva oscura, ché la diritta via era smarrita."

Dante Alighieri. La Divina Commedia. Canto I.

"I must be gone and live, or stay and die." William Shakespeare. *Romeo and Juliet.* 3.5.11.

"Un voyage se passe de motifs. Il ne tarde pas à prouver qu'il se suffit à lui-même. On croit qu'on va faire un voyage, mais bientôt c'est le voyage qui vous fait, ou vous défait."

Nicolas Bouvier. L'Usage du monde.

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#### Préambule

Dans cette thèse, nous examinons plusieurs méthodes d'approximations stochastiques à la fois pour le calcul de mesures de risques financiers et pour le pricing de produits dérivés. Comme les formules explicites sont rarement disponibles pour de telles quantités, le besoin d'approximations analytiques rapides, efficaces et fiables est d'une importance capitale pour les institutions financières. Nous visons ainsi à donner un large aperçu de ces méthodes d'approximation et nous nous concentrons sur trois approches distinctes.

Dans la première partie, nous étudions plusieurs méthodes d'approximation Monte Carlo multi-niveaux et les appliquons à deux problèmes pratiques : l'estimation de quantités impliquant des espérances imbriquées (comme la marge initiale) ainsi que la discrétisation des intégrales apparaissant dans les modèles rough pour la variance forward pour le pricing d'options sur le VIX. Dans les deux cas, nous analysons les propriétés d'optimalité asymptotique des estimateurs multi-niveaux correspondants et démontrons numériquement leur supériorité par rapport à une méthode de Monte Carlo classique.

Dans la deuxième partie, motivés par les nombreux exemples issus de la modélisation en risque de crédit, nous proposons un cadre général de méta-modélisation pour de grandes sommes de variables aléatoires de Bernoulli pondérées, qui sont conditionnellement indépendantes par rapport à un facteur commun X. Notre approche générique est basée sur la décomposition en polynômes du chaos du facteur commun et sur une approximation gaussienne. Les estimations d'erreur  $L_2$  sont données lorsque le facteur X est associé à des polynômes orthogonaux classiques.

Enfin, dans la dernière partie de cette thèse, nous nous intéressons aux asymptotiques en temps court de la volatilité implicite américaine et les prix d'options américaines dans les modèles à volatilité locale. Nous proposons également une approximation en loi de l'indice VIX dans des modèles rough pour la variance forward, exprimée en termes de proxys log-normaux et dérivons des résultats d'expansion pour les options sur le VIX dont les coefficients sont explicites.

#### Preamble

The present work investigates several stochastic approximation methods for both the computation of financial risk measures and the pricing of derivatives. As closed-form expressions are scarcely available for such quantity, the need for fast, efficient, and reliable analytic approximation formulas is of primal importance to financial institutions.

This thesis aims at giving a broad overview of such approximation methods and focuses on three distinct approaches. In the first part, we study some Multilevel Monte Carlo approximation methods – recently formalized by Giles [74] – and apply them for two practical problems: the estimation of quantities involving nested expectations (such as the initial margin) along with the discretization of integrals arising in rough forward variance models for the pricing of VIX derivatives. For both cases, we analyze the properties of the corresponding multilevel estimators, provide results of asymptotical optimality and numerically demonstrate the superiority of multilevel methods compared to a standard Monte Carlo.

In the second part, motivated by the numerous examples arising in credit risk modeling, we propose a general meta-model framework for large sums of weighted Bernoulli random variables which are conditional independent on a common factor X. Our generic approach in based on a Polynomial Chaos Expansion on the common factor together with some Gaussian approximation.  $L_2$  error estimates are given when the factor X is associated with classical orthogonal polynomials.

Finally, in the last part of this dissertation, we deal with small-time asymptotics and provide asymptotic expansions for both American implied volatility and American option prices in local volatility models. We also investigate a weak approximations for the VIX index in rough forward variance models expressed in terms of lognormal proxys, and derive expansion results for VIX derivatives.

#### List of publications

Here is a list of articles (accepted or submitted) and working papers that were written during this thesis:

- [35] F. Bourgey, S. De Marco, E. Gobet, and A. Zhou. Multilevel Monte Carlo methods and lower-upper bounds in initial margin computations. *Monte Carlo Methods and Applications*, 26(2):131–161, 2020.
- [34] F. Bourgey, E. Gobet, and C. Rey. Meta-model of a large credit risk portfolio in the Gaussian copula model. Under minor revision for the SIAM Journal of Financial Mathematics.
- F. Bourgey, E. Gobet, and C. Rey. Polynomial chaos expansion and meta-model of large sums of dependent random variables. *Working paper*.
- F. Bourgey, S. De Marco. Small-time asymptotics for American options in local volatility models. *Working paper*.
- F. Bourgey, S. De Marco. Multilevel Monte Carlo for rough forward variance models. Working paper.
- F. Bourgey, S. De Marco, and E. Gobet. Weak approximations and VIX option price expansions in rough forward variances models. *Working paper*.

#### **Keywords**

Multilevel Monte Carlo; Initial Margin; Risk management; Credit risk measures; Lower–upper bounds; Asymptotic methods; Meta-modeling; Polynomial Chaos Expansion; Orthogonal polynomials; American options; Implied volatility; Heat kernel expansion; VIX; Weak approximations; Rough volatility; Forward Variance;

#### Notations

#### **General Notation**

- $\mathbb{N} = \{0, 1, \dots, \}$  and  $\mathbb{N}^* = \mathbb{N} \setminus \{0\}$  for the nonnegative and positive integers.
- $\delta_{nm} = 1$  if n = m and 0 otherwise for all  $n, m \in \mathbb{N}$  (Kronecker delta).
- $X \stackrel{d}{=} Y$  stands for equality in distribution of the random vectors (or processes) X and Y.
- $\xrightarrow{d}$  denotes the convergence in distribution of random vectors.
- $\mathcal{N}(\mu, \Sigma)$  denotes the distribution of a Gaussian vector with mean  $\mu$  and covariance matrix  $\Sigma$ .
- The acronym c.d.f. stands for *cumulative distribution function*.
- The acronym i.i.d. stands for independent identically distributed.
- The acronym p.d.f. stands for probability distribution function.
- The acronym w.r.t. stands for with respect to.
- The acronym resp. stands for *respectively*.

#### **Special functions**

• Let  $n \in \mathbb{N}^*$ ,  $\mu \in \mathbb{R}^n$ ,  $\Sigma \in \mathbb{R}^{n \times n}$  positive definite. The c.d.f. of  $X \stackrel{d}{=} \mathcal{N}(\mu, \Sigma)$  is given for all  $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$ ,

$$\Phi_{\Sigma}(x) := \mathbb{P}(X \le x) = \int_{-\infty}^{x_1} \dots \int_{-\infty}^{x_n} \frac{e^{-\frac{1}{2}(t-\mu)^{\top}\Sigma^{-1}(t-\mu)}}{(2\pi)^{\frac{n}{2}} (\det(\Sigma))^{\frac{1}{2}}} dt_1 \dots dt_n$$

In the case n = 1 and  $\Sigma = 1$ , we simply write  $\Phi$  for  $\Phi_{\Sigma}$  i.e.

$$\Phi(x) = \int_{-\infty}^{x} \frac{e^{-\frac{t^2}{2}}}{\sqrt{2\pi}} \mathrm{d}t, \quad x \in \mathbb{R}.$$

• Upper incomplete gamma and lower incomplete beta function:

$$\Gamma_a(z) = \int_z^\infty t^{a-1} e^{-t} dt, \quad z \ge 0, \ a > 0,$$
  
$$B_{a,b}(x) = \int_0^x t^{a-1} (1-t)^{b-1} dt, \quad x \in [0,1], \ a, b > 0$$

When z = 0 (resp. x = 1) we drop the dependence in z (resp. x) and simply write  $\Gamma_a = \Gamma_a(0)$  (resp.  $B_{a,b} = B_{a,b}(1)$ ) for the usual Gamma (resp. Beta) function.

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### INTRODUCTION

#### 0.1 Multilevel Monte Carlo approximation methods

#### 0.1.1 Motivation

The popularity of Monte Carlo methods, especially in the financial community, is indisputable. Though known to converge slowly, it undoubtedly remains among the most general, reliable, and powerful approach (especially in high-dimensional settings) when dealing with the estimation of expectations (see e.g. Hammersley [99] for a nice introduction to the study of Monte Carlo methods, Asmussen and Glynn [12], Kalos and Whitlock [120] for a broad focus on Monte Carlo algorithms and stochastic simulation). Such methods have become an essential tool in computational finance, notably for the pricing of derivatives security, and in risk management for which practitioners have to compute daily risk indicators using huge samples of data – see Glasserman [81] for a review of Monte Carlo methods in financial engineering or more recently Pagès [147] for a broad overview of numerical probability and Monte Carlo methods with applications to mathematical finance.

In most cases, we are interested in numerically approximating a quantity

$$p = \mathbb{E}\left[P\right],$$

for a very general integrable real random variable  $P : (\Omega, \mathcal{A}, \mathbb{P}) \to \mathbb{R}^d$ . For the sake of clarity, we focus here only on the one-dimensional case i.e. d = 1, though the extension to d > 1 is straightforward. In most applications, simulating P cannot be achieved at a reasonable computational cost or is simply unfeasible. However, we may assume that it can be approximated (in a sense to be made precise later) by a family of random variables  $(P_h)_{h>0}$  where h refers to some small approximation (or bias) parameter. We further suppose that the random variable  $P_h$  can be simulated with a computational complexity of  $\operatorname{Cost}(P_h)$ . A natural estimator for the quantity  $\mathbb{E}[P_h] \approx \mathbb{E}[P]$  is the following crude Monte Carlo estimator

$$\widehat{P}_{M,h} = \frac{1}{M} \sum_{m=1}^{M} P_h^{(m)}, \qquad (0.1.1)$$

where M is the number of Monte Carlo samples and  $\left(P_h^{(m)}\right)_{1 \le m \le M}$  are independent copies of  $P_h$ . Assuming that  $P_h$  is integrable for all h > 0, and that the weak error converges to 0, that is

$$\mathbb{E}\left[P_{h}\right] \xrightarrow[h \to 0]{} \mathbb{E}\left[P\right], \qquad (0.1.2)$$

the Strong Law of Large Numbers ensures that almost surely, as  $h \to 0$  and  $M \to +\infty$ ,

$$\widehat{P}_{M,h} \to p = \mathbb{E}[P].$$

The (weak) rate of convergence in the Strong Law of Large Numbers is ruled by the Central Limit Theorem, which states that if  $P_h$  is square-integrable, then

$$\sqrt{M}\left(\widehat{P}_{M,h} - \mathbb{E}\left[P_{h}\right]\right) \xrightarrow{d} \mathcal{N}\left(0, \sigma_{h}^{2}\right),$$

where  $\sigma_h^2 = \text{Var}(P_h) = \mathbb{E}[P_h^2] - \mathbb{E}[P_h]^2$  is the variance of  $P_h$ . In practice, we have to fix the discretization parameter h and the number of Monte Carlo samples M which produces two types of errors: one due to the approximation of the random variable P with  $P_h$  (discretization error or bias), and one due to the Monte Carlo simulation (statistical error). More precisely, suppose we are quantifying the accuracy of our approximation method by use of the mean-square error MSE, or equivalently the root-mean-square RMSE, both defined as

$$RMSE = MSE^{\frac{1}{2}} = \mathbb{E}\left[\left(\mathbb{E}\left[P\right] - \mathbb{E}\left[\widehat{P}_{M,h}\right]\right)^{2}\right]^{\frac{1}{2}}.$$
(0.1.3)

Then, from the (well-known) bias-variance decomposition, we have

$$MSE = \left(\mathbb{E}\left[P\right] - \mathbb{E}\left[\widehat{P}_{M,h}\right]\right)^{2} + Var\left(\widehat{P}_{M,h}\right)$$
$$= \underbrace{\left(\mathbb{E}\left[P\right] - \mathbb{E}\left[P_{h}\right]\right)^{2}}_{\text{discretization error or bias}} + \underbrace{\frac{Var\left(P_{h}\right)}{M}}_{\text{statistical error}}, \qquad (0.1.4)$$

where the last equality results from the independence of the  $\left(P_h^{(m)}\right)_{1 \le m \le M}$ . A natural question arising is then:

**Question.** For a given accuracy  $\varepsilon > 0$ , how do we need to set the parameters M, h so that we achieve the constraint RMSE  $\leq \varepsilon$ ?

From (0.1.4), we observe that if the bias (or weak error) is of order 1, i.e.  $|\mathbb{E}[P] - \mathbb{E}[P_h]| = \mathcal{O}(h)$ , and  $\operatorname{Var}(P_h) = \mathcal{O}(1)$ , then

$$RMSE = \mathcal{O}(h) + \mathcal{O}(M^{-\frac{1}{2}}).$$

Consequently, for the RMSE to be proportional to  $\varepsilon$ , we then have to choose  $M = \mathcal{O}(\varepsilon^{-2})$  and  $h = \mathcal{O}(\varepsilon)$  which leads to a total computational cost of

$$\operatorname{Cost}(\widehat{P}_{M,h}) = \operatorname{Cost}(P_h) \times M = \operatorname{Cost}(P_h) \times \mathcal{O}\left(\varepsilon^{-2}\right), \qquad (0.1.5)$$

for the crude Monte Carlo estimator (0.1.1). Observe that if P can be simulated exactly (i.e. no bias) then the mean-square error and the total computational complexity reduce to

$$MSE = \frac{Var(P)}{M}, \quad Cost(\widehat{P}_M) = Cost(P) \times M = Cost(P) \times \mathcal{O}(\varepsilon^{-2}).$$

This is the optimal complexity available for standard unbiased Monte Carlo estimators. As discussed in more detail below, the Multilevel Monte Carlo algorithm attains (under appropriate conditions) such an optimal order.

#### 0.1.2 The multilevel approach

Heinrich was the first to formalize the multilevel idea as a variance reduction technique (Heinrich and Sindambiwe [106], Heinrich [102, 103, 104, 105]). In his seminal works, Heinrich developed Multilevel Monte Carlo methods for parametric integration, the evaluation of functional arising from the solution of integral equations, and weakly singular integral operators. For the former,

the author was interested in estimating the value of  $\mathbb{E}[f(x,\lambda)]$  where X is some finite-dimensional random variable and  $\lambda$  a parameter. If  $\lambda$  takes values in [0,1], then having estimated  $\mathbb{E}[f(X,0)]$ and  $\mathbb{E}[f(X,1)]$ , one can use  $\frac{1}{2}(f(X,0) + f(X,1))$  as a control variate for the estimation of  $\mathbb{E}[f(X,\frac{1}{2})]$ . The intuition being that the variance of  $f(X,\frac{1}{2}) - \frac{1}{2}(f(X,0) + f(X,1))$  will most likely be less than that of  $f(X,\frac{1}{2})$ . Such a procedure can then be recursively applied for the estimation of all values for  $\lambda$ , provided  $f(X, \cdot)$  is sufficiently smooth, and will result in large savings in terms of computational complexity.

In [74], Giles generalized Heinrich's ideas and investigated infinite-dimensional random variables such as Brownian paths. Yet, as explained below, the reduction variance technique is very similar: coarse paths (large h) are used as control variates for the estimation of more refined paths (smaller h).

This multilevel approach is also an extension of the two-level method of Kebaier [123], also known as the statistical Romberg method. This in turn was inspired by yet another work on multi-grid ideas for iterative solutions of partial differential equation approximations for statistical physics applications (see Brandt, Galun, and Ron [37], Brandt and Ilyin [36]).

**Multilevel Monte Carlo theorem.** We now come back to our general problem i.e. estimating  $p = \mathbb{E}[P]$  for which the random variable P can only be approximated with  $P_h$  at some order h > 0. Note that the smaller h, the better the approximation but the higher the computational cost.

Let us fix  $L \in \mathbb{N}^*$  (number of levels) and consider a sequence  $\mathbf{h} = (h_0, \ldots, h_L)$  of decreasing  $h_L < \cdots < h_0$  approximation parameters with increasing accuracy but increasing cost. With a slight abuse of notation, we now write

$$P_l = P_{h_l}, \quad \text{for all } l = 1, \dots, L,$$

and we wish to estimate the fine approximation  $\mathbb{E}[P_{h_L}]$ . The level l = 0 refers to the coarsest approximate while the level l = L is the finest. To fix ideas, suppose we are dealing with the simulation of a solution from a given stochastic differential equation (in short SDE) on a time interval [0, T] with T > 0. The parameter  $h_l$  represents here the time-step for the SDE and one possible choice is uniform time-steps, namely  $h_l = 2^{-l}T$  for all  $l = 0, \ldots, L$ . The higher the level l, the lower the time-step.

From the telescopic sum

$$\mathbb{E}\left[P_L\right] = \mathbb{E}\left[P_0\right] + \sum_{l=1}^{L} \mathbb{E}\left[P_l - P_{l-1}\right], \qquad (0.1.6)$$

the multilevel idea is to independently estimate the expectation for the coarsest level  $\mathbb{E}[P_0]$  with a high number of Monte Carlo samples  $M_0$  and the expectation of the difference  $\mathbb{E}[P_l - P_{l-1}]$ with a decreasing number of Monte Carlo samples  $M_l$  for all levels  $l = 0, \ldots, L$ , that is consider the estimator

$$\widehat{P}_{l,M_l} = \frac{1}{M_l} \sum_{m=1}^{M_l} \left( P_l^{(m)} - P_{l-1}^{(m)} \right), \quad P_{-1} = 0.$$

Introducing the decreasing sequence  $M = (M_0, \ldots, M_L)$ , the multilevel estimator is then defined as:

$$\widehat{P}_{\boldsymbol{M},\boldsymbol{h}}^{\mathrm{ML}} = \sum_{l=1}^{L} \widehat{P}_{l,M_{l}} = \frac{1}{M_{0}} \sum_{m=1}^{M_{0}} P_{0}^{(0,m)} + \sum_{l=1}^{L} \frac{1}{M_{l}} \sum_{m=1}^{M_{l}} \left( P_{l}^{(l,m)} - P_{l-1}^{(l,m)} \right), \qquad (0.1.7)$$

where

1. for all l,  $\left(P_l^{(l,m)}\right)_{1 \le m \le M_l}$  and  $\left(P_{l-1}^{(l,m)}\right)_{1 \le m \le M_l}$  are i.i.d. samples, distributed according to  $P_l$  and  $P_{l-1}$  respectively.

- 2. The levels are independent.
- 3. Inside each level l,  $P_l^{(l,m)}$  and  $P_{l-1}^{(l,m)}$  are constructed with the same common random numbers. The intuition is that, due to the strong convergence, the difference  $P_l^{(l,m)} P_{l-1}^{(l,m)}$  becomes smaller and smaller, and thus its variance, as the number of levels l increases.

Recall that  $P_{-1} = 0$  and denote for all  $l = 1, \ldots, L$ ,

$$C_{l} = \text{Cost}(P_{l} - P_{l-1}), \quad V_{l} = \text{Var}(P_{l} - P_{l-1}),$$

the cost and variance of one  $P_l - P_{l-1}$ . The total computational complexity of the multilevel estimator (0.1.7) is  $\sum_{l=0}^{L} M_l C_l$  and from the independence between levels, it holds:

$$\mathbb{E}\left[\widehat{P}_{\boldsymbol{M},\boldsymbol{h}}^{\mathrm{ML}}\right] = \mathbb{E}\left[P_{L}\right], \quad \mathrm{Var}\left(\widehat{P}_{\boldsymbol{M},\boldsymbol{h}}^{\mathrm{ML}}\right) = \sum_{l=0}^{L} \frac{V_{l}}{M_{l}}.$$
(0.1.8)

We now recall Giles' multilevel theorem [75, Theorem 1].

**Theorem 0.1.1.** Let P denotes a random variable, and let  $P_l$  denotes the corresponding level lnumerical approximation. If there exist independent estimators  $\widehat{P}_{l,M_l}$  based on  $M_l$  Monte Carlo samples, each with expected cost  $C_l$  and variance  $V_l$ , and positive constants  $\alpha, \beta, \gamma, c_1, c_2, c_3, c_4$ such that  $\alpha \geq \frac{1}{2} \min(\beta, \gamma)$  and

1.  $|\mathbb{E}[P_l - P]| \leq c_1 2^{-\alpha l},$ 2.  $\mathbb{E}\left[\widehat{P}_{l,M_l}\right] = \mathbb{E}[P_l - P_{l-1}], \quad P_{-1} = 0,$ 3.  $V_l \leq c_2 2^{-\beta l},$ 4.  $C_l \leq c_2 2^{\gamma l}$ 

4. 
$$C_l \leq c_3 2^{\mu}$$
,

then there exists a positive constant  $c_4$  such that for any  $\varepsilon < e^{-1}$  there are values L and  $M_l$  for which the multilevel estimator

$$\widehat{P}_{\boldsymbol{M},\boldsymbol{h}}^{\mathrm{ML}} = \sum_{l=0}^{L} \widehat{P}_{l,M_l},$$

has a mean-square error with bound

$$MSE = \mathbb{E}\left[\left(\widehat{P}_{\boldsymbol{M},\boldsymbol{h}}^{ML} - \mathbb{E}\left[P\right]\right)^{2}\right] < \varepsilon^{2},$$

with a computational complexity C with bound

$$\mathbb{E}[C] \leq \begin{cases} c_4 \varepsilon^{-2}, & \beta > \gamma, \\ c_4 \varepsilon^{-2} (\ln \varepsilon)^2, & \beta = \gamma, \\ c_4 \varepsilon^{-2 - \frac{\gamma - \beta}{\alpha}}, & \beta < \gamma. \end{cases}$$

Let us also mention that when a polynomial expansion in  $h^{\alpha}$  ( $\alpha > 0$ ) holds for the bias i.e.

$$\mathbb{E}[P_h] = \mathbb{E}[P] + \sum_{k=1}^{R} c_k h^{\alpha k} + o(h^{\alpha R}), \quad R \in \mathbb{N}^*,$$

a weighted version, which both improve and generalize the estimator (0.1.7) (the so-called Multilevel Richardson–Romberg weighted estimator), was introduced by Lemaire and Pagès [134] (see also Giorgi [78], Giorgi, Lemaire, and Pagès [79, 80]).

#### 0.1.3 Multilevel Monte Carlo for nested expectations and lower–upper bounds in nested risk computations.

In Chapter 1, we apply Multilevel Monte Carlo methods to the evaluation of nested expectations, that is quantity of the form

$$p = \mathbb{E}\left[g\left(\mathbb{E}\left[f\left(X,Y\right)|X\right]\right)\right],\tag{0.1.9}$$

where X, Y are two independent random variables with values respectively in  $\mathbb{R}^d$  and  $\mathbb{R}^{d'}$ , and  $f: \mathbb{R}^d \times \mathbb{R}^{d'} \to \mathbb{R}$  and  $g: \mathbb{R} \to \mathbb{R}$  are two measurable functions. By independence, the conditional expectation (0.1.9) rewrites as

$$\mathbb{E}\left[f\left(X,Y\right)|X\right] = E_f\left(X\right),\tag{0.1.10}$$

where for every  $x \in \mathbb{R}^d$ ,  $E_f(x) := \mathbb{E}[f(x, Y)]$ . The random variable  $E_f(X)$  can thus only be approximated, and as  $E_f(\cdot)$  writes as an expectation, a natural unbiased estimator for (0.1.10) is given by

$$\widehat{E}_{f,n}\left(X\right) = \frac{1}{n} \sum_{i=1}^{n} f\left(X, Y_{i}\right), \quad n \in \mathbb{N}^{*},$$

where the  $(Y_i)_{1 \le i \le n}$  are i.i.d. samples of Y independent of X. The regularity of the outer function g drives the bias of the random variable  $g(\hat{E}_{f,n}(X))$ : there exists a trade-off between the smoothness of the function g and that of the probability distribution of the underlying random variables – the less regularity on g, the stronger the requirements on the underlying distributions.

Let us also mention that this is exactly the setting of Section 0.1.1: here the random variable  $P = g(E_f(X))$  can only be approximated by  $P_n = g(\widehat{E}_{f,n}(X))$  for which  $\frac{1}{n}$  plays the role of the approximation parameter h.

Nested expectations of the form (0.1.9) are ubiquitous in computational finance (see e.g. Gordy and Juneja [89]). Possible examples are the pricing of American-type derivatives (Lamberton and Lapeyre [129]), the estimation of a large variety of risk valuations as VaR or CVaR of a portfolio (McNeil, Frey, and Embrechts [140]) or CVA (Abbas-Turki, Crépey, and Diallo [1]) or the assessment of margin costs for centrally cleared portfolios ([17]). Mathematically, most of those computations require either the estimation of an expected exposure of a portfolio for which:

$$p = \mathbb{E}\Big[\Big(\mathbb{E}[f(X_{t_2})|X_{t_1}]\Big)_+\Big],\tag{0.1.11}$$

where  $(X_{t_1}, X_{t_2})$  is some market risk factor at dates  $t_1 < t_2$  and  $g(x) = x_+$ , or the estimation of the tail distribution of a loss process for which:

$$p = \mathbb{P}\left(L(X_{t_1}) \ge a\right) = \mathbb{E}\left[\mathbf{1}_{\mathbb{E}\left[f\left(X_{t_2}\right)|X_{t_1}\right] \ge a}\right],\tag{0.1.12}$$

where  $L(X_{t_1}) = \mathbb{E}[f(X_{t_2})|X_{t_1}]$  denotes the loss of a portfolio conditional on the value of the risk factor  $X_{t_1}$  at time  $t_1$  (see Chapter 3), and  $g(x) = \mathbf{1}_{x \geq a}$  is an indicator function. When dealing with step functions as in (0.1.12), most of the authors (see e.g. Gordy and Juneja [89] or Giorgi, Lemaire, and Pagès [80]) assume rather strong and (in some cases) unverifiable hypothesis on the distribution of the underlying random variables. Most precisely, they require some smoothness assumptions on the p.d.f. of the couple  $(\mathbb{E}[f(X,Y)|X],X)$  and

 $\left(\mathbb{E}[f(X,Y)|X], \frac{1}{n}\sum_{j=1}^{n}f(X,Y_j) - \mathbb{E}[f(X,Y)|X]\right)$ . Motivated by the application of Initial Margin computation for which g is of the form g(x) = |x| or  $g(x) = (x - a)_+$  for some real a, we focus our attention to a continuous and piecewise  $C_b^1$  function for g. Being in a situation of intermediate regularity for the function g – less than  $C^2$ , but more regular than a step function – allows us to bypass the restrictive assumptions stated above on the underlying distribution. We rather suppose that the following mild assumptions hold:

**Assumption 0.1.2.** The function g is continuous, and there exists a finite set of points  $-\infty = d_0 < d_1 < ... < d_\theta < d_{\theta+1} = \infty$  such that on each open interval  $(d_i, d_{i+1}), 0 \le i \le \theta, g$  is of class  $C^1, g'$  is bounded and Hölder continuous for some exponent  $\eta \in (0, 1]$ .

We will also need to be able to control the probability that the random variable  $E_f(X) = \mathbb{E}[f(X, Y) | X]$  takes values in a neighborhood of the singularities of g (Assumption 0.1.4), and requires finiteness of some moment of order p > 2 for the random variable f(X, Y) (Assumption 0.1.3), a condition which is met in most of the examples of practical interest.

Assumption 0.1.3. There exists p > 2 such that  $\mathbb{E}\left[|f(X,Y)|^p\right] < \infty$ .

Assumption 0.1.4 (Small ball estimate around the singularities). There exist some positive constants  $\nu$ ,  $K_{\nu}$  and  $z_0$  such that

$$\mathbb{P}\left(\operatorname{dist}(E_f(X), D) \le z\right) \le K_{\nu} z^{\nu}, \qquad \forall z < z_0, \qquad (0.1.13)$$

where  $\operatorname{dist}(y, D) := \min_{1 \le i \le \theta} |y - d_i|.$ 

Approximating both the inner and outer conditional expectations of (0.1.9) with independent Monte Carlo samples leads to the following plain Nested Monte Carlo (NMC) estimator

$$\widehat{P}_{M,N} = \frac{1}{M} \sum_{m=1}^{M} g\left(\frac{1}{N} \sum_{j=1}^{N} f\left(X_m, Y_j^m\right)\right), \qquad (0.1.14)$$

where  $M, N \in \mathbb{N}^*$ , and  $(X_m)_{m \in \mathbb{N}^*}$ ,  $(Y_j^m)_{j,m \in \mathbb{N}^*}$  are independent i.i.d. families having the same distribution as X and Y respectively, and whose complexity is stated in the following proposition.

**Proposition 0.1.5** (Complexity of the Nested Monte Carlo estimator (0.1.14)). Let Assumptions 0.1.2, 0.1.3 and 0.1.4 hold true, and consider an error tolerance  $\varepsilon > 0$ . As  $\varepsilon \to 0$ , the bound MSE =  $\mathcal{O}(\varepsilon^2)$  for the estimator (0.1.14), is achieved with a computational complexity  $\mathcal{O}\left(\varepsilon^{-2\left(1+\frac{1}{1+\frac{(p-1)\nu}{p+\nu}\wedge\eta}\right)}\right)$  with the choice  $M \sim \varepsilon^{-2}$  and  $N \sim \varepsilon^{-\frac{2}{1+\frac{(p-1)\nu}{p+\nu}\wedge\eta}}$ .

Note that in the smooth case where we can take  $\eta = 1$ ,  $\nu = \infty$  and assuming  $p \ge 2$ , the ratio for N simplifies as  $\frac{(p-1)\nu}{p+\nu} \land \eta = (p-1) \land \eta = 1$ , and we retrieve the standard computational complexity  $\mathcal{O}(\varepsilon^{-3})$  for nested estimators involving smooth functions. This time-consuming estimator can be improved using a specific multilevel Monte Carlo estimator which is able to reach an optimal complexity of order  $\mathcal{O}(\varepsilon^{-2})$ .

An antithetic Multilevel estimator for nested expectations. Following (0.1.7), we construct an antithetic multilevel Monte Carlo estimator combining estimators of the form of  $\widehat{P}_{M,N}$ . More precisely, let us consider two independent families of i.i.d. random variables  $(X_m^l)_{l,m\in\mathbb{N}^*}$ and  $(Y_j^{l,m})_{j,l,m\in\mathbb{N}^*}$ , distributed according to X and Y respectively. Let  $L \in \mathbb{N}^*$  denotes the number of levels,  $\mathbf{M} = (M_0, ..., M_L) \in (\mathbb{N}^*)^{L+1}$ , respectively  $\mathbf{n} = (n_0, ..., n_L) \in (\mathbb{N}^*)^{L+1}$ , be multi-indexes representing the number of samples used to approximate the outer expectation, respectively the inner conditional expectation in (0.1.9) at the different levels. Finally, we set the number of samples for the inner conditional expectation to

$$n_l = n_0 2^l, \qquad 0 \le l \le L$$

The antithetic multilevel estimator of p is then defined by

$$\widehat{P}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}} = \frac{1}{M_0} \sum_{m=1}^{M_0} g\left(\frac{1}{n_0} \sum_{j=1}^{n_0} f\left(X_m^0, Y_j^{0,m}\right)\right) + \sum_{l=1}^{L} \frac{1}{M_l} \sum_{m=1}^{M_l} \left\{g\left(\frac{1}{n_l} \sum_{j=1}^{n_l} f\left(X_m^l, Y_j^{l,m}\right)\right) - \frac{1}{2} \left(g\left(\frac{1}{n_{l-1}} \sum_{j=1}^{n_{l-1}} f\left(X_m^l, Y_j^{l,m}\right)\right) + g\left(\frac{1}{n_{l-1}} \sum_{j=n_{l-1}+1}^{n_l} f\left(X_m^l, Y_j^{l,m}\right)\right)\right)\right\}.$$
(0.1.15)

Note that, in the expression inside the curly brackets, the function g is evaluated more than once on different empirical means, constructed using the samples  $X_m^l$  and  $Y_j^{l,m}$  at level l only. The remaining degrees of freedom of the estimator lie in the choices of  $n_0$ , L, and of the sample size  $M_l$  for every l, and the multilevel estimator (0.1.15) achieves asymptotic optimality.

**Theorem 0.1.6.** Let Assumptions 0.1.2, 0.1.3, and 0.1.4 hold true, and consider an error tolerance  $\varepsilon > 0$ . There exist  $n_0, M_0, L$  such that as  $\varepsilon \to 0$  the bound MSE =  $\mathcal{O}(\varepsilon^2)$  for the estimator (0.1.15) is achieved with a computational complexity  $\mathcal{O}(\varepsilon^{-2})$  with the choice:

$$n_l = n_0 2^l$$
,  $M_l = M_0 2^{-\left(1 + \frac{(p-2)\nu}{4(p+\nu)} \wedge \frac{\eta}{2}\right)l}$ ,  $0 \le l \le L$ .

Non-nested upper and lower bounds. In American-type option pricing, one has to estimate nested expectations when dealing with the dual approach proposed by Andersen and Broadie [7]. At each time-step, the estimation of conditional expectations using many sub-paths is required. Building on their idea, and a recent work from Guo and Loeper [93] we provide lower and upper non-nested bounds, that we tackle with a regression-based procedure, along with error estimates for the estimation of p.

**Theorem 0.1.7.** Let  $\mathcal{R}$  be a real integrable random variable and  $g : \mathbb{R} \to \mathbb{R}$  a convex function such that  $g(\mathcal{R})$  is integrable. Then, the following identity holds

$$\sup_{\varphi} J_{\varphi} = \mathbb{E}\left[g(\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right])\right] = \inf_{\varepsilon} \mathbb{E}\left[g(\mathcal{R}-\varepsilon)\right], \qquad (0.1.16)$$

where

$$J_{\varphi} = g(z) + g'(z)(\mathbb{E}\left[\mathcal{R}\right] - z) + \int_{z}^{\infty} \mathbb{E}\left[(\mathcal{R} - u)\mathbf{1}_{\varphi(\mathcal{O}) \ge u}\right] \mu(\mathrm{d}u) + \int_{-\infty}^{z} \mathbb{E}\left[(u - \mathcal{R})\mathbf{1}_{\varphi(\mathcal{O}) \le u}\right] \mu(\mathrm{d}u),$$

and the inf is taken over the set of random variables { $\varepsilon$  is integrable and such that  $\mathbb{E}[\varepsilon|\mathcal{O}] = 0$ }. Equality is attained for  $\varphi^{\star}(\mathcal{O}) = \mathbb{E}[\mathcal{R}|\mathcal{O}]$  and for  $\varepsilon^{\star} = \mathcal{R} - \mathbb{E}[\mathcal{R}|\mathcal{O}]$ . Moreover, the following error estimate holds:

$$0 \le J_{\varphi^{\star}} - J_{\varphi} \le 2 \mathbb{E} \big[ \big| \varphi^{\star}(\mathcal{O}) - \varphi(\mathcal{O}) \big| \mu([\varphi^{\star}(\mathcal{O}), \varphi(\mathcal{O})]) \big], \qquad (0.1.17)$$

where  $\mu([a,b])$  stands for the measure of the interval [a,b] if  $a \leq b$  or [b,a] if b < a. If g is Lipschitz with Lipschitz constant  $L_q$ , the error estimate

$$0 \le \mathbb{E}\left[g(\mathcal{R} - \varepsilon)\right] - \mathbb{E}\left[g(\mathcal{R} - \varepsilon^{\star})\right] \le L_g \left\|\varepsilon^{\star} - \varepsilon\right\|_1.$$
(0.1.18)

is straightforward. Finally, if g is improved to  $C^2$  with bounded second derivative, the upper bound in (0.1.18) can be replaced by  $\frac{1}{2} \|g''\|_{\infty} \|\varepsilon^* - \varepsilon\|_2^2$ .

Application to initial margin computations. For several types of trades, banks and financial institutions have to post collateral to a central counterparty (CCP, also called clearing house) to secure their positions. Every day, the CCP requires each market member to deposit a certain capital according to the risk exposure of their contracts. One of these protection capitals is the Initial Margin (IM) deposit: in case of default of one of the CCP members, this capital aims to cover potential losses experienced by the hedging portfolio during the liquidation period of the defaulted member – concretely, the IM is materialized by the value-at-risk or conditional value-at-risk (CVaR) of the member's portfolio over a time period  $\Delta$ . Since the time window  $\Delta$ is small in year units (typically, one week), the usual approach in view of the computations is to apply an asymptotic expansion for the solution of the involved stochastic equation as  $\Delta$  becomes small, see Henry-Labordère [108, Section 4.2] and Agarwal et al. [3]. More precisely, in a Black–Scholes framework for which the price asset is modeled as  $S_t = S_0 e^{\left(r - \frac{\sigma^2}{2}\right)t + \sigma W_t}$  where W is a Brownian motion and the initial price  $S_0 > 0$ , the interest rate r > 0 and the volatility  $\sigma > 0$  are constant, IM computation requires the estimation of nested expectation for which Theorem 0.1.6 applies.

Following the methodology of Agarwal et al. [3], the IM correction for an option with payoff  $\varphi(S_T)$  is computed according to the CVaR of the future evolution of the replicating portfolio over a small time interval  $\Delta > 0$ . When  $\Delta = 0$  (that is: no IM correction), the price at time t is given by the classical Black–Scholes price,  $\mathbb{E}\left[e^{-r(T-t)}\varphi(S_T)|S_t\right]$ , with first derivative  $\delta(t,S) = \partial_s \mathbb{E}\left[e^{-r(T-t)}\varphi(S_T)|S_t=s\right]$ . As shown in Agarwal et al. [3], for small values of  $\Delta$ , a first-order correction to this Black–Scholes price leads to considering the quantity:

$$RC_{\alpha} \mathbb{E}\left[\int_{0}^{T} e^{-rt} \sqrt{(t+\Delta) \wedge T - t} |Z_{t}| \,\mathrm{d}t\right], \qquad (0.1.19)$$

where R is the funding cost net interest rate,  $C_{\alpha} := \text{CVaR}^{\alpha} \left( \mathcal{N}(0,1) \right) = \left. \frac{e^{-\frac{x^2}{2}}}{(1-\alpha)\sqrt{2\pi}} \right|_{x=\Phi^{-1}(\alpha)}$  is the CVaR of a standard Gaussian random variable, and

$$Z_t = z(t, S_t) := \sigma S_t \,\delta(t, S_t). \tag{0.1.20}$$

Using the likelihood ratio method of Broadie and Glasserman [38], we can restore an expression of Z in terms of an expectation:

$$z^{BS}(t,s) = \sigma s \,\partial_s \mathbb{E}\left[ e^{-r(T-t)} \varphi(S_T) \middle| S_t = s \right]$$
$$= \mathbb{E}\left[ e^{-r(T-t)} \left( \varphi(S_T) - \varphi(S_t) \right) \frac{W_T - W_t}{T-t} \middle| S_t = s \right].$$
(0.1.21)

In the last expression, the conditionally centered term  $-\varphi(S_t)\frac{W_T-W_t}{T-t}$  that we have artificially introduced allows to reduce variance in the simulation, by playing the role of a control variate (see [147, Chapter 3]).

Assuming that every hedging operation is performed before  $\tilde{T} := T - \Delta$ , we have  $\sqrt{(t+\Delta) \wedge T - t} = \sqrt{\Delta}$  inside (0.1.19), which allows us to consider the slightly modified quantity:

$$R C_{\alpha} \sqrt{\Delta} \tilde{T} \mathbb{E} \left[ \frac{1}{\tilde{T}} \int_{0}^{\tilde{T}} e^{-rt} |z(t, S_{t})| dt \right] = R C_{\alpha} \sqrt{\Delta} \tilde{T} \mathbb{E} \left[ e^{-rU} |z(U, S_{U})| \right] =: R C_{\alpha} \sqrt{\Delta} \tilde{T} \times I,$$

$$(0.1.22)$$

where instead of discretizing the time integral over  $[0, \tilde{T}]$  – which would produce a bias – we have introduced an independent random variable U with a uniform distribution over  $[0, \tilde{T}]$ . Ignoring the product of constants  $R C_{\alpha} \sqrt{\Delta} \tilde{T}$  (which can be fixed once and for all), the quantity I in (0.1.22) can be cast under the form of a nested expectation as in (0.1.9). We particularly focus our attention on a butterfly option with payoff

$$\varphi(s) = (s - (K + a))_{+} + (s - (K - a))_{+} - 2(s - K)_{+},$$

and whose delta changes sign (see Figure 1).



Figure 1 – Delta  $S \to \Delta_t(S)$  of call (red), put (orange) and butterfly (blue) option prices w.r.t. the variable price S in a Black–Scholes model with parameters  $S_0 = K = 100, a = \frac{K}{2}, T = 1, t = \frac{T}{5}, r = 0.1, \sigma = 0.3$ .

Since  $\delta^{butterfly}$  changes its sign and because the absolute value function g has a singular point at zero, we need to study the behavior of  $\delta^{butterfly}$  around zero to check that Assumption 0.1.4 holds.

**Theorem 0.1.8.** Assumptions 0.1.2, 0.1.3, 0.1.4 hold true in the butterfly case for  $\eta = 1$ , any p > 2 and  $\nu = \frac{1}{2} \left( 1 \wedge \frac{T - \tilde{T}}{\tilde{T}(1+A)} \right)$  for any A > 0. Therefore, Theorem 0.1.6 applies.

#### 0.1.4 Multilevel Monte Carlo in rough forward variance models

In Chapter 2, we investigate Multilevel Monte Carlo approximation methods for the pricing of variance options under rough forward variance models. Before giving more details, we recall some basic concepts of forward variance modeling, whose first appearance is due to Dupire [57], and was later extensively studied by Bergomi [26, 27, 28, 29].

Variance swaps and forward variance. By definition, the annualized realized variance of an asset price S for a period [t, T] with n business days  $t_0 = t < \cdots < t_n = T$  is defined as

$$\mathrm{RV}^{[t,T]} = \frac{1}{T-t} \sum_{i=1}^{n} \ln\left(\frac{S_{t_i}}{S_{t_{i-1}}}\right)^2, \qquad (0.1.23)$$

where T - t is expressed in years unit. A variance swap over the period [t, T] is a contract that pays out the realized variance for the period [t, T]. A forward variance over [t, T] (or implied variance of the variance swap), denoted  $V_t^T$ , is defined as the fair strike of the variance swap, that is

$$V_t^T = \operatorname{price}_t^{\operatorname{mkt}} \left( \operatorname{RV}^{[t,T]} \right), \qquad (0.1.24)$$

where price  $t^{\text{mkt}}(\cdot)$  refers to the market price at time t.

**Instantaneous forward variance.** By analogy with instantaneous forward rates from bond prices, we define the instantaneous forward variance observed at time t and for a maturity T > t as

$$\xi_t^T = \frac{\mathrm{d}}{\mathrm{d}T} \left( (T - t) V_t^T \right), \quad t < T,$$

so that the forward variance rewrites as

$$V_t^T = \frac{1}{T - t} \int_t^T \xi_t^\alpha \mathrm{d}\alpha, \quad t < T.$$

The natural question arising is then:

**Question.** What kind of models should we specify for  $(\xi_t^T)_{t < T}$ ?

Forward variances over  $[T_1, T_2]$ . It is possible to construct a forward variance over the future period  $[T_1, T_2]$ . Indeed consider  $t < T_1 < T_2$ . At time t, we can build the payoff

$$\operatorname{RV}^{[T_1, T_2]} - V_t^{T_1, T_2}, \quad T_2 > T_1,$$

by summing up (long and short) positions in variance swaps over both periods  $[t, T_1]$  and  $[t, T_2]$ .  $V_t^{T_1,T_2}$  is then referred to as the forward variance over  $[T_1, T_2]$  and because realized variance is additive,  $V_t^{T_1,T_2}$  is given by

$$V_t^{T_1,T_2} = \frac{(T_2 - t) V_t^{T_2} - (T_1 - t) V_t^{T_1}}{T_2 - T_1},$$

so that

$$W_t^{T_1, T_2} = \frac{1}{T_2 - T_1} \int_{T_1}^{T_2} \xi_t^{\alpha} \mathrm{d}\alpha, \qquad t < T_1 < T_2.$$

We can then observe that forward variances  $V^{T_1,T_2}$  can be traded. Indeed, when considering another time  $t' \geq t$ , we can enter the opposite payoff

$$-\mathrm{RV}^{[T_1,T_2]} + V_{t'}^{T_1,T_2},$$

and our net position at time  $T_2$  is given by forward variance increment

$$V_{t'}^{T_1,T_2} - V_t^{T_1,T_2}$$

Summing up, we have materialized a portfolio containing the increments of the forward variance  $V^{T_1,T_2}$ , and can thus be used as hedging instrument. Hence, since entering the variance swap has zero cost i.e.

$$\operatorname{price}_{t}\left(V_{t'}^{T_{1},T_{2}}-V_{t}^{T_{1},T_{2}}\right)=0,$$

we infer that, under a pricing measure,  $(V_t^{T_1,T_2})_{0 \le t \le T_1}$  are driftless martingales. Notice also that if  $T_2 = T_1 + \Delta$  for a small time interval  $\Delta \approx 0$ , then  $V_t^{T_1,T_1+\Delta} \approx \xi_t^{T_1}$ . Consequently, the forward variance  $V_t^{T_1,T_1+\Delta}$  over  $[T_1,T_1+\Delta]$  (which can be traded) is close (up to some correction order) to the instantaneous forward variance  $\xi_t^{T_1}$  observed at t for a maturity  $T_1$  (which cannot be traded).

A class of models based on Gaussian processes. From the previous analysis, instantaneous forward variances  $(\xi_t^T)_{T \ge t}$  have to be positive martingales under a given pricing measure. Having this in mind, we model the instantaneous forward variance as

$$\begin{aligned} \xi_t^T &= \xi_0^T \mathcal{E} \left( \int_0^t K^T \left( s \right)^\top \mathrm{d} W_s \right) \\ &= \xi_0^T e^{-\frac{1}{2} \int_0^t K(T-s)^\top \Omega K(T-s) \mathrm{d} s + \int_0^t K(T-s)^\top \mathrm{d} W_s} \\ &= \xi_0^T e^{-\frac{1}{2} \sum_{i,j=1}^n \int_0^T \Omega_{i,j} K_i(T-s) K_j(T-s) \mathrm{d} s + \sum_{i=1}^n \int_0^T K_i(T-s) \mathrm{d} W_s^{(i)}}, \end{aligned}$$
(0.1.25)

where  $\mathcal{E}(X)$  is a shorthand notation for  $e^{X-\frac{1}{2}\operatorname{Var}(X)}$ ,  $(\xi_0^T)_{T\geq 0}$  is the initial instantaneous forward variance curve (market parameter),  $W = (W^{(1)}, \ldots, W^{(n)})$  is an *n*-dimensional Brownian motion (we talk of *n* factors) associated with a correlation matrix  $\Omega$  i.e. for all  $1 \leq i, j \leq n$ , we have  $d \langle W^{(i)}, W^{(j)} \rangle_t = \Omega_{i,j} dt$  and  $K = (K_1, \ldots, K_n)$  are deterministic locally square-integrable kernels i.e. for all  $1 \leq i \leq n$ ,  $K_i(\cdot) \in L_{2,\operatorname{loc}}(\mathbb{R}_+, \mathbb{R}^*_+)$  and  $K^T(s) = K(T-s)$ . From the model (0.1.25), observe that for all *T*, the instantaneous forward variance  $(\xi_t^T)_{t\leq T}$  is both a Gaussian process and a martingale i.e.  $\mathbb{E}\left[\xi_t^T | \mathcal{F}_s^W\right] = \xi_s^T$  for  $s \leq t$  where  $(\mathcal{F}_s^W)_{s\geq 0}$  is the natural filtration of *W*. Observe also that  $(\xi_t^T)_{t\leq T}$  solves the following SDE

$$\mathrm{d}\xi_t^T = \xi_t^T K \left(T - t\right)^\top \mathrm{d}W_t, \quad t \le T,$$

so that  $(\xi_t^T)_{t\leq T}$  is lognormal. From a calibration and simulation point of view, such models are quite popular among practitioners as they only involve Gaussian random variables. In practice, the deterministic kernels are chosen so that the map  $\tau \to K(\tau)$  is nonincreasing; the intuition is that as the kernels appear as instantaneous volatility of instantaneous forward variance, we want instantaneous forward variances associated with longer maturities to move less than the ones with shorter maturities as this is what is observed in market data.

A first parametric example: the one-factor Bergomi model (exponential kernels). The so-called one-factor (i.e. n = 1) Bergomi's model [27] considers exponential kernels, that is

$$K(\tau) = \omega e^{-k\tau}, \quad \omega, \, k > 0. \tag{0.1.26}$$

In this particular example, the instantaneous forward variance rewrites as

$$\begin{aligned} \xi_t^T &= \xi_0^T \mathcal{E} \left( \omega \int_0^t e^{-k(T-s)} \mathrm{d}W_s \right) \\ &= \xi_0^T \mathcal{E} \left( \omega e^{-k(T-t)} \int_0^t e^{-k(t-s)} \mathrm{d}W_s \right) \\ &= \xi_0^T e^{K(T-t)Z_t - \frac{1}{2}K(T-t)^2 \operatorname{Var}(Z_t)}, \end{aligned}$$

where Z is the Ornstein–Uhlenbeck process which follows the Markov dynamics:  $dZ_t = -kZ_t dt + dW_t$ . Consequently, there exists a map  $\Psi(\cdot, \cdot)$  such that for all  $t, \xi_t^T = \Psi(T - t, Z_t)$  so that the instantaneous forward variance curve  $\xi^T$  is a function of only one single Markov factor Z. The extension to the *n*-factor Bergomi's model [27] naturally leads to considering exponential power kernels of the form:

$$K_i(\tau) = \omega_i e^{-k_i \tau}, \qquad \omega_i, k_i > 0, \quad \text{for all} \quad 1 \le i \le n$$

A second parametric example: the rough Bergomi model (power kernels). The rough Bergomi model, recently introduced by Bayer, Friz, and Gatheral [18], considers power kernels of the form

$$K(\tau) = \eta \tau^{H - \frac{1}{2}}, \qquad H \in (0, 1), \, \eta > 0.$$

*H* is the so-called Hurst parameter or exponent. Observe that for all  $H \in (0, \frac{1}{2}), \eta > 0$ , the kernel explodes at 0 i.e.  $K(\tau) \xrightarrow[\tau \to 0^+]{} +\infty$ . Here,  $(\xi_t^T)_{t \leq T}$  takes the form:

$$\xi_t^T = \xi_0^T e^{-\frac{\eta^2}{2} \int_0^T (T-s)^{2H-1} \mathrm{d}s + \eta \int_0^T (T-s)^{H-\frac{1}{2}} \mathrm{d}W_s}.$$
 (0.1.27)

Consequently, as opposed to Bergomi's model, the curve  $T \to \xi_t^T$  does not admit a lowdimensional Markov representation. It is worth mentioning that so far, nothing is rough since in all the models considered, the processes  $(\xi_t^T)_{t < T}$  remain martingales for every T.

**Static replication of log-contracts.** Let us now consider a general stochastic volatility model of the form

$$\mathrm{d}S_t = \mu_t S_t \mathrm{d}t + \sigma_t S_t \mathrm{d}W_t^{\mathrm{hist}},\tag{0.1.28}$$

where  $(\mu_t)_{t\geq 0}$  is a deterministic process,  $(\sigma_t)_{t\geq 0}$  is an adapted square-integrable process and  $(W_t^{\text{hist}})_{t>0}$  a standard Brownian motion all defined on a given filtered probability space

 $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{0 \le t \le T}, \mathbb{P})$ . The sigma-field  $\mathcal{F}_t$  corresponds to the market information available up to time t. We also assume zero interest rate, repo, and dividend. We now recall that realized variance can be replicated with both the underlying S and a log-contract.

Using that  $(T-t) \times \mathrm{RV}^{[t,T]}$  is a consistent estimator of the quadratic variation (see e.g. Barndorff-Nielsen and Shephard [16]), that is as  $\sup_{i=1,...,n} |t_i - t_{i-1}| \xrightarrow[n\to\infty]{} 0$ , we have  $(T-t) \times \mathrm{RV}^{[t,T]} \xrightarrow{\mathrm{P}} \langle \ln S \rangle_T - \langle \ln S \rangle_t$  where  $\xrightarrow{\mathrm{P}}$  refers to the convergence in probability of random variables (actually this result holds for any continuous semimartingale  $(S_t)$ ), the forward variance also equals

$$V_t^T = \text{price}_t \left( \frac{1}{T - t} \left( \langle \ln S \rangle_T - \langle \ln S \rangle_t \right) \right), \qquad (0.1.29)$$

where  $\operatorname{price}_t(\cdot)$  denotes now the model price at time t. From a direct application of Itô's formula, it holds:

$$\ln\left(\frac{S_T}{S_t}\right) = \int_t^T \frac{\mathrm{d}S_\alpha}{S_\alpha} - \frac{1}{2} \int_t^T \sigma_\alpha^2 \mathrm{d}\alpha$$

The quantity  $\int_t^T \frac{\mathrm{d}S_\alpha}{S_\alpha}$  represents the payoff of a hedging strategy which involves maintaining a constant dollar amount up to the maturity T, so that  $\operatorname{price}_t \left( \int_t^T \frac{\mathrm{d}S_\alpha}{S_\alpha} \right) = 0$ . On the contrary, the second term at the r.h.s. corresponds to half the quadratic variation of the stock process  $(S_t)_{t\geq 0}$  i.e.  $\int_t^T \sigma_\alpha^2 \mathrm{d}\alpha = \langle \ln S \rangle_T - \langle \ln S \rangle_t$ , so that the forward variance is given by

$$\begin{split} V_t^T &= \operatorname{price}_t \left( \frac{1}{T-t} \left[ \langle \ln S \rangle_T - \langle \ln S \rangle_t \right] \right) \\ &= \operatorname{price}_t \left( \frac{1}{T-t} \int_t^T \sigma_\alpha^2 \mathrm{d}\alpha \right) \\ &= \operatorname{price}_t \left( -\frac{2}{T-t} \ln \left( \frac{S_T}{S_t} \right) \right), \end{split}$$

where the last quantity corresponds to the price at time t of a log-contract which pays  $\ln\left(\frac{S_T}{S_t}\right)$ .

A consistent model for the stock price  $S_t$ . Consequently, for a given model on the instantaneous forward variance  $\xi_t^T$ , we can build a consistent stochastic volatility model for the stock price S of the form

$$\mathrm{d}S_t = S_t \sqrt{\xi_t^t} \mathrm{d}B_t,$$

where  $(B_t)_{t\geq 0}$  is a standard Brownian motion. Observe here that  $\xi_t^t = \lim_{T\to t} \xi_t^T$  plays the role of an instantaneous volatility. Let us suppose that our pricing function at time t writes as a conditional expectation i.e. price<sub>t</sub>  $(\cdot) = \mathbb{E}[\cdot|\mathcal{F}_t]$  where  $(\mathcal{F}_t)_{t\geq 0} = (\mathcal{F}_t^{W,B})_{t\geq 0}$  is the natural filtration of the random process  $(B_t, W_t)_{t\geq 0}$ . Such a model is consistent in the sense that the price of log-contracts is given by

$$\operatorname{price}_{t} \left( -\frac{2}{T-t} \ln \left( \frac{S_{T}}{S_{t}} \right) \right) = \mathbb{E} \left[ \frac{1}{T-t} \int_{t}^{T} \xi_{u}^{u} \mathrm{d}u \middle| \mathcal{F}_{t} \right]$$
$$= \frac{1}{T-t} \int_{t}^{T} \mathbb{E} \left[ \xi_{u}^{u} \middle| \mathcal{F}_{t} \right] \mathrm{d}u$$
$$= \frac{1}{T-t} \int_{t}^{T} \xi_{t}^{u} \mathrm{d}u.$$

The roughness of such models thus only appear at the stock price level. Indeed, considering the rough Bergomi model, we have:

$$\mathrm{d}S_t = S_t \sqrt{\xi_t^t} \mathrm{d}B_t,$$

where the instantaneous volatility  $\xi_t^t$  of  $S_t$  is said to be rough since

$$\xi_t^t = \mathcal{E}\left(\eta \mathcal{V}_t^t\right), \qquad \mathcal{V}_t^t = \eta \int_0^t \left(t - s\right)^{H - \frac{1}{2}} \mathrm{d}W_s,$$

where  $\mathcal{V}_t^t$  is a Volterra process that admits a  $\beta$ -Hölder modification for  $\beta < H$ .

The VIX index. The VIX index is by definition the implied volatility of the 30-day variance swap on the S&P500 (see [47]). From the analysis above, the volatility index VIX<sub>T</sub> at a future date T can be equivalently defined as the implied volatility of a log-contract that delivers  $\ln\left(\frac{S_{T+\Delta}}{S_T}\right)$  at a future date  $T + \Delta$  where  $\Delta = 30$  days and  $S_T$  (resp.  $S_{T+\Delta}$ ) is the S&P500 at date T (resp.  $T + \Delta$ ) i.e.

$$\text{VIX}_T = \sqrt{\text{price}_T^{\text{mkt}} \left(-\frac{2}{\Delta} \ln \left(\frac{S_{T+\Delta}}{S_T}\right)\right)}.$$

The VIX index is quoted by the Chicago Board Options Exchange [47] by static replication of the payoff  $\ln(S)$ . More precisely, from Carr–Madan's formula [43] the VIX can be replicated with an infinite strip of European options in a completely model-independent way, that is

$$\operatorname{VIX}_{T} = \sqrt{\frac{2}{\Delta} \left( \int_{0}^{S_{T}} \frac{P_{T} \left( T + \Delta, \kappa \right)}{\kappa^{2}} \mathrm{d}\kappa + \int_{S_{T}}^{\infty} \frac{C_{T} \left( T + \Delta, \kappa \right)}{\kappa^{2}} \mathrm{d}\kappa \right)}, \qquad (0.1.30)$$

where  $C_T(T + \Delta, \kappa)$  and  $P_T(T + \Delta, \kappa)$  denote market prices at time T of respectively call and put options on the stock S for a maturity  $T + \Delta$  and strike  $\kappa$ . It should be noted that in general, VIX and forward variances of variance swap are different i.e.  $\text{VIX}_T^2 \neq V_T^{T+\Delta} = \frac{1}{\Delta} \int_T^{T+\Delta} \xi_T^{\alpha} d\alpha$ , but match (as shown above) when assuming a stochastic volatility model.

Derivatives on the VIX in the rough Bergomi model. We now come back to general models of the form (0.1.25) for which  $VIX_T^2 = V_T^{T+\Delta}$ . The price at time t of a VIX option with payoff  $\varphi$  is then given by

$$p_t = \mathbb{E}\left[\left.\varphi\left(\frac{1}{\Delta}\int_T^{T+\Delta}\xi_T^{\alpha}\mathrm{d}\alpha\right)\right|\mathcal{F}_t\right] = \phi\left(t, (\xi_t^{\alpha})_{T\leq\alpha\leq T+\Delta}\right),$$

where we recall that  $(\mathcal{F}_t)_{t\geq 0}$  is the natural filtration of W and  $\phi$  is a deterministic map from  $[0,T] \times L^2([T,T+\Delta])$  to  $\mathbb{R}$  defined by

$$\phi(t,z) = \mathbb{E}\left[\varphi\left(\frac{1}{\Delta}\int_{T}^{T+\Delta} z^{\alpha}e^{-\frac{1}{2}\int_{0}^{T}K(\alpha-t)^{\top}\Omega K(\alpha-t)\mathrm{d}t + \int_{0}^{T}K(\alpha-t)^{\top}\mathrm{d}W_{t}}\mathrm{d}\alpha\right)\right].$$

In particular for the one-factor (i.e. n = 1) rough Bergomi model, writing the kernel as  $K^{\alpha}(t) = \eta(\alpha - t)^{H-\frac{1}{2}}$  the option price at time t = 0 reads as

$$p_{0} = \mathbb{E}\left[\varphi\left(\frac{1}{\Delta}\int_{T}^{T+\Delta}\xi_{0}^{\alpha}e^{-\frac{1}{2}\int_{0}^{T}K^{\alpha}(t)^{2}\mathrm{d}t+\int_{0}^{T}K^{\alpha}(t)\mathrm{d}W_{t}}\mathrm{d}\alpha\right)\right]$$
$$= \mathbb{E}\left[\varphi\left(\frac{1}{\Delta}\int_{T}^{T+\Delta}e^{X_{T}^{\alpha}}\mathrm{d}\alpha\right)\right],$$
$$= \mathbb{E}\left[\varphi\left(P\right)\right],$$
$$(0.1.31)$$

where we have introduced the instantaneous log-forward variance  $X_t^{\alpha} = \ln(\xi_t^{\alpha})$  which equals

$$X_T^{\alpha} = X_0^{\alpha} - \frac{1}{2} \int_0^T K^{\alpha} (t)^2 \, \mathrm{d}t + \int_0^T K^{\alpha} (t) \, \mathrm{d}W_t, \qquad (0.1.32)$$

and set  $P = \frac{1}{\Delta} \int_T^{T+\Delta} e^{X_T^{\alpha}} d\alpha$ . To evaluate VIX derivatives, we thus need to compute integrals over a family a lognormal random variables. As it will be discussed in details in both Chapters 2 and 6, this is very close in spirit to Asian option pricing (see Kemna and Vorst [124]).

In Chapter 2, we study the right-point rectangle discretization of (0.1.31) i.e. for  $n \in \mathbb{N}^*$  discretization points, we approximate

$$P = \frac{1}{\Delta} \int_{T}^{T+\Delta} e^{X_{T}^{\alpha}} \mathrm{d}\alpha \approx P_{n} = \frac{1}{n} \sum_{i=1}^{n} e^{X_{T}^{t_{i}}}$$

where for every  $0 \leq i \leq n$ , we consider uniform time-steps of the form  $t_i = T + ih$  with  $h = \frac{\Delta}{n}$ . The sequence of random variables  $(X_T^{t_i})_{i=0,\dots,n}$  forms a Gaussian vector with mean vector  $\mu = (\mu(t_i))_{i=0,\dots,n}$  and covariance matrix  $C = (C(t_i, t_j))_{0 \leq i,j \leq n}$  where for all  $0 \leq i, j \leq n$ ,

$$\mu(t_i) = \mathbb{E}\left[X_T^{t_i}\right] = X_0^{t_i} - \frac{1}{2} \int_0^T K^{t_i}(s)^2 \,\mathrm{d}s,$$
$$C(t_i, t_j) = \mathbb{C}\operatorname{ov}\left(X_T^{t_i}, X_T^{t_j}\right) = \int_0^T K^{t_i}(s) \,K^{t_j}(s) \,\mathrm{d}s.$$

The option price  $p_0 = \mathbb{E}[\varphi(P)] \approx \mathbb{E}[\varphi(P_n)]$  is then estimated with the crude Monte Carlo estimator:

$$\widehat{P}_{M,n} = \frac{1}{M} \sum_{m=1}^{M} \varphi\left(P_n^{(m)}\right), \qquad (0.1.33)$$

where  $(P_n^{(m)})_{1 \le m \le M}$  are independent copies of  $P_n$  and M is the number of Monte Carlo samples. This is once again exactly the setting of Section 0.1.1: here the random variable  $P = \text{VIX}_T^2 = \frac{1}{\Delta} \int_T^{T+\Delta} e^{X_T^{\alpha}} d\alpha$  is approximated by  $P_n = \frac{1}{n} \sum_{i=1}^n e^{X_T^{t_i}}$  for which  $\frac{1}{n}$  plays the role of the approximation parameter h.

The total computational cost for the estimator (0.1.33) can be decomposed as follows: one Cholesky decomposition of the covariance matrix C with complexity  $\mathcal{O}(n^3)$ , the sampling of an *n*-dimensional Gaussian vector  $\mathcal{O}(n^2)$  together with the sum over its components  $\mathcal{O}(n)$ . Consequently, the overall computational cost for the crude Monte Carlo is given by:

$$\operatorname{Cost}(\widehat{P}_{M,n}) = \mathcal{O}\left(n^{3}\right) + \left(\mathcal{O}\left(n^{2}\right) + \mathcal{O}\left(n\right)\right) \times M = \mathcal{O}\left(\varepsilon^{-4}\right).$$

We show how the total complexity can be reduced to  $\mathcal{O}\left(\ln(\varepsilon)^2 \varepsilon^{-2}\right)$  by use of a multilevel scheme. We first need to estimate both the strong and weak error for the right-point rectangle scheme.

**Theorem 0.1.9** ( $L_2$  strong error). Assume an initial flat instantaneous forward variance i.e.  $X_0^{\alpha} = X_0$  for all  $\alpha \in [T, T + \Delta]$ . As  $n \to \infty$ , it holds:

$$\left(\mathbb{E}\left[|P-P_n|^2\right]\right)^{\frac{1}{2}} \sim \frac{\Lambda\left(X_0, T, \Delta, H\right)}{n},\tag{0.1.34}$$

where

$$\Lambda\left(X_{0}, T, \Delta, H\right) = \frac{e^{X_{0}}}{2} \left( e^{\eta^{2} \frac{T^{2H}}{2H}} + e^{\eta^{2} \frac{(T+\Delta)^{2H} - \Delta^{2H}}{2H}} - 2e^{\eta^{2} \int_{0}^{T} t^{H-\frac{1}{2}} (\Delta+t)^{H-\frac{1}{2}} dt} \right)^{\frac{1}{2}}.$$

As a direct consequence of Cauchy–Schwartz inequality, if the payoff  $\varphi$  is Lipschitz then the weak error is of order 1 i.e.

$$\left|\mathbb{E}\left[\varphi\left(P\right) - \varphi\left(P_{n}\right)\right]\right| = \mathcal{O}\left(n^{-1}\right). \tag{0.1.35}$$

**Multilevel scheme.** Let  $L \in \mathbb{N}^*$  be the number of levels and  $\mathbf{M} = (M_0, \ldots, M_L)$ ,  $\mathbf{n} = (n_0, \ldots, n_L) \in (\mathbb{N}^*)^{L+1}$  be multi-indexes representing respectively the decreasing number of samples used to approximate the expectation and the increasing number of time-steps used to approximate the integral. For all  $l = 0, \ldots, L$ , we introduce the short-hand notation

$$P_l = \varphi\left(\frac{1}{n_l}\sum_{i=1}^{n_l} e^{X_T^{T+\Delta\frac{i}{n_l}}}\right),$$

where the discretization points are of the form  $n_l = n_0 2^l$  for a given  $n_0 \in \mathbb{N}^*$ . The multilevel estimator is defined as:

$$\widehat{P}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}} = \frac{1}{M_0} \sum_{m=1}^{M_0} P_0^{(0,m)} + \sum_{l=1}^L \frac{1}{M_l} \sum_{m=1}^{M_l} \left( P_l^{(l,m)} - P_{l-1}^{(l,m)} \right), \qquad (0.1.36)$$

where for every l, the random variables  $(P_l^{(l,m)})_{1 \le m \le M_l}$  and  $(P_{l-1}^{(l,m)})_{1 \le m \le M_l}$  are independent copies of  $P_l$  and  $P_{l-1}$  respectively. Note that for a fixed level l, the random variables  $P_l^{(l,m)}$ ,  $P_{l-1}^{(l,m)}$  are constructed using the same Brownian paths.

**Theorem 0.1.10.** Suppose that the payoff function  $\varphi$  is Lipschitz, and consider an error tolerance  $\varepsilon > 0$ . Then, there exist  $M_0, L \in \mathbb{N}^*$  such that the multilevel estimator (0.1.36) has a mean-square error with bound MSE =  $\mathcal{O}(\varepsilon^2)$  and a computational complexity  $\mathcal{O}\left(\ln(\varepsilon)^2 \varepsilon^{-2}\right)$ with the choice:

$$n_l = n_0 2^l, \qquad M_l = M_0 2^{-2l}, \qquad 0 \le l \le L.$$

#### 0.2 Meta-modeling and Polynomial Chaos Expansion

In the second part, we are concerned with large sums of the form

$$\mathcal{L}_K = \sum_{k=1}^K l_k \mathbf{1}_{Y_k \le X},\tag{0.2.1}$$

where  $X, Y_1, \ldots, Y_K$  are random variables whose marginal distributions have densities and  $(Y_k)_{k=0...K}$  are independent and independent of X. The  $(l_k)_{k=1,...,K}$  are deterministic and the parameter

 $K \in \mathbb{N}^*$  is assumed finite but large. Observe that when the common factor X is known,  $\mathcal{L}_K$  writes as a sum of weighted independent Bernoulli random variables. More precisely,

 $\mathbf{1}_{Y_k < X} | X = x \stackrel{d}{=} \mathcal{B}(F_{Y_k}(x)), \text{ where for every } x, F_{Y_k}(x) = \mathbb{P}(Y_k \le x).$ 

Though our motivation for studying large sums of the form of (0.2.1) comes from the vast examples of credit risk literature (see more details below), we believe it to be a relevant approach to tackle certain functionals of large sums arising in other branches of applied mathematics such as reliability methods (see e.g. Melchers and Beck [141]), telecommunication, social network modeling etc.

In most applications, one may be interested in estimating tail probabilities  $\mathbb{P}(\mathcal{L}_K > L)$  for  $\mathcal{L}_K$ , especially at large values of L, or more generally expectations of functionals of the loss,  $\mathbb{E}[f(\mathcal{L}_K)]$ . To estimate such quantity, Monte Carlo methods are often the preferred choice. However, as K is supposed large and because we are dealing with tail events any Monte Carlo simulation scheme will be quite time-consuming. For instance, suppose we want to estimate  $\mathbb{E}[f(\mathcal{L}_K)]$ , for some function f, using a Monte Carlo method. Then, to reach an error tolerance of  $\varepsilon > 0$  for the root mean squared error, we would need to sample  $N = \mathcal{O}(\varepsilon^{-2})$  times the loss  $\mathcal{L}_K$ . Each simulation of  $\mathcal{L}_K$  requires to generate  $(Y_1, \ldots, Y_K)$  and apply the sum (0.2.1). Consequently, if the simulation cost of one  $Y_k$  is taken to be one unit basis, the global simulation cost (to reach an accuracy of  $\varepsilon$ ) is  $\mathcal{O}(K\varepsilon^{-2})$ . For instance, if the number K is quite large (say a million), and the error tolerance is one percent, this would lead to a cost of ten billion unit operations. Needless to say that the more accurate the estimation (i.e. smaller  $\varepsilon$ ), the higher the number of samples N. Quite imprecise estimations of the expectation of interest could then be the only option available under a given computational time constraint.

To alleviate this problem, we propose a meta-model for the large sum  $\mathcal{L}_K$ . A meta-model is an approximation of a true model and has the advantage of being much faster to evaluate. Our procedure for deriving the proposed meta-model is two-fold:

- 1. We first apply a Polynomial Chaos Expansion on the common factor X, and obtain the associated truncated loss  $\mathcal{L}_{K,N}$  at some order  $N \in \mathbb{N}^*$ .
- 2. We then provide a Gaussian-based approximation  $\mathcal{L}_{K,N}^{\mathrm{G}}$  of the truncated loss  $\mathcal{L}_{K,N}$  with explicit characteristics.

Reminder on Orthogonal Polynomials. Let  $\nu(dx) = w(x)dx$  be a probability measure defined on a finite or infinite open interval  $I_w = (a, b)$  in  $\mathbb{R}$ . The nonnegative weight function w(x) is continuous or piecewise continuous or integrable, and such that  $0 < \int_{I_w} x^{2n} w(x) dx$  for all n. The set of polynomial functions  $(p_n)_{n \in \mathbb{N}}$  is said to be an orthogonal polynomials set (OPS) associated with the weight function w(x) (or equivalently with the probability measure  $\nu$ ), if for all  $n, m \in \mathbb{N}$ ,

$$\int_{I_w} p_n(x) p_m(x) w(x) \mathrm{d}x = h_n \delta_{nm}, \qquad (0.2.2)$$

where  $\delta_{nm} = 1$  if n = m or 0 otherwise, and  $h_n := \int_a^b p_n(x)^2 w(x) dx < \infty$ . When  $h_n = 1$ , we say that the polynomials are orthonormalized.

**Recurrence relation.** A remarkable property of orthogonal polynomials is that they necessarily solve a three-term recurrence relation of the form ([157, Theorem 3.2.1]):

$$p_{n+1}(x) = (A_n x + B_n) p_n(x) - C_n p_{n-1}(x), \quad n \in \mathbb{N}^*,$$
(0.2.3)

where  $A_n, B_n, C_n$  are constants with  $A_n > 0, C_n > 0$ .
**Polynomial Chaos Expansion (PCE) of an indicator function.** Let  $(p_n)_{n \in \mathbb{N}}$  be an OPS for a probability measure  $\nu(dx) = w(x)dx$  and introduce the threshold  $c \in \mathbb{R}$ . As soon as  $X \stackrel{d}{=} \nu$ , the following PCE holds

$$\mathbf{1}_{c \le X} \stackrel{L_2(\nu)}{=} \sum_{n=0}^{\infty} \gamma_n(c) p_n(X), \quad \gamma_n(c) = \frac{\mathbb{E}\left[\mathbf{1}_{c \le X} p_n(X)\right]}{h_n} = \frac{\int_c^b p_n(x) w(x) \mathrm{d}x}{\int_a^b p_n^2(x) w(x) \mathrm{d}x}.$$
(0.2.4)

Because the sum (0.2.4) requires the computation of an infinite number of parameters, in practice we have no choice be to truncate it at some order  $N \in \mathbb{N}^*$ , and approximate it with

$$\sum_{n=0}^{\infty} \gamma_n(c) p_n(X) \approx \sum_{n=0}^{N} \gamma_n(c) p_n(X).$$
(0.2.5)

We will also be interested in estimating the  $L_2$  error between  $\mathbf{1}_{c\leq X}$  and  $\sum_{n=0}^{N} \gamma_n(c) p_n(X)$  i.e.

$$\mathcal{E}_{N}(c) = \mathbb{E}\left[\left|\mathbf{1}_{c \le X} - \sum_{n=0}^{N} \gamma_{n}(c)p_{n}(X)\right|^{2}\right]^{\frac{1}{2}} = \left|\sum_{n=N+1}^{\infty} h_{n}\gamma_{n}(c)^{2}\right|^{\frac{1}{2}}, \quad (0.2.6)$$

where the last equality results from the orthogonality condition (0.2.2).

Classical orthogonal polynomials set or COPS. Rather than considering any orthogonal polynomial, we study a subclass of continuous orthogonal polynomials commonly referred to as the classical orthogonal polynomials set or COPS. The COPS includes only the Hermite, Laguerre (with parameter  $\alpha > -1$ ), and the Jacobi (with parameters  $\alpha, \beta > -1$ ) orthogonal polynomials, for which some of the properties are gathered in Table 1 (see e.g. [146, Chapter 18] for an extensive review of their characteristics). The Legendre polynomials are particular Jacobi polynomials with parameters  $\alpha = \beta = 0$  and they play a key role in our study. These polynomials are the only ones to satisfy to Rodrigues' formula, that is

$$p_n(x) = \frac{1}{\kappa_n w(x)} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left[ F(x)^n w(x) \right], \qquad (0.2.7)$$

where F is a polynomial with deg  $(F) \leq 2$  and  $\kappa_n$  some coefficients, and their weight function  $w(\cdot)$  satisfies the following Pearson's type differential equation

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[F(x)w(x)\right] = G(x)w(x),\tag{0.2.8}$$

where G is a polynomial with  $\deg(G) = 1$  and the following limit conditions hold

$$\lim_{x \to a} w(x)F(x) = \lim_{x \to b} w(x)F(x) = 0.$$

Both properties are essential to derive closed-form expressions and recurrence relations for the chaos coefficients  $\gamma_n$ , and motivate our choice to focus only on the COPS (see [6, Theorem 1.2] for a full characterization).

Name	Hermite	Laguerre	Jacobi	Legendre
Remark		$\alpha > -1$	$\alpha,\beta>-1$	$\text{Jacobi} \left( \alpha = \beta = 0 \right)$
$p_n(x)$	$\operatorname{He}_n(x)$	$\mathcal{L}_n^{(\alpha)}(x)$	$\mathrm{P}_n^{(lpha,eta)}(x)$	$P_n(x)$
(a,b)	$(-\infty,\infty)$	$(0,\infty)$	(-1,1)	(-1,1)
w(x)	$\frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}$	$\frac{x^{\alpha}e^{-x}}{\Gamma_{\alpha+1}}$	$\frac{(1-x)^{lpha}(1+x)^{eta}}{2^{lpha+eta+1}\mathrm{B}_{lpha+1,eta+1}}$	$\frac{1}{2}$
ν	$\mathcal{N}\left(0,1 ight)$	$\operatorname{Gamma}\left(\alpha+1,1\right)$	$1 - 2 \text{Beta}\left(\alpha + 1, \beta + 1\right)$	$\mathcal{U}\left(-1,1 ight)$
$p_0(x)$	1	1	1	1
$p_1(x)$	x	$1 + \alpha - x$	$\alpha + 1 + \frac{(\alpha + \beta + 2)(x - 1)}{2}$	x

Table 1 – Some properties for the classical orthogonal polynomials.

**Theorem 0.2.1** ( $L_2$  error estimates). There exists a positive constant A, independent of N and c, such that the following global estimates hold:

$$e^{-\frac{c^2}{4}}N^{-\frac{1}{4}}, \quad c \in \left[-N^{\frac{1}{2}}, N^{\frac{1}{2}}\right], \nu = \mathcal{N}(0, 1),$$

$$(0.2.9)$$

$$\mathcal{E}_{N}(c) \leq A \left\{ \begin{array}{ll} c^{\frac{\alpha}{2} + \frac{1}{4}} e^{-\frac{c}{2}} N^{-\frac{1}{4}}, & c \in [0, N], \ \alpha \notin \mathbb{N}, \ \nu = \text{Gamma}\left(\alpha + 1, 1\right), \end{array} \right.$$
(0.2.10)

$$(1-c)^{\frac{\alpha}{2}+\frac{1}{4}}(1+c)^{\frac{\nu}{2}+\frac{1}{4}}N^{-\frac{1}{4}}, \quad c \in [-1,1], \ \nu = 1-2\text{Beta}\left(\alpha+1,\beta+1\right), \ (0.2.11)$$

$$(1-c)^{\frac{1}{2}+\frac{1}{4}}N^{-\frac{1}{2}}, \quad c \in [-1,1], \ \nu = 2/(-1,1), \ (0.2.12)$$

$$\left( (1-c^2)^{\frac{4}{9}} N^{-\frac{1}{2}}, \quad c \in [-1,1], \, \nu = \mathcal{U}(-1,1). \right)$$
(0.2.12)

For no extreme values of c, that is  $c = \pm \infty$  for the Hermite polynomials, c = 0 or  $c = +\infty$  for the Laguerre polynomials,  $c = \pm 1$  for the Jacobi polynomials, we have an  $L_2$  error of order  $\mathcal{O}\left(N^{-\frac{1}{4}}\right)$  for all polynomials except the Legendre polynomials which exhibit and faster decrease of order  $\mathcal{O}\left(N^{-\frac{1}{2}}\right)$  (see Figure 2). The order  $\mathcal{O}\left(N^{-\frac{1}{4}}\right)$  seems rather poor for the truncation to be effective. Yet, the principal significance of Theorem 0.2.1 lies in the fact that it keeps track of the dependence on the parameter c (see Figure 3). It reveals an exponential factor  $e^{-\frac{c^2}{4}}$  (resp.  $e^{-\frac{c}{2}}$ ) for the Hermite (resp. Laguerre) polynomials which ensures a faster decrease for large values of c (see Figure 3)

More precisely, to assess and compare the performance of each polynomial in terms of  $L_2$  error, we consider the problem of approximating the indicator function

$$\mathbf{1}_{q \leq U} \stackrel{d}{=} \mathbf{1}_{F^{-1}(q) \leq F^{-1}(U)},$$

where the quantile  $q \in (0, 1)$ ,  $U \stackrel{d}{=} \mathcal{U}(0, 1)$ , and  $F(\cdot)$  may refer to the c.d.f. of  $\mathcal{U}(-1, 1)$  (Legendre polynomials) or  $\mathcal{N}(0, 1)$  (Hermite polynomials) or Gamma  $(\alpha + 1, 1)$  (Laguerre polynomials) or  $1 - 2\text{Beta}(\alpha + 1, \beta + 1)$  (Jacobi polynomials). The PCE of the indicator function  $\mathbf{1}_{q \leq U}$  for the COPS is displayed for "standard quantiles" in Figure 2 in which we observe that indeed the Legendre polynomials perform best. This is different for "extreme quantiles" (Figure 3) where we note that the Legendre (resp. Jacobi) polynomials seem to provide the highest (resp. lowest)  $L_2$  error.



Figure 2 –  $L_2$  error for the COPS w.r.t.  $q \in (0, 1)$  with truncation parameter N = 40.



Figure 3 –  $L_2$  error for the COPS w.r.t. small quantiles  $q \in (10^{-4}, 10^{-3})$  (left) and large quantiles  $q \in (1 - 10^{-3}, 1 - 10^{-4})$  (right).

Gaussian-based approximation and Central Limit Theorem. We now come back to our original problem i.e. giving a meta-model for the large sum (0.2.1). In light of the previous section, it seems natural to split the sum into three different clusters depending on the value of  $Y_k$ . For instance, supposing that  $X \stackrel{d}{=} \Gamma(\alpha + 1, 1)$  and denoting  $F(\cdot)$  its c.d.f., we would get three different groups in which the  $Y_k$  are close to 0 (extreme low quantiles), the  $Y_k$  are close to  $\infty$  (extreme high quantiles), and the  $Y_k$  take "normal" values on  $(0, \infty)$ . For the latter, noting that  $\mathbf{1}_{Y_k \leq X} = \mathbf{1}_{2F(Y_k)-1 \leq 2F(X)-1} \stackrel{d}{=} \mathbf{1}_{2F(Y_k)-1 \leq \mathcal{U}(-1,1)}$ , we could then perform a PCE of  $\mathbf{1}_{2F(Y_k)-1 \leq 2F(X)-1}$  instead of  $\mathbf{1}_{Y_k \leq X}$  using the Legendre polynomials. For the other two groups, a similar procedure could be used though we would not use the Legendre polynomials (see Lemma 4.3.1 and Remark 11 for more details).

We then suppose that early transformations have been made according to the values of  $(Y_k)_{k=1,...K}$ . From the PCE of  $\mathbf{1}_{Y_k \leq X}$  (0.2.4), and because  $X, Y_1, \ldots, Y_K$  are random variables having densities, it holds almost surely that

$$\mathcal{L}_{K} = \sum_{k=1}^{K} \left( \sum_{n=0}^{\infty} l_{k} \gamma_{n} \left( Y_{k} \right) \right) p_{n}(X) = \sum_{n=0}^{\infty} \varepsilon_{K,n} p_{n}(X),$$

where we define the new random variable

$$\varepsilon_{K,n} := \sum_{k=1}^{K} l_k \gamma_n \left( Y_k \right). \tag{0.2.13}$$

Our meta-model for  $\mathcal{L}_K$  consists in considering only the first terms of the chaos decomposition of the indicator function combined with a Gaussian-based approximation. For a truncation order  $N \in \mathbb{N}^*$ , we define the truncated version of  $\mathcal{L}_K$  as

$$\mathcal{L}_{K,N} := \sum_{n=0}^{N} \varepsilon_{K,n} p_n(X). \tag{0.2.14}$$

We further introduce the expectation  $\boldsymbol{\mu}_{K} = (\mu_{K,n})_{0 \leq n \leq N}$  and the covariance matrix  $\Sigma_{K} = (\Sigma_{K,n,m})_{0 \leq n,m \leq N}$  of the vector  $\boldsymbol{\varepsilon}_{K} = (\varepsilon_{K,n} : n = 0, \dots, N)$  where for every  $n, m \in \{0, \dots, N\}$ ,

$$\mu_{K,n} = \mathbb{E}\left[\varepsilon_{K,n}\right] = \sum_{k=1}^{K} l_k \mathbb{E}\left[\gamma_n\left(Y_k\right)\right],$$

$$\Sigma_{K,n,m} = \mathbb{C}\operatorname{ov}\left(\varepsilon_{K,n}, \varepsilon_{K,m}\right) = \sum_{k,k'=1}^{K} l_k l_{k'} \mathbb{C}\operatorname{ov}\left(\gamma_n\left(Y_k\right), \gamma_m\left(Y_{k'}\right)\right).$$
(0.2.15)

Replacing the vector  $\boldsymbol{\varepsilon}_{K}$  by its Gaussian approximation

$$\boldsymbol{\varepsilon}_{K}^{\mathrm{G}} = \left(\varepsilon_{K,n}^{\mathrm{G}} : n = 0, \dots, N\right) \stackrel{d}{=} \mathcal{N}\left(\mu_{K}, \Sigma_{K}\right), \qquad (0.2.16)$$

leads to the meta-model  $\mathcal{L}_{K,N}^{\mathrm{G}}$  for the initial model  $\mathcal{L}_{K}$  defined by:

$$\mathcal{L}_{K,N}^{\mathrm{G}} = \mathcal{L}_{K,N}^{\mathrm{G}}(X) = \sum_{n=0}^{N} \varepsilon_{K,n}^{\mathrm{G}} p_n(X).$$
(0.2.17)

Hence when X is known,  $\mathcal{L}_{K,N}^{\mathrm{G}}(x) \stackrel{d}{=} \mathcal{N}\left(\mu_{\mathcal{L}_{K,N}}(x), \sigma_{\mathcal{L}_{K,N}}^{2}(x)\right)$  with for every  $x \in \mathbb{R}$ ,

$$\mu_{\mathcal{L}_{K,N}}(x) = \sum_{n=0}^{N} \mu_{K,n} p_n(x), \quad \sigma_{\mathcal{L}_{K,N}}^2(x) = \sum_{n,m=0}^{N} \Sigma_{K,n,m} p_n(x) p_m(x).$$

The striking property is that the coefficients  $(\varepsilon_{K,n})_{n \in 0,...,N}$  write as a sum of independent random variables. The next result gives a sufficient condition so that one can replace the coefficients by a Gaussian random vector with explicit characteristics.

**Theorem 0.2.2** (Central Limit Theorem). Assume that the following Lindeberg condition holds

$$\|\Sigma_K^{-1}\| \sup_{1 \le k \le K} l_k^2 \xrightarrow[K \to +\infty]{} 0 \quad with \quad \|\Sigma_K^{-1}\| := \sup_{\boldsymbol{x} \in \mathbb{R}^{N+1}, x \ne 0} \frac{|\Sigma_K^{-1} \boldsymbol{x}|}{|\boldsymbol{x}|}.$$
(0.2.18)

Then, the vector  $\boldsymbol{\varepsilon}_K$  satisfies the following Central Limit Theorem

$$\Sigma_{K}^{-\frac{1}{2}}(\boldsymbol{\varepsilon}_{K}-\boldsymbol{\mu}_{K}) \xrightarrow[K\to\infty]{d} \mathcal{N}(0, \mathrm{Id}_{N+1}).$$
(0.2.19)

-1

Meta-model for large credit risk portfolio in the Gaussian copula model. In Chapter 3, we focus on large credit risk portfolios in the Gaussian copula model (see Li [135]). We study the one-year total loss from defaults (without any provision) defined as:

$$\mathcal{L}_K = \sum_{k=1}^K l_k D_k$$

where  $D_k$  represents the default indicator for the kth obligor at one-year i.e.  $D_k = 1$  if the kth obligor defaults or 0 otherwise. We assume that the defaults obey to the Gaussian copula model, namely

$$D_k = \mathbf{1}_{G_k \ge c_k} \tag{0.2.20}$$

with stochastic factors  $G_k$ , thresholds (or default boundaries)  $c_k$ , and in which the dependence among obligors is achieved through a multivariate normal vector  $(G_1, \ldots, G_K)$  with standardized entries  $G_k \stackrel{d}{=} \mathcal{N}(0, 1)$  for every k. More precisely, in a one-dimensional Gaussian copula model,  $G_k$  can be decomposed as:

$$G_k = \rho_k Z + \sqrt{1 - \rho_k^2} \varepsilon_k, \qquad (0.2.21)$$

where the random variable  $Z \stackrel{d}{=} \mathcal{N}(0,1)$  represents a systemic risk factor (common to every obligor),  $\varepsilon_k \stackrel{d}{=} \mathcal{N}(0,1)$  is an idiosyncratic risk (specific to every obligor) associated with the kth obligor (independent of Z), and  $\rho_k \in (-1,1)$  a correlation parameter. We stress that the  $(\varepsilon_k)_{1 \leq k \leq K}$  are independent and independent of Z, and we assume that  $\rho_k \neq 0$  since (from an economic point of view) there always exists a dependency between the default of an obligor and the systemic risk factor.

Setting the default boundary  $c_k := \Phi^{-1}(1-p_k) = -\Phi^{-1}(p_k)$  so that it matches the constraint  $p_k = \mathbb{P}(D_k = 1)$ , we infer that

$$\mathbb{P}(D_k = 1) = \mathbb{P}(G_k \ge c_k) = \Phi(-c_k) = p_k.$$

Then, the default event writes (remembering that we exclude the case  $\rho_k = 0$ ):

$$\left\{G_k \ge c_k\right\} = \left\{-\frac{\sqrt{1-\rho_k^2}}{|\rho_k|}\varepsilon_k - \frac{\Phi^{-1}(p_k)}{|\rho_k|} \le \frac{\rho_k}{|\rho_k|}Z\right\}.$$
 (0.2.22)

Here, we emphasize that both random variables are normally distributed and observe that the credit risk sum is of the form (0.2.1) with:

$$X = \frac{\rho_k}{|\rho_k|} Z \stackrel{d}{=} \mathcal{N}(0, 1), \qquad Y_k = -\frac{\sqrt{1 - \rho_k^2}}{|\rho_k|} \varepsilon_k - \frac{\Phi^{-1}(p_k)}{|\rho_k|} \stackrel{d}{=} \mathcal{N}\left(-\frac{\Phi^{-1}(p_k)}{|\rho_k|}, \frac{1 - \rho_k^2}{\rho_k^2}\right).$$

Remark 1. Models of the form (0.2.21) fall into the category of the so-called "threshold models" which are extremely popular in credit risk modeling (see e.g. McNeil, Frey, and Embrechts [140, Section 8.3]). One of the most well-known extensions to the Gaussian copula model (0.2.21) is the Student t copula model (see [140, Example 8.21]) for which  $G_k = W\left(\rho_k Z + \sqrt{1-\rho_k^2}\varepsilon_k\right)$  and W is an Inverse Gamma distribution.

**Theorem 0.2.3.** Under the assumption that  $(\varepsilon_k)_{k=1,...,K}$  is independent of Z, the N-truncated chaos decomposition of order  $N \in \mathbb{N}$  of the loss  $\mathcal{L}_K$  w.r.t. Z (see (0.2.14)) is given by:

$$\mathcal{L}_{K,N} = \sum_{n=0}^{N} \left\{ \sum_{k=1}^{K} l_k \gamma_n \left( -\frac{\sqrt{1-\rho_k^2}}{|\rho_k|} \varepsilon_k - \frac{\Phi^{-1}(p_k)}{|\rho_k|} \right) \frac{\rho_k^n}{|\rho_k|^n} \right\} \operatorname{He}_n(Z), \qquad (0.2.23)$$

where the coefficients  $\gamma_n(c)$  (see (0.2.4)) associated with the Hermite polynomials write as

$$\gamma_0(c) = \Phi(-c), \quad \gamma_n(c) = \frac{e^{-\frac{c^2}{2}} \operatorname{He}_{n-1}(c)}{n! \sqrt{2\pi}}, \quad (n \in \mathbb{N}^*).$$

Applying the Central Limit Theorem 0.2.2, our meta-model consists of sampling an (N + 1)dimensional Gaussian vector. Further, as the c.d.f. of Y (Gaussian here) is known in closed-form and thanks to (0.2.3), efficient recurrence relations are satisfied by the mean vector  $\mu$  and covariance matrix  $\Sigma$ . Considering M Monte Carlo samples, our meta-model requires  $\mathcal{O}(KN^2)$ (offline cost for computing the Gaussian vector characteristics) +  $\mathcal{O}(MN^2)$  (sampling of an (N + 1)-dimensional Gaussian vector) operations which entails a total computational cost of  $\mathcal{O}(KN^2) + \mathcal{O}(MN^2)$ . Remembering that  $K \geq 10^5$  and because for most applications, a truncation parameter  $N \leq 50$  leads to satisfactory results, the complexity  $\mathcal{O}(MK)$ , required for a standard Monte Carlo, is much bigger.

## 0.3 Weak approximations, options prices expansions, and smalltime asymptotics

For many years, small-time asymptotics for stochastic volatility models has attracted both practitioners and academics in the financial community (see e.g. Berestycki, Busca, and Florent [25], Henry-Labordère [107], Forde and Jacquier [65], Feng, Forde, and Fouque [63], Gatheral et al. [71], Friz et al. [69]). Building on the small-time expansion of the transition density of a general diffusion process, expressed in terms of a distance function on a Riemannian manifold whose metric is proportional to the inverse of the diffusion coefficient (see the seminal works of Varadhan [162, 161] or Henry-Labordère [107]), all of these references examine and derive asymptotics for the European implied-volatility in a small-time regime. For instance, consider a time-homogeneous local volatility model on a non-dividend stock price S,

$$\mathrm{d}S_t = rS_t \mathrm{d}t + S_t \sigma(S_t) \mathrm{d}W_t, \qquad (0.3.1)$$

or equivalently for the logarithmic stock price  $X_t := \ln S_t$ ,

$$dX_t = \left(r - \frac{1}{2}\sigma^2(e^{X_t})\right)dt + \sigma\left(e^{X_t}\right)dW_t.$$
(0.3.2)

The heat-kernel expansion for the transition density of the process  $X_t$  starting at  $X_0 = x$  is then given by ([71, Proposition 2.1]):

$$f_X(t,y|x) = \frac{e^{-\frac{d^2(x,y)}{2t}}}{\sqrt{2\pi t}} \left( u_0(x,y) + \mathcal{O}(t;x,y) \right), \quad (t \to 0^+),$$

where the squared distance function and the coefficient  $u_0$  are respectively defined as

$$d(x,y)^{2} = \left(\int_{x}^{y} \frac{dp}{\sigma(e^{p})}\right)^{2}, \quad u_{0}(x,y) := \sigma(e^{x})^{\frac{1}{2}} \sigma(e^{y})^{-\frac{3}{2}} e^{-\frac{1}{2}(y-x)+r\int_{x}^{y} \frac{dp}{\sigma^{2}(e^{p})}},$$

and there exists a positive constant C (independent of x and y) such that  $|\mathcal{O}(t; x, y)| \leq Ct$  for every t > 0.

European put price and European implied volatility expansions. A put option written on the stock price  $S_t$  with time-to-maturity  $\tau$ , strike K, and initial price  $S_0 = s$  can thus be expressed as a Laplace-type integral of the form

$$P(\tau, s, K) = \mathbb{E}\left[e^{-r\tau}(K - S_{\tau})_{+}\right]$$
$$= \frac{Ke^{-r\tau}}{\sqrt{2\pi\tau}} \int_{-\infty}^{0} \left(1 - e^{z}\right) \left(u_{0}\left(\ln s, \ln K + z\right) + \mathcal{O}\left(\tau\right)\right) e^{-\frac{\mathrm{d}^{2}\left(\ln s, z + \ln K\right)}{2\tau}} \mathrm{d}z.$$

Using Laplace's method (see e.g. Bender and Orszag [22, Chapter 6]) and depending on whether s > K (out-the-money), s = K (at-the-money) or s < K (in-the-money), the European put price admits the following small-time expansion,

$$\int \frac{s\sigma(s)}{\sqrt{2\pi}}\sqrt{\tau} - \frac{rs}{2}\tau + A_1(s)\frac{s}{\sqrt{2\pi}}\tau\sqrt{\tau}, \quad \text{if } s = K, \tag{0.3.3}$$

$$\frac{P(\tau, s, K)}{\tau \to 0} \approx \begin{cases} A_2(s) e^{-\frac{\mathrm{d}^2(\ln K, \ln s)}{2\tau}} \tau \sqrt{\tau}, & \text{if } s > K, \\ \mathrm{d}^2(\ln K \ln s) \end{cases} \tag{0.3.4}$$

$$\left( K \left( 1 - e^{-r\tau} \right) - A_2(s) e^{-\frac{d^2(\ln K, \ln s)}{2\tau}} \tau \sqrt{\tau}, \quad \text{if } s < K.$$
 (0.3.5)

where  $A_1(s)$  depends only on  $\sigma(\cdot)$  and  $A_2(s) = \frac{u_0(\ln s, \ln K)K\sigma(K)^2}{\sqrt{2\pi}d^2(\ln K, \ln s)}$ .

Defining the European implied volatility  $\sigma_{\rm E}(\tau,s,K)$  as solution to:

$$P(\tau, s, K) = P_{\rm BS}(\tau, s, K; \sigma_{\rm E}(\tau, s, K)),$$

where  $P_{\rm BS}$  refers to the Black–Scholes put price (i.e.  $\sigma(s) = \sigma$  for every s), and using the expansions (0.3.3), (0.3.4), (0.3.5) lead to a polynomial expansion for the European implied volatility of the form (see e.g. [71, Section 2.2]),

$$\sigma_{\mathrm{E}}\left(\tau, s, K\right) = \sigma_{0}\left(s, K\right) + \sigma_{1}\left(s, K\right)\tau + \mathcal{O}\left(\tau^{2}\right),$$

where

$$\sigma_0(s,K) = \frac{\ln\left(\frac{s}{K}\right)}{d\left(\ln K,\ln s\right)},$$
  
$$\sigma_1(s,K) = \frac{\sigma_0^3(s,K)}{\ln\left(\frac{s}{K}\right)^2} \ln\left(\frac{u_0\left(\ln s,\ln K\right)\sigma^2\left(K\right)}{\sigma_0\left(s,K\right)}\right) - \frac{\sigma_0^3\left(s,K\right)}{2\ln\left(\frac{s}{K}\right)} + \frac{r\sigma_0\left(s,K\right)}{\ln\left(\frac{s}{K}\right)},$$

#### 0.3.1 Small-time asymptotics for American options in local volatility models

American put in a time-homogeneous local volatility model. In Chapter 5, following the same methodology, we study the American put price (denoted  $A(\tau, s, K)$  for an initial stock price  $S_0 = s$ , strike K, and time-to-maturity  $\tau$ ) and implied volatility asymptotic expansions for a model of the form (0.3.1).

As opposed to a European option that can only be exercised at maturity, an American option gives its owner the right to exercise any time prior or at maturity (see Bensoussan [24] and Karatzas [121] for an optimal stopping problem representation). It is well-known (see McKean [139] and Van Moerbeke [160]) that  $A(\tau, s, K)$  solves the following backward parabolic obstacle PDE:

$$\begin{cases}
-\partial_{\tau}A + \frac{\sigma^{2}(s)s^{2}}{2}\partial_{ss}A + rs\partial_{s}A - rA = 0, \quad \tau > 0, \quad s > \bar{s}(\tau), \\
A(\tau, s, K) > (K - s)_{+}, \quad \tau > 0, \quad s > \bar{s}(\tau), \\
A(\tau, s, K) = (K - s)_{+}, \quad \tau > 0, \quad s \le \bar{s}(\tau), \\
A(0, s, K) = (K - s)_{+}, \quad \tau = 0, \quad s > 0,
\end{cases}$$
(0.3.6)

where the function  $\tau \to \bar{s}(\tau)$  in (0.3.6) is the so-called exercise boundary which completely characterizes the American price. Observe that in the continuation region  $\{s > 0 \mid s > \bar{s}(\tau)\}$ , the American put price solves the Black–Scholes PDE while on the exercise region  $\{s > 0 \mid s \le \bar{s}(\tau)\}$ , it matches the payoff. The optimal stopping time for an American option can thus be viewed as the first hitting time of the stock price at the exercise boundary.

The exercise boundary and the early premium formula. The exercise boundary has been extensively studied in the literature, and we recall its main properties (see e.g. Karatzas and Shreve [122]): the map  $\tau \to \bar{s}(\tau)$  is continuous and decreasing on  $\mathbb{R}_+$ , continuously differentiable on every interval  $[\alpha, \infty)$  for  $\alpha > 0$ ,  $\bar{s}(0) = K$  and  $\lim_{\tau \to 0} \bar{s}(\tau) = -\infty$ .



Figure 4 – Exercise boundary in a Black–Scholes model w.r.t. the time-to-maturity  $\tau$ .

The relation between the American and European put price is given by the following integral representation, the so-called early premium formula (see Kim [125], Jacka [114], Carr, Jarrow, and Myneni [44], Huang, Subrahmanyam, and Yu [113]),

$$A(\tau, s, K) = P(\tau, s, K) + rK \int_0^\tau e^{-ru} \mathbb{P}_{0,s} \Big( S_u \le \bar{s} (\tau - u) \Big) \mathrm{d}u, \qquad (0.3.7)$$

where the last term at the r.h.s. of (0.3.7) is referred to as the American premium. Economically, this positive term quantifies the right of exercising the option earlier than expiration. To numerically approximate the exercise boundary, note that setting  $s = \bar{s}(\tau)$  in (0.3.7) and using the continuity condition (0.3.6),  $A(\tau, \bar{s}(\tau), K) = K - \bar{s}(\tau)$ , the following convolution-type integral equation holds

$$\bar{s}(\tau) - K + P(\tau, \bar{s}(\tau), K) + rK \int_0^\tau e^{-ru} \mathbb{P}_{0,\bar{s}(\tau)} \left( S_u \le \bar{s}(\tau - u) \right) du = 0.$$

The exercise boundary  $\bar{s}(\tau)$  can then be recursively approximated discretizing the integral with initial point  $\bar{s}(0) = K$  (see Section 5.2.3 for a detailed discussion).

In view of (0.3.7), to study the small time-to-maturity behavior of the American put price, we need to understand how the exercise boundary behaves close to maturity in a model (0.3.1). A refined asymptotic was proposed by De Marco and Henry-Labordère [53] who showed that as  $\tau \to 0^+$ ,

$$\ln \bar{s}(\tau) = \ln K - \sigma(K) \sqrt{\tau \ln\left(\frac{\gamma(K)}{\tau}\right)} \left(1 + \frac{1}{\ln^2\left(\frac{\gamma(K)}{\tau}\right)} + \mathcal{O}\left(\frac{1}{\ln^3\left(\frac{1}{\tau}\right)}\right)\right),\tag{0.3.8}$$

where  $\gamma(K) = \frac{\sigma^2(K)}{8\pi(rK)^2}$  plays the role of a time-scale. In view of (0.3.8), note that the exercise boundary essentially exhibits a parabolic behavior  $\sqrt{\tau}$  along with some logarithmic correction terms (see Ahn et al. [4, Section 7] and references therein for a detailed survey on the asymptotic expansion of the exercise boundary close to maturity).

Combining (0.3.8), Laplace's method, and defining the American implied volatility  $\sigma_A(\tau, s, K)$  as solution to:

$$A(\tau, s, K) = A_{\rm BS}(\tau, s, K; \sigma_A(\tau, s, K)),$$

we obtain the following results.

**Theorem 0.3.1** (Small-time expansions for the American premium). Let  $l(\tau) = \ln\left(\frac{\sigma(K)^2}{8\pi r^2 \tau}\right)$ . If s = K, as  $\tau \to 0^+$ ,

$$p(\tau, s) = \frac{rs}{2}\tau \frac{C_0}{l(\tau)} + C_1 \frac{\ln^2(l(\tau))}{l^2(\tau)} + C_2 \frac{\ln(l(\tau))}{l^2(\tau)} + \frac{C_3}{l^2(\tau)}(1+o(1))$$

where  $C_0, C_1, C_2, C_3$  are universal constants, and if s > K,

$$p(\tau, s, K) = p_0(s, K) \frac{\tau^{\frac{5}{2}}}{l(\tau)} e^{-\frac{d^2(\ln K, \ln s)}{2\tau}} (1 + o(1)),$$

where  $p_0(s, K) = \frac{2rKu_0(\ln s, \ln K)\sigma(K)}{\sqrt{2\pi}d^3(\ln K, \ln s)}$ . Consequently, the difference between the American and European implied volatility is of order

$$\sigma_{\rm A}(\tau, s, K) - \sigma_{\rm E}(\tau, s, K) = \begin{cases} \mathcal{O}\left(\frac{\tau}{l(\tau)}\right), & \text{if } s = K, \end{cases}$$
(0.3.9)

$$\left( \mathcal{O}\left(\frac{\tau^2}{l\left(\tau\right)}\right), \text{ if } s > K. \right.$$
 (0.3.10)

## 0.3.2 Weak approximation in rough forward variance models, and VIX option prices expansion

We now come back to the pricing of VIX derivatives in rough forward variance models (see (0.1.31)). Rather than discretizing the VIX as in Chapter 2, we propose to study its approximation in law (or weak approximation) in the rough Bergomi model (0.1.27). More precisely, motivated by the fact that  $\Delta = \frac{1}{12}$  is small, we introduce the new probability measure

$$\nu_0\left(\mathrm{d}\alpha\right) = \frac{\frac{e^{X_0^\alpha}}{\Delta}\mathrm{d}\alpha}{\int_T^{T+\Delta} e^{X_0^\alpha}\frac{\mathrm{d}\alpha}{\Delta}},$$

and study weak approximations regarding functionals of the

$$\begin{aligned} \operatorname{VIX}_{T}^{2} &= \frac{1}{\Delta} \int_{T}^{T+\Delta} e^{X_{T}^{\alpha}} \mathrm{d}\alpha \\ &= \int_{T}^{T+\Delta} e^{X_{T}^{\alpha} - X_{0}^{\alpha}} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta} \\ &= \left( \int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta} \right) \times \int_{T}^{T+\Delta} e^{-\frac{1}{2} \int_{0}^{T} K^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K^{\alpha}(t) \mathrm{d}W_{t}} \nu_{0}\left(\mathrm{d}\alpha\right), \end{aligned}$$
(0.3.11)

expressed in terms of the following lognormal proxy (exponential of the arithmetic mean)

$$\operatorname{VIX}_{T,P}^{2} = \left(\int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta}\right) \times e^{\int_{T}^{T+\Delta} \left[-\frac{1}{2} \int_{0}^{T} K^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K^{\alpha}(t) \mathrm{d}W_{t}\right] \nu_{0}(\mathrm{d}\alpha)}.$$
 (0.3.12)

The connection between  $\text{VIX}_T^2$  and its proxy  $\text{VIX}_{T,P}^2$  is made through the interpolation ( $\varepsilon \in [0,1]$ ),

$$I(\varepsilon) = \left(\int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta}\right) \int_{T}^{T+\Delta} e^{\int_{T}^{T+\Delta} \left[-\frac{1}{2} \int_{0}^{T} K^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K^{\alpha}(t) \mathrm{d}W_{t}\right] \nu_{0}(\mathrm{d}\alpha)} \times e^{\varepsilon \left(-\frac{1}{2} \int_{0}^{T} K^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K^{\alpha}(t) \mathrm{d}W_{t} - \int_{T}^{T+\Delta} \left[-\frac{1}{2} \int_{0}^{T} K^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K^{\alpha}(t) \mathrm{d}W_{t}\right] \nu_{0}(\mathrm{d}\alpha)}\right) \nu_{0}(\mathrm{d}\alpha),$$

for which by a direct application of Taylor's formula with integral remainder  $I(1) - I(0) = \text{VIX}_T^2 - \text{VIX}_{T,P}^2 = \int_0^1 (1-\varepsilon)I^2(\varepsilon)d\varepsilon \ge 0$  i.e. the lognormal proxy (0.3.12) always underestimates the  $\text{VIX}_T^2$  (0.3.11). Following the methodology of Gobet and Miri [85], we derive option price approximations under the form of explicit combinations of Black–Scholes prices and greeks (see (0.3.13)) which do not rely on small-time asymptotics and are valid for any option maturity.

**Theorem 0.3.2** (Option price expansion in the rough Bergomi model). The price at time 0 of an option on the  $VIX_T^2$  with (smooth) payoff  $\varphi$  can be approximated by

$$\mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T}^{2}\right)\right] = \mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T,\mathrm{P}}^{2}\right)\right] + \sum_{i=1}^{3}\gamma_{i}\,\partial_{\varepsilon}^{i}\mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T,\mathrm{P}}^{2}\times e^{\varepsilon}\right)\right]\Big|_{\varepsilon=0} + \mathcal{O}\left(\Delta^{3H}\right),\qquad(0.3.13)$$

where the coefficients  $(\gamma_i)_{i=1,2,3}$  depend only on  $T, \eta, H$ .



Figure 5 – VIX smiles in the rough Bergomi model (left) for T = 1, 3, 6 months and relative error approximations in % (right) for an initial flat instantaneous log-forward variance  $X_0 =$  $\ln (0.235^2), \eta = 1, H = 0.1, \Delta = \frac{1}{12}$ . The "+" (resp. "\*") corresponds to the zeroth-order (resp. third-order) approximation.

Figure 5 compares the VIX smile and its zeroth-order and third-order approximation (see (0.3.13)) for different maturities (1, 3 and 6 months), and shows that our expansion formula (0.3.13) is quite accurate (less than -2% in relative error for the third-order approximation). Note also that as the proxy (0.3.12) is lognormal, the zeroth-order VIX smile is flat.

Mixed one-factor rough Bergomi model. In order to alleviate the inconsistent VIX smile (which exhibits a pronounced positive skew in the market) generated by the rough Bergomi model, we study the mixed one-factor rough Bergomi model (simultaneously introduced by De Marco [52] and Guyon [95]) defined as

$$\xi_T^{\alpha} = \xi_0^{\alpha} \Big[ \lambda \mathcal{E} \Big( \int_0^T K_1^{\alpha}(t) \mathrm{d}W_t \Big) + (1 - \lambda) \, \mathcal{E} \Big( \int_0^T K_2^{\alpha}(t) \mathrm{d}W_t \Big) \Big], \tag{0.3.14}$$

where  $\mathcal{E}(X)$  is a shorthand notation for  $e^{X-\frac{1}{2}\operatorname{Var}(X)}$ ,  $K_i^{\alpha}(t) = \eta_i (\alpha - t)^{H-\frac{1}{2}}$  for  $i = 1, 2, \eta_1, \eta_2 > 0$  can be different volatility-of-volatility parameters, and  $\lambda \in [0, 1]$  is a mixing parameter. Proxy is now modeled by the exponential mean of a convex combination of lognormal random variables:

$$VIX_{T,P}^{2} = \left(\int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta}\right) \times \left(\lambda e^{\int_{T}^{T+\Delta} \left[-\frac{1}{2}\int_{0}^{T} K_{1}^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K_{1}^{\alpha}(t) \mathrm{d}W_{t}\right]} \nu_{0}(\mathrm{d}\alpha) + (1-\lambda) e^{\int_{T}^{T+\Delta} \left[-\frac{1}{2}\int_{0}^{T} K_{2}^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K_{2}^{\alpha}(t) \mathrm{d}W_{t}\right]} \nu_{0}(\mathrm{d}\alpha)\right). \quad (0.3.15)$$

Following the same strategy used for Theorem 0.3.2 leads to the following option price approximation formula in the mixed one-factor rough Bergomi model (0.3.14).

**Theorem 0.3.3** (Option price expansion in the mixed one-factor rough Bergomi model). The price at time 0 of an option on the VIX<sub>T</sub><sup>2</sup> with (smooth) payoff  $\varphi$  can be approximated by

$$\mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T}^{2}\right)\right] = P_{0} + \sum_{i=1}^{3} \gamma_{i}(\eta_{1})P_{i,1} + \gamma_{i}(\eta_{2})P_{i,2} + \mathcal{O}(\Delta^{3H})$$
(0.3.16)

and

$$P_{0} = \mathbb{E}\left[\varphi\left(\ln\left(\int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta}\right) \left[\lambda e^{\mu_{1}+\sigma_{1}Z} + (1-\lambda) e^{\mu_{2}+\sigma_{2}Z}\right]\right)\right],$$

where  $Z \stackrel{d}{=} \mathcal{N}(0,1)$ , and mean and variance (for j = 1,2) defined as

$$\mu_j = -\frac{1}{2} \int_0^T \left( \int_T^{T+\Delta} K_j^{\alpha}(t)^2 \nu_0(\mathrm{d}\alpha) \right) \mathrm{d}t,$$
  
$$\sigma_j^2 = \int_0^T \left( \int_T^{T+\Delta} K_j^{\alpha}(t)^2 \nu_0(\mathrm{d}\alpha) \right)^2 \mathrm{d}t,$$

and for all i = 1, 2, 3,

$$P_{i,1} = \partial_{\varepsilon}^{i-1} \mathbb{E} \left[ \Psi_1 \left( \mu_1 + \sigma_1 + Z + \varepsilon \right) \right]_{\varepsilon=0}, \qquad P_{i,2} = \partial_{\varepsilon}^{i-1} \mathbb{E} \left[ \Psi_2 \left( \mu_2 + \sigma_2 + Z + \varepsilon \right) \right]_{\varepsilon=0}$$

and

$$\Psi_{1}(x) = \partial_{\omega} \varphi \left( \ln \left( \int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta} \right) \left[ \lambda e^{x+\omega} + (1-\lambda) e^{\frac{\eta_{2}}{2}(\eta_{1}-\eta_{2})\int_{0}^{T} \int_{T}^{T+\Delta} K_{0}^{\alpha}(t)^{2}\nu_{0}(\mathrm{d}\alpha)\mathrm{d}t + \frac{\eta_{2}}{\eta_{1}}x} \right] \right) \Big|_{\omega=0},$$

$$\Psi_{2}(x) = \partial_{\omega} \varphi \left( \ln \left( \int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta} \right) \left[ \lambda e^{\frac{\eta_{1}}{2}(\eta_{2}-\eta_{1})\int_{0}^{T} \int_{T}^{T+\Delta} K_{0}^{\alpha}(t)^{2}\nu_{0}(\mathrm{d}\alpha)\mathrm{d}t + \frac{\eta_{1}}{\eta_{2}}x} + (1-\lambda) e^{x+\omega} \right] \right) \Big|_{\omega=0}.$$



Figure 6 – VIX smiles in the mixed one-factor rough Bergomi model (left) for T = 1, 3, 6 months and relative error approximations in % (right) for an initial flat instantaneous log-forward variance  $X_0 = \ln(0.235^2)$ ,  $\eta_1 = 0.9$ ,  $\eta_2 = 0.7$ ,  $\lambda = 0.3$ , H = 0.1,  $\Delta = \frac{1}{12}$ . The "+" (resp. "\*") corresponds to the zeroth-order (resp. third-order) approximation.

# INTRODUCTION (EN FRANÇAIS)

### 0.4 Méthodes d'approximation de Monte Carlo multi-niveaux

#### 0.4.1 Motivation

La popularité des méthodes de Monte Carlo, en particulier dans la communauté financière, est incontestable. Bien que connues pour converger lentement, elle reste sans aucun doute parmi l'approche la plus générale, la plus fiable et la plus puissante (en particulier pour des problèmes en grande dimension) lorsqu'il s'agit d'estimer des espérances (voir par exemple Hammersley [99] pour une excellente introduction aux méthodes de Monte Carlo, Asmussen et Glynn [12], Kalos et Whitlock [120] pour une étude détaillée des algorithmes de Monte Carlo et de la simulation stochastique). Ces méthodes sont devenues un outil essentiel en finance quantitative, notamment pour la tarification de produits dérivés et la gestion des risques pour lesquelles les praticiens doivent calculer quotidiennement des indicateurs de risque à partir de vastes échantillons de données - voir Glasserman [81] pour une revue des méthodes de Monte Carlo en ingénierie financière ou plus récemment Pagès [147] pour un aperçu général en probabilité numérique et des méthodes de Monte Carlo avec applications aux mathématiques financières.

Dans la plupart des cas, nous souhaitons approximer numériquement une quantité

$$p = \mathbb{E}\left[P\right],$$

pour une variable aléatoire réelle intégrable très générale  $P : (\Omega, \mathcal{A}, \mathbb{P}) \to \mathbb{R}^d$ . Par souci de clarté, nous nous concentrons ici uniquement sur le cas unidimensionnel, c'est-à-dire d = 1, bien que l'extension au cas multidimensionnel (d > 1) soit directe. Dans la majorité des cas, simuler Pne peut être réalisé qu'avec un coût de calcul raisonnable ou est tout simplement impossible. Faisons cependant l'hypothèse que la variable aléatoire P puisse être approchée (dans un sens à préciser plus tard) par une famille de variables aléatoires  $(P_h)_{h>0}$  où h fait référence à un (petit) paramètre d'approximation (ou de biais) et que la variable aléatoire  $P_h$  puisse être simulée avec une complexité de calcul  $\text{Cost}(P_h)$ . Un estimateur naturel pour la quantité  $\mathbb{E}[P_h] \approx \mathbb{E}[P]$  est l'estimateur Monte Carlo standard

$$\widehat{P}_{M,h} = \frac{1}{M} \sum_{m=1}^{M} P_h^{(m)}, \qquad (0.4.1)$$

où M est le nombre de tirages Monte Carlo et  $\left(P_h^{(m)}\right)_{1 \le m \le M}$  sont des copies indépendantes de  $P_h$ . En supposant que  $P_h$  reste intégrable pour tout h > 0, et que l'erreur faible converge vers 0, c'est-à-dire

$$\mathbb{E}\left[P_{h}\right] \xrightarrow[h \to 0]{} \mathbb{E}\left[P\right], \qquad (0.4.2)$$

la loi forte des grands nombres assure que, presque sûrement, pour  $h \to 0$  et  $M \to +\infty$ ,

$$\widehat{P}_{M,h} \to p = \mathbb{E}\left[P\right].$$

La vitesse de convergence (faible) dans la loi forte des grands nombres est régie par le théorème de la limite centrale, qui stipule que si  $P_h$  est de carré intégrable, alors

$$\sqrt{M}\left(\widehat{P}_{M,h} - \mathbb{E}\left[P_{h}\right]\right) \xrightarrow{d} \mathcal{N}\left(0, \sigma_{h}^{2}\right),$$

où  $\sigma_h^2 = \text{Var}(P_h) = \mathbb{E}[P_h^2] - \mathbb{E}[P_h]^2$  est la variance de  $P_h$ . En pratique, nous devons choisir le paramètre de discrétisation h et le nombre de tirages M ce qui engendre deux types d'erreur : une en raison de l'approximation de la variable aléatoire P avec  $P_h$  (erreur de discrétisation ou biais), et une due à la simulation de Monte Carlo (erreur statistique). Plus précisément, supposons que la précision de notre méthode d'approximation soit quantifiée au travers de l'erreur quadratique moyenne MSE, ou de manière équivalente de la racine de l'erreur quadratique moyenne RMSE, tous deux définies comme

$$RMSE = MSE^{\frac{1}{2}} = \mathbb{E}\left[\left(\mathbb{E}\left[P\right] - \mathbb{E}\left[\widehat{P}_{M,h}\right]\right)^{2}\right]^{\frac{1}{2}}.$$
(0.4.3)

Alors, à partir de la (fameuse) décomposition biais-variance, nous avons

$$MSE = \left(\mathbb{E}\left[P\right] - \mathbb{E}\left[\widehat{P}_{M,h}\right]\right)^{2} + \operatorname{Var}\left(\widehat{P}_{M,h}\right)$$
$$= \underbrace{\left(\mathbb{E}\left[P\right] - \mathbb{E}\left[P_{h}\right]\right)^{2}}_{\text{erreur de discrétisation ou biais}} + \underbrace{\frac{\operatorname{Var}\left(P_{h}\right)}{M}}_{\text{erreur statistique}}, \qquad (0.4.4)$$

où la dernière égalité résulte de l'indépendance de  $\left(P_h^{(m)}\right)_{1 \le m \le M}$ . Une question naturelle qui se pose est alors :

**Question.** Pour une précision donnée  $\varepsilon > 0$ , comment devons-nous choisir les paramètres M, h dans le but de satisfaire à la contrainte RMSE  $\leq \varepsilon$ ?

À partir de (0.4.4), nous observons que si le biais (ou erreur faible) est d'ordre 1, i.e.  $|\mathbb{E}[P] - \mathbb{E}[P_h]| = \mathcal{O}(h)$ , et que Var $(P_h) = \mathcal{O}(1)$ , alors

$$RMSE = \mathcal{O}(h) + \mathcal{O}(M^{-\frac{1}{2}}).$$

Par conséquent, pour que la RMSE soit proportionnelle à  $\varepsilon$ , il nous faut choisir  $M = \mathcal{O}(\varepsilon^{-2})$  et  $h = \mathcal{O}(\varepsilon)$  ce qui conduit à un coût de calcul total de

$$\operatorname{Cost}(\widehat{P}_{M,h}) = \operatorname{Cost}(P_h) \times M = \operatorname{Cost}(P_h) \times \mathcal{O}\left(\varepsilon^{-2}\right), \qquad (0.4.5)$$

pour l'estimateur Monte Carlo standard (0.4.1). Notons que si P peut être simulée exactement (c'est-à-dire sans biais) alors l'erreur quadratique moyenne et la complexité de calcul totale se réduisent à

$$MSE = \frac{Var(P)}{M}, \quad Cost(\widehat{P}_M) = Cost(P) \times M = Cost(P) \times \mathcal{O}\left(\varepsilon^{-2}\right).$$

Il s'agit de la complexité optimale pour les estimateurs standards de Monte Carlo sans biais. Comme expliqué plus en détail ci-dessous, l'algorithme de Monte Carlo multi-niveaux atteint (dans des conditions appropriées) un telle complexité optimale.

#### 0.4.2 L'approche multi-niveaux

Heinrich a été le premier à utiliser l'idée multi-niveaux en tant que technique de réduction de variance (Heinrich et Sindambiwe [106], Heinrich [102, 103, 104, 105]). Dans ses travaux fondateurs, Heinrich a développé des méthodes de Monte Carlo multi-niveaux pour l'intégration numérique, l'évaluation fonctionnelle découlant de la solution d'équations intégrales et pour les opérateurs intégraux faiblement singuliers. Pour le premier cas, l'auteur souhaitait estimer la valeur de  $\mathbb{E} [f(X,\lambda)]$  où X est une variable aléatoire de dimension finie et  $\lambda$  un paramètre. Si  $\lambda$  appartient à [0,1], alors ayant estimé  $\mathbb{E} [f(X,0)]$  et  $\mathbb{E} [f(X,1)]$ , nous pouvons utiliser  $\frac{1}{2} (f(X,0) + f(X,1))$  comme variable de contrôle pour l'estimation de  $\mathbb{E} [f(X,\frac{1}{2})]$ . L'intuition étant que la variance de  $f(X,\frac{1}{2}) - \frac{1}{2} (f(X,0) + f(X,1))$  sera probablement plus petite que celle de  $f(X,\frac{1}{2})$ . Une telle procédure peut ensuite être appliquée récursivement pour l'estimation de toutes les valeurs de  $\lambda$ , à condition que  $f(X, \cdot)$  soit suffisamment régulière et se traduira par de grandes économies en termes de temps calcul.

Dans [74], Giles généralise les idées de Heinrich et utilise l'approche multi-niveaux pour le mouvement brownien (variable aléatoire infini-dimensionnel). Pourtant, comme expliqué cidessous, la technique de réduction de variance est très similaire : les trajectoires grossières (grandes valeurs de h) sont utilisées comme variables de contrôle pour l'estimation des trajectoires plus fines (petites valeurs de h).

Cette approche multi-niveaux est également une extension de la méthode à deux niveaux de Kebaier [123], aussi connue sous le nom de méthode statistique de Romberg. Cela a été inspiré, à son tour, par un autre travail portant sur les multi-réseaux pour des solutions itératives d'approximations d'équations aux dérivées partielles pour certaines applications en physique statistique (voir Brandt, Galun et Ron [37], Brandt et Ilyin [36]).

**Théorème pour l'estimateur Monte Carlo multi-niveaux.** Nous revenons maintenant à notre problème général, à savoir estimer la quantité  $p = \mathbb{E}[P]$  pour laquelle la variable aléatoire P peut seulement être approximée par  $P_h$  à un certain ordre h > 0. Notons que plus h est petit, meilleure est l'approximation mais plus le coût de calcul est élevé.

Fixons une constante  $L \in \mathbb{N}^*$  (nombre de niveaux) et considérons un vecteur de paramètres d'approximation  $\mathbf{h} = (h_0, \ldots, h_L)$  dont les composantes sont décroissantes  $(h_L < \cdots < h_0)$ , avec une précision croissante mais un coût de plus en plus élevé. Avec un léger abus de notation, nous écrivons maintenant

$$P_l = P_{h_l}$$
, pour tout  $l = 1, \ldots, L$ ,

et nous souhaitons estimer l'approximation fine  $\mathbb{E}[P_{h_L}]$ . Le niveau l = 0 fait référence à l'approximation la plus grossière tandis que le niveau l = L est la plus fine. Par exemple, supposons que nous voulions simuler la solution d'une équation différentielle stochastique (EDS) sur un intervalle de temps [0, T] avec T > 0. Le paramètre  $h_l$  représenterait le pas de temps de la discrétisation de l'EDS pour lequel un choix possible pourrait être un pas de temps uniforme de la forme  $h_l = 2^{-l}T$  pour tout  $l = 0, \ldots, L$ . Plus le niveau l serait élevé et plus le pas de temps serait petit.

À partir de la somme télescopique,

$$\mathbb{E}\left[P_L\right] = \mathbb{E}\left[P_0\right] + \sum_{l=1}^{L} \mathbb{E}\left[P_l - P_{l-1}\right], \qquad (0.4.6)$$

l'approche multi-niveaux consiste à estimer indépendamment l'espérance du niveau le plus grossier  $\mathbb{E}[P_0]$  avec un nombre important de tirages Monte Carlo  $M_0$  et l'espérance de la différence  $\mathbb{E}[P_l - P_{l-1}]$  avec un nombre décroissant de tirages Monte Carlo  $M_l$  pour tous les niveaux  $l = 0, \ldots, L$ , c'est-à-dire considérer l'estimateur

$$\widehat{P}_{l,M_l} = \frac{1}{M_l} \sum_{m=1}^{M_l} \left( P_l^{(m)} - P_{l-1}^{(m)} \right), \quad P_{-1} = 0.$$

En introduisant le vecteur de tirages Monte Carlo (décroissants)  $\mathbf{M} = (M_0, \ldots, M_L)$ , l'estimateur multi-niveaux est ainsi défini comme :

$$\widehat{P}_{\boldsymbol{M},\boldsymbol{h}}^{\mathrm{ML}} = \sum_{l=1}^{L} \widehat{P}_{l,M_{l}} = \frac{1}{M_{0}} \sum_{m=1}^{M_{0}} P_{0}^{(0,m)} + \sum_{l=1}^{L} \frac{1}{M_{l}} \sum_{m=1}^{M_{l}} \left( P_{l}^{(l,m)} - P_{l-1}^{(l,m)} \right), \qquad (0.4.7)$$

où

- 1. Pour tout l,  $\left(P_l^{(l,m)}\right)_{1 \le m \le M_l}$  et  $\left(P_{l-1}^{(l,m)}\right)_{1 \le m \le M_l}$  sont indépendants, identiquement distribués et ayant la même loi que  $P_l$  et  $P_{l-1}$  respectivement.
- 2. Les niveaux sont indépendants entre eux.
- 3. Pour chaque niveau l,  $P_l^{(l,m)}$  et  $P_{l-1}^{(l,m)}$  sont construits avec les mêmes nombres aléatoires communs. L'intuition étant que que, en conséquence de la convergence forte, la différence  $P_l^{(l,m)} P_{l-1}^{(l,m)}$  devient de plus en plus petite, et donc sa variance, à mesure que le nombre des niveaux l augmente.

Rappelons que  $P_{-1} = 0$  et désignons pour tout  $l = 1, \ldots, L$ ,

$$C_{l} = \text{Cost}(P_{l} - P_{l-1}), \quad V_{l} = \text{Var}(P_{l} - P_{l-1}),$$

le coût et la variance d'un échantillon  $P_l - P_{l-1}$ . La complexité totale de l'estimateur multiniveaux (0.4.7) est  $\sum_{l=0}^{L} M_l C_l$  et grâce à l'indépendance entre les niveaux, nous avons que :

$$\mathbb{E}\left[\widehat{P}_{\boldsymbol{M},\boldsymbol{h}}^{\mathrm{ML}}\right] = \mathbb{E}\left[P_{L}\right], \quad \operatorname{Var}\left(\widehat{P}_{\boldsymbol{M},\boldsymbol{h}}^{\mathrm{ML}}\right) = \sum_{l=0}^{L} \frac{V_{l}}{N_{l}}.$$
(0.4.8)

Nous rappelons maintenant le théorème de Giles [75, Théorème 1].

**Theorem 0.4.1.** Soit P une variable aléatoire et  $P_l$  son approximation au niveau l correspondante S'il existe des estimateurs indépendants  $\widehat{P}_{l,M_l}$  basés sur  $M_l$  tirages Monte Carlo, chacun avec coût calcul  $C_l$ , une variance  $V_l$ , des constantes positives  $\alpha, \beta, \gamma, c_1, c_2, c_3, c_4$  tels que  $\alpha \geq \frac{1}{2} \min(\beta, \gamma)$  et

1.  $|\mathbb{E}[P_l - P]| \le c_1 2^{-\alpha l},$ 2.  $\mathbb{E}[\widehat{P}_{l,M_l}] = \mathbb{E}[P_l - P_{l-1}], \quad P_{-1} = 0,$ 3.  $V_l \le c_2 2^{-\beta l},$ 4.  $C_l \le c_3 2^{\gamma l},$ 

alors il existe une constante positive  $c_4$  telle que pour tout  $\varepsilon < e^{-1}$ , il existe des valeurs L et  $M_l$ pour lesquelles l'estimateur multi-niveaux

$$\widehat{P}_{\boldsymbol{M},\boldsymbol{h}}^{\mathrm{ML}} = \sum_{l=0}^{L} \widehat{P}_{l,M_l},$$

a une erreur quadratique moyenne avec borne

$$MSE = \mathbb{E}\left[\left(\widehat{P}_{\boldsymbol{M},\boldsymbol{h}}^{ML} - \mathbb{E}\left[P\right]\right)^{2}\right] < \varepsilon^{2}$$

et une complexité C inférieure à

$$\mathbb{E}[C] \leq \begin{cases} c_4 \varepsilon^{-2}, & \beta > \gamma, \\ c_4 \varepsilon^{-2} \left( \ln \varepsilon \right)^2, & \beta = \gamma, \\ c_4 \varepsilon^{-2 - \frac{\gamma - \beta}{\alpha}}, & \beta < \gamma. \end{cases}$$

Mentionnons également que lorsqu'une expansion polynomiale en  $h^{\alpha}~(\alpha>0)$  existe pour le biais, c'est-à-dire

$$\mathbb{E}[P_h] = \mathbb{E}[P] + \sum_{k=1}^{R} c_k h^{\alpha k} + o(h^{\alpha R}), \quad R \in \mathbb{N}^*,$$

une version pondérée, qui à la fois améliore et généralise l'estimateur (0.4.7) (l'estimateur multiniveaux pondéré de Richardson-Romberg), a été introduite par Lemaire et Pagès [134] (voir également Giorgi [78], Giorgi, Lemaire et Pagès [79, 80]).

## 0.4.3 Monte Carlo multi-niveaux pour les espérance imbriquées et bornes inférieures et supérieures pour les calculs de risques imbriqués.

Dans le Chapitre 1, nous appliquons des méthodes de Monte Carlo multi-niveaux pour l'évaluation d'espérances imbriquées, c'est-à-dire pour des quantités de la forme

$$p = \mathbb{E}\left[g\left(\mathbb{E}\left[f\left(X,Y\right)|X\right]\right)\right],\tag{0.4.9}$$

où X, Y sont deux variables indépendantes à valeurs dans  $\mathbb{R}^d$  et  $\mathbb{R}^{d'}$ , et  $f : \mathbb{R}^d \times \mathbb{R}^{d'} \to \mathbb{R}$  et  $g : \mathbb{R} \to \mathbb{R}$  sont deux fonction mesurables. Par indépendance, l'espérance conditionnelle (0.4.9) est égale à

$$\mathbb{E}\left[f\left(X,Y\right)|X\right] = E_f\left(X\right),\tag{0.4.10}$$

où pour tout  $x \in \mathbb{R}^d$ ,  $E_f(x) := \mathbb{E}[f(x, Y)]$ . La variable aléatoire  $E_f(X)$  peut alors uniquement être approchée et comme  $E_f(\cdot)$  s'écrit comme une espérance, un estimateur sans biais naturel pour (0.4.10) est donné par

$$\widehat{E}_{f,n}\left(X\right) = \frac{1}{n} \sum_{i=1}^{n} f\left(X, Y_{i}\right), \quad n \in \mathbb{N}^{*},$$

où les  $(Y_i)_{1 \le i \le n}$  sont i.i.d. de loi Y et indépendants de X. Le biais de la variable aléatoire  $g(\widehat{E}_{f,n}(X))$  dépend de la régularité de la fonction externe g: il existe un compromis entre la régularité de la fonction g et celle de la distribution de probabilité des variables aléatoires sous-jacentes - moins il y a de régularité pour g, plus les exigences relatives aux distributions sous-jacentes sont importantes.

Mentionnons également que ceci est exactement le formalisme de la Section 0.4.1 : ici la variable aléatoire  $P = g(E_f(X))$  peut seulement être approchée par  $P_n = g(\widehat{E}_{f,n}(X))$  pour laquelle  $\frac{1}{n}$  joue le rôle du paramètre d'approximation h.

Les espérance imbriquées de la forme (0.4.9) sont omniprésentes en finance quantitative (voir par exemple Gordy et Juneja [89]). De possibles exemples sont la tarification des produits dérivés de type américain (Lamberton et Lapeyre [129]), l'estimation de risques financiers comme la VaR ou CVaR pour un portefeuille (McNeil, Frey et Embrechts [140]) ou la CVA (Abbas-Turki, Crépey et Diallo [1]) ou l'évaluation de marge pour les portefeuilles qui font l'objet d'une compensation centrale ([17]). Mathématiquement, la plupart de ces calculs nécessitent soit l'estimation d'une espérance pour l'exposition d'un portefeuille pour laquelle :

$$p = \mathbb{E}\Big[\Big(\mathbb{E}[f(X_{t_2})|X_{t_1}]\Big)_+\Big],\tag{0.4.11}$$

où  $(X_{t_1}, X_{t_2})$  est un facteur de risque de marché aux dates  $t_1 < t_2$  et  $g(x) = x_+$ , ou soit l'estimation de la distribution finale d'un processus de perte pour laquelle :

$$p = \mathbb{P}\left(L(X_{t_1}) \ge a\right) = \mathbb{E}\left[\mathbf{1}_{\mathbb{E}\left[f\left(X_{t_2}\right)|X_{t_1}\right] \ge a}\right],\tag{0.4.12}$$

où  $L(X_{t_1}) = \mathbb{E}[f(X_{t_2})|X_{t_1}]$  indique la perte d'un portefeuille conditionnellement à la valeur du facteur de risque  $X_{t_1}$  au temps  $t_1$  (voir Chapitre 3), et  $g(x) = \mathbf{1}_{x \geq a}$  est une fonction indicatrice. Lorsqu'il s'agit de fonctions indicatrices comme dans (0.4.12), la plupart des auteurs (voir par exemple Gordy et Juneja [89] ou Giorgi, Lemaire et Pagès [80]) supposent d'exigeantes et (dans certains cas) d'invérifiables hypothèses sur la distribution des variables aléatoires sous-jacentes. Plus précisément, ils requièrent des hypothèses de régularité pour la densité du couple  $\left(\mathbb{E}[f(X,Y)|X], X\right)$  et  $\left(\mathbb{E}[f(X,Y)|X], \frac{1}{n}\sum_{j=1}^{n} f(X,Y_j) - \mathbb{E}[f(X,Y)|X]\right)$ . Motivés par l'application du calcul de la marge initiale pour laquelle g est de la forme g(x) = |x|ou  $g(x) = (x - a)_+$  pour un réel a, nous portons notre attention aux fonctions  $C_b^1$  pour g. Le fait d'être en situation de régularité intermédiaire pour la fonction g - moins que  $C^2$ , mais plus régulière qu'une fonction échelon - nous permet de contourner les hypothèses restrictives énoncées ci-dessus sur la distribution sous-jacente. Nous supposons plutôt que les hypothèses moins restrictives suivantes soient valables :

**Assumption 0.4.2.** La fonction g est continue, et il existe un nombre fini de points  $-\infty = d_0 < d_1 < ... < d_\theta < d_{\theta+1} = \infty$  tels que sur chaque intervalle ouvert  $(d_i, d_{i+1}), 0 \le i \le \theta$ , g est de classe  $C^1$ , g' est bornée, continue et Hölder pour un certain exposant  $\eta \in (0, 1]$ .

Nous devons également pouvoir contrôler la probabilité que la variable aléatoire  $E_f(X) = \mathbb{E}[f(X,Y)|X]$  puisse prendre des valeurs dans un voisinage des singularités de g (Hypothèse 0.4.4) et l'existence des moments d'ordre p > 2 pour la variable aléatoire f(X,Y) (Hypothèse 0.4.3), une condition qui est vérifiée dans la plupart des exemples en pratique.

Assumption 0.4.3. Il existe p > 2 tel que  $\mathbb{E}\left[|f(X,Y)|^p\right] < \infty$ .

Assumption 0.4.4 (Estimées autour des singularités). Il existe des constantes positives  $\nu$ ,  $K_{\nu}$  et  $z_0$  telles que

$$\mathbb{P}\left(\operatorname{dist}(E_f(X), D) \le z\right) \le K_{\nu} z^{\nu}, \qquad \forall z < z_0, \qquad (0.4.13)$$

 $o\dot{u} \operatorname{dist}(y, D) := \min_{1 \le i \le \theta} |y - d_i|.$ 

Nous approchons l'espérances extérieure et intérieure de (0.4.9) avec des échantillons indépendants de Monte Carlo en considérant l'estimateur Monte Carlo imbriqué (NMC),

$$\widehat{P}_{M,N} = \frac{1}{M} \sum_{m=1}^{M} g\left(\frac{1}{N} \sum_{j=1}^{N} f\left(X_m, Y_j^m\right)\right), \qquad (0.4.14)$$

où  $M, N \in \mathbb{N}^*$ , et  $(X_m)_{m \in \mathbb{N}^*}, (Y_j^m)_{j,m \in \mathbb{N}^*}$  sont i.i.d. ayant la même loi que X et Y respectivement, et dont la complexité est donnée par la proposition ci-dessous.

**Proposition 0.4.5** (Complexité de l'estimateur Monte Carlo imbriqué (0.4.14)). Supposons que les Hypothèses 0.4.2, 0.4.3 et 0.4.4 soient vérifiées, et considérons une précision  $\varepsilon > 0$ . Quand  $\varepsilon \to 0$ , la borne MSE =  $\mathcal{O}(\varepsilon^2)$  pour l'estimateur (0.4.14), est atteinte avec complexité  $\mathcal{O}\left(\varepsilon^{-2\left(1+\frac{1}{1+\frac{(p-1)\nu}{p+\nu}\wedge\eta}\right)}\right)$  en choisissant  $M \sim \varepsilon^{-2}$  et  $N \sim \varepsilon^{-\frac{2}{1+\frac{(p-1)\nu}{p+\nu}\wedge\eta}}$ .

Notons que dans le cas où la fonction est régulière, nous pouvons prendre  $\eta = 1$ ,  $\nu = \infty$  et supposer  $p \geq 2$ , le quotient pour N se simplifie alors en  $\frac{(p-1)\nu}{p+\nu} \wedge \eta = (p-1) \wedge \eta = 1$ , et on retrouve la complexité habituelle  $\mathcal{O}(\varepsilon^{-3})$  pour les estimateurs imbriqués avec fonctions régulières. Cet estimateur coûteux en temps calcul peut être amélioré en utilisant un estimateur Monte Carlo multi-niveaux spécifique capable d'atteindre une complexité optimale en  $\mathcal{O}(\varepsilon^{-2})$ .

Un estimateur multi-niveaux antithétique pour les espérances imbriquées. Par (0.4.7), nous construisons un estimateur Monte Carlo multi-niveaux antithétique en combinant des estimateurs de la forme  $\hat{P}_{M,N}$ . Plus précisément, soient deux familles de variables aléatoires indépendantes et i.i.d.  $(X_m^l)_{l,m\in\mathbb{N}^*}$  et  $(Y_j^{l,m})_{j,l,m\in\mathbb{N}^*}$ , distribuées selon X et Y respectivement. Soit  $L \in \mathbb{N}^*$  le nombre de niveaux,  $\mathbf{M} = (M_0, ..., M_L) \in (\mathbb{N}^*)^{L+1}$ , respectivement  $\mathbf{n} = (n_0, ..., n_L) \in$  $(\mathbb{N}^*)^{L+1}$ , être des multi-indices représentant le nombre de tirages utilisés pour approximer l'espérance externe, respectivement l'espérance conditionnelle interne dans (0.4.9) aux différents niveaux. Enfin, nous définissons le nombre de tirages pour l'espérance conditionnelle interne par

$$n_l = n_0 2^l, \qquad 0 \le l \le L.$$

L'estimateur antithétique multi-niveaux de p est défini comme

$$\widehat{P}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}} = \frac{1}{M_0} \sum_{m=1}^{M_0} g\left(\frac{1}{n_0} \sum_{j=1}^{n_0} f\left(X_m^0, Y_j^{0,m}\right)\right) + \sum_{l=1}^{L} \frac{1}{M_l} \sum_{m=1}^{M_l} \left\{g\left(\frac{1}{n_l} \sum_{j=1}^{n_l} f\left(X_m^l, Y_j^{l,m}\right)\right) - \frac{1}{2} \left(g\left(\frac{1}{n_{l-1}} \sum_{j=1}^{n_{l-1}} f\left(X_m^l, Y_j^{l,m}\right)\right) + g\left(\frac{1}{n_{l-1}} \sum_{j=n_{l-1}+1}^{n_l} f\left(X_m^l, Y_j^{l,m}\right)\right)\right)\right\}.$$
(0.4.15)

Notons que, dans l'expression entre accolades, la fonction g est évaluée plus d'une fois sur différentes moyennes empiriques, construites à partir des échantillons  $X_m^l$  et  $Y_j^{l,m}$  au niveau lseulement. Les degrés de liberté restants de l'estimateur résident dans les choix de  $n_0$ , L, et de la taille du nombre de tirages  $M_l$  pour chaque l, et l'estimateur multi-niveaux (0.4.15) atteint l'optimalité asymptotique.

**Theorem 0.4.6.** Supposons vérifiées les Hypothèses 0.4.2, 0.4.3 et 0.4.4, et considérons une erreur  $\varepsilon > 0$ . Alors, il existe  $n_0, M_0, L$  tels que pour  $\varepsilon \to 0$  la borne MSE =  $\mathcal{O}(\varepsilon^2)$  pour l'estimateur (0.4.15) soit atteinte avec complexité  $\mathcal{O}(\varepsilon^{-2})$  en choisissant :

$$n_l = n_0 2^l, \quad M_l = M_0 2^{-\left(1 + \frac{(p-2)\nu}{4(p+\nu)} \wedge \frac{\eta}{2}\right)l}, \quad 0 \le l \le L.$$

Limites supérieures et inférieures non imbriquées. Pour la tarification d'options américaines, l'approche duale proposée par Andersen et Broadie [7] requiert l'estimation d'espérances imbriquées à chaque pas de temps en utilisant de nombreuses trajectoires. S'appuyant sur leur idée et un papier récent de Guo et Loeper [93], nous fournissons des bornes inférieures et supérieures non-imbriquées, que nous abordons avec une procédure fondée sur des techniques de régression, ainsi que des estimations d'erreur pour l'estimation de p.

**Theorem 0.4.7.** Soit  $\mathcal{R}$  une variable aléatoire réelle et intégrable et  $g : \mathbb{R} \to \mathbb{R}$  une fonction convexe telle que  $g(\mathcal{R})$  soit intégrable. L'identité suivante est satisfaite

$$\sup_{\varphi} J_{\varphi} = \mathbb{E}\left[g(\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right])\right] = \inf_{\varepsilon} \mathbb{E}\left[g(\mathcal{R}-\varepsilon)\right], \qquad (0.4.16)$$

оù

$$J_{\varphi} = g(z) + g'(z)(\mathbb{E}\left[\mathcal{R}\right] - z) + \int_{z}^{\infty} \mathbb{E}\left[(\mathcal{R} - u)\mathbf{1}_{\varphi(\mathcal{O}) \ge u}\right] \mu(\mathrm{d}u) + \int_{-\infty}^{z} \mathbb{E}\left[(u - \mathcal{R})\mathbf{1}_{\varphi(\mathcal{O}) \le u}\right] \mu(\mathrm{d}u),$$

et l' inf est pris sur l'ensemble des variables aléatoires { $\varepsilon$  est intégrable et telle que  $\mathbb{E}[\varepsilon|\mathcal{O}] = 0$ }. L'égalité est atteinte pour  $\varphi^*(\mathcal{O}) = \mathbb{E}[\mathcal{R}|\mathcal{O}]$  et pour  $\varepsilon^* = \mathcal{R} - \mathbb{E}[\mathcal{R}|\mathcal{O}]$ . De plus, nous avons l'estimation d'erreur suivante

$$0 \le J_{\varphi^{\star}} - J_{\varphi} \le 2 \mathbb{E} \Big[ \big| \varphi^{\star}(\mathcal{O}) - \varphi(\mathcal{O}) \big| \mu([\varphi^{\star}(\mathcal{O}), \varphi(\mathcal{O})]) \Big], \qquad (0.4.17)$$

où  $\mu([a,b])$  correspond à la mesure [a,b] si  $a \leq b$  ou [b,a] si b < a. Si g est Lipschitz avec constante de Lipschitz  $L_q$ , l'estimation d'erreur

$$0 \le \mathbb{E}\left[g(\mathcal{R} - \varepsilon)\right] - \mathbb{E}\left[g(\mathcal{R} - \varepsilon^{\star})\right] \le L_g \left\|\varepsilon^{\star} - \varepsilon\right\|_1.$$
(0.4.18)

est directe. Enfin, si g est de classe  $C^2$  avec dérivée seconde bornée, la borne supérieure dans (0.4.18) peut être remplacée par  $\frac{1}{2} \|g''\|_{\infty} \|\varepsilon^* - \varepsilon\|_2^2$ .

Application aux calculs de marge initiale. Pour plusieurs types de transactions, les banques et institutions financières doivent déposer des garanties auprès d'une contrepartie centrale (CCP, également appelée chambre de compensation) pour sécuriser leurs positions. Chaque jour, la CCP demande à chaque membre du marché de déposer un certain capital en fonction de l'exposition au risque de ses contrats. L'un de ces capitaux de protection est le dépôt de marge initiale (IM) : en cas de défaut de l'un des membres de la CCP, ce capital vise à couvrir les pertes potentielles subies par le portefeuille de couverture pendant la période de liquidation du membre défaillant - concrètement, l'IM est matérialisée par la VaR ou la CVaR du portefeuille du membre sur une période de temps  $\Delta$ . Puisque l'intervalle de temps  $\Delta$  est petit en nombre d'années (typiquement, une semaine), l'approche usuelle est d'appliquer une expansion asymptotique pour la solution de l'équation stochastique impliquée lorsque  $\Delta$  devient petit, voir Henry-Labordère [108, Section 4.2] et Agarwal et al. [3].

Plus précisément, dans un cadre Black–Scholes pour lequel l'actif est modélisé comme  $S_t = S_0 e^{\left(r - \frac{\sigma^2}{2}\right)t + \sigma W_t}$  où W est un mouvement brownien et le prix initial  $S_0 > 0$ , le taux d'intérêt r > 0 et la volatilité  $\sigma > 0$  sont constants, le calcul de la marge initiale nécessite l'estimation d'espérances imbriquées pour laquelle le Théorème 0.4.6 s'applique.

Suivant la méthodologie de Agarwal et al. [3], la correction de marge initiale pour une option avec payoff  $\varphi(S_T)$  est calculée selon la CVaR de l'évolution future du portefeuille répliquant sur un petit intervalle de temps  $\Delta > 0$ . Quand  $\Delta = 0$  (pas de correction de marge initiale), le prix à la date t est donné par le prix classique Black–Scholes  $\mathbb{E}\left[e^{-r(T-t)}\varphi(S_T)|S_t\right]$ , avec comme derivée première  $\delta(t, S) = \partial_s \mathbb{E}\left[e^{-r(T-t)}\varphi(S_T)|S_t = s\right]$ . Comme montré dans Agarwal et al. [3], pour de petites valeurs de  $\Delta$ , une correction au premier ordre de ce prix Black–Scholes conduit à considérer la quantité :

$$R C_{\alpha} \mathbb{E}\left[\int_{0}^{T} e^{-rt} \sqrt{(t+\Delta) \wedge T - t} |Z_{t}| \,\mathrm{d}t\right], \qquad (0.4.19)$$

où R est le taux d'intérêt du coût de financement,  $C_{\alpha} := \text{CVaR}^{\alpha} \left( \mathcal{N}(0,1) \right) = \left. \frac{e^{-\frac{x^2}{2}}}{(1-\alpha)\sqrt{2\pi}} \right|_{x=\Phi^{-1}(\alpha)}$  est la CVaR d'une variable aléatoire gaussienne, et

$$Z_t = z(t, S_t) := \sigma S_t \,\delta(t, S_t). \tag{0.4.20}$$

En utilisant la méthode du rapport de vraisemblance de Broadie et Glasserman [38], nous pouvons exprimer Z comme une espérance

$$z^{BS}(t,s) = \sigma s \,\partial_s \mathbb{E}\left[ e^{-r(T-t)} \varphi(S_T) \middle| S_t = s \right]$$
$$= \mathbb{E}\left[ e^{-r(T-t)} \left( \varphi(S_T) - \varphi(S_t) \right) \frac{W_T - W_t}{T-t} \middle| S_t = s \right].$$
(0.4.21)

Dans la dernière expression, le terme conditionnellement centré  $-\varphi(S_t)\frac{W_T-W_t}{T-t}$ , que nous avons artificiellement introduit, permet de réduire la variance de l'estimateur associé, en jouant le rôle d'une variable de contrôle (voir [147, Chapitre 3]).

En supposant que chaque opération de couverture soit effectuée avant  $\tilde{T} := T - \Delta$ , nous avons  $\sqrt{(t + \Delta) \wedge T - t} = \sqrt{\Delta}$  dans (0.4.19), ce qui permet de considérer la quantité légèrement mod-

 $\sqrt{(t+\Delta)} \wedge T - t = \sqrt{\Delta} \text{ dans } (0.4.19), \text{ ce qui permet de considérer la quantité légèrement mod$ ifiée :

$$RC_{\alpha}\sqrt{\Delta}\,\tilde{T}\,\mathbb{E}\left[\frac{1}{\tilde{T}}\int_{0}^{T}e^{-rt}\left|z(t,S_{t})\right|\,\mathrm{d}t\right] = RC_{\alpha}\sqrt{\Delta}\,\tilde{T}\,\mathbb{E}\left[e^{-rU}\left|z(U,S_{U})\right|\right] =:RC_{\alpha}\sqrt{\Delta}\,\tilde{T}\times I,$$

$$(0.4.22)$$

où au lieu de discrétiser l'intégrale en temps sur  $[0, \tilde{T}]$  - ce qui produirait un biais - nous avons introduit une variable aléatoire indépendante U avec une distribution uniforme sur  $[0, \tilde{T}]$ . En ignorant le produit de constantes  $R C_{\alpha} \sqrt{\Delta} \tilde{T}$  (qui peut être fixé une fois pour toute), la quantité I dans (0.4.22) peut être mise sous la forme d'une espérance conditionnelle comme dans (0.4.9). Nous nous intéressons plus particulièrement à une option butterfly dont le payoff est donné par

 $\varphi(s) = (s - (K + a))_{+} + (s - (K - a))_{+} - 2(s - K)_{+},$ 

et dont le delta change de signe (voir Figure 7).



Figure 7 – Delta  $S \to \Delta_t(S)$  d'un Call (rouge), Put (orange) et Butterfly (bleu) en fonction du spot S dans un modèle Black–Scholes avec paramètres  $S_0 = K = 100, a = \frac{K}{2}, T = 1, t = \frac{T}{5}, r = 0.1, \sigma = 0.3.$ 

Puisque  $\delta^{butterfly}$  change de signe et parce que la fonction valeur absolue g a un point singulier en zéro, nous devons étudier le comportement de  $\delta^{butterfly}$  autour du zéro pour vérifier si l'Hypothèse 0.4.4 tient.

**Theorem 0.4.8.** Les Hypothèses 0.4.2, 0.4.3, 0.4.4 sont vérifiées dans le calcul d'une option Butterfly avec  $\eta = 1$ , tout p > 2 et  $\nu = \frac{1}{2} \left( 1 \wedge \frac{T - \tilde{T}}{\tilde{T}(1+A)} \right)$  pour tout A > 0. Ainsi, le Théorème 0.4.6 s'applique.

## 0.4.4 Monte Carlo multi-niveaux dans les modèles rough pour la variance forward

Dans le Chapitre 2, nous étudions des méthodes d'approximation de Monte Carlo multi-niveaux pour la tarification d'options sur la variance dans des modèles rough pour la variance forward. Avant de donner plus de détails, nous rappelons quelques concepts de base de la modélisation de la variance forward, dont la première apparition est due à Dupire [57], et a ensuite été largement étudiée par Bergomi [26, 27, 28, 29].

Swaps de variance et variance forward. Par définition, la variance réalisée annualisée d'un d'actif S pour une période [t, T] avec n jours ouvrables  $t_0 = t < \cdots < t_n = T$  est définie comme

$$\mathrm{RV}^{[t,T]} = \frac{1}{T-t} \sum_{i=1}^{n} \ln\left(\frac{S_{t_i}}{S_{t_{i-1}}}\right)^2, \qquad (0.4.23)$$

où T - t est exprimé en années. Un swap de variance sur la période [t, T] est un contrat qui paie l'écart réalisé pour la période [t, T]. Une variance forward sur [t, T] (ou variance implicite du swap de variance), dénotée  $V_t^T$ , est définie comme

$$V_t^T = \text{price}_t^{\text{mkt}} \left( \text{RV}^{[t,T]} \right), \qquad (0.4.24)$$

où price $_t^{\text{mkt}}(\cdot)$  fait référence au prix du marché au moment t.

Variance forward instantanée. Par analogie avec les taux forward instantanés des prix d'obligations, nous définissons la variance forward instantanée observée au temps t et pour une maturité T > t comme

$$\xi_t^T = \frac{\mathrm{d}}{\mathrm{d}T} \left( (T - t) \, V_t^T \right), \quad t < T,$$

de sorte que la variance forward se réécrit comme

$$V_t^T = \frac{1}{T-t} \int_t^T \xi_t^\alpha \mathrm{d}\alpha, \quad t < T.$$

La question naturelle qui se pose est alors :

**Question.** Par quel type de modèles devrions-nous modéliser la quantité  $(\xi_t^T)_{t < T}$ ?

Variances forward sur  $[T_1, T_2]$ . Il est possible de construire une variance forward sur la période future  $[T_1, T_2]$ . En effet, soient  $t < T_1 < T_2$ . Au temps t, nous pouvons construire le payoff

$$\operatorname{RV}^{[T_1, T_2]} - V_t^{T_1, T_2}, \quad T_2 > T_1,$$

en ajoutant des positions (d'achat et de vente) en swaps de variance sur les périodes  $[t, T_1]$  et  $[t, T_2]$ .  $V_t^{T_1, T_2}$  est alors appelée la variance forward sur  $[T_1, T_2]$  et puisque la variance réalisée est additive,  $V_t^{T_1, T_2}$  est donnée par

$$V_t^{T_1,T_2} = \frac{(T_2 - t) V_t^{T_2} - (T_1 - t) V_t^{T_1}}{T_2 - T_1}$$

de sorte que

$$V_t^{T_1, T_2} = \frac{1}{T_2 - T_1} \int_{T_1}^{T_2} \xi_t^{\alpha} \mathrm{d}\alpha, \qquad t < T_1 < T_2.$$

Nous observons alors que la variance forward  $V^{T_1,T_2}$  peut être achetée. En effet, en considérant un autre temps  $t' \ge t$ , nous pouvons considérer le payoff inverse

$$-\mathrm{RV}^{[T_1,T_2]} + V_{t'}^{T_1,T_2},$$

et notre position au moment  $T_2$  est donnée par l'incrément de variance forward

$$V_{t'}^{T_1,T_2} - V_t^{T_1,T_2}.$$

En résumé, nous avons matérialisé un porte feuille contenant les incréments de la variance forward  $V^{T_1,T_2}$ , et peut donc être utilisé comme instrument de couverture. Par conséquent, acheter un swap de variance a un coût nul i.e.

$$\operatorname{price}_{t} \left( V_{t'}^{T_{1},T_{2}} - V_{t}^{T_{1},T_{2}} \right) = 0,$$

et nous déduisons que, pour une mesure de pricing donnée,  $\left(V_t^{T_1,T_2}\right)_{0 \le t \le T_1}$  sont des martingales sans dérive. Remarquons aussi que si  $T_2 = T_1 + \Delta$  pour un petit intervalle de temps  $\Delta \approx 0$ , alors  $V_t^{T_1,T_1+\Delta} \approx \xi_t^{T_1}$ . Ainsi, la variance forward  $V_t^{T_1,T_1+\Delta}$  sur la période  $[T_1, T_1 + \Delta]$  (qui peut être échangée) est proche (jusqu'à un certain ordre de correction) de la variance forward instantanée  $\xi_t^{T_1}$  observée au temps t pour une maturité  $T_1$  (qui ne peut être échangée).

Une classe de modèles basée sur des processus gaussiens. Grâce à l'analyse précédente, les variances forward instantanées  $(\xi_t^T)_{T \ge t}$  doivent être des martingales positives pour une mesure de prix donnée. Ayant cela à l'esprit, nous modélisons la variance forward instantanée comme

$$\begin{aligned} \xi_t^T &= \xi_0^T \mathcal{E}\left(\int_0^t K^T \left(s\right)^\top \mathrm{d}W_s\right) \\ &= \xi_0^T e^{-\frac{1}{2}\int_0^t K(T-s)^\top \Omega K(T-s)\mathrm{d}s + \int_0^t K(T-s)^\top \mathrm{d}W_s} \\ &= \xi_0^T e^{-\frac{1}{2}\sum_{i,j=1}^n \int_0^T \Omega_{i,j} K_i(T-s)K_j(T-s)\mathrm{d}s + \sum_{i=1}^n \int_0^T K_i(T-s)\mathrm{d}W_s^{(i)}}, \end{aligned}$$
(0.4.25)

où  $\mathcal{E}(X)$  est une notation abrégée pour  $e^{X-\frac{1}{2}\operatorname{Var}(X)}$ ,  $(\xi_0^T)_{T\geq 0}$  est la courbe initiale de variance forward instantanée (paramètre de marché),  $W = (W^{(1)}, \ldots, W^{(n)})$  est un mouvement brownien de dimension n (on parle de n facteurs) associé à une matrice de corrélation  $\Omega$  i.e. pour tout  $1 \leq i, j \leq n$ , nous avons d $\langle W^{(i)}, W^{(j)} \rangle_t = \Omega_{i,j} dt$  et  $K = (K_1, \ldots, K_n)$  sont des noyaux déterministes de carré localement intégrable i.e. pour tout  $1 \leq i \leq n, K_i$  (·)  $\in L_{2,\operatorname{loc}}(\mathbb{R}_+, \mathbb{R}^*_+)$  et  $K^T(s) = K(T-s)$ . À partir du modèle (0.4.25), notons que pour tout T, la variance forward instantanée  $(\xi_t^T)_{t\leq T}$  est un processus gaussien et une martingale i.e.  $\mathbb{E}\left[\xi_t^T \middle| \mathcal{F}_s^W\right] = \xi_s^T$  pour  $s \leq t$  où  $(\mathcal{F}_s^W)_{s\geq 0}$ est la filtration naturelle de W. Notons aussi que  $(\xi_t^T)_{t\leq T}$  est solution de l'EDS

$$\mathrm{d}\xi_t^T = \xi_t^T K \left(T - t\right)^\top \mathrm{d}W_t, \quad t \le T,$$

de sorte que  $(\xi_t^T)_{t \leq T}$  soit log-normale. D'un point de vue de la calibration et de la simulation, ces modèles sont très populaires parmi les praticiens car ils n'impliquent que des variables aléatoires gaussiennes. En pratique, les noyaux déterministes sont choisis de sorte que l'application  $\tau \to K(\tau)$  soit décroissante; l'intuition étant que puisque les noyaux apparaissent comme volatilité instantanée de la variance forward instantanée, nous voulons que les variances forward associées à des échéances plus longues bougent moins que celles avec des maturités plus courtes pour être en adéquation avec ce qui est observé sur le marché.

Un premier exemple paramétrique : le modèle de Bergomi à un facteur (noyau exponentiel). Le modèle de Bergomi à un facteur (i.e. n = 1) [27] considère un noyau exponentiel, c'est-à-dire

$$K(\tau) = \omega e^{-k\tau}, \quad \omega, \, k > 0. \tag{0.4.26}$$

Dans cet exemple précis, la variance forward instantanée s'écrit comme

$$\xi_t^T = \xi_0^T \mathcal{E}\left(\omega \int_0^t e^{-k(T-s)} \mathrm{d}W_s\right)$$

$$=\xi_0^T \mathcal{E}\left(\omega e^{-k(T-t)} \int_0^t e^{-k(t-s)} \mathrm{d}W_s\right)$$
$$=\xi_0^T e^{K(T-t)Z_t - \frac{1}{2}K(T-t)^2 \operatorname{Var}(Z_t)},$$

où Z est un processus d'Ornstein-Uhlenbeck qui suit la dynamique markovienne :  $dZ_t = -kZ_t dt + dW_t$ . En conséquence, il existe une application  $\Psi(\cdot, \cdot)$  telle que pour tout  $t, \xi_t^T = \Psi(T - t, Z_t)$  de sorte que la courbe de variance forward instantanée  $\xi_{\cdot}^T$  soit fonction d'un seul facteur markovien Z. L'extension au modèle de Bergomi à *n* facteurs [27] conduit naturellement à considérer des noyaux exponentielles de la forme :

$$K_i(\tau) = \omega_i e^{-k_i \tau}, \qquad \omega_i, k_i > 0, \quad \text{pour tout} \quad 1 \le i \le n.$$

Un deuxième exemple paramétrique : le modèle rough Bergomi (noyau puissance). Le modèle rough Bergomi, introduit récemment par Bayer, Friz et Gatheral [18], considère un noyau puissance de la forme

$$K(\tau) = \eta \tau^{H - \frac{1}{2}}, \qquad H \in (0, 1), \, \eta > 0.$$

*H* est le paramètre ou l'exposant de Hurst. Notons que pour tout  $H \in (0, \frac{1}{2}), \eta > 0$ , le noyau explose en 0 i.e.  $K(\tau) \xrightarrow[\tau \to 0^+]{} +\infty$ . Ici,  $(\xi_t^T)_{t \leq T}$  prend la forme

$$\xi_t^T = \xi_0^T e^{-\frac{\eta^2}{2} \int_0^T (T-s)^{2H-1} \mathrm{d}s + \eta \int_0^T (T-s)^{H-\frac{1}{2}} \mathrm{d}W_s}.$$
 (0.4.27)

Par conséquent, contrairement au modèle de Bergomi, la courbe  $T \to \xi_t^T$  n'admet pas de représentation markovienne de faible dimension. Il convient de mentionner que jusqu'à présent, rien n'est rough car dans tous les modèles considérés, les processus  $(\xi_t^T)_{t\leq T}$  restent des martingales pour chaque T.

**Réplication statique des log-contrats.** Considérons maintenant un modèle de volatilité stochastique général de la forme

$$\mathrm{d}S_t = \mu_t S_t \mathrm{d}t + \sigma_t S_t \mathrm{d}W_t^{\mathrm{hist}},\tag{0.4.28}$$

où  $(\mu_t)_{t\geq 0}$  est un processus déterministe,  $(\sigma_t)_{t\geq 0}$  est un processus adapté de carré intégrable et  $(W_t^{\text{hist}})_{t\geq 0}$  un mouvement brownien standard défini sur un espace de probabilité filtré donné  $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{0\leq t\leq T}, \mathbb{P})$ . La tribu  $\mathcal{F}_t$  correspond à l'informations du marché disponible au temps t. Nous supposons également que les taux d'intérêt, repo et dividendes sont nuls. Nous rappelons maintenant que la variance réalisée peut être répliquée avec le sous-jacent S et un log-contrat.

En utilisant que  $(T - t) \times \mathrm{RV}^{[t,\tilde{T}]}$  est un estimateur consistant de la variation quadratique (voir par exemple Barndorff-Nielsen et Shephard [16]), lorsque  $\sup_{i=1,...,n} |t_i - t_{i-1}| \xrightarrow[n \to \infty]{} 0$ , nous avons  $(T - t) \times \mathrm{RV}^{[t,T]} \xrightarrow{\mathrm{P}} \langle \ln S \rangle_T - \langle \ln S \rangle_t$  où  $\xrightarrow{\mathrm{P}}$  fait référence à la convergence en probabilité (ce résultat est vrai pour toute semi-martingale continue)  $(S_t)$ ), la variance forward est aussi égale à

$$V_t^T = \operatorname{price}_t \left( \frac{1}{T-t} \left( \langle \ln S \rangle_T - \langle \ln S \rangle_t \right) \right), \qquad (0.4.29)$$

où price<sub>t</sub>(·) dénote maintenant le prix modèle au temps t. Par une application directe de la formule d'Itô, nous avons :

$$\ln\left(\frac{S_T}{S_t}\right) = \int_t^T \frac{\mathrm{d}S_\alpha}{S_\alpha} - \frac{1}{2} \int_t^T \sigma_\alpha^2 \mathrm{d}\alpha.$$

La quantité  $\int_t^T \frac{dS_{\alpha}}{S_{\alpha}}$  représente le payoff d'une stratégie de couverture qui consiste à maintenir un dollar jusqu'à l'échéance T, de sorte que price<sub>t</sub>  $\left(\int_t^T \frac{dS_{\alpha}}{S_{\alpha}}\right) = 0$ . Au contraire, le second terme correspond à la moitié la variation quadratique du processus de prix  $(S_t)_{t\geq 0}$  i.e.  $\int_t^T \sigma_{\alpha}^2 d\alpha = \langle \ln S \rangle_T - \langle \ln S \rangle_t$ , de sorte que la variance forward est donnée par

$$\begin{split} V_t^T &= \operatorname{price}_t \left( \frac{1}{T-t} \left[ \langle \ln S \rangle_T - \langle \ln S \rangle_t \right] \right) \\ &= \operatorname{price}_t \left( \frac{1}{T-t} \int_t^T \sigma_\alpha^2 \mathrm{d}\alpha \right) \\ &= \operatorname{price}_t \left( -\frac{2}{T-t} \ln \left( \frac{S_T}{S_t} \right) \right), \end{split}$$

où la dernière quantité correspond au prix à l'instant t du log-contrat dont le payoff est égal à  $\ln\left(\frac{S_T}{S_t}\right)$ .

Un modèle consistent pour le sous-jacent  $S_t$ . Par conséquent, pour un modèle donné sur la variance forward instantanée  $\xi_t^T$ , nous pouvons construire un modèle de volatilité stochastique cohérent pour le prix S de la forme

$$\mathrm{d}S_t = S_t \sqrt{\xi_t^t} \mathrm{d}B_t,$$

où  $(B_t)_{t\geq 0}$  est un mouvement brownien standard. Notons qu'ici  $\xi_t^t = \lim_{T\to t} \xi_t^T$  joue le rôle d'une volatilité instantanée. Supposons que notre fonction de pricing au temps t s'écrive comme une espérance conditionnelle i.e. price<sub>t</sub>  $(\cdot) = \mathbb{E}[\cdot|\mathcal{F}_t]$  où  $(\mathcal{F}_t)_{t\geq 0} = (\mathcal{F}_t^{W,B})_{t\geq 0}$  est la filtration naturelle du processus aléatoire  $(B_t, W_t)_{t\geq 0}$ . Un tel modèle est cohérent en ce sens que le prix des log-contrats est donné par

$$\operatorname{price}_{t} \left( -\frac{2}{T-t} \ln \left( \frac{S_{T}}{S_{t}} \right) \right) = \mathbb{E} \left[ \frac{1}{T-t} \int_{t}^{T} \xi_{u}^{u} \mathrm{d}u \middle| \mathcal{F}_{t} \right]$$
$$= \frac{1}{T-t} \int_{t}^{T} \mathbb{E} \left[ \xi_{u}^{u} \middle| \mathcal{F}_{t} \right] \mathrm{d}u$$
$$= \frac{1}{T-t} \int_{t}^{T} \xi_{t}^{u} \mathrm{d}u.$$

Le caractère rough de tels modèles n'apparaît donc qu'au niveau du processus de prix. En effet, compte tenu du modèle rough Bergomi, nous avons :

$$\mathrm{d}S_t = S_t \sqrt{\xi_t^t} \mathrm{d}B_t,$$

où la volatilité instantanée  $\xi_t^t$  de  $S_t$  est dite rough puisque

$$\xi_t^t = \mathcal{E}\left(\eta \mathcal{V}_t^t\right), \qquad \mathcal{V}_t^t = \eta \int_0^t (t-s)^{H-\frac{1}{2}} \,\mathrm{d}W_s,$$

où  $\mathcal{V}_t^t$  est un processus de Volterra qui admet une modification  $\beta$ -Hölderienne pour  $\beta < H$ .

**L'indice** VIX. L'indice VIX est par définition la volatilité implicite d'un swap de variance de maturité 30 jours sur le S&P500 (voir [47]). À partir de l'analyse précédente, l'indice de volatilité VIX<sub>T</sub> à une date future T peut être défini de façon équivalente comme la volatilité implicite d'un

log-contrat qui livre  $\ln\left(\frac{S_{T+\Delta}}{S_T}\right)$  à une date future  $T + \Delta$  où  $\Delta = 30$  jours et  $S_T$  (resp.  $S_{T+\Delta}$ ) est le S&P500 à la date T (resp.  $T + \Delta$ ) i.e.

$$\text{VIX}_T = \sqrt{\text{price}_T^{\text{mkt}} \left(-\frac{2}{\Delta} \ln\left(\frac{S_{T+\Delta}}{S_T}\right)\right)}.$$

L'indice VIX est établi par le Chicago Board Options Exchange [47] par réplication statique du payoff  $\ln(S)$ . Plus précisement, par la formule de Carr-Madan [43], le VIX peut être répliqué par une infinité d'options européennes de manière complètement indépendante du modèle, c'est-à-dire

$$\operatorname{VIX}_{T} = \sqrt{\frac{2}{\Delta} \left( \int_{0}^{S_{T}} \frac{P_{T} \left( T + \Delta, \kappa \right)}{\kappa^{2}} \mathrm{d}\kappa + \int_{S_{T}}^{\infty} \frac{C_{T} \left( T + \Delta, \kappa \right)}{\kappa^{2}} \mathrm{d}\kappa \right)}, \qquad (0.4.30)$$

où  $C_T(T + \Delta, \kappa)$  et  $P_T(T + \Delta, \kappa)$  dénotent les prix marché à la date T de respectivement un Call et Put sur S de maturité  $T + \Delta$  et strike  $\kappa$ . Il convient de noter qu'en général, le VIX et la variance forward d'un swap de variance sont différents i.e.  $\operatorname{VIX}_T^2 \neq V_T^{T+\Delta} = \frac{1}{\Delta} \int_T^{T+\Delta} \xi_T^{\alpha} d\alpha$ , mais correspondent (comme indiqué ci-dessus) en supposant un modèle à volatilité stochastique.

**Produits dérivés sur le** VIX **dans le modèle rough Bergomi.** Nous revenons maintenant aux modèles généraux de la forme (0.4.25) pour lesquels  $\text{VIX}_T^2 = V_T^{T+\Delta}$ . Le prix au temps td'une option sur le VIX avec payoff  $\varphi$  est donné par

$$p_t = \mathbb{E}\left[\varphi\left(\frac{1}{\Delta}\int_T^{T+\Delta}\xi_T^{\alpha}\mathrm{d}\alpha\right)\middle|\mathcal{F}_t\right] = \phi\left(t, (\xi_t^{\alpha})_{T\leq\alpha\leq T+\Delta}\right),$$

où nous rappelons que  $(\mathcal{F}_t)_{t\geq 0}$  est la filtration naturelle de W et  $\phi$  est une application de  $[0, T] \times L^2([T, T + \Delta])$  dans  $\mathbb{R}$  définie par

$$\phi(t,z) = \mathbb{E}\left[\varphi\left(\frac{1}{\Delta}\int_{T}^{T+\Delta} z^{\alpha}e^{-\frac{1}{2}\int_{0}^{T}K(\alpha-t)^{\top}\Omega K(\alpha-t)\mathrm{d}t + \int_{0}^{T}K(\alpha-t)^{\top}\mathrm{d}W_{t}}\mathrm{d}\alpha\right)\right].$$

En particulier, pour le modèle rough Bergomi à un facteur (i.e. n = 1), en écrivant le noyau comme  $K^{\alpha}(t) = \eta(\alpha - t)^{H-\frac{1}{2}}$ , le prix de l'option à t = 0 est donné par

$$p_{0} = \mathbb{E}\left[\varphi\left(\frac{1}{\Delta}\int_{T}^{T+\Delta}\xi_{0}^{\alpha}e^{-\frac{1}{2}\int_{0}^{T}K^{\alpha}(t)^{2}\mathrm{d}t+\int_{0}^{T}K^{\alpha}(t)\mathrm{d}W_{t}}\mathrm{d}\alpha\right)\right]$$
$$= \mathbb{E}\left[\varphi\left(\frac{1}{\Delta}\int_{T}^{T+\Delta}e^{X_{T}^{\alpha}}\mathrm{d}\alpha\right)\right],$$
$$= \mathbb{E}\left[\varphi\left(P\right)\right],$$
$$(0.4.31)$$

où nous avons introduit la variance log-forward instantanée  $X_t^{\alpha} = \ln(\xi_t^{\alpha})$  qui est égale à

$$X_T^{\alpha} = X_0^{\alpha} - \frac{1}{2} \int_0^T K^{\alpha} (t)^2 \, \mathrm{d}t + \int_0^T K^{\alpha} (t) \, \mathrm{d}W_t, \qquad (0.4.32)$$

et défini  $P = \frac{1}{\Delta} \int_T^{T+\Delta} e^{X_T^{\alpha}} d\alpha$ . La tarification de produits dérivés sur le VIX requiert donc le calcul d'intégrales sur une famille à variables aléatoires log-normales. Comme il sera discuté en détail dans les deux Chapitres 2 et 6, l'approche est similaire à la tarification des options asiatiques (voir Kemna et Vorst [124]).

Dans le Chapitre 2, nous étudions la discrétisation par la méthode des rectangles à droite de (0.4.31) i.e. pour  $n \in \mathbb{N}^*$  points de discrétisation, nous approchons

$$P = \frac{1}{\Delta} \int_{T}^{T+\Delta} e^{X_{T}^{\alpha}} \mathrm{d}\alpha \approx P_{n} = \frac{1}{n} \sum_{i=1}^{n} e^{X_{T}^{t_{i}}},$$

où pour tout  $0 \le i \le n$ , nous considérons des pas de temps uniformes de la forme  $t_i = T + ih$ avec  $h = \frac{\Delta}{n}$ . Le vecteur  $(X_T^{t_i})_{i=0,\dots n}$  défini un vecteur gaussien avec moyenne  $\mu = (\mu(t_i))_{i=0,\dots,n}$ et matrice de covariance  $C = (C(t_i, t_j))_{0 \le i,j \le n}$  où pour tout  $0 \le i, j \le n$ ,

$$\mu(t_i) = \mathbb{E}\left[X_T^{t_i}\right] = X_0^{t_i} - \frac{1}{2} \int_0^T K^{t_i}(s)^2 \,\mathrm{d}s,$$
$$C(t_i, t_j) = \mathbb{C}\mathrm{ov}\left(X_T^{t_i}, X_T^{t_j}\right) = \int_0^T K^{t_i}(s) \,K^{t_j}(s) \,\mathrm{d}s$$

Le prix de l'option  $p_0 = \mathbb{E}\left[\varphi\left(P\right)\right] \approx \mathbb{E}\left[\varphi\left(P_n\right)\right]$  est alors estimé avec l'estimateur Monte Carlo :

$$\widehat{P}_{M,n} = \frac{1}{M} \sum_{m=1}^{M} \varphi\left(P_n^{(m)}\right), \qquad (0.4.33)$$

où  $(P_n^{(m)})_{1 \le m \le M}$  sont des copies indépendantes de  $P_n$  et M est le nombre de tirages Monte Carlo. Ceci correspond une nouvelle fois au formalisme de la Section 0.4.1 : ici la variable aléatoire  $P = \text{VIX}_T^2 = \frac{1}{\Delta} \int_T^{T+\Delta} e^{X_T^{\alpha}} d\alpha$  est approchée par  $P_n = \frac{1}{n} \sum_{i=1}^n e^{X_T^{t_i}}$  pour laquelle  $\frac{1}{n}$  joue le rôle du paramètre d'approximation h.

Le coût de calcul total de l'estimateur (0.4.33) peut être décomposé comme suit : une décomposition de Cholesky de la matrice de covariance C avec complexité  $\mathcal{O}(n^3)$ , l'échantillonnage d'un vecteur gaussien de dimension n avec complexité  $\mathcal{O}(n^2)$  et la somme sur ses composantes avec complexité  $\mathcal{O}(n)$ . Par conséquent, le coût de calcul global de l'estimateur Monte Carlo est donné par :

$$\operatorname{Cost}(\widehat{P}_{M,n}) = \mathcal{O}(n^3) + (\mathcal{O}(n^2) + \mathcal{O}(n)) \times M = \mathcal{O}(\varepsilon^{-4}).$$

Nous montrons comment la complexité totale peut être réduite à  $\mathcal{O}\left(\ln(\varepsilon)^2 \varepsilon^{-2}\right)$  en utilisant un schéma multi-niveaux. Nous devons d'abord estimer les erreurs forte et faible pour le schéma de discrétisation.

**Theorem 0.4.9** (Erreur forte  $L_2$ ). Supposons une variance forward instantanée initiale constante i.e.  $X_0^{\alpha} = X_0$  pour tout  $\alpha \in [T, T + \Delta]$ . Pour  $n \to \infty$ , nous avons

$$\left(\mathbb{E}\left[|P-P_n|^2\right]\right)^{\frac{1}{2}} \sim \frac{\Lambda\left(X_0, T, \Delta, H\right)}{n},\tag{0.4.34}$$

оù

$$\Lambda\left(X_{0}, T, \Delta, H\right) = \frac{e^{X_{0}}}{2} \left(e^{\eta^{2} \frac{T^{2H}}{2H}} + e^{\eta^{2} \frac{(T+\Delta)^{2H} - \Delta^{2H}}{2H}} - 2e^{\eta^{2} \int_{0}^{T} t^{H-\frac{1}{2}} (\Delta+t)^{H-\frac{1}{2}} dt}\right)^{\frac{1}{2}}$$

Par application directe de l'inégalité de Cauchy–Schwartz, si le payoff  $\varphi$  est Lipschitz alors l'erreur faible est d'ordre 1 i.e.

$$\left|\mathbb{E}\left[\varphi\left(P\right) - \varphi\left(P_{n}\right)\right]\right| = \mathcal{O}\left(n^{-1}\right). \tag{0.4.35}$$

Schéma multi-niveaux. Soit  $L \in \mathbb{N}^*$  le nombre de niveaux et  $\mathbf{M} = (M_0, \dots, M_L)$ ,  $\mathbf{n} = (n_0, \dots, n_L) \in (\mathbb{N}^*)^{L+1}$  des multi-indices représentant respectivement le nombre décroissant de tirages utilisés pour approximer l'espérance et le nombre croissant des pas de temps utilisés pour approcher l'intégrale. Pour tout  $l = 0, \dots, L$ , nous introduisons la notation abrégée

$$P_l = \varphi\left(\frac{1}{n_l}\sum_{i=1}^{n_l} e^{X_T^{T+\Delta\frac{i}{n_l}}}\right),$$

où les points de discrétisation sont de la forme  $n_l = n_0 2^l$  pour un  $n_0 \in \mathbb{N}^*$  donné. L'estimateur multi-niveaux est défini comme :

$$\widehat{P}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}} = \frac{1}{M_0} \sum_{m=1}^{M_0} P_0^{(0,m)} + \sum_{l=1}^{L} \frac{1}{M_l} \sum_{m=1}^{M_l} \left( P_l^{(l,m)} - P_{l-1}^{(l,m)} \right), \qquad (0.4.36)$$

où pour tout l, les variables aléatoires  $(P_l^{(l,m)})_{1 \le m \le M_l}$  et  $(P_{l-1}^{(l,m)})_{1 \le m \le M_l}$  sont des copies indépendantes de  $P_l$  et  $P_{l-1}$  respectivement. Notons que pour un niveau fixé l, les variables aléatoires  $P_l^{(l,m)}, P_{l-1}^{(l,m)}$  sont construites en utilisant les mêmes trajectoires browniennes.

**Theorem 0.4.10.** Supposons que le payoff  $\varphi$  soit Lipschitz, et considérons une erreur  $\varepsilon > 0$ . Alors, il existe  $M_0, L \in \mathbb{N}^*$  tel que l'estimateur multi-niveaux (0.4.36) ait une erreur quadratique moyenne avec borne  $MSE = \mathcal{O}(\varepsilon^2)$  et une complexité de  $\mathcal{O}\left(\ln(\varepsilon)^2 \varepsilon^{-2}\right)$  en choisissant :

$$m_l = n_0 2^l, \qquad M_l = M_0 2^{-2l}, \qquad 0 \le l \le L$$

### 0.5 Méta-modélisation et décomposition en polynômes du chaos

Dans la deuxième partie, nous nous intéressons aux grandes sommes de la forme

$$\mathcal{L}_K = \sum_{k=1}^K l_k \mathbf{1}_{Y_k \le X},\tag{0.5.1}$$

où  $X, Y_1, \ldots, Y_K$  sont des variables aléatoires à densité et  $(Y_k)_{k=0\ldots K}$  sont indépendantes et indépendantes de X. Les  $(l_k)_{k=1,\ldots,K}$  sont déterministes et le paramètre  $K \in \mathbb{N}^*$  est supposé fini mais grand. Lorsque le facteur commun X est connu,  $\mathcal{L}_K$  s'écrit comme une somme de variables aléatoires indépendantes et pondérées de Bernoulli. Plus précisément,

$$\mathbf{1}_{Y_k \leq X} | X = x \stackrel{d}{=} \mathcal{B}\left(F_{Y_k}(x)\right), \quad \text{où pour tout } x, \quad F_{Y_k}(x) = \mathbb{P}\left(Y_k \leq x\right).$$

Bien que notre motivation pour étudier les grandes sommes de la forme (0.5.1) provienne des nombreux exemples en risque de crédit (voir plus de détails ci-dessous), nous pensons que notre approche est pertinente pour s'attaquer à certaines fonctionnelles de grandes sommes apparaissant dans d'autres branches des mathématiques appliquées telles que les méthodes de fiabilité (voir e.g. Melchers and Beck [141]), télécommunication, modélisation de réseaux sociaux, etc.

Dans la plupart des applications, nous nous intéressons à l'estimation de probabilités extrêmes  $\mathbb{P}(\mathcal{L}_K > L)$  pour de grandes valeurs de L, ou plus généralement à des espérances de la forme  $\mathbb{E}[f(\mathcal{L}_K)]$  pour une certaine fonction f. Pour estimer de telles quantités, l'estimation par des méthodes de Monte Carlo est souvent l'approche privilégiée. Cependant, comme K est supposé grand et parce que nous avons affaire à des évènements extrêmes, toute simulation de Monte Carlo sera coûteuse. Par exemple, supposons que nous voulions estimer  $\mathbb{E}[f(\mathcal{L}_K)]$ , pour une certaine fonction f, en utilisant une méthode de Monte Carlo. Alors, pour atteindre une erreur  $\varepsilon > 0$ pour la racine de l'erreur quadratique moyenne, nous aurions besoin de tirer  $N = \mathcal{O}(\varepsilon^{-2})$  fois la perte  $\mathcal{L}_K$ . Chaque simulation de  $\mathcal{L}_K$  nécessitant la génération de  $(Y_1, \ldots, Y_K)$  et d'appliquer la somme (0.5.1) et si la simulation d'un  $Y_k$  est d'une unité de temps calcul, le coût total (pour atteindre une précision de  $\varepsilon$ ) est alors de  $\mathcal{O}(K\varepsilon^{-2})$ . Par exemple, si le nombre K est très grand (disons un million), et la tolérance d'erreur est de un pour cent, cela entraînerait un coût de dix milliards d'opérations unitaires. Inutile de dire que plus l'estimation est précise (c'est-à-dire une faible valeur de  $\varepsilon$ ), plus le nombre de tirages N est élevé. Des estimations assez imprécises de l'espérance peuvent alors être la seule option disponible sous une contrainte de temps de calcul donnée.

Pour pallier à ce problème, nous proposons un méta-modèle pour la grande somme  $\mathcal{L}_K$ . Un méta-modèle est une approximation d'un vrai modèle et a l'avantage d'être beaucoup plus rapide à évaluer. Notre approche de méta-modélisation proposée est double :

- 1. Nous appliquons d'abord une décomposition en polynômes du chaos sur le facteur commun X, et obtenons la perte tronquée associée  $\mathcal{L}_{K,N}$  à un certain ordre  $N \in \mathbb{N}^*$ .
- 2. Nous fournissons alors une approximation gaussienne  $\mathcal{L}_{K,N}^{\mathrm{G}}$  de la perte tronquée  $\mathcal{L}_{K,N}$  dont les caractéristiques sont explicites.

**Rappels sur les polynômes orthogonaux.** Soit  $\nu(dx) = w(x)dx$  une mesure de probabilité définie sur un intervalle ouvert fini ou infini  $I_w = (a, b)$  dans  $\mathbb{R}$ . La fonction de poids positive w(x) est continue ou continue par morceaux ou intégrable, et telle que  $0 < \int_{I_w} x^{2n} w(x) dx$  pour tout n. L'ensemble des fonctions polynomiales  $(p_n)_{n \in \mathbb{N}}$  est dit être un ensemble de polynômes orthogonaux (OPS) associé à la fonction de poids w(x) (ou de manière équivalente à la mesure de probabilité  $\nu$ ), si pour tout  $n, m \in \mathbb{N}$ ,

$$\int_{I_w} p_n(x) p_m(x) w(x) \mathrm{d}x = h_n \delta_{nm}, \qquad (0.5.2)$$

où  $\delta_{nm} = 1$  si n = m ou 0 sinon, et  $h_n := \int_a^b p_n(x)^2 w(x) dx < \infty$ . Lorsque  $h_n = 1$ , nous parlons de polynômes orthonormaux.

**Relation de récurrence.** Une propriété remarquable des polynômes orthogonaux est qu'ils satisfont nécessairement une relation de récurrence à trois termes de la forme ([157, Théorème 3.2.1]):

$$p_{n+1}(x) = (A_n x + B_n) p_n(x) - C_n p_{n-1}(x), \quad n \in \mathbb{N}^*, \tag{0.5.3}$$

où  $A_n, B_n, C_n$  sont des constantes et  $A_n > 0, C_n > 0$ .

Décomposition en polynômes du chaos (PCE) d'une fonction indicatrice. Soit  $(p_n)_{n \in \mathbb{N}}$ un OPS pour la mesure de probabilité  $\nu(dx) = w(x)dx$  et introduisons le seuil  $c \in \mathbb{R}$ . Lorsque  $X \stackrel{d}{=} \nu$ , la PCE suivante est vérifiée

$$\mathbf{1}_{c \le X} \stackrel{L_2(\nu)}{=} \sum_{n=0}^{\infty} \gamma_n(c) p_n(X), \quad \gamma_n(c) = \frac{\mathbb{E}\left[\mathbf{1}_{c \le X} p_n(X)\right]}{h_n} = \frac{\int_c^b p_n(x) w(x) \mathrm{d}x}{\int_a^b p_n^2(x) w(x) \mathrm{d}x}.$$
(0.5.4)

Puisque la somme (0.5.4) nécessite le calcul d'un nombre infini de paramètres, dans la pratique, nous ne pouvons que tronquer à un certain ordre  $N \in \mathbb{N}^*$ , et l'approximer avec

$$\sum_{n=0}^{\infty} \gamma_n(c) p_n(X) \approx \sum_{n=0}^{N} \gamma_n(c) p_n(X).$$
(0.5.5)

Nous serons également intéressés à estimer l'erreur  $L_2$  entre  $\mathbf{1}_{c\leq X}$  et  $\sum_{n=0}^{N} \gamma_n(c) p_n(X)$  i.e.

$$\mathcal{E}_{N}(c) = \mathbb{E}\left[\left|\mathbf{1}_{c \le X} - \sum_{n=0}^{N} \gamma_{n}(c)p_{n}(X)\right|^{2}\right]^{\frac{1}{2}} = \left|\sum_{n=N+1}^{\infty} h_{n}\gamma_{n}(c)^{2}\right|^{\frac{1}{2}}, \quad (0.5.6)$$

où la dernière égalité résulte de la condition d'orthogonalité (0.5.2).

Ensemble des polynômes orthogonaux classiques ou COPS. Plutôt que de considérer tous les polynôme orthogonaux, nous étudions une sous-classe de polynômes orthogonaux continus communément appelé ensemble de polynômes orthogonaux classiques ou COPS. Le COPS ne comprend que les polynômes orthogonaux d'Hermite, de Laguerre (avec paramètre  $\alpha > -1$ ) et de Jacobi (avec paramètres  $\alpha, \beta > -1$ ), dont certaines des propriétés sont rassemblées dans le Tableau 2 (voir e.g. [146, Chapitre 18] pour un résumé détaillé de leurs caractéristiques). Les polynômes de Legendre sont des polynômes de Jacobi particuliers avec paramètres  $\alpha = \beta = 0$ et jouent un rôle clé dans notre étude. Ces polynômes sont les seuls à satisfaire à la formule de Rodrigues, c'est-à-dire

$$p_n(x) = \frac{1}{\kappa_n w(x)} \frac{d^n}{dx^n} \left[ F(x)^n w(x) \right], \qquad (0.5.7)$$

où F est un polynôme avec degré deg $(F) \leq 2$ ,  $\kappa_n$  certains coefficients et leur fonction de poids  $w(\cdot)$  satisfait l'équation différentielle (de Pearson) suivante

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[F(x)w(x)\right] = G(x)w(x),\tag{0.5.8}$$

où G est un polynôme avec degré deg(G) = 1 et dont les conditions limites suivantes sont satisfaites

$$\lim_{x \to a} w(x)F(x) = \lim_{x \to b} w(x)F(x) = 0.$$

Les deux propriétés sont essentielles pour trouver des formules fermées et des relations de récurrence pour les coefficients du chaos  $\gamma_n$ , et motivent notre choix de nous concentrer uniquement sur le COPS (voir [6, Théorème 1.2] pour une caractérisation complète).

Nom	Hermite	Laguerre	Jacobi	Legendre
Remarque		$\alpha > -1$	$\alpha,\beta>-1$	Jacobi ( $\alpha = \beta = 0$ )
$p_n(x)$	$\operatorname{He}_n(x)$	$\mathcal{L}_n^{(\alpha)}(x)$	$\mathrm{P}_n^{(lpha,eta)}(x)$	$P_n(x)$
(a,b)	$(-\infty,\infty)$	$(0,\infty)$	(-1,1)	(-1,1)
w(x)	$\frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}$	$\frac{x^{\alpha}e^{-x}}{\Gamma_{\alpha+1}}$	$\frac{(1-x)^{\alpha}(1+x)^{\beta}}{2^{\alpha+\beta+1}\mathcal{B}_{\alpha+1,\beta+1}}$	$\frac{1}{2}$
ν	$\mathcal{N}\left(0,1 ight)$	$\operatorname{Gamma}\left(\alpha+1,1\right)$	$1 - 2 \text{Beta}\left(\alpha + 1, \beta + 1\right)$	$\mathcal{U}\left(-1,1 ight)$
$p_0(x)$	1	1	1	1
$p_1(x)$	x	$1 + \alpha - x$	$\alpha + 1 + \frac{(\alpha + \beta + 2)(x - 1)}{2}$	x

Table 2 – Quelques propriétés des polynômes orthogonaux classiques.

**Theorem 0.5.1** (Estimées d'erreur  $L_2$ ). Il existe une constante positive A, indépendante de N et c, de sorte que les estimations globales suivantes tiennent :

$$\left( \begin{array}{cc} e^{-\frac{c^2}{4}} N^{-\frac{1}{4}}, & c \in \left[ -N^{\frac{1}{2}}, N^{\frac{1}{2}} \right], \nu = \mathcal{N}(0, 1), \end{array} \right)$$
(0.5.9)

$$\mathcal{E}_{N}(c) \leq A \left\{ \begin{array}{ll} c^{\frac{\alpha}{2} + \frac{1}{4}} e^{-\frac{c}{2}} N^{-\frac{1}{4}}, & c \in [0, N], \ \alpha \notin \mathbb{N}, \ \nu = \text{Gamma}\left(\alpha + 1, 1\right), \end{array} \right.$$
(0.5.10)

$$(1-c)^{\frac{\alpha}{2}+\frac{1}{4}}(1+c)^{\frac{\beta}{2}+\frac{1}{4}}N^{-\frac{1}{4}}, \quad c \in [-1,1], \ \nu = 1-2\text{Beta}\left(\alpha+1,\beta+1\right), \ (0.5.11)$$

$$\left(1-c^2\right)^{\frac{1}{4}}N^{-\frac{1}{2}}, \quad c \in [-1,1], \ \nu = \mathcal{U}(-1,1).$$
 (0.5.12)

Pour des valeurs non-extrêmes de c, c'est-à-dire  $c = \pm \infty$  pour les polynômes de Hermite, c = 0 ou  $c = +\infty$  pour les polynômes de Laguerre,  $c = \pm 1$  pour les polynômes de Jacobi, nous avons une erreur  $L_2$  d'ordre  $\mathcal{O}\left(N^{-\frac{1}{4}}\right)$  pour tous les polynômes sauf les polynômes de Legendre qui présentent une décroissance d'ordre plus rapide  $\mathcal{O}\left(N^{-\frac{1}{2}}\right)$  (voir Figure 8). L'ordre  $\mathcal{O}\left(N^{-\frac{1}{4}}\right)$  semble plutôt médiocre pour que la troncature soit efficace. Pourtant, l'intérêt principal du Théorème 0.5.1 réside dans le fait qu'il garde une trace en la dépendance du paramètre c (voir Figure 9). Il révèle un facteur exponentiel  $e^{-\frac{c^2}{4}}$  (resp.  $e^{-\frac{c}{2}}$ ) pour les polynômes d'Hermite (resp. de Laguerre) ce qui assure une décroissance plus rapide pour les grandes valeurs de c (voir Figure 9)

Plus précisément, pour évaluer et comparer les performances de chaque polynôme en termes d'erreur  $L_2$ , nous considérons le problème d'approximation de la fonction indicatrice

$$\mathbf{1}_{q \leq U} \stackrel{d}{=} \mathbf{1}_{F^{-1}(q) \leq F^{-1}(U)},$$

où le quantile  $q \in (0, 1)$ ,  $U \stackrel{d}{=} \mathcal{U}(0, 1)$ , et  $F(\cdot)$  fait référence à la c.d.f. de  $\mathcal{U}(-1, 1)$  (polynômes de Legendre) ou  $\mathcal{N}(0, 1)$  (polynômes d'Hermite) ou Gamma ( $\alpha + 1, 1$ ) (polynômes de Laguerre) ou 1 - 2Beta ( $\alpha + 1, \beta + 1$ ) (polynômes de Jacobi). La PCE de la fonction indicatrice  $\mathbf{1}_{q \leq U}$  pour le COPS est affiché par les "quantiles standards" en Figure 8 dans laquelle on observe, qu'en effet, les polynômes de Legendre sont les plus performants. Ceci est différent pour les "quantiles extrêmes" (Figure 9) où nous notons que les polynômes de Legendre (resp. Jacobi) semblent fournir l'erreur  $L_2$  la plus élevée (resp. la plus faible).



Figure 8 – Erreur  $L_2$  pour le COPS en fonction de  $q \in (0,1)$  avec paramètre de troncation N = 40.



Figure 9 – Erreur  $L_2$  pour le COPS en fonction des petits quantiles  $q \in (10^{-4}, 10^{-3})$  (gauche) et grands quantiles  $q \in (1 - 10^{-3}, 1 - 10^{-4})$  (droite).

Approximation gaussienne et théorème de la limite centrale. Nous revenons maintenant à notre problème initial, c'est-à-dire proposer un méta-modèle pour la grande somme (0.5.1). Au vue de la section précédente, il semble naturel de diviser la somme en trois groupes différents selon la valeur de  $Y_k$ . Par exemple, en supposant que  $X \stackrel{d}{=} \Gamma(\alpha+1,1)$  et en dénotant  $F(\cdot)$ leur c.d.f., nous aurions trois groupes différents dans lesquels les  $Y_k$  sont proches de 0 (quantiles extrêmement bas), les  $Y_k$  sont proches de  $\infty$  (quantiles extrêmement élevés), et les  $Y_k$  prennent des valeurs "normales" sur  $(0, \infty)$ . Pour ce dernier, notant que  $\mathbf{1}_{Y_k \leq X} = \mathbf{1}_{2F(Y_k)-1 \leq 2F(X)-1} \stackrel{d}{=} \mathbf{1}_{2F(Y_k)-1 \leq \mathcal{U}(-1,1)}$ , nous pourrions alors effectuer une PCE de  $\mathbf{1}_{2F(Y_k)-1 \leq 2F(X)-1}$  au lieu de  $\mathbf{1}_{Y_k \leq X}$ en utilisant les polynômes de Legendre. Pour les deux autres groupes, une procédure similaire pourrait être utilisée bien que nous n'utiliserions pas les polynômes de Legendre (voir Lemme 4.3.1 et Remarque 11 pour plus de détails).

Nous supposons donc maintenant que des transformations aient été faites au préalable selon les valeurs de  $(Y_k)_{k=1,...K}$ . À partir de la PCE  $\mathbf{1}_{Y_k \leq X}$  (0.5.4), et puisque  $X, Y_1, \ldots, Y_K$  sont des variables aléatoires à densité, nous avons presque sûrement que

$$\mathcal{L}_{K} = \sum_{k=1}^{K} \left( \sum_{n=0}^{\infty} l_{k} \gamma_{n} \left( Y_{k} \right) \right) p_{n}(X) = \sum_{n=0}^{\infty} \varepsilon_{K,n} p_{n}(X),$$

où nous définissons la nouvelle variable aléatoire

$$\varepsilon_{K,n} := \sum_{k=1}^{K} l_k \gamma_n \left( Y_k \right). \tag{0.5.13}$$

Notre méta-modèle pour  $\mathcal{L}_K$  consiste à considérer seulement les premiers termes de la décomposition en chaos de la fonction indicatrice combinée avec une approximation gaussienne. Pour un ordre de troncature  $N \in \mathbb{N}^*$ , nous définissons donc la version tronquée de  $\mathcal{L}_K$  comme

$$\mathcal{L}_{K,N} := \sum_{n=0}^{N} \varepsilon_{K,n} p_n(X). \tag{0.5.14}$$

Nous introduisons en outre l'espérance  $\boldsymbol{\mu}_K = (\mu_{K,n})_{0 \le n \le N}$  et la matrice de covariance  $\Sigma_K = (\Sigma_{K,n,m})_{0 \le n,m \le N}$  du vecteur  $\boldsymbol{\varepsilon}_K = (\varepsilon_{K,n} : n = 0, \dots, N)$  où pour tout  $n, m \in \{0, \dots, N\}$ ,

$$\mu_{K,n} = \mathbb{E}\left[\varepsilon_{K,n}\right] = \sum_{k=1}^{K} l_k \mathbb{E}\left[\gamma_n\left(Y_k\right)\right],$$

$$\Sigma_{K,n,m} = \mathbb{C}\text{ov}\left(\varepsilon_{K,n}, \varepsilon_{K,m}\right) = \sum_{k,k'=1}^{K} l_k l_{k'} \mathbb{C}\text{ov}\left(\gamma_n\left(Y_k\right), \gamma_m\left(Y_{k'}\right)\right).$$
(0.5.15)

Remplacer le vecteur  $\boldsymbol{\varepsilon}_{K}$  par l'approximation gaussienne

$$\boldsymbol{\varepsilon}_{K}^{\mathrm{G}} = \left(\boldsymbol{\varepsilon}_{K,n}^{\mathrm{G}} : n = 0, \dots, N\right) \stackrel{d}{=} \mathcal{N}\left(\boldsymbol{\mu}_{K}, \boldsymbol{\Sigma}_{K}\right), \qquad (0.5.16)$$

conduit au méta-modèle  $\mathcal{L}_{K,N}^{\mathrm{G}}$  pour le modèle initial  $\mathcal{L}_{K}$  défini comme :

$$\mathcal{L}_{K,N}^{\mathrm{G}} = \mathcal{L}_{K,N}^{\mathrm{G}}(X) = \sum_{n=0}^{N} \varepsilon_{K,n}^{\mathrm{G}} p_n(X).$$
(0.5.17)

Ainsi lorsque le facteur commun X est connu,  $\mathcal{L}_{K,N}^{\mathrm{G}}(x) \stackrel{d}{=} \mathcal{N}\left(\mu_{\mathcal{L}_{K,N}}(x), \sigma_{\mathcal{L}_{K,N}}^{2}(x)\right)$  avec pour tout  $x \in \mathbb{R}$ ,

$$\mu_{\mathcal{L}_{K,N}}(x) = \sum_{n=0}^{N} \mu_{K,n} p_n(x), \quad \sigma_{\mathcal{L}_{K,N}}^2(x) = \sum_{n,m=0}^{N} \Sigma_{K,n,m} p_n(x) p_m(x).$$

L'avantage principal de cette approche est que les coefficients  $(\varepsilon_{K,n})_{n \in 0,...,N}$  s'écrivent comme une somme de variables aléatoires indépendantes. Le résultat suivant donne une condition suffisante pour que l'on puisse remplacer les coefficients par un vecteur gaussien dont les caractéristiques sont explicites.

**Theorem 0.5.2** (Théorème centrale limite). Supposons que la condition de Lindeberg suivante soit vérifiée

$$\|\Sigma_K^{-1}\| \sup_{1 \le k \le K} l_k^2 \xrightarrow[K \to +\infty]{} 0 \quad with \quad \|\Sigma_K^{-1}\| := \sup_{\boldsymbol{x} \in \mathbb{R}^{N+1}, x \ne 0} \frac{|\Sigma_K^{-1} \boldsymbol{x}|}{|\boldsymbol{x}|}. \tag{0.5.18}$$

Alors, le vecteur  $\boldsymbol{\varepsilon}_K$  vérifie le théorème centrale limite

$$\Sigma_K^{-\frac{1}{2}}(\boldsymbol{\varepsilon}_K - \boldsymbol{\mu}_K) \xrightarrow[K \to \infty]{d} \mathcal{N}(0, \mathrm{Id}_{N+1}).$$
(0.5.19)

Méta-modèle pour de grand portefeuille de risque de crédit dans le modèle de copule gaussienne. Dans le Chapitre 3, nous nous concentrons sur le risque de crédit pour de grands portefeuilles dans un modèle à copule gaussienne (voir Li [135]). Nous étudions la perte totale par défaut sur un an (sans provision) définie comme :

$$\mathcal{L}_K = \sum_{k=1}^K l_k D_k,$$

où  $D_k$  représente l'indice de défaut pour le kième débiteur sur un an i.e.  $D_k = 1$  si le kième fait défaut ou 0 sinon. On suppose que les défauts obéissent à un modèle à copule gaussienne, à savoir

$$D_k = \mathbf{1}_{G_k \ge c_k} \tag{0.5.20}$$

avec facteurs stochastiques  $G_k$ , seuils (ou limites par défaut)  $c_k$ , et dans lequel la dépendance entre les débiteurs est traduite via un vecteur normal  $(G_1, \ldots, G_K)$  avec  $G_k \stackrel{d}{=} \mathcal{N}(0, 1)$  centré et réduit pour tout k. Plus précisément, dans un modèle de copule gaussienne unidimensionnel,  $G_k$ peut être décomposé en :

$$G_k = \rho_k Z + \sqrt{1 - \rho_k^2} \varepsilon_k, \qquad (0.5.21)$$

où la variable aléatoire  $Z \stackrel{d}{=} \mathcal{N}(0, 1)$  représente un facteur de risque systémique (commun à tous les débiteurs),  $\varepsilon_k \stackrel{d}{=} \mathcal{N}(0, 1)$  est un risque idiosyncratique (propre à chaque débiteur) associé au kième débiteur (indépendant de Z) et  $\rho_k \in (-1, 1)$  un paramètre de corrélation. Nous soulignons que les  $(\varepsilon_k)_{1 \leq k \leq K}$  sont indépendants et indépendants de Z, et nous supposons que  $\rho_k \neq 0$  puisque (d'un point de vue économique), il existe toujours une dépendance entre la valeur par défaut d'un débiteur et le facteur de risque systémique.

En définissant la limite par défaut comme  $c_k := \Phi^{-1}(1 - p_k) = -\Phi^{-1}(p_k)$  pour qu'elle satisfasse à la contrainte  $p_k = \mathbb{P}(D_k = 1)$ , nous en déduisons que

$$\mathbb{P}\left(D_{k}=1\right)=\mathbb{P}\left(G_{k}\geq c_{k}\right)=\Phi\left(-c_{k}\right)=p_{k}$$

Ensuite, l'événement par défaut s'écrit (en gardant à l'esprit que nous excluons le cas  $\rho_k = 0$ ) :

$$\left\{G_k \ge c_k\right\} = \left\{-\frac{\sqrt{1-\rho_k^2}}{|\rho_k|}\varepsilon_k - \frac{\Phi^{-1}(p_k)}{|\rho_k|} \le \frac{\rho_k}{|\rho_k|}Z\right\}.$$
 (0.5.22)

Ici, nous soulignons que les deux variables aléatoires sont gaussiennes et observons que la somme du risque de crédit est de la forme (0.5.1) avec :

$$X = \frac{\rho_k}{|\rho_k|} Z \stackrel{d}{=} \mathcal{N}(0,1), \qquad Y_k = -\frac{\sqrt{1-\rho_k^2}}{|\rho_k|} \varepsilon_k - \frac{\Phi^{-1}(p_k)}{|\rho_k|} \stackrel{d}{=} \mathcal{N}\left(-\frac{\Phi^{-1}(p_k)}{|\rho_k|}, \frac{1-\rho_k^2}{\rho_k^2}\right).$$

*Remark* 2. Les modèles de la forme (0.5.21) entrent dans la catégorie des "modèles à seuil" qui sont extrêmement populaires dans la modélisation du risque de crédit (voir e.g. [140, Section 8.3]). Une des extensions les plus connues de la copule gaussienne (0.5.21) est la copule de Student t (voir [140, Exemple 8.21]) pour laquelle  $G_k = W\left(\rho_k Z + \sqrt{1 - \rho_k^2}\varepsilon_k\right)$  et W est une distribution gamma inverse.

**Theorem 0.5.3.** Sous l'hypothèse que les  $(\varepsilon_k)_{k=1,...,K}$  soient indépendants de Z, la décomposition en chaos à l'ordre  $N \in \mathbb{N}$  de la perte  $\mathcal{L}_K$  en fonction de Z (voir (0.5.14)) est donnée par :

$$\mathcal{L}_{K,N} = \sum_{n=0}^{N} \left\{ \sum_{k=1}^{K} l_k \gamma_n \left( -\frac{\sqrt{1-\rho_k^2}}{|\rho_k|} \varepsilon_k - \frac{\Phi^{-1}(p_k)}{|\rho_k|} \right) \frac{\rho_k^n}{|\rho_k|^n} \right\} \operatorname{He}_n(Z), \quad (0.5.23)$$

où les coefficients  $\gamma_n(c)$  (voir (0.5.4)) associés aux polynômes d'Hermite s'écrivent comme

$$\gamma_0(c) = \Phi(-c), \quad \gamma_n(c) = \frac{e^{-\frac{c^2}{2}} \operatorname{He}_{n-1}(c)}{n! \sqrt{2\pi}}, \quad (n \in \mathbb{N}^*).$$

Par application du théorème central limite 0.5.2, notre méta-modèle consiste à tirer un vecteur gaussien de dimension (N+1). De plus, comme la c.d.f. de Y (ici gaussien) est analytique et grâce à (0.5.3), des relations de récurrence efficaces sont satisfaites pour le vecteur moyen  $\mu$  et la matrice de covariance  $\Sigma$ . En considérant M tirages Monte Carlo, notre méta-modèle requiert  $\mathcal{O}(KN^2)$ (coût hors ligne pour le calcul des caractéristiques du vecteur gaussien) +  $\mathcal{O}(MN^2)$  (tirage d'un vecteur gaussien de dimension (N + 1)) opérations ce qui entraîne un coût de calcul total de  $\mathcal{O}(KN^2) + \mathcal{O}(MN^2)$ . En se souvenant que  $K \ge 10^5$  et puisque pour la plupart des applications, un paramètre de troncature  $N \le 50$  conduit à des résultats satisfaisants, la complexité  $\mathcal{O}(MK)$ , requise pour un Monte Carlo standard, est beaucoup plus grande.

### 0.6 Approximations faibles, expansion des prix d'options et asymptotiques en temps court

Depuis de nombreuses années, les asymptotiques en temps court pour les modèles à volatilité stochastique ont attiré aussi bien les praticiens que le milieu universitaire en mathématiques financières (voir e.g. Berestycki, Busca et Florent [25], Henry-Labordère [107], Forde et Jacquier [65], Feng, Forde et Jacquier [63], Gatheral et al. [71], Friz et al. [69]). S'appuyant sur l'expansion en temps court de la densité de transition d'un processus général de diffusion, exprimée en termes d'une fonction de distance sur une variété riemannienne dont la métrique est proportionnelle à l'inverse du coefficient de diffusion (voir les travaux fondateurs de Varadhan [162, 161] ou Henry-Labordère [107]), toutes ces références examinent et proposent des asymptotiques pour la volatilité implicite européenne en temps court. Par exemple, considérons un modèle à volatilité locale homogène pour une action sans dividende S,

$$dS_t = rS_t dt + S_t \sigma(S_t) dW_t, \qquad (0.6.1)$$

ou de façon équivalente pour le log prix  $X_t := \ln S_t$ ,

$$dX_t = \left(r - \frac{1}{2}\sigma^2(e^{X_t})\right)dt + \sigma\left(e^{X_t}\right)dW_t.$$
(0.6.2)

L'expansion du noyau de la chaleur pour la densité de transition du processus  $X_t$  à partir de  $X_0 = x$  est alors donnée par ([71, Proposition 2.1]) :

$$f_X(t,y|x) = \frac{e^{-\frac{d^2(x,y)}{2t}}}{\sqrt{2\pi t}} \left( u_0(x,y) + \mathcal{O}(t;x,y) \right), \quad (t \to 0^+),$$

où la fonction de distance au carré et le coefficient  $u_0$  sont respectivement définis comme

$$d(x,y)^{2} = \left(\int_{x}^{y} \frac{dp}{\sigma(e^{p})}\right)^{2}, \quad u_{0}(x,y) := \sigma(e^{x})^{\frac{1}{2}} \sigma(e^{y})^{-\frac{3}{2}} e^{-\frac{1}{2}(y-x)+r\int_{x}^{y} \frac{dp}{\sigma^{2}(e^{p})}},$$

et il existe une constante positive C (indépendante de x et y) telle que  $|\mathcal{O}(t;x,y)| \leq Ct$  pour tout t > 0.

Expansions du prix du Put européen et de la volatilité implicite européenne. Un Put sur le sous-jacent  $S_t$  avec temps à maturité  $\tau$ , strike K et prix initial  $S_0 = s$  peut donc être exprimé comme une intégrale de Laplace de la forme

$$P(\tau, s, K) = \mathbb{E}\left[e^{-r\tau}(K - S_{\tau})_{+}\right]$$
$$= \frac{Ke^{-r\tau}}{\sqrt{2\pi\tau}} \int_{-\infty}^{0} \left(1 - e^{z}\right) \left(u_{0}\left(\ln s, \ln K + z\right) + \mathcal{O}\left(\tau\right)\right) e^{-\frac{\mathrm{d}^{2}(\ln s, z + \ln K)}{2\tau}} \mathrm{d}z.$$

En utilisant la méthode de Laplace (voir e.g. Bender et Orszag [22, Chapitre 6]) et si s > K(en dehors de la monnaie), s = K (à la monnaie) or s < K (dans la monnaie), le prix du Put européen admet l'expansion en temps court suivante,

$$\int \frac{s\sigma(s)}{\sqrt{2\pi}}\sqrt{\tau} - \frac{rs}{2}\tau + A_1(s)\frac{s}{\sqrt{2\pi}}\tau\sqrt{\tau}, \quad \text{if } s = K, \tag{0.6.3}$$

$$P(\tau, s, K) \underset{\tau \to 0}{\sim} \left\{ A_2(s) e^{-\frac{\mathrm{d}^2(\ln K, \ln s)}{2\tau}} \tau \sqrt{\tau}, \quad \text{if } s > K, \right.$$
(0.6.4)

$$\left( K \left( 1 - e^{-r\tau} \right) - A_2(s) e^{-\frac{d^2(\ln K, \ln s)}{2\tau}} \tau \sqrt{\tau}, \quad \text{if } s < K.$$
 (0.6.5)

où  $A_1(s)$  dépend seulement de  $\sigma(\cdot)$  et  $A_2(s) = \frac{u_0(\ln s, \ln K)K\sigma(K)^2}{\sqrt{2\pi}d^2(\ln K, \ln s)}$ . En définissant la volatilité implicite européenne  $\sigma_{\rm E}(\tau, s, K)$  comme solution de :

 $P(\tau, s, K) = P_{\rm BS}(\tau, s, K; \sigma_{\rm E}(\tau, s, K)),$ 

où  $P_{\rm BS}$  fait référence au prix d'un Put dans le modèle de Black-Scholes (i.e.  $\sigma(s) = \sigma$  pour tout s), et en utilisant les expansions (0.6.3), (0.6.4), (0.6.5), il existe une expansion polynomiale pour la volatilité implicite européenne de la forme (voir e.g. [71, Section 2.2]),

$$\sigma_{\mathrm{E}}\left(\tau, s, K\right) = \sigma_{0}\left(s, K\right) + \sigma_{1}\left(s, K\right)\tau + \mathcal{O}\left(\tau^{2}\right),$$

où

$$\sigma_0(s,K) = \frac{\ln\left(\frac{s}{K}\right)}{\mathrm{d}\left(\ln K,\ln s\right)},$$
  
$$\sigma_1(s,K) = \frac{\sigma_0^3(s,K)}{\ln\left(\frac{s}{K}\right)^2} \ln\left(\frac{u_0\left(\ln s,\ln K\right)\sigma^2\left(K\right)}{\sigma_0\left(s,K\right)}\right) - \frac{\sigma_0^3\left(s,K\right)}{2\ln\left(\frac{s}{K}\right)} + \frac{r\sigma_0\left(s,K\right)}{\ln\left(\frac{s}{K}\right)},$$

#### 0.6.1Asymptotiques en temps court pour les options américaines dans les modèles à volatilité locale.

Put américain dans un modèle à volatilité locale homogène en temps. Dans le Chapitre 5, en suivant la même méthodologie, nous étudions le prix du Put américain (noté  $A(\tau, s, K)$  pour un prix initial  $S_0 = s$ , strike K et temps à maturité  $\tau$ ) et des expansions asymptotiques de la volatilité implicite pour un modèle de la forme (0.6.1).

Contrairement à une option européenne qui ne peut être exercée qu'à l'échéance, une option américaine donne à son propriétaire le droit d'exercer à tout moment avant ou à l'échéance (voir Bensoussan [24] et Karatzas [121] pour une représentation en un problème d'un temps arrêt optimal). Il est connu (voir McKean [139] et Van Moerbeke [160]) que  $A(\tau, s, K)$  est solution de l'équation aux dérivées partielles (EDP) parabolique avec obstacle suivante :

o .

$$\begin{cases}
-\partial_{\tau}A + \frac{\sigma^{2}(s)s^{2}}{2}\partial_{ss}A + rs\partial_{s}A - rA = 0, \quad \tau > 0, \quad s > \bar{s}(\tau), \\
A(\tau, s, K) > (K - s)_{+}, \quad \tau > 0, \quad s > \bar{s}(\tau), \\
A(\tau, s, K) = (K - s)_{+}, \quad \tau > 0, \quad s \le \bar{s}(\tau), \\
A(0, s, K) = (K - s)_{+}, \quad \tau = 0, \quad s > 0,
\end{cases}$$
(0.6.6)

où la fonction  $\tau \to \bar{s}(\tau)$  dans (0.6.6) est la frontière d'exercice qui caractérise complètement le prix américain. Observons que dans la région de continuation  $\{s > 0 \mid s > \bar{s}(\tau)\}$ , le prix du Put américain est solution de l'EDP de Black–Scholes tandis que dans la région d'exercice  $\{s > 0 \mid s \leq \bar{s}(\tau)\}$ , il est égal au payoff. Le temps d'arrêt optimal pour une option américaine peut ainsi être considéré comme le premier moment pour lequel le cours de l'action franchit la frontière d'exercice.

La frontière d'exercice et la formule de prime anticipée. La frontière d'exercice a été largement étudiée dans la littérature, et nous rappelons ses propriétés principales (voir e.g. Karatzas et Shreve [122]) : la fonction  $\tau \to \bar{s}(\tau)$  est continue et décroissante sur  $\mathbb{R}_+$ ,  $C^1$  sur chaque intervalle  $[\alpha, \infty)$  avec  $\alpha > 0$ ,  $\bar{s}(0) = K$  et  $\lim_{\tau \to 0} \bar{s}'(\tau) = -\infty$ .



Figure 10 – Frontière d'exercice dans un modèle de Black–Scholes en fonction du temps à maturité  $\tau$ .

La relation entre le prix de vente américain et européen est donnée par la représentation intégrale suivante, la formule dite de prime anticipée (voir Kim [125], Jacka [114], Carr, Jarrow et Myneni [44], Huang, Subrahmanyam et Yu [113]),

$$A(\tau, s, K) = P(\tau, s, K) + rK \int_0^\tau e^{-ru} \mathbb{P}_{0,s} \Big( S_u \le \bar{s} (\tau - u) \Big) \mathrm{d}u, \qquad (0.6.7)$$

où le dernier terme à droite de (0.6.7) est appelée prime américaine. Économiquement, ce terme positif quantifie le droit d'exercer l'option avant l'expiration. Pour approximer numériquement
la frontière d'exercice, en prenant  $s = \bar{s}(\tau)$  dans (0.6.7) et en utilisant la condition de continuité  $(0.6.6), A(\tau, \bar{s}(\tau), K) = K - \bar{s}(\tau)$ , nous avons l'équation intégrale de convolution suivante :

$$\bar{s}(\tau) - K + P(\tau, \bar{s}(\tau), K) + rK \int_0^\tau e^{-ru} \mathbb{P}_{0,\bar{s}(\tau)} \Big( S_u \le \bar{s}(\tau - u) \Big) du = 0.$$

La frontière d'exercice  $\bar{s}(\tau)$  peut alors être récursivement approchée en discrétisant l'intégrale avec le point initial  $\bar{s}(0) = K$  (voir Section 5.2.3 pour une discussion détaillée).

Pour étudier le comportement en temps court du prix du Put américain et au vue de (0.6.7), nous devons comprendre comment la frontière d'exercice se comporte près de la maturité dans un modèle (0.6.1). Une asymptotique fine a été proposée par De Marco et Henry-Labordère [53], pour laquelle les auteurs ont montré que pour  $\tau \to 0^+$ ,

$$\ln \bar{s}(\tau) = \ln K - \sigma(K) \sqrt{\tau \ln\left(\frac{\gamma(K)}{\tau}\right)} \left(1 + \frac{1}{\ln^2\left(\frac{\gamma(K)}{\tau}\right)} + \mathcal{O}\left(\frac{1}{\ln^3\left(\frac{1}{\tau}\right)}\right)\right),\tag{0.6.8}$$

où  $\gamma(K) = \frac{\sigma^2(K)}{8\pi(rK)^2}$  joue le rôle d'une échelle de temps. Au vue de (0.6.8), notons que la frontière d'exercice présente essentiellement un comportement parabolique  $\sqrt{\tau}$  avec quelques termes de correction logarithmique (voir Ahn et al. [4, Section 7] et les références associées pour une étude détaillée sur l'expansion asymptotique de la frontière d'exercice près de la maturité).

En combinant (0.6.8), la méthode de Laplace et en définissant la volatilité implicite américaine  $\sigma_{\mathbf{A}}(\tau, s, K)$  comme solution de :

$$A(\tau, s, K) = A_{\rm BS}(\tau, s, K; \sigma_A(\tau, s, K)),$$

nous obtenons les résultats suivants.

**Theorem 0.6.1** (Expansions en temps court de la prime américaine). Soit  $l(\tau) = \ln\left(\frac{\sigma(K)^2}{8\pi r^2 \tau}\right)$ . Si s = K, pour  $\tau \to 0^+$ ,

$$p(\tau,s) = \frac{rs}{2}\tau \frac{C_0}{l(\tau)} + C_1 \frac{\ln^2(l(\tau))}{l^2(\tau)} + C_2 \frac{\ln(l(\tau))}{l^2(\tau)} + \frac{C_3}{l^2(\tau)} \left(1 + o(1)\right),$$

où  $C_0, C_1, C_2, C_3$  sont des constantes universelles, et si s > K,

 $\sigma_{\rm A}$ 

$$p(\tau, s, K) = p_0(s, K) \frac{\tau^{\frac{5}{2}}}{l(\tau)} e^{-\frac{d^2(\ln K, \ln s)}{2\tau}} (1 + o(1)),$$

 $où \ p_0(s,K) = \frac{2rKu_0(\ln s,\ln K)\sigma(K)}{\sqrt{2\pi}d^3(\ln K,\ln s)}.$  Par conséquent, la différence entre la volatilité implicite américaine et européenne est d'ordre

$$(\tau, s, K) - \sigma_{\rm E}(\tau, s, K) = \begin{cases} \mathcal{O}\left(\frac{\tau}{l(\tau)}\right), & \text{if } s = K, \end{cases}$$
(0.6.9)

$$\left( \mathcal{O}\left(\frac{\tau^2}{l\left(\tau\right)}\right), \text{ if } s > K. \right.$$
 (0.6.10)

#### 0.6.2Approximations faibles dans les modèles rough pour la variance forward et expansions des prix d'options sur le VIX

Nous revenons maintenant à la tarification de produits dérivés sur le VIX dans les modèles rough pour la variance forward (voir (0.4.31)). Plutôt que de discrétiser le VIX comme dans le Chapitre 2, nous proposons d'étudier son approximation en loi (ou approximation faible) dans le modèle rough Bergomi (0.4.27). Plus précisément, motivés par le fait que  $\Delta = \frac{1}{12}$  est faible, nous introduisons la nouvelle mesure de probabilité

$$\nu_{0}\left(\mathrm{d}\alpha\right) = \frac{\frac{e^{X_{0}^{\alpha}}}{\Delta}\mathrm{d}\alpha}{\int_{T}^{T+\Delta} e^{X_{0}^{\alpha}}\frac{\mathrm{d}\alpha}{\Delta}},$$

et étudions les approximations faibles de fonctionnels du

$$\begin{aligned} \operatorname{VIX}_{T}^{2} &= \frac{1}{\Delta} \int_{T}^{T+\Delta} e^{X_{T}^{\alpha}} d\alpha \\ &= \int_{T}^{T+\Delta} e^{X_{T}^{\alpha} - X_{0}^{\alpha}} e^{X_{0}^{\alpha}} \frac{d\alpha}{\Delta} \\ &= \left( \int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{d\alpha}{\Delta} \right) \times \int_{T}^{T+\Delta} e^{-\frac{1}{2} \int_{0}^{T} K^{\alpha}(t)^{2} dt + \int_{0}^{T} K^{\alpha}(t) dW_{t}} \nu_{0} \left( \mathrm{d} \alpha \right), \end{aligned}$$
(0.6.11)

exprimées en termes du proxy log-normal suivant (exponentielle de la moyenne arithmétique)

$$\operatorname{VIX}_{T,P}^{2} = \left(\int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta}\right) \times e^{\int_{T}^{T+\Delta} \left[-\frac{1}{2} \int_{0}^{T} K^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K^{\alpha}(t) \mathrm{d}W_{t}\right] \nu_{0}(\mathrm{d}\alpha)}.$$
 (0.6.12)

La connexion entre  $VIX_T^2$  et son proxy  $VIX_{T,P}^2$  est faite au travers de l'interpolation ( $\varepsilon \in [0,1]$ ),

$$\begin{split} I\left(\varepsilon\right) &= \left(\int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta}\right) \int_{T}^{T+\Delta} e^{\int_{T}^{T+\Delta} \left[-\frac{1}{2} \int_{0}^{T} K^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K^{\alpha}(t) \mathrm{d}W_{t}\right] \nu_{0}(\mathrm{d}\alpha)} \\ &\times e^{\varepsilon \left(-\frac{1}{2} \int_{0}^{T} K^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K^{\alpha}(t) \mathrm{d}W_{t} - \int_{T}^{T+\Delta} \left[-\frac{1}{2} \int_{0}^{T} K^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K^{\alpha}(t) \mathrm{d}W_{t}\right] \nu_{0}(\mathrm{d}\alpha)}\right) \nu_{0}\left(\mathrm{d}\alpha\right), \end{split}$$

pour laquelle, par une application directe de la formule de Taylor avec reste intégral, nous avons que  $I(1) - I(0) = \text{VIX}_T^2 - \text{VIX}_{T,\text{P}}^2 = \int_0^1 (1 - \varepsilon) I^2(\varepsilon) d\varepsilon \ge 0$  i.e. le proxy log-normal (0.6.12) sous-estime toujours le  $\text{VIX}_T^2$  (0.6.11). Suivant la méthodologie de Gobet et Miri [85], nous proposons des approximations de prix d'options sous la forme de combinaisons explicites de prix Black–Scholes et de grecs (voir (0.6.13)), ne reposant pas sur des asymptotiques en temps court et étant ainsi valables pour toute maturité.

**Theorem 0.6.2** (Expansion de prix d'option dans le modèle rough Bergomi). Le prix au temps 0 d'une option sur le  $VIX_T^2$  avec payoff régulier  $\varphi$  peut être approché par

$$\mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T}^{2}\right)\right] = \mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T,\mathrm{P}}^{2}\right)\right] + \sum_{i=1}^{3}\gamma_{i} \partial_{\varepsilon}^{i}\mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T,\mathrm{P}}^{2} \times e^{\varepsilon}\right)\right]\Big|_{\varepsilon=0} + \mathcal{O}\left(\Delta^{3H}\right), \quad (0.6.13)$$

où les coefficients  $(\gamma_i)_{i=1,2,3}$  dépendent seulement de  $T, \eta, H$ .



Figure 11 – Smiles du VIX dans le modèle rough Bergomi à un facteur (gauche) pour T = 1, 3, 6 mois et les approximations en erreur relative en % (droite) pour une log-variance forward instantanée plate  $X_0 = \ln (0.235^2), \eta = 1, H = 0.1, \Delta = \frac{1}{12}$ . Le "+" (resp. "\*") fait référence à l'approximation d'ordre zéro (resp. d'ordre trois).

Le Figure 11 compare le smile du VIX et ses approximations d'ordre zéro et du troisième ordre (voir (0.6.13)) pour différentes maturités (1, 3 et 6 mois), et montre que notre formule d'expansion (0.6.13) est tout à fait exact (moins de -2% en erreur relative pour l'approximation du troisième ordre). Notons également que puisque le proxy (0.6.12) est log-normal, l'approximation du smile du VIX à l'ordre zéro est constante.

Le modèle rough Bergomi mixte à un facteur. Afin de palier au smile inconsistant du VIX (qui présente un skew positif prononcé sur le marché) généré par le modèle rough Bergomi, nous étudions le modèle rough Bergomi mixte à un facteur (introduit simultanément par De Marco [52] et Guyon [95]) défini comme

$$\xi_T^{\alpha} = \xi_0^{\alpha} \Big[ \lambda \mathcal{E} \Big( \int_0^T K_1^{\alpha}(t) \mathrm{d}W_t \Big) + (1 - \lambda) \, \mathcal{E} \Big( \int_0^T K_2^{\alpha}(t) \mathrm{d}W_t \Big) \Big], \tag{0.6.14}$$

où  $\mathcal{E}(X)$  est une notation abrégée pour  $e^{X-\frac{1}{2}\operatorname{Var}(X)}$ ,  $K_i^{\alpha}(t) = \eta_i (\alpha - t)^{H-\frac{1}{2}}$  pour  $i = 1, 2, \eta_1, \eta_2 > 0$  qui peuvent être différents paramètres de volatilité-de-volatilité, et  $\lambda \in [0, 1]$  est un paramètre de mélange. La variance forward instantanée est maintenant modélisée par la moyenne exponentielle d'une combinaison convexe de variables aléatoires log-normales :

$$VIX_{T,P}^{2} = \left(\int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta}\right) \times \left(\lambda e^{\int_{T}^{T+\Delta} \left[-\frac{1}{2} \int_{0}^{T} K_{1}^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K_{1}^{\alpha}(t) \mathrm{d}W_{t}\right] \nu_{0}(\mathrm{d}\alpha)} + (1-\lambda) e^{\int_{T}^{T+\Delta} \left[-\frac{1}{2} \int_{0}^{T} K_{2}^{\alpha}(t)^{2} \mathrm{d}t + \int_{0}^{T} K_{2}^{\alpha}(t) \mathrm{d}W_{t}\right] \nu_{0}(\mathrm{d}\alpha)}\right). \quad (0.6.15)$$

En suivant la même stratégie que celle utilisée pour le Théorème 0.6.2, nous obtenons l'approximation suivante pour les prix d'option dans le modèle rough Bergomi mixte à un facteur (0.6.14).

**Theorem 0.6.3** (Expansion de prix d'option dans le modèle rough Bergomi mixte). Le prix au temps 0 d'une option sur le  $VIX_T^2$  avec payoff régulier  $\varphi$  peut être approché par

$$\mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{T}^{\cdot}\right)\right)\right] = P_{0} + \sum_{i=1}^{3} \gamma_{i}(\eta_{1})P_{i,1} + \gamma_{i}(\eta_{2})P_{i,2} + \mathcal{O}\left(\Delta^{3H}\right), \qquad (0.6.16)$$

$$P_{0} = \mathbb{E}\left[\varphi\left(\ln\left(\int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta}\right) \left[\lambda e^{\mu_{1}+\sigma_{1}Z} + (1-\lambda) e^{\mu_{2}+\sigma_{2}Z}\right]\right)\right],$$

où  $Z\stackrel{d}{=}\mathcal{N}\left(0,1
ight)$  et moyenne et variance (pour j=1,2) définies comme

$$\begin{split} \mu_j &= -\frac{1}{2} \int_0^T \Bigl( \int_T^{T+\Delta} K_j^{\alpha}(t)^2 \nu_0(\mathrm{d}\alpha) \Bigr) \mathrm{d}t \\ \sigma_j^2 &= \int_0^T \Bigl( \int_T^{T+\Delta} K_j^{\alpha}(t)^2 \nu_0(\mathrm{d}\alpha) \Bigr)^2 \mathrm{d}t, \end{split}$$

*et pour tout* i = 1, 2, 3,

$$P_{i,1} = \partial_{\varepsilon}^{i-1} \mathbb{E} \left[ \Psi_1 \left( \mu_1 + \sigma_1 + Z + \varepsilon \right) \right] |_{\varepsilon=0}, \qquad P_{i,2} = \partial_{\varepsilon}^{i-1} \mathbb{E} \left[ \Psi_2 \left( \mu_2 + \sigma_2 + Z + \varepsilon \right) \right] |_{\varepsilon=0},$$

et

$$\Psi_{1}(x) = \partial_{\omega} \varphi \left( \ln \left( \int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta} \right) \left[ \lambda e^{x+\omega} + (1-\lambda) e^{\frac{\eta_{2}}{2}(\eta_{1}-\eta_{2})\int_{0}^{T} \int_{T}^{T+\Delta} K_{0}^{\alpha}(t)^{2}\nu_{0}(\mathrm{d}\alpha)\mathrm{d}t + \frac{\eta_{2}}{\eta_{1}}x} \right] \right) \Big|_{\omega=0},$$

$$\Psi_{2}(x) = \partial_{\omega} \varphi \left( \ln \left( \int_{T}^{T+\Delta} e^{X_{0}^{\alpha}} \frac{\mathrm{d}\alpha}{\Delta} \right) \left[ \lambda e^{\frac{\eta_{1}}{2}(\eta_{2}-\eta_{1})\int_{0}^{T} \int_{T}^{T+\Delta} K_{0}^{\alpha}(t)^{2}\nu_{0}(\mathrm{d}\alpha)\mathrm{d}t + \frac{\eta_{1}}{\eta_{2}}x} + (1-\lambda) e^{x+\omega} \right] \right) \Big|_{\omega=0}.$$



Figure 12 – Smiles du VIX dans le modèle rough Bergomi mixte à un facteur (gauche) pour T = 1, 3, 6 mois et les approximations en erreur relative en % (droite) pour une log-variance forward instantanée plate  $X_0 = \ln (0.235^2), \eta_1 = 0.9, \eta_2 = 0.7, \lambda = 0.3, H = 0.1, \Delta = \frac{1}{12}$ . Le "+" (resp. "\*") fait référence à l'approximation d'ordre zéro (resp. d'ordre trois).

et

## Part I

# Multilevel Monte Carlo approximation methods

## CHAPTER 1

# MULTILEVEL MONTE CARLO METHODS AND LOWER–UPPER BOUNDS IN INITIAL MARGIN COMPUTATIONS

Note. The results of this chapter are based on the paper [35].

Abstract. The Multilevel Monte Carlo (MLMC) method developed by Giles [74] has a natural application to the evaluation of *nested* expectation of the form  $\mathbb{E}\left[g(\mathbb{E}\left[f(X,Y)|X\right])\right]$ , where f,g are functions and (X,Y) a couple of independent random variables. Apart from the pricing of American-type derivatives, such computations arise in a large variety of risk valuations (VaR or CVaR of a portfolio, CVA), and in the assessment of margin costs for centrally cleared portfolios. In this work, we focus on the computation of Initial Margin. We analyze the properties of the corresponding MLMC estimators, for which we provide results of asymptotical optimality; at the technical level, we have to deal with limited regularity of the outer function g (which might fail to be everywhere differentiable). Parallel to this, we investigate upper and lower bounds for nested expectations as above, in the spirit of primal-dual algorithms for stochastic control problems.

## 1.1 Introduction

Nested expectations – to be understood as expectations of functionals of conditional expectations – are ubiquitous in the field of financial risk assessment: from standard risk management computations, where a market factor is simulated up to a certain time horizon and then the performance of a portfolio is evaluated conditionally on the value of the factor, to dynamic hedging of derivatives products, in particular nowadays after the widespread establishment of the so-called *valuation adjustments* to derivative trades.

The paradigm of linear risk-neutral pricing of financial contracts has indeed changed in the last years, under the influence of market regulators: for several types of trades, banks and financial institutions have to post collateral to a central counterparty (CCP, also called clearing house) in order to secure their positions. Every day, the CCP requires each market member to deposit a certain capital according to the risk exposure of their contracts. From the modeling

point of view, taking into account this type of regulatory capitals in the valuation of a derivative trade gives rise to non-linear (backward stochastic- or partial-) differential equations.

One of these protection capitals is the Initial Margin (IM) deposit: in case of default of one of the CCP members, the aim of this capital is to cover potential losses experienced by the hedging portfolio during the liquidation period of the defaulted member – concretely, the IM is materialized by the Value-at-risk or Conditional value-at-risk (CVaR) of the member's portfolio over a time period  $\Delta$ . Since the time window  $\Delta$  is small in year units (typically, one week), the usual approach in view of the computations is to apply an asymptotic expansion for the solution of the involved stochastic equation as  $\Delta$  becomes small, see Henry-Labordère [108, Section 4.2] and Agarwal et al. [3]. To be more precise, let us borrow the mathematical setting from [3]: assuming for the underlying asset price the stochastic model  $dS_t = \mu_t S_t dt + \sigma_t S_t dW_t^{\text{hist}}$ , the value V of the hedging portfolio replicating a claim  $\xi$  solves the (eventually) linear Backward Stochastic Differential Equation (BSDE)

$$\begin{aligned} V_t &= \xi + \int_t^T \left( -r_s V_s + Z_s \sigma_s^{-1} \left( r_s - \mu_s \right) + R C_\alpha \sqrt{(s+\Delta) \wedge T - s} \left| Z_s^{\text{ref}} \right| \right) \mathrm{d}s \\ &- \int_t^T Z_s \mathrm{d}W_s^{\text{hist}}, \end{aligned}$$

where  $r_t$  is a risk-free rate. Recall from BSDE theory that the solution to the equation above is the couple of processes  $(V_t, Z_t)$ ; using standard notation in derivative pricing theory, the wealth  $\delta_t S_t$  invested in the asset at time t is related to the Z component via  $\delta_t S_t = Z_t \sigma_t^{-1}$ ,  $\delta_t$  being the number of shares of the asset S contained in the portfolio at time t (a.k.a. the portfolio's delta). The second term inside the time integral appears due to the aforementioned asymptotic expansion as  $\Delta$  becomes small (note that the argument of the square root is equal to  $\Delta$  for every  $s \leq T - \Delta$ ), and corresponds to the additional IM cost, computed using a reference value  $\delta_t^{\text{ref}}$ of the delta via  $Z_t^{\text{ref}} = \delta_t^{\text{ref}} S_t \sigma_t$ . The constant  $C_{\alpha}$  is related to the CVaR of a standard normal distribution (we refer to Section 1.3 for more details), and R denotes the net interest rate of the account used to fund the IM cost. The reference value  $\delta^{\text{ref}}$  is fixed by some external source, and often corresponds to the delta of a standard risk-neutral portfolio (in the simplest case, the Black–Scholes portfolio - but other choices are possible). When  $\xi = \varphi(S_T)$ ,  $r_t$  is deterministic,  $\sigma_t$  and  $\delta_t^{\text{ref}}$  are both functions of time and the underlying price  $S_t$ , we have the following classical Feynman-Kac representation for the initial price  $V_0$ 

$$V_0 = \mathbb{E}\left[e^{-\int_0^T r_s \mathrm{d}s}\varphi(S_T) + R C_\alpha \int_0^T e^{-\int_0^t r_s \mathrm{d}s} \sqrt{(t+\Delta) \wedge T - t} \left| Z^{\mathrm{ref}}(t,S_t) \right| \mathrm{d}t\right], \qquad (1.1.1)$$

where the expectation is computed under a probability measure such that  $dS_t = r_t S_t dt + \sigma_t S_t dW_t$ . The function  $Z^{\text{ref}}(\cdot)$  being defined via a conditional expectation, the problem of computing the price  $V_0$  requires, in general, to evaluate a nested expectation. This is our motivation for tackling expectations of the form

$$I := \mathbb{E}\left[g\left(\mathbb{E}\left[f\left(X,Y\right)|X\right]\right)\right],\tag{1.1.2}$$

by Monte Carlo simulation, notably in situations where the function g has the regularity of the absolute value function  $z \mapsto |z|$ , as in (1.1.1). Precisely, we consider the formulation in this setting of the Multi-level Monte Carlo method, introduced by Giles in [74]. For a detailed survey of the MLMC method and various recent extensions and generalizations, see also Giles [75]. Our main result in this direction (Theorem 1.2.6) is to prove that the so-called antithetic Multi-level nested estimator Giles [75, Section 9] asymptotically achieves the performance of an unbiased estimator (that is: complexity  $\mathcal{O}(\varepsilon^{-2})$  for a tolerance  $\varepsilon^2$  on the mean-squared error), even in this setting of limited regularity for the function g. On the other hand, in the (practically interesting) case where g is convex, we introduce and analyze a representation of (1.1.2) as the solution of a (primal-dual) optimization problem. In the spirit of American option pricing, this representation leads to upper and lower biased non-nested estimators, that we tackle with a regression-based procedure.

In the general setting, X, Y are two independent random variables with values respectively in  $\mathbb{R}^d$  and  $\mathbb{R}^{d'}$ , and  $f: \mathbb{R}^d \times \mathbb{R}^{d'} \to \mathbb{R}$  and  $g: \mathbb{R} \to \mathbb{R}$  are two measurable functions. By independence, the conditional expectation in (1.1.2) can be rewritten as:

$$\mathbb{E}\left[f\left(X,Y\right)|X\right] = E_f(X),\tag{1.1.3}$$

where for every  $x \in \mathbb{R}^d$ ,  $E_f(x) := \mathbb{E}[f(x, Y)]$ . A natural estimator of the conditional expectation in (1.1.3) is, for  $n \ge 1$ ,

$$\widehat{E}_{f,n}(X) := \frac{1}{n} \sum_{i=1}^{n} f(X, Y_i)$$

where the  $(Y_i)_{1 \leq i \leq n}$  are i.i.d. samples of Y independent of X. Conditional on the value of X, the estimator  $\widehat{E}_{f,n}(X)$  is, of course, unbiased; the regularity of the outer function g will determine the bias of the random variable  $g(\widehat{E}_{f,n}(X))$  and therefore of related nested estimators – see Section 1.2 for precise definitions. In order to estimate the bias and overall the performance of such estimators, there is a trade-off between the smoothness of the function g and that of the probability distribution of the underlying random variables – the less regularity on g, the stronger the requirements on the underlying distribution. As mentioned above, the precise regularity conditions we are going to impose on the function g, motivated by the applicability to (1.1.1), together with the assumptions on the law of the underlying random variables, represent the core of our study and the main difference with other works (as we discuss more in details below).

In the existing literature, efforts have been made to evaluate the nested expectation I in (1.1.2) in the case of limited regularity, where g is a step function  $g = 1_{[a,\infty)}$ . This setting appears when evaluating tail distributions and quantiles; in the financial context,  $\mathbb{E}\left[f(X,Y)|X\right]$ will typically represent the loss of a portfolio, conditional on the value of some market factor X. To our knowledge, in early papers dealing with this problem using nested Monte Carlo methods, such as the seminal paper of Gordy and Juneja [89] or Broadie, Du, and Moallemi [39], it is assumed that for  $n \geq 1$ , the couple of random variables  $(E_f(X), \sqrt{n}(E_{f,n}(X) - E_f(X)))$  has a joint density  $g_n$  w.r.t. the two-dimensional Lebesgue measure, and that the partial derivatives  $\partial_y g_n(y,\cdot)$  and  $\partial_y^2 g_n(y,\cdot)$  admit finite moments (up to order 4), uniformly in n. Under these conditions, the authors obtain an expansion of the bias of the nested estimator at order 1. Assumptions of this kind may look rather strong<sup>1</sup> and overall do not seem obvious to check: notably, a control on the moments of the joint law that is uniform over n does not seem easy to achieve. The analysis of the bias is pushed forward in the nice paper by Giorgi, Lemaire, and Pagès [80], where a higher-order expansion is derived. These authors work, on the one hand, with a setting where q is smooth, and on the other hand with an opposite setting where g is a step function: in the latter case, it is assumed that both couples of random variables  $(E_f(X), E_f(X) - \widehat{E}_{f,n}(X))$  and  $(E_f(X), X)$  admit smooth densities on  $\mathbb{R}^2$  for  $n \ge 1$ , and again that a certain number of their partial derivatives with respect to the first variable exist and are continuous<sup>2</sup>. As a comparison with our setting, our Assumption 1.2.3 does not require the existence of densities and their derivatives.

Let us mention some works where other types of functions g have been considered. In Bujok, Hambly, and Reisinger [40], the authors consider the pricing of CDO tranches and face the

<sup>&</sup>lt;sup>1</sup>As an example, one can check that in the case where X is Gaussian, Y is a Bernoulli random variable with  $\mathbb{P}(Y = 1) = 1 - \mathbb{P}(Y = -1) = p$  with p > 0.5, and f(X,Y) = XY, we have  $E_f(X) = (2p - 1)X$ ,  $\widehat{E}_{f,1}(X) - E_f(X) = (Y_1 - 2p + 1)X$ , so that the couple ((2p - 1)X, (Y - 2p + 1)X) does not have a density with respect to the two-dimensional Lebesgue measure.

<sup>&</sup>lt;sup>2</sup>More precisely, denoting respectively  $p_1$  and  $p_2$  the two densities, in order to derive a bias expansion at order  $R \in \mathbb{N}$ , [80] assumes existence of the partial derivatives  $\partial_x^{(l)} p_1(x, y)$  for  $l = 0, ..., 2R+1, \partial_x^{(l)} p_2(x, y)$  for l = 0, ..., 2R, and that  $\partial_x^{(2R+1)} p_1(x, y)$  is continuous.

problem of estimating  $\mathbb{E}[g(\mathbb{E}[Z|X])]$  in the precise case where g is piecewise linear and Z a Bernoulli random variable depending on some economic factor  $X \in [0, 1]$ , while in the survey paper [75], the case where g is twice differentiable is discussed, thus allowing for more general assumptions on X. In Giles and Goda [76], the aim is to estimate  $\mathbb{E}[\max_{d \in D} \mathbb{E}[f_d(X, Y)|X]]$ where D is a finite set; similar assumptions to ours, though more restrictive, are made (see further below for more details). In both papers, the tolerance  $\varepsilon^2$  on the mean-squared error is achieved with complexity  $\mathcal{O}(\varepsilon^{-2})$ , using an antithetic Multi-level estimator.

In our setting, the function g would typically be the absolute value – and more generally, a continuous and piecewise  $C_b^1$  function (see Assumption 1.2.1). With respect to the works cited above, we are in a situation of intermediate regularity of the function g – less than  $C^2$ , but more regular than a step function – thus allowing to drop restrictive assumptions on the distribution of the underlying random variables. It will be sufficient for us to only exploit some (mild) regularity of the law of  $E_f(X)$  in the neighborhood of the singularities of g, instead of considering the joint law of  $E_f(X)$  and its estimator. The arguments used in this work are close to those in Giles and Haji-Ali [77], where g is a step function and the authors assume that in a neighborhood of the discontinuity point of the step function, the random variable  $\frac{E_f(X)}{\sqrt{\operatorname{Var}(f(X,Y)|X)}}$ 

has a bounded density; the resulting Multi-level estimator achieves mean-squared error  $\varepsilon^2$  with complexity  $\mathcal{O}(\varepsilon^{-2}|\log \varepsilon|^2)$ . Once again, we would like to point out that such conditions on the underlying distributions are stronger than ours. In fact, our setting allows us to treat the case of a butterfly option payoff (see Section 1.3.2), for which the assumption of the existence of a bounded density seems out of reach, while our milder assumption (Assumption 1.2.3) proves to be checkable in financially meaningful cases.

The paper is organized as follows. In Section 1.2, we study the generic problem of estimating I. Here we compare theoretically and numerically different nested estimators. In particular, we show that using the MLMC method, the tolerance  $\varepsilon^2$  on the mean-squared error can be achieved with complexity  $\mathcal{O}(\varepsilon^{-2})$  for a function g satisfying Assumption 1.2.1, provided that the probability that the conditional expectation  $\mathbb{E}[f(X,Y)|X]$  is close to the singular points of g can be controlled polynomially. In Section 1.2.3 we introduce an algorithm computing lower and upper bounds using non-nested Monte Carlo simulations. In Section 1.3 we show that the problem of evaluating the option price  $V_0$  (1.1.1) with initial margin correction fits in the framework of our generic problem, and we numerically compare the results obtained using the different methods.

**Notations.** We denote  $||f||_{\infty}$  the sup-norm for bounded functions, and  $||A||_p := \mathbb{E}[|A|^p]^{\frac{1}{p}}$ , p > 0, the  $L^p$  norm for vector-valued random variables. For a function  $f : \mathbb{R} \to \mathbb{R}$ , its Total-Variation semi-norm is defined by  $||f||_{\mathsf{TV}} := \sup \sum_{i=1}^{N} |f(x_i) - f(x_{i-1})|$ , where the supremum is taken over finite sequences of increasing points  $(x_i)_i$ .

### 1.2 Theoretical methodology

As mentioned in the introduction, we want to design optimal Multilevel estimators in situations where the function g is of the form g(x) = |x| or  $g(x) = (x-a)^+$  for some  $a \in \mathbb{R}$ . Such examples enter in the class of functions covered by the following assumption: essentially, we are asking that the function g be continuous and piecewise  $C_b^1$ .

**Assumption 1.2.1.** The function g is continuous, and there exists a finite set of points  $-\infty = d_0 < d_1 < ... < d_\theta < d_{\theta+1} = \infty$  such that on each open interval  $(d_i, d_{i+1}), 0 \le i \le \theta$ , g is of class  $C^1$ , g' is bounded and Hölder continuous for some exponent  $\eta \in (0, 1]$ .

We will also need to be able to control the probability that the random variable  $E_f(X) = \mathbb{E}[f(X, Y)|X]$  takes values in a neighborhood of the singularities of g; Assumption 1.2.3 below

precisely takes care of this. Finally, Assumption 1.2.2 requires finiteness of some moment of order p > 2 for the random variable f(X, Y), a condition that is met in most of the examples of practical interest.

Assumption 1.2.2. There exists p > 2 such that  $\mathbb{E}\left[|f(X,Y)|^p\right] < \infty$ .

Assumption 1.2.3 (Small ball estimate around the singularities). There exist some positive constants  $\nu$ ,  $K_{\nu}$  and  $z_0$  such that

$$\mathbb{P}\left(\operatorname{dist}(E_f(X), D) \le z\right) \le K_{\nu} z^{\nu}, \qquad \forall z < z_0, \qquad (1.2.1)$$

where  $\operatorname{dist}(y, D) := \min_{1 \le i \le \theta} |y - d_i|.$ 

Note that, if the random variable  $E_f(X)$  has a bounded density p, then Assumption 2.3 trivially holds true with  $\nu = 1$ , since in this case  $\mathbb{P}(\operatorname{dist}(E_f(X), D) \leq z) \leq \sum_{i=1}^{\theta} \mathbb{P}(|E_f(X) - d_i| \leq z) \leq 2\theta ||p||_{\infty} z$ . On the other hand, Assumption 1.2.3 is more general: it is stated in terms of the distribution of  $E_f(X)$  and does not require existence or regularity of a density for  $E_f(X)$ .

The basic estimator of the nested expectation (1.1.2) approximates the inner conditional expectation and the outer expectation with independent Monte Carlo samples; we obtain the plain Nested Monte Carlo (NMC) estimator

$$\widehat{I}_{M,N} = \frac{1}{M} \sum_{m=1}^{M} g\left(\frac{1}{N} \sum_{j=1}^{N} f\left(X_m, Y_j^m\right)\right), \qquad (1.2.2)$$

where  $M, N \in \mathbb{N}^*$ , and  $(X_m)_{m \in \mathbb{N}^*}$ ,  $(Y_j^m)_{j,m \in \mathbb{N}^*}$  are independent i.i.d. families having the same distribution as X and Y respectively. Multilevel (ML) estimators are obtained by combining estimators of the form of  $\widehat{I}_{M,N}$ . In the following section, we consider the so-called *antithetic* ML estimator, for which we show that it achieves the asymptotically unbiased setting; another "standard" (and sub-optimal, then) ML estimator is also analyzed in Section 1.2.2, see (1.2.8).

#### **1.2.1** Multilevel Monte Carlo estimator

Let us consider two independent families of i.i.d. random variables  $(X_m^l)_{l,m\in\mathbb{N}^*}$  and  $(Y_j^{l,m})_{j,l,m\in\mathbb{N}^*}$ , distributed according to X and Y respectively. We denote  $L \in \mathbb{N}^*$  the number of levels in the estimator. Let  $\mathbf{M} = (M_0, ..., M_L) \in (\mathbb{N}^*)^{L+1}$ , respectively  $\mathbf{n} = (n_0, ..., n_L) \in (\mathbb{N}^*)^{L+1}$ , be multiindexes representing the number of samples used to approximate the outer expectation, respectively the inner conditional expectation in (1.1.2) at the different levels. We assume  $n_l > n_{l-1}$ for every l = 1, ..., L. The antithetic Multilevel estimator of I is defined by

$$\widehat{I}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}} = \frac{1}{M_0} \sum_{m=1}^{M_0} g\left(\frac{1}{n_0} \sum_{j=1}^{n_0} f\left(X_m^0, Y_j^{0,m}\right)\right) + \sum_{l=1}^{L} \frac{1}{M_l} \sum_{m=1}^{M_l} \left\{g\left(\frac{1}{n_l} \sum_{j=1}^{n_l} f\left(X_m^l, Y_j^{l,m}\right)\right) - \frac{1}{2} \left(g\left(\frac{1}{n_{l-1}} \sum_{j=1}^{n_{l-1}} f\left(X_m^l, Y_j^{l,m}\right)\right) + g\left(\frac{1}{n_{l-1}} \sum_{j=n_{l-1}+1}^{n_l} f\left(X_m^l, Y_j^{l,m}\right)\right)\right)\right\}.$$
(1.2.3)

Note that, in the expression inside the curly brackets, the function g is evaluated more than once on different empirical means, constructed using the samples  $X_m^l$  and  $Y_j^{l,m}$  at level l only. From now on, we set

$$n_l = n_0 2^l, \qquad 0 \le l \le L;$$

the remaining degrees of freedom of the estimator lie in the choices of  $n_0$ , L, and of the sample size  $M_l$  for every l.

The mean-squared error of  $\widehat{I}_{M,n}^{\mathrm{ML}}$  can (as usual) be decomposed into bias and variance

$$MSE := \mathbb{E}\left[\left(\widehat{I}_{\boldsymbol{M},\boldsymbol{n}}^{ML} - I\right)^2\right] = \left(\mathbb{E}\left[\widehat{I}_{\boldsymbol{M},\boldsymbol{n}}^{ML}\right] - I\right)^2 + \operatorname{Var}\left(\widehat{I}_{\boldsymbol{M},\boldsymbol{n}}^{ML}\right).$$
(1.2.4)

Under Assumptions 1.2.1, 1.2.2 and 1.2.3, we separately estimate the bias and variance terms in (1.2.4).

**Proposition 1.2.4** (Bias estimate). Let  $(Y_j)_{j \in \mathbb{N}^*}$  be an i.i.d. family of random variables distributed according to Y and independent of X. Under Assumptions 1.2.1, 1.2.2 and 1.2.3, there exists a positive constant  $\kappa$  such that

$$\forall n \ge 1, \quad \left| \mathbb{E}\left[ g\left(\frac{1}{n} \sum_{j=1}^{n} f(X, Y_j)\right) - g\left(E_f(X)\right) \right] \right| \le \frac{\kappa}{n^{\frac{1}{2}\left(1 + \frac{(p-1)\nu}{p+\nu} \land \eta\right)}}.$$
 (1.2.5)

Note that the smooth case with no singularities (that is,  $g \in C_b^1$  with Lipschitz continuous derivative) corresponds to  $\eta = 1$  and  $\nu = \infty$ . In this case, the exponent for n at the denominator of (1.2.5) becomes  $\frac{1}{2}(1 + (p - 1) \wedge 1)$ . If  $p \ge 2$ , this number is worth  $\frac{1}{2}2 = 1$ . Therefore, in this case Proposition 1.2.4 provides the standard  $\mathcal{O}\left(\frac{1}{n}\right)$  estimate for the bias in the presence of a smooth function.

We now turn to an estimate of the variance term. Proposition 1.2.5 estimates the contribution to the global variance of the ML estimator coming from level l. To do so, let us introduce the notation

$$\begin{split} V_{l} &:= \operatorname{Var} \left( g\left( \frac{1}{n_{l}} \sum_{j=1}^{n_{l}} f\left( X, Y_{j} \right) \right) - \frac{1}{2} g\left( \frac{1}{n_{l-1}} \sum_{j=1}^{n_{l-1}} f\left( X, Y_{j} \right) \right) \\ &- \frac{1}{2} g\left( \frac{1}{n_{l-1}} \sum_{j=n_{l-1}+1}^{n_{l}} f\left( X, Y_{j} \right) \right) \right). \end{split}$$

**Proposition 1.2.5** (Variance estimate). Under Assumptions 1.2.1, 1.2.2 and 1.2.3, there exists a positive constant  $\tilde{\kappa}$  such that

$$V_l \le \frac{\tilde{\kappa}}{n_l^{1+\frac{(p-2)\nu}{2(p+\nu)}\wedge\eta}},\tag{1.2.6}$$

holds for every  $l \geq 1$ .

Once again, note that in the smooth case (that is:  $g \in C_b^1$  with Lipschitz derivative, no singularities), we can take  $\eta = 1$  and  $\nu = \infty$ . The exponent for  $n_l$  in (1.2.6) then becomes  $1 + \frac{p-2}{2} \wedge 1$ . If we are allowed to take  $p \to \infty$ , this number tends to 1 + 1 = 2, which corresponds to a  $\mathcal{O}\left(\frac{1}{n_l^2}\right)$ estimate of the variance at level l.

We are now in a position to apply the Multilevel Theorem of Giles [75] and conclude on global convergence rates. Since we wish to keep track of the constants arising from our assumptions (for numerical purposes), we also provide a brief proof of the theorem.

**Theorem 1.2.6.** Let Assumptions 1.2.1, 1.2.2 and 1.2.3 hold true, and consider an error tolerance  $\varepsilon > 0$ . There exist  $n_0, M_0, L$  such that the bound MSE =  $\mathcal{O}(\varepsilon^2)$  as  $\varepsilon \to 0$  is achieved with a computational complexity  $\mathcal{O}(\varepsilon^{-2})$  with the choice:

$$n_l = n_0 2^l$$
,  $M_l = M_0 2^{-\left(1 + \frac{(p-2)\nu}{4(p+\nu)} \wedge \frac{\eta}{2}\right)l}$ ,  $0 \le l \le L$ .

As a comment on Theorem 1.2.6, note that it states an existence result for an optimal set of ML parameters L,  $n_l$  and  $M_l$  achieving the performance of the unbiased setting. Unfortunately, the question of how to set numerically the constants  $n_0, M_0, L$  remains open – this is a usual situation in MLMC literature: we know how to optimize convergence rates, but some constants remain implicitly defined. However, supposing that we knew the constant  $\kappa$  (resp.  $\tilde{\kappa}$ ) in Proposition 1.2.4 (resp. Propositon 1.2.5), then we could choose the following optimal values for  $n_0, M_0, L$  (see the proof of Theorem 1.2.6 for further details): for any  $n_0 \in \mathbb{N}^*$ , set

$$L = \left[\frac{\log\left(\frac{\sqrt{2}\kappa}{n_0^{\alpha}\varepsilon}\right)}{\alpha\log 2}\right], \quad M_0 = \left[\frac{2}{\varepsilon^2}\,\tilde{\kappa}\,n_0^{-\beta}\frac{1-2^{-\frac{L+1}{2}(\beta-\gamma)}}{1-2^{\frac{1}{2}(\beta-\gamma)}}\right].$$
(1.2.7)

Remark 3. Note also that the optimal number of Monte Carlo samples at level l is of the form  $M_l = M_0 2^{-(1+a)l}$  for a positive constant a, so that the computational cost at level l is proportional to  $n_l M_l = n_0 M_0 2^{-al} = \mathcal{O}(\varepsilon^{-2}) 2^{-al}$ : as usual in the ML framework, the most expensive levels are the coarsest ones. As we have done for Propositions 1.2.4 and 1.2.5, it is instructive to consider the case corresponding to  $\eta = 1$  in Assumption 1.2.1. If we can take p to be large in Assumption 1.2.2,  $M_l$  approaches  $M_0 2^{-\left(1+\frac{\nu}{4}\wedge\frac{1}{2}\right)}$ . When there are no singularities, then we can take  $\nu \to \infty$  in the small ball estimate (1.2.1) and obtain  $M_l = M_0 2^{-\frac{3}{2}l}$ . When there is at least one singularity but we can still take  $\nu = 1$ , then we obtain  $M_l = M_0 2^{-\frac{3}{4}l}$ . Overall, Theorem 1.2.6 tells that, as soon as  $\nu > 0$  and p > 2, we can make the choice  $M_l = M_0 2^{-(1+a)l}$  for some positive a, which is still enough to achieve an overall cost of order  $\mathcal{O}(\varepsilon^{-2})$  for the ML estimator.

Proof of Theorem 1.2.6. We start from decomposition (1.2.4). Due to the telescopic sum property of ML estimator (1.2.3), it is clear that  $\mathbb{E}\left[\widehat{I}_{M,n}^{\mathrm{ML}}\right] = \mathbb{E}\left[g\left(\frac{1}{n_L}\sum_{j=1}^{n_L} f\left(X_1^L, Y_j^{L,1}\right)\right)\right]$ . By Proposition 1.2.4, there exists a positive constant  $\kappa$ , independent of  $\boldsymbol{n}$ , such that

$$\left|\mathbb{E}\left[\widehat{I}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}}-I\right]\right| = \left|\mathbb{E}\left[g\left(\frac{1}{n_{L}}\sum_{j=1}^{n_{L}}f\left(X,Y_{j}\right)\right)\right]-I\right| \leq \frac{\kappa}{n_{L}^{\alpha}} = \kappa n_{0}^{-\alpha} 2^{-\alpha L},$$

with  $\alpha := \frac{1}{2} \left( 1 + \frac{(p-1)\nu}{p+\nu} \wedge \eta \right)$ . This estimate drives our choice of the number of levels; we want the squared bias to be smaller than  $\frac{\varepsilon^2}{2}$ , which gives:

$$\kappa^2 \, n_0^{-2\alpha} \, 2^{-2\alpha L} \le \frac{\varepsilon^2}{2} \iff L \ge \frac{\log\left(\frac{\sqrt{2\kappa}}{n_0^\alpha \varepsilon}\right)}{\alpha \log 2}$$

We therefore choose L as in (1.2.7).

On the other hand, Proposition 1.2.5 states that

$$V_l \le \tilde{\kappa} \, n_0^{-\beta} 2^{-\beta l}, \qquad \forall \ 1 \le l \le L,$$

where  $\beta = 1 + \frac{(p-2)\nu}{2(p+\nu)} \wedge \eta$ . The computational cost  $C_l$  for one single sample in the layer l is proportional to  $n_l$ , hence bounded by a constant times  $2^{\gamma l}$  with  $\gamma = 1$ . The hypotheses of Giles [75, Theorem 1] are therefore satisfied: in particular, it is easy to check that  $\alpha \geq \frac{1}{2} \min(\beta, \gamma)$ and that p > 2 implies  $\beta > \gamma$ . Hence, we are in the first case of Giles [75, Theorem 1], which states that the overall complexity of the ML estimator behaves as  $\mathcal{O}(\varepsilon^{-2})$ .

The optimal number of Monte Carlo samples  $M_l$  can be set by minimizing the computational cost of the ML estimator under the constraint that the global variance is smaller than  $\frac{\varepsilon^2}{2}$ . The solution is of the form  $M_l = M_0 2^{\frac{-(\beta+\gamma)l}{2}}$  where  $M_0$  is a constant chosen so that the variance

is smaller than  $\frac{\varepsilon^2}{2}$ . More precisely, by independence  $\operatorname{Var}\left(\widehat{I}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}}\right) = \sum_{l=0}^{L} \frac{V_l}{M_l}$ , and the following estimate holds:

$$\sum_{l=0}^{L} \frac{V_l}{M_l} \le \sum_{l=0}^{L} \frac{\tilde{\kappa} n_0^{-\beta} 2^{-\beta l}}{M_0 2^{-\frac{l}{2}(\beta+\gamma)}} = \frac{\tilde{\kappa} n_0^{-\beta}}{M_0} \frac{1 - 2^{-\frac{L+1}{2}(\beta-\gamma)}}{1 - 2^{-\frac{1}{2}(\beta-\gamma)}},$$

where we recall that  $\beta > \gamma$ . Hence, setting  $M_0 = \left[\frac{2}{\varepsilon^2} \tilde{\kappa} n_0^{-\beta} \frac{1-2^{-\frac{L+1}{2}(\beta-\gamma)}}{1-2^{-\frac{1}{2}(\beta-\gamma)}}\right]$  yields  $\operatorname{Var}\left(\widehat{I}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}}\right) \leq \frac{\varepsilon^2}{2}$ and evoking (1.2.4), we obtain MSE  $\leq \frac{\varepsilon^2}{2} + \frac{\varepsilon^2}{2} = \varepsilon^2$ . It is sufficient to note that  $\frac{\beta+\gamma}{2} = 1 + \frac{(p-2)\nu}{4(p+\nu)} \wedge \frac{\eta}{2}$  to conclude the proof to conclude the proof.

One can notice that, once the quantitative bias and variance estimates (1.2.5) and (1.2.6)have been established, the proof of Theorem 1.2.6 is relatively straightforward. The most difficult part lies indeed in proving Propositions 1.2.4 and 1.2.5; their proofs are provided in Sections 1.2.4 and 1.2.5.

#### 1.2.2Other nested estimators

We analyze in this section alternative nested or MLMC estimators that will be tested in our numerical experiments. Some simulation-based lower and upper bounds on I that do not require nested simulations will be presented in the following section. The first is the plain Nested Monte Carlo estimator (1.2.2). We denote

$$MSE^{NMC} := \mathbb{E}\left[\left(\widehat{I}_{M,N} - I\right)^2\right]$$

the associated mean-squared error.

**Proposition 1.2.7** (Complexity of the Nested Monte Carlo estimator (1.2.2)). Let Assumptions 1.2.1, 1.2.2 and 1.2.3 hold true, and consider an error tolerance  $\varepsilon > 0$ . As  $\varepsilon \to 0$ , the bound  $MSE^{NMC} = \mathcal{O}(\varepsilon^2) \text{ is achieved with a computational complexity } \mathcal{O}\left(\varepsilon^{-2\left(1 + \frac{1}{1 + \frac{(p-1)\nu}{p+\nu} \land \eta}\right)}\right) \text{ with the }$ 

choice  $M \sim \varepsilon^{-2}$  and  $N \sim \varepsilon^{-\frac{2}{1+\frac{(p-1)\nu}{p+\nu}\wedge\eta}}$ 

Note that in the smooth case where we can take  $\eta = 1$  and  $\nu = \infty$ , the exponent in the definition of N becomes  $\frac{(p-1)\nu}{p+\nu} \wedge \eta = (p-1) \wedge \eta$ . If  $p \ge 2$ , we retrieve the standard computational complexity  $\mathcal{O}(\varepsilon^{-3})$  for nested estimators involving smooth functions.

In addition to the antithetic ML estimator  $\widehat{I}_{M,n}^{\text{ML}}$  considered in Section 1.2.1, we introduce a non-antithetic "standard" ML estimator  $\widehat{I}_{M,n}^{\text{ML2}}$ , ML2 estimator in short, defined by

$$\widehat{I}_{\boldsymbol{M},\boldsymbol{n}}^{\text{ML2}} = \frac{1}{M_0} \sum_{m=1}^{M_0} g\left(\frac{1}{n_0} \sum_{j=1}^{n_0} f\left(X_m^0, Y_j^{0,m}\right)\right) + \sum_{l=1}^{L} \frac{1}{M_l} \sum_{m=1}^{M_l} \left\{g\left(\frac{1}{n_l} \sum_{j=1}^{n_l} f\left(X_m^l, Y_j^{l,m}\right)\right) - g\left(\frac{1}{n_{l-1}} \sum_{j=1}^{n_{l-1}} f\left(X_m^l, Y_j^{l,m}\right)\right)\right\},$$
(1.2.8)

where the notation is the same as in Section 1.2.1. Let  $MSE^{ML2} = \mathbb{E}\left[\left(\widehat{I}_{M,n}^{ML2} - I\right)^2\right]$  be the associated mean-squared error.

**Proposition 1.2.8** (Complexity of the non-antithetic ML estimator (1.2.8)). Let Assumptions 1.2.1, 1.2.2 and 1.2.3 hold true, and consider an error tolerance  $\varepsilon > 0$ . There exist  $n_0, M_0, L$ such that the bound MSE<sup>ML2</sup> =  $\mathcal{O}(\varepsilon^2)$  as  $\varepsilon \to 0$  is achieved with a computational complexity  $\mathcal{O}((\log \varepsilon)^2 \varepsilon^{-2})$  with the choice:

$$n_l = n_0 2^l$$
,  $M_l = M_0 2^{-l}$ ,  $0 \le l \le L$ .

As our main theorem (Theorem 1.2.6), Propositions 1.2.7 and 1.2.8 are also based on the bias and variance estimates derived in Section 1.2.1; their proofs are postponed to Section 1.5.

Observe that in terms of complexity for a given error tolerance, the two estimators considered in this section are theoretically less efficient than the antithetic MLMC estimator (1.2.3). They will all be compared in our numerical tests.

#### 1.2.3 Non-nested upper and lower bounds

Following common practice in American option pricing (see Haugh and Kogan [101]), another way of estimating nested expectations is to approach their value through lower and upper bounds which are computed using non-nested Monte Carlo algorithms. Using Legendre–Fenchel transforms, a similar result has been proved (though their statements, proof and applications differ from ours) in the recent paper Guo and Loeper [93, Theorem 2.1] where the authors provide non-nested bounds for  $\mathbb{E}\left[g\left(\mathbb{E}\left[H|\mathcal{F}_t\right]\right)\right]$  where  $(\mathcal{F}_t)_{t\in[0,T]}$  denotes a filtration, H an  $\mathcal{F}_T$ -measurable random variable and g is convex. Our upper bound in Theorem 1.2.10 looks similar to that of Guo and Loeper [93, Theorem 2.1]), while our lower bound has a different representation from theirs. Furthermore, here we complement our lower–upper bounds with theoretical error estimates (see Theorem 1.2.10).

**Lemma 1.2.9.** Let  $K \in \mathbb{R}$ , and let  $\mathcal{R}$  be a real integrable random variable. For any measurable function  $\varphi : \mathbb{R} \to \mathbb{R}$  and random variable  $\mathcal{O}$ , we have

$$\mathbb{E}\left[(\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right]-K)_{+}\right] \geq \mathbb{E}\left[(\mathcal{R}-K)\mathbf{1}_{\varphi(\mathcal{O})\geq K}\right] =: C_{\varphi}(K),\\ \mathbb{E}\left[(K-\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right])_{+}\right] \geq \mathbb{E}\left[(K-\mathcal{R})\mathbf{1}_{\varphi(\mathcal{O})\leq K}\right] =: P_{\varphi}(K).$$

*Proof.* Let  $\varphi$  and  $\mathcal{O}$  be as above. Since

$$\mathbb{E}\left[(\mathcal{R}-K)\mathbf{1}_{\varphi(\mathcal{O})\geq K}\right] = \mathbb{E}\left[(\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right]-K)\mathbf{1}_{\varphi(\mathcal{O})\geq K}\right]$$

and  $(\mathbb{E}[\mathcal{R}|\mathcal{O}] - K)_+ = (\mathbb{E}[\mathcal{R}|\mathcal{O}] - K)\mathbf{1}_{\mathbb{E}[\mathcal{R}|\mathcal{O}] \ge K}$ , we deduce that

$$\mathbb{E}\left[(\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right]-K)_{+}\right]-\mathbb{E}\left[(\mathcal{R}-K)\mathbf{1}_{\varphi(\mathcal{O})\geq K}\right]$$
$$=\mathbb{E}\left[(\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right]-K)(\mathbf{1}_{\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right]>K}-\mathbf{1}_{\varphi(\mathcal{O})>K})\right].$$

Note that the random variable inside the expectation on the right-hand side above is always non-negative, from which we obtain the first inequality. The second inequality is obtained with a similar argument.  $\hfill \Box$ 

Given a convex function  $g : \mathbb{R} \to \mathbb{R}$ , g is differentiable except on a countable set of points. For a differentiable point  $z \in \mathbb{R}$  of g, we have

$$\forall x \in \mathbb{R}, \ g(x) = g(z) + g'(z)(x - z) + \int_{z}^{\infty} (x - u)^{+} \mu(\mathrm{d}u) + \int_{-\infty}^{z} (u - x)^{+} \mu(\mathrm{d}u), \qquad (1.2.9)$$

where  $\mu(du)$  corresponds to the second derivative of g in the sense of distributions. Let us define, for a measurable function  $\varphi : \mathbb{R} \to \mathbb{R}$ , the functional

$$J_{\varphi} = g(z) + g'(z)(\mathbb{E}\left[\mathcal{R}\right] - z) + \int_{z}^{\infty} C_{\varphi}(u)\mu(\mathrm{d}u) + \int_{-\infty}^{z} P_{\varphi}(u)\mu(\mathrm{d}u).$$
(1.2.10)

Although  $J_{\varphi}$  also depends on z, we omit this dependence in our notation, for the sake of simplicity.

**Theorem 1.2.10.** Let  $\mathcal{R}$  be a real integrable random variable and  $g : \mathbb{R} \to \mathbb{R}$  a convex function such that  $g(\mathcal{R})$  is integrable. The following identity holds

$$\sup_{\varphi} J_{\varphi} = \mathbb{E}\left[g(\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right])\right] = \inf_{\varepsilon} \mathbb{E}\left[g(\mathcal{R}-\varepsilon)\right], \qquad (1.2.11)$$

where the inf is taken over the set of random variables { $\varepsilon$  is integrable and such that  $\mathbb{E}[\varepsilon|\mathcal{O}] = 0$ }. Equality is attained for  $\varphi^{\star}(\mathcal{O}) = \mathbb{E}[\mathcal{R}|\mathcal{O}]$  and for  $\varepsilon^{\star} = \mathcal{R} - \mathbb{E}[\mathcal{R}|\mathcal{O}]$ . Moreover, the following error estimate holds:

$$0 \le J_{\varphi^{\star}} - J_{\varphi} \le 2 \mathbb{E} \big[ \big| \varphi^{\star}(\mathcal{O}) - \varphi(\mathcal{O}) \big| \mu([\varphi^{\star}(\mathcal{O}), \varphi(\mathcal{O})]) \big].$$
(1.2.12)

If g is Lipschitz with Lipschitz constant  $L_q$ , the error estimate

$$0 \le \mathbb{E}\left[g(\mathcal{R} - \varepsilon)\right] - \mathbb{E}\left[g(\mathcal{R} - \varepsilon^{\star})\right] \le L_g \left\|\varepsilon^{\star} - \varepsilon\right\|_1.$$
(1.2.13)

is straightforward. Finally, if g is improved to  $C^2$  with bounded second derivative, the upper bound in (1.2.13) can be replaced by  $\frac{1}{2} \|g''\|_{\infty} \|\varepsilon^* - \varepsilon\|_2^2$ .

In (1.2.12),  $\mu([a, b])$  stands for the measure of the interval [a, b] if  $a \leq b$  or [b, a] if b < a. When  $g(x) = x_+$  ( $\mu$  is the Dirac measure at 0) as in our numerical experiments, the bounds (1.2.12) and (1.2.13) are replaced by  $2\mathbb{E}\left[|\varphi^*(\mathcal{O}) - \varphi(\mathcal{O})|\right]$  and  $\mathbb{E}\left[|\varepsilon^* - \varepsilon|\right]$ , with no hope to significantly improve them. If g were  $C^2$  with bounded second derivative,  $2\|g''\|_{\infty}\mathbb{E}\left[|\varphi^*(\mathcal{O}) - \varphi(\mathcal{O})|^2\right]$  would be a better estimate for (1.2.12).

*Proof.* To obtain the inequality  $\mathbb{E}\left[g(\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right])\right] \geq J_{\varphi}$  for every  $\varphi$ , it is sufficient to replace x by  $\mathbb{E}\left[\mathcal{R}|\mathcal{O}\right]$  in (1.2.9) and then apply Lemma 1.2.9 and Fubini's theorem. Optimality of  $\varphi^{\star}(\mathcal{O}) = \mathbb{E}\left[\mathcal{R}|\mathcal{O}\right]$  is also implied by Lemma 1.2.9, and the equality on the left-hand side of (1.2.11) follows.

The identity on the right-hand side of (1.2.11) is also straightforward to prove: for any integrable random variable  $\varepsilon$  such that  $\mathbb{E}[\varepsilon|\mathcal{O}] = 0$ , we have  $\mathbb{E}[g(\mathcal{R} - \varepsilon)] \ge \mathbb{E}[g([\mathbb{E}[\mathcal{R} - \varepsilon|\mathcal{O}])] = \mathbb{E}[g(\mathbb{E}[\mathcal{R}|\mathcal{O}])]$  by Jensen's inequality. It is immediate to check that equality is reached for  $\varepsilon^* = \mathcal{R} - \mathbb{E}[\mathcal{R}|\mathcal{O}]$ , which concludes this part of the proof.

We now move to the error estimates. From the identities,  $C_{\varphi}(u) = \mathbb{E}\left[\left(\mathcal{R}-u\right)\mathbf{1}_{\varphi(O)\geq u}\right] = \mathbb{E}\left[\left(\varphi^{\star}(\mathcal{O})-u\right)\mathbf{1}_{\varphi(O)\geq u}\right] \text{ and } P_{\varphi}(u) = \mathbb{E}\left[\left(u-\varphi^{\star}(\mathcal{O})\right)\mathbf{1}_{\varphi(O)\leq u}\right],$ we get

$$J_{\varphi^{\star}} - J_{\varphi} = \int_{z}^{\infty} \mathbb{E}\left[\left(\varphi^{\star}(\mathcal{O}) - u\right) \left(\mathbf{1}_{\varphi^{\star}(\mathcal{O}) \ge u} - \mathbf{1}_{\varphi(\mathcal{O}) \ge u}\right)\right] \mu(\mathrm{d}u)$$
(1.2.14)

$$+ \int_{-\infty}^{z} \mathbb{E}\left[ \left( u - \varphi^{\star}(\mathcal{O}) \right) \left( \mathbf{1}_{\varphi^{\star}(\mathcal{O}) \leq u} - \mathbf{1}_{\varphi(\mathcal{O}) \leq u} \right) \right] \mu(\mathrm{d}u).$$
(1.2.15)

Now, if  $\varphi^{\star}(\mathcal{O}) \geq u > \varphi(\mathcal{O})$ , we have

$$0 \leq (\varphi^{\star}(\mathcal{O}) - u) \left( \mathbf{1}_{\varphi^{\star}(\mathcal{O}) \geq u} - \mathbf{1}_{\varphi(\mathcal{O}) \geq u} \right) = (\varphi^{\star}(\mathcal{O}) - u) \mathbf{1}_{\varphi^{\star}(\mathcal{O}) \geq u > \varphi(\mathcal{O})}$$
$$\leq (\varphi^{\star}(\mathcal{O}) - \varphi(\mathcal{O})) \mathbf{1}_{\varphi^{\star}(\mathcal{O}) \geq u > \varphi(\mathcal{O})}.$$

Similarly, if  $\varphi(\mathcal{O}) \ge u > \varphi^{\star}(\mathcal{O})$ ,

$$0 \le (\varphi^{\star}(\mathcal{O}) - u) \left( \mathbf{1}_{\varphi^{\star}(\mathcal{O}) \ge u} - \mathbf{1}_{\varphi(\mathcal{O}) \ge u} \right) \le (\varphi(\mathcal{O}) - \varphi^{\star}(\mathcal{O})) \mathbf{1}_{\varphi(\mathcal{O}) \ge u > \varphi^{\star}(\mathcal{O})}.$$

Otherwise, we have  $(\varphi^{\star}(\mathcal{O}) - u) \left( \mathbf{1}_{\varphi^{\star}(\mathcal{O}) \geq u} - \mathbf{1}_{\varphi(\mathcal{O}) \geq u} \right) = 0$  and overall we get (applying the positivity of the measure  $\mu$ )

$$\left| \int_{z}^{\infty} \mathbb{E} \left[ \left( \varphi^{\star}(\mathcal{O}) - u \right) \left( \mathbf{1}_{\varphi^{\star}(\mathcal{O}) \geq u} - \mathbf{1}_{\varphi(\mathcal{O}) \geq u} \right) \right] \mu(\mathrm{d}u) \right|$$

$$\leq \mathbb{E}\left[|\varphi^{\star}(\mathcal{O}) - \varphi(\mathcal{O})|\mu([\varphi^{\star}(\mathcal{O}),\varphi(\mathcal{O})])\right].$$

Using analogous arguments, the second integral in (1.2.14) can be bounded by the same upper bound as above; estimate (1.2.12) follows.

Finally, assuming that g'' exists and is bounded, we can apply Taylor's theorem with Lagrange remainder and get

$$g(\mathcal{R}-\varepsilon) - g(\mathcal{R}-\varepsilon^{\star}) \leq g'(\mathcal{R}-\varepsilon^{\star})(\varepsilon^{\star}-\varepsilon) + \frac{\|g''\|_{\infty}}{2}(\varepsilon^{\star}-\varepsilon)^{2}.$$

Taking expectations and using that  $\mathbb{E}\left[\mathbb{E}\left[g'(\mathcal{R}-\varepsilon^{\star})(\varepsilon^{\star}-\varepsilon) \mid \mathcal{O}\right]\right] = 0$  since  $g'(\mathcal{R}-\varepsilon^{\star})$  is  $\mathcal{O}$ -measurable and  $\varepsilon^{\star}, \varepsilon$  are centered conditionally on  $\mathcal{O}$ , we obtain the announced improvement of estimate (1.2.13).

#### Upper and lower biased estimators

We set  $\mathcal{R} = f(X, Y)$  and  $\mathcal{O} = X$  to restore our main setting. Note that any choice of admissible  $\varphi$  and  $\varepsilon$  in (1.2.11) leads to a lower bound  $J_{\varphi}$  and an upper bound  $\mathbb{E}[g(f(X, Y) - \varepsilon)]$  for the nested expectation  $\mathbb{E}[g(\mathbb{E}[f(X, Y)|X])]$ . The optimal choices  $\varphi^*(\mathcal{O}) = \mathbb{E}[\mathcal{R}|\mathcal{O}]$  and  $\varepsilon^* = \mathcal{R} - \mathbb{E}[\mathcal{R}|\mathcal{O}]$  would require to exactly evaluate the conditional expectation itself; we can actually approach these optimal choices by approximating conditional expectations, as we do below, based on a (linear) regression algorithm.

Let  $(p_i)_{i\geq 0}$  (resp.  $(q_i)_{i\geq 0}$ ) be a basis of  $L^2(X)$  (resp.  $L^2(Y)$ ). Given  $N \in \mathbb{N}^*$  and  $k, d \in \mathbb{N}$ , we solve the following Ordinary Least Squares minimization problem

$$(l_{j}^{*})_{j} = \underset{\substack{l_{j} \in \mathbb{R} \\ 0 \le j \le k}}{\operatorname{arg\,min}} \frac{1}{N} \sum_{i=1}^{N} \left( f(\tilde{X}_{i}, \tilde{Y}_{i}) - \sum_{j=0}^{k} l_{j} p_{j}(\tilde{X}_{i}) \right)^{2},$$
(1.2.16)

$$(u_{ab}^{*})_{a,b} = \underset{\substack{u_{ab} \in \mathbb{R} \\ 0 \le a, b \le d}}{\arg\min} \frac{1}{N} \sum_{i=1}^{N} \left( f(\tilde{X}_{i}, \tilde{Y}_{i}) - \sum_{a,b=0}^{d} u_{ab} p_{a}(\tilde{X}_{i}) \left( q_{b}(\tilde{Y}_{i}) - \mathbb{E} \left[ q_{b}(\tilde{Y}_{i}) \right] \right) \right)^{2}, \quad (1.2.17)$$

where for  $1 \leq i \leq N$ , each  $(\tilde{X}_i, \tilde{Y}_i)$  is an independent copy of (X, Y). We then define:

$$\varphi_k^*(X) := \sum_{j=0}^k l_j^* p_j(X), \qquad \qquad \varepsilon_d^* := \sum_{a,b=0}^d u_{ab}^* p_a(X)(q_b(Y) - \mathbb{E}\left[q_b(Y)\right]). \tag{1.2.18}$$

Notice that the coefficients  $(l_j^*)_{0 \le j \le k}$  and  $(u_{ab}^*)_{0 \le a, b \le d}$  are random and independent of (X, Y), being functions of the sample  $(\tilde{X}_i, \tilde{Y}_i)_{1 \le i \le N}$ . This property allows us to obtain the following result.

**Proposition 1.2.11.** The following inequalities hold

$$\mathbb{E}\left[J_{\varphi_k^*}\right] \le \mathbb{E}\left[g(\mathbb{E}\left[f(X,Y)|X\right]\right)\right] \le \mathbb{E}\left[g(f(X,Y) - \varepsilon_d^*)\right].$$
(1.2.19)

*Proof.* In order to obtain the inequality on the left-hand side, it is sufficient to take conditional expectation with respect to  $(\tilde{X}_i, \tilde{Y}_i)_{i \leq N}$ , then exploit the independence with respect to (X, Y) and proceed as in the first part of the proof of Theorem 1.2.10. Similarly, since the coefficients  $l^*$  and  $u^*$  are independent of (X, Y), it is easy to check that  $\mathbb{E}[\varepsilon_d^*|X] = 0$ , so that  $\varepsilon_d^*$  is admissible for (1.2.11), and the inequality on the right-hand side follows.

When  $k, d, N \to +\infty$  (see Györfi, Kohler, Krzyżak, and Walk [96, Chapter XI] for precise conditions),  $\varphi_k^*$  and  $\varepsilon_d^*$  converge in  $L_2$  to the optimal  $\varphi^*$  and  $\varepsilon^*$ . Owing to the error estimates in Theorem 1.2.10, the lower-upper estimators in Proposition 1.2.11 converge to the true value of

the nested expectation  $\mathbb{E}\left[g(\mathbb{E}\left[f(X,Y)|X\right])\right]$ . Even if we do not derive here precise convergence rates (though this is theoretically possible, building on the reference above), the practical interest of the estimators in Proposition 1.2.11 is clear: we can replace the expectations on the left-hand and right-hand side of (1.2.19) with standard (non-nested) Monte Carlo estimates based on i.i.d. samples of (X,Y) (see Section 1.3.3 for details about the final simulation algorithm). This provides an upper and a lower bound for the nested expectation; by observing the size of the interval between the two bounds, we decide whether the precision of this estimation procedure is acceptable for our purposes.

#### 1.2.4 Proof of the bias estimate in Proposition 1.2.4

For  $x \in \mathbb{R}^d$  and  $n \ge 1$ , let us define

$$\widehat{E}_{f,n}(x) = \frac{1}{n} \sum_{j=1}^{n} f(x, Y_j)$$
 and  $\delta E_n(x) = \widehat{E}_{f,n}(x) - E_f(x)$ .

We first control the moments of  $\delta E_n(X)$ .

**Lemma 1.2.12.** Assume that there exists  $p \ge 2$  such that  $\mathbb{E}[|f(X,Y)|^p] < \infty$ . Then, there exists a positive constant  $C_p$  independent of n such that

$$\forall n \ge 1, \ \forall q \in (0, p], \qquad ||\delta E_n(X)||_q \le \frac{C_p}{\sqrt{n}}.$$

Proof. Since  $||\delta E_n(X)||_q \leq ||\delta E_n(X)||_p$  for  $q \in (0, p]$ , it is sufficient to deal with the case q = p. Let us define  $Z_j = f(X, Y_j) - E_f(X)$  and, for  $n \geq 1$ ,  $S_n = \sum_{i=1}^n Z_i$ . Conditional with respect to X, S is a martingale, since the variables  $Y_j$  are i.i.d. and independent of X. By Burkhölder's inequality (see Hall and Heyde [98, Theorem 2.10]), there exists a constant  $c_p$  only depending on p such that, almost surely,

$$\mathbb{E}\left[|S_n|^p|X\right] \le c_p \mathbb{E}\left[\left|\sum_{i=1}^n Z_i^2\right|^{\frac{p}{2}}|X\right] \le c_p n^{\frac{p}{2}} \mathbb{E}\left[|Z_1|^p|X\right],$$

where in the last inequality we have used that  $\left|\sum_{i=1}^{n} Z_{i}^{2}\right|^{\frac{p}{2}} \leq n^{\frac{p}{2}-1} \sum_{i=1}^{n} |Z_{i}|^{p}$ . Since  $\delta E_{n}(X) = \frac{S_{n}}{n}$ , we obtain  $\left|\left|\delta E_{n}(X)\right|\right|_{p} = \frac{1}{n} \mathbb{E}\left[\left|S_{n}\right|^{p}\right]^{\frac{1}{p}} \leq \frac{C_{p}}{\sqrt{n}}$ , where  $C_{p} = c_{p}^{\frac{1}{p}} \left|\left|Z_{1}\right|\right|_{p}$ .

In order to prove estimate (1.2.5), we expand g around the point  $E_f(X)$ , using a Taylor expansion with integral remainder. To cope with the non-smooth character of g, let us introduce the generalized derivative of g which is equal to 0 on the set  $\{d_1, \ldots, d_\theta\}$ , and to g' elsewhere. By a slight abuse of notation, we will also denote this function by g'. The following lemma is standard: we provide a short proof for completeness.

**Lemma 1.2.13.** Under Assumption 1.2.1, for any  $x \notin \{d_1, ..., d_\theta\}$  and any  $y \in \mathbb{R}$ , we have

$$g(y) - g(x) = g'(x)(y - x) + (y - x) \int_0^1 \left[g'(x + \lambda(y - x)) - g'(x)\right] d\lambda.$$
 (1.2.20)

Moreover, for every  $x, y \in (d_k, d_{k+1})$ ,

$$|g(y) - g(x) - g'(x)(y - x)| \le \frac{[g']_{\eta}}{1 + \eta} |y - x|^{1 + \eta}, \qquad (1.2.21)$$

where  $[g']_{\eta} = \max_{0 \le k \le \theta} \sup_{z_1, z_2 \in (d_k, d_{k+1}), z_1 \ne z_2} \frac{|g'(z_1) - g'(z_2)|}{|z_1 - z_2|^{\eta}}.$ 

Proof. Without loss of generality, we assume that x < y and consider the finite set  $(e_1, \dots, e_k) = [x, y] \cap \{d_1, \dots, d_\theta\}$ , in ascending order. Let us also denote  $e_0 = x$  and  $e_{k+1} = y$  if  $e_k < y$ . Since g is continuous on  $\mathbb{R}$  and  $C^1$  with Hölder continuous derivative on each interval  $(e_i, e_{i+1})$ , we have  $g(e_{i+1}) - g(e_i) = \int_{e_i}^{e_{i+1}} g'(s) ds$ . Summing over the index i, we obtain  $g(y) - g(x) = \int_x^y g'(s) ds$ . We then obtain (1.2.20) adding and subtracting g'(x) inside the integral and then applying the change of variable  $s = x + \lambda(y - x)$ . To prove (1.2.21), it is sufficient to use (1.2.20) and the Hölder property of g' on the interval  $(d_k, d_{k+1})$ .

We are now ready to prove Proposition 1.2.4. By Lemma 1.2.13, applying (1.2.20), we have that the identity

$$g\left(\widehat{E}_{f,n}(X)\right) - g\left(E_{f}(X)\right) = \delta E_{n}(X)g'\left(E_{f}(X)\right) + \delta E_{n}(X)\int_{0}^{1} \left(g'\left(E_{f}(X) + \lambda\delta E_{n}(X)\right) - g'\left(E_{f}(X)\right)\right) d\lambda := T_{1} + T_{2}, \quad (1.2.22)$$

holds on the set  $E_f(X) \notin \{d_1, \ldots, d_\theta\}$ . By Assumption 1.2.3, this set has probability equal to one. Using the tower property of the conditional expectation, we have

$$\mathbb{E}[T_1] = \mathbb{E}\left[\delta E_n(X)g'(E_f(X))\right] = 0,$$

since  $\mathbb{E}[\delta E_n(X)|X] = \mathbb{E}\left[\widehat{E}_{f,n}(X)|X\right] - E_f(X) = 0$  almost surely, and g' is bounded.

We now control the term  $\mathbb{E}[T_2]$ . We have to consider separately the cases where  $E_f(X)$  is close to, respectively far from, the singularities of g. To do so, let us set  $h = \frac{1}{2} \min_{1 \le i \ne j \le \theta} (|d_i - d_j|)$ and introduce a parameter  $z \in (0, h)$  to be fixed later. We consider the following partition:

$$\Omega_1 = \left\{ \min_{1 \le j \le \theta} |E_f(X) - d_j| \le z \right\},\$$
  
$$\Omega_2 = \Omega_1^c \cap \{ |\delta E_n(X)| > z \},\$$
  
$$\Omega_3 = \Omega_1^c \cap \{ |\delta E_n(X)| \le z \}.$$

We upper bound the values of the three expectations  $\mathbb{E}[T_2\mathbf{1}_{\Omega_1}]$ ,  $\mathbb{E}[T_2\mathbf{1}_{\Omega_2}]$ , and  $\mathbb{E}[T_2\mathbf{1}_{\Omega_3}]$ . For the first term, note that since g' is bounded, we have

$$\left|\mathbb{E}\left[T_{2}\mathbf{1}_{\Omega_{1}}\right]\right| \leq 2\left\|g'\right\|_{\infty} \mathbb{E}\left[\left|\delta E_{n}(X)\right|\mathbf{1}_{\Omega_{1}}\right] \leq 2\left\|g'\right\|_{\infty} \mathbb{P}\left(\Omega_{1}\right)^{\frac{1}{q}} \left\|\delta E_{n}(X)\right\|_{q^{*}}, \qquad (1.2.23)$$

where we have applied Hölder's inequality with  $q, q^* \ge 1$  such that  $\frac{1}{q} + \frac{1}{q^*} = 1$  and  $q^* \le p$ , where p is the exponent appearing in Assumption 1.2.2. Assumption 1.2.3 ensures that  $\mathbb{P}(\Omega_1) \le K_{\nu} z^{\nu}$ . Then, it follows from Lemma 1.2.12 that

$$\left|\mathbb{E}\left[T_{2}\mathbf{1}_{\Omega_{1}}\right]\right| \leq 2\left\|g'\right\|_{\infty}K_{\nu}^{\frac{1}{q}}z^{\frac{\nu}{q}}\frac{C_{p}}{\sqrt{n}}$$

For the second term, note that  $\mathbf{1}_{\Omega_2} \leq \left(\frac{|\delta E_n(X)|}{z}\right)^r$  for any r > 0. Therefore

$$\begin{aligned} |\mathbb{E}\left[T_{2}\mathbf{1}_{\Omega_{2}}\right]| &\leq 2\frac{\|g'\|_{\infty}}{z^{r}} \mathbb{E}\left[|\delta E_{n}(X)|^{r+1}\right] = 2\frac{\|g'\|_{\infty}}{z^{r}} \|\delta E_{n}(X)\|_{r+1}^{r+1} \\ &\leq 2\frac{\|g'\|_{\infty} C_{p}^{r+1}}{z^{r}n^{\frac{r+1}{2}}}, \end{aligned}$$

where we applied Lemma 1.2.12 in the last inequality, under the condition that  $r + 1 \leq p$ . For the third term, note that on the set  $\Omega_3$ , both  $E_f(X)$  and  $\widehat{E}_{f,n}(X)$  belong to the same interval  $(d_i, d_{i+1})$ . Applying estimate (1.2.21), we obtain:

$$|\mathbb{E}[T_{2}\mathbf{1}_{\Omega_{3}}]| \leq \frac{[g']_{\eta}}{1+\eta} \mathbb{E}\left[|\delta E_{f}(X)|^{1+\eta} \mathbf{1}_{\Omega_{3}}\right] \leq \frac{[g']_{\eta}}{1+\eta} \frac{C_{p}^{1+\eta}}{n^{\frac{1+\eta}{2}}},$$

where we have applied Lemma 1.2.12 in the last inequality. Putting things together, we have shown that the inequality

$$\begin{aligned} \left| \mathbb{E} \left[ g \left( \widehat{E}_{f,n}(X) \right) - g \left( E_f(X) \right) \right] \right| \\ &\leq 2 \left\| g' \right\|_{\infty} K_{\nu}^{\frac{1}{q}} z^{\frac{\nu}{q}} \frac{C_p}{\sqrt{n}} + 2 \frac{\|g'\|_{\infty} C_p^{r+1}}{z^r n^{\frac{r+1}{2}}} + \frac{[g']_{\eta}}{1+\eta} \frac{C_p^{1+\eta}}{n^{\frac{1+\eta}{2}}}, \end{aligned}$$

holds for all  $z \in (0, h)$ ,  $r \leq p - 1$  and q such that  $q^* \leq p$ .

The minimum point of the right-hand side corresponds to the minimum point of the function

$$z \in \mathbb{R} \to \Psi(z) := \Gamma_q z^{\frac{\nu}{q}} n^{-\frac{1}{2}} + \Lambda_r z^{-r} n^{-\frac{r+1}{2}},$$

where  $\Gamma_q = 2 \|g'\|_{\infty} K_{\nu}^{\frac{1}{q}} C_p$  and  $\Lambda_r = 2 \|g'\|_{\infty} C_p^{r+1}$ . The minimum of  $\Psi$  is achieved at  $z^* = \left(\frac{\Lambda_r rq}{\nu \Gamma_q}\right)^{\frac{q}{rq+\nu}} n^{-\frac{1}{2}\frac{rq}{rq+\nu}}$ , which is smaller than h for n large enough. The value  $\Psi(z^*)$  at the minimum point is proportional to  $n^{-\frac{1}{2}\left(1+\frac{r\nu}{rq+\nu}\right)}$ . In order to maximize  $\frac{r\nu}{rq+\nu}$  under the constraints  $r+1 \leq p$ ,  $\frac{1}{q} + \frac{1}{q^*} = 1$  and  $q^* \leq p$ , we set r = p-1 and  $q = \frac{p}{p-1}$ , which finally yields the estimate

$$\left|\mathbb{E}\left[g\left(\widehat{E}_{f,n}(X)\right) - g\left(E_f(X)\right)\right]\right| \leq \frac{\kappa_1}{n^{\frac{1}{2}\left(1 + \frac{(p-1)\nu}{p+\nu} \wedge \eta\right)}},$$

for all  $n \ge h^{-2\left(1+\frac{\nu}{rq}\right)} \left(\frac{\Lambda_r rq}{\nu\Gamma_q}\right)^{\frac{2}{r}} =: N$ , where  $\kappa_1 = \Gamma_q \left(\frac{\Lambda_r rq}{\nu\Gamma_q}\right)^{\frac{\nu}{rq+\nu}} + \Lambda_r \left(\frac{\Lambda_r rq}{\nu\Gamma_q}\right)^{\frac{-rq}{rq+\nu}} + \frac{[g']_{\eta}}{1+\eta} C_p^{1+\eta}$ . We conclude the proof of estimate (1.2.5) for all  $n \ge 1$  (and not only for  $n \ge N$ )

 $+ \frac{g_{1+\eta}}{1+\eta} C_p \quad \forall \text{ we conclude the proof of estimate (1.2.5) for all } n \ge 1 \text{ (and not only for } n \ge N)$ by improving the constant  $\kappa_1$  to  $\kappa = \kappa_1 + \kappa_2 N^{\frac{1}{2}\left(1 + \frac{(p-1)\nu}{p+\nu} \land \eta\right)}$ , where  $\kappa_2$  is a uniform bound on  $|\mathbb{E}\left[g(\widehat{E}_{f,n}(X)) - g\left(E_f(X)\right)\right] | \text{ for } 1 \le n \le N.$ 

#### 1.2.5 Proof of the variance estimate in Proposition 1.2.5

For simplicity, let us define

$$\widehat{Z}_{1} := \frac{1}{n_{l-1}} \sum_{j=1}^{n_{l-1}} f(X, Y_{j}), \quad \widehat{Z}_{2} := \frac{1}{n_{l-1}} \sum_{j=n_{l-1}+1}^{n_{l}} f(X, Y_{j}), \quad (1.2.24)$$

$$\widehat{Z} := \frac{\widehat{Z}_{1} + \widehat{Z}_{2}}{2} = \frac{1}{n_{l}} \sum_{j=1}^{n_{l}} f(X, Y_{j}),$$

so that  $V_l = \operatorname{Var}\left(g(\widehat{Z}) - \frac{1}{2}g(\widehat{Z}_1) - \frac{1}{2}g(\widehat{Z}_2)\right)$ . Let us also define

$$\delta \widehat{Z}_1 = \widehat{Z}_1 - E_f(X), \qquad \delta \widehat{Z}_2 = \widehat{Z}_2 - E_f(X),$$
  
$$\delta \widehat{Z} = \frac{1}{2} (\delta \widehat{Z}_1 + \delta \widehat{Z}_2) = \widehat{Z} - E_f(X).$$

Recall that  $h = \frac{1}{2} \min_{1 \le i \ne j \le \theta} (|d_i - d_j|)$ , and introduce a parameter  $z \in (0, h)$ , to be fixed later. We consider a partition of  $\Omega$  into disjoint sets, analogous to the one used in the proof of Proposition 1.2.4:

$$\tilde{\Omega}_1 = \left\{ \min_{1 \le j \le \theta} |E_f(X) - d_j| \le z \right\} = \Omega_1, \\ \tilde{\Omega}_2 = \tilde{\Omega}_1^c \cap \left\{ \max\left( |\delta \widehat{Z}_1|, |\delta \widehat{Z}_2| \right) > z \right\},$$

$$\tilde{\Omega}_3 = \tilde{\Omega}_1^c \cap \left\{ \max\left( |\delta \widehat{Z}_1|, |\delta \widehat{Z}_2| \right) \le z \right\}.$$

We bound  $V_l$  from above using the second moment  $\mathbb{E}\left[\left(g(\widehat{Z}) - \frac{1}{2}g(\widehat{Z}_1) - \frac{1}{2}g(\widehat{Z}_2)\right)^2\right]$ . For  $A \in \{\widehat{Z}, \widehat{Z}_1, \widehat{Z}_2\}$ , it follows from (1.2.20) and Assumption 1.2.3 that

$$g(A) = g(E_f(X)) + \delta A \int_0^1 g'(E_f(X) + \lambda \,\delta A) \,\mathrm{d}\lambda \qquad \text{with } \delta A = A - E_f(X),$$

and therefore, using the identity  $\delta \widehat{Z} = \frac{\delta \widehat{Z}_1 + \delta \widehat{Z}_2}{2}$ , we get:

$$\begin{split} & \left(g(\widehat{Z}) - \frac{1}{2}g(\widehat{Z}_1) - \frac{1}{2}g(\widehat{Z}_2)\right)^2 \\ & \leq 2\left(\frac{\delta\widehat{Z}_1}{2}\int_0^1 \left(g'\left(E_f(X) + \lambda\delta\widehat{Z}\right) - g'\left(E_f(X) + \lambda\delta\widehat{Z}_1\right)\right) \mathrm{d}\lambda\right)^2 \\ & \quad + 2\left(\frac{\delta\widehat{Z}_2}{2}\int_0^1 \left(g'\left(E_f(X) + \lambda\delta\widehat{Z}\right) - g'\left(E_f(X) + \lambda\delta\widehat{Z}_2\right)\right) \mathrm{d}\lambda\right)^2 \\ & \leq 2||g'||_\infty^2 \left((\delta\widehat{Z}_1)^2 + (\delta\widehat{Z}_2)^2\right). \end{split}$$

We first focus on the set  $\tilde{\Omega}_1$ . According to Lemma 1.2.12, there exists a positive constant  $C_p$  such that

$$\mathbb{E}\left[\left((\delta\widehat{Z}_{1})^{2}+(\delta\widehat{Z}_{2})^{2}\right)\mathbf{1}_{\tilde{\Omega}_{1}}\right] \leq ||\delta\widehat{Z}_{1}||_{2q^{*}}^{2}\mathbb{P}\left(\tilde{\Omega}_{1}\right)^{\frac{1}{q}}+||\delta\widehat{Z}_{2}||_{2q^{*}}^{2}\mathbb{P}\left(\tilde{\Omega}_{1}\right)^{\frac{1}{q}} \leq 2\frac{C_{p}^{2}}{n_{l-1}}K_{\nu}^{\frac{1}{q}}z^{\frac{\nu}{q}},$$

where we have applied Hölder's inequality twice with conjugate exponents  $q, q^* \ge 1$  such that  $2q^* \le p$ , and we have used  $n_l - n_{l-1} = n_{l-1}$ . On the set  $\tilde{\Omega}_2$ , since  $\mathbf{1}_{\tilde{\Omega}_2} < \frac{\max(|\delta \hat{Z}_1|, |\delta \hat{Z}_2|)^r}{z^r}$  for any r > 0, we obtain:

$$\mathbb{E}\left[\left((\delta\widehat{Z}_1)^2 + (\delta\widehat{Z}_2)^2\right)\mathbf{1}_{\tilde{\Omega}_2}\right] \le \frac{2}{z^r} \mathbb{E}\left[\max\left(|\delta\widehat{Z}_1|, |\delta\widehat{Z}_2|\right)^{r+2}\right] \le \frac{4}{z^r} \frac{C_p^{r+2}}{n_{l-1}^{\frac{r+2}{2}}},$$

for any positive r such that  $r + 2 \leq p$ , again owing to Lemma 1.2.12. Finally, in order to control the term  $\mathbb{E}\left[(g(\widehat{Z}) - \frac{1}{2}g(\widehat{Z}_1) - \frac{1}{2}g(\widehat{Z}_2))^2\mathbf{1}_{\widetilde{\Omega}_3}\right]$ , we use the fact that, on the set  $\widetilde{\Omega}_3$ , all the variables  $\widehat{Z}_1, \ \widehat{Z}_2, \ \widehat{Z}$ , and  $E_f(X)$  belong to the same interval  $(d_i, d_{i+1})$ . Using the fact that g' is Hölder continuous together with the identity  $\delta \widehat{Z} = \frac{1}{2}(\delta \widehat{Z}_1 + \delta \widehat{Z}_2)$ , on the set  $\widetilde{\Omega}_3$ , we have

$$\begin{split} &\left(g(\widehat{Z}) - \frac{1}{2}g(\widehat{Z}_1) - \frac{1}{2}g(\widehat{Z}_2)\right)^2 \\ &\leq 2\frac{(\delta\widehat{Z}_1)^2}{4} \int_0^1 \left|g'\left(E_f(X) + \lambda\delta\widehat{Z}\right) - g'\left(E_f(X) + \lambda\delta\widehat{Z}_1\right)\right|^2 \mathrm{d}\lambda \\ &\quad + 2\frac{(\delta\widehat{Z}_2)^2}{4} \int_0^1 \left|g'\left(E_f(X) + \lambda\delta\widehat{Z}\right) - g'\left(E_f(X) + \lambda\delta\widehat{Z}_2\right)\right|^2 \mathrm{d}\lambda \\ &\leq 2\frac{[g']_\eta^2}{4^{\eta+1}\left(1+2\eta\right)} \left((\delta\widehat{Z}_2)^2 + (\delta\widehat{Z}_1)^2\right) \left|\delta\widehat{Z}_2 - \delta\widehat{Z}_1\right|^{2\eta}. \end{split}$$

$$\begin{split} \text{Using } \left| \delta \widehat{Z}_2 - \delta \widehat{Z}_1 \right|^{2\eta} &\leq 2^{2\eta} \left( |\delta \widehat{Z}_2|^{2\eta} + |\delta \widehat{Z}_1|^{2\eta} \right), \ |\delta \widehat{Z}_1|^{2\eta} |\delta \widehat{Z}_2|^2 \\ &+ |\delta \widehat{Z}_1|^2 |\delta \widehat{Z}_2|^{2\eta} \leq |\delta \widehat{Z}_1|^{2\eta+2} + |\delta \widehat{Z}_2|^{2\eta+2} \text{ together with Lemma 1.2.12 one more time, we obtain:} \\ & \mathbb{E} \left[ \left( g(\widehat{Z}) - \frac{1}{2} g(\widehat{Z}_1) - \frac{1}{2} g(\widehat{Z}_2) \right)^2 \mathbf{1}_{\tilde{\Omega}_3} \right] \leq 2 \frac{[g']_{\eta}^2 C_p^{2\eta+2}}{(1+2\eta) n_{l-1}^{1+\eta}}. \end{split}$$

Gathering the estimates obtained so far, we have shown that the upper bound

$$\begin{split} V_l &\leq \mathbb{E}\left[\left(g(\widehat{Z}) - \frac{1}{2}g(\widehat{Z}_1) - \frac{1}{2}g(\widehat{Z}_2)\right)^2\right] \\ &\leq 8||g'||_{\infty}^2 K_{\nu}^{\frac{1}{q}} z^{\frac{\nu}{q}} C_p^2 \frac{1}{n_l} + \frac{8||g'||_{\infty}^2 C_p^{r+2} 2^{\frac{r+2}{2}}}{z^r} \frac{1}{n_l^{\frac{r+2}{2}}} + 2\frac{[g']_{\eta}^2 C_p^{2\eta+2} 2^{1+\eta}}{(1+2\eta)} \frac{1}{n_l^{1+\eta}} \end{split}$$

holds for every z < h,  $r \le p-2$  and q such that  $2q^* \le p$ . We conclude by minimizing the right-hand side with respect to z, and setting r = p-2 and  $q = \frac{\frac{p}{2}}{\frac{p}{2}-1}$ .

#### 1.2.6 An alternative set of hypotheses

We can formulate a version of Theorem 1.2.6 under an alternative set of hypotheses, where we relax the assumption on the regularity of g, at the price of strengthening the condition on the law of the random variable  $\mathbb{E}[f(X, Y)|X]$ . We obtain the following result, which may present interest in its own. Note that, as a difference with Assumption 1.2.1, here g' may fail to be Hölder continuous.

**Theorem 1.2.14.** Let us assume that g admits a derivative g' in the sense of distributions which has bounded variation. Let us assume that  $E_f(X)$  has a bounded density  $\chi_E$  w.r.t. the Lebesgue measure and that there exists p > 2 such that  $\mathbb{E}[|f(X,Y)|^p] < \infty$ . Then the tolerance  $\varepsilon^2$  on the MSE of the antithetic ML estimator (1.2.3) can be achieved with complexity  $\mathcal{O}(\varepsilon^{-2})$ .

The proof of Theorem 1.2.14 mimics the one of Theorem 1.2.6; once again, we need to rely on an estimate of the bias and of the variance at each level, which is the content of the two propositions below.

Under the boundedness assumption on the density of  $E_f(X)$ , we manage to relax the regularity hypothesis on the function g' by exploiting the arguments of Avikainen [13, Theorem 2.4 (i)].

**Proposition 1.2.15** (Bias estimate under bounded variation condition for g'). Under the assumptions of Theorem 1.2.14, there exists a constant  $\kappa > 0$  such that

$$\left|\mathbb{E}\left[g\left(\widehat{E}_{f,n}(X)\right)\right] - g\left(E_{f}(X)\right)\right| \leq \frac{\kappa}{n^{1 - \frac{1}{p+1}}}$$

*Proof.* Proceeding as in the beginning of the proof of Proposition 1.2.4 (see equation (1.2.22)), we have

$$\mathbb{E}\left[g\left(\widehat{E}_{f,n}(X)\right) - g\left(E_f(X)\right)\right] = \mathbb{E}\left[T_2\right],$$

where  $T_2 := \delta E_n(X) \int_0^1 (g'(E_f(X) + \lambda \delta E_n(X)) - g'(E_f(X))) d\lambda$ . Applying Hölder's inequality with  $q, q^*$  in the interval [1, p] such that  $\frac{1}{q} + \frac{1}{q^*} = 1$ , we obtain

$$\left|\mathbb{E}\left[T_{2}\right]\right| \leq \int_{0}^{1} \left\|\delta E_{n}(X)\right\|_{q^{*}} \left\|\left(g'\left(E_{f}(X)+\lambda\delta E_{n}(X)\right)-g'\left(E_{f}(X)\right)\right)\right\|_{q} \mathrm{d}\lambda\right\|_{q^{*}}$$

By Lemma 1.2.12, we have  $\|\delta E_n(X)\|_{q^*} \leq \frac{C_p}{\sqrt{n}}$ . For the second term, it follows from Avikainen [13, Thm 2.4(i)] that for every  $0 \leq \lambda \leq 1$  and  $r \leq p$ ,

$$\left\|g'\left(E_f(X) + \lambda\delta E_n(X)\right) - g'\left(E_f(X)\right)\right\|_q$$

$$\leq 3^{1+\frac{1}{q}} ||g'||_{\mathrm{TV}} \, \|\chi_E\|_{\infty}^{\frac{r}{q(r+1)}} \, \|\delta E_n(X)\|_r^{\frac{r}{q(r+1)}}.$$

Now applying again Lemma 1.2.12 to the last term on the right-hand side and maximizing the exponent  $\frac{r}{q(r+1)}$  by choosing  $q = \frac{p}{p-1}$  (corresponding to  $q^* = p$ ) and r = p, we obtain

$$\mathbb{E}\left[g\left(\widehat{E}_{f,n}(X)\right) - g\left(E_f(X)\right)\right] \le \frac{\kappa}{n^{1-\frac{1}{p+1}}}$$

where  $\kappa = 3^{1+\frac{1}{q}} ||g'||_{\text{TV}} ||\chi_E||_{\infty}^{\frac{r}{q(r+1)}} C_p$ , and this concludes the proof.

**Proposition 1.2.16** (Variance estimate under bounded variation condition for g'). Under the assumptions of Theorem 1.2.14, there exists a constant  $\tilde{\kappa}$  such that

$$V_l \le \frac{\tilde{\kappa}}{n_l^{1+\frac{p-2}{2(p+1)}}},$$

for every  $l \geq 1$ .

*Proof.* We restore the notation of Proposition 1.2.5. Applying the Taylor expansion (1.2.20) to  $x = E_f(X)$  and  $y \in \{\hat{Z}_1, \hat{Z}_2, \hat{Z}\}$  defined in (1.2.24), we have

$$\left(g(\widehat{Z}) - \frac{g(\widehat{Z}_{1}) + g(\widehat{Z}_{2})}{2}\right)^{2} \leq 3 \left(\delta\widehat{Z} \int_{0}^{1} \left(g'(E_{f}(X) + \lambda\delta\widehat{Z}) - g'(E_{f}(X))\right) d\lambda\right)^{2} + \frac{3}{4} \left(\delta\widehat{Z}_{1} \int_{0}^{1} \left(g'(E_{f}(X) + \lambda\delta\widehat{Z}_{1}) - g'(E_{f}(X))\right) d\lambda\right)^{2} + \frac{3}{4} \left(\delta\widehat{Z}_{2} \int_{0}^{1} \left(g'(E_{f}(X) + \lambda\delta\widehat{Z}_{2}) - g'(E_{f}(X))\right) d\lambda\right)^{2}.$$
(1.2.25)

The expectation of the first term on the right-hand side of (1.2.25) can be bounded by

$$\mathbb{E}\left[\left(\int_0^1 \left(g'(E_f(X) + \lambda\delta\widehat{Z}) - g'(E_f(X))\right) \mathrm{d}\lambda\right)^{2q}\right]^{\frac{1}{q}} \mathbb{E}\left[(\delta\widehat{Z})^{2q^*}\right]^{\frac{1}{q^*}}, \qquad (1.2.26)$$

where we used Hölder's inequality with q > 1 and  $q^*$  such that  $\frac{1}{q} + \frac{1}{q^*} = 1$  and  $2q^* \le p$ . By Lemma 1.2.12, the second factor in (1.2.26) is bounded by  $\frac{C_p}{n_l}$ . Moreover, by Jensen's inequality and Avikainen [13, Theorem 2.4(i)],

$$\mathbb{E}\left[\left(\int_{0}^{1} \left(g'(E_{f}(X) + \lambda\delta\widehat{Z}) - g'(E_{f}(X))\right) d\lambda\right)^{2q}\right]$$
  
$$\leq \int_{0}^{1} \mathbb{E}\left[\left(g'(E_{f}(X) + \lambda\delta\widehat{Z}) - g'(E_{f}(X))\right)^{2q}\right] d\lambda$$
  
$$\leq 3^{2q+1}||g'||_{\mathrm{TV}}^{2q}||\chi_{E}||_{\infty}^{\frac{p}{p+1}}||\delta\widehat{Z}||_{p}^{\frac{p}{p+1}}.$$

We proceed as in the proof of Proposition 1.2.15: we apply again Lemma 1.2.12 to  $||\delta \widehat{Z}||_{p}^{\frac{p}{p+1}}$  and then optimize the resulting  $n_l^{-\frac{p}{2q(p+1)}}$  over q under the constraint  $q^* \leq \frac{p}{2}$ , which leads to the choice  $q = \frac{p}{p-2}$ . Overall, we have just shown that the expectation of the first term on the right-hand side of (1.2.25) is bounded by a constant times  $n_l^{-1-\frac{p-2}{2(p+1)}}$ . Similar computations for the two other terms in (1.2.25) lead to the same upper bound, which concludes the proof.

The proof of Theorem 1.2.14 now boils down to the application of Giles [75, Theorem 1] with coefficients  $\alpha = 1 - \frac{1}{p+1}$ ,  $\beta = 1 + \frac{p-2}{2(p+1)}$ , and  $\gamma = 1$ , which satisfy  $\alpha > \frac{1}{2} \max(\beta, \gamma)$  and  $\beta > \gamma$ .

#### **1.3** Application to initial margin computations

In the following, we work on a probability space  $(\Omega, \mathcal{A}, \mathbb{P})$  and consider the augmented filtration  $\mathcal{F}$  of a Brownian motion W, that is  $\mathcal{F}_t := \sigma(W_s, 0 \le s \le t, \mathcal{N}_{\mathbb{P}})$  where  $\mathcal{N}_{\mathbb{P}}$  denotes the family of  $\mathbb{P}$ -negligible sets of  $\mathcal{A}$ . In this section, we consider examples of IM computation where Theorem 1.2.6 applies. More precisely, we generate expectations by means of a Black–Scholes (BS) model

$$S_t = S_0 e^{\left(r - \frac{\sigma^2}{2}\right)t + \sigma W_t}, \quad S_0 > 0,$$
 (1.3.1)

where the interest rate r > 0 and the volatility  $\sigma > 0$  are constant. Model (1.3.1) provides a simple (yet meaningful) setting where we can evaluate explicit reference values (or unbiased estimates) for some of the involved nested expectations (see Proposition 1.3.2 and Section 1.3.3 for a detailed discussion of several financial examples), which we can use to test the multi-level estimators.

In [3], the IM correction for an option with payoff  $\varphi(S_T)$  is computed according to the CVaR of the future evolution of the replicating portfolio over a small time interval  $\Delta > 0$ . When  $\Delta = 0$  (that is: no IM correction), the price at time t is given by the classical BS price,  $\mathbb{E}\left[e^{-r(T-t)}\varphi(S_T) | S_t\right]$ , with first derivative  $\delta(t, S) = \partial_s \mathbb{E}\left[e^{-r(T-t)}\varphi(S_T) | S_t = s\right]$ . As shown in [3], for small values of  $\Delta$ , a first-order correction to this BS price is given precisely by the integral term in (1.1.1), Z<sup>ref</sup> being computed according to the same BS model:

$$R C_{\alpha} \mathbb{E}\left[\int_{0}^{T} e^{-rt} \sqrt{(t+\Delta) \wedge T - t} |Z_{t}| \,\mathrm{d}t\right], \qquad (1.3.2)$$

where: R is the funding cost net interest rate,  $C_{\alpha} := \text{CVaR}^{\alpha} \left( \mathcal{N}(0,1) \right) = \left. \frac{e^{-\frac{x^2}{2}}}{(1-\alpha)\sqrt{2\pi}} \right|_{x=\Phi^{-1}(\alpha)}$  is the CVaR of a standard Gaussian random variable, and

$$Z_t = z(t, S_t) := \sigma S_t \,\delta(t, S_t). \tag{1.3.3}$$

Using the likelihood ratio method of Broadie and Glasserman [38], we can restore an expression of Z in terms of an expectation:

$$z^{BS}(t,s) = \sigma s \partial_s \mathbb{E} \left[ e^{-r(T-t)} \varphi(S_T) \middle| S_t = s \right]$$
  
=  $\mathbb{E} \left[ e^{-r(T-t)} \varphi(S_T) \frac{W_T - W_t}{T-t} \middle| S_t = s \right]$   
=  $\mathbb{E} \left[ e^{-r(T-t)} \left( \varphi(S_T) - \varphi(S_t) \right) \frac{W_T - W_t}{T-t} \middle| S_t = s \right].$  (1.3.4)

In the last expression, the conditionally centered term  $-\varphi(S_t)\frac{W_T-W_t}{T-t}$  that we have artificially introduced allows us to reduce variance in the simulation, by playing the role of a control variate.

Assuming that every hedging operation is performed before  $\tilde{T} := T - \Delta$ , we have

$$\sqrt{(t+\Delta)\wedge T-t} = \sqrt{\Delta}$$

inside (1.3.2), which allows us to consider the slightly modified quantity:

$$R C_{\alpha} \sqrt{\Delta} \tilde{T} \mathbb{E} \left[ \frac{1}{\tilde{T}} \int_{0}^{\tilde{T}} e^{-rt} |z(t, S_{t})| dt \right] =: R C_{\alpha} \sqrt{\Delta} \tilde{T} \times I.$$
(1.3.5)

The proposition below, whose proof is elementary, shows that (1.3.5) can be cast under the form of a nested expectation as (1.1.2). In particular, instead of discretizing the time integral over  $[0, \tilde{T}]$  – which would produce a bias – we introduce an independent random variable with uniform distribution over  $[0, \tilde{T}]$ . Note that the product of constants  $R C_{\alpha} \sqrt{\Delta} \tilde{T}$  is fixed once and for all; in the following, we therefore focus on the evaluation of the expectation  $I = \mathbb{E} \left[ \frac{1}{\tilde{T}} \int_{0}^{\tilde{T}} e^{-rt} |z(t, S_t)| dt \right]$ .

**Proposition 1.3.1.** Let Y,  $\tilde{Z}$  and U be three independent random variables such that  $Y, \tilde{Z} \stackrel{d}{=} \mathcal{N}(0,1)$  and  $U \stackrel{d}{=} \mathcal{U}([0,\tilde{T}])$ , and consider the function  $g : x \in \mathbb{R} \to |x|$ . Then the vector  $X = (U, S_0 e^{(r - \frac{\sigma^2}{2})U + \sigma\sqrt{U}\tilde{Z}})$  is independent of Y, and the expectation I in (1.3.5) satisfies

$$I = \mathbb{E}\left[g\left(E_f(X)\right)\right] = \mathbb{E}\left[\left|\mathbb{E}\left[f\left(X,Y\right)|X\right]\right|\right],$$

where f is defined by

$$f:((t,s),y) \in ([0,\tilde{T}] \times (0,\infty)) \times \mathbb{R}$$

$$\to e^{-rT} \frac{\left(\varphi\left(s e^{(r-\frac{\sigma^2}{2})(T-t)+\sigma\sqrt{T-t}y}\right) - \varphi\left(s\right)\right)y}{\sqrt{T-t}}. \quad (1.3.6)$$

*Proof.* Using the fact that  $S_t$  and  $W_T - W_t$  are independent, we have:

$$I = \frac{1}{\tilde{T}} \int_0^{\tilde{T}} \mathbb{E} \left[ e^{-rt} \left| z(t, S_t) \right| \right] dt$$
  
=  $\frac{1}{\tilde{T}} \int_0^{\tilde{T}} \mathbb{E} \left[ \left| \mathbb{E} \left[ e^{-rT} \left( \varphi \left( s e^{(r - \frac{\sigma^2}{2})(T - t) + \sigma(W_T - W_t)} \right) - \varphi \left( s \right) \right) \right. \right. \\ \left. \left. \left. \left. \left. \frac{W_T - W_t}{T - t} \right]_{s = S_t} \right| \right] dt.$ 

Since  $W_T - W_t \stackrel{d}{=} \sqrt{T - t} Y$  and  $U \stackrel{d}{=} \mathcal{U}([0, \tilde{T}])$  is independent of Z, we can write

$$\begin{split} I &= \mathbb{E}\bigg[\bigg|\mathbb{E}\bigg[e^{-rT}\frac{\left(\varphi\left(se^{(r-\frac{\sigma^{2}}{2})(T-t)+\sigma\sqrt{T-t}Y}\right)-\varphi\left(s\right)\right)Y}{\sqrt{T-t}}\bigg]_{(t,s)}\bigg|\bigg] \\ &= \mathbb{E}\bigg[g\left(\mathbb{E}\left[f\left((t,s),Y\right)\right]_{(t,s)}\right)\bigg], \end{split}$$

where all the expressions are computed over  $t = U, s = S_0 e^{\left(r - \frac{\sigma^2}{2}\right)U + \sigma\sqrt{U}\tilde{Z}}$ . Now, using the independence of  $X = (U, S_0 e^{\left(r - \frac{\sigma^2}{2}\right)U + \sigma\sqrt{U}\tilde{Z}})$  and Y, the argument of g in the last expression is precisely  $\mathbb{E}\left[f\left(X,Y\right)|X\right]$ .

From now on, the function g will correspond to the absolute value, g(x) = |x|.

Additional notation. In the rest of this section we will make use of the following notation, specific to the BS framework: for every T > 0, K > 0, r > 0, s > 0, every  $t \in [0,T)$  and  $a \in [0, K)$ , we define:

$$\Phi: x \in \mathbb{R} \to \int_{-\infty}^{x} \frac{e^{-\frac{z^2}{2}}}{\sqrt{2\pi}} \mathrm{d}z, \qquad \text{(the c.d.f. of the standard normal distribution)}, \qquad (1.3.7)$$

$$d_1(t,T,s,K) := \frac{\log\left(\frac{s}{K}\right) + \left(r + \frac{\sigma^2}{2}\right)(T-t)}{\sigma\sqrt{T-t}},\tag{1.3.8}$$

$$A(t) := \frac{\log\left(\frac{K}{K-a}\right)}{\sigma\sqrt{T-t}}, \quad B(t) := \frac{\log\left(\frac{K+a}{K}\right)}{\sigma\sqrt{T-t}}, \tag{1.3.9}$$

$$\delta_t : x \in \mathbb{R} \to \Phi\left(x - B(t)\right) + \Phi\left(x + A(t)\right) - 2\Phi(x), \tag{1.3.10}$$

$$H_t: x \in \mathbb{R} \to e^{-\frac{A(t)^2}{2}} e^{-A(t)x} + e^{-\frac{B(t)^2}{2}} e^{B(t)x} - 2.$$
(1.3.11)

For future purposes, it is important to observe the identity

$$\sqrt{2\pi}\,\delta_t'(x)\,e^{\frac{x^2}{2}} = H_t(x). \tag{1.3.12}$$

Remark 4. Notice that A(t) > B(t) > 0, since  $\frac{K^2}{K^2 - a^2} > 1$ . We will also make use of the following well-known asymptotic expansion for the c.d.f. of the

standard normal distribution (see e.g. Gordon [86]):  

$$\exp\left(-\frac{z^2}{2}\right)$$

$$\Phi(z) \underset{z \to -\infty}{\sim} -\frac{\exp\left(-\frac{z^{-}}{2}\right)}{z\sqrt{2\pi}}.$$
(1.3.13)

#### **1.3.1** Call and put options

The usual price at time  $0 \le t \le T$  of a call option of maturity T > 0 and strike K > 0 is defined by:

$$v^{call}(t, S_t) = \mathbb{E}\left[ \left. e^{-r(T-t)} \varphi^{call}(S_t) \right| S_t \right], \qquad (1.3.14)$$

where  $\varphi^{call}(s) = (s - K)_+$ . Similarly, we define  $v^{put}$  from  $\varphi^{put}(s) = (K - s)_+$  for a put option. Recall that the delta of a call option is positive: in the BS case (1.3.1),

$$\delta^{call}(t, S_t) = \Phi\left(d_1\left(t, T, S_t, K\right)\right) > 0, \tag{1.3.15}$$

while for a put option, the delta is negative:

$$\delta^{put}(t, S_t) = -\Phi\left(-d_1\left(t, T, S_t, K\right)\right) < 0.$$
(1.3.16)

Hence, we are in a situation where the conditional expectation  $\mathbb{E}[f(X,Y)|X]$  has constant sign and the function g, here the absolute value function, does not induce any nonlinearity. It is also possible to derive closed formulas for the expectation I.

**Proposition 1.3.2.** Denote  $I^{call} = \mathbb{E}\left[\left|E_f^{call}(X)\right|\right]$  resp.  $I^{put} = \mathbb{E}\left[\left|E_f^{put}(X)\right|\right]$  the expectation I in (1.3.5) associated to a call resp. put option, where X and  $E_f^{call}(X)$  are given in Proposition 1.3.1. Then,

$$I^{call} = S_0 \sigma \Phi \left( d_1 \left( 0, T, S_0, K \right) \right), \qquad I^{put} = S_0 \sigma \Phi \left( -d_1 \left( 0, T, S_0, K \right) \right). \tag{1.3.17}$$

As a comment, note that  $I^{call}$  and  $I^{put}$  do not depend on  $\tilde{T}$ .

*Proof.* We justify the first expression in (1.3.17). We follow the arguments of Gobet and Makhlouf [84, Lemma 2.2]: using the martingale property of  $(e^{-rt}v^{call}(t,S_t))_{t\leq \tilde{T}}$ , it is possible to show (by differentiating w.r.t.  $S_0$ ) that the process  $e^{-rt}\delta^{call}(t,S_t)\sigma S_t = e^{-rt}Z_t^{call}$  is also a martingale. Since the sign of  $Z_t^{call}$  is positive (see (1.3.15)), we obtain:

$$I^{call} = \frac{1}{\tilde{T}} \int_0^{\tilde{T}} e^{-rt} \mathbb{E}\left[ \left| Z_t^{call} \right| \right] \mathrm{d}t = \frac{1}{\tilde{T}} \int_0^{\tilde{T}} \mathbb{E}\left[ e^{-rt} Z_t^{call} \right] \mathrm{d}t = \frac{1}{\tilde{T}} \int_0^{\tilde{T}} \mathbb{E}\left[ Z_0^{call} \right] \mathrm{d}t = \sigma S_0 \Phi\left( d_1\left(0, T, S_0, K\right) \right).$$

The proof for the second expression in (1.3.17) is analogous.

#### 1.3.2 The butterfly option

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In this section, we focus on a butterfly option -a non-trivial case for which we will show that Theorem 1.2.6 applies. Note that the delta of such an option does change sign (see Figure 1.1) and thus, the simple arguments of Proposition 1.3.2 do not hold. The butterfly option payoff, price and delta are respectively defined by:

$$\varphi^{butterfly}(s) = (s - (K + a))_{+} + (s - (K - a))_{+} - 2(s - K)_{+}, \qquad (1.3.18)$$

$$v_{T,K,a}^{butterfly}(t,S_t) = v_{T,K+a}^{call}(t,S_t) + v_{T,K-a}^{call}(t,S_t) - 2v_{T,K}^{call}(t,S_t),$$
(1.3.19)

$$\delta^{butterfly}(t, S_t) := \Delta_t(S_t) = \left. \frac{\partial v_{T,K,a}^{butterfly}(t,s)}{\partial s} \right|_{s=S_t}$$

$$= \Phi\left( d_1\left(t, T, S_t, K+a\right) \right) + \Phi\left( d_1\left(t, T, S_t, K-a\right) \right)$$
(1.3.20)

$$-2\Phi(d_1(t,T,S_t,K)),$$

for a given strike K > 0 and parameter a > 0. Note that we now make the maturity and strike parameters appear explicitly in the notation for the call option price  $v_{T,K}^{call}$ .

To fix ideas, we plot in Figure 1.1 the delta of a call, put and butterfly option where  $S_0 = K = 100, a = \frac{K}{2}, T = 1, t = \frac{T}{5}, r = 0.1, \sigma = 0.3$ . Observe that (as expected) while the call and put deltas have a constant sign, the delta of the butterfly takes values of both signs.



Figure 1.1 – Delta  $S \to \Delta_t(S)$  of call (red), put (orange) and butterfly (blue) option prices with respect to the variable price S.

The aim of this section will be to show that Assumptions 1.2.1, 1.2.2, and 1.2.3 are satisfied for such a butterfly option. Since  $\delta^{butterfly}$  changes its sign and the absolute value function ghas a singular point at zero, we will need to study the behavior of  $\delta^{butterfly}$  around zero in order to check that Assumption 1.2.3 is verified. Although the computations we are going to perform are specific to the butterfly payoff, we believe that the same arguments can be used to check Assumptions 1.2.1, 1.2.2 and 1.2.3 for more general payoffs, such as the ones we are going to consider in our numerical experiments in Section 1.3.3.

**Theorem 1.3.3.** Assumptions 1.2.1, 1.2.2, 1.2.3 hold true in the butterfly case for  $\eta = 1$ , any p > 2 and  $\nu = \frac{1}{2} \left( 1 \wedge \frac{T - \tilde{T}}{\tilde{T}(1+A)} \right)$  for any A > 0. Therefore, Theorem 1.2.6 applies.

The proof of Theorem 1.3.3 relies on a set of technical results, that we collect in the following section.

#### Technical results required in the proof of Theorem 1.3.3

Notice that we can rewrite the butterfly delta as (see (1.3.10))

$$\Delta_t(S_t) = \delta_t \left( d_1(t, T, S_t, K) \right).$$
(1.3.21)

**Lemma 1.3.4.** Let  $\mu \in \mathbb{R}$ ,  $\sigma \in \mathbb{R}^*$ , and let  $Z \stackrel{d}{=} \mathcal{N}(0,1)$ . Then for every A > 0, there exists  $z_0(A) > 0$  such that,

$$\forall 0 < z < z_0(A), \qquad \mathbb{P}\left(\Phi\left(\mu + \sigma Z\right) < z\right) \le z^{\frac{1}{(1+A)\sigma^2}}.$$

The proof of Lemma 1.3.4 is postponed to Section 1.5.3.

**Lemma 1.3.5.** Denote  $s \in (0, \infty) \rightarrow p_t(s)$  the density function of  $S_t$  defined in (1.3.1). Then

$$\forall s \in (0, \infty), \quad p_t(s) := \frac{e^{-\frac{\left(\log(s) - \left(\log(S_0) + (r - \frac{\sigma^2}{2})t\right)\right)^2}{2\sigma^2 t}}}{s\sigma\sqrt{t}\sqrt{2\pi}} \\ \leq \overline{p}_t := \frac{e^{\left(\sigma^2 - r\right)t}}{S_0\sigma\sqrt{t}\sqrt{2\pi}} \in L^1([0, \tilde{T}]). \quad (1.3.22)$$

*Proof.* For  $t \in (0, \tilde{T}]$ , the derivative of  $p_t$  is

$$p_t'(s) = \frac{1}{\sigma\sqrt{t}\sqrt{2\pi}s^2} e^{-\frac{\left(\log\left(\frac{s}{S_0}\right) - (r - \frac{\sigma^2}{2})t\right)^2}{2\sigma^2 t}} \left[-\frac{\log\left(\frac{s}{S_0}\right) - (r - \frac{\sigma^2}{2})t}{\sigma^2 t} - 1\right].$$

It is easy to check that the density has a single maximum, located at  $s_0(t) := S_0 e^{\left(r - 3\frac{\sigma^2}{2}\right)t}$  where  $p'_t(s_0(t)) = 0$ . Therefore,

$$\overline{p}_t := p_t\left(s_0(t)\right) = \frac{e^{-\frac{\left(-\sigma^2 t\right)^2}{2\sigma^2 t}}}{S_0 e^{\left(r-3\frac{\sigma^2}{2}\right)t} \sigma \sqrt{t}\sqrt{2\pi}} = \frac{e^{\left(\sigma^2 - r\right)t}}{S_0 \sigma \sqrt{t}\sqrt{2\pi}} \in L^1([0,\tilde{T}]).$$

The rather lengthy proofs of the following two Propositions are postponed to Section 1.5.4 and 1.5.5.

**Proposition 1.3.6.** For every  $t \in [0, \tilde{T}]$ , the following statements hold.

- 1. The function  $H_t$  defined in (1.3.11) has exactly two zeros denoted  $\alpha(t), \beta(t)$  such that  $t \to \alpha(t)$  and  $t \to \beta(t)$  are  $\mathcal{C}^{\infty}([0,T))$  and  $\alpha(t) < 0 < \beta(t)$ .
- 2. The function  $\Gamma_t : s \in (0,\infty) \to \Delta'_t(s)$  has two zeros denoted  $\tilde{\alpha}(t), \tilde{\beta}(t)$  given by

$$\tilde{\alpha}(t) = K e^{\sigma\alpha(t)\sqrt{T-t} - \left(r + \frac{\sigma^2}{2}\right)(T-t)}, \quad \tilde{\beta}(t) = K e^{\sigma\beta(t)\sqrt{T-t} - \left(r + \frac{\sigma^2}{2}\right)(T-t)}.$$
(1.3.23)

In particular,  $t \to \tilde{\alpha}(t)$  and  $t \to \tilde{\beta}(t) \in \mathcal{C}^{\infty}([0,T))$ .

3. The delta of the butterfly option  $s \in (0,\infty) \to \Delta_t(s)$  is increasing for  $s \in (0,\tilde{\alpha}(t)) \cup (\tilde{\beta}(t),\infty)$ , decreasing for  $s \in (\tilde{\alpha}(t),\tilde{\beta}(t))$  and has a unique zero denoted  $\gamma(t)$ . Furthermore,  $t \to \gamma(t) \in \mathcal{C}^{\infty}([0,T))$  is bounded by

$$\forall t \in [0,T), \quad \tilde{\alpha}(t) < Ke^{-\left(r + \frac{\sigma^2}{2}\right)(T-t)} < \gamma(t) < \tilde{\beta}(t).$$
(1.3.24)

Remark 5 (Geometric butterfly option). The geometric butterfly option corresponds to the purchase of two calls with strike  $Ke^{-a}$  and  $Ke^{a}$  (a > 0) and the sale of two puts with strike K. In other words, K is the geometric mean of  $Ke^{-a}$  and  $Ke^{a}$  while for a plain butterfly option, it is the arithmetic mean. For the geometric butterfly option, we can obtain an explicit formula for the unique zero of the delta

$$\Delta_t^{\text{geom}}(T, K, a) = \Phi\left(d_1(t, T, S_t, K) + \tilde{A}(t)\right) + \Phi\left(d_1(t, T, S_t, K) - \tilde{B}(t)\right) - 2\Phi\left(d_1(t, T, S_t, K)\right),$$

 $\tilde{A}(t) = \tilde{B}(t) = \frac{a}{\sigma\sqrt{T-t}}$ , which is now given by  $\gamma(t) = Ke^{-\left(r + \frac{\sigma^2}{2}\right)(T-t)}$ . Unfortunately, for the more realistic case of the arithmetic butterfly option (1.3.18), we do not have such an explicit expression for the zero of the delta function; but the estimates provided in Proposition 1.3.6 will be sufficient for the remaining part of our analysis.

**Proposition 1.3.7.** For every  $t \in [0, \tilde{T}]$ , denote  $\mathcal{V}(t)$  the neighborhood of  $\gamma(t)$  defined by  $\mathcal{V}(t) = (\gamma(t) - \varepsilon(t), \gamma(t) + \varepsilon(t))$  where  $\varepsilon(t) := \left(\frac{\gamma(t) - \tilde{\alpha}(t)}{2}\right) \wedge \left(\frac{\tilde{\beta}(t) - \gamma(t)}{2}\right)$ , and denote  $\chi_t$  the density function of the random variable  $\Delta_t(S_t)$ . Then,  $\chi_t$  is bounded on  $\mathcal{W}(t) := \Delta_t(\mathcal{V}(t))$ , more precisely for all  $y \in \mathcal{W}(t)$ ,  $\chi_t(y) \leq C(t) < \infty$  where  $C \in L^1([0, \tilde{T}])$ .

Note that Proposition 1.3.7 provides an upper bound for the density of the random variable  $\Delta_t(S_t)$  (related to the nested expectation problem via  $\mathbb{E}[f(X,Y)|X] = e^{-rU}\sigma S_U\Delta_U(S_U)$ , see Proposition 1.3.1 for notations) only on the bounded interval  $\Delta_t(\mathcal{V}(t))$ . Unfortunately, this will not be enough to justify Assumption 1.2.3: in the butterfly option case, additional contributions to the "small" probability  $\mathbb{P}(\operatorname{dist}(E_f(X), D) \leq z)$  will also come from the left and right tails of the function  $s \mapsto \Delta_t(s)$ , which tend to zero exponentially fast as  $s \to 0$  and  $s \to \infty$ , see Figure 1.1. In the proof of Theorem 1.3.3, we precisely have to take care of this fact. As a result, the estimate we obtain on the probability  $\mathbb{P}(\operatorname{dist}(E_f(X), D) \leq z)$  is of order  $z^{\nu}$  with  $\nu < 1$ , which is *worse* than what we would obtain if we knew that the random variable  $\operatorname{dist}(E_f(X), D)$  had a bounded density around zero.

#### Proof of Theorem 1.3.3

 $\triangleright$  Since g(x) = |x| and  $g'(x) = \operatorname{sgn}(x)$ , g has only one singular point  $d_1 = 0$  and Assumption 1.2.1 holds true with  $\eta = 1$ .

 $\triangleright \text{ We now check Assumption 1.2.2. Recall that } f \text{ is defined in (1.3.6), that } S_t = S_0 e^{\left(r - \frac{\sigma^2}{2}\right)t + \sigma\sqrt{t}\tilde{Z}}$ and  $\tilde{S}_t = S_t e^{\left(r - \frac{\sigma^2}{2}\right)(T-t) + \sigma\sqrt{T-t}Y}$ , where  $\tilde{Z} \stackrel{d}{=} \mathcal{N}(0,1), Y \stackrel{d}{=} \mathcal{N}(0,1), U \stackrel{d}{=} \mathcal{U}([0,\tilde{T}])$  are independent. First, notice that  $\frac{e^{-rT}}{\sqrt{T-U}} \leq \frac{e^{-rT}}{\sqrt{T-\tilde{T}}}$  and  $\varphi(s) = (s - (K+a))_+ + (s - (K-a))_+ - 2(s - K)_+ \in [0, a]$ . Therefore, we get

$$|f(X,Y)| \le 2\frac{e^{-rT}}{\sqrt{T-\tilde{T}}}a|Y|,$$

and Assumption 1.2.2 is obviously fulfilled for any positive p.

 $\triangleright$  Let us now deal with Assumption 1.2.3. From (1.3.3), (1.3.5), and (1.3.20), we have  $E_f(X) =$  $e^{-rU}S_U\sigma\Delta_U(S_U)$ . Therefore, dist $(E_f(X), D) = |E_f(X)| = e^{-rU}S_U\sigma|\Delta_U(S_U)|$ . Since

$$\mathbb{P}\left(e^{-rU}\sigma S_U \left|\Delta_U(S_U)\right| < z\right) \le \mathbb{P}\left(\sigma S_U \left|\Delta_U(S_U)\right| < \frac{ze^{r\bar{T}}}{\sigma}\right),\tag{1.3.25}$$

it is sufficient to study (writing z instead of  $\frac{ze^{r\tilde{T}}}{\sigma}$ )  $\mathbb{P}(S_U |\Delta_U(S_U)| < z)$ . We have

$$\mathbb{P}\left(S_U \left| \Delta_U(S_U) \right| < z\right) \le \mathbb{P}\left(S_U < \sqrt{z}\right) + \mathbb{P}\left(\left| \Delta_U(S_U) \right| < \sqrt{z}\right)$$
$$\le \frac{1}{\tilde{T}} \int_0^{\tilde{T}} \int_0^{\sqrt{z}} p_t\left(s\right) \mathrm{d}s \mathrm{d}t + \mathbb{P}\left(\left| \Delta_U(S_U) \right| < \sqrt{z}\right),$$

and by Lemma 1.3.5

$$\frac{1}{\tilde{T}} \int_0^{\tilde{T}} \int_0^{\sqrt{z}} p_t(s) \,\mathrm{d}s \,\mathrm{d}t \le \frac{\sqrt{z}}{\tilde{T}} \int_0^{\tilde{T}} \frac{e^{(\sigma^2 - r)t}}{S_0 \sigma \sqrt{t} \sqrt{2\pi}} \mathrm{d}t \le \frac{2e^{|\sigma^2 - r|\tilde{T}}}{\sqrt{\tilde{T}} S_0 \sigma \sqrt{2\pi}} \sqrt{z}. \tag{1.3.26}$$

Furthermore, defining the sets

$$\mathcal{S}_1(t) := (0, \tilde{\alpha}(t)), \quad \mathcal{S}_2(t) := \left(\tilde{\alpha}(t), \tilde{\beta}(t)\right), \quad \mathcal{S}_3(t) := \left(\tilde{\beta}(t), \infty\right)$$

one has

$$\mathbb{P}\left(|\Delta_U(S_U)| < \sqrt{z}\right) = \mathbb{P}\left(\Delta_U(S_U) < \sqrt{z}, S_U \in \mathcal{S}_1(U)\right) \\ + \mathbb{P}\left(|\Delta_U(S_U)| < \sqrt{z}, S_U \in \mathcal{S}_2(U)\right) \\ + \mathbb{P}\left(-\Delta_U(S_U) < \sqrt{z}, S_U \in \mathcal{S}_3(U)\right) \\ =: p_1 + p_2 + p_3.$$

Estimate of the second term  $p_2$ . Taking  $\sqrt{z} < \min_{t \in [0,\tilde{T}]} \left\{ \left| \Delta_t \left( \gamma(t) + \frac{\tilde{\beta}(t) - \gamma(t)}{2} \right) \right| \land \left| \Delta_t \left( \gamma(t) - \frac{\gamma(t) - \tilde{\alpha}(t)}{2} \right) \right| \right\} := \sqrt{z_2}, \text{ using } \left\{ \left| \Delta_t(S_t) \right| < 1 \right\}$  $\sqrt{z}, S_t \in \mathcal{S}_2(t) \} \subset \{S_t \in \mathcal{V}(t)\}$  and Proposition 1.3.7, we get

$$p_{2} = \frac{1}{\tilde{T}} \int_{0}^{T} \mathbb{P}\left( |\Delta_{t}(S_{t})| < \sqrt{z}, S_{t} \in \mathcal{S}_{2}(t) \right) dt$$
$$\leq \frac{1}{\tilde{T}} \int_{0}^{\tilde{T}} \int_{-\sqrt{z}}^{\sqrt{z}} \chi_{t}(y) dy dt \leq \left( \frac{2}{\tilde{T}} \int_{0}^{\tilde{T}} C(t) dt \right) \sqrt{z}.$$
(1.3.27)

Estimate of the first term  $p_1$ .

Recall (1.3.10) and (1.3.21), so that  $\Delta_t(S_t) = \delta_t (d_1(t, T, S_t, K))$ . Using (1.3.13), we have:

$$\frac{\Phi\left(y-B(t)\right)}{\Phi\left(y+A(t)\right)} \approx \frac{\exp\left(-\frac{\left(y-B(t)\right)^2}{2}\right)}{\exp\left(-\frac{\left(y+A(t)\right)^2}{2}\right)} \frac{y+A(t)}{y-B(t)}$$
$$\approx \exp\left(\frac{1}{2}\left(A(t)+B(t)\right)\left(2y-B(t)+A(t)\right)\right) \xrightarrow[y\to-\infty]{} 0,$$
$$\frac{\Phi(y)}{\Phi\left(y+A(t)\right)} \approx \exp\left(\frac{A(t)}{2}\left(2y+A(t)\right)\right) \xrightarrow[y\to-\infty]{} 0.$$

Consequently,  $\delta_t(y) \underset{y \to -\infty}{\sim} \Phi(y + A(t))$  and using that  $\forall t \in [0, \tilde{T}]$ ,

 $\Phi(y + A(t)) > \Phi(y)$ , we deduce the existence of  $\theta_1 < 0$  such that

$$t \in [0, \tilde{T}], \quad y < \theta_1 \implies \delta_t(y) > \frac{1}{2}\Phi(y).$$

Without loss of generality, we can assume that  $\theta_1 < \inf_{t \in [0,\tilde{T}]} \tilde{\alpha}(t)$ , possibly taking a smaller  $\theta_1$ . Set  $\sqrt{z_1} := \min_{t \in [0,\tilde{T}]} \delta_t(\theta_1)$ . Combining the estimate above yields (for  $\sqrt{z} \leq \sqrt{z_1}$ ),

$$\begin{aligned} \{\Delta_U(S_U) &= \delta_U(d_1(U, T, S_U, K)) < \sqrt{z}, S_U \in \mathcal{S}_1(U)\} \\ &\subset \left\{ \frac{1}{2} \Phi(d_1(U, T, S_U, K)) < \sqrt{z} \right\}, \end{aligned}$$

i.e.  $p_1 \leq \mathbb{P}\left(\Phi\left(d_1(U, T, S_U, K)\right) < 2\sqrt{z}\right)$ . Furthermore, noticing that  $d_1(U, T, S_U, K) | U \stackrel{d}{=} \Phi\left(\mu_U, \sigma_U^2\right)$  where:

$$\mu := \frac{\log\left(\frac{S_0}{K}\right) + rT + \sigma^2\left(\frac{T}{2} - \tilde{T}\right)}{\sigma\sqrt{T}} < \mu_U := \frac{\log\left(\frac{S_0}{K}\right) + \left(r + \frac{\sigma^2}{2}\right)T - \sigma^2U}{\sigma\sqrt{T - U}}$$
$$< \bar{\mu} := \frac{\log\left(\frac{S_0}{K}\right) + \left(r + \frac{\sigma^2}{2}\right)T}{\sigma\sqrt{T - \tilde{T}}},$$
$$0 < \sigma_U := \sqrt{\frac{U}{T - U}} < \sigma_{\tilde{T}} := \sqrt{\frac{\tilde{T}}{T - \tilde{T}}} < \infty,$$

we obtain:

$$\mathbb{P}\left(\Phi\left(d_{1}(U,T,S_{U},K)\right)<2\sqrt{z}\right)=\mathbb{P}\left(\Phi\left(\mu_{U}+\sigma_{U}N\right)<2\sqrt{z},N>0\right)$$
$$+\mathbb{P}\left(\Phi\left(\mu_{U}+\sigma_{U}N\right)<2\sqrt{z},N<0\right)$$
$$\leq\mathbb{P}\left(\Phi\left(\underline{\mu}-\sigma_{\tilde{T}}N\right)<2\sqrt{z},N>0\right)$$
$$+\mathbb{P}\left(\Phi\left(\underline{\mu}+\sigma_{\tilde{T}}N\right)<2\sqrt{z},N<0\right)$$
$$\leq2\mathbb{P}\left(\Phi\left(\underline{\mu}+\sigma_{\tilde{T}}N\right)<2\sqrt{z}\right),$$

with  $N \stackrel{d}{=} \mathcal{N}(0,1)$  independent of U. Hence, from Lemma 1.3.4 we obtain that for every A > 0, there exists  $z_{0,1} > 0$  such that

$$\forall 0 < z < z_{0,1} \land z_1, \quad p_1 \le 2^{1 + \frac{1}{(1+A)\sigma_T^2}} z^{\frac{1}{2(1+A)\sigma_T^2}} = 2^{1 + \frac{T-\tilde{T}}{\tilde{T}(1+A)}} z^{\frac{T-\tilde{T}}{2\tilde{T}(1+A)}}.$$
(1.3.28)

Estimate of the third term  $p_3$ . Using the identity  $\Phi(y) + \Phi(-y) = 1$ , the function  $-\delta_t$  can be written as

$$-\delta_t(y) = \Phi(-y - A(t)) + \Phi(-y + B(t)) - 2\Phi(-y).$$

Note that we now have

$$\frac{\Phi\left(-y-A(t)\right)}{\Phi\left(-y+B(t)\right)} \underset{y \to +\infty}{\sim} \exp\left(\frac{1}{2}\left(A(t)+B(t)\right)\left(-2y-A(t)+B(t)\right)\right) \xrightarrow[y \to +\infty]{} 0,$$

$$\frac{\Phi\left(-y\right)}{\Phi\left(-y+B(t)\right)} \underset{y \to +\infty}{\sim} \exp\left(\frac{1}{2}B(t)\left(-2y+B(t)\right)\right) \xrightarrow[y \to +\infty]{} 0.$$

Hence, there exists  $\theta_3 > 0$  such that  $\forall y > \theta_3$ ,  $-\delta_t(y) > \frac{1}{2}\Phi(-y + B(t)) > \frac{1}{2}\Phi(-y) > 0$ . We can assume without loss of generality that  $\theta_3 > \sup_{t \in [0,\tilde{T}]} \tilde{\beta}(t)$  and set  $\sqrt{z_3} := \min_{t \in [0,\tilde{T}]} -\delta_t(\theta_3)$ . Then, with similar arguments to the analysis of the term  $p_1$  above, we get (for  $z < z_3$ )

$$p_3 = \mathbb{P}\left(-\delta_U\left(d_1(U, T, S_U, K)\right) < \sqrt{z}, S_U \in \mathcal{S}_3(U)\right)$$

$$\leq \mathbb{P}\left(\Phi\left(-d_1(U,T,S_U,K)\right) < 2\sqrt{z}\right) \\ = \mathbb{P}\left(\Phi\left(-\mu_U - \sigma_U N\right) < 2\sqrt{z}\right) \leq 2\mathbb{P}\left(\Phi\left(-\bar{\mu} + \sigma_{\bar{T}} N\right) < 2\sqrt{z}\right).$$

Therefore, owing to Lemma 1.3.4, for any A > 0 there exists  $z_{0,3} > 0$  such that

$$\forall 0 < z < z_{0,3} \land z_3, \quad p_3 \le 2^{1 + \frac{T - \tilde{T}}{\tilde{T}(1+A)}} z^{\frac{T - \tilde{T}}{2\tilde{T}(1+A)}}.$$
(1.3.29)

Finally, putting estimates (1.3.26), (1.3.27), (1.3.28) and (1.3.29) together, we obtain an upper bound for (1.3.25): defining  $\bar{z} := (z_{0,1} \wedge z_1 \wedge z_2 \wedge z_3 \wedge z_{0,3}) \frac{e^{r\tilde{T}}}{\sigma}$ , we conclude that for every  $0 < z < \bar{z} \wedge 1 := z_0$ ,

$$\mathbb{P}\left(|E_f(X)| < z\right) \le \left(\frac{2}{\tilde{T}} \int_0^{\tilde{T}} C(t) \mathrm{d}t + \frac{2e^{\left|\sigma^2 - r\right|\tilde{T}}}{\sqrt{\tilde{T}}S_0\sigma\sqrt{2\pi}}\right) \left(\frac{z}{\sigma e^{-r\tilde{T}}}\right)^{\frac{1}{2}} + 2^{2 + \frac{T - \tilde{T}}{\tilde{T}(1+A)}} \left(\frac{z}{\sigma e^{-r\tilde{T}}}\right)^{\frac{T - \tilde{T}}{2\tilde{T}(1+A)}} \le K_{\nu} z^{\nu},$$

for  $\nu$  as in the statement of the Theorem. Assumption 1.2.3 is therefore proved, and the proof of Theorem 1.3.3 follows.

#### **1.3.3** Numerical experiments

In this section, we test and compare numerically the antithetic ML estimator (1.2.3), the nonantithetic ML estimator (1.2.8), the NMC estimator (1.2.2) and the upper and lower bounds (1.2.19) for the estimation of the initial margin correction (1.3.5) in different situations: a single call/ put/ butterfly option, and several portfolios containing different combinations of butterfly options. In order to evaluate the MSE of the different estimators, we will make use of the available closed formulas  $I^{call}$  and  $I^{put}$  (1.3.17) in the single call and put cases. Unfortunately, we do not possess analogous formulas for the expectation  $I^{butterfly}$  associated to the butterfly option, or to butterfly option portfolios. In this case, since we still have an explicit expression for the conditional expectation  $E_f(X)$  (based on (1.3.20)), we can construct a benchmark value by applying an intensive standard Monte Carlo method to evaluate  $\mathbb{E}[g(E_f(X))] = \mathbb{E}[|E_f(X)|]$ .

#### The nested estimators

We estimate the mean-squared errors (denoted resp.  $\text{MSE}^{\text{ML}}$ ,  $\text{MSE}^{\text{ML2}}$  and  $\text{MSE}^{\text{NMC}}$ ) with  $\frac{1}{n_{\text{MSE}}} \sum_{j=1}^{n_{\text{MSE}}} \left(\widehat{I}_j - I\right)^2$ , where  $(\widehat{I}_j)_{1 \leq j \leq n_{\text{MSE}}}$  are independent copies of the respective estimator and  $n_{\text{MSE}} = 200$ . We will denote the related computational complexities  $\mathbf{C}^{\text{ML}}$ ,  $\mathbf{C}^{\text{ML2}}$  and  $\mathbf{C}^{\text{NMC}}$ .

In order to achieve MSE =  $\mathcal{O}(\varepsilon^2)$  for  $\varepsilon > 0$ , Theorem 1.2.6, Propositions 1.2.8 and 1.2.7 provide the following optimal choices of parameters for each estimator.

**Construction of the antithetic ML estimator.** The optimal ML estimator obtained in Theorem 1.2.6 depends on some problem-specific parameters  $\nu, \eta, p$ . In our application to IM computation presented in Section 1.3, we can take  $\eta = 1$ , p arbitrary large and  $\nu = \frac{1}{2} \left( 1 \wedge \frac{T - \tilde{T}}{\tilde{T}(1+A)} \right)$  for any A > 0.

If  $\tilde{T} < \frac{T}{2}$ , then  $\frac{T-\tilde{T}}{\tilde{T}} > 1$ , and choosing  $A = \frac{1}{2} \left( \frac{T-\tilde{T}}{\tilde{T}} - 1 \right)$  we get  $\frac{T-\tilde{T}}{\tilde{T}(1+A)} > 1$ . As a consequence,  $\nu = \frac{1}{2}$ . Since  $1 + \frac{(p-2)\nu}{4(p+\nu)} \wedge \frac{\eta}{2} \to \frac{9}{8}$  as  $p \uparrow +\infty$ , following Theorem 1.2.6 we choose the outer Monte Carlo samples  $M_l$  as

$$M_l = M_0 2^{-\frac{9}{8}l}.$$

If  $\tilde{T} \geq \frac{T}{2}$ , then  $\frac{T-\tilde{T}}{\tilde{T}(1+A)} < 1$  for any A > 0, yielding  $\nu = \frac{T-\tilde{T}}{2\tilde{T}(1+A)}$ . Since  $1 + \frac{(p-2)\nu}{4(p+\nu)} \wedge \frac{\eta}{2} \rightarrow 1 + \frac{T-\tilde{T}}{8\tilde{T}(1+A)}$  as  $p \uparrow +\infty$ , again following Theorem 1.2.6 we can choose

$$M_l = M_0 2^{-\left(1 + \frac{T - \tilde{T}}{8\tilde{T}(1+A)}\right)l}, \qquad A > 0.$$

For such choices of  $M_l$ , the overall computational complexity is  $\mathbf{C}^{\mathrm{ML}} = \sum_{l=0}^{L} n_l M_l$ =  $\frac{1-2^{-\frac{(L+1)\nu}{4}}}{1-2^{-\frac{\nu}{4}}} M_0 n_0$  where  $\nu = \frac{1}{2}$  if  $\tilde{T} < \frac{T}{2}$  and  $\nu = \frac{T-\tilde{T}}{2\tilde{T}(1+A)}$  if  $\tilde{T} \geq \frac{T}{2}$ . In our experiments, we will consider options with maturity T = 1 and set  $\tilde{T} = \frac{252-5}{252}T$  (1 week before the maturity, 252 trading days in a year) and A = 0.05. As a consequence, we have  $\tilde{T} \geq \frac{T}{2}$  and  $\nu = \frac{T-\tilde{T}}{2\tilde{T}(1+A)}$ .

Construction of the two other estimators. The NMC estimator (1.2.2) only depends on the two sample sizes N and M; its complexity is  $\mathbf{C}^{\text{NMC}} = MN$ . The non-antithetic ML estimator ML2 is fixed by Propositions 1.2.8: recall that we make the choice  $\tilde{M}_l = \tilde{M}_0 2^{-l}$ , which implies that the product  $\tilde{n}_l \tilde{M}_l = \tilde{n}_0 \tilde{M}_0$  is independent of l. The resulting computational complexity is  $\mathbf{C}^{\text{ML2}} = \tilde{n}_0 \tilde{M}_0 (\tilde{L} + 1)$ .

We fix the model parameters r = 0.1,  $\sigma = 0.3$  in (1.3.1) and consider four different Portfolios  $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}$ , described below. To estimate a reference value for I, we use an unbiased Monte Carlo estimation of  $\mathbb{E}[g(E_f(X))]$  (recall that  $E_f(X)$  is explicit in the examples below) with  $n_{\mathrm{MC}} = 5 \times 10^7$  samples, and provide the associated 95%-confidence interval. Denote  $\varphi(s, K, a) = (s - (K - a))_+ + (s + (K + a))_+ - 2(s - K)_+$  the butterfly option payoff with strikes K - a, K, and K + a.

**Portfolio**  $\mathcal{A}$ . We consider one butterfly option with payoff  $\varphi(s, 100, 50)$ , and set  $S_0 = 90$ . Here we have that  $I_{\mathcal{A}} = \mathbb{E}\left[g(E_f^{butterfly}(X))\right]$  is worth  $10.720 \pm 0.002$ .

**Portfolio**  $\mathcal{B}$ . We choose Portfolio  $\mathcal{A}$ , but now with  $S_0 = 30$ , which implies  $S_0 \ll K = 100$ , and therefore the resulting samples will be far from the singularity of g with high probability (see Figure 1.2). Here  $I_{\mathcal{B}} = 0.998 \pm 5 \times 10^{-4}$ .

**Portfolio** C. We choose a more diversified portfolio, made of a linear combination of five different butterfly options. The final payoff is of the form

 $2\varphi(s, 10, 1) + 2\varphi(s, 20, 2) + 2\varphi(s, 40, 4) + \varphi(s, 50, 5) + 1.5\varphi(s, 80, 8)$ . In Figure 1.3 one can observe that the Portfolio delta, as a function of s, now has several zeros (playing the role of singularities for g(z) = |z|). We set  $S_0 = 20$  (close to the singularities) and get  $I_{\mathcal{C}} = 0.507 \pm 0.0002$  as a reference value.

**Portfolio**  $\mathcal{D}$ . We choose Portfolio  $\mathcal{C}$ , but now setting  $S_0 = 100$  (further away from the singularities of the option's delta, see Figure 1.3 again). Here  $I_{\mathcal{D}} = 1.263 \pm 0.0004$ .



Figure 1.2 – Functions  $s \to 0.1\Delta_t(s)$  (blue) and  $s \to p_t(s)$  for the Portfolios  $\mathcal{A}$  (orange) and  $\mathcal{B}$  (green) at different values of t.



Figure 1.3 – Functions  $s \to \Delta_t(s)$  (blue) and  $s \to p_t(s)$  for the Portfolios  $\mathcal{C}$  (red) and  $\mathcal{D}$  (black) at different values of t.

In Figures 1.2 and 1.3 we plot the Portfolio delta (as a function of s) for different times t, together with the probability density function of  $S_t$ , denoted  $p_t$ . Note that in Figure 1.2, we have re-scaled the delta so to fit all the functions on the same graph. Observing the support of  $p_t$ , we see that in Portfolios  $\mathcal{A}$  and  $\mathcal{C}$  there is a high probability that  $\Delta_t(S_t)$  will change sign, as opposed to Portfolios  $\mathcal{B}$  and  $\mathcal{D}$ .

In Figure 1.4, we plot the MSE's of the different estimators in terms of their respective computational costs, on a log-log plot. We have to fix their (free) parameters: (M, N) for the NMC estimator,  $(M_0, n_0, L)$  for the ML estimator and  $(\tilde{M}_0, \tilde{n}_0, \tilde{L})$  for the ML2 estimator. Recall from the analysis above that  $\mathbf{C}^{\mathrm{ML}} = \frac{1-2^{-\frac{(L+1)\nu}{4}}}{1-2^{-\frac{\nu}{4}}} M_0 n_0$ ,  $\mathbf{C}^{\mathrm{ML2}} = \tilde{n}_0 \tilde{M}_0 (\tilde{L}+1)$  and  $\mathbf{C}^{\mathrm{NMC}} = MN$ . For a fixed value of the cost  $\mathbf{C}$  (here ranging from  $5 \times 10^5$  to  $1 \times 10^6$ ), we look for values of  $M, M_0, \tilde{M}_0$  on a grid of evenly spaced values between  $10^3$  and  $10^4$  and for values of  $L, \tilde{L}$  in  $\{2, 3, 4, 5\}$  that minimize the estimated MSE. We fix the corresponding parameters  $N, n_0, \tilde{n}_0$  using the identities

$$N = \frac{\mathbf{C}}{M}, \ n_0 = \frac{(1 - 2^{-\frac{\nu}{4}})\mathbf{C}}{(1 - 2^{-(L+1)\frac{\nu}{4}})M_0}, \ \tilde{n_0} = \frac{\mathbf{C}}{(\tilde{L} + 1)\tilde{M_0}}$$



Figure 1.4 – log (MSE) against log of the computational cost for the Portfolios  $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}$ . ML (red) stands for the antithetic Multi-level estimator (1.2.3), ML2 (orange) for the non-antithetic ML estimator (1.2.8), and NMC (blue) for the plain nested estimator (1.2.2). The green straight line has a slope of -1.

We observe that the antithetic ML estimator gives the best results in terms of the size of the MSE for a fixed cost **C** for the Portfolios  $\mathcal{A}, \mathcal{C}$ , and  $\mathcal{D}$ , for which we have singularities in the delta. We retrieve a slope close to -1 for the ML estimator, whereas the other estimators show a slightly smaller slope (in absolute value), which is in line with the theoretical results. On the other side, recall that Portfolio  $\mathcal{B}$  was constructed in such a way that the probability of hitting the zeros of the delta function is very small, so that the function g essentially does not introduce any bias. In this case, the three estimators provide similar results (and the antithetic ML estimator actually does not display the best results anymore): the use of a multilevel estimator in this setting does not seem to provide a concrete advantage with respect to a plain nested MC procedure. In all the other situations, the antithetic MLMC estimator has the best performance.

#### Non-nested lower and upper estimators

With reference to the notation of Section 1.2.3 and Proposition 1.3.1, we have to evaluate the regression coefficients (1.2.16) and (1.2.17) with respect to  $X = (U, Z) \in \mathbb{R}^2$ . To do so, we choose as a projection basis the tensor product of (first-kind) Chebychev polynomials  $T_i$  and Hermite polynomials  $H_i$ , precisely: we set  $L_{X,k_X} := L_{U,k_U} \otimes L_{Z,k_Z}$  for  $k_U \ge 0$  and  $k_Z \ge 0$ , where

$$k_X := k_U \times k_Z, \quad L_{U,k_U} := \operatorname{span}\left(T_i(\frac{U}{\tilde{T}}) : 0 \le i \le k_U\right)$$
$$L_{Z,k_Z} := \operatorname{span}\left(H_i(Z) : 0 \le i \le k_Z\right),$$
where the polynomials  $T_i$  and  $H_i$  are defined by

$$T_0(x) = 1, \quad T_1(x) = x, \quad \forall i \ge 1, \\ T_{i+1}(x) = 2x T_i(x) - T_{i-1}(x), \\ H_0(x) = 1, \quad H_1(x) = x, \quad \forall i \ge 1, \\ H_{i+1}(x) = x H_i(x) - i H_{i-1}(x).$$

Choosing such smooth basis functions is motivated by the intuition that, in the present setting,  $\mathbb{E}_f(X)$  is a reasonably smooth function of X. For every  $0 \le j_u \le k_U$  and  $0 \le j_z \le k_Z$ , we solve the least-squares problems introduced in Section 1.2.3, the first one being

$$(l_{j_u j_z}^*) = \underset{\substack{l_{j_u j_z} \in \mathbb{R}, \\ 0 \le j_u \le k_U, \\ 0 \le j_z \le k_z}}{\operatorname{arg\,min}} \frac{1}{N} \sum_{i=1}^N \left( f(\tilde{X}_i, \tilde{Y}_i) - \sum_{\substack{0 \le j_u \le k_U, \\ 0 \le j_z \le k_z}} l_{j_u j_z} T_{j_u} \left( \frac{\tilde{U}_i}{\tilde{T}} \right) H_{j_z}(\tilde{Z}_i) \right)^2$$

For the construction of the random variable  $\varepsilon_d^*$ , we use the same kind of basis for X, i.e.  $L_{X,d_X} = L_{U,d_U} \otimes L_{Z,d_Z}$  (possibly with different values of  $d_U \ge 0, d_Z \ge 0$ ), and choose as an approximation space for Y the space  $L_{Y,d_Y} = \text{span}(H_i(Y): 0 \le i \le d_Y), d_Y \ge 0$ . For every  $0 \le a_u \le d_U$ ,  $0 \le a_z \le d_Z$  and  $0 \le b_y \le d_Y$ , we have to solve the least-squares problem

$$\begin{aligned} &(u_{a_{u}a_{z}b_{y}}^{*}) = \\ & \underset{\substack{u_{a_{u}a_{z}b_{y}} \in \mathbb{R}, \\ 0 \leq a_{u} \leq d_{U}, \\ 0 \leq a_{z} \leq d_{Z}, \\ 0 < b_{y} \leq d_{Y}}}{\underset{\substack{u_{a_{u}a_{z}b_{y}} \in \mathbb{R}, \\ 0 \leq a_{z} \leq d_{Z}, \\ 0 < b_{y} \leq d_{Y}}}{\underset{u_{a_{u}a_{z}b_{y}} \in \mathbb{R}, \\ 0 \leq a_{z} \leq d_{Z}, \\ 0 < b_{y} \leq d_{Y}}} \frac{1}{N} \sum_{i=1}^{N} \left( f(\tilde{X}_{i}, \tilde{Y}_{i}) - \sum_{\substack{0 \leq a_{u} \leq d_{U}, \\ 0 \leq a_{z} \leq d_{Z}, \\ 0 < b_{y} \leq d_{Y}}} u_{a_{u}a_{z}b_{y}} T_{a_{u}} \left( \frac{\tilde{U}_{i}}{\tilde{T}} \right) H_{a_{z}} \left( \tilde{Z}_{i} \right) H_{b_{y}} \left( \tilde{Y}_{i} \right) \right)^{2}, \end{aligned}$$

where we have used the zero-mean property  $H_{b_y}(\tilde{Y}) - \mathbb{E}\left[H_{b_y}(\tilde{Y})\right] = \mathbf{1}_{b_y \neq 0} H_{b_y}(\tilde{Y})$  following from the orthogonality of the Hermite polynomials with respect to the Gaussian measure Abramowitz and Stegun [2, 22.2.15, p.775], which means that we can restrict the sum to  $0 < b_y \leq d_Y$ .

To construct the upper and lower biased estimators, we generate N independent copies  $\left(\tilde{X}_i, \tilde{Y}_i\right)_{1 \le i \le N}$  of (X, Y) in order to solve both least-squares problems above, and define the regression functions  $\varphi_k^*$  and  $\varepsilon_d^*$  from (1.2.18). Once these functions are fixed, we generate another sample of  $\tilde{N}$  independent copies of (X, Y) and estimate the left and right expectations in (1.2.19) with a standard Monte Carlo procedure.

Impact and choice thereof of the polynomial degrees. In Tables 1.1, 1.2, we list the resulting values of the lower-upper bounds together with their 95% confidence interval, for different choices of the polynomial degrees  $(k_U, k_Z)$  and  $(d_U, d_Z, d_Y)$ . The sample sizes are respectively  $N = 10^5$  and  $\tilde{N} = 5 \times 10^6$ . We have run the algorithm on call and put options with parameters  $S_0 = K = 100$ , T = 1, r = 0.1,  $\sigma = 0.3$ . In Tables 1.3, 1.4 we provide the corresponding lower-upper bounds obtained for Portfolios  $\mathcal{A}$  and  $\mathcal{C}$ . Sample sizes are this time  $N = 10^6$ ,  $\tilde{N} = 2 \times 10^6$ .

$(k_U, k_Z)$	Call	Put
(1,1)	$20.52\pm0.033$	$9.415 \pm 0.014$
(2,2)	$20.551 \pm 0.033$	$9.421 \pm 0.014$
(3, 3)	$20.551 \pm 0.033$	$9.396 \pm 0.014$
(4, 4)	$20.554\pm0.033$	$9.424 \pm 0.015$
(5,5)	$20.535 \pm 0.073$	$9.409 \pm 0.032$
(6, 6)	$20.548 \pm 0.033$	$9.429 \pm 0.015$

Table 1.1 – Lower bound for the call  $(I^{call} = 20.567)$  and put  $(I^{put} = 9.433)$  options.

$(d_U, d_Z, d_Y)$	Call $(I^{call} = 20.567)$	Put $(I^{put} = 9.433)$
(1, 1, 1)	$22.963 \pm 0.028$	$11.066 \pm 0.012$
(2, 2, 2)	$22.461 \pm 0.012$	$10.969 \pm 0.006$
(3,3,3)	$21.104\pm0.009$	$10.177 \pm 0.005$
(4, 4, 4)	$20.909\pm0.01$	$9.924 \pm 0.005$
(5, 5, 5)	$20.883 \pm 0.01$	$9.859 \pm 0.006$
(6, 6, 6)	$20.874\pm0.02$	$9.797 \pm 0.009$

Table 1.2 – Upper bound for the call  $(I^{call} = 20.567)$  and put  $(I^{put} = 9.433)$  options.

$(k_U,k_Z)$	Portfolio $\mathcal{A}$	Portfolio $\mathcal{C}$
(6, 6)	$10.686 \pm 0.036$	$0.467 \pm 0.004$
(7,7)	$10.689 \pm 0.036$	$0.495 \pm 0.004$
(8,8)	$10.702 \pm 0.036$	$0.498 \pm 0.004$
(9,9)	$10.707 \pm 0.036$	$0.503 \pm 0.004$

Table 1.3 – Lower bound for Portfolio  $\mathcal{A}$  ( $I_{\mathcal{A}} = 10.720 \pm 0.002$ ) and  $\mathcal{C}$  ( $I_{\mathcal{C}} = 0.507 \pm 0.0002$ ).

$(d_U, d_Z, d_Y)$	Portfolio $\mathcal{A}$	Portfolio $\mathcal{C}$
(6, 6, 6)	$11.695 \pm 0.013$	$1.424\pm0.003$
(7, 7, 7)	$11.342 \pm 0.038$	$1.415\pm0.005$
(8, 8, 8)	$11.207 \pm 0.017$	$1.383\pm0.004$
(9, 9, 9)	$11.142 \pm 0.04$	$1.375\pm0.007$

Table 1.4 – Upper bound for Portfolios  $\mathcal{A}$  ( $I_{\mathcal{A}} = 10.720 \pm 0.002$ ) and  $\mathcal{C}$  ( $I_{\mathcal{C}} = 0.507 \pm 0.0002$ ).

Notice that an automatic choice of the degrees  $(k_U, k_Z)$  and  $(d_U, d_Z, d_Y)$  could be done through a cross-validation procedure so that the out-of-sample regression error is minimized, see Györfi et al. [96, Chapter 8] and Hastie, Tibshirani, and Friedman [100, Chapter 8] for instance. A minimal out-of-sample regression error (a.k.a. generalization error) should intuitively give the best bounds. Here, since we evaluate both bounds at once, we can also make a choice based on the difference between their values: we choose polynomial degrees  $(k_U, k_Z)$  and  $(d_U, d_Z, d_Y)$ such that the distance between the two estimated bounds is minimized. In Table 1.2 this would correspond to the highest degree  $d_U = d_Z = d_Y = 6$  for the upper bound; the lower bound does not seem to be very sensitive to the value of  $k_U, k_Z$  and is well estimated already with  $k_U = k_Z = 1$ . Using the reference explicit values of  $I^{call}$  and  $I^{put}$ , we can see that the results are overall very accurate; when  $k_U = k_Z = d_U = d_Z = d_Y = 6$ , the relative error between the two bounds is  $\frac{20.874-20.548}{20.567} = 1.6\%$  for the call option and  $\frac{9.797-9.429}{9.433} = 3.9\%$  for the put option. In Table 1.4, we observe a similar behavior for Portfolio  $\mathcal{A}$ ; here the relative error for the higher tested degree is  $\frac{11.142-10.707}{10.720} = 4.0\%$ . Note that we had to use higher polynomial degrees and larger sample size N than in Table 1.2 in order to obtain comparable relative errors, which we can attribute to the more singular behavior of this portfolio. For Portfolio  $\mathcal{C}$  (containing even more singularities), we see that the two bounds are still quite far from each other; notably, while the lower bounds provide accurate results, the upper bounds remain relatively far from the true value. Obtaining tighter bounds in this case would require higher values for  $N, \tilde{N}$  and the polynomial degrees.

# 1.4 Conclusion

For the evaluation of  $\mathbb{E}\left[g(\mathbb{E}\left[f(X,Y)|X\right]\right)\right]$  with a piece-wise  $C^1$  function g, we have designed an antithetic Multi-Level Monte Carlo estimator and lower-upper biased non-nested Monte Carlo estimators. Theoretical results support the convergence of all these estimators (Theorem 1.2.6 and Theorem 1.2.10). Globally, our numerical experiments show better performance of the antithetic MLMC estimator compared to the non-antithetic one and to a plain nested Monte Carlo estimator (as expected). The lower-upper bounds can be implemented using empirical regression methods, and this leads to a scheme for "sandwiching" the quantity of interest, provided that the conditional expectation  $x \mapsto \mathbb{E}\left[f(X,Y)|X=x\right]$  can be efficiently approximated over a space of basis functions.

# 1.5 Technical proofs

# 1.5.1 Proof of Proposition 1.2.7 on the complexity of the NMC estimator

First notice that by independence,  $\mathbb{E}\left[\widehat{I}_{M,N}\right] = \mathbb{E}\left[g\left(\frac{1}{N}\sum_{j=1}^{N}f\left(X,Y_{j}\right)\right)\right]$  and by Proposition 1.2.4 there exists a positive constant  $\kappa$  such that

$$\forall N \ge 1, \quad \left| \mathbb{E} \left[ \widehat{I}_{M,N} - g\left( E_f(X) \right) \right] \right| \le \frac{\kappa}{N^{\frac{1}{2} \left( 1 + \frac{(p-1)\nu}{p+\nu} \land \eta \right)}}.$$

By Lemma 1.2.13, applying (1.2.20), the identity

$$g\left(\widehat{E}_{f,N}(X)\right) = g\left(E_f(X)\right) + \delta E_N(X) \int_0^1 \left(g'\left(E_f(X) + \lambda \delta E_N(X)\right)\right) \mathrm{d}\lambda$$

holds on the set  $E_f(X) \notin \{d_1, \ldots, d_\theta\}$  with probability one by Assumption 1.2.3. Whence, we have:

$$\mathbb{E}\left[g\left(\widehat{E}_{f,N}(X)\right)^{2}\right] \leq 2\left(\mathbb{E}\left[g\left(E_{f}(X)\right)^{2}\right] + ||g'||_{\infty}^{2}\mathbb{E}\left[\left(\delta E_{N}(X)\right)^{2}\right]\right)$$
$$\leq 2\left(\mathbb{E}\left[g\left(E_{f}(X)\right)^{2}\right] + ||g'||_{\infty}^{2}\frac{C_{p}^{2}}{N}\right),$$

using Lemma 1.2.12. By independence, we get the following estimate for the variance:

$$\operatorname{Var}\left(\widehat{I}_{M,N}\right) = \frac{1}{M} \operatorname{Var}\left(g\left(\widehat{E}_{f,N}(X)\right)\right)$$
$$\leq \frac{1}{M} \mathbb{E}\left[g\left(\widehat{E}_{f,N}(X)\right)^{2}\right]$$
$$\leq \frac{2}{M} \left(\mathbb{E}\left[g\left(E_{f}(X)\right)^{2}\right] + ||g'||_{\infty}^{2} \frac{C_{p}^{2}}{N}\right).$$

Finally, by the bias-variance decomposition of  $MSE^{NMC}$ , we get:

$$\mathrm{MSE}^{\mathrm{NMC}} \le C_{NMC} \left( \frac{1}{N^{\left(1 + \frac{(p-1)\nu}{p+\nu} \land \eta\right)}} + \frac{1}{MN} + \frac{1}{M} \right),$$

where  $C_{NMC} = \kappa^2 \vee \left( 2\mathbb{E} \left[ g \left( E_f(X) \right)^2 \right] \right) \vee \left( 2||g'||_{\infty}^2 C_p^2 \right)$ . The statement on the complexity of the NMC estimator finally follows from the fact that the computational cost is of order  $\mathcal{O}(MN)$ .  $\Box$ 

# 1.5.2 Proof of Proposition 1.2.8 on the complexity of the Multi level estimator ML2

Since g is Lipschitz continuous, proceeding as in the proof of Proposition 1.2.7, there exists a constant  $C_p > 0$  such that

$$\mathbb{E}\left[\left(g(\widehat{Z}) - g(\widehat{Z}_1)\right)^2\right] \le ||g'||_{\infty}^2 \mathbb{E}\left[\left(\frac{\delta\widehat{Z}_2 - \delta\widehat{Z}_1}{2}\right)^2\right] \le ||g'||_{\infty}^2 \frac{C_p^2}{n_l}$$

Now noticing that the variance at level l for the estimator (1.2.8) is given by

$$V_{l} = \operatorname{Var}\left(g\left(\frac{1}{n_{l}}\sum_{j=1}^{n_{l}}f\left(X,Y_{j}\right)\right) - g\left(\frac{1}{n_{l-1}}\sum_{j=1}^{n_{l-1}}f\left(X,Y_{j}\right)\right)\right)$$
$$= \operatorname{Var}\left(g(\widehat{Z}) - g(\widehat{Z}_{1})\right),$$

we conclude as in the Proof of Theorem 1.2.6, now using the estimate  $V_l \leq C n_l^{-1}$  for a positive constant C and the case  $\beta = \gamma$  in Giles [75, Theorem 1].

### 1.5.3 Proof of Lemma 1.3.4

Since  $\Phi(\cdot)$  is increasing on  $\mathbb{R}$ , we have  $\mathbb{P}\left(\Phi\left(\mu + \sigma Z\right) < z\right) = \Phi\left(\frac{\Phi^{-1}(z) - \mu}{\sigma}\right)$  for every z > 0. For given A > 0, define  $\sigma' := (1 + \frac{A}{2})^{\frac{1}{2}}\sigma$  and note that, owing to (1.3.13)),

$$\frac{\Phi\left(\frac{\Phi^{-1}(z)-\mu}{\sigma}\right)}{\Phi\left(\frac{\Phi^{-1}(z)}{\sigma'}\right)} \approx \frac{\sigma}{\sigma'} \frac{\exp\left(-\frac{1}{2}\left(\frac{\Phi^{-1}(z)-\mu}{\sigma}\right)^2\right)}{\exp\left(-\frac{1}{2}\left(\frac{\Phi^{-1}(z)}{\sigma'}\right)^2\right)} \frac{1}{1-\frac{\mu}{\Phi^{-1}(z)}}$$
$$\approx \frac{\sigma}{z \to 0} \frac{\sigma}{\sigma'} \exp\left(-\frac{1}{2}\left(\frac{\sigma'-\sigma}{\sigma\sigma'}\Phi^{-1}(z)-\frac{\mu}{\sigma}\right)\left(\frac{\sigma'+\sigma}{\sigma\sigma'}\Phi^{-1}(z)-\frac{\mu}{\sigma}\right)\right).$$

Then, using  $\sigma' > \sigma > 0$  and  $\Phi^{-1}(z) \xrightarrow[z \to 0^+]{} -\infty$ , we obtain  $\frac{\Phi\left(\frac{\Phi^{-1}(z)-\mu}{\sigma}\right)}{\Phi\left(\frac{\Phi^{-1}(z)}{\sigma'}\right)} \xrightarrow[z \to 0^+]{} 0$ . Hence, there exists  $\lambda_0(A) > 0$  such that for every  $0 < z < \lambda_0(A)$ :

$$\Phi\left(\frac{\Phi^{-1}(z)-\mu}{\sigma}\right) < \Phi\left(\frac{\Phi^{-1}(z)}{\sigma'}\right).$$

Now, using the fact that, for every  $z \in (0, \frac{1}{2}], \Phi^{-1}(z) \leq 0$ , we have that for every  $z \in (0, 2^{-(1+A)\sigma^2}]$ ,

$$\begin{split} \Phi\left(\frac{\Phi^{-1}\left(z\right)}{\sigma'}\right) &\leq z^{\frac{1}{(1+A)\sigma^2}} \iff \frac{\Phi^{-1}\left(z\right)}{\sigma'} \leq \Phi^{-1}\left(z^{\frac{1}{(1+A)\sigma^2}}\right) \leq 0\\ &\iff \left(\frac{\Phi^{-1}\left(z\right)}{\sigma'}\right)^2 \geq \left(\Phi^{-1}\left(z^{\frac{1}{(1+A)\sigma^2}}\right)\right)^2 \end{split}$$

Now using the asymptotic expansion for the inverse c.d.f. of the standard normal distribution (see Dominici [56]),

$$\left(\Phi^{-1}\left(z\right)\right)^{2} \underset{z \to 0^{+}}{\sim} \log\left(\frac{1}{2\pi z^{2}}\right) - \log\left(\log\left(\frac{1}{2\pi z^{2}}\right)\right) \underset{z \to 0^{+}}{\sim} - 2\log\left(z\right),$$

the following limit holds:

$$\frac{\left(\frac{\Phi^{-1}(z)}{\sigma'}\right)^2}{\left(\Phi^{-1}\left(z^{\frac{1}{(1+A)\sigma^2}}\right)\right)^2} \xrightarrow[z \to 0^+]{} \frac{1}{z^{1+A}\sigma^2} \left(\sigma'\right)^2 = \frac{1+A}{1+\frac{A}{2}} > 1.$$

0

We have just shown that there exists  $\lambda_1(A) > 0$  such that for every  $0 < z < \lambda_1(A)$ , one has  $\left(\frac{\Phi^{-1}(z)}{\sigma'}\right)^2 \ge \left(\Phi^{-1}\left(z^{\frac{1}{(1+A)\sigma^2}}\right)\right)^2$ . Finally, choosing  $z_0(A) := \lambda_0(A) \land \lambda_1(A) \land 2^{-\frac{1}{(1+A)\sigma^2}}$ , we obtain the announced claim.

### 1.5.4 Proof of Proposition 1.3.6

 $\triangleright$  Let us justify point 1. For notational simplicity, we omit the dependence with respect to t of the functions A and B. Taking the derivative of  $H_t$  yields

$$H'_t(x) = -Ae^{-\frac{A^2}{2}}e^{-Ax} + Be^{-\frac{B^2}{2}}e^{Bx}.$$

Now

$$H'_t(x) = 0 \iff x = x_0(t) := \frac{\log\left(\frac{A}{B}\right)}{A+B} - \frac{1}{2}\left(A-B\right), \tag{1.5.1}$$

 $H'_t(x) > 0$  for  $x > x_0(t)$  and  $H'_t(x) < 0$  for  $x < x_0(t)$ . Recall that A > B > 0. Using  $H_t(x) \xrightarrow[x \to \pm\infty]{} +\infty, H_t$  is decreasing on  $(-\infty, x_0(t))$  and increasing on  $(x_0(t), +\infty)$ . Furthermore, let us show that

$$H_t(x_0(t)) = e^{-A\frac{\log(\frac{A}{B})}{A+B} - \frac{AB}{2}} + e^{B\frac{\log(\frac{A}{B})}{A+B} - \frac{AB}{2}} - 2 < 0.$$

Let us define  $y := \frac{A}{B} > 1$  so that  $H_t(x_0(t)) = e^{-\frac{AB}{2}} \left( e^{-\frac{y \log(y)}{1+y}} + e^{\frac{\log(y)}{1+y}} - 2 \right) := e^{-\frac{AB}{2}} (h(y) - 2).$ Since  $e^{\frac{-AB}{2}} < 1$ , it is now sufficient to prove that

$$\forall y > 1, \quad h(y) < 2.$$

Set  $g(y) := \frac{y \log(y)}{1+y}$  so that  $h(y) = \frac{1+y}{e^{y \log(y)}} = \frac{1+y}{e^{g(y)}}$ . A direct computation yields  $g'(y) = \frac{\log(y)}{(1+y)^2} + \frac{1}{(1+y)}$  and  $h'(y) = e^{-g(y)} (1 - (1+y)g'(y)) = \frac{-\log(y)e^{-g(y)}}{(1+y)} < 0$  for y > 1. Hence h is continuous and decreasing on  $(1, \infty)$ , thus strictly upper bounded by h(1) = 2, which is the announced claim.

Now using the intermediate value theorem, there exist only two roots  $\alpha(t), \beta(t) \in \mathbb{R}$  of  $H_t$ . Summing up, we have:

$$\alpha(t) < x_0(t) < \beta(t), \qquad H_t\left(\alpha(t)\right) = H_t\left(\beta(t)\right) = 0.$$

Using  $H_t(0) = e^{-\frac{A^2}{2}} + e^{-\frac{B^2}{2}} - 2 < 0$ , we finally get:

$$\alpha(t) < 0 < \beta(t). \tag{1.5.2}$$

Let us now prove that  $\alpha \in \mathcal{C}^{\infty}([0,T))$  (similar arguments can be used for  $\beta$ ). Note that H which is  $\mathcal{C}^{\infty}$  can be defined for negative t as well, say on  $(-\eta, T)$  with  $\eta > 0$  and we keep writing H for this extended definition. The roots  $\alpha$  and  $\beta$  are also well defined on  $(-\eta, T)$ . Now let  $t_1 \in (-\eta, T)$  and using  $\forall t \in (-\eta, T)$ ,  $x_0(t) \neq \alpha(t)$ , we have:

$$H\left(t_1, \alpha\left(t_1\right)\right) = 0,$$

$$\frac{\partial H}{\partial x}\left(t_{1},\alpha\left(t_{1}\right)\right) = -A\left(t_{1}\right)e^{-\frac{A\left(t_{1}\right)^{2}}{2}}e^{-A\left(t_{1}\right)\alpha\left(t_{1}\right)} + B\left(t_{1}\right)e^{-\frac{B\left(t_{1}\right)^{2}}{2}}e^{B\left(t_{1}\right)\alpha\left(t_{1}\right)} \neq 0.$$

Using the implicit function theorem (see Dieudonné [55, Thereom 10.2.2]), there exist neighborhoods  $\mathcal{U}_{t_1}$  and  $\mathcal{U}_{\alpha(t_1)}$  of  $t_1$  and  $\alpha(t_1)$ , a function  $\chi: \mathcal{U}_{t_1} \to \mathcal{U}_{\alpha(t_1)}$  of class  $\mathcal{C}^{\infty}$  such that

$$\forall t \in \mathcal{U}_{t_1}, \ H(t, \chi(t)) = 0.$$

Hence  $\alpha(t_1) = \chi(t_1)$  and  $\alpha$  is  $\mathcal{C}^{\infty}$  at  $t_1$  (for every  $t_1 \in (-\eta, T)$ ), so that  $\alpha \in \mathcal{C}^{\infty}((-\eta, T))$  and consequently  $\alpha \in \mathcal{C}^{\infty}([0, T))$ .

▷ We now prove point 2. Let us denote  $d_1(t,s)$  instead of  $d_1(t,T,s,K)$ . Notice that  $\forall t \in [0,T), s \in (0,\infty) \rightarrow d_1(t,s) = \frac{\log(\frac{s}{K}) + \left(r + \frac{\sigma^2}{2}\right)(T-t)}{\sigma\sqrt{T-t}}$  is increasing and:

$$x = d_1(t, s) \iff s = K e^{\sigma \sqrt{T - t}x - \left(r + \frac{\sigma^2}{2}\right)(T - t)},$$
  

$$\Gamma_t(S_t) := \Delta_t'(S_t) \stackrel{(1.3.21)}{=} \delta_t'(d_1(t, T, S_t, K)) \frac{1}{S_t \sigma \sqrt{T - t}}.$$
(1.5.3)

In view of relation (1.3.12) (i.e.  $\sqrt{2\pi}\delta'_t(x) = e^{-\frac{y^2}{2}}H_t(x)$ ), the zeros  $\alpha(t), \beta(t)$  of  $H_t(\cdot)$  transfer to those of  $\delta'_t(d_1(t,.))$  (and thus  $\Gamma_t(\cdot)$ ) via (1.5.3). This leads to the announced expression (1.3.23) of two zeros  $\tilde{\alpha}(t), \tilde{\beta}(t)$  for  $\Gamma_t(\cdot)$ . The time-smoothness of  $\alpha(t), \beta(t)$  is clearly transferred to that of  $t \to \tilde{\alpha}(t), \tilde{\beta}(t)$ .

 $\begin{aligned} & \succ \text{Finally, let us prove point 3. The function } x \to \delta_t(x) \text{ is increasing on } (-\infty, \alpha(t)) \\ & \cup (\beta(t), \infty) \text{ and decreasing on } (\alpha(t), \beta(t)) \text{ since } H_t \text{ is positive on } (-\infty, \alpha(t)) \cup (\beta(t), \infty), \text{ negative on } (\alpha(t), \beta(t)) \text{ and has two unique zeros } \alpha(t), \beta(t). \text{ Using that } s \to d_1(t, s) \text{ is an increasing function and by } (1.3.21), \text{ we conclude that } s \to \Delta_t(s) \text{ is increasing on } (0, \tilde{\alpha}(t)) \cup (\tilde{\beta}(t), \infty) \text{ and } \\ & \text{decreasing on } (\tilde{\alpha}(t), \tilde{\beta}(t)). \text{ Noticing that, for all } t \in [0, T), \Delta_t(s) \xrightarrow[s \to 0^+]{} 0 \text{ and } \Delta_t(s) \xrightarrow[s \to +\infty]{} 0, \\ & \text{by the intermediate value theorem, there exists a unique function } t \in [0, T) \to \gamma(t) \text{ such that } \end{aligned}$ 

$$\forall t \in [0,T), \quad \tilde{\alpha}(t) < \gamma(t) < \tilde{\beta}(t), \quad \Delta_t(\gamma(t)) = 0.$$

Also, using the monotonicity of  $\Phi$ , the definitions (1.3.9) and  $\delta_t(0) = \Delta_t \left( K e^{-\left(r + \frac{\sigma^2}{2}\right)(T-t)} \right) = \Phi \left( A(t) \right) - \Phi \left( B(t) \right) > 0$ , we obtain:  $\forall t \in [0, T), \ \tilde{\alpha}(t) < K e^{-\left(r + \frac{\sigma^2}{2}\right)(T-t)} < \gamma(t).$ 

It remains to justify that  $t \to \gamma(t) \in \mathcal{C}^{\infty}([0,T))$ : this can be done using the implicit function theorem, exactly as we have done for point 1.

#### 1.5.5 Proof of Proposition 1.3.7

By Proposition 1.3.6,  $s \in \mathcal{V}(t) \to \Delta_t(s)$  is decreasing and takes its values in  $\mathcal{W}(t)$ , hence we can define  $\Delta_t^{-1}$  (the inverse function of  $\Delta_t(\cdot)$ ) and  $\Delta_t$  is a  $C^1$ - diffeomorphism from  $\mathcal{V}(t)$  to  $\mathcal{W}(t)$ . Keeping on with the notation  $p_t$  used in Lemma 1.3.5, the density  $\chi_t$  restricted to  $\mathcal{W}(t)$  is defined as:

$$\forall t \in [0,T), \ \forall y \in \mathcal{W}(t), \quad \chi_t(y) = \left. \frac{p_t(s)}{|\Delta'_t(s)|} \right|_{s = \Delta_t^{-1}(y)}$$

where for the sake of clarity we write  $d_1(t, s)$  instead of  $d_1(t, T, s, K)$  and (see (1.5.3) and (1.3.12))

$$\left|\Delta_{t}'(s)\right| = \frac{e^{-\frac{d_{1}(t,s)^{2}}{2}}}{s\sigma\sqrt{T-t}\sqrt{2\pi}}\left|H_{t}\left(d_{1}\left(t,s\right)\right)\right|.$$

Proposition 1.3.6 gives us all information about the sign and the variation of  $H_t(\cdot)$ . Combining the previous remark and the fact that  $s \to d_1(t,s)$  is increasing on  $(0,\infty)$ , we easily deduce that for  $t \in [0, \tilde{T}]$  the function  $s \to |H_t(d_1(t, s))|$  is increasing on  $(\tilde{\alpha}(t), \tilde{x}_0(t))$  and decreasing on  $(\tilde{x}_0(t), \tilde{\beta}(t))$  where  $\tilde{x}_0(t) := K e^{\sigma \sqrt{T-t}x_0(t) - \left(r + \frac{\sigma^2}{2}\right)(T-t)}$ . Consequently,  $\forall s \in \mathcal{V}(t)$ ,

$$|H_t(d_1(t,s))| \ge |H_t(d_1(t,\gamma(t)+\varepsilon(t)))| \wedge |H_t(d_1(t,\gamma(t)-\varepsilon(t)))| := C_1(t).$$

Observe that on  $[0, \tilde{T}]$ ,  $C_1(\cdot)$  is continuous and positive because of the choice of  $\varepsilon(t)$ .

Using that 
$$s \in (0,\infty) \to e^{-\frac{d_1(t,s)^2}{2}}$$
 is increasing on  $\left(0, Ke^{-(r+\frac{\sigma^2}{2})(T-t)}\right)$ , decreasing on  $\left(Ke^{-(r+\frac{\sigma^2}{2})(T-t)},\infty\right)$  and the inequality  $\frac{1}{s\sqrt{T-t}} \ge \frac{1}{\sqrt{T}(\gamma(t)+\varepsilon(t))}$  on  $\mathcal{V}(t)$ , we have:  
 $\forall s \in \mathcal{V}(t), \quad \frac{e^{-\frac{d_1(t,s)^2}{2}}}{\sqrt{T}(t)} \ge \frac{e^{-\frac{d_1(t,\gamma(t)+\varepsilon(t))^2}{2}} \wedge e^{-\frac{d_1(t,\gamma(t)-\varepsilon(t))^2}{2}}}{\sqrt{T}(t)} := C_2(t).$ 

$$\forall s \in \mathcal{V}(t), \quad \frac{e^{-\frac{d_1(t,s)}{2}}}{s\sigma\sqrt{T-t}\sqrt{2\pi}} \ge \frac{e^{-\frac{d_1(t,\gamma(t)+\varepsilon(t))}{2}} \wedge e^{-\frac{d_1(t,\gamma(t)-\varepsilon(t))}{2}}}{\sqrt{T}(\gamma(t)+\varepsilon(t))\sigma\sqrt{2\pi}} := C_2(t)$$

It is clear that  $C_2(\cdot)$  is also continuous and positive on  $[0, \tilde{T}]$ . Owing to Lemma 1.3.5, we finally obtain the following upper bound for  $\chi_t$ :

$$\forall y \in \mathcal{W}(t), \ \chi_t(y) \le \frac{e^{(\sigma^2 - r)t}}{S_0 \sigma \sqrt{2\pi} \sqrt{t}} \frac{1}{C_1(t)C_2(t)} := C(t).$$

Summing up, we have shown that the function  $C(\cdot)$  is bounded by  $\frac{1}{\sqrt{t}}$  up to a constant. Therefore,  $C(\cdot)$  is in  $L^1([0, \tilde{T}])$ , and this concludes the proof.

# CHAPTER 2

# DISCRETIZATION AND MULTILEVEL MONTE CARLO SIMULATION OF ROUGH FORWARD VARIANCES

**Note.** Working paper with Stefano De Marco.

Abstract. We focus on the pricing of VIX derivatives in rough forward variance models. The computation of such options requires both the discretization in time of an integral and a standard Monte Carlo simulation which leads to a computational complexity of  $\mathcal{O}(\varepsilon^{-4})$  for Lipschitz payoffs. We demonstrate that it can be reduced to  $\mathcal{O}(\ln(\varepsilon)^2 \varepsilon^{-2})$  using a Multilevel estimator. The exact asymptotic expansion for the  $L_2$  strong error associated with the right-point rectangle scheme is also provided along with some numerical experiments.

# 2.1 Introduction

For many problems in computational finance, as the distribution of the quantity of interest is unknown, closed-form expressions are unavailable and approximation methods may then be the only options available. One typical example of such problems is the pricing of derivatives regarding integrals over the maturity of the underlying asset. It requires both the discretization of an integral in time and a Monte Carlo method which often leads to deal with computationally expensive estimators. The most well-known example is Asian options pricing, which has attracted much attention for the last thirty years. As it is closed in spirit to our work, we recall its definition and main properties.

For a Black–Scholes asset,  $S_t = S_0 e^{(r - \frac{\sigma^2}{2})t + \sigma W_t}$  where  $S_0 > 0$  is the initial spot price, r > 0 the interest rate,  $\sigma > 0$  the volatility and  $W_t$  the standard Brownian motion, an Asian option with payoff  $\varphi$  is defined as

$$\mathbb{E}\left[\varphi\left(\frac{1}{T}\int_{0}^{T}S_{u}\mathrm{d}u\right)\right].$$
(2.1.1)

We emphasize again that the distribution of  $\frac{1}{T} \int_0^T S_u du$  is unknown, and thus closed-form expressions for (2.1.1) do not exist. Kemna and Vorst [124] were the first to investigate Monte Carlo methods for Asian options, and Lapeyre and Temam [130] provided a precise study of the associated rectangle and trapezoidal scheme for the discretization of the integral in (2.1.1). More

precisely, they showed that both the weak and  $L_2$  strong error were of order 1 for the rectangle and trapezoidal schemes. Consequently, for a positive error tolerance  $\varepsilon$ , if we wish the meansquare error MSE to satisfy the bound MSE  $\leq \varepsilon^2$ , the resulting computational complexity will be of order  $\mathcal{O}(\varepsilon^{-3})$ . Later, Ben Alaya and Kebaier [21] showed that using a multilevel scheme, the complexity can be reduced to  $\mathcal{O}(\varepsilon^{-2})$  and proposed a central limit theorem of Lindeberg–Feller type for the associated multilevel estimator. A different approach was proposed by Gobet and Miri [85] in which the authors derived a weak approximation for the mean process  $\frac{1}{T} \int_0^T S_u du$ (see Chapter 6).

In this work, we focus on the pricing of derivatives on the Chicago Board Options Exchange volatility index (VIX) in rough forward variance models. As opposed to Asian options, the VIX writes as an integral over the maturity of the instantaneous variance forward rather than over its time. Even though VIX and Asian options are different objects mathematically speaking, the methodology and theoretical study used for the pricing of VIX derivatives will be shown to be quite similar to that of Asian options.

This chapter is structured as follows. In Section 2.2, we analyze the right-point rectangle scheme associated with the VIX discretization focusing on the rough Bergomi model of Bayer, Friz, and Gatheral [18], and provide some numerical tests. In Section 2.3, we investigate a multilevel estimator and demonstrate that it can reduce the complexity to  $\mathcal{O}\left(\ln(\varepsilon)^2 \varepsilon^{-2}\right)$ .

# 2.2 Rough forward variance models

Let T and  $\Delta$  be positive real numbers. Recall that in the rough Bergomi model, the instantaneous log-forward variance solves the following stochastic differential equation:

$$X_T^{\alpha} - X_0^{\alpha} = -\frac{1}{2} \int_0^T K^{\alpha} (t)^2 + \int_0^T K^{\alpha} (t) \, \mathrm{d}W_t, \quad \alpha \ge T,$$

where for all  $t < \alpha$ ,  $K^{\alpha}(t) = \eta (\alpha - t)^{H - \frac{1}{2}}$  and  $H \in (0, 1)$ ,  $\eta > 0$ . In this work, we are concerned with the evaluation of options on the

$$\mathrm{VIX}_T^2 = \frac{1}{\Delta} \int_T^{T+\Delta} \xi_T^{\alpha} \mathrm{d}\alpha = \frac{1}{\Delta} \int_T^{T+\Delta} e^{X_T^{\alpha}} \mathrm{d}\alpha,$$

with payoff  $\varphi$ , that is quantity of the form

$$p = \mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T}^{2}\right)\right] = \mathbb{E}\left[\varphi\left(\frac{1}{\Delta}\int_{T}^{T+\Delta}e^{X_{T}^{\alpha}}\mathrm{d}\alpha\right)\right].$$

If  $\varphi(x) = (\sqrt{x} - \kappa)_+$  (resp.  $\varphi(x) = (\kappa - \sqrt{x})_+$ ), the quantity above refers to a call (resp. put) option with strike  $\kappa$  on the VIX<sub>T</sub>. We choose to divide the interval  $[T, T + \Delta]$  into  $n \in \mathbb{N}^*$  uniform time-steps i.e. we consider a discretization grid  $\mathcal{D}_n = \{t_0 = T + ih, i = 0, \ldots, n\}$  with uniform time-step  $h = \frac{\Delta}{n}$ . To approach the desired quantity, we consider the right-point rectangle scheme whose definition is given below.

**Definition 2.2.1** (Right-point rectangle scheme). The right-point rectangle scheme of order  $n \in \mathbb{N}^*$  for the VIX<sub>T</sub><sup>2</sup> is defined as:

$$\operatorname{VIX}_{T}^{2,\mathcal{R}_{n}} = \frac{1}{n} \sum_{i=1}^{n} e^{X_{T}^{t_{i}}}.$$
(2.2.1)

Observe that the sequence of random variables  $(X_T^{t_i})_{i=0,\dots,n}$  forms a Gaussian vector with mean  $\mu = (\mu(t_i))_{i=0,\dots,n}$  and covariance  $C = (C(t_i, t_j))_{0 \le i,j \le n}$  where for all  $0 \le i, j \le n$ ,

$$\mu(t_i) = \mathbb{E}\left[X_T^{t_i}\right] = X_0^{t_i} - \frac{1}{2} \int_0^T K^{t_i}(s)^2 \, \mathrm{d}s = X_0^{t_i} - \frac{\eta^2}{4H} \left(t_i^{2H} - (t_i - T)^{2H}\right), \qquad (2.2.2)$$

and

$$C(t_i, t_j) = \mathbb{C}\operatorname{ov}\left(X_T^{t_i}, X_T^{t_j}\right) = \int_0^T K^{t_i}(s) \, K^{t_j}(s) \, \mathrm{d}s = \eta^2 \int_0^T (t_i - s)^{H - \frac{1}{2}} (t_j - s)^{H - \frac{1}{2}} \, \mathrm{d}s.$$
(2.2.3)

If i = j, a direct computation gives

$$C(t_i, t_i) = \frac{\eta^2}{2H} \left( t_i^{2H} - (t_i - T)^{2H} \right),$$

while if i < j,

$$C(t_i, t_j) = \frac{\eta^2 (t_j - t_i)^{H - \frac{1}{2}}}{H + \frac{1}{2}} \Big[ t_i^{2H} {}_2F_1 \Big( \frac{1}{2} - H, \frac{1}{2} + H, \frac{3}{2} + H, -\frac{t_i}{t_j - t_i} \Big) - (t_i - T)^{2H} {}_2F_1 \Big( \frac{1}{2} - H, \frac{1}{2} + H, \frac{3}{2} + H, -\frac{t_i - T}{t_j - t_i} \Big) \Big],$$

where  ${}_{2}F_{1}(\cdot, \cdot, \cdot, \cdot)$  is the hypergeometric function (see e.g. Olver et al. [146]).

# 2.2.1 Strong convergence

**Theorem 2.2.1** ( $L_2$  strong error). Assume an initial flat instantaneous forward variance i.e.  $X_0^{\alpha} = X_0$  for all  $\alpha \in [T, T + \Delta]$ . As  $n \to \infty$ , it holds:

$$\left(\mathbb{E}\left[\left|\mathrm{VIX}_{T}^{2}-\mathrm{VIX}_{T}^{2,\mathcal{R}_{n}}\right|^{2}\right]\right)^{\frac{1}{2}} \sim \frac{\Lambda\left(X_{0},T,\Delta,H\right)}{n},\tag{2.2.4}$$

where

$$\Lambda\left(X_{0}, T, \Delta, H\right) = \frac{e^{X_{0}}}{2} \left(e^{\eta^{2} \frac{T^{2H}}{2H}} + e^{\eta^{2} \frac{(T+\Delta)^{2H} - \Delta^{2H}}{2H}} - 2e^{\eta^{2} \int_{0}^{T} t^{H-\frac{1}{2}} (\Delta+t)^{H-\frac{1}{2}} dt}\right)^{\frac{1}{2}}$$

Proof of Theorem 2.2.1. The squared  $L_2$  strong error rewrites as

$$\begin{split} \mathbb{E}\left[\left|\operatorname{VIX}_{T}^{2}-\operatorname{VIX}_{T}^{2,\mathcal{R}_{n}}\right|^{2}\right] &= \mathbb{E}\left[\left(\frac{1}{\Delta}\sum_{i=1}^{n}\int_{t_{i-1}}^{t_{i}}\left(e^{X_{T}^{\alpha}}-e^{X_{T}^{t_{i}}}\right)\mathrm{d}\alpha\right)^{2}\right] \\ &= \frac{1}{\Delta^{2}}\mathbb{E}\left[\sum_{i,j=1}^{n}\int_{t_{i-1}}^{t_{i}}\left(e^{X_{T}^{\alpha}}-e^{X_{T}^{t_{i}}}\right)\mathrm{d}\alpha\int_{t_{j-1}}^{t_{j}}\left(e^{X_{T}^{\beta}}-e^{X_{T}^{t_{j}}}\right)\mathrm{d}\beta\right] \\ &= \frac{h^{2}}{\Delta^{2}}\sum_{i,j=1}^{n}\int_{0}^{1}\int_{0}^{1}\mathbb{E}\left[\left(e^{X_{T}^{t_{i}-uh}}-e^{X_{T}^{t_{i}}}\right)\left(e^{X_{T}^{t_{j}-vh}}-e^{X_{T}^{t_{j}}}\right)\right]\mathrm{d}u\mathrm{d}v, \end{split}$$

where we have introduced the new variables  $u = \frac{t_i - \alpha}{h}$ ,  $v = \frac{t_j - \beta}{h}$ . Evoking the moment-generating function of the normal distribution, it holds for all  $a, b \in [T, T + \Delta]$ ,

$$\mathbb{E}\left[e^{X_T^a + X_T^b}\right] = e^{X_0^a + X_0^b} \mathbb{E}\left[e^{-\frac{1}{2}\int_0^T \left(K^a(t)^2 + K^b(t)^2\right) \mathrm{d}t + \int_0^T \left(K^a(t) + K^b(t)\right) \mathrm{d}W_t}\right]$$
$$= e^{X_0^a + X_0^b} e^{\int_0^T K^a(t) K^b(t) \mathrm{d}t}.$$

The expectation in the integrand then simplifies to

$$\mathbb{E}\left[\left(e^{X_T^{t_i-uh}}-e^{X_T^{t_i}}\right)\left(e^{X_T^{t_j-vh}}-e^{X_T^{t_j}}\right)\right]$$

$$= e^{X_0^{t_i - uh} + X_0^{t_j - vh}} e^{\int_0^T K^{t_i - uh}(t)K^{t_j - vh}(t)dt} - e^{X_0^{t_i - uh} + X_0^{t_j}} e^{\int_0^T K^{t_i - uh}(t)K^{t_j}(t)dt} - e^{X_0^{t_i} + X_0^{t_j}} e^{\int_0^T K^{t_i}(t)K^{t_j - vh}(t)dt} + e^{X_0^{t_i} + X_0^{t_j}} e^{\int_0^T K^{t_i}(t)K^{t_j}(t)dt}.$$

Using that for all  $\alpha$ ,  $X_0^{\alpha} = X_0$ , we then get that

$$\begin{split} \frac{n^2}{e^{2X_0}} \mathbb{E}\left[ \left| \mathrm{VIX}_T^2 - \mathrm{VIX}_T^{2,\mathcal{R}_n} \right|^2 \right] &= \sum_{i,j=1}^n \int_0^1 \int_0^1 \left( e^{\int_0^T K^{t_i - uh}(t)K^{t_j - vh}(t)\mathrm{d}t} - e^{\int_0^T K^{t_i - uh}(t)K^{t_j}(t)\mathrm{d}t} - e^{\int_0^T K^{t_i}(t)K^{t_j}(t)\mathrm{d}t} - e^{\int_0^T K^{t_i}(t)K^{t_j}(t)\mathrm{d}t} + e^{\int_0^T K^{t_i}(t)K^{t_j}(t)\mathrm{d}t} \right) \mathrm{d}u\mathrm{d}v. \\ &= \sum_{i,j=1}^n \Psi\left(ih, jh\right), \end{split}$$

where we have introduced the new variable s = T - t and set for every  $x, y \in [0, \Delta], s \in [0, T], u, v \in [0, 1],$ 

$$\Psi: (x,y) \in [0,\Delta]^2 \to \int_{u=0}^1 \int_{v=0}^1 \left( e^{\eta^2 \int_0^T (s+x-uh)^{H-\frac{1}{2}} (s+y-vh)^{H-\frac{1}{2}} \mathrm{d}s} - e^{\eta^2 \int_0^T (s+ih-uh)^{H-\frac{1}{2}} (s+jh)^{H-\frac{1}{2}} \mathrm{d}s} - e^{\eta^2 \int_0^T (s+ih)^{H-\frac{1}{2}} (s+jh)^{H-\frac{1}{2}} \mathrm{d}s} + e^{\eta^2 \int_0^T (s+ih)^{H-\frac{1}{2}} (s+jh)^{H-\frac{1}{2}} \mathrm{d}s} \right) \mathrm{d}u \mathrm{d}v.$$

Noticing that  $\Psi$  is continuous and as the double sum in the last equality is a Riemann sum, it holds that as  $n \to \infty$ ,

$$\frac{n^2}{e^{2X_0}} \mathbb{E}\left[ \left| \mathrm{VIX}_T^2 - \mathrm{VIX}_T^{2,\mathcal{R}_n} \right|^2 \right] \sim h^{-2} \int_{x=0}^{\Delta} \int_{y=0}^{\Delta} \Psi(x,y) \, \mathrm{d}x \mathrm{d}y \\ \sim h^{-2} \int_{x=0}^{\Delta} \int_{y=0}^{\Delta} \int_{u=0}^{1} \int_{v=0}^{1} \left( e^{\eta^2 \int_0^T (s+x-uh)^{H-\frac{1}{2}} (s+y-vh)^{H-\frac{1}{2}} \mathrm{d}s} - e^{\eta^2 \int_0^T (s+x-uh)^{H-\frac{1}{2}} (s+y)^{H-\frac{1}{2}} \mathrm{d}s} - e^{\eta^2 \int_0^T (s+x)^{H-\frac{1}{2}} (s+y)^{H-\frac{1}{2}} \mathrm{d}s} - e^{\eta^2 \int_0^T (s+x)^{H-\frac{1}{2}} \mathrm{d}s} + e^{\eta^2 \int_0^T (s+x)^{H-\frac{1}{2}} (s+y)^{H-\frac{1}{2}} \mathrm{d}s} \right) \mathrm{d}u \mathrm{d}v \mathrm{d}x \mathrm{d}y.$$

Omitting the dependence on x and y, the asymptotic expansion of the map

$$F_{u,v}: h \to e^{\eta^2 \int_0^T (s+x-uh)^{H-\frac{1}{2}} (s+y-vh)^{H-\frac{1}{2}} \mathrm{d}s},$$

up to  $h^2$  is

$$F_{u,v}(h) \sim F_{u,v}(0) + F'_{u,v}(0)h + F''_{u,v}(0)h^2,$$

where

$$F_{u,v}(0) = F(0) = e^{\eta^2 \int_0^T (s+x)^{H-\frac{1}{2}} (s+y)^{H-\frac{1}{2}} \mathrm{d}s},$$

and

$$\frac{F'_{u,v}(0)}{F(0)} = -\left(H - \frac{1}{2}\right)\eta^2 \int_0^T \left[v(s+x)^{H - \frac{1}{2}}(s+y)^{H - \frac{3}{2}} + u(s+x)^{H - \frac{3}{2}}(s+y)^{H - \frac{1}{2}}\right] \mathrm{d}s,$$

and

$$\begin{aligned} \frac{F_{u,v}^{''}\left(0\right)}{F\left(0\right)} &= \left(H - \frac{1}{2}\right) \left(H - \frac{3}{2}\right) \eta^2 \int_0^T \left[v^2 (s+x)^{H - \frac{1}{2}} (s+y)^{H - \frac{5}{2}} + u^2 (s+x)^{H - \frac{5}{2}} (s+y)^{H - \frac{1}{2}}\right] \mathrm{d}s \\ &+ \left(H - \frac{1}{2}\right)^2 \eta^2 uv \int_0^T (s+x)^{H - \frac{3}{2}} (s+y)^{H - \frac{3}{2}} \mathrm{d}s \end{aligned}$$

$$+\left(H-\frac{1}{2}\right)^{2}\eta^{4}\left(\int_{0}^{T}\left[v(s+x)^{H-\frac{1}{2}}(s+y)^{H-\frac{3}{2}}+u(s+x)^{H-\frac{3}{2}}(s+y)^{H-\frac{1}{2}}\right]\mathrm{d}s\right)^{2}.$$

Further, observe that the following identities for the first and second derivatives hold:

$$F'_{u,v}(0) - F'_{0,v}(0) - F'_{u,0}(0) = 0$$

and

$$\begin{split} F_{u,v}''(0) - F_{0,v}''(0) - F_{u,0}''(0) &= \left(H - \frac{1}{2}\right)^2 uv \left[\eta^2 \int_0^T (s+x)^{H - \frac{3}{2}} (s+y)^{H - \frac{3}{2}} \mathrm{d}s \\ &+ \eta^4 \int_0^T (s+x)^{H - \frac{1}{2}} (s+y)^{H - \frac{3}{2}} \mathrm{d}s \int_0^T (s+x)^{H - \frac{3}{2}} (s+y)^{H - \frac{1}{2}} \mathrm{d}s \right]. \end{split}$$

Consequently, using that  $\int_0^1 \int_0^1 uv du dv = \frac{1}{4}$  and setting  $g(x, y) = \eta^2 \int_0^T (s+x)^{H-\frac{1}{2}} (s+y)^{H-\frac{1}{2}} ds$ , the squared  $L_2$  strong error is asymptotic to:

$$\begin{split} \mathbb{E}\Big[\Big|\mathrm{VIX}_{T}^{2}-\mathrm{VIX}_{T}^{2,\mathcal{R}_{n}}\Big|^{2}\Big] & \underset{n \to \infty}{\sim} \frac{e^{2X_{0}}}{4n^{2}} \int_{0}^{\Delta} \int_{0}^{\Delta} e^{g(x,y)} \Big[\partial_{x}g\left(x,y\right)\partial_{y}g\left(x,y\right) + \partial_{x,y}g\left(x,y\right)\Big]\mathrm{d}x\mathrm{d}y \\ &= \frac{e^{2X_{0}}}{4n^{2}} \int_{0}^{\Delta} \int_{0}^{\Delta} \frac{\partial^{2}e^{g(x,y)}}{\partial x\partial y} \mathrm{d}x\mathrm{d}y \\ &= \frac{e^{2X_{0}}}{4n^{2}} \left[e^{g(\Delta,\Delta)} - 2e^{g(\Delta,0)} + e^{g(0,0)}\right] \\ &= \frac{e^{2X_{0}}}{4n^{2}} \left[e^{\frac{(T+\Delta)^{2H}-\Delta^{2H}}{2H}} - 2e^{\int_{0}^{T}t^{H-\frac{1}{2}}(t+\Delta)^{H-\frac{1}{2}}\mathrm{d}t} + e^{\frac{T^{2H}}{2H}}\right], \end{split}$$

and this concludes the proof.

Remark 6 (Weak error). As a direct consequence of Theorem 2.2.1 and Cauchy–Schwarz inequality, if the payoff function  $\varphi$  is Lipschitz, then the weak error is of order 1 that is:

$$\left| \mathbb{E} \left[ \varphi \left( \mathrm{VIX}_T^2 \right) - \varphi \left( \mathrm{VIX}_T^{2,\mathcal{R}_n} \right) \right] \right| = \mathcal{O} \left( n^{-1} \right).$$
(2.2.5)

#### 2.2.2Control variate

Observing that the VIX<sup>2</sup> is defined as a small-time integral over a family of lognormal random variables, we approximate  $\text{VIX}_T^{2,\mathcal{R}_n} = \frac{1}{n} \sum_{i=1}^n e^{X_T^{i_i}}$  with  $e^{\frac{1}{n} \sum_{i=1}^n X_T^i}$ . The key ingredient is that the control variate  $e^{\frac{1}{n} \sum_{i=1}^n X_T^i}$  is lognormal, that is  $\frac{1}{n} \sum_{i=1}^n X_T^i \stackrel{d}{=} \mathcal{N}\left(\mu_{\mathrm{P}}^n, (\sigma_{\mathrm{P}}^n)^2\right)$  with characteristics (see (2.2.2), (2.2.3)),

$$\mu_{\rm P}^n = \frac{1}{n} \sum_{i=1}^n \mu(t_i) = \frac{1}{n} \sum_{i=1}^n \left( X_0^{t_i} - \frac{1}{2} \int_0^T K^{t_i}(t)^2 \, \mathrm{d}t \right),$$
  
$$\sigma_{\rm P}^n = \sqrt{\frac{1}{n} \sum_{i,j=1}^n C(t_i, t_j)} = \sqrt{\int_0^T \left(\frac{1}{n} \sum_{i=1}^n K^{t_i}(t)\right)^2 \, \mathrm{d}t}.$$
(2.2.6)

Consequently, for M Monte Carlo samples, we estimate option prices on the VIX<sup>2</sup> with

$$\mathbb{E}\left[\varphi\left(\frac{1}{n}\sum_{i=1}^{n}e^{X_{T}^{t_{i}}}\right)\right] \approx \frac{1}{M}\sum_{m=1}^{M}\varphi\left(\frac{1}{n}\sum_{i=1}^{n}e^{X_{T}^{t_{i},m}} - e^{\frac{1}{n}\sum_{i=1}^{n}X_{T}^{t_{i},m}}\right) + CV_{n},$$

where  $\left(X_T^{t_1,m},\ldots,X_T^{t_n,m}\right)_{1\leq m\leq M}$  are independent copies of the Gaussian vector  $\left(X_T^{t_1},\ldots,X_T^{t_n}\right)$ and  $\operatorname{CV}_n = \mathbb{E}\left[\varphi\left(e^{\frac{1}{n}\sum_{i=1}^n X_T^i}\right)\right]$ . The control variate price  $\operatorname{CV}_n$  can be explicitly computed as

$$CV_n = \begin{cases} C_{BS} \left( e^{\frac{\mu_P^n}{2} + \frac{(\sigma_P^n)^2}{8}}, \kappa, \frac{\sigma_P^n}{2} \right) & \text{if } \varphi \left( x \right) = \left( \sqrt{x} - \kappa \right)_+, \\ P_{BS} \left( e^{\frac{\mu_P^n}{2} + \frac{(\sigma_P^n)^2}{8}}, \kappa, \frac{\sigma_P^n}{2} \right) & \text{if } \varphi \left( x \right) = \left( \kappa - \sqrt{x} \right)_+, \\ e^{\frac{\mu_P^n}{2} + \frac{(\sigma_P^n)^2}{8}} & \text{if } \varphi \left( x \right) = \sqrt{x}, \end{cases}$$

where for all x, y, z > 0,  $C_{\text{BS}}(\cdot, \cdot, \cdot)$ ,  $P_{\text{BS}}(\cdot, \cdot, \cdot)$  are the usual call and put prices, that is

$$C_{\rm BS}(x,y,z) = x\Phi\left(\frac{\ln\left(\frac{x}{y}\right)}{z} + \frac{z}{2}\right) - y\Phi\left(\frac{\ln\left(\frac{x}{y}\right)}{z} - \frac{z}{2}\right),$$
$$P_{\rm BS}(x,y,z) = y\Phi\left(-\frac{\ln\left(\frac{x}{y}\right)}{z} + \frac{z}{2}\right) - x\Phi\left(-\frac{\ln\left(\frac{x}{y}\right)}{z} - \frac{z}{2}\right)$$

### 2.2.3 Numerical tests

To check the asymptotic expansion given in (2.2.4) for the  $L_2$  strong error, we consider three sets of parameters for  $X_0, \eta, T, H$  (specified in the legend) and choose  $\Delta = \frac{1}{12}$ . Since we cannot simulate exactly the random variable  $\operatorname{VIX}_T^2$ , we have no choice but to approximate  $\operatorname{VIX}_T^2 \approx$  $\operatorname{VIX}_T^{2,\mathcal{R}_{n_{\mathrm{ref}}}}$  with a very high number of discretization points, and the strong error is replaced with  $\mathbb{E}\left[\left|\operatorname{VIX}_T^2 - \operatorname{VIX}_T^{2,\mathcal{R}_n}\right|^2\right]^{\frac{1}{2}} \approx \mathbb{E}\left[\left|\operatorname{VIX}_T^{2,\mathcal{R}_{n_{\mathrm{ref}}}} - \operatorname{VIX}_T^{2,\mathcal{R}_n}\right|^2\right]^{\frac{1}{2}}$ . We choose  $n_{\mathrm{ref}} = 2000$  discretization points and take  $M = 10^5$  Monte Carlo samples. Similarly, we want to check the order obtained for the weak error when dealing with call options (the payoff being Lipschitz in that case). We estimate the weak error for a call option with parameters  $X_0 = \ln(0.235^2)$ ,  $\eta = 0.5$ , H = 0.3,  $T = \frac{1}{4}$ ,  $\kappa = 0.1$ . The reference price 0.13093742 ± 5 × 10<sup>-8</sup> is estimated with 400 discretization points and  $3 \times 10^6$  Monte Carlo samples (using our control variate).



Figure 2.1 – Log-log plot for the  $L_2$  strong error of  $\text{VIX}_T^{2,\mathcal{R}_n}$  with marker "+" and its asymptotic expansion with marker " $\circ$ " (left) and weak error (right) of call option w.r.t. n.

Figure 2.1 confirms the theoretical asymptotic expansion for the  $L_2$  strong error advertised in Theorem 2.2.1 and the weak error of order 1 i.e. (slope of -1 in a log-log plot) for Lipschitz payoffs.

# 2.3 Multilevel Monte Carlo

### 2.3.1 Bias-variance decomposition

Let us now come back to our initial problem i.e. estimating the price of an option on the  $\operatorname{VIX}_T^2$  with payoff  $\varphi$ , namely  $p = \mathbb{E}\left[\varphi\left(\operatorname{VIX}_T^2\right)\right]$ . To price such an option, we saw that we first need to discretize the integral  $\operatorname{VIX}_T^2 = \frac{1}{\Delta} \int_T^{T+\Delta} e^{X_T^\alpha} d\alpha$  with some discretization scheme (the right-point rectangle scheme  $\operatorname{VIX}_T^{2,\mathcal{R}_n}$  as an example). We then approximate the expectation  $\mathbb{E}\left[\varphi\left(\operatorname{VIX}_T^{2,\mathcal{R}_n}\right)\right]$  with the crude Monte Carlo estimator:

$$\widehat{P}_{M,n} = \frac{1}{M} \sum_{m=1}^{M} \varphi \left( \text{VIX}_{T,m}^{2,\mathcal{R}_n} \right),$$

where  $\left(\operatorname{VIX}_{T,m}^{2,\mathcal{R}_n}\right)_{1 \leq m \leq M}$  are independent copies of  $\operatorname{VIX}_T^{2,\mathcal{R}_n}$  and M is the number of Monte Carlo samples. Such approximation leads to two kind of errors, namely a discretization error and a statistical error

$$\left| \mathbb{E} \left[ \varphi \left( \mathrm{VIX}_T^2 \right) - \varphi \left( \mathrm{VIX}_T^{2,\mathcal{R}_n} \right) \right] \right|, \quad \frac{1}{M} \sum_{m=1}^M \left( \varphi \left( \mathrm{VIX}_{T,m}^{2,\mathcal{R}_n} \right) - \mathbb{E} \left[ \mathrm{VIX}_T^{2,\mathcal{R}_n} \right] \right)$$

From the bias-variance decomposition, the mean-squared error can be decomposed as

$$MSE = \mathbb{E}\left[\left(\mathbb{E}\left[\varphi\left(VIX_{T}^{2}\right)\right] - \widehat{P}_{M,n}\right)^{2}\right]$$
$$= \mathbb{E}\left[\varphi\left(VIX_{T}^{2}\right) - \varphi\left(VIX_{T}^{2,\mathcal{R}_{n}}\right)\right]^{2} + \frac{\operatorname{Var}\left(\varphi\left(VIX_{T}^{2,\mathcal{R}_{n}}\right)\right)}{M}.$$

Suppose now that we want the mean-square error to satisfy MSE  $\leq \varepsilon^2$  for a given accuracy  $\varepsilon > 0$ . If  $\varphi$  is Lipschitz then from the weak error in Theorem 2.2.1, we observe that  $M = \mathcal{O}(\varepsilon^{-2})$ . From now on, we assume that we have computed beforehand any desired Cholesky decomposition for any desired discretization grid  $\mathcal{D}_n$ , so that sampling an *n*-dimensional Gaussian vector only requires  $\mathcal{O}(n^2)$  operations.

The total computational cost then requires the sampling of an *n*-dimensional Gaussian vector  $\mathcal{O}(n^2)$  together with the sum over its components  $\mathcal{O}(n)$ . Consequently, the overall computational cost for the crude Monte Carlo is given by:

$$\operatorname{Cost}_{\mathrm{MC}} = \left( \mathcal{O}\left(n^{2}\right) + \mathcal{O}\left(n\right) \right) \times M = \mathcal{O}\left(\varepsilon^{-4}\right).$$

We will now show how the total complexity can be reduced to  $\mathcal{O}\left(\ln(\varepsilon)^2 \varepsilon^{-2}\right)$  by use of a multilevel scheme.

### 2.3.2 Multilevel scheme

Let  $L \in \mathbb{N}^*$  denote the number of levels and let  $\mathbf{M} = (M_0, \ldots, M_L)$ ,  $\mathbf{n} = (n_0, \ldots, n_L) \in (\mathbb{N}^*)^{L+1}$ be multi-indexes representing respectively the decreasing number of samples used to approximate the expectation and the increasing number of time-steps used to approximate the integral. For the ease of notation, we set for all  $l = 0, \ldots, L$ ,

$$P_l = \varphi \left( \text{VIX}_T^{2,\mathcal{R}_{n_l}} \right) = \varphi \left( \frac{1}{n_l} \sum_{i=1}^{n_l} e^{X_T^{T+\Delta} \frac{i}{n_l}} \right).$$

From the telescopic sum

$$\mathbb{E}[P_L] = \mathbb{E}[P_0] + \sum_{l=1}^{L} \mathbb{E}[P_l - P_{l-1}],$$

the multilevel estimator is naturally defined as:

$$\widehat{P}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}} = \frac{1}{M_0} \sum_{m=1}^{M_0} P_0^{(0,m)} + \sum_{l=1}^L \frac{1}{M_l} \sum_{m=1}^{M_l} \left( P_l^{(l,m)} - P_{l-1}^{(l,m)} \right), \qquad (2.3.1)$$

where for every l, the random variables  $(P_l^{(l,m)})_{1 \le m \le M_l}$  and  $(P_{l-1}^{(l,m)})_{1 \le m \le M_l}$  are independent copies of  $P_l$  and  $P_{l-1}$  respectively. Note that for a fixed level l, the random variables  $P_l^{(l,m)}, P_{l-1}^{(l,m)}$  are constructed using the same Brownian paths. Observe that by independence,

$$\mathbb{E}\left[\widehat{P}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}}\right] = \mathbb{E}\left[P_{L}\right], \quad \operatorname{Var}\left(\widehat{P}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}}\right) = \sum_{l=0}^{L} \frac{V_{l}}{M_{l}}$$

where  $V_0 = \operatorname{Var}(P_0)$  and for all  $l = 1, \ldots, L$ ,

$$V_l = \operatorname{Var}\left(P_l - P_{l-1}\right)$$

Further, we denote the cost of one sample  $P_l - P_{l-1}$  by

$$C_l = \operatorname{Cost} \left( P_l - P_{l-1} \right), \quad 0 \le l \le L,$$

and for a given  $n_0 \in \mathbb{N}^*$ , we set the discretization parameters to

$$n_l = n_0 2^l, \qquad 0 \le l \le L.$$

Applying Giles [75, Theorem 1], we now prove that the multilevel estimator (2.3.1) achieves the constraint MSE  $\leq \varepsilon^2$  with complexity  $\mathcal{O}\left(\ln(\varepsilon)^2 \varepsilon^{-2}\right)$ .

**Theorem 2.3.1.** Suppose that the payoff function  $\varphi$  is Lipschitz, and consider an error tolerance  $\varepsilon > 0$ . Then, there exist  $M_0, L \in \mathbb{N}^*$  such that the multilevel estimator (2.3.1) has a mean-square error with bound MSE =  $\mathcal{O}(\varepsilon^2)$  and a computational complexity  $\mathcal{O}\left(\ln(\varepsilon)^2 \varepsilon^{-2}\right)$  with the choice:

$$n_l = n_0 2^l, \qquad M_l = M_0 2^{-2l}, \qquad 0 \le l \le L$$

Remark 7 (On the free parameters  $n_0, M_0, L$ ). Actually, let us set (see the proof below for more details) the level at  $L = \left[\frac{\ln(\sqrt{2}c_1\varepsilon^{-1})}{\ln(2)}\right]$ , the initial number of Monte Carlo samples at  $M_0 = \left[\frac{2}{\varepsilon^2}c_2(L+1)\right]$  where  $c_1 = L_{\varphi}\Lambda(X_0, T, \Delta, H) n_0^{-1}, c_2 = 10L_{\varphi}^2\Lambda(X_0, T, \Delta, H)^2 n_0^{-2}$  and  $L_{\varphi}$ is the Lipschitz constant of the payoff function. Then, the associated multilevel estimator has an  $MSE = \mathcal{O}(\varepsilon^2)$  with complexity  $\mathcal{O}\left(\ln(\varepsilon)^2\varepsilon^{-2}\right)$ . This is quite unusual in the multilevel literature as one usually only has the existence of such free parameters. Numerically, it means that one generally has to run a grid-search procedure to find the "approximate" optimal free parameters i.e. the ones that achieve the lowest MSE for a given computational cost. The fact that we know how to set exactly  $M_0$  and L is a direct consequence of Theorem 2.2.1 which provides an expansion for the  $L_2$  strong error.

Proof of Theorem 2.3.1. We follow the proof of Giles [75, Theorem 1] and borrow the mathematical notations. As for the crude Monte Carlo and because we assumed that any Cholesky decomposition has been computed beforehand, the computational cost  $C_l$  for each level l is of order  $\mathcal{O}(n_l^2)$ , and so we have  $\gamma = 2$ . For the variance, using that  $\varphi$  is Lipschitz (with Lipschitz constant  $L_{\varphi}$ ) along with the strong error (2.2.4), we have

$$\begin{split} V_{l} &\leq \mathbb{E}\left[\left(P_{l}-P_{l-1}\right)^{2}\right] \\ &= \mathbb{E}\left[\left(\varphi\left(\mathrm{VIX}_{T}^{2,\mathcal{R}_{l}}\right)-\varphi\left(\mathrm{VIX}_{T}^{2}\right)+\varphi\left(\mathrm{VIX}_{T}^{2}\right)-\varphi\left(\mathrm{VIX}_{T}^{2,\mathcal{R}_{l-1}}\right)\right)^{2}\right] \\ &\leq 2\mathrm{L}_{\varphi}^{2}\mathbb{E}\left[\left(\mathrm{VIX}_{T}^{2}-\mathrm{VIX}_{T}^{2,\mathcal{R}_{l}}\right)^{2}+\left(\mathrm{VIX}_{T}^{2}-\mathrm{VIX}_{T}^{2,\mathcal{R}_{l-1}}\right)^{2}\right] \\ &\leq 2\mathrm{L}_{\varphi}^{2}\Lambda\left(X_{0},T,\Delta,H\right)^{2}\left(n_{l}^{-2}+n_{l-1}^{-2}\right) \\ &=c_{2}2^{-\beta l}, \end{split}$$

where we have set  $c_2 = 10 L_{\varphi}^2 \Lambda (X_0, T, \Delta, H)^2 n_0^{-2}$  and  $\beta = 2$ . We then know that the optimal number of samples  $M_l$  on level l is of the form  $M_l = M_0 2^{-\frac{(\beta+\gamma)}{2}l} = M_0 2^{-2l}$ . The constant of proportionality  $M_0$  is fixed so that  $\operatorname{Var}\left(\widehat{P}_{M,n}^{\mathrm{ML}}\right) \leq \frac{\varepsilon^2}{2}$  i.e. as

$$\operatorname{Var}\left(\widehat{P}_{\boldsymbol{M},\boldsymbol{n}}^{\mathrm{ML}}\right) = \sum_{l=0}^{L} \frac{V_{l}}{M_{l}} \le \frac{c_{2}}{M_{0}} \sum_{l=0}^{L} 2^{-2l+2l} = \frac{c_{2}\left(L+1\right)}{M_{0}},$$

we choose  $M_0 = \left\lceil \frac{2}{\varepsilon^2} c_2 (L+1) \right\rceil$ . For the bias, a direct application of Cauchy–Schwarz inequality gives

$$\left|\mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T}^{2,\mathcal{R}_{l}}\right)-\varphi\left(\mathrm{VIX}_{T}^{2}\right)\right]\right|\leq\mathbb{E}\left[\left|\varphi\left(\mathrm{VIX}_{T}^{2,\mathcal{R}_{l}}\right)-\varphi\left(\mathrm{VIX}_{T}^{2}\right)\right|^{2}\right]^{\frac{1}{2}}\leq c_{1}2^{-\alpha l},$$

where we have set  $c_1 = L_{\varphi} \Lambda(X_0, T, \Delta, H) n_0^{-1}$  and  $\alpha = 1$ . It follows that

$$\left| \mathbb{E} \left[ \varphi \left( \mathrm{VIX}_T^{2, \mathcal{R}_L} \right) - \varphi \left( \mathrm{VIX}_T^2 \right) \right] \right| \le c_1 2^{-L},$$

and as we wish the squared bias to be smaller than  $\frac{\varepsilon^2}{2}$  i.e.

$$c_1^2 2^{-2L} \le \frac{\varepsilon^2}{2} \iff L \ge \frac{\ln\left(\sqrt{2}c_1\varepsilon^{-1}\right)}{\ln\left(2\right)},$$

we choose this time  $L = \left\lceil \frac{\ln(\sqrt{2}c_1\varepsilon^{-1})}{\ln(2)} \right\rceil$ . Finally, evoking Giles [75, Theorem 1] and observing that  $\alpha \ge \frac{1}{2} \min(\gamma, \beta)$  and  $\gamma = \beta$ , we infer that the complexity for the multilevel estimator (2.3.1) is of order  $\mathcal{O}\left(\ln(\varepsilon)^2\varepsilon^{-2}\right)$ .

#### 2.3.3 Numerical test

As the costs of the crude and multilevel Monte Carlo estimators are respectively given by  $\operatorname{Cost}_{\mathrm{MC}} = \mathcal{O}\left(\varepsilon^{-4}\right)$ ,  $\operatorname{Cost}_{\mathrm{ML}} = \mathcal{O}\left(\ln\left(\varepsilon\right)^{2}\varepsilon^{-2}\right)$  and  $\mathrm{MSE} = \mathcal{O}\left(\varepsilon^{2}\right)$ , we infer that  $\ln\left(\mathrm{MSE}\right) \approx -\frac{1}{2}\ln\left(\operatorname{Cost}_{\mathrm{MC}}\right) + \operatorname{Cst}$  and  $\ln\left(\mathrm{MSE}\right) \approx -\ln\left(\operatorname{Cost}_{\mathrm{ML}}\right) + \operatorname{Cst}$  up to some logarithmic terms. To check the theoretical slope of  $-\frac{1}{2}$  (resp. -1) for the crude (resp. multilevel) Monte Carlo, we price a call option on the VIX with parameters T = 0.5,  $\Delta = \frac{1}{12}$ , H = 0.1,  $\eta = 0.5$ ,  $X_{0} = \ln\left(0.235^{2}\right)$ ,  $\kappa = 0.1$ . The reference price is set at  $0.121971 \pm 6 \times 10^{-7}$  (computed by a crude Monte Carlo simulation with  $1 \times 10^{7}$  samples and a rectangle discretization with 500 discretization points).

For a grid of 10 evenly-spaced  $\varepsilon \in [0.075, 0.094]$ , we choose  $M = \lceil \varepsilon^{-2} \rceil$  and  $n = \lceil \varepsilon^{-1} \rceil$ for the crude Monte Carlo. For the multilevel estimator, we take a grid of 10 evenly-spaced  $\varepsilon \in [0.011, 0.018]$ , we set  $n_0 = 6$  and choose  $L = \left\lceil \frac{\ln(\sqrt{2}c_1\varepsilon^{-1})}{\ln(2)} \right\rceil$  and  $M_0 = \left\lceil \frac{2}{\varepsilon^2}c_2(L+1) \right\rceil$ (see Remark 7) where  $L_{\varphi} = \frac{1}{2\kappa}$  (call option i.e.  $\varphi'(x) = \frac{1}{2\sqrt{x}}\mathbf{1}_{\sqrt{x}\geq\kappa} \leq \frac{1}{2\kappa}$ ) and we recall that  $c_1 = L_{\varphi}\Lambda(X_0, T, \Delta, H) n_0^{-1}, c_2 = 10L_{\varphi}^2\Lambda(X_0, T, \Delta, H)^2 n_0^{-2}$ . We estimate the mean-squared error MSE for both methods with  $\frac{1}{N_{\text{MSE}}}\sum_{j=1}^{N_{\text{MSE}}} (\hat{p}_j - p)$ , where  $(\hat{p}_j)_{1\leq n_{\text{MSE}}}$  are  $N_{\text{MSE}} = 400$  independent copies of either the multilevel or crude Monte Carlo estimator, along with its associated 95%confidence interval. The cost of both methods are computed with the identities  $\text{Cost}_{\text{MC}} = n^2 M$ and  $\text{Cost}_{\text{ML}} = \sum_{l=0}^{L} n_l^2 M_l = n_0^2 M_0 (L+1)$ .



Figure  $2.2 - \ln (MSE)$  w.r.t.  $\ln (Cost)$  for the Monte Carlo and multilevel estimators.

As expected, in Figure 2.2 we approximately retrieve the theoretical slopes of order  $-\frac{1}{2}$  and -1 for both the crude and multilevel Monte Carlo estimators, and observe that for a given cost, the estimated MSE is significantly smaller for the multilevel estimator than that of the crude estimator.

# 2.4 Conclusion

In this work, we have built a Multilevel Monte Carlo estimator for the evaluation of VIX options in rough forward variance models. With a complexity of  $\mathcal{O}\left(\ln(\varepsilon)^2 \varepsilon^{-2}\right)$ , we have shown that such an estimator significantly reduces the computational time required compared to that of a standard Monte Carlo with complexity  $\mathcal{O}\left(\varepsilon^{-4}\right)$ . To further our research, we intend to study other discretization schemes (e.g. trapezoidal scheme) and provide the associated strong error expansion. We will also explore other Multilevel estimators which hopefully achieve the optimal complexity of order  $\mathcal{O}\left(\varepsilon^{-2}\right)$ .

# Part II

# Meta-modeling and Polynomial Chaos Expansion

# CHAPTER 3

# META-MODEL OF A LARGE CREDIT RISK PORTFOLIO IN THE GAUSSIAN COPULA MODEL

Note. The results of this chapter are based on [34].

Abstract. We design a meta-model for the loss distribution  $\mathcal{L}$  of a large credit risk portfolio in the Gaussian copula model. Our procedure is twofold. We first apply the Wiener chaos decomposition on the normal systemic economic factor, and derive a truncated loss  $\mathcal{L}_I$  at some order I. Then, we provide a Gaussian approximation  $\mathcal{L}_I^G$  of the associated truncated loss. Such an approach is motivated by the fact that we are dealing with large portfolios. Our procedure significantly reduces the computational time needed for sampling the loss, and therefore for estimating risk measures. The accuracy and effectiveness of our method are confirmed by numerical examples.

# 3.1 Introduction

This paper is concerned with credit risk losses arising in large portfolios of loans, bonds, and other instruments. Credit risk refers to the risk of incurring losses due to unexpected changes in the credit quality of a counterparty. Effective measurement of such risk is a great deal of importance for financial institutions. In this work, we examine credit risk portfolio losses of the form

$$\mathcal{L} := \sum_{k=1}^{K} l_k Y_k. \tag{3.1.1}$$

The number K (assumed fixed) denotes the large number (commonly  $K \geq 10^5$ ) of obligors considered. The default indicators  $Y_1, \ldots, Y_K$  describe the default  $Y_k = 1$  or not  $Y_k = 0$  of the kth obligor, and  $l_k$  refers to its related deterministic Loss Given Default (LGD). Estimating tail probabilities  $\mathbb{P}(\mathcal{L} > x)$  for such losses, especially at large values of x, or more generally expectations of functionals of the loss,  $\mathbb{E}[f(\mathcal{L})]$ , is essential to credit risk measures such as VaR, CVaR, etc (see Artzner et al. [10], Cherubini, Luciano, and Vecchiato [46], McNeil, Frey, and Embrechts [140], Bielecki and Rutkowski [31] for extensive references on risk measures and credit risk). To estimate the aforementioned risk measures, Monte Carlo methods are undoubtedly among the most widely used computational tools available. However, as credit risk deals with tail events and because we deal with large portfolios, any Monte Carlo simulation scheme is often quite time-consuming. Indeed, generating a single sample of  $\mathcal{L}$  requires to compute all the terms of the sum (3.1.1). For instance, suppose we want to estimate  $\mathbb{E}[f(\mathcal{L})]$ , for some function f, using a Monte Carlo method. Then, in order to reach an error tolerance of  $\varepsilon > 0$  for the root mean squared error, we would need to sample  $N = \mathcal{O}(\varepsilon^{-2})$  times the Loss  $\mathcal{L}$ . Each simulation of  $\mathcal{L}$  requires to generate  $(Y_1, \ldots, Y_K)$  and apply the sum (3.1.1). Consequently, if the simulation cost of one  $Y_k$  is taken to be one unit basis, the global simulation cost (to reach an accuracy of  $\varepsilon$ ) is  $\mathcal{O}(K\varepsilon^{-2})$ . For instance, if the number of obligors is quite large (say a million), and the error tolerance is one percent, this would lead to a cost of ten billion unit operations. Needless to say that the more accurate the estimation (i.e. smaller  $\varepsilon$ ), the higher the number of samples N. Quite imprecise estimations of the expectation of interest could then be the only option available under a given computational time constraint.

**Our contributions.** The main contribution of the paper is to provide a new meta-model for sampling the loss. Based on the Wiener chaos decomposition, it will be shown – see our numerical experiments reported in Subsection 3.3.2 – to be approximately 17 times faster than a standard Monte Carlo approach. A meta-model is an approximation of the true model and has the advantage of being much faster to evaluate. It is then more suitable for massive Monte Carlo simulations and asymptotic statistical error analysis. As it will be explained, the order of approximation for  $\mathcal{L}$  can be tuned as the user wants, so that we obtain a full range of meta-models from exact to rough, with decreasing accuracy but increasing speed-up.

About copula modeling. A key feature of any credit risk portfolio is a mechanism for capturing dependence between obligors. Here, we choose to derive our metal-model in the Gaussian copula model for the default indicators  $Y_1, \ldots, Y_K$ . Copula modeling is a major area of interest for risk management. Its ability to capture – in a flexible way – interdependence between financial variables makes it an attractive tool. The first work related to dependence modeling probably dates back to Fréchet's work [68]. In his seminal work, Fréchet studied the following problem: given the cumulative distribution functions  $F_1, F_2$  of two random variables  $X_1, X_2$  on some probability space, what can be said about the set  $\Gamma(F_1, F_2)$  of the bivariate distribution function whose marginals are respectively  $F_1$  and  $F_2$ ? But it was Sklar who introduced the name *copula*, formalized the concept, and proved the theorem that now bears his name [156, 155]. A vast literature has emerged since those seminal works (some classical references are for instance Joe [116], Nelsen [142]).

In the late 90s, the probabilistic modeling of dependencies emerged in credit risk management. Owing to methodologies like J.P. Morgan's CreditMetrics [94], the KMV model (see Vasicek [163] available in [164]), or Credit Suisse Creditrisk+ [33], the goal was to take into account risk dependencies within portfolios. A comparative analysis of these methodologies is proposed in Gordy [87]. In the context of risk management, the terminology *Gaussian copula* first appeared in Li's work [135] who related risk dependencies to Sklar's approach. For standard references on the application of copulas in risk management, the reader may refer to [46] or [140]. According to the recent report [15] from the Bank of International Settlements about Risk-Weighted Assets, "among various modeling choices, the normal copula is often chosen for its simplicity (for example within the regulatory IRB framework)". For detailed approaches about Internal ratings-based (IRB) see e.g. Wilde [167], Rutkowski and Tarca [152], and references therein.

In Gaussian copula models, every default depends on some common variables Z which model systemic risk factors and act as macro-economic variables. They are modeled as standard normal random variables, and conditionally on Z defaults are independent. In particular, the Loss is expressed as a sum of dependent defaults which are triggered as soon as some Gaussian variable (which is correlated to the other standard Gaussian default variables) is above a given threshold. See also Andersen, Sidenius, and Basu [8] where such a copula model is used for the CDO do not claim that such a Gaussian copula mode

(Collateralised Debt Obligation) pricing. We do not claim that such a Gaussian copula model is the best for practical use. As any risk model, it may not be used uncritically and the impact of such modeling choice must be analyzed in the context where it is used. We refer to Section 3.2 for a precise description of the one-factor Gaussian copula model (corresponding to a univariate Z). The multi-factor extension of our model is discussed in Subsection 3.3.3.

In the one-factor Gaussian copula model, the meta-model  $\mathcal{L}_{I}^{G}$  proposed for  $\mathcal{L}$  takes the following form (see Theorem 3.3):

$$\mathcal{L}(\omega) \approx \mathcal{L}_{I}^{\mathrm{G}}(\omega) := \sum_{i=0}^{I} \varepsilon_{K,i}(\omega) \operatorname{He}_{i}(Z(\omega)), \qquad (3.1.2)$$

where

- $(\text{He}_i(\cdot): i \ge 0)$  is the family of probabilists' Hermite polynomials.
- *I* is a truncation parameter tuning the accuracy of the meta-model.
- the (random) coefficients  $\varepsilon_{K,i}$  form a normal vector with explicit characteristics (depending on the LGD and other default parameters), and independent of Z. The significant gain is that these characteristics can be computed offline. Sampling from the meta-model thus reduces to only sample from an *I*-dimensional normal vector together with the systemic risk factor Z. Instead of sampling from K terms, we essentially sample from I terms with  $I \ll K$ .

The meta-model (3.1.2) writes as a (truncated) Wiener chaos decomposition of  $\mathcal{L}$  in the Z variable.

Background mathematical results. In the early 2000s, many works focused on the numerical approximation of CDO pricing (before the 2007-crisis, these products were very popular). It requires the computation of the tranche function  $\mathbb{E}\left[(\mathcal{L}-x)_{+}\right]$ , for many attachment levels x, and for some loss  $\mathcal{L}$  of the form (3.1.1). The usual methodology was to derive explicit approximations for conditional quantities  $\mathbb{E}\left[(\mathcal{L}-x)_+ \mid Z\right]$ , and then integrate over  $Z^{-1}$ . The problem is simpler since the conditional loss writes as a sum of independent random variables. For instance, Vasicek [163] proposed a Gaussian approximation using the central limit theorem principle. In El Karoui, Jiao, and Kurtz [61], the authors significantly improved the zeroth-order Gaussian approximation by identifying some correction terms thanks to Stein method. Together with Gaussian approximations for some specific parameter regime, they also provided Poisson approximations. Still taking advantage of the independence of the random variables, some works promoted explicit characteristic functions for some conditional losses. Applying saddle-point techniques, they derived approximations for the tranche function, see e.g. Yang, Hurd, and Zhang [169]. In Dembo, Deuschel, and Duffie [54], the authors employed large deviation estimation techniques for the tail distribution of  $\mathcal{L}$ . Here again, the strategy is to solve first the conditional problem with respect to (w.r.t.) Z, and then perform the integration. As opposed to our setting where Z has a continuous distribution, the authors supposed that Z takes only a finite number of values, which makes the integration straightforward. All these references (and others therein) provide approximations for the conditional loss using a probability distribution with parameters  $\theta$  depending on Z. For a large portfolio  $(K \to +\infty)$ , this may be computationally very intensive. Indeed, for any sampled risk factor Z (usually many for computing the outer non-conditional expectation), the parameters  $\theta(Z)$  have to be re-evaluated each time, using the recomputations of all the K terms in (3.1.1) conditionally on Z.

Taking advantage of the conditional independence, granularity adjustments (GA) methods have been proposed as an alternative for approximating risk measures such as the VaR. GA

<sup>&</sup>lt;sup>1</sup>which is standard using Monte Carlo method or any numerical integration method

techniques rely on an asymptotic expansion of a large portfolio loss  $\mathcal{L}$  using its conditional loss  $\mathbb{E}[\mathcal{L}|Z]$  as a proxy. The asymptotic is understood in the limit of perfectly fine-grained (a.k.a. infinitely granular) portfolio. The granularity of a portfolio can be measured owing to its Herfindahl-Hirschman Index (first introduced by Hirschman [109, Chap. 7] to measure the concentration of the market)

$$\operatorname{HHI}_{K} := \frac{\sum_{k=1}^{K} l_{k}^{2}}{(\sum_{k=1}^{K} l_{k})^{2}}.$$
(3.1.3)

Asymptotically infinitely granular portfolio corresponds to  $\lim_{K\to+\infty} \operatorname{HHI}_K = 0$ . For an overview of granularity measure, see Lütkebohmert [136, Chapter 8]. In infinitely granular portfolios, any idiosyncratic risk is eliminated through diversification (as a consequence of the Law of Large Numbers), and the loss depends only on the systemic risk Z i.e.  $\mathcal{L} = \mathbb{E}[\mathcal{L} \mid Z]$ . As a consequence, computing the VaR is dramatically simplified as the  $\alpha$  quantile of  $\mathcal{L}$  is replaced by that of  $\mathbb{E}[\mathcal{L}|Z]$ . To account for non-perfect fine-granularity, some granularity adjustments can be computed. GA techniques rely on the seminal studies concerning Credit modeling and sensitivity analysis for VaR proposed respectively in Gordy [87] and Gouriéroux, Laurent, and Scaillet [91] before the GA approach was formalized in Gordy [88]. The GA method for VaR relies on the following parametrization between the loss  $\mathcal{L}$  and its infinitely granular approximation  $\mathbb{E}[\mathcal{L}|Z]$ :  $\mathcal{L}(\varepsilon) = \mathbb{E}[\mathcal{L} \mid Z] + \varepsilon(\mathcal{L} - \mathbb{E}[\mathcal{L} \mid Z]), \ \varepsilon \in [0,1]$  (noticing that  $\mathcal{L}(1) = \mathcal{L}$  and  $\mathcal{L}(0) = \mathbb{E}[\mathcal{L} \mid Z]$ ). Invoking Taylor's formula, the VaR<sub> $\alpha$ </sub> (at a fixed level  $\alpha \in [0,1]$ ) is then approximated by:

$$\operatorname{VaR}_{\alpha}(\mathcal{L}) \approx \operatorname{VaR}_{\alpha}(\mathbb{E}\left[\mathcal{L}|Z\right]) + \frac{\partial \operatorname{VaR}_{\alpha}(\mathcal{L}(\varepsilon))}{\partial \varepsilon}\Big|_{\varepsilon=0} + \frac{1}{2} \frac{\partial^{2} \operatorname{VaR}_{\alpha}(\mathcal{L}(\varepsilon))}{\partial \varepsilon^{2}}\Big|_{\varepsilon=0}.$$

It is shown by Gouriéroux, Laurent, and Scaillet [91, Lemma 1] that  $\frac{\partial \operatorname{VaR}_{\alpha}(\mathcal{L}(\varepsilon))}{\partial \varepsilon}\Big|_{\varepsilon=0} = 0$ , so that the granularity adjustment terms come from the second-order derivative w.r.t.  $\varepsilon$ . A rigorous study of GA formula and remaining terms is provided in Fermanian [64] by the use of Fourier techniques. After the Basel II proposals, many authors (evoking GA techniques) derived closedform approximations for the VaR. Examples are Wilde [167] for the CreditRisk+ model [33] and Emmer and Tasche [62], Gordy and Lütkebohmert [90] for CreditMetrics. We refer to Lütkebohmert [136] for an overview of the subject. Following Fermanian [64], GA techniques are particularly effective when the systemic risk factor Z is one-dimensional and all the defaults are positively correlated to it. As a difference, these two assumptions are not necessary in our approach. However, our approximation also relies indirectly on the assumption of an infinitely granular portfolio. We refer to Section 3.3.2 for a more specific discussion and comparison between GA and the proposed approach.

Our approach (based on the Wiener chaos decomposition) is different since we are able to factorize the dependence w.r.t. Z from the other variables (see Theorem 3.3), and thus greatly reduce the computational time. We derive an approximation directly on the  $\mathcal{L}$ , independently of the threshold x appearing in the tranche function  $\mathbb{E}[(\mathcal{L} - x)_+]$  or in the survival function  $\mathbb{P}(\mathcal{L} > x)$  or in the expectation  $\mathbb{E}[f(\mathcal{L})]$  for a test function f. We aim at approximating the loss distribution rather than its statistics (through test functions). Our method is closer to a simulation-based experience that a risk manager could wish to have, with visualization of loss histograms or Q-Q plots.

Another family of numerical methods to sample from  $\mathcal{L}$ , and efficiently compute their statistics is the Monte Carlo method with importance sampling (IS). This is quite efficient, especially for extreme loss thresholds x. An important reference is Glasserman and Li [82] where the authors apply IS conditionally on Z (the common factors affecting obligors), and IS to the factors themselves. The tuning of this approach depends on x, and the computational time suffers also from the large number of obligors  $(K \to +\infty)$ . Our work takes a different route as we wish to approximate the full distribution of  $\mathcal{L}$ , especially as  $K \to +\infty$ . Regarding the financial community, Polynomial Chaos Expansion (PCE) has been recently used (for two different problems) in [133] and [20]. Lelong [133] uses PCE for pricing Bermudan options by directly solving the dual minimization problem of Rogers [151] and approximating the set of uniformly square integrable martingales by a finite dimensional Wiener chaos expansion. In Belomestny et al. [20], the authors use PCE to construct control variates for stochastic differential equation simulation using a Wiener-chaos type decomposition as well. Yet, we are not aware of any of its use for assessing portfolio credit risk. For a recent account on meta-modeling with PCE and Gaussian processes, see Le Gratiet, Marelli, and Sudret [131]. In our case where polynomials are of Hermite type, we prefer to use the terminology Wiener chaos decomposition than PCE, in reference to the seminal work of Wiener [166].

**Organization of the paper.** In Section 3.2, we briefly recall the Gaussian copula model of Li [135], state known properties on probabilists' Hermite polynomials and the Wiener chaos decomposition. Then, we compute the chaos decomposition of the indicator function  $\mathbf{1}_{c\leq Z}$  where Z is standard normal and c a constant, and apply this to obtain a stochastic chaos decomposition of order I (denoted  $\mathcal{L}_I$ ) for the portfolio loss  $\mathcal{L}$ . We then show how the coefficients of this decomposition can be well approximated by suitable multidimensional normal distributions. We provide also the  $L_2$  error and a central limit theorem for the approximation  $\mathcal{L}_I$ . Technicalities are postponed to Section 3.5. In Section 3.3, we give explicit expressions to compute the characteristics of the normal vector needed for the approximation, and test our approach on different portfolio scenarios. We summarize our main contributions and conclude in Section 3.4.

#### Notations.

- $\mathbb{N} = \{0, 1, \dots, \}$  for the non-negative integers.
- Let  $n \in \mathbb{N}^*$ ,  $x \in \mathbb{R}^n$ ,  $\Sigma \in \mathbb{R}^{n \times n}$  positive definite and  $X \stackrel{d}{=} \mathcal{N}(0, \Sigma)$ , set

$$\Phi_{\Sigma}(x) := \mathbb{P}(X \le x) = \int_{-\infty}^{x_1} \dots \int_{-\infty}^{x_n} \frac{e^{-\frac{1}{2}t^{\top}\Sigma^{-1}t}}{(2\pi)^{\frac{n}{2}} (\det(\Sigma))^{\frac{1}{2}}} dt_1 \dots dt_n.$$

In the case n = 1 and  $\Sigma = 1$ , we simply write  $\Phi$  for  $\Phi_{\Sigma}$ .

• For  $n, m \in \mathbb{N}$ ,  $\delta_{nm}$  denotes the Kronecker delta i.e.  $\delta_{nm} = 1$  if n = m and 0 otherwise.

# 3.2 Gaussian copula model, Wiener chaos decomposition and main results on meta-models

# 3.2.1 Gaussian copula model for the portfolio credit risk problem

We are concerned with the one-year loss of a large portfolio composed of K obligors, each having a deterministic LGD  $l_k \geq 0$ . The marginal default probability of the kth obligor is denoted by  $p_k$ . It is assumed to be known either from credit ratings, market prices, corporate bonds or credit default swaps. In this framework, the one-year total loss from defaults (without any provision) is defined as:

$$\mathcal{L} := \sum_{k=1}^{K} l_k Y_k, \tag{3.2.1}$$

where  $Y_k$  represents the default indicator for the kth obligor at one-year i.e.  $Y_k = 1$  if the kth obligor defaults or 0 otherwise. We assume that the defaults obey to the Gaussian copula model, namely

$$Y_k = \mathbf{1}_{X_k \ge c_k} \tag{3.2.2}$$

with stochastic factors  $X_k$  and thresholds  $c_k$  (referred to as a default boundary), and the dependence among obligors is achieved through a multivariate normal vector  $(X_1, \ldots, X_K)$  with standardized entries  $(X_k \stackrel{d}{=} \mathcal{N}(0, 1))$ .

We choose to first focus our analysis on a one-dimensional factor model where  $X_k$  takes the form:

$$X_k = \rho_k Z + \sqrt{1 - \rho_k^2} \varepsilon_k.$$

The random variable  $Z \stackrel{d}{=} \mathcal{N}(0,1)$  is a systemic risk factor,  $\varepsilon_k \stackrel{d}{=} \mathcal{N}(0,1)$  is an idiosyncratic risk associated with the *k*th obligor (independent of *Z*), and  $\rho_k \in (-1,1)$  a correlation parameter. The  $(\varepsilon_k)_{1 \leq k \leq K}$  are independent and independent of *Z*. The extension to a multi-factor model is presented in Section 3.3.3.

We assume from now on that  $\rho_k \neq 0$ . Indeed, from an economic point of view, there always exists a dependency between the default of an obligor and the systemic risk factor. From a mathematical point of view, the set of random variables  $Y_k$  associated to  $\rho_k = 0$  forms an independent sequence, and independent of the other  $Y_k$ . Their marginal distributions are just Bernoulli distributions, and thus can be easily treated separately from the dependent  $Y_k$ .

The default boundary  $c_k := \Phi^{-1}(1 - p_k) = -\Phi^{-1}(p_k)$  is set so that it matches the constraint  $p_k = \mathbb{P}(Y_k = 1)$ , and we have that

$$\mathbb{P}(Y_k = 1) = \mathbb{P}(X_k \ge c_k) = \Phi(-c_k) = p_k.$$

Then, the default event writes (remembering that we exclude the case  $\rho_k = 0$ ):

$$\{X_k \ge c_k\} = \left\{a_k \varepsilon_k + b_k \le \frac{\rho_k}{|\rho_k|} Z\right\}, \quad \text{where} a_k = \frac{-\sqrt{1 - \rho_k^2}}{|\rho_k|}, \ b_k = \frac{-\Phi^{-1}(p_k)}{|\rho_k|}.$$
(3.2.3)

Here, we emphasize that both random variables are normally distributed:

$$\frac{\rho_{k}}{\left|\rho_{k}\right|}Z \stackrel{d}{=} \mathcal{N}\left(0,1\right), \qquad a_{k}\varepsilon_{k} + b_{k} \stackrel{d}{=} \mathcal{N}\left(b_{k},a_{k}^{2}\right).$$

#### 3.2.2 Wiener chaos decomposition of the indicator function

We first recall some well-known results on the probabilists' Hermite polynomials of degree  $i \in \mathbb{N}$ . See Szegő [157, Chapter V] and Funaro [70] for extensive references on orthogonal polynomials. For (3.2.4)-(3.2.5)-(3.2.7)-(3.2.13), we refer to Le Maître and Knio [132, Section B.1.2]. For (3.2.11) and (3.2.12), see Nualart [145, Chapter 1] and Bailey [14] respectively. Equalities (3.2.6) and (3.2.9) readily follow from (3.2.7). Equality (3.2.8) is derived from the exact Taylor expansion w.r.t. x at point y, combined with  $\operatorname{He}_{i}^{(m)}(y) = \frac{i!}{(i-m)!}\operatorname{He}_{m}(y)$  ( $0 \leq m \leq i$ ) which follows from (3.2.11). Equality (3.2.10) is a direct consequence of (3.2.5) and (3.2.11). The exponential generating function (3.2.14) is obtained from the series expansion of  $e^{xw-\frac{w^2}{2}} = \sum_{i\geq 0} \frac{c_i}{i!}w^i$  with  $c_i = \frac{\partial^i}{\partial w^i} \left( e^{xw-\frac{w^2}{2}} \right) \bigg|_{w=0} = \operatorname{He}_i(x)$ .

**Proposition 3.2.1.** For every  $i \in \mathbb{N}$ , the following properties hold for the probabilists' Hermite polynomials:

$$\operatorname{He}_{i}(x) = (-1)^{i} e^{\frac{x^{2}}{2}} \frac{\mathrm{d}^{i}}{\mathrm{d}x^{i}} \left(e^{-\frac{x^{2}}{2}}\right), \qquad (3.2.4)$$

$$\operatorname{He}_{0}(x) = 1, \quad \operatorname{He}_{1}(x) = x, \quad \operatorname{He}_{i+2}(x) = x \operatorname{He}_{i+1}(x) - (i+1) \operatorname{He}_{i}(x), \quad (3.2.5)$$

$$\operatorname{He}_{i}(-x) = (-1)^{i} \operatorname{He}_{i}(x), \qquad (3.2.6)$$

$$\operatorname{He}_{i}(x) = i! \sum_{m=0}^{\left\lfloor \frac{i}{2} \right\rfloor} \frac{(-1)^{m}}{m! (i-2m)!} \frac{x^{i-2m}}{2^{m}},$$
(3.2.7)

$$\operatorname{He}_{i}\left(x+y\right) = \sum_{m=0}^{i} \begin{pmatrix} i\\m \end{pmatrix} x^{i-m} \operatorname{He}_{m}\left(y\right), \qquad (3.2.8)$$

$$\operatorname{He}_{2i}(0) = (-1)^{i} \frac{(2i)!}{2^{i}i!}, \quad \operatorname{He}_{2i+1}(0) = 0, \tag{3.2.9}$$

$$He_i''(x) - xHe_i'(x) + iHe_i(x) = 0, \qquad (3.2.10)$$

$$\operatorname{He}_{i+1}^{\prime}(x) - (i+1)\operatorname{He}_{i}(x) = 0, \qquad (3.2.11)$$

$$\forall A \in \mathbb{R}, \quad \operatorname{He}_{i}(Ax) = \sum_{m=0}^{\lfloor \frac{i}{2} \rfloor} A^{i-2m} \left(A^{2}-1\right)^{m} \frac{i!}{m!(i-2m)!} 2^{-m} \operatorname{He}_{i-2m}(x), \quad (3.2.12)$$

$$\forall i, j \in \mathbb{N}, \quad \int_{\mathbb{R}} \operatorname{He}_{i}(x) \operatorname{He}_{j}(x) \frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}x = i! \delta_{ij}, \qquad (3.2.13)$$

$$\forall x, w \in \mathbb{R}, \quad e^{xw - \frac{w^2}{2}} = \sum_{i=0}^{\infty} \operatorname{He}_i(x) \frac{w^i}{i!}.$$
(3.2.14)

We recall that any measurable function  $\varphi : \mathbb{R} \to \mathbb{R}$ , such that  $\mathbb{E}[\varphi^2(Z)] < +\infty$ , can be decomposed into  $L_2$  (chaos decomposition) as

$$\varphi(Z) = \sum_{i=0}^{\infty} \alpha_i \operatorname{He}_i(Z)$$

with  $\alpha_i = \frac{\mathbb{E}[\varphi(Z) \operatorname{He}_i(Z)]}{i!}$ . Before applying this result to the indicator function on the event (3.2.3), we need the following proposition.

**Proposition 3.2.2.** Let Z be a standard normal random variable and  $c \in \mathbb{R}$ . Then the following chaos decomposition holds:

$$\mathbf{1}_{c \le Z} = \sum_{i=0}^{\infty} \alpha_i(c) \operatorname{He}_i(Z)$$
(3.2.15)

with  $\alpha_0(c) = \Phi(-c)$  and for  $i \in \mathbb{N}^*$ ,

$$\alpha_i(c) = \frac{e^{-\frac{c^2}{2}} \operatorname{He}_{i-1}(c)}{i!\sqrt{2\pi}} = \frac{e^{-\frac{c^2}{2}}}{i\sqrt{2\pi}} \sum_{m=0}^{\lfloor \frac{i-1}{2} \rfloor} \frac{(-1)^m}{m! (i-1-2m)!} \frac{c^{i-1-2m}}{2^m}.$$
 (3.2.16)

Furthermore, the following relations between coefficients hold:

$$\forall i \in \mathbb{N}, \quad \alpha_{i+2}(c) = \frac{c}{i+2} \alpha_{i+1}(c) - \frac{i}{(i+1)(i+2)} \alpha_i(c). \tag{3.2.17}$$

Equality (3.2.15) holds in  $L_2$ , and thus for almost every Z. Actually (see the discussion below), the equality holds for  $Z \neq c$ .

# 3.2.3 Wiener chaos decomposition of the loss

At this point, in view of (3.2.3) and since  $\frac{\rho_k}{|\rho_k|}Z \stackrel{d}{=} Z \stackrel{d}{=} \mathcal{N}(0,1)$ , we would like to apply (3.2.15) with  $c = a_k \varepsilon_k + b_k$ . However, as (3.2.15) holds almost surely (i.e. except on a set of zero measure  $\mathcal{E}_c$ ), and the c's are to be chosen as random, one has to be careful. Fortunately, the convergence

in (3.2.15) does not hold only for almost every Z, but for all  $Z \neq c$ . This is a consequence of the Uspensky's criterion [159] for pointwise convergence of Hermite series. Moreover, the series on the right-hand side of (3.2.15) converges to the left-hand side uniformly on any compact set of Z-values that does not contain c. For the special case Z = c, it converges to  $\frac{1}{2}$  (Runge's phenomenon), see Sansone [153, Section IV.10]. It implies that on the complement of the set  $\mathcal{E} = \bigcup_{k=1}^{K} \left\{ a_k \varepsilon_k + b_k = \frac{\rho_k}{|\rho_k|} Z \right\}$ , the equality (3.2.15) holds simultaneously for  $c = a_k \varepsilon_k + b_k$  for all  $k \in \{1, \ldots, K\}$ . Since the sequence  $(\varepsilon_k)_{k=1,\ldots,K}$  is independent of  $\frac{\rho_k}{|\rho_k|} Z$  and the distribution of  $\frac{\rho_k}{|\rho_k|} Z$  has no atoms, the set  $\mathcal{E}$  has zero probability. It implies that we have almost surely

$$\mathcal{L}^{(3.2.3)} \sum_{k=1}^{K} l_k \mathbf{1}_{\{a_k \varepsilon_k + b_k \le \frac{\rho_k}{|\rho_k|}Z\}}$$
(3.2.18)  
$$= \sum_{k=1}^{K} l_k \sum_{i=0}^{\infty} \alpha_i \left(a_k \varepsilon_k + b_k\right) \operatorname{He}_i \left(\frac{\rho_k}{|\rho_k|}Z\right)$$
$$= \sum_{i=0}^{\infty} \left\{ \sum_{k=1}^{K} l_k \alpha_i \left(a_k \varepsilon_k + b_k\right) \frac{\rho_k^i}{|\rho_k|^i} \right\} \operatorname{He}_i (Z) .$$

The last equality can easily be obtained noticing that:

$$\operatorname{He}_{i}\left(\frac{\rho_{k}}{|\rho_{k}|}Z\right) = \operatorname{He}_{i}\left(Z\right)\mathbf{1}_{\rho_{k}>0} + \operatorname{He}_{i}\left(-Z\right)\mathbf{1}_{\rho_{k}<0}$$

$$\stackrel{(3.2.6)}{=}\operatorname{He}_{i}\left(Z\right)\mathbf{1}_{\rho_{k}>0} + \left(-1\right)^{i}\operatorname{He}_{i}\left(Z\right)\mathbf{1}_{\rho_{k}<0}$$

$$= \frac{\rho_{k}^{i}}{|\rho_{k}|^{i}}\operatorname{He}_{i}\left(Z\right).$$

$$(3.2.19)$$

Truncating the sum over i at I gives the so-called I-chaos decomposition of the loss. This is our first main result.

**Theorem 3.1.** Under the assumption that  $(\varepsilon_k)_{k=1,...,K}$  is independent of Z, the chaos decomposition of the loss  $\mathcal{L}$  with respect to Z is given by:

$$\mathcal{L} = \sum_{i=0}^{\infty} \left\{ \sum_{k=1}^{K} l_k \alpha_i \left( a_k \varepsilon_k + b_k \right) \frac{\rho_k^i}{|\rho_k|^i} \right\} \operatorname{He}_i(Z), \qquad (3.2.20)$$

where the  $\alpha_i(\cdot)$ 's are given in Proposition 3.2.2. Then, the associated truncated chaos decomposition of order  $I \in \mathbb{N}$  of the loss  $\mathcal{L}$ , or I-chaos decomposition, is defined by:

$$\mathcal{L}_{I} = \sum_{i=0}^{I} \left\{ \sum_{k=1}^{K} l_{k} \alpha_{i} \left( a_{k} \varepsilon_{k} + b_{k} \right) \frac{\rho_{k}^{i}}{\left| \rho_{k} \right|^{i}} \right\} \operatorname{He}_{i} \left( Z \right).$$
(3.2.21)

The analysis of the truncation error is made possible by a better understanding of how fast the coefficients  $\alpha_i$  decrease to 0. It will be handled by the next two results.

**Lemma 3.2.3.** For every  $n \in \mathbb{N}$ , the successive relative maxima of  $x \in \mathbb{R} \to e^{-\frac{x^2}{2}} |\text{He}_n(x)|$  form a decreasing (resp. increasing) sequence for  $x \ge 0$  (resp. for  $x \le 0$ ).

**Corollary 3.2.4.** For every  $n \in \mathbb{N}$ , define  $M_n := \max_{x \in \mathbb{R}} \left( \frac{e^{-x^2} \operatorname{He}_n^2(x)}{(n+1)!} \right)$  then:

$$M_n = \begin{cases} \frac{(2m)!}{(2m+1)(m!)^2 2^{2m}} & \text{if } n = 2m\\ \frac{e^{-x_{1,2m+2}^2 \operatorname{He}_{2m+1}^2}(x_{1,2m+1})}{(2m+2)!} & \text{if } n = 2m+1 \end{cases}$$



Figure 3.1 – Plot of  $x \mapsto e^{-\frac{x^2}{2}} |\text{He}_n(x)|$  for n = 1, ..., 5 to illustrate Lemma 3.2.3.

$$M_{2m+1} < M_{2m}, (3.2.22)$$

where  $m \in \mathbb{N}$  and  $x_{1,2m+2} > 0$  denotes the first positive zero of He<sub>2m+2</sub>.

For the reader interested in estimates on the maximum of weighted Hermite polynomials, see the work of Krasikov [127]. Notice that his estimates are different as he considers physicists' Hermite polynomials  $H_i(\cdot)$  which are linked to the probabilists' Hermite polynomials through the relation  $H_i(x) = 2^{\frac{i}{2}} \text{He}_i(\sqrt{2}x)$ . Yet the upper bound obtained in Krasikov [127, Theorem 1] is not equivalent to that of our Corollary 3.2.4 (even after the above rescaling). Our above upper bound is tight and customized to our setting.



Figure 3.2 – Plot of  $x \mapsto \frac{e^{-x^2} \operatorname{He}_n^2(x)}{(n+1)!}$  for  $n = 1, \dots, 5$ , to illustrate the inequality (3.2.22).

We are now in a position to analyze the truncation error related to the chaos decomposition of Proposition 3.2.2 and Theorem 3.1. We recall that the  $(\varepsilon_k)_{k=1...K}$  are independent of Z.

**Theorem 3.2.** Let  $I \in \mathbb{N}^*, c \in \mathbb{R}$  and Z be a standard normal random variable. Then, there exists  $C_{(3,2,23)} \geq 0$  which does not depend on I and K, such that:

$$\sup_{c \in \mathbb{R}} \mathbb{E} \left[ \left| \mathbf{1}_{c \leq Z} - \sum_{i=0}^{I} \alpha_i(c) \operatorname{He}_i(Z) \right|^2 \right] \leq \frac{C_{(3.2.23)}}{\sqrt{I}},$$

$$and \quad \mathbb{E} \left[ \left| \mathcal{L} - \mathcal{L}_I \right|^2 \right] \leq C_{(3.2.23)} \frac{\left( \sum_{k=1}^{K} l_k \right)^2}{\sqrt{I}}.$$

$$(3.2.23)$$

A careful analysis of the proof shows that this result holds without assuming that

 $(\varepsilon_k)_{k=1...K}$  forms an independent sequence, only the independence w.r.t. Z is required. This property is interesting in view of the further extension to the multi-factor model (see the discussion in Section 3.3.3). According to the numerical experiments reported in Figure 3.6, it seems that the above estimates are tight (one can not improve the convergence rate).

Proof of Theorem 3.2. We first note that the second estimate is a direct consequence of the first one. Indeed, starting from (3.2.18)-(3.2.19)-(3.2.21), along with the positivity of  $l_k$ , and the Cauchy–Schwarz inequality, and the fact that  $\frac{\rho_k}{|\rho_k|}Z \stackrel{d}{=} Z \stackrel{d}{=} \mathcal{N}(0,1)$  and the first estimate, we have:

$$\begin{split} \mathbb{E}\left[\left|\mathcal{L}-\mathcal{L}_{I}\right|^{2}\right] = \mathbb{E}\left[\left|\sum_{k=1}^{K} l_{k}\left(\mathbf{1}_{\left\{a_{k}\varepsilon_{k}+b_{k}\leq\frac{\rho_{k}}{|\rho_{k}|}Z\right\}}-\sum_{i=0}^{I}\alpha_{i}\left(a_{k}\varepsilon_{k}+b_{k}\right)\operatorname{He}_{i}\left(\frac{\rho_{k}}{|\rho_{k}|}Z\right)\right)\right|^{2}\right] \\ &\leq \sum_{k,k'=1}^{K} l_{k}l_{k'}\mathbb{E}\left[\left|\mathbf{1}_{\left\{a_{k}\varepsilon_{k}+b_{k}\leq\frac{\rho_{k}}{|\rho_{k}|}Z\right\}}-\sum_{i=0}^{I}\alpha_{i}\left(a_{k}\varepsilon_{k}+b_{k}\right)\operatorname{He}_{i}\left(\frac{\rho_{k}}{|\rho_{k}|}Z\right)\right|\right] \\ &\times\left|\mathbf{1}_{\left\{a_{k'}\varepsilon_{k'}+b_{k'}\leq\frac{\rho_{k}}{|\rho_{k}|}Z\right\}}-\sum_{i=0}^{I}\alpha_{i}\left(a_{k'}\varepsilon_{k'}+b_{k'}\right)\operatorname{He}_{i}\left(\frac{\rho_{k}}{|\rho_{k}|}Z\right)\right|^{2}\right]^{\frac{1}{2}} \\ &\leq \sum_{k,k'=1}^{K} l_{k}l_{k'}\mathbb{E}\left[\left|\mathbf{1}_{\left\{a_{k}\varepsilon_{k}+b_{k}\leq\frac{\rho_{k}}{|\rho_{k}|}Z\right\}}-\sum_{i=0}^{I}\alpha_{i}\left(a_{k'}\varepsilon_{k'}+b_{k'}\right)\operatorname{He}_{i}\left(\frac{\rho_{k'}}{|\rho_{k'}|}Z\right)\right|^{2}\right]^{\frac{1}{2}} \\ &\times \mathbb{E}\left[\left|\mathbf{1}_{\left\{a_{k'}\varepsilon_{k'}+b_{k'}\leq\frac{\rho_{k'}}{|\rho_{k'}|}Z\right\}}-\sum_{i=0}^{I}\alpha_{i}\left(a_{k'}\varepsilon_{k'}+b_{k'}\right)\operatorname{He}_{i}\left(Z\right)\right|^{2}\right]^{\frac{1}{2}} \\ &=\sum_{k,k'=1}^{K} l_{k}l_{k'}\mathbb{E}\left[\left|\mathbf{1}_{\left\{a_{k}\varepsilon_{k}+b_{k}\leq Z\right\}}-\sum_{i=0}^{I}\alpha_{i}\left(a_{k'}\varepsilon_{k'}+b_{k'}\right)\operatorname{He}_{i}\left(Z\right)\right|^{2}\right]^{\frac{1}{2}} \\ &\times \mathbb{E}\left[\left|\mathbf{1}_{\left\{a_{k'}\varepsilon_{k'}+b_{k'}\leq Z\right\}}-\sum_{i=0}^{I}\alpha_{i}\left(a_{k'}\varepsilon_{k'}+b_{k'}\right)\operatorname{He}_{i}\left(Z\right)\right|^{2}\right]^{\frac{1}{2}} \\ &\leq \frac{C(3.2.23)}{\sqrt{I}}\left(\sum_{k=1}^{K} l_{k}\right)^{2}. \end{split}$$

Now, let us prove the first estimate. The quadratic error of the truncated projection is equal to:

$$\mathbb{E}\left[\left|\mathbf{1}_{c\leq Z} - \sum_{i=0}^{I} \alpha_{i}(c) \operatorname{He}_{i}(Z)\right|^{2}\right] \stackrel{(3.2.15)}{=} \mathbb{E}\left[\left|\sum_{i=I+1}^{\infty} \alpha_{i}(c) \operatorname{He}_{i}(Z)\right|^{2}\right] \\ \stackrel{(3.2.13)}{=} \sum_{i=I+1}^{\infty} \sum_{i=I+1}^{i! \alpha_{i}(c)^{2}} \frac{(3.5.2)}{2\pi(i+1)!} \sum_{i=I}^{\infty} \frac{e^{-c^{2}} \operatorname{He}_{i}^{2}(c)}{2\pi(i+1)!}.$$

Since the above upper bound is decreasing in I and in view of the advertised upper bound of Theorem 3.2, it is enough to consider the case of I even, i.e. I = 2N for some  $N \in \mathbb{N}^*$ . For such

I, by Corollary 3.2.4, we have

$$\sum_{i=2N}^{\infty} \frac{e^{-c^2} \operatorname{He}_i^2(c)}{2\pi(i+1)!} = \frac{1}{2\pi} \sum_{p=N}^{\infty} \left( \frac{e^{-c^2} \operatorname{He}_{2p}^2(c)}{(2p+1)!} + \frac{e^{-c^2} \operatorname{He}_{2p+1}^2(c)}{(2p+2)!} \right)$$
$$\leq \frac{1}{2\pi} \sum_{p=N}^{\infty} (M_{2p} + M_{2p+1})$$
$$\leq \frac{1}{\pi} \sum_{p=N}^{\infty} M_{2p} = \frac{1}{\pi} \sum_{p=N}^{\infty} \frac{(2p)!}{(2p+1)(p!)^2 2^{2p}}.$$

Now, using Stirling's formula  $p! \underset{p \to \infty}{\sim} \sqrt{2\pi p} \left(\frac{p}{e}\right)^p$ , we have:

$$\frac{(2p)!}{(2p+1)(p!)^2 \, 2^{2p}} \underset{p \to \infty}{\sim} \frac{\sqrt{2\pi 2p} \left(\frac{2p}{e}\right)^{2p}}{(2p+1)2\pi p \left(\frac{p}{e}\right)^{2p} 2^{2p}} \underset{p \to \infty}{\sim} \frac{1}{2\sqrt{\pi}p^{\frac{3}{2}}}$$

Standard computations about comparing tails of series and integrals show that, for any  $\alpha > 1$ ,

$$\sum_{k=N}^{\infty} \frac{1}{p^{\alpha}} \underset{N \to \infty}{\sim} \frac{1}{\alpha - 1} \frac{1}{N^{\alpha - 1}}.$$

Applying the above with  $\alpha = \frac{3}{2}$  directly gives

$$\frac{1}{\pi} \sum_{p=N}^{\infty} \frac{(2p)!}{\left(2p+1\right) \left(p!\right)^2 2^{2p}} \underset{N \to \infty}{\sim} \frac{\operatorname{Cst}}{\sqrt{N}},$$

whence the announced result.

Owing to (3.2.21), we can write

$$\mathcal{L}_{I} = \sum_{i=0}^{I} \varepsilon_{K,i} \operatorname{He}_{i}(Z) \quad \text{with} \quad \varepsilon_{K,i} = \sum_{k=1}^{K} l_{k} \alpha_{i} \left( a_{k} \varepsilon_{k} + b_{k} \right) \frac{\rho_{k}^{i}}{|\rho_{k}|^{i}}, \quad (3.2.24)$$

where  $(\varepsilon_k)_{k=1...K}$  are i.i.d. standard normal random variables and independent of Z. The striking property is that the coefficients  $(\varepsilon_{K,i})_{i \in 0,...,I}$  write as a sum of independent random variables. The next result gives a sufficient condition so that one can replace the coefficients by a Gaussian random vector with explicit characteristics.

**Theorem 3.3.** Let  $I \in \mathbb{N}$ . For every  $k \in \{1, \ldots, K\}$ , recall the definitions from (3.2.3):

$$a_k = \frac{-\sqrt{1-\rho_k^2}}{|\rho_k|}, \ b_k = \frac{-\Phi^{-1}(p_k)}{|\rho_k|},$$

and set for every  $i, j \in \{0, \ldots, I\}$ :

$$m_{K,i} := \sum_{k=1}^{K} l_k \frac{\rho_k^i}{|\rho_k|^i} \mu_i(a_k, b_k), \quad s_{K,i,j} := \sum_{k=1}^{K} l_k^2 \frac{\rho_k^i}{|\rho_k|^i} \frac{\rho_k^j}{|\rho_k|^j} \sigma_{i,j}(a_k, b_k), \quad (3.2.25)$$

with  $\mu_i(a,b) := \mathbb{E}[\alpha_i(aX+b)]$  and  $\sigma_{i,j}(a,b) := \mathbb{C}ov(\alpha_i(aX+b),\alpha_j(aX+b))$  for  $a \in \mathbb{R}, b \in \mathbb{R}$ and  $X \stackrel{d}{=} \mathcal{N}(0, 1)$ .

Now, assume that the matrix  $s_K = (s_{K,i,j} : 0 \le i, j \le I)$  is invertible for large K and that

$$\|s_K^{-1}\| \sup_{1 \le k \le K} l_k^2 \xrightarrow[K \to +\infty]{} 0 \quad \text{with} \quad \|s_K^{-1}\| := \sup_{x \in \mathbb{R}^{I+1}, x \ne 0} \frac{|s_K^{-1}x|}{|x|}.$$
(3.2.26)

Then, the random chaos coefficients vector  $\varepsilon_K = (\varepsilon_{K,i})_{i \in \{0,...,I\}}$  satisfies the following Central Limit Theorem (CLT):

$$s_K^{-\frac{1}{2}}(\varepsilon_K - m_K) \xrightarrow{d} \mathcal{N}(0, \mathrm{Id}_{I+1}) \quad \text{where} \quad m_K = (m_{K,i})_{i \in \{0, \dots, I\}}.$$
(3.2.27)

Assumption 3.2.26 is rather a theoretical condition which is not easy to simplify, since it links the losses given default  $l_k$ , the correlations  $\rho_k$  and the unconditional default probabilities  $p_k$ . If we ignore the covariance term  $\sigma_{i,j}(\cdot)$  and simplify the variance to 1 then  $s_K = \left(\sum_{k=1}^K l_k^2\right) \operatorname{Id}_{I+1}$ . Condition 3.2.26 becomes

$$\frac{\sup_{1 \le k \le K} l_k^2}{\sum_{k=1}^K l_k^2} \xrightarrow[K \to +\infty]{} 0, \qquad (3.2.28)$$

which is, to our opinion, the main take-home message of (3.2.26): the Gaussian approximation holds if none of the individual square loss is significantly too large compared to the global sum. *Remark* 1 (About granularity measurement). Condition 3.2.28 can be related to conditions on infinitely granular portfolios, like the Herfindahl–Hirschman Index (3.1.3) presented in the introduction. Actually (3.2.28) implies that asymptotically, the portfolio is perfectly fine-grained, in the sense that  $\text{HHI}_K \to 0$  as  $K \to +\infty$  since

$$\mathtt{HHI}_{K} = \frac{\sum_{k=1}^{K} l_{k}^{2}}{(\sum_{k=1}^{K} l_{k})^{2}} \le \frac{\sup_{1 \le k \le K} l_{k}}{\sum_{k=1}^{K} l_{k}} \le \frac{\sup_{1 \le k \le K} l_{k}^{2}}{\sum_{k=1}^{K} l_{k}^{2}}.$$

Besides, our condition (3.2.28) is different from that of Gordy [88, Proposition 1] which writes

$$\sum_{k\geq 1} l_k = +\infty \quad \text{and} \quad \sum_{K\geq 1} \left(\frac{l_K}{\sum_{k=1}^K l_k}\right)^2 < +\infty.$$
(3.2.29)

Under this condition, the idiosyncratic risk can be eliminated through diversification leading to GA techniques described in the introduction. It is easy to check (using the Kronecker lemma) that the Gordy condition (3.2.29) also implies  $\text{HHI}_K \to 0$  as  $K \to +\infty$ . On the other hand, there is no clear general implication between our condition and that of Gordy, although on usual examples of  $(l_k : k \ge 1)$  the condition (3.2.28) is stronger than (3.2.29) – which is compatible with the intuition since (3.2.29) is used to establish almost-sure results while (3.2.28) is used to study random fluctuations.

From (3.2.27), as K is assumed to be large, it is natural to approximate the vector  $\varepsilon_K = (\varepsilon_{K,i})_{i \in \{0,\dots,I\}}$  with a normal vector of mean  $m_K$  and covariance matrix  $s_K$ . The larger the number of obligors K, the better the normal approximation will be. Besides, explicit formulas for  $\mu_i(\cdot)$ ,  $\sigma_{i,j}(\cdot)$  are given in Section 3.3.1, yielding explicit expressions for  $m_K$  and  $s_K$ . As these characteristics can be computed offline, sampling the meta-model thus reduces to sampling an *I*-dimensional Gaussian vector and the systemic risk factor Z, making our approach much faster (see Section 3.3.2 for further details and remarks on the implementation of our model).

Proof of Theorem 3.3. We take K large enough, so that  $s_K$  is invertible and we can define properly  $s_K^{-\frac{1}{2}}$ .

It is then straightforward to check that the vector  $\varepsilon_K$  has mean  $m_K$  and covariance matrix

 $s_K$ . Since  $s_K^{-\frac{1}{2}}(\varepsilon_k - m_K)$  is a sum of independent vectors, has zero mean and unit covariance matrix, the announced CLT (3.2.27) is a direct consequence of the CLT for arrays of sums of independent random variables as soon as we check the Lindeberg condition (see Bhattacharya and Rao [30, Theorem 18.2] or Jacod and Shiryaev [115, Theorem VII.5.2]): i.e. for any  $\varepsilon > 0$  and  $i \in \{0, \ldots, I\}$ , we need:

$$\sum_{k=1}^{K} l_k^2 \mathbb{E} \left[ \left| s_K^{-\frac{1}{2}} \alpha_i(a_k \varepsilon_k + b_k) - s_K^{-\frac{1}{2}} \mu(a_k, b_k) \right|^2 \right]$$
$$\mathbf{1}_{\mathbb{R}_+} \left( l_k^2 \left| s_K^{-\frac{1}{2}} \alpha_i(a_k \varepsilon_k + b_k) - s_K^{-\frac{1}{2}} \mu(a_k, b_k) \right|^2 - \varepsilon \right) \xrightarrow{K \to \infty} 0. \quad (3.2.30)$$

On the one hand, observe that

$$\left\{ l_k^2 \left| s_K^{-\frac{1}{2}} \alpha_i(a_k \varepsilon_k + b_k) - s_K^{-\frac{1}{2}} \mu(a_k, b_k) \right|^2 \ge \varepsilon \right\}$$
$$\subset \left\{ l_k^2 \| s_K^{-1} \| \left| \alpha_i(a_k \varepsilon_k + b_k) - \mu(a_k, b_k) \right|^2 \ge \varepsilon \right\}$$
$$\subset \left\{ \| s_K^{-1} \| \sup_{1 \le k \le K} l_k^2 \sup_{c,a,b} |\alpha_i(c) - \mu(a, b)|^2 \ge \varepsilon \right\}$$

where we have used that  $\alpha$  and  $\mu$  are bounded (by a constant depending only on the number of coefficients I + 1). On the other hand, owing to (3.2.26), for large K the above event is empty. Therefore, the Lindeberg condition is obviously satisfied and this concludes the proof.

In light of the above Theorem, we define the Gaussian approximation of the *I*-chaos decomposition by:

$$\mathcal{L}_{I}^{\mathrm{G}} = \sum_{i=0}^{I} \varepsilon_{K,i}^{\mathrm{G}} \mathrm{He}_{i}\left(Z\right) \quad \text{where} \quad \varepsilon_{K}^{\mathrm{G}} = \left(\varepsilon_{K,i}^{\mathrm{G}}\right)_{i=0...I} \stackrel{d}{=} \mathcal{N}\left(m_{K}, s_{K}\right), \tag{3.2.31}$$

where we recall that both  $m_K = (m_{K,i})_{i=0...I}$  and  $s_K = (s_{K,i,j})_{i,j=0...I}$  have been defined in (3.2.25).

# 3.3 Implementation of the model

#### 3.3.1 Main analytical formulas

**Proposition 3.3.1.** Let  $a \in \mathbb{R}^*, b \in \mathbb{R}$  and X a standard normal random variable. For every  $i, j \in \mathbb{N}$ , define

$$\mu_i(a,b) := \mathbb{E} \left[ \alpha_i(aX+b) \right],$$
  
$$\sigma_{i,j}(a,b) := \mathbb{C} \text{ov} \left( \alpha_i(aX+b), \alpha_j(aX+b) \right).$$

Then the following recursive relations hold:

$$\begin{cases} \mu_0(a,b) = \Phi\left(-\frac{b}{\sqrt{1+a^2}}\right), \quad \mu_1(a,b) = \frac{e^{-\frac{b^2}{2(1+a^2)}}}{\sqrt{2\pi}\sqrt{1+a^2}}, \\ \mu_{i+2}(a,b) = \frac{b}{(i+2)(1+a^2)}\mu_{i+1}(a,b) - \frac{i}{(i+2)(i+1)(1+a^2)}\mu_i(a,b), \end{cases}$$
(3.3.1)

$$\begin{aligned} \sigma_{0,0}(a,b) &= \Phi_{\Sigma} \left( (-b,-b)^{\top} \right) - \mu_0(a,b)^2, \quad \Sigma = \left( \frac{1+a^2}{a^2} \frac{a^2}{1+a^2} \right), \\ \sigma_{0,1}(a,b) &= \mu_1(a,b) \left( \mu_0 \left( \frac{a}{\sqrt{1+a^2}}, \frac{b}{1+a^2} \right) - \mu_0(a,b) \right), \\ \sigma_{0,i+2}(a,b) &= \frac{b}{(i+2)(1+a^2)} \sigma_{0,i+1}(a,b) - \frac{i}{(i+1)(i+2)(1+a^2)} \sigma_{0,i}(a,b) \\ &\qquad - \frac{a^2}{(i+2)(1+a^2)} \mu_1(a,b) \mu_{i+1} \left( \frac{a}{\sqrt{1+a^2}}, \frac{b}{1+a^2} \right), \\ \sigma_{i+1,j+1}(a,b) &= \frac{1}{a^2(i+1)} \left[ -\left( 1+a^2 \right) (j+2) \sigma_{i,j+2}(a,b) + b \sigma_{i,j+1}(a,b) - \frac{j}{j+1} \sigma_{i,j}(a,b) \right] \\ &\qquad - \mu_{i+1}(a,b) \mu_{j+1}(a,b). \end{aligned}$$

$$(3.3.2)$$

We exclude the case a = 0 from the statement since in that case we directly get  $\mu_i(a, b) = \alpha_i(b)$ ,  $\sigma_{i,j}(a, b) = 0$ . In the non-trivial case  $a \neq 0$ , the above result gives an effective scheme to compute all the metal-model parameters. If the coefficients related to  $i, j \in \{0, \ldots, I\}$  are sought, then one shall start with getting  $\mu_i(a, b)$  from i = 0 to I using the above initialization and iteration. Then, one shall compute  $\sigma_{0,j}(a, b)$  from j = 0 to I. The computation of  $\sigma_{i+1,j}(a, b)$  from the  $\sigma_{i,.}(a, b)$  is more difficult since one needs (in particular)  $\sigma_{i,j+2}(a, b)$ , and by iteration  $\sigma_{i-l,j+l+2}(a, b)$  for l = 0 to i. It means that the previous computations for  $\mu_i(a, b)$  and  $\sigma_{0,j}(a, b)$  have to be carried out for  $i, j = 0, \ldots, 2I$ , in order to be able, at the end, to get  $\sigma_{i,j}(a, b)$  for all  $i, j = 0, \ldots, I$ .

Proposition 3.3.1 allows us to recursively compute the means  $\mu_i(a, b)$ , the variances  $\sigma_{i,i}(a, b)$ and the covariances  $\sigma_{i,j}(a, b)$ . This is very simple from an algorithmic point of view. However, for evaluations with I large and for many different (a, b) (the default parameters), we may prefer to have explicit formulas, in order to get possibly more efficient schemes according to the way this is implemented on a computer. The following results are aimed at giving explicit representations of these coefficients as multiple sums, that are straightforward to compute without induction. Note that the expressions below need only to be stated for  $i, j \neq 0$ . Indeed, from Proposition 3.3.1, the case i = 0 and/or j = 0 has already been treated as we have derived a closed-form expression for  $\mu_0(a, b)$  and a recurrence relation for  $\sigma_{0,j}(a, b) = \sigma_{j,0}(a, b)$  for  $j \in \{0, \ldots, I\}$ .

**Lemma 3.3.2.** For every  $i, j \in \mathbb{N}^*$ ,  $\mu_i(a, b)$ ,  $\sigma_{i,j}(a, b)$  can be expressed explicitly as:

$$\begin{split} \mu_i(a,b) &= \frac{e^{-\frac{b^2}{2(1+a^2)}}}{i\sqrt{2\pi}} \sum_{k=0}^{\lfloor \frac{i-1}{2} \rfloor} \frac{a^{2k} \operatorname{He}_{i-1-2k}\left(\frac{b}{1+a^2}\right)}{2^k k! \left(i-1-2k\right)! \left(1+a^2\right)^{k+\frac{1}{2}}}, \\ \sigma_{i,j}\left(a,b\right) &= \frac{e^{-\frac{b^2}{1+2a^2}}}{2\pi i! j! \sqrt{1+2a^2}} \\ &\times \left( \sum_{k=0}^{\lfloor \frac{i-1}{2} \rfloor} \sum_{p=0}^{\lfloor \frac{i-1}{2} \rfloor} \left(\frac{i-1}{2k}\right) \left(\frac{j-1}{2p}\right) \frac{a^{2(k+p)} \left(2\left(k+p\right)\right)! \operatorname{He}_{i-1-2k}\left(\frac{b}{1+2a^2}\right) \operatorname{He}_{j-1-2p}\left(\frac{b}{1+2a^2}\right)}{\left(1+2a^2\right)^{k+p} 2^{k+p} \left(k+p\right)!} \\ &+ \sum_{k=0}^{\lfloor \frac{i-2}{2} \rfloor} \sum_{p=0}^{\lfloor \frac{i-2}{2} \rfloor} \left(\frac{i-1}{2k+1}\right) \left(\frac{j-1}{2p+1}\right) \frac{a^{2(k+p+1)} \left(2\left(k+p+1\right)\right)! \operatorname{He}_{i-2k-2}\left(\frac{b}{1+2a^2}\right) \operatorname{He}_{j-2p-2}\left(\frac{b}{1+2a^2}\right)}{\left(1+2a^2\right)^{k+p+1} 2^{k+p+1} \left(k+p+1\right)!} \\ &- \mu_i\left(a,b\right) \mu_j\left(a,b\right). \end{split}$$

#### 3.3.2 Numerical tests

All the numerical tests were performed on a MacBook Pro laptop (2,7 GHz Intel Core i5) using the programming language Python 3.7.2.

We first focus on the approximation of the indicator function  $\mathbf{1}_{c\leq Z} \approx \sum_{i=0}^{I} \alpha_i(c) \operatorname{He}_i(Z)$  and illustrate it with several plots. Keeping in mind that the random variable Z is standard normal, we restrict our attention to [-3, 3] for the possible values of Z (more precisely  $\mathbb{P}(Z \in [-3, 3]) \approx$  0.997). Concerning the threshold c, note that in our framework it takes values in  $\mathbb{R}$ . Indeed, in light of (3.2.3),

$$c = a_k \varepsilon_k + b_k \stackrel{d}{=} \mathcal{N}\left(b_k, a_k^2\right)$$

The values taken by the normally distributed threshold c thus fully depend on both the values of the default probability  $p_k$  and the correlation  $\rho_k$  for the kth obligor.

### Values taken by the threshold c



Figure 3.3 – On the left,  $\rho \mapsto \frac{1-\rho^2}{\rho^2}$ . On the right,  $(\rho, p) \mapsto \frac{-\Phi^{-1}(p)}{\rho}$ .

On Figure 3.3, we plot (omitting the dependence of k) the mean  $(\rho, p) \mapsto \frac{-\Phi^{-1}(p)}{|\rho|}$  and the variance  $\rho \mapsto \frac{1-\rho^2}{\rho^2}$  for positive correlations (a similar analysis would be obtained for negative correlation). From both plots, we see that extreme values are obtained with either small correlation and/or small default probability. Economically, this can be interpreted as follows: under such regimes (high values for c), for the event  $\{c \leq Z\}$  to occur, one needs to have an extreme economic scenario (high values for Z). Indeed, as the obligor would (almost) not depend on the economy and/or would have a very small default probability, only extreme values of Z (most likely during a crisis) may lead to default.

### Approximation of the indicator $\mathbf{1}_{c < Z}$ w.r.t. Z

To visualize the approximation for the indicator function, in Figure 3.4 we plot for 4 different values of fixed  $c \in \{-1, 0, 1, 2\}$ , the *I*-chaos decomposition associated where  $I \in \{5, 20, 50, 80\}$ . As the parameter *I* increases, the quality of the approximation improves together with an increasing number of oscillations and lower amplitudes. The  $L_2$  convergence does not imply uniform convergence (Runge's phenomenon at the discontinuity point, see Sansone [153, Section IV.10]). We notice also that the value *c* introduces a dissymmetry on the quality of the approximation. Indeed, if c < 0 (resp. c > 0), the approximation seems much accurate for Z > c (resp. Z < c) while for c = 0 the approximation remains the same.

There is another phenomenon worth mentioning when one approximates the indicator function (bounded function) using the Wiener chaos decomposition. As we are approximating the indicator function with a sum of Hermite polynomials (non-bounded functions) for large values of Z, the quality of the approximation deteriorates completely as we are getting extreme amplitudes (see Figure 3.5). However, as said before, Z is standard normal and such values for Zare very unlikely. Let us also notice that the rough estimate obtained in Theorem 3.2 allows us to cover a large range of values for the threshold c, although the estimate could presumably be refined for a certain range of values.

Finally, in order to illustrate the  $L_2$  error in Theorem 3.2, we provide the log-log plot of the mean square error MSE =  $\mathbb{E}\left[\left|\mathbf{1}_{c\leq Z} - \sum_{i=0}^{I} \alpha_i(c) \operatorname{He}_i(Z)\right|^2\right]$  w.r.t. I for 4 different values


Figure 3.4 – *I*-chaos decomposition for  $\mathbf{1}_{c \leq Z}$  with  $I \in \{5, 20, 50, 80\}$  and  $c \in \{-1, 0, 1, 2\}$ .

of fixed  $c \in \{-1, 0, 1, 2\}$ . More precisely, we fix I = 50, generate  $N = 5 \times 10^5$  i.i.d. samples  $(Z_n)_{1 \le n \le N} \stackrel{d}{=} \mathcal{N}(0, 1)$  and estimate the MSE by Monte Carlo simulation. As expected, we retrieve the order  $\mathcal{O}(\frac{\text{Cst}}{\sqrt{I}})$  since log(MSE) is a linear function w.r.t. log(I) with a slope of  $-\frac{1}{2}$  (see Figure 3.6). Actually note that in light of Theorem 3.2, we have a closed formula for the MSE i.e. MSE =  $\sum_{i=I+1}^{\infty} i! \alpha_i(c)^2$ . However, in order to avoid numerical instability by trying to compute Hermite polynomials of very high degrees (over i = 200, errors are returned), we prefer to use a Monte Carlo simulation to evaluate numerically the MSE.



Figure 3.5 – *I*-chaos decomposition for  $\mathbf{1}_{0 \leq Z}$  with  $I \in \{5, 20, 50, 80\}$  to illustrate extreme amplitudes in the tails.



#### The portfolio loss and its chaos decomposition

Let us recall that the *I*-chaos decomposition (3.2.21) and its Gaussian-based approximation (3.2.31) for the portfolio loss are given by

$$\mathcal{L}_{I} = \sum_{i=0}^{I} \varepsilon_{K,i} \operatorname{He}_{i}(Z) = \sum_{i=0}^{I} \left\{ \sum_{k=1}^{K} l_{k} \alpha_{i} (a_{k} \varepsilon_{k} + b_{k}) \frac{\rho_{k}^{i}}{|\rho_{k}^{i}|} \right\} \operatorname{He}_{i}(Z), \quad \mathcal{L}_{I}^{\mathrm{G}} = \sum_{i=0}^{I} \varepsilon_{K,i}^{\mathrm{G}} \operatorname{He}_{i}(Z),$$

where  $a_k \varepsilon_k + b_k \stackrel{d}{=} \mathcal{N}(b_k, a_k^2)$ ,  $a_k = -\frac{\sqrt{1-\rho_k^2}}{|\rho_k|}$ ,  $b_k = -\frac{\Phi^{-1}(p_k)}{|\rho_k|}$  and  $\varepsilon_K^{\mathrm{G}} \stackrel{d}{=} \mathcal{N}(m_K, s_K)$ . To fix ideas, we give below the algorithm to generate N samples from the Gaussian-based

To fix ideas, we give below the algorithm to generate N samples from the Gaussian-based approximation  $\mathcal{L}_{I}^{G}$ . As stated before, the only needed parameters (which can be computed offline) are the mean vector  $m_{K}$  and covariance matrix  $s_{K}$  that can be either computed using the recurrence relations in Proposition 3.3.1 or by explicit expressions stated in Lemma 3.3.2. The costly step (with respect to K) is made offline when computing  $m_{K}$  and  $s_{K}$ , this is a very significant improvement compared to the crude algorithm where new sums over k have to be computed at each sample of  $\mathcal{L}$ . More precisely, the Gaussian-based approximation allows us to bypass the computation of the sum over all obligors needed in a naive approach for the sampling of  $\mathcal{L}$  (see Algorithms 1, 2, and Remark 2). Note that we actually take advantage of the fact that K is very large since the larger the number of obligors, the better the Gaussian-based approximation will be.

Algorithm 1: Gaussian-based approximation for the loss  $\mathcal{L}$ 

Input: N (nonnegative integer),  $m_K$  (vector of size I + 1),  $s_K$  (covariance matrix of size (I + 1, I + 1)) Output:  $\mathcal{L}_I^{G,(1:N)} = \left(\left(\mathcal{L}_I^G\right)^{(1)}, \dots, \left(\mathcal{L}_I^G\right)^{(N)}\right)$ 1  $\mathcal{L}_I^{G,(1:N)} = \left(\left(\mathcal{L}_I^G\right)^{(1)}, \dots, \left(\mathcal{L}_I^G\right)^{(N)}\right) \leftarrow (0, \dots, 0)$  (vector of size N) 2 for  $n = 1 \dots N$  do 3 Generate  $Z^{(n)} \sim \mathcal{N}(0, 1)$  (scalar) 4 Generate  $(\varepsilon_K^G)^{(n)} \sim \mathcal{N}(m_K, s_K)$  (vector of size I + 1 independent of  $Z^{(n)}$ ) 5  $\left(\mathcal{L}_I^G\right)^{(n)} \leftarrow 0$  (scalar) 6 for  $i = 0 \dots I$  do 7  $\left(\mathcal{L}_I^G\right)^{(n)} \leftarrow \left(\mathcal{L}_I^G\right)^{(n)} + \left(\varepsilon_{K,i}^G\right)^{(n)}$  He<sub>i</sub>  $(Z^{(n)})$ 

### Algorithm 2: Naive algorithm to sample from $\mathcal{L}$

**Input**: N (nonnegative integer),  $(a_1, \ldots, a_K)$  (vector of size K),  $(b_1, \ldots, b_K)$  (vector of size K),  $(\rho_1, \ldots, \rho_K)$  (vector of size K),  $(l_1, \ldots, l_K)$  (vector of size K) **Output**:  $\mathcal{L}^{(1:N)} = (\mathcal{L}^{(1)}, \dots, \mathcal{L}^{(N)})$ 1  $\mathcal{L}^{(1:N)} = (\mathcal{L}^{(1)}, \dots, \mathcal{L}^{(N)}) \leftarrow (0, \dots, 0)$  (vector of size N) **2** for n = 1 ... N do Generate  $Z^{(n)} \sim \mathcal{N}(0,1)$  (scalar) 3 Generate  $(\varepsilon_K)^{(n)} = \left(\varepsilon_{K,1}^{(n)}, \dots, \varepsilon_{K,K}^{(n)}\right) \sim \mathcal{N}(0, \mathrm{Id}_K)$  (vector of size K independent of  $\mathbf{4}$  $Z^{(n)}$ )  $\mathcal{L}^{(n)} \leftarrow 0 \; (\text{scalar})$  $\mathbf{5}$ for  $k = 1 \dots K$  do 6  $\mathcal{L}^{(n)} \leftarrow \mathcal{L}^{(n)} + l_k \mathbf{1}_{a_k \varepsilon_{K,k}^{(n)} + b_k \leq \frac{\rho_k}{|\rho_k|} Z^{(n)}}$ 7

Remark 2. To assess the efficiency of our method, we provide both complexity of the two algorithms, in terms of elementary operations. We assume that any Hermite polynomial of degree ican be computed at one unit cost  $\mathcal{O}(1)$ : this is a reasonable assumption since one usually needs to compute these polynomials at once from degree 0 to I, which can be done by the recursive relation (3.2.5). In order to evaluate the complexity of Algorithm 1, we separate the offline/online parts for the approximation.

 $\triangleright$  Offline computational cost. From Proposition 3.3.1, note that  $\mu_0, \mu_1$  are explicit (unit cost) and each  $(\mu_i)_{i\geq 2}$  requires one unit cost  $\mathcal{O}(1)$  owing to the recursive relation (3.3.1). Hence from the Definition 3.2.25, computing  $m_K$  requires  $\mathcal{O}(KI)$  operations. A similar analysis gives that the computational cost for  $s_K$  using (3.3.2) is  $\mathcal{O}(KI^2)$  and  $\mathcal{O}(I^3)$  for having a Cholesky decomposition of  $s_K$ . Overall the offline cost is  $\mathcal{O}(KI) + \mathcal{O}(KI^2) + \mathcal{O}(I^3) = \mathcal{O}(KI^2)$ , using that usually  $K \gg I$ .

 $\triangleright$  Online computational cost. Once the Cholesky decomposition of  $s_K$  is obtained, sampling  $(\varepsilon_{K,i}^{\mathrm{G}})_{i=0,\ldots,I}$  can be done at cost  $\mathcal{O}(I^2)$ , which implies that our Gaussian-based algorithm for N samples only requires  $\mathcal{O}(NI^2)$  operations.

The total cost of Algorithm 1 is then  $\mathcal{O}(KI^2) + \mathcal{O}(NI^2)$ . On the contrary, the naive Algorithm 2 would require  $\mathcal{O}(NK)$  operations. Remembering that  $K \ge 10^5$  and  $I \le 50$  (which is enough in most cases), the computational cost of Algorithm 1 is much smaller.

This numerical analysis thus shows a significant improvement of the computational cost compared to a naive Monte Carlo scheme. At this point, we try to expose how implementing the GA methodology differs from our approach.

**Comparison with GA approach.** As pointed out in the aforementioned literature, the GA methodology relies on the estimation of the VaR of  $\mathcal{L}$  by that of  $\mathbb{E}[\mathcal{L}|Z]$  which is much easier to compute. More particularly, Fermanian [64, Corollary 3] states that, if Z is one-dimensional, we have:

$$\operatorname{VaR}(\mathcal{L}) \approx \operatorname{VaR}(\mathbb{E}\left[\mathcal{L}|Z\right]) - \frac{1}{2f_{\mathbb{E}[\mathcal{L}|Z]}\left(\operatorname{VaR}(\mathbb{E}\left[\mathcal{L}|Z\right])\right)} \sum_{k=1}^{K} l_k^2 \kappa_k'(\operatorname{VaR}(\mathbb{E}\left[\mathcal{L}|Z\right]))$$
(3.3.3)

with  $\kappa_k(v) = \mathbb{E}[V_k(Z) | \nu_K(Z) = v] f_{\mathbb{E}[\mathcal{L}|Z]}(v), v \in \mathbb{R}, V_k(z) = \text{Var}[Y_k | Z = z], \nu_K(z) = \mathbb{E}[\mathcal{L} | Z = z], z \in \mathbb{R}$ . Here  $f_Y(\cdot)$  stands for the density of the distribution of a scalar random variable Y. As pointed out by the author in the proof of this result, the derivatives of  $\kappa_k$ are explicit because  $\nu_K$  is assumed to be monotonic (the correlations  $\rho_k$  all have the same sign) and Z is one-dimensional. In particular,  $\kappa'_k(v) = \frac{\partial}{\partial v}[V_k(\nu_K^{-1}(v))f_{\mathbb{E}[\mathcal{L}|Z]}(v)]$ . Consequently, the computational cost for calculating the sum of the r.h.s. of the estimation above is  $\mathcal{O}(K)$ . As a result, in this one-factor copula model with positive correlations, the GA approach is quite effective to evaluate one quantile of order  $\alpha$ . Repeating this procedure for many  $\alpha$  gives an approximation of the full distribution of  $\mathcal{L}$ .

In our approach  $\rho_k \in (-1, 1)$ , so that there is no monotonic limitation for  $\nu_K$ . Moreover, had we extended the above GA formula (3.3.3) to the multi-dimensional case for Z, the conditional expectations ( $\mathbb{E}[V_k(Z) | \nu_K(Z) = v] : k \geq 1$ ), the density of  $\nu_K(Z) = \mathbb{E}[\mathcal{L}|Z]$  and their derivatives would not be easily computed. In this case, we would resort to another Monte Carlo scheme (combined with techniques from non-parametric statistics), using N samples of loss, to numerically compute those quantities. However, it changes drastically the global complexity since the computational cost becomes (at least)  $\mathcal{O}(NK)$ . It is comparable to a crude Monte Carlo scheme and therefore is much larger than the one using our meta-model approach (see Subsection 3.3.3 for more details about our meta-model extension to the multi-factor case with the same complexity). To summarize, in the case of correlations with different signs and of multi-factor copula model, the efficiency of GA approach (when K is large) is not guaranteed anymore contrary to the current meta-model approach.

We now want to test such a decomposition and see how well it approximates the true portfolio loss  $\mathcal{L}$ . More precisely, we consider different portfolio scenarios  $\{A, B\}$  as choices need to be made for the *k*th obligor correlation  $\rho_k$ , default probability  $p_k$ , the loss  $l_k$  and the values taken by the macro-economic factor Z. We fix the (large) number of obligors at  $K = 5 \times 10^5$ . For each scenario, we provide:

- The histogram of  $N = 10^4$  samples  $\varepsilon_{K,i}$  together with the normal probability density centered at  $m_{K,i}$  and with variance  $s_{K,i,i}$  for different  $i \in \{1,3,6,8\}$ . Indeed, for a fixed  $i \in \{0, \ldots, I\}$ , we know from Theorem 3.3 that  $\mathbb{E}[\varepsilon_{K,i}] = m_{K,i}$ ,  $\operatorname{Var}[\varepsilon_{K,i}] = s_{K,i,i}$ . We thus want to test how well the  $\varepsilon_{K,i}$  marginals are close to a normal  $\mathcal{N}(m_{K,i}, s_{K,i,i})$ .
- The kernel density estimation (KDE) of  $\mathcal{L}_I$  conditionally on Z from  $N = 10^4$  samples  $\mathcal{L}_I | Z$ and the "true" conditional loss  $\mathcal{L} | Z$  for different economic scenarios  $Z \in \{-1, 0, 1, 2\}$  and truncation parameters  $I \in \{1, 3, 6, 9\}$ .
- The KDE of  $\mathcal{L}$  and  $\mathcal{L}_{I}^{G}$  for  $I \in \{1, 3, 6, 9\}$  with  $N = 10^{5}$  samples.
- In order to assess if  $\mathcal{L}_{I}^{G}$  succeeds in approximating  $\mathcal{L}$  in the tails, we provide the quantilequantile plot of  $\mathcal{L}_{I}^{G}$  w.r.t.  $\mathcal{L}$  for  $I \in \{1, 3, 6, 9, 12, 15\}$  with  $N = 10^{5}$  samples.

<u>Portfolio A</u>: We consider both homogeneous correlation and default probability i.e.  $\forall k \in \{1, \dots, K\}, p_k = 0.01, \rho_k = 0.1$  and take the kth loss of the form  $l_k = \frac{1}{\sqrt{k}}$ . Note that in that

case, we have that  $a_k = \frac{-\sqrt{1-\rho^2}}{|\rho|} = a$ ,  $b_k = \frac{-\Phi^{-1}(p)}{|\rho|} = b$  and for every  $i, j \in \{0, \dots, I\}$ ,  $m_{K,i} = \mu_i(a, b) \frac{\rho^i}{|\rho|^i} \sum_{k=1}^K l_k$ ,  $s_{K,i,j} = \sigma_{i,j}(a, b) \sum_{k=1}^K l_k^2$ . The simplified Lindeberg condition (3.2.28) easily holds as  $\sup_{1 \le k \le K} l_k^2 = 1$  and  $\sum_{k=1}^K \frac{1}{k} \xrightarrow{K \to +\infty} +\infty$ .



Figure 3.7 – Histograms of  $\varepsilon_{K,i}$  with the p.d.f. of  $\mathcal{N}(\mathbb{E}[\varepsilon_{K,i}], \operatorname{Var}[\varepsilon_{K,i}])$  for  $i \in \{1, 3, 6, 9\}$  for the Portfolio A.



Figure 3.8 – KDE of  $\mathcal{L}_{I}^{G}$  for  $I \in \{1, 3, 6, 9\}$  and  $\mathcal{L}$  conditionally on  $Z \in \{-1, 0, 1, 2\}$  for the Portfolio A.



Figure 3.9 – Loss of Portfolio A.



Figure 3.10 – Q-Q plots of  $\mathcal{L}_I^G$  w.r.t.  $\mathcal{L}$  for the Portfolio A.

In Figure 3.7, all marginals  $\varepsilon_{K,i}$  for i = 1, 3, 6, 9 seem to be very close to a normal distribution centered at  $m_{K,i}$  and with variance  $s_{K,i}$  indicating that a Gaussian approximation seems legit. In both Figures 3.8 and 3.9, we see that the Gaussian-based approximation  $\mathcal{L}_I^{\mathrm{G}}$  quickly converges to the 'true' loss  $\mathcal{L}$  for small I as both densities are indistinguishable from I = 3. As for the previous graphs, the Q-Q plot in Figure 3.10 shows a poor approximation for I = 1. From I = 6, the two distributions have almost the same estimated quantiles with an error of approximately  $\frac{2}{N} \times 100 = 0.002\%$  (2 quantiles differ totally when  $\mathcal{L} \geq 36$ ). Notice also that increasing the truncating parameter from I = 6 to I = 9 does not seem to yield any improvement which probably indicates that the error (for those I) comes from the Gaussian approximation of the  $\varepsilon_{K,i}$ .

Simulation of  $\mathcal{L}_3^{\mathrm{G}}$  (with I = 3, the Q-Q plot shows an error of approximately  $\approx 0.002\%$ ) took 112.77 seconds (offline part) + 0.03 seconds (online part) = 112.80 seconds, compared to 1880.44 seconds for the naive Monte Carlo approach. The meta-model being  $\frac{1880.44}{112.80} \approx 17$  times faster, this clearly highlights the benefits of our method in terms of running time compared to a naive Monte Carlo. Note that once we have access to the characteristics  $m_K, s_K$  (most computationally intensive part in our approach), sampling the Gaussian vector is extremely fast (0.03 seconds). This corroborates our computational complexity discussion in Remark 2.

Portfolio B: We consider the same portfolio as in Glasserman and Li [82] i.e.  $\forall k \in \{1, \ldots, K\}$ ,  $p_k = 0.01(1 + \sin(\frac{16\pi k}{K})) + 0.001$ ,  $\rho_k \stackrel{d}{=} \mathcal{U}([0, 1/\sqrt{10}]) + 0.001$  (we add 0.001 so that  $p_k \neq 0$  and  $\rho_k \neq 0$  for every obligor k) and  $l_k = (\lceil \frac{5k}{K} \rceil)^2$ . Note that the marginal default probabilities vary between 0.001% and 2.001% with a mean 1.0005%. The losses  $l_k$  are 1, 4, 9, 16, 25 with  $\frac{K}{5}$  at each level. Notice also that the simplified Lindeberg condition (3.2.28) holds since  $\sup_{1 \leq k \leq K} l_k^2 = 25$  and  $\sum_{k=1}^{K} (\lceil \frac{5k}{K} \rceil)^2 \geq \frac{25}{K^2} \sum_{k=1}^{K} k^2 = \frac{25}{K^2} \frac{K(K+1)(2K+1)}{6} \sim \frac{25}{3} K^2 \xrightarrow[K \to +\infty]{K \to +\infty} +\infty$ . We recall that

 $K = 5 \times 10^5.$ 



Figure 3.11 – Histograms of  $l_k, p_k, \rho_k$  for the Portfolio B.



Figure 3.12 – Histograms of  $\varepsilon_{K,i}$  with the p.d.f. of  $\mathcal{N}(\mathbb{E}[\varepsilon_{K,i}], \operatorname{Var}[\varepsilon_{K,i}])$  for  $i \in \{1, 3, 6, 9\}$  for the Portfolio B.



Figure 3.13 – KDE of  $\mathcal{L}_{I}^{G}$  for  $I \in \{1,3,6,9\}$  and  $\mathcal{L}$  conditionally on  $Z \in \{-1,0,1,2\}$  for the Portfolio B.



Figure 3.14 – Loss of Portfolio B.

In the simplified portfolio A, our approximation seems to give excellent results. We now want to challenge our method by conducting the same analysis with a less homogeneous (and thus more realistic) portfolio. Figures 3.12, 3.13, and 3.14 essentially give the same results as for the Portfolio A where we see that a small I seems to already give satisfactory results. For the Q-Q plot of Figure 3.15 however, we notice that for I = 1, 3 our method is unable to approach accurately the true loss. From I = 6, our approximation provides quite satisfactory results with an error of approximately  $(\frac{10}{N}) \times 100 = 0.01\%$  (10 quantiles differ totally when  $\mathcal{L} \geq 250000$ ). Hence, our approach can be used for the computation of risk measures (such as VaR) up to 99.99% which is probably more than enough for the current regulation. Again notice that increasing the truncating parameter from I = 6 does not seem to give a better approximation. This is probably due to the lack of perfect accuracy of the Gaussian approximation, that is it seems like the global approximation error is only due to the Gaussian approximation error (or central limit error) that we do not control here as K is assumed to be fixed.

Simulation of  $\mathcal{L}_9^{\mathrm{G}}$  (with I = 9, the Q-Q plot shows an error of approximately  $\approx 0.01\%$ ) took 110.50 seconds (offline part) + 0.07 seconds (online part) = 110.57 seconds, compared to 1926.51 seconds for the naive Monte Carlo approach. The meta-model is this time  $\frac{1926.51}{110.57} \approx 17$  times faster.



Figure 3.15 – Q-Q plots of  $\mathcal{L}_{I}^{\mathrm{G}}$  w.r.t.  $\mathcal{L}$  for the Portfolio B.

#### 3.3.3 Extension to the *d*-factor credit model

In this section, we extend our results obtained so far to a *d*-factor Gaussian copula model. For the sake of clarity, we introduce the following standard multi-index notation. For multi-indices  $\mathbf{i} = (i_1, \ldots, i_d), \mathbf{j} = (b_1, \ldots, b_d) \in \mathbb{N}_0^d$  and vector  $\mathbf{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d$ , we write:

- $\mathbf{i} \pm \mathbf{j} = (i_1 \pm j_1, \dots, i_d \pm j_d)$  (component-wise sum and difference).
- $|\mathbf{i}| = i_1 + \dots + i_d$  (sum of components).
- $\mathbf{i}! = i_1! \dots i_d!$  (factorial).
- $\begin{pmatrix} |\mathbf{i}| \\ \mathbf{i} \end{pmatrix} = \frac{|\mathbf{i}|}{\mathbf{i}!} = \frac{|\mathbf{i}|}{i_1!\dots i_d!}$  (multinomial coefficient).
- $\mathbf{x}^{\mathbf{i}} = x_1^{i_1} \dots x_d^{i_d}$  (power).
- $\|\mathbf{x}\| = \sqrt{x_1^2 + \dots + x_d^2}$  (Euclidean norm).

So far our analysis was built on a one-factor (d = 1) model. The extension to a *d*-factor credit model goes as follows (see Glasserman and Li [82]). The default event indicator remains  $Y_k = \mathbf{1}_{\{X_k \ge c_k\}}$  (as for (3.2.2)), with a stochastic factor  $X_k$  given by

$$X_k = \boldsymbol{\rho}_k \cdot \boldsymbol{Z} + \beta_k \varepsilon_k = \sum_{j=1}^d \rho_{kj} Z_j + \beta_k \varepsilon_k,$$

where the *d* systemic factors (each representing an industry sector or a geographic zone)  $\mathbf{Z} = (Z_1, \ldots, Z_d)$  are independent standard normal random variables, and  $\varepsilon_k$  is an idiosyncratic risk factor. The sequence  $(\varepsilon_k)_{k=1,\ldots,K}$  is made of independent standard normal random variables, and independent of the *d* systemic factors.

Without loss of generality, we can assume that the coefficients are adjusted so that the stochastic factor  $X_k$  is standard normal. The factor loadings vector (correlations to the systemic factors) for the *k*th obligor are denoted by  $\boldsymbol{\rho}_k = (\rho_{k1}, \dots, \rho_{kd})$ . Since  $X_k$  is standard normal, we can set  $\beta_k = \sqrt{1 - \|\boldsymbol{\rho}_k\|^2}$ . The constraint  $p_k = \mathbb{P}(Y_k = 1)$  gives again

$$c_k = -\Phi^{-1}(p_k).$$

We now give the extension to both Theorem 3.2 and 3.3 in the *d*-factor Gaussian copula model. **Theorem 3.1.** Let  $d \in \mathbb{N}^*$  and  $I \in \mathbb{N}$ . For every  $k \in \{1, \ldots, K\}$ , define

$$a_k = -\frac{\sqrt{1 - \|\boldsymbol{\rho}_k\|^2}}{\|\boldsymbol{\rho}_k\|}, \quad b_k = -\frac{\Phi(p_k)}{\|\boldsymbol{\rho}_k\|},$$

and set for every multi-indices  $\mathbf{i} = (i_1, \ldots, i_d), \mathbf{j} = (j_1, \ldots, j_d) \in \{0, \ldots, I\}^d$ 

$$\varepsilon_{K,\mathbf{i}} = \sum_{k=1}^{K} l_k \left( \frac{\boldsymbol{\rho}_k}{\|\boldsymbol{\rho}_k\|} \right)^{\mathbf{i}} \left( \begin{array}{c} |\mathbf{i}| \\ \mathbf{i} \end{array} \right) \alpha_{|\mathbf{i}|} \left( a_k \varepsilon_k + b_k \right),$$

where  $\alpha(\cdot)$  has been defined in Proposition 3.2.2. Then, in the d-factor model, the loss  $\mathcal{L}$  and  $\mathcal{L}_I$  write as:

$$\mathcal{L} = \sum_{i=0}^{\infty} \sum_{|\mathbf{i}|=i} \varepsilon_{K,\mathbf{i}} \operatorname{He}_{i_1}(Z_1) \dots \operatorname{He}_{i_d}(Z_d), \quad \mathcal{L}_I = \sum_{i=0}^{I} \sum_{|\mathbf{i}|=i} \varepsilon_{K,\mathbf{i}} \operatorname{He}_{i_1}(Z_1) \dots \operatorname{He}_{i_d}(Z_d).$$
(3.3.4)

The  $L_2$  error for the I-truncated chaos decomposition is the same as in Theorem 3.2 i.e. there exists C > 0,

$$\mathbb{E}\left[\left|\mathcal{L}-\mathcal{L}_{I}\right|^{2}\right] \leq \frac{C}{\sqrt{I}} \left(\sum_{k=1}^{K} l_{k}\right)^{2}.$$
(3.3.5)

Before giving the proof, note that an extension to the CLT (3.2.27) holds also in the *d*-factor Gaussian copula model. For every multi-indices  $\mathbf{i} = (i_1, \ldots, i_d), \mathbf{j} = (j_1, \ldots, j_d) \in \{0, \ldots, I\}^d$ , let

$$m_{K,\mathbf{i}} = \mathbb{E}\left[\varepsilon_{K,\mathbf{i}}\right] = \sum_{k=1}^{K} l_k \left(\frac{\boldsymbol{\rho}_k}{\|\boldsymbol{\rho}_k\|}\right)^{\mathbf{i}} \left(\begin{array}{c}|\mathbf{i}|\\\mathbf{i}\end{array}\right) \mu_{|\mathbf{i}|}\left(a_k, b_k\right),$$
$$s_{K,\mathbf{i},\mathbf{j}} = \mathbb{C}\mathrm{ov}\left(\varepsilon_{K,\mathbf{i}}, \varepsilon_{K,\mathbf{j}}\right) = \sum_{k=1}^{K} l_k^2 \left(\frac{\boldsymbol{\rho}_k}{\|\boldsymbol{\rho}_k\|}\right)^{\mathbf{i}+\mathbf{j}} \left(\begin{array}{c}|\mathbf{i}|\\\mathbf{i}\end{array}\right) \left(\begin{array}{c}|\mathbf{j}|\\\mathbf{j}\end{array}\right) \sigma_{|\mathbf{i}|,|\mathbf{j}|}\left(a_k, b_k\right)$$

and define the associated mean and covariance matrix:

$$m_K = (m_{K,\mathbf{i}} : |\mathbf{i}| = i; i \in \{0, \dots, I\}), \quad s_K = (s_{K,\mathbf{i},\mathbf{j}} : |\mathbf{i}| = i; |\mathbf{j}| = j; i, j \in \{0, \dots, I\}).$$

Under the same assumption (3.2.26), it is natural to approximate the vector

$$\varepsilon_K = (\varepsilon_{K,\mathbf{i}} : |\mathbf{i}| = i; i \in \{0, \dots, I\})$$

with a Gaussian vector  $\varepsilon_K^{\mathbf{G}}$  with mean  $m_K$  and covariance matrix  $s_K$ .

Proof of Theorem 3.1. Remembering that  $c_k = -\Phi^{-1}(p_k)$ , in the *d*-multi-factor model the default event rewrites as:

$$\{X_k \ge c_k\} = \left\{\boldsymbol{\rho}_k \cdot \boldsymbol{Z} + \sqrt{1 - \|\boldsymbol{\rho}_k\|^2} \varepsilon_k \ge c_k\right\} = \left\{\frac{\boldsymbol{\rho}_k}{\|\boldsymbol{\rho}_k\|} \cdot \boldsymbol{Z} \ge a_k \varepsilon_k + b_k\right\},\$$

where  $\frac{\rho_k}{\|\rho_k\|} \cdot \mathbf{Z} = \sum_{j=1}^d \frac{\rho_{kj}}{\sqrt{\rho_{k_1}^2 + \dots + \rho_{k_j}^2}} Z_j \stackrel{d}{=} \mathcal{N}(0,1)$  since the  $(Z_j)_{j=1,\dots,d}$  are i.i.d. standard normal. We can thus apply Proposition 3.2.2 with  $c = a_k \varepsilon_k + b_k$  and  $Z = \frac{\rho_k}{\|\rho_k\|} \cdot \mathbf{Z}$  so that:

$$\mathbf{1}_{X_k \ge c_k} = \sum_{i=0}^{\infty} \alpha_i \left( a_k \varepsilon_k + b_k \right) \operatorname{He}_i \left( \frac{\boldsymbol{\rho}_k}{\|\boldsymbol{\rho}_k\|} \cdot \boldsymbol{Z} \right),$$

at any  $\mathbf{Z}$  such that  $\frac{\boldsymbol{\rho}_k}{\|\boldsymbol{\rho}_k\|} \cdot \mathbf{Z} \neq a_k \varepsilon_k + b_k$ . We now need the following Lemma to proceed with the expansion of the term  $\operatorname{He}_i\left(\frac{\boldsymbol{\rho}_k}{\|\boldsymbol{\rho}_k\|} \cdot \mathbf{Z}\right)$ .

**Lemma 3.3.3.** Let  $d \in \mathbb{N}^*$ ,  $i \in \mathbb{N}$  and  $\mathbf{a} = (a_1, \ldots, a_d)$ ,  $\mathbf{b} = (b_1, \ldots, b_d) \in \mathbb{R}^d$  with  $\|\mathbf{a}\| = 1$ . Then, the following decomposition holds:

$$\operatorname{He}_{i}\left(\mathbf{a}\cdot\mathbf{b}\right) = \sum_{|\mathbf{i}|=i} \mathbf{a}^{\mathbf{i}} \begin{pmatrix} i\\ \mathbf{i} \end{pmatrix} \operatorname{He}_{i_{1}}\left(b_{1}\right) \dots \operatorname{He}_{i_{d}}\left(b_{d}\right)$$

*Proof.* Taking  $x = \mathbf{a} \cdot \mathbf{b}$  in (3.2.14), we first get:

$$e^{\mathbf{a}\cdot\mathbf{b}\,w-\frac{w^2}{2}} = \sum_{i=0}^{\infty} \operatorname{He}_i\left(\mathbf{a}\cdot\mathbf{b}\right)\frac{w^i}{i!}.$$
(3.3.6)

Since  $\|\mathbf{a}\| = 1$ , notice that the exponential rewrites also as:

$$e^{\mathbf{a}\cdot\mathbf{b}\,w-\frac{w^2}{2}} = \prod_{j=1}^d e^{b_j a_j w - \frac{\left(a_j w\right)^2}{2}} = \prod_{j=1}^d \sum_{i_j=0}^\infty \operatorname{He}_{i_j}\left(b_j\right) a_j^{i_j} \frac{w^{i_j}}{i_j!},\tag{3.3.7}$$

where we have applied (3.2.14) with w as  $a_j w$  and x as  $b_j$ . We identify each term of both series and obtain the announced claim by successively taking the derivative w.r.t. w and setting w = 0.

Applying Lemma 3.3.3 with  $\mathbf{a} = \frac{\boldsymbol{\rho}_k}{\|\boldsymbol{\rho}_k\|}$  and  $\mathbf{b} = \mathbf{Z}$ , we obtain:

$$\mathbf{1}_{X_k \ge c_k} = \sum_{i=0}^{\infty} \alpha_i \left( a_k \varepsilon_k + b_k \right) \sum_{|\mathbf{i}|=i} \left( \frac{\boldsymbol{\rho}_k}{\|\boldsymbol{\rho}_k\|} \right)^{\mathbf{i}} \begin{pmatrix} i \\ \mathbf{i} \end{pmatrix} \operatorname{He}_{i_1}(Z_1) \dots \operatorname{He}_{i_d}(Z_d),$$

and this gives (3.3.4). Estimate (3.3.5) remains the same as in Theorem 3.2 noticing that  $\mathcal{L} = \sum_{i=0}^{\infty} \alpha_i (a_k \varepsilon_k + b_k) \operatorname{He}_i \left( \frac{\rho_k}{\|\rho_k\|} \cdot \mathbf{Z} \right)$  with  $\frac{\rho_k}{\|\rho_k\|} \cdot \mathbf{Z} \stackrel{d}{=} \mathcal{N}(0,1)$ . Indeed, as in the proof of Theorem 3.2, we only need the  $(\varepsilon_k)_{1 \leq k \leq K}$  to be independent of Z.

# 3.4 Conclusion

By use of the Wiener chaos decomposition, we have designed a meta-model that significantly reduces the computational effort needed to sample from the loss distribution of a very large credit portfolio. Instead of going over all K obligors, we essentially sum over an I + 1 Gaussian vector whose characteristics can be computed offline. Our approach gives accurate and fast results that have been numerically tested on two different portfolios. We have seen that even with a small I, the approximation performs well even in the tails (up to 99.99% quantile). Such a method can, therefore, be used to estimate risk measures as VaR and CVaR which need to be computed often for regulatory purposes. To further our research, we intend to give an estimate of the Gaussian approximation error between  $\mathcal{L}_I$  and  $\mathcal{L}_I^G$ , so that we could get an estimate of the full error between  $\mathcal{L}$  and  $\mathcal{L}_I^G$ . This is a difficult issue as the Gaussian dimension is asymptotically infinite (as  $I \to +\infty$ ).

# 3.5 Technical proofs

#### 3.5.1 Proof of Proposition 3.2.2

By definition  $\alpha_i(c) = \frac{1}{i!} \mathbb{E} [\mathbf{1}_{c \leq Z} \operatorname{He}_i(Z)]$ . Hence

$$\alpha_0(c) = \mathbb{P}\left(Z \ge c\right) = \Phi\left(-c\right),\tag{3.5.1}$$

and using Equation (3.2.4), we have for every  $i \in \mathbb{N}^*$ :

$$\alpha_{i}(c) = \frac{1}{i!} \int_{c}^{\infty} \operatorname{He}_{i}(z) \frac{e^{-\frac{z^{2}}{2}}}{\sqrt{2\pi}} dz = \frac{(-1)^{i}}{i!\sqrt{2\pi}} \int_{c}^{\infty} \frac{d^{i}}{dz^{i}} \left(e^{-\frac{z^{2}}{2}}\right) dz = \frac{(-1)^{i-1}}{i!\sqrt{2\pi}} \frac{d^{i-1}}{dz^{i-1}} \left(e^{-\frac{z^{2}}{2}}\right) \Big|_{z=c} = \frac{e^{-\frac{c^{2}}{2}} \operatorname{He}_{i-1}(c)}{i!\sqrt{2\pi}}.$$
(3.5.2)

Consequently  $\alpha_1(c) = \frac{e^{-\frac{c^2}{2}}}{\sqrt{2\pi}}$  and using Equation (3.2.5), one has:

$$\alpha_{i+2}(c) = \frac{e^{-\frac{c^2}{2}} \operatorname{He}_{i+1}(c)}{(i+2)!\sqrt{2\pi}} = \frac{e^{-\frac{c^2}{2}}}{(i+2)!\sqrt{2\pi}} \left(c\operatorname{He}_i(c) - i\operatorname{He}_{i-1}(c)\right)$$
$$= \frac{c}{i+2}\alpha_{i+1}(c) - \frac{i}{(i+1)(i+2)}\alpha_i(c).$$

Finally, the explicit expression for  $\alpha$  is a direct consequence of the relation  $\alpha_i(c) = \frac{e^{-\frac{c^2}{2}} \operatorname{He}_{i-1}(c)}{i!\sqrt{2\pi}}$ and Equation (3.2.7).

#### 3.5.2 Proof of Lemma 3.2.3

We proceed as in Szegő [157, Theorem 7.6.1]. Using Equation (3.2.10), a direct computation shows that the function  $z(x) := \text{He}_n(x)e^{-\frac{x^2}{2}}$  solves the following ordinary differential equation (ODE):

$$z''(x) + xz'(x) + (n+1)z(x) = 0.$$

Now let  $(n+1)f(x) := (n+1)\left(\operatorname{He}_n(x)e^{-\frac{x^2}{2}}\right)^2 + \left(\frac{\mathrm{d}}{\mathrm{d}x}\left\{\operatorname{He}_n(x)e^{-\frac{x^2}{2}}\right\}\right)^2$  and notice that  $f(x) = \left(\operatorname{He}_n(x)e^{-\frac{x^2}{2}}\right)^2$  when  $\left(\frac{\mathrm{d}}{\mathrm{d}x}\left\{\operatorname{He}_n(x)e^{-\frac{x^2}{2}}\right\}\right)^2 = 0$ . Further, using the ODE above, we have:

$$(n+1)f'(x) = 2(n+1)\left(\operatorname{He}_n(x)e^{-\frac{x^2}{2}}\right)\frac{\mathrm{d}}{\mathrm{d}x}\left\{\operatorname{He}_n(x)e^{-\frac{x^2}{2}}\right\}$$
$$+ 2\frac{\mathrm{d}}{\mathrm{d}x}\left\{\operatorname{He}_n(x)e^{-\frac{x^2}{2}}\right\}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left\{\operatorname{He}_n(x)e^{-\frac{x^2}{2}}\right\}$$
$$= -2x\left(\frac{\mathrm{d}}{\mathrm{d}x}\left\{\operatorname{He}_n(x)e^{-\frac{x^2}{2}}\right\}\right)^2.$$

For x > 0 (resp. x < 0) the derivative of f is strictly negative (resp. positive) except at a finite number of points. Hence f(x) is (strictly) decreasing on  $x \ge 0$  (resp. increasing on  $x \le 0$ ). Remind that at the points of maxima of  $x \mapsto z^2(x)$ , f(x) and  $z^2(x)$  coincide, whence the announced result.

# 3.5.3 Proof of Corollary 3.2.4

Let us define  $z_n : x \in \mathbb{R} \to \frac{e^{-\frac{x^2}{2}} \operatorname{He}_n(x)}{\sqrt{(n+1)!}}$  and notice that  $z_n^2$  is an even function owing to (3.2.6). We thus restrict our attention to  $x \ge 0$ . It is known that zeros of orthogonal polynomials are both real and distinct (see Szegő [157, Theorem 3.3.1]). Therefore, for any  $m \in \mathbb{N}^*$  we can denote the 2m (resp. 2m-1) zeros of  $\operatorname{He}_{2m}(x)$  (resp.  $\operatorname{He}_{2m-1}(x)$ ) by  $x_{-m,2m} < \cdots < x_{-1,2m} < 0 < x_{1,2m} < \cdots < x_{m,2m}$  (resp.  $x_{-(m-1),2m-1} < \cdots < x_{0,2m-1} = 0 < \cdots < x_{m-1,2m-1}$ ). Also, the derivative of  $z_n^2$  is given by:

$$(z_n^2(x))' \stackrel{(3.2.11)}{=} \frac{1}{(n+1)!} \left( -2xe^{-x^2} \operatorname{He}_n^2(x) + 2e^{-x^2} n \operatorname{He}_n(x) \operatorname{He}_{n-1}(x) \right)$$
  
=  $\frac{2e^{-x^2} \operatorname{He}_n(x)}{(n+1)!} \left( -x \operatorname{He}_n(x) + n \operatorname{He}_{n-1}(x) \right) \stackrel{(3.2.5)}{=} - \frac{2e^{-x^2} \operatorname{He}_n(x) \operatorname{He}_{n+1}(x)}{(n+1)!}.$ 

Therefore, the critical points of  $z_n^2$  are the zeros of He<sub>n</sub> and He<sub>n+1</sub>. But  $z_n^2$  is non-negative, vanishes at the *n* zeros of He<sub>n</sub>, and converges to 0 at  $\pm \infty$ . Therefore, the points of maxima of  $z_n^2$  must be the n + 1 zeros of He<sub>n+1</sub>. By Lemma 3.2.3, the maxima of  $z_n^2$  is achieved at  $x_{0,n} = 0$  (resp.  $x_{1,n}$ ) if *n* is odd (resp. even). In view of (3.2.9), we obtain for any  $n \in \mathbb{N}$ ,

$$M_n = \begin{cases} \frac{\text{He}_{2m}^2(0)}{(2m+1)!} = \frac{(2m)!}{(2m+1)(m!)^2 2^{2m}}, & \text{if } n = 2m, \\ \frac{e^{-(x_{1,2m+2})^2 \text{He}_{2m+1}^2(x_{1,2m+2})}}{(2m+2)!}, & \text{if } n = 2m+1 \end{cases}$$

Let us now prove that  $M_{2m+1} < M_{2m}$  for every  $m \in \mathbb{N}$ . First notice that the following recursive relations for  $z_n$  hold:

$$z_{n+2}(x) = \frac{\operatorname{He}_{n+2}(x) e^{-\frac{x^2}{2}}}{\sqrt{(n+3)!}}$$

$$\begin{array}{l} (3.2.5) & \frac{(x \operatorname{He}_{n+1}(x) - (n+1) \operatorname{He}_{n}(x)) e^{-\frac{x^{2}}{2}}}{\sqrt{(n+3)!}} \\ &= \frac{x \operatorname{He}_{n+1}(x) e^{-\frac{x^{2}}{2}}}{\sqrt{n+3}\sqrt{(n+2)!}} - \frac{(n+1) \operatorname{He}_{n}(x) e^{-\frac{x^{2}}{2}}}{\sqrt{(n+3)(n+2)}\sqrt{(n+1)!}} \\ &= \frac{x}{\sqrt{n+3}} z_{n+1}(x) - \frac{n+1}{\sqrt{(n+3)(n+2)}} z_{n}(x) , \\ z_{n}'(x) \stackrel{(3.2.11)}{=} \frac{(n \operatorname{He}_{n-1}(x) - x \operatorname{He}_{n}(x)) e^{-\frac{x^{2}}{2}}}{\sqrt{(n+1)!}} \\ & \stackrel{(3.2.5)}{=} -\sqrt{n+2} z_{n+1}(x) , \\ z_{n}''(x) \stackrel{(3.5.4)}{=} -\sqrt{n+2} z_{n+1}'(x) \end{array}$$
(3.5.4)

$$\begin{aligned} & \overset{(3.5.4)}{=} -\sqrt{n+2} z_{n+1}(x) \\ & \overset{(3.5.4)}{=} \sqrt{(n+2)(n+3)} z_{n+2}(x) \\ & \overset{(3.5.3)}{=} x\sqrt{n+2} z_{n+1}(x) - (n+1) z_n(x) \\ & \overset{(3.5.4)}{=} -x z'_n(x) - (n+1) z_n(x) . \end{aligned}$$

$$(3.5.5)$$

Now define the map  $f_n : x \to (z_n(x))^2 + \frac{1}{n+1} (z'_n(x))^2 \stackrel{(3.5.4)}{=} (z_n(x))^2 + \frac{n+2}{n+1} (z_{n+1}(x))^2$  whose derivative equals:

$$f'_{n}(x) = 2z'_{n}(x)\left(z_{n}(x) + \frac{z''_{n}(x)}{n+1}\right) \stackrel{(3.5.5)}{=} -\frac{2x}{n+1}\left(z'_{n}(x)\right)^{2}.$$

Hence  $f_n$  is (strictly) decreasing on  $[0, +\infty)$  ( $z'_n$  vanishes only at a finite number of points). Now consider the case where n is even, i.e. n = 2m for  $m \in \mathbb{N}$ . Using that  $x_{1,2m+2} > 0$  we have:

$$f_{2m}(x_{1,2m+2}) < f_{2m}(0).$$
(3.5.6)

On the other hand,  $f_{2m}(0) = (z_{2m}(0))^2 + \frac{2m+2}{2m+1}(z_{2m+1}(0))^2 \stackrel{(3.2.9)}{=} (z_{2m}(0))^2 = M_{2m}$  and  $f_{2m}(x_{1,2m+2}) = (z_{2m}(x_{1,2m+2}))^2 + \frac{2m+2}{2m+1}(z_{2m+1}(x_{1,2m+2}))^2 > M_{2m+1}$ . Finally, owing to (3.5.6) we get:

$$M_{2m+1} < M_{2m},$$

which concludes the proof.

### 3.5.4 Proof of Proposition 3.3.1

In the proof, X, Y, Z are independent standard normal random variables.  $\triangleright$  Results on the mean  $\mu_{\cdot}(\cdot, \cdot)$ . By definition of  $\alpha_0$  (see (3.5.1)), we get:

$$\mu_0(a,b) = \mathbb{E}\left[\Phi\left(-aX - b\right)\right] = \mathbb{E}\left[\mathbb{P}\left(Y < -aX - b \mid X\right)\right].$$

Using that  $aX + Y \stackrel{d}{=} \mathcal{N}(0, 1 + a^2)$ , we get:

$$\mathbb{E}\left[\alpha_0(aX+b)\right] = \Phi\left(-\frac{b}{\sqrt{1+a^2}}\right).$$

Now we compute  $\mu_1(a, b)$ . Invoking the expression of  $\alpha_1(\cdot)$  from (3.5.2), we have:

$$\mu_1(a,b) = \int_{\mathbb{R}} \frac{e^{-\frac{(aX+b)^2}{2}}}{\sqrt{2\pi}} \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} dx = \frac{e^{-\frac{b^2}{2(1+a^2)}}}{\sqrt{2\pi}} \int_{\mathbb{R}} \frac{e^{-\frac{1+a^2}{2}\left(x+\frac{ab}{1+a^2}\right)^2}}{\sqrt{2\pi}} dx = \frac{e^{-\frac{b^2}{2(1+a^2)}}}{\sqrt{2\pi}\sqrt{1+a^2}}.$$

We turn to the derivation of the three-term recurrence relation for  $\mu_i(a, b)$ . From Proposition 3.2.2, it follows that

$$\mu_{i+2}(a,b) = \mathbb{E}\left[\frac{aX+b}{i+2}\alpha_{i+1}(aX+b) - \frac{i}{(i+1)(i+2)}\alpha_i(aX+b)\right]$$
$$= \frac{a}{i+2}\mathbb{E}\left[X\alpha_{i+1}(aX+b)\right] + \frac{b}{i+2}\mu_{i+1}(a,b) - \frac{i}{(i+1)(i+2)}\mu_i(a,b).$$
(3.5.7)

An integration by parts gives

$$\mathbb{E}\left[X\alpha_{i+1}(aX+b)\right] = \frac{(-1)^i}{(i+1)!\sqrt{2\pi}} \int_{\mathbb{R}} x \left.\frac{\mathrm{d}^i}{\mathrm{d}z^i} \left(e^{-\frac{z^2}{2}}\right)\right|_{z=ax+b} \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} \mathrm{d}x$$
$$= \frac{(-1)^i}{(i+1)!\sqrt{2\pi}} a \int_{\mathbb{R}} \left.\frac{\mathrm{d}^{i+1}}{\mathrm{d}z^{i+1}} \left(e^{-\frac{z^2}{2}}\right)\right|_{z=ax+b} \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} \mathrm{d}x$$
$$= -a(i+2)\mu_{i+2}(a,b).$$

Plugging the above into (3.5.7) readily gives

$$(1+a^2)\mu_{i+2}(a,b) = \frac{b}{i+2}\mu_{i+1}(a,b) - \frac{i}{(i+1)(i+2)}\mu_i(a,b).$$

 $\triangleright$  Initialization of the variance/covariance terms. First, we have:

$$\sigma_{0,0}(a,b) = \mathbb{E}\left[\Phi\left(-aX-b\right)^2\right] - \mathbb{E}\left[\Phi\left(-aX-b\right)\right]^2.$$

Now notice that:

$$\mathbb{E}\left[\Phi\left(-aX-b\right)^{2}\right] = \int_{\mathbb{R}} \left(\int_{\mathbb{R}^{2}} \mathbf{1}_{y < -ax-b} \frac{e^{-\frac{y^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}y \mathbf{1}_{z < -ax-b} \frac{e^{-\frac{z^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}z\right) \frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}x$$
$$= \mathbb{E}\left[\mathbf{1}_{Y+aX < -b} \mathbf{1}_{Z+aX < -b}\right]$$

using that X, Y, Z are i.i.d. Whence, since  $Y + aX \stackrel{d}{=} \mathcal{N}(0, 1 + a^2), Z + aX \stackrel{d}{=} \mathcal{N}(0, 1 + a^2)$  and  $\mathbb{C}$ ov  $(Y + aX, Z + aX) = a^2$ , we get

$$\mathbb{E}\left[\Phi\left(-aX-b\right)^{2}\right] = \Phi_{\Sigma}\left(\left(-b,-b\right)^{\top}\right),$$

where  $\Sigma = \begin{pmatrix} 1+a^2 & a^2 \\ a^2 & 1+a^2 \end{pmatrix}$ .

Consider now the covariance. For the sake of clarity, we introduce the notation

$$\rho_{i,j}(a,b) := \mathbb{E}\left[\alpha_i(aX+b)\alpha_j(aX+b)\right] \Longleftrightarrow \sigma_{i,j}(a,b) = \rho_{i,j}(a,b) - \mu_i(a,b)\mu_j(a,b).$$
(3.5.8)

Then, we have:

$$\begin{split} \rho_{0,1}(a,b) &= \mathbb{E} \left[ \alpha_0 (aX+b) \alpha_1 (aX+b) \right] \\ &= \int_{\mathbb{R}} \alpha_0 (aX+b) \alpha_1 (aX+b) \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} \mathrm{d}x \\ &= \int_{\mathbb{R}} \Phi \left( -ax-b \right) \frac{e^{-\frac{(aX+b)^2}{2}}}{\sqrt{2\pi}} \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} \mathrm{d}x \\ &= \frac{e^{-\frac{b^2}{2(1+a^2)}}}{\sqrt{2\pi}} \int_{\mathbb{R}} \Phi \left( -ax-b \right) \frac{e^{-\frac{1+a^2}{2} \left( x + \frac{ab}{1+a^2} \right)^2}}{\sqrt{2\pi}} \mathrm{d}x \end{split}$$

$$= \frac{e^{-\frac{b^2}{2(1+a^2)}}}{\sqrt{2\pi}\sqrt{1+a^2}} \int_{\mathbb{R}} \Phi\left(-\frac{a}{\sqrt{1+a^2}}y - \frac{b}{1+a^2}\right) \frac{e^{-\frac{y^2}{2}}}{\sqrt{2\pi}} dy \qquad (3.5.9)$$
$$= \frac{e^{-\frac{b^2}{2(1+a^2)}}}{\sqrt{2\pi}\sqrt{1+a^2}} \mu_0\left(\frac{a}{\sqrt{1+a^2}}, \frac{b}{1+a^2}\right)$$
$$= \mu_1(a,b)\mu_0\left(\frac{a}{\sqrt{1+a^2}}, \frac{b}{1+a^2}\right),$$

where we have set  $y = \sqrt{1 + a^2}x + \frac{ab}{\sqrt{1+a^2}}$ . We get the announced result for  $\sigma_{0,1}(a,b)$  owing to (3.5.8).

 $\triangleright$  Three-term recurrence relation on variance/covariance. Similarly, using (3.2.17) in Proposition 3.2.2 yields:

$$\begin{aligned} \rho_{0,i+2}(a,b) &= \mathbb{E} \left[ \alpha_0 (aX+b) \alpha_{i+2} (aX+b) \right] \\ &= \frac{a}{i+2} \mathbb{E} \left[ X \alpha_0 (aX+b) \alpha_{i+1} (aX+b) \right] + \frac{b}{i+2} \rho_{0,i+1}(a,b) - \frac{i}{(i+1)(i+2)} \rho_{0,i}(a,b). \end{aligned}$$

Integrating by parts as before gives:

$$\mathbb{E}\left[X\alpha_{0}(aX+b)\alpha_{i+1}(aX+b)\right] = \frac{(-1)^{i}}{(i+1)!\sqrt{2\pi}} \int_{\mathbb{R}} x\Phi\left(-ax-b\right) \frac{\mathrm{d}^{i}}{\mathrm{d}z^{i}} \left(e^{-\frac{z^{2}}{2}}\right) \Big|_{z=ax+b} \frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}x$$
$$= \frac{(-1)^{i}}{(i+1)!\sqrt{2\pi}} \int_{\mathbb{R}} \left(-a\frac{e^{-\frac{(aX+b)^{2}}{2}}}{\sqrt{2\pi}} \frac{\mathrm{d}^{i}}{\mathrm{d}z^{i}} \left(e^{-\frac{z^{2}}{2}}\right) \Big|_{z=ax+b}$$
$$+a\Phi\left(-ax-b\right) \frac{\mathrm{d}^{i+1}}{\mathrm{d}z^{i+1}} \left(e^{-\frac{z^{2}}{2}}\right) \Big|_{z=ax+b} \frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}x. \quad (3.5.10)$$

Using the new variable  $y = \sqrt{1 + a^2}x + \frac{ab}{\sqrt{1+a^2}}$ , we show (similar computations to (3.5.9)) that the first integral is equal to

$$-\frac{a(-1)^{i}e^{-\frac{b^{2}}{2(1+a^{2})}}}{(i+1)!\sqrt{2\pi}\sqrt{1+a^{2}}}\int_{\mathbb{R}}\frac{1}{\sqrt{2\pi}}\left.\frac{\mathrm{d}^{i}}{\mathrm{d}z^{i}}\left(e^{-\frac{z^{2}}{2}}\right)\right|_{z=\frac{a}{\sqrt{1+a^{2}}}y+\frac{b}{1+a^{2}}}\frac{e^{-\frac{y^{2}}{2}}}{\sqrt{2\pi}}\mathrm{d}y$$
$$=-a\mu_{1}(a,b)\mu_{i+1}\left(\frac{a}{\sqrt{1+a^{2}}},\frac{b}{1+a^{2}}\right).$$
(3.5.11)

Besides, the second integral at the right-hand side of (3.5.10) is

$$-\frac{a(-1)^{i+1}(i+2)}{(i+2)!\sqrt{2\pi}}\int_{\mathbb{R}}\Phi\left(-ax-b\right)\left.\frac{\mathrm{d}^{i+1}}{\mathrm{d}z^{i+1}}\left(e^{-\frac{z^2}{2}}\right)\right|_{z=ax+b}\frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}\mathrm{d}x=-a(i+2)\rho_{0,i+2}(a,b)$$

All in all, (3.5.10) becomes finally:

$$(1+a^2) \rho_{0,i+2}(a,b) = -\frac{a^2}{i+2} \mu_1(a,b) \mu_{i+1} \left(\frac{a}{\sqrt{1+a^2}}, \frac{b}{1+a^2}\right) + \frac{b}{i+2} \rho_{0,i+1}(a,b) - \frac{i}{(i+1)(i+2)} \rho_{0,i}(a,b). \quad (3.5.12)$$

Owing to (3.5.8), and by subtracting  $(1 + a^2)\mu_0(a, b)$  times the recursive relation (3.3.1) on  $\mu_1(a, b)$ , the above is equivalent to

$$(1+a^2)\sigma_{0,i+2}(a,b) = -\frac{a^2}{i+2}\mu_1(a,b)\mu_{i+1}\left(\frac{a}{\sqrt{1+a^2}},\frac{b}{1+a^2}\right) + \frac{b}{i+2}\sigma_{0,i+1}(a,b) - \frac{i}{(i+1)(i+2)}\sigma_{0,i}(a,b).$$
 (3.5.13)

The proof of the iterative equation (3.3.2) for  $\sigma_{0,.}(a, b)$  is complete. We now handle the relation on  $\sigma_{i,j}(a, b)$  where  $i, j \in \mathbb{N}$  and proceed analogously. Starting from (3.2.17), write

$$\rho_{i,j+2}(a,b) = \mathbb{E} \left[ \alpha_i (aX+b)\alpha_{j+2}(aX+b) \right]$$
  
=  $\frac{a}{j+2} \mathbb{E} \left[ X \alpha_i (aX+b)\alpha_{j+1}(aX+b) \right] + \frac{b\rho_{i,j+1}(a,b)}{j+2} - \frac{j\rho_{i,j}(a,b)}{(j+1)(j+2)}.$ 

Next, we derive

$$\begin{split} & \mathbb{E}\left[X\alpha_{i}(aX+b)\alpha_{j+1}(aX+b)\right] \\ = & \frac{(-1)^{i-1}}{i!\sqrt{2\pi}} \frac{(-1)^{j}}{(j+1)!\sqrt{2\pi}} \int_{\mathbb{R}} x \frac{\mathrm{d}^{i-1}}{\mathrm{d}z^{i-1}} \left(e^{-\frac{z^{2}}{2}}\right) \Big|_{z=ax+b} \frac{\mathrm{d}^{j}}{\mathrm{d}z^{j}} \left(e^{-\frac{z^{2}}{2}}\right) \Big|_{z=ax+b} \frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}x \\ = & \frac{(-1)^{i-1}}{i!\sqrt{2\pi}} \frac{(-1)^{j}a}{(j+1)!\sqrt{2\pi}} \int_{\mathbb{R}} \left(\frac{\mathrm{d}^{i}}{\mathrm{d}z^{i}} \left(e^{-\frac{z^{2}}{2}}\right) \Big|_{z=ax+b} \frac{\mathrm{d}^{j}}{\mathrm{d}z^{j}} \left(e^{-\frac{z^{2}}{2}}\right) \Big|_{z=ax+b} \\ & \quad + \frac{\mathrm{d}^{i-1}}{\mathrm{d}z^{i-1}} \left(e^{-\frac{z^{2}}{2}}\right) \Big|_{z=ax+b} \frac{\mathrm{d}^{j+1}}{\mathrm{d}z^{j+1}} \left(e^{-\frac{z^{2}}{2}}\right) \Big|_{z=ax+b} \right) \frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}x \\ = & - a\left((i+1)\rho_{i+1,j+1}(a,b) + (j+2)\rho_{i,j+2}(a,b)\right). \end{split}$$

Therefore, all in all, we get

$$(1+a^2)\rho_{i,j+2}(a,b) = -\frac{a^2(i+1)}{j+2}\rho_{i+1,j+1}(a,b) + \frac{b}{j+2}\rho_{i,j+1}(a,b) - \frac{j}{(j+1)(j+2)}\rho_{i,j}(a,b).$$

Accounting for (3.2.17), we obtain

$$(1+a^2)\sigma_{i,j+2}(a,b) = -\frac{a^2(i+1)}{j+2}\rho_{i+1,j+1}(a,b) + \frac{b}{j+2}\sigma_{i,j+1}(a,b) - \frac{j}{(j+1)(j+2)}\sigma_{i,j}(a,b).$$

Now, express  $\rho_{i+1,j+1}(a, b)$  as a function of the other terms and this gives the announced result in (3.3.2).

#### 3.5.5 Proof of Lemma 3.3.2

Let  $A, B \in \mathbb{R}$  and  $X \stackrel{d}{=} \mathcal{N}(0, 1)$ . It is well-known that the moments of the standard normal distribution are given by:

$$\mathbb{E}\left[X^{m}\right] = \int_{\mathbb{R}} x^{m} \frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}x = \begin{cases} 0 & \text{if } m = 2k+1, \ (k \in \mathbb{N}) \\ \frac{(2k)!}{2^{k}k!} & \text{if } m = 2k, \ (k \in \mathbb{N}) \end{cases}.$$
(3.5.14)

From the above relation, we obtain:

$$\mathbb{E}\left[\operatorname{He}_{i}\left(AX+B\right)\right] \stackrel{(3.2.8)}{=} \sum_{m=0}^{i} \binom{i}{m} A^{m}\operatorname{He}_{i-m}\left(B\right) \int_{\mathbb{R}} x^{m} \frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}x$$

$$\stackrel{(3.5.14)}{=} \sum_{k=0}^{\left\lfloor \frac{i}{2} \right\rfloor} \frac{i! A^{2k} \operatorname{He}_{i-2k}\left(B\right)}{2^{k} k! \left(i-2k\right)!}.$$
(3.5.15)

By the identity  $-\frac{(ax+b)^2}{2} - \frac{x^2}{2} = -\frac{1}{2} \left(\sqrt{1+a^2}x + \frac{ab}{\sqrt{1+a^2}}\right)^2 - \frac{b^2}{2(1+a^2)}$ , we have:

$$\mu_i(a,b) \stackrel{(3.2.16)}{=} \frac{1}{\sqrt{2\pi}i!} \int_{\mathbb{R}} \operatorname{He}_{i-1}(ax+b) e^{-\frac{(ax+b)^2}{2}} \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} \mathrm{d}x$$
$$= \frac{e^{-\frac{b^2}{2(1+a^2)}}}{\sqrt{2\pi}i!} \int_{\mathbb{R}} \operatorname{He}_{i-1}(ax+b) \frac{e^{-\frac{1}{2}\left(\sqrt{1+a^2}x + \frac{ab}{\sqrt{1+a^2}}\right)^2}}{\sqrt{2\pi}} \mathrm{d}x$$
$$= \frac{e^{-\frac{b^2}{2(1+a^2)}}}{\sqrt{2\pi}i!\sqrt{1+a^2}} \int_{\mathbb{R}} \operatorname{He}_{i-1}\left(\frac{a}{\sqrt{1+a^2}}y + \frac{b}{1+a^2}\right) \frac{e^{-\frac{y^2}{2}}}{\sqrt{2\pi}} \mathrm{d}y$$

where we have introduced the new variable  $y = \sqrt{1 + a^2}x + \frac{ab}{\sqrt{1+a^2}}$  in the last equality. The expression for  $\mu_i(a, b)$  is then a direct consequence of (3.5.15) with  $A = \frac{a}{\sqrt{1+a^2}}$  and  $B = \frac{b}{1+a^2}$ . Similarly, we get:

$$\mathbb{E}\left[\operatorname{He}_{i}\left(AX+B\right)\operatorname{He}_{j}\left(AX+B\right)\right] \tag{3.5.16}$$

$$= \sum_{m=0}^{i} \sum_{n=0}^{j} \binom{i}{m} \binom{j}{n} A^{m+n}\operatorname{He}_{i-m}\left(B\right)\operatorname{He}_{j-n}\left(B\right) \int_{\mathbb{R}} x^{m+n} \frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}} dx$$

$$= \sum_{k=0}^{\left\lfloor\frac{i}{2}\right\rfloor} \sum_{p=0}^{\left\lfloor\frac{j}{2}\right\rfloor} \binom{i}{2k} \binom{j}{2p} \frac{A^{2(k+p)}\operatorname{He}_{i-2k}\left(B\right)\operatorname{He}_{j-2p}\left(B\right)\left(2\left(k+p\right)\right)!}{2^{k+p}\left(k+p\right)!}$$

$$+ \sum_{k=0}^{\left\lfloor\frac{i-1}{2}\right\rfloor} \sum_{p=0}^{\left\lfloor\frac{j-1}{2}\right\rfloor} \binom{i}{2k+1} \binom{j}{2p+1} \frac{A^{2(k+p+1)}\operatorname{He}_{i-2k-1}\left(B\right)\operatorname{He}_{j-2p-1}\left(B\right)\left(2\left(k+p+1\right)\right)!}{2^{k+p+1}\left(k+p+1\right)!}.$$

From the identity  $-(ax+b)^2 - \frac{x^2}{2} = -\frac{1}{2} \left( \sqrt{1+2a^2}x + \frac{2ab}{\sqrt{1+2a^2}} \right)^2 - \frac{b^2}{1+2a^2}$ , the covariance rewrites as:

$$\begin{split} \sigma_{i,j}\left(a,b\right) &= \frac{1}{2\pi i! j!} \int_{\mathbb{R}} \operatorname{He}_{i-1}(ax+b) \operatorname{He}_{j-1}(ax+b) e^{-(ax+b)^2} \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} \mathrm{d}x - \mu_i\left(a,b\right) \mu_j\left(a,b\right) \\ &= \frac{e^{-\frac{b^2}{1+2a^2}}}{2\pi i! j! \sqrt{1+2a^2}} \int_{\mathbb{R}} \operatorname{He}_{i-1}\left(\frac{a}{\sqrt{1+2a^2}}y + \frac{b}{1+2a^2}\right) \operatorname{He}_{j-1}\left(\frac{a}{\sqrt{1+2a^2}}y + \frac{b}{1+2a^2}\right) \frac{e^{-\frac{y^2}{2}}}{\sqrt{2\pi}} \mathrm{d}y \\ &- \mu_i\left(a,b\right) \mu_j\left(a,b\right), \end{split}$$

where we have introduced this time  $y = \sqrt{1 + 2a^2}x + \frac{2ab}{\sqrt{1+2a^2}}$ . We conclude using (3.5.16) with  $A = \frac{a}{\sqrt{1+2a^2}}$  and  $B = \frac{b}{1+2a^2}$ .

# CHAPTER 4

# POLYNOMIAL CHAOS EXPANSION AND META-MODEL OF LARGE SUMS OF DEPENDENT RANDOM VARIABLES

Note. Working paper with Emmanuel Gobet and Clément Rey.

# 4.1 Introduction

This work proposes a meta-model for the distribution

$$\mathcal{L}_K = \sum_{k=1}^K l_k \mathbf{1}_{Y_k \le X},\tag{4.1.1}$$

where  $X, Y_1, \ldots, Y_K$  are random variables having densities and  $(Y_k)_{k=0...K}$  are independent and independent of X. The parameter K is assumed finite but large. We notice that when X is known,  $\mathcal{L}_K$  writes as a sum of weighted independent Bernoulli random variables i.e. for every  $k \in 1, \ldots, K$ ,

$$\mathbf{1}_{Y_k \leq X} | \, X = x \stackrel{d}{=} \mathcal{B}\left(F_{Y_k}(x)\right), \quad \text{where for every } x, \quad F_{Y_k}(x) = \mathbb{P}\left(Y_k \leq x\right).$$

We are going to build an approximation for  $\mathcal{L}_K$  based on some Gaussian approximation of the random coefficients of a specific chaos decomposition of the random variables  $\mathbf{1}_{Y_k \leq X}$ .

**Standard results.** We will make extensive use of the following tail asymptotic expansion result.

$$\sum_{n=N}^{\infty} \frac{1}{p^m} \underset{N \to \infty}{\sim} \frac{1}{m-1} \frac{1}{N^{m-1}}, \quad \text{for all } m > 1.$$
(4.1.2)

**Special functions** ([146, Chapter 5]).

• Upper incomplete gamma and regularized lower incomplete gamma function:

$$\Gamma_a(z) = \int_z^\infty t^{a-1} e^{-t} dt, \quad \mathscr{G}_a(z) = \frac{1}{\Gamma_a} \int_0^z t^{a-1} e^{-t} dt, \quad a > 0, \ z \ge 0.$$
(4.1.3)

When z = 0, we drop the dependence in z and simply write  $\Gamma_a = \Gamma_a(0)$  for the usual Gamma function.

• Lower incomplete beta and its regularized version:

$$B_{a,b}(x) = \int_0^x t^{a-1} (1-t)^{b-1} dt, \quad \mathscr{B}_{a,b}(x) = \frac{B_{a,b}(x)}{B_{a,b}}, \quad a, b > 0, \ x \in [0,1], \qquad (4.1.4)$$

When x = 1, we drop the dependence in x and simply write  $B_{a,b} = B_{a,b}(1)$  for the usual Beta function. It is well known that the beta function can be expressed in terms of the Gamma function:

$$\mathbf{B}_{a,b} = \frac{\Gamma_a \Gamma_b}{\Gamma_{a+b}}$$

**Probability distributions** (see e.g. Johnson, Kotz, and Balakrishnan [117, Chapters 17, 18] [118, Chapter 25]).

• The random variable X has a Beta distribution with parameters a, b > 0, written  $X \stackrel{d}{=} Beta(a, b)$ , if its density is

$$f(x) = \frac{1}{B_{a,b}} x^{a-1} \left( 1 - x \right)^{b-1}, \quad x \in [0,1].$$
(4.1.5)

Its c.d.f. is given by  $\mathbb{P}(X \leq x) = \mathscr{B}_{a,b}(x)$ .

• The random variable X has a Gamma distribution with parameters a, b > 0, written  $X \stackrel{d}{=} \text{Gamma}(a, b)$ , if its density is

$$f(x) = \frac{b^a}{\Gamma_a} x^{a-1} e^{-bx}, \quad x > 0,$$
(4.1.6)

Its c.d.f. is given by  $\mathbb{P}(X \leq x) = \mathscr{G}_a(bx)$  and for any  $\lambda > 0$ , we have  $\lambda X \stackrel{d}{=} \text{Gamma}(a, \frac{b}{\lambda})$ .

# 4.2 Orthogonal polynomials and polynomial chaos expansion

We start by recalling the definition and some of the main results on orthogonal polynomials. General references are Szegő [157], Chihara [48] and for extensive reviews of their characterizations and main properties see e.g. Al-Salam [5] and Olver et al. [146, Chapter 18].

Let  $\nu(dx) = w(x)dx$  be a probability measure defined on a finite or infinite open interval  $I_w = (a, b)$  in  $\mathbb{R}$ . The nonnegative weight function w(x) is continuous or piecewise continuous or integrable, and such that  $0 < \int_{I_w} x^{2n} w(x) dx$  for all n. The set of polynomial functions  $(p_n)_{n \in \mathbb{N}}$  is said to be an orthogonal polynomials set (OPS) associated with the weight function w(x) (or equivalently with the probability measure  $\nu$ ), if for all  $n, m \in \mathbb{N}$ ,

$$\int_{I_w} p_n(x) p_m(x) w(x) \mathrm{d}x = h_n \delta_{nm}, \qquad (4.2.1)$$

where  $\delta_{nm} = 1$  if n = m or 0 otherwise, and  $h_n := \int_a^b p_n(x)^2 w(x) dx < \infty$ . When  $h_n = 1$ , we say that the polynomials are orthonormalized. Note that the choice of taking  $\nu$  to be a probability measure is specific to our case, and orthogonal polynomials can be defined for any positive measure  $d\alpha(x)$ , where  $\alpha(x)$  is a bounded nondecreasing function on the closure of (a, b)with an infinite number of points of increase and such that  $0 < \int_a^b x^{2n} d\alpha(x)$  (see [157, Sec 2.2]). When the measure  $\nu$  is nonatomic, we talk of continuous orthogonal polynomials. **Orthogonal polynomials of a discrete variable.** In the case when w(x) is a piecewise constant function with jumps  $w_i$  at the points  $X = \{x_i, i \in \mathbb{N}\}$ , the orthogonality condition (4.2.1) rewrites as

$$\sum_{x \in X} p_n(x) p_m(x) w_x = h_n \delta_{nm}.$$

Observe that X can be either a finite or countable infinite set of distinct points on  $\mathbb{R}$ . The polynomials  $p_n(x)$  satisfying such relations are called the orthogonal polynomials of a discrete variable (see Nikiforov, Suslov, and Uvarov [144] for a general reference on discrete orthogonal polynomials).

Askey-scheme. Let us mention that (continuous and discrete) orthogonal polynomials can be listed according to the so-called Askey-scheme of hypergeometric orthogonal polynomials. All of such polynomials can be expressed in terms of hypergeometric functions  ${}_{p}F_{q}(\cdot)$  and are listed according to their free real parameters (see [146, Figure 18.21.1] and Koekoek, Lesky, and Swarttouw [126]). For the continuous (resp. discrete) orthogonal polynomials, the most general polynomials are the Wilson (resp. Racah) polynomials which depend on four parameters. Then, the Continuous dual Hahn and Continuous Hahn (resp. Hahn and Dual Hahn) with three parameters, the Meixner–Pollaczek and Jacobi polynomials (resp. Meixner and Krawtchouk) with two parameters, the Laguerre polynomials (resp. Charlier) with one parameter, and finally the Hermite polynomials.

**Recurrence relation.** A remarkable property of orthogonal polynomials is that they necessarily solve a three-term recurrence relation of the form ([157, Theorem 3.2.1]):

$$p_{n+1}(x) = (A_n x + B_n) p_n(x) - C_n p_{n-1}(x), \quad n \in \mathbb{N}^*,$$
(4.2.2)

where  $A_n, B_n, C_n$  are constants with  $A_n > 0, C_n > 0$ . Note that the converse is also true and is known as Favard's Theorem (see Chihara [48]).

Classical orthogonal polynomials set or COPS. In this work, we will consider a subclass of continuous orthogonal polynomials commonly referred to as the classical orthogonal polynomials set or COPS. These polynomials are the only ones to satisfy to Rodrigues' formula (4.2.3) and the limit conditions (4.2.4), which will be essential to derive closed-form expressions and recurrence relations for the chaos coefficients  $\gamma_n$  (see Propositions 4.2.1 and 4.2.2). This motivates our choice to focus on the COPS which can be completely characterized as follows.

**Theorem 4.1.** (see Al-Salam [5, Section 5], Alvarez Nodarse [6, Theorem 1.2]) The set of orthogonal polynomials  $(p_n(x) : n \in \mathbb{N})$  associated with some measure  $\nu(dx) = w(x)dx$  is said to be a classical orthogonal polynomials set (COPS) if and only if it satisfies one of the following equivalent assertions:

1. For any  $n \ge 0$ ,  $p_n(\cdot)$  satisfies a second order linear differential equation of the Sturm-Liouville type:

$$F(x)\frac{\mathrm{d}^2 p_n}{\mathrm{d}x^2}(x) + G(x)\frac{\mathrm{d}p_n}{\mathrm{d}x}(x) + \lambda_n p_n(x) = 0,$$

where F is a polynomial with deg  $(F) \leq 2$  and G with deg (G) = 1, and are both independent of n, and  $\lambda_n$  is a constant independent of x.

2. The family of polynomials  $\left(\frac{dp_n}{dx}(x), n \in \mathbb{N}\right)$  forms also a COPS.

3. They all satisfy a Rodrigues' type formula of the form:

$$p_n(x) = \frac{1}{\kappa_n w(x)} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left[ F(x)^n w(x) \right], \qquad (4.2.3)$$

for some coefficients  $\kappa_n$ .

4. The weight function  $w(\cdot)$  satisfies the following Pearson's type differential equation

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[F(x)w(x)\right] = G(x)w(x),\tag{4.2.4}$$

with the limit conditions  $\lim_{x\to a} w(x)F(x) = \lim_{x\to b} w(x)F(x) = 0.$ 

In view of this characterization, observe that the only classical orthogonal polynomials are the Hermite, Laguerre (with parameter  $\alpha > -1$ ) and the Jacobi (with parameters  $\alpha, \beta > -1$ ) orthogonal polynomials, for which some of the properties are gathered in Table 4.1 (see e.g. [146]). Special cases of the Jacobi polynomials are the Ultraspherical or Gegenbauer polynomials with  $\alpha = \beta = \lambda$  with  $\lambda > -\frac{1}{2}$  and  $\lambda \neq 0$ , Chebyshev polynomials with  $\alpha = \beta = -\frac{1}{2}$  (first kind),  $\alpha = \beta = \frac{1}{2}$  (second kind),  $\alpha = -\beta = \frac{1}{2}$  (third kind) and  $\beta = -\alpha = \frac{1}{2}$  (fourth kind). Finally, the Legendre polynomials are particular Jacobi polynomials with  $\alpha = \beta = 0$  and they will play a key role in our study.

Name	Hermite	Laguerre	Jacobi	Legendre
Remark		$\alpha > -1$	$\alpha,\beta>-1$	$\text{Jacobi} \left( \alpha = \beta = 0 \right)$
$p_n(x)$	$\operatorname{He}_n(x)$	$\mathcal{L}_n^{(\alpha)}(x)$	$\mathrm{P}_n^{(lpha,eta)}(x)$	$P_n(x)$
(a,b)	$(-\infty,\infty)$	$(0,\infty)$	(-1,1)	(-1,1)
w(x)	$\frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}$	$\frac{x^{\alpha}e^{-x}}{\Gamma_{\alpha+1}}$	$rac{(1-x)^lpha(1+x)^eta}{2^{lpha+eta+1}\mathrm{B}_{lpha+1,eta+1}}$	$\frac{1}{2}$
ν	$\mathcal{N}\left(0,1 ight)$	$Gamma(\alpha+1,1)$	$1 - 2 \text{Beta}  (\alpha + 1, \beta + 1)^1$	$\mathcal{U}\left(-1,1 ight)$
$p_0(x)$	1	1	1	1
$p_1(x)$	x	$1 + \alpha - x$	$\alpha + 1 + \frac{(\alpha + \beta + 2)(x - 1)}{2}$	x
$h_n$	n!	$\frac{1}{n!} \frac{\Gamma_{n+\alpha+1}}{\Gamma_{\alpha+1}}$	$\frac{\Gamma_{n+\alpha+1}\Gamma_{n+\beta+1}}{(2n+\alpha+\beta+1)\Gamma_{n+\alpha+\beta+1}n!B_{\alpha+1,\beta+1}}$	$\frac{2}{2n+1}$
$A_n$	1	$-\frac{1}{n+1}$	$\frac{(\alpha+\beta+2n+1)(\alpha+\beta+2n+2)}{2(n+1)(\alpha+\beta+n+1)}$	$\frac{2n+1}{n+1}$
$B_n$	0	$\frac{2n+\alpha+1}{n+1}$	$\frac{\left(\alpha^2 - \beta^2\right)(\alpha + \beta + 2n + 1)}{2(n+1)(\alpha + \beta + n + 1)(\alpha + \beta + 2n)}$	0
$C_n$	n	$\frac{n+\alpha}{n+1}$	$\frac{(\alpha+n)(\beta+n)(\alpha+\beta+2n+2)}{(n+1)(\alpha+\beta+n+1)(\alpha+\beta+2n)}$	$\frac{n}{n+1}$
F(x)	1	x	$1-x^2$	$1 - x^2$
G(x)	-x	$\alpha + 1 - x$	$\beta - \alpha - (\alpha + \beta + 2) x$	-2x
$\kappa_n$	$(-1)^n$	n!	$(-2)^n  n!$	$(-2)^n n!$

Table 4.1 – Some properties for the classical orthogonal polynomials.

Remark 8. From (4.1.5), the density function of the random variable  $X \stackrel{d}{=} \text{Beta}(\alpha + 1, \beta + 1)$  is given by  $f_X(x; \alpha, \beta) = \frac{x^{\alpha}(1-x)^{\beta}}{B_{\alpha+1,\beta+1}} \mathbf{1}_{x\in[0,1]}$ . Hence, the probability density function of Y = 1 - 2X is equal to  $f_Y(y; \alpha, \beta) = \frac{2^{-\alpha-\beta-1}}{B_{\alpha+1,\beta+1}} (1-y)^{\alpha} (1+y)^{\beta} \mathbf{1}_{y\in[-1,1]}$ . Indeed, for every bounded positive function g,

$$\mathbb{E}\left[g\left(1-2X\right)\right] = \int_{0}^{1} g\left(1-2x\right) \frac{x^{\alpha} \left(1-x\right)^{\beta}}{B_{\alpha+1,\beta+1}} dx \stackrel{y=1-2x}{=} \frac{2^{-\alpha-\beta-1}}{B_{\alpha+1,\beta+1}} \int_{-1}^{1} g\left(y\right) \left(1-y\right)^{\alpha} \left(1+y\right)^{\beta} dy.$$

1

**Polynomial Chaos Expansion (PCE).** Let  $(p_n)_{n \in \mathbb{N}}$  be an OPS for a probability measure  $\nu(dx) = w(x)dx$  and introduce  $c \in \mathbb{R}$ . As soon as  $X \stackrel{d}{=} \nu$ , the following PCE holds

$$\mathbf{1}_{c \le X} \stackrel{L_2(\nu)}{=} \sum_{n=0}^{\infty} \gamma_n(c) p_n(X), \quad \gamma_n(c) = \frac{\mathbb{E}\left[\mathbf{1}_{c \le X} p_n(X)\right]}{h_n} = \frac{\int_c^b p_n(x) w(x) \mathrm{d}x}{\int_a^b p_n^2(x) w(x) \mathrm{d}x}, \tag{4.2.5}$$

where we recall that  $h_n = \mathbb{E}\left[p_n(X)^2\right]$ . In practice, one has to truncate the sum above at some order  $N \in \mathbb{N}^*$ , and consider

$$\sum_{n=0}^{N} \gamma_n(c) p_n(X).$$

We will also be interested in estimating the  $L_2$  error between  $\mathbf{1}_{c \leq X}$  and  $\sum_{n=0}^{N} \gamma_n(c) p_n(X)$  i.e.

$$\mathcal{E}_{N}(c) = \mathbb{E}\left[\left|\mathbf{1}_{c\leq X} - \sum_{n=0}^{N} \gamma_{n}(c)p_{n}(X)\right|^{2}\right]^{\frac{1}{2}}$$
$$= \mathbb{E}\left[\left|\sum_{n=N+1}^{\infty} \gamma_{n}(c)p_{n}(X)\right|^{2}\right]^{\frac{1}{2}}$$
$$= \left|\sum_{n=N+1}^{\infty} h_{n}\gamma_{n}(c)^{2}\right|^{\frac{1}{2}}, \qquad (4.2.6)$$

where we have used the orthogonality condition (4.2.1) for the last equality.

#### 4.2.1 Chaos decomposition of the indicator function for the COPS.

We restrict our attention to the COPS associated with a probability measure  $\nu(dx) = w(x)dx$ and assume that  $X \stackrel{d}{=} \nu$ . As explained above, w(x) can refer to the Hermite or Laguerre or Jacobi polynomials which are associated with the Normal or Gamma or Beta distributions. For the COPS, equality (4.2.5) holds not only in  $L_2(\nu)$  but for all  $X \neq c$  with  $c \in I_w$ . Recall that  $I_w = (-\infty, \infty)$  for the Hermite polynomials,  $I_w = (0, \infty)$  for the Laguerre polynomials, and  $I_w = (-1, 1)$  for the Jacobi polynomials. Furthermore, all coefficients  $\gamma_n(c)$  admit a closed-form representation and they all satisfy a three-term recurrence relation.

**Proposition 4.2.1.** Let  $(p_n)_{n \in \mathbb{N}}$  be a COPS w.r.t.  $\nu$ ,  $\nu(dx) = w(x)dx$ ,  $X \stackrel{d}{=} \nu$  and let  $c \in I_w$ . Then,

$$\forall X \neq c, \quad \mathbf{1}_{c \leq X} = \sum_{n=0}^{\infty} \gamma_n(c) p_n(X).$$

where the coefficients  $\gamma_n(\cdot)$  have been defined in (4.2.5). Furthermore, for every  $n \in \mathbb{N}^*$ ,

• If  $\nu = \mathcal{N}(0, 1)$ ,

$$\gamma_0(c) = \Phi(-c), \quad \gamma_1(c) = \frac{e^{-\frac{c^2}{2}}}{\sqrt{2\pi}}, \quad \gamma_n(c) = \frac{e^{-\frac{c^2}{2}} \operatorname{He}_{n-1}(c)}{n!\sqrt{2\pi}}.$$
 (4.2.7)

• If 
$$\nu = \text{Gamma}(\alpha + 1, 1)$$
,

$$\gamma_{0}(c) = \frac{\Gamma_{\alpha+1}(c)}{\Gamma_{\alpha+1}}, \quad \gamma_{1}(c) = -\frac{c^{1+\alpha}e^{-c}}{\Gamma_{\alpha+2}},$$
$$\gamma_{n}(c) = -\frac{(n-1)!}{\Gamma_{n+\alpha+1}}c^{\alpha+1}e^{-c}\mathcal{L}_{n-1}^{(\alpha+1)}(c) = \frac{(n-1)!}{\Gamma_{n+\alpha+1}}c^{\alpha}e^{-c}\left(n\mathcal{L}_{n}^{(\alpha)}(c) - (n+\alpha)\mathcal{L}_{n-1}^{(\alpha)}(c)\right).$$
(4.2.8)

• If  $\nu = 1 - 2 \text{Beta} (\alpha + 1, \beta + 1)$ ,

$$\gamma_{0}(c) = \mathscr{B}_{\alpha+1,\beta+1}\left(\frac{1-c}{2}\right),$$

$$\gamma_{1}(c) = \frac{\alpha+\beta+3}{(\alpha+1)(\beta+1)} \frac{(\alpha+1)B_{\alpha+1,\beta+1}\left(\frac{1-c}{2}\right) - (\alpha+\beta+2)B_{\alpha+2,\beta+1}\left(\frac{1-c}{2}\right)}{B_{\alpha+1,\beta+1}},$$

$$\gamma_{n}(c) = C(n,\alpha,\beta)(1-c)^{\alpha+1}(1+c)^{\beta+1}P_{n-1}^{(\alpha+1,\beta+1)}(c) \qquad (4.2.9)$$

$$= \frac{2C(n,\alpha,\beta)(1-c)^{\alpha}(1+c)^{\beta}}{(2n+\alpha+\beta)(n+\alpha+\beta+1)} \times \left(n(\alpha-\beta-(2n+\alpha+\beta)c)P_{n}^{(\alpha,\beta)}(c) + 2(n+\alpha)(n+\beta)P_{n-1}^{(\alpha,\beta)}(c)\right),$$
where  $C(n,\alpha,\beta) = \frac{(2n+\alpha+\beta+1)\Gamma_{n+\alpha+\beta+1}(n-1)!}{2^{\alpha+\beta+2}\Gamma_{n+\alpha+1}\Gamma_{n+\beta+1}} = \frac{1}{2^{\alpha+\beta+2}B_{\alpha+1,\beta+1}nh_{n}(\alpha,\beta)}.$ 
If  $\nu = \mathcal{U}(-1,1) = 1 - 2\text{Beta}(1,1),$ 

$$\gamma_{0}(c) = \frac{1-c}{2}, \quad \gamma_{1}(c) = \frac{3}{4} - \frac{c^{2}}{4},$$

$$\gamma_{n}(c) = \frac{2n+1}{2(n+1)}(-cP_{n}(c) + P_{n-1}(c))$$

$$= (1-c^{2}) \frac{2n+1}{2(n+1)} \frac{dP_{n}(c)}{d(n+1)} \qquad (4.2.10)$$

$$= (1 - c^{2}) \frac{2(n+1)n}{2(n+1)n} \frac{dc}{\sum_{j=0}^{\lfloor \frac{n-1}{2} \rfloor}} (2(n-1-2j)+1) P_{n-1-2j}(c).$$

This second result gives a three-term recurrence relation for the chaos coefficients  $\gamma_n(c)$ . The main interest of this result relies in the fact that the implementation of the meta-model (see Theorem 4.2.5) may be computationally intensive.

**Proposition 4.2.2** (Recurrence relation for the  $\gamma_n(\cdot)$ ). For every  $n \in \mathbb{R}$ , the following recurrence relation holds for the parameters  $\gamma_n(c)$ ,

$$\gamma_{n+2}(c) = (B_{n+1} + A_{n+1}c) \frac{h_{n+1}}{h_{n+2}} \gamma_{n+1}(c) - C_{n+1} \frac{h_n}{h_{n+2}} \gamma_n(c) + \frac{h_{n+1}}{h_{n+2}} A_{n+1} \int_c^b \gamma_{n+1}(x) \mathrm{d}x. \quad (4.2.11)$$

Consequently for the COPS,

• If  $\nu = \mathcal{N}(0, 1)$ ,

- $\gamma_{n+2}(c) = \frac{c}{(n+2)}\gamma_{n+1}(c) \frac{n}{(n+1)(n+2)}\gamma_n(c).$ (4.2.12)
- If  $\nu = \text{Gamma}(\alpha + 1, 1)$ ,

$$\gamma_{n+2}(c) = \frac{2n+\alpha+2-c}{n+\alpha+2}\gamma_{n+1}(c) - \frac{n}{n+\alpha+2}\gamma_n(c).$$
(4.2.13)

• If  $\nu = 1 - 2 \text{Beta} (\alpha + 1, \beta + 1)$ ,

$$\gamma_{n+2}(c) = D(n,\alpha,\beta)\gamma_{n+1}(c) + E(n,\alpha,\beta)\gamma_n(c), \qquad (4.2.14)$$

where

$$D(n, \alpha, \beta) = \frac{(\alpha + \beta + n + 2)(\alpha + \beta + 2n + 5) [(\alpha - \beta)(\alpha + \beta + 2) + c(\alpha + \beta + 2n + 2)(\alpha + \beta + 2n + 4)]}{2(\alpha + n + 2)(\beta + n + 2)(\alpha + \beta + n + 3)(\alpha + \beta + 2n + 2)},$$
$$E(n, \alpha, \beta) = -\frac{n(\alpha + \beta + n + 1)(\alpha + \beta + n + 2)(\alpha + \beta + n + 3)(\alpha + \beta + 2n + 4)(\alpha + \beta + 2n + 5)}{(\alpha + n + 2)(\beta + n + 2)(\alpha + \beta + n + 3)(\alpha + \beta + 2n + 1)(\alpha + \beta + 2n + 2)}.$$

• If  $\nu = \mathcal{U}(-1, 1)$ ,

$$\gamma_{n+2}(c) = \frac{2n+5}{n+3}c\gamma_{n+1}(c) - \frac{(2n+5)n}{(n+3)(2n+1)}\gamma_n(c).$$
(4.2.15)

**Extension to**  $l(X)\mathbf{1}_{X\leq c}$ . Following the approach of (4.2.5), we now consider the chaos decomposition of  $l(X)\mathbf{1}_{X\leq c}$ . More precisely when  $X \stackrel{d}{=} \nu$ , it holds that for every measurable function  $l \in L_2(\nu)$ ,

$$l(X)\mathbf{1}_{c\leq X} \stackrel{L_2(\nu)}{=} \sum_{n=0}^{\infty} \Gamma_{l,n}(c)p_n(X), \quad \Gamma_{l,n}(c) = \frac{\mathbb{E}[l(X)\mathbf{1}_{c\leq X}p_n(X)]}{h_n}.$$
 (4.2.16)

Observe that performing a second chaos decomposition on l(X) leads to the following equivalent formulation for the coefficients  $\Gamma_{f,n}(c)$ ,

$$\Gamma_{l,n}(c) = \sum_{m=0}^{\infty} \frac{\mathbb{E}\left[\mathbf{1}_{c \leq X} p_n(X) p_m(X)\right]}{h_n h_m} \mathbb{E}\left[l(X) p_m(X)\right].$$

In order to express  $\Gamma_{f,n}(c)$  as a function of  $\gamma_n(c)$ , we need a linearization-type formula for the product of two orthogonal polynomials (see [11, Lecture 5]). Doing so for the COPS leads to the following extended formulas.

**Proposition 4.2.3.** For the COPS, the following assertions hold:

- If  $\nu = \mathcal{N}(0, 1)$ ,  $\Gamma_{f,n}(c) = \sum_{m=0}^{\infty} \left( \sum_{r=0}^{m \wedge n} \frac{\gamma_{m+n-2r}(c)}{(m+n-2r)!r!(n-r)!(m-r)!} \right) \mathbb{E}\left[ l(X) \operatorname{He}_{m}(X) \right].$
- If  $\nu = \text{Gamma}(\alpha + 1, 1)$ ,

$$\Gamma_{f,n}(c) = \sum_{m=0}^{\infty} \left( \sum_{r=|m-n|}^{m+n} C_{r,m,n}^{\mathrm{L}} \gamma_r(c) \right) \mathbb{E} \left[ l(X) \mathcal{L}_m^{(\alpha)}(X) \right],$$

where

$$C_{r,m,n}^{L} = {}_{3}F_{2} \left( \begin{array}{c} \alpha + r + 1, \frac{1}{2} \left( r - m - n \right), \frac{1}{2} \left( r - m - n + 1 \right) \\ r - m + 1, r - n + 1 \end{array} ; 1 \right) \frac{\left( -1 \right)^{m+n-r} 2^{m+n-r} n! m!}{\left( r - m \right)! \left( r - n \right)! \left( m + n - r \right)!} \frac{\Gamma_{r+\alpha+1} \Gamma_{\alpha+1}}{\Gamma_{n+\alpha+1} \Gamma_{m+\alpha+1}},$$

and  $_{3}F_{2}(\cdot)$  denotes the generalized hypergeometric series <sup>2</sup> ([146, Chapter 16]).

• If  $\nu = 1 - 2 \text{Beta} (\alpha + 1, \beta + 1)$ ,

$$\Gamma_{f,n}(c) = \sum_{m=0}^{\infty} \left( \sum_{r=0}^{m+n} C^{\mathbf{J}}_{r,m,n} \gamma_r(c) \right) \mathbb{E} \left[ l(X) \mathbf{P}_m^{(\alpha,\beta)}(X) \right],$$

where  $h_n = \frac{\Gamma_{n+\alpha+1}\Gamma_{n+\beta+1}}{(2n+\alpha+\beta+1)\Gamma_{n+\alpha+\beta+1}n!B_{\alpha+1,\beta+1}}$  (see Table 4.1) and  $C_{r,m,n}^{\rm J} = \frac{(\alpha+\beta+1)_{n+m-r}(\alpha+1)_{n+m}(2(n+m-r)+\alpha+\beta+1)}{(\alpha+1)_{n+m-r}(\alpha+\beta+1)_{2(n+m)-r+1}}$ 

 $\overline{\left[\begin{array}{c} 2 \\ p F_q \left(\begin{array}{c} a_1, \dots, a_p \\ b_1, \dots, b_q \end{array}; z\right) = \sum_{k=0}^{\infty} \frac{(a_1)_k \dots (a_p)_k}{(b_1)_k \dots (b_q)_k} \frac{z^k}{k!}. \text{ where } (x)_n = \frac{\Gamma(x+n)}{\Gamma(x)} = x \, (x+1) \dots (x+n-1), \, x > 0, n \in \mathbb{N}^*, \text{ denote the rising factorial or Pochhammer symbol.} \end{array}\right]$ 

$$\times \frac{(-1)^{r} (n+m)! (\alpha + \beta + 1)_{2n} (\alpha + \beta + 1)_{2m}}{n!m!r! (\alpha + \beta + 1)_{n} (\alpha + \beta + 1)_{m}} \\ \times F_{2:1}^{2:2} \left( \begin{array}{c} -r, -\alpha - \beta - 1 - 2 (n+m) + r : -n, -\alpha - n; -m; -\alpha - m; \\ -(n+m), -\alpha - (n+m) : -2n - \alpha - \beta; -2j - \alpha - \beta \end{array} \right) \\ \times \frac{h_{n+m-r}}{h_{n}h_{m}},$$

where  $F_{2:1}^{2:2}(\cdot)$  is Kampé de Fériet's <sup>3</sup> function (see Ragab [150]).

Remark 9. Suppose that l(x) writes as a power series  $l(x) = \sum_{p=0}^{\infty} l_p x^p$  for every  $x \in I_w$ . In light of Proposition 4.2.3, it suffices to simplify the term  $\mathbb{E}[l(X)p_m(X)] = \sum_{p=0}^{\infty} l_p \mathbb{E}[X^p p_m(X)]$ . This is easily achieved thanks to the orthogonality condition (4.2.1) along with the Connection Formulas (see [146, 18.18(iv)]) i.e. for every  $p \in \mathbb{N}$ ,

$$x^{p} = p! \sum_{l=0}^{\left\lfloor \frac{p}{2} \right\rfloor} \frac{\operatorname{He}_{p-2l}(x)}{2^{l}l! (p-2l)!} = (\alpha+1)_{p} \sum_{l=0}^{p} \frac{(-p)_{l}}{(\alpha+1)_{l}} \mathcal{L}_{l}^{(\alpha)}(x),$$
$$\left(\frac{1+x}{2}\right)^{p} = \frac{(\beta+1)_{p}}{(\alpha+\beta+2)_{p}} \sum_{l=0}^{p} \frac{\alpha+\beta+2l+1}{\alpha+\beta+1} \frac{(\alpha+\beta+1)_{l} (p-l+1)_{l}}{(\beta+1)_{l} (p+\alpha+\beta+2)_{l}} \mathcal{P}_{l}^{(\alpha,\beta)}(x).$$

For example when  $\nu = \mathcal{N}(0, 1)$ , we have for all  $m \in \mathbb{N}$ ,

$$\mathbb{E}\left[l(X)\operatorname{He}_{m}(X)\right] = \sum_{p=0}^{\infty} l_{p}\mathbb{E}\left[X^{p}\operatorname{He}_{m}(X)\right] = \sum_{p=0}^{\infty} l_{p}p! \sum_{l=0}^{\lfloor \frac{p}{2} \rfloor} \frac{\mathbb{E}\left[\operatorname{He}_{p-2l}(X)\operatorname{He}_{m}(X)\right]}{2^{l}l! (p-2l)!}$$

#### **4.2.2** $L_2$ error

 $\mathcal{E}_N$ 

In this section, we provide estimates for the  $L_2$  error between  $\mathbf{1}_{c \leq X}$  and  $\sum_{n=0}^{N} \gamma_n(c) p_n(X)$  which is given by (see (4.2.6)),

$$\mathcal{E}_N(c) = \left| \sum_{n=N+1}^{\infty} h_n \gamma_n(c)^2 \right|^{\frac{1}{2}}.$$

We will explicit the dependence of the basis for the  $L_2$  error i.e. we write  $\mathcal{E}_N^{\text{He}}(\cdot)$  for the Hermite polynomials,  $\mathcal{E}_N^{\text{Le}}(\cdot)$  for the Legendre polynomials,  $\mathcal{E}_N^{\text{J}}(\cdot)$  for the Jacobi polynomials and  $\mathcal{E}_N^{\text{La}}(\cdot)$  for the Laguerre polynomials.

**Theorem 4.2.4.** There exists a positive constant A, independent of N and c, such that the following global estimates hold:

$$\left(1 \vee |c|^{\frac{1}{6}} \vee |c|^{\frac{4}{3}} N^{-\frac{7}{3}}\right) e^{-\frac{c^2}{4}} N^{-\frac{1}{4}} =: \mathcal{E}_N^{\mathrm{He}}(c), \ c \in \mathbb{R}, \nu = \mathcal{N}(0, 1),$$

$$(4.2.17)$$

$$(c) \leq A \left\{ \begin{array}{c} c^{\frac{\alpha}{2} + \frac{1}{4}} \left( 1 \lor c^{\frac{5}{4}} N^{-\frac{1}{4}} \right) e^{-\frac{c}{2}} N^{-\frac{1}{4}} =: \mathcal{E}_{N}^{\mathrm{La}}(c), \ c \in [0, \infty), \alpha \notin \mathbb{N}, \nu = \mathrm{Gamma}\left(\alpha + 1, 1\right), \ (4.2.18) \right\} \right\}$$

$$(1-c)^{\frac{\alpha}{2}+\frac{1}{4}}(1+c)^{\frac{\beta}{2}+\frac{1}{4}}N^{-\frac{1}{4}} =: E_N^J(c), \ c \in [-1,1], \nu = 1-2\text{Beta}(\alpha+1,\beta+1), \ (4.2.19)$$

$$\left( (1-c^2)^{\frac{1}{4}} N^{-\frac{1}{2}} =: \mathcal{E}_N^{\text{Le}}(c), \ c \in [-1,1], \nu = \mathcal{U}(-1,1). \right)$$
(4.2.20)

Furthermore, the following localized estimates hold. For the Hermite polynomials: let a > 0 and  $0 < \eta < 2$ , then there exists a positive constant B (depending on a and  $\eta$ ) such that:

$$\mathcal{E}_{N}^{\text{He}}(c) \le B(a,\eta) \begin{cases} c^{\frac{1}{3}}e^{-\frac{c^{2}}{4}}N^{-\frac{1}{4}}, & |c| \in [a,\infty), \\ c^{-\frac{c^{2}}{4}}N^{-\frac{1}{4}}, & |c| \in [a,\infty), \end{cases}$$
(4.2.21)

$$(4.2.22)$$

$${}^{3}F_{r:s}^{p:q}\left(\begin{array}{c}a_{1},\ldots,a_{p}:b_{1},b_{1}';\ldots;b_{q},b_{q}';\\c_{1},\ldots,c_{r}:d_{1},d_{1}';\ldots;d_{s},d_{s}';\end{array};x,y\right)=\sum_{m,n=0}^{\infty}\frac{(a_{1})_{m+n}\cdots(a_{p})_{m+n}}{(c_{1})_{m+n}\cdots(c_{r})_{m+n}}\frac{(b_{1})_{m}(b_{1}')_{n}\cdots(b_{q})_{m}(b_{q}')_{n}}{(d_{1})_{m}(d_{1}')_{n}\cdots(d_{q})_{m}(d_{q}')_{n}}\frac{x^{m}y^{n}}{m!n!}.$$

For the Laguerre polynomials: let a > 0 and  $0 < \eta < 4$ , then there exists a positive constant C (depending on a and  $\eta$ ) such that:

$$\mathcal{E}_{N}^{\text{La}}(c) \le C(a,\eta) \begin{cases} c^{\frac{\alpha}{2} + \frac{5}{12}} e^{-\frac{c}{2}} N^{-\frac{1}{4}}, & |c| \in [a,\infty), \\ a + 1 - c - 1 & |c| \in [a,\infty), \end{cases}$$
(4.2.23)

$$V(r) = V(r) \left( c^{\frac{\alpha}{2} + \frac{1}{4}} e^{-\frac{c}{2}} N^{-\frac{1}{4}}, \quad |c| \in [a, (4 - \eta)N].$$
(4.2.24)

Remark 10. Let us briefly comment on each of these truncation orders.

- The order  $\mathcal{O}\left(N^{-\frac{1}{4}}\right)$  for the Jacobi polynomials take into account large values of  $\alpha$  and  $\beta$ . More precisely, for small enough values of  $\alpha, \beta$  the  $L_2$  error for the Jacobi polynomials will be similar to that of the Legendre case (see Figure 4.1 for the Jacobi polynomials with  $\alpha = 3, \beta = 4$ ).
- For no extreme values of c, that is  $c = \pm \infty$  for the Hermite polynomials, c = 0 and  $c = +\infty$  for the Laguerre polynomials and  $c = \pm 1$  for the Jacobi polynomials, we have an  $L_2$  error of order  $\mathcal{O}\left(N^{-\frac{1}{4}}\right)$  for all polynomials except the Legendre polynomials which exhibit and faster decrease of order  $\mathcal{O}\left(N^{-\frac{1}{2}}\right)$ . The order  $\mathcal{O}\left(N^{-\frac{1}{4}}\right)$  seems rather poor for the truncation to be effective. Yet, the principal significance of Theorem 4.2.4 lies in the fact that it keeps track of the dependence on the parameter c. More precisely, it reveals an exponential factor  $e^{-\frac{c^2}{4}}$  (resp.  $e^{-\frac{c}{2}}$ ) for the Hermite (resp. Laguerre) polynomials which ensures a faster decrease for large values of c (see Section 4.3.2).
- Combining (4.2.22) with a = 1,  $\eta = 1$  and (4.2.17), we have the existence of an independent positive constant  $A_1$  such that

$$\mathcal{E}_N^{\text{He}}(c) \le A_1 e^{-\frac{c^2}{4}} N^{-\frac{1}{4}}, \quad |c| \in \left[0, N^{\frac{1}{2}}\right].$$
 (4.2.25)

Similarly, combining (4.2.24) with a = 1,  $\eta = 3$ , and (4.2.18), we have the existence of an independent positive constant  $A_2$  such that

$$\mathcal{E}_N^{\text{La}}(c) \le A_2 c^{\frac{\alpha}{2} + \frac{1}{4}} e^{-\frac{c}{2}} N^{-\frac{1}{4}}, \quad |c| \in [0, N].$$
(4.2.26)

• Finally, it is worth highlighting that in most cases, the  $L_2$  truncation error goes to 0 for extreme values of c, that is when  $\mathbf{1}_{c\leq X} = 1$  or 0, More precisely, for any fixed N, in view of (4.2.17), (4.2.18), and (4.2.19) we have  $\mathcal{E}_N^{\text{He}}(c) \to 0$  as  $c \to \pm \infty$ ,  $\mathcal{E}_N^{\text{La}}(c) \to 0$  as  $c \to +\infty$  and  $\mathcal{E}_N^{\text{La}}(c) \to 0$  as  $c \to 0^+$  for  $\alpha \ge -\frac{1}{2}$ ,  $\mathcal{E}_N^{\text{J}}(c) \to 0$  as  $c \to \pm 1$  when  $\alpha, \beta \ge -\frac{1}{2}$ .

#### 4.2.3 Central limit theorem

We now come back to our original problem i.e. giving a meta-model for the large sum (4.1.1). In light of the previous section, it seems natural to split the sum into three different clusters depending on the value of  $Y_k$ . For instance, supposing that  $X \stackrel{d}{=} \Gamma(\alpha + 1, 1)$  and denoting  $F(\cdot)$  its c.d.f., we would get three different groups in which the  $Y_k$  are close to 0 (extreme low quantiles) the  $Y_k$  are close to  $\infty$  (extreme high quantiles), and the  $Y_k$  take "normal" values on  $(0, \infty)$ . For the latter, noting that  $\mathbf{1}_{Y_k \leq X} = \mathbf{1}_{2F(Y_k)-1 \leq 2F(X)-1} \stackrel{d}{=} \mathbf{1}_{2F(Y_k)-1 \leq \mathcal{U}(-1,1)}$ , we could then perform a PCE of  $\mathbf{1}_{2F(Y_k)-1 \leq 2F(X)-1}$  instead of  $\mathbf{1}_{Y_k \leq X}$  using the Legendre polynomials. For the other two groups, a similar procedure could be used though we would either use the Hermite or the Jacobi polynomials depending on the values of the Jacobi polynomials parameters  $\alpha, \beta$  (see Lemma 4.3.1 and Remark 11 for more details).

From now on, we then suppose that early transformations have been made according to the values of  $(Y_k)_{k=1,...K}$ . Let us introduce the conditional mean and variance of  $\mathcal{L}_K$  w.r.t. X i.e. for every  $x \in \mathbb{R}$ ,

$$\mu_{\mathcal{L}_K}(x) = \sum_{k=1}^{K} l_k F_{Y_k}(x), \quad \sigma_{\mathcal{L}_K}^2(x) = \sum_{k=1}^{K} l_k F_{Y_k}(x) \bar{F}_{Y_k}(x), \quad (4.2.27)$$

where  $\bar{F}_Y(\cdot)$  denotes the survival function of Y, that is  $\bar{F}_Y(x) = 1 - F_Y(x)$ . We are going to build an approximation for  $\mathcal{L}_K$  based on a Gaussian approximation of the random coefficients of a specific chaos decomposition of the random variables  $\mathbf{1}_{Y_k \leq X}$ . Since  $X, Y_1, \ldots, Y_K$  are random variables having densities, it holds almost surely that

$$\mathcal{L}_{K} = \sum_{k=1}^{K} \left( \sum_{n=0}^{\infty} l_{k} \gamma_{n} \left( Y_{k} \right) \right) p_{n}(X) = \sum_{n=0}^{\infty} \varepsilon_{K,n} p_{n}(X),$$

where we define the new random variable

$$\varepsilon_{K,n} := \sum_{k=1}^{K} l_k \gamma_n \left( Y_k \right). \tag{4.2.28}$$

We now introduce our meta-model for  $\mathcal{L}_K$  which consists in considering only the first terms of the chaos decomposition of the indicator function combined with a Gaussian approximation. Let  $N \in \mathbb{N}^*$  be the chaos decomposition truncation order. In particular, we consider  $\mathcal{L}_{K,N}$ , the truncated version of  $\mathcal{L}_K$  as

$$\mathcal{L}_{K,N} := \sum_{n=0}^{N} \varepsilon_{K,n} p_n(X).$$
(4.2.29)

We further introduce the expectation  $\boldsymbol{\mu}_{K} = (\mu_{K,n})_{0 \leq n \leq N}$  and the covariance matrix  $\Sigma_{K} = (\Sigma_{K,n,m})_{0 \leq n,m \leq N}$  of the vector  $\boldsymbol{\varepsilon}_{K} = (\varepsilon_{K,n} : n = 0, \dots, N)$  where for every  $n \in \{0, \dots, N\}$ ,

$$\mu_{K,n} = \mathbb{E}\left[\varepsilon_{K,n}\right] = \sum_{k=1}^{K} l_k \mathbb{E}\left[\gamma_n\left(Y_k\right)\right],$$

$$\Sigma_{K,n,m} = \mathbb{C}\mathrm{ov}\left(\varepsilon_{K,n}, \varepsilon_{K,m}\right) = \sum_{k,k'=1}^{K} l_k l_{k'} \mathbb{C}\mathrm{ov}\left(\gamma_n\left(Y_k\right), \gamma_m\left(Y_{k'}\right)\right).$$
(4.2.30)

Replacing the vector  $\boldsymbol{\varepsilon}_{K}$  by its Gaussian approximation

$$\boldsymbol{\varepsilon}_{K}^{\mathrm{G}} = \left(\boldsymbol{\varepsilon}_{K,n}^{\mathrm{G}} : n = 0, \dots, N\right) \stackrel{d}{=} \mathcal{N}\left(\boldsymbol{\mu}_{K}, \boldsymbol{\Sigma}_{K}\right), \qquad (4.2.31)$$

leads to the meta-model  $\mathcal{L}_{K,N}^{\mathrm{G}}$  for the initial model  $\mathcal{L}_{K}$  defined by:

$$\mathcal{L}_{K,N}^{\mathrm{G}} = \mathcal{L}_{K,N}^{\mathrm{G}}(X) = \sum_{n=0}^{N} \varepsilon_{K,n}^{\mathrm{G}} p_n(X).$$
(4.2.32)

Hence when X is known,  $\mathcal{L}_{K,N}^{\mathrm{G}}(x) \stackrel{d}{=} \mathcal{N}\left(\mu_{\mathcal{L}_{K,N}}(x), \sigma_{\mathcal{L}_{K,N}}^{2}(x)\right)$  with for every  $x \in \mathbb{R}$ ,

$$\mu_{\mathcal{L}_{K,N}}(x) = \sum_{n=0}^{N} \mu_{K,n} p_n(x), \quad \sigma_{\mathcal{L}_{K,N}}^2(x) = \sum_{n,m=0}^{N} \Sigma_{K,n,m} p_n(x) p_m(x).$$

Observe also,

$$\mu_{\mathcal{L}_{K,N}}(x) = \mathbb{E}\left[\sum_{k=1}^{K} l_k \sum_{n=0}^{N} \gamma_n\left(Y_k\right) p_n(x)\right] \xrightarrow[N \to +\infty]{} \mu_{\mathcal{L}_K}(x),$$
  
$$\sigma_{\mathcal{L}_{K,N}}^2(x) = \sum_{k,k'=1}^{K} l_k l_{k'} \mathbb{C}\mathrm{ov}\left(\sum_{n=0}^{N} \gamma_n\left(Y_k\right) p_n(x), \sum_{m=0}^{N} \gamma_m\left(Y_{k'}\right) p_m(x)\right)$$
  
$$= \operatorname{Var}\left(\sum_{k=1}^{K} l_k \sum_{n=0}^{N} \gamma_n\left(Y_k\right) p_n(x)\right) \xrightarrow[N \to +\infty]{} \sigma_{\mathcal{L}_K}^2(x).$$

We then also introduce the random variable  $\mathcal{L}_{K,\infty}^{\mathrm{G}}(x)$  for which conditionally on X = x,

$$\mathcal{L}_{K,\infty}^{\mathrm{G}}(X) | X = x \stackrel{d}{=} \mathcal{N}\left(\mu_{\mathcal{L}_{K}}(x), \sigma_{\mathcal{L}_{K}}^{2}(x)\right).$$

We emphasize that our meta-model is inspired by the following central limit theorem on the random coefficients of the chaos decomposition whose proof is similar to that of [34, Theorem 7].

Theorem 4.2.5 (Central limit theorem). Assume that

$$\|\Sigma_{K}^{-1}\| \sup_{1 \le k \le K} l_{k}^{2} \xrightarrow[K \to +\infty]{} 0 \quad with \quad \|\Sigma_{K}^{-1}\| := \sup_{\boldsymbol{x} \in \mathbb{R}^{N+1}, x \ne 0} \frac{|\Sigma_{K}^{-1}\boldsymbol{x}|}{|\boldsymbol{x}|}.$$
 (4.2.33)

Then, the vector  $\boldsymbol{\varepsilon}_K$  satisfies the following central limit theorem

$$\Sigma_{K}^{-\frac{1}{2}}(\boldsymbol{\varepsilon}_{K}-\boldsymbol{\mu}_{K}) \xrightarrow{d} \mathcal{N}(0, \mathrm{Id}_{N+1}).$$
(4.2.34)

# 4.3 Numerical tests

## **4.3.1** $L_2$ errors comparison w.r.t. N

To illustrate Theorem 4.2.4, we try to retrieve the order  $\mathcal{O}\left(N^{-\frac{1}{2}}\right)$  for the Legendre polynomials and  $\mathcal{O}\left(N^{-\frac{1}{4}}\right)$  for the other orthogonal polynomials. We then plot  $\log\left(\mathcal{E}_N(c)\right)$  w.r.t.  $\log\left(N\right)$  for different fixed values of c and truncating parameters in  $N \in [1, 30]$ . Note that even if we have explicit formulas for all  $L_2$  errors of the COPS, this would result in numerical instability as we would need to evaluate polynomials at very high degrees and large values. To overcome this issue, we proceed with a Monte Carlo simulation and directly estimate the expectation (4.2.6) with  $M = 3 \times 10^5$  samples. We do not report the confidence interval as the error is negligible (less than 0.1% in relative error).



Figure 4.1 – log  $\mathcal{E}_N(c)$  w.r.t. log N for the COPS for different parameters c.

## **4.3.2** $L_2$ errors comparison w.r.t. q

In this section, we compare all  $L_2$  errors w.r.t. a common quantile  $q \in (0,1)$ . To do so, let us introduce  $q \in (0,1)$ ,  $U \stackrel{d}{=} \mathcal{U}(0,1)$  and consider the problem of approximating the indicator function

 $\mathbf{1}_{q\leq U}$ .

Introduce  $L \stackrel{d}{=} \mathcal{U}(-1,1)$ ,  $N \stackrel{d}{=} \mathcal{N}(0,1)$ ,  $G \stackrel{d}{=} \text{Gamma}(\alpha + 1, 1)$ ,  $J \stackrel{d}{=} 1 - 2\text{Beta}(\alpha + 1, \beta + 1)$  and recall that for all x (see (4.1.3)),

$$\mathbb{P}(N \le x) = \Phi(x), \quad \mathbb{P}(G \le x) = \mathscr{G}_{\alpha+1}(x) \quad \mathbb{P}(J \le x) = \mathscr{B}_{\alpha+1,\beta+1}\left(\frac{1+x}{2}\right).$$

The last equality is a direct consequence of (4.1.4) along with the symmetry property  $1 - \text{Beta}(\alpha + 1, \beta + 1) \stackrel{d}{=} \text{Beta}(\beta + 1, \alpha + 1)$ . Finally, we introduce:

$$c_{\rm He}(q) = \Phi^{-1}(q) \in (-\infty, \infty), \quad c_{\rm Le}(q) = 2q - 1 \in (-1, 1),$$
  
$$c_{\rm La}(q) = \mathscr{G}_{\alpha+1}^{-1}(q) \in (0, \infty), \quad c_{\rm J}(q) = 2\mathscr{B}_{\alpha+1,\beta+1}^{-1}(q) - 1 \in (-1, 1)$$

where the superscript  $\cdot^{-1}$  refers to the inverse function w.r.t. x for all three c.d.f.s. (the free parameters being fixed). Observing that

$$\mathbf{1}_{q \leq U} \stackrel{d}{=} \mathbf{1}_{c_{\mathrm{Le}}(q) \leq L} \stackrel{d}{=} \mathbf{1}_{c_{\mathrm{He}}(q) \leq N} \stackrel{d}{=} \mathbf{1}_{c_{\mathrm{La}}(q) \leq G} \stackrel{d}{=} \mathbf{1}_{c_{\mathrm{J}}(q) \leq J},$$

the indicator function can be decomposed using the Legendre or Hermite or Laguerre or Jacobi polynomials. We then have to compare  $\mathcal{E}_N^{\text{Le}}(c_{\text{Le}}(q))$ ,  $\mathcal{E}_N^{\text{He}}(c_{\text{He}}(q))$ ,  $\mathcal{E}_N^{\text{La}}(c_{\text{La}}(q))$ ,  $\mathcal{E}_N^{\text{J}}(c_{\text{J}}(q))$  for all  $q \in (0, 1)$ . We will see that depending on the value q, it might be more adequate (in terms of  $L_2$  error) to decompose on one basis compare to another. Again we choose  $M = 3 \times 10^5$  samples for the Monte Carlo simulation and we plot each  $L_2$  error w.r.t. the quantile  $q \in (0, 1)$ .



Figure 4.2 –  $L_2$  error for the COPS w.r.t.  $q \in (0, 1)$  and for  $N \in \{10, 20, 30, 40\}$ .

As expected, we observe that the Legendre polynomials provide the smaller  $L_2$  error compared to the other orthogonal polynomials, and that the Jacobi polynomials seem to be more efficient than both the Hermite and Laguerre polynomials though they share the same order  $\mathcal{O}(N^{-\frac{1}{4}})$ (see the remarks of Theorem 4.2.4).

To illustrate the tightness of the estimates found in Theorem 4.2.4, we plot the ratio between the  $L_2$  error and the corresponding error estimate for every orthogonal polynomial, and expect this ratio to be constant for all quantiles  $q \in (0,1)$ . More precisely, as a function of  $q \in (0,1)$ , we plot

$$\begin{split} R_{\rm He}(q) &= e^{\frac{c_{\rm He}(q)^2}{4}} N^{\frac{1}{4}} \mathcal{E}_N^{\rm He}\left(c_{\rm He}(q)\right),\\ R_{\rm La}(q) &= c_{\rm La}(q)^{-\frac{\alpha}{2} - \frac{1}{4}} e^{\frac{c_{\rm La}(q)}{2}} N^{\frac{1}{4}} \mathcal{E}_N\left(c_{\rm La}(q)\right),\\ R_{\rm J}(q) &= \frac{\mathcal{E}_N^{\rm J}\left(c_{\rm J}\left(q\right)\right)}{E_N^{\rm J}\left(c_{\rm J}\left(q\right)\right)} = (1 - c_{\rm J}(q))^{-\frac{\alpha}{2} - \frac{1}{4}} \left(1 + c_{\rm J}(q)\right)^{-\frac{\beta}{2} - \frac{1}{4}} N^{\frac{1}{4}} \mathcal{E}_N^{\rm J}\left(c_{\rm J}(q)\right)\\ R_{\rm Le}(q) &= \frac{\mathcal{E}_N^{\rm Le}\left(c_{\rm Le}\left(q\right)\right)}{E_N^{\rm Le}\left(c_{\rm Le}\left(q\right)\right)} = \left(1 - c_{\rm Le}(q)^2\right)^{-\frac{1}{4}} N^{\frac{1}{2}} \mathcal{E}_N^{\rm Le}\left(c_{\rm Le}(q)\right), \end{split}$$

where we recall that the notation  $\mathbf{E}_N^{\cdot}$  refers to one of the global estimates found in Theorem 4.2.4. Note that for the Hermite (resp. Laguerre) polynomials, the global estimate (4.2.17) (resp. (4.2.18)) being too large when q is close to 1, we use the second localized estimate (4.2.22) (resp. (4.2.24)) valid for  $|c| \in [0, N^{\frac{1}{2}}]$  (resp.  $|c| \in [0, N]$ ), see (4.2.25) (resp. (4.2.26)). Actually, if we set N = 10 (which is a typical truncation parameter in practice), we have  $\Phi(10^{\frac{1}{2}}) \approx 0.999217$  and setting  $\alpha = 1$ ,  $\mathscr{G}_{\alpha+1}(10) \approx 0.999501$ . Consequently, the probability of N and G to be outside the range of values of  $[0, N^{\frac{1}{2}}]$  and [0, N] respectively is extremely small, and the localized estimates exposed in (4.2.25) and (4.2.26) seem satisfactory enough (see Figure 4.3).



Figure 4.3 – Ratio between the  $L_2$  error and the error estimates of Theorem 4.2.4 w.r.t. the quantile  $q \in (0, 1)$  for different truncation parameters  $N \in \{10, 20, 30, 40\}$ .

Finally, in Figure 4.4, we plot the estimates (4.2.19), (4.2.20), (4.2.22), (4.2.24), and observe that we are able to recover the same order displayed in Figure 4.2 for the true  $L_2$  error though



a higher number of truncation parameter N is needed.

Figure 4.4 – Estimates (4.2.19), (4.2.20), (4.2.22), (4.2.24) w.r.t.  $q \in (0,1)$  for  $N \in \{40, 70, 100, 130\}$ .

#### Extreme quantiles

The Legendre polynomials seem to provide the smallest error for not-too-extreme values of q. As displayed in Figure 4.2, this seems different when dealing with extremely small  $(q \to 0^+)$  or large  $(q \to 1^-)$  quantiles as it is shown in the next lemma.

**Lemma 4.3.1.** Let us fix  $N \in \mathbb{N}^*$ . We have as  $q \to 0^+$ ,

$$\begin{split} \mathbf{E}_{N}^{\mathrm{Le}}\left(c_{\mathrm{Le}}(q)\right) &\sim 2^{\frac{1}{2}}N^{-\frac{1}{2}}q^{\frac{1}{4}},\\ \mathbf{E}_{N}^{\mathrm{He}}\left(c_{\mathrm{He}}(q)\right) &\sim 2^{\frac{7}{12}}\pi^{\frac{1}{4}}N^{-\frac{1}{4}}q^{\frac{1}{2}}|\ln(q)|^{\frac{1}{3}},\\ \mathbf{E}_{N}^{\mathrm{La}}\left(c_{\mathrm{La}}(q)\right) &\sim \Gamma_{\alpha+2}^{\frac{2\alpha+1}{4(\alpha+1)}}N^{-\frac{1}{4}}q^{\frac{2\alpha+1}{4(\alpha+1)}},\\ \mathbf{E}_{N}^{\mathrm{J}}\left(c_{\mathrm{J}}(q)\right) &\sim 2^{\frac{\alpha+\beta+1}{2}}\left((\alpha+1)\mathbf{B}_{\alpha+1,\beta+1}\right)^{\frac{2\beta+1}{4(\alpha+1)}}N^{-\frac{1}{4}}q^{\frac{2\beta+1}{4(\alpha+1)}}, \end{split}$$

and as  $q \to 1^-$ ,

$$\begin{split} \mathbf{E}_{N}^{\mathrm{Le}}\left(c_{\mathrm{Le}}(q)\right) &\sim 2^{\frac{1}{2}}N^{-\frac{1}{2}}(1-q)^{\frac{1}{4}},\\ \mathbf{E}_{N}^{\mathrm{He}}\left(c_{\mathrm{He}}(q)\right) &\sim 2^{\frac{7}{6}}\pi^{\frac{1}{4}}N^{-\frac{31}{12}}(1-q)^{\frac{1}{2}}|\ln(1-q)|^{\frac{11}{12}},\\ \mathbf{E}_{N}^{\mathrm{La}}\left(c_{\mathrm{La}}(q)\right) &\sim \Gamma_{\alpha+1}^{\frac{1}{2}}N^{-\frac{1}{2}}(1-q)^{\frac{1}{2}}\left|\ln(1-q)\right|^{\frac{3}{2}},\\ \mathbf{E}_{N}^{\mathrm{J}}\left(c_{\mathrm{J}}(q)\right) &\sim 2^{\frac{\alpha+\beta+1}{2}}\left((\beta+1)\mathbf{B}_{\beta+1,\alpha+1}\right)^{\frac{2\alpha+1}{4(\beta+1)}}N^{-\frac{1}{4}}(1-q)^{\frac{2\alpha+1}{4(\beta+1)}} \end{split}$$

Remark 11. Denote  $\alpha_{\rm J}$ ,  $\beta_{\rm J}$  the parameters associated with the Jacobi polynomials. In light of Lemma 4.3.1, we observe that for small quantiles  $(q \to 0^+)$ , the smaller  $L_2$  error is either achieved by the Jacobi polynomials, when  $-1 < \alpha_{\rm J} < \beta_{\rm J} - \frac{1}{2}$ , or the Hermite polynomials when  $\frac{1}{2} + \alpha_{\rm J} > \beta_{\rm J} > -\frac{1}{2}$  or  $-1 < \beta_{\rm J} \leq -\frac{1}{2}$  Similarly for large quantiles  $(q \to 1^{-1})$ , we note that the Hermite (resp. Jacobi) polynomials attain the smallest error when  $\alpha_{\rm J} < \beta_{\rm J} + \frac{1}{2}$  (resp.  $\alpha_{\rm J} > \beta_{\rm J} + \frac{1}{2}$ ).

To illustrate Lemma 4.3.1, let us plot the  $L_2$  error for small values of q, namely  $q \in (10^{-4}, 10^{-3})$ . Set  $\alpha_{\text{La}} = 3.5$  so that  $E_N^{\text{La}}(c) = \mathcal{O}\left(q^{\frac{4}{9}}\right)$  and  $\alpha_{\text{J}} = 1, \beta_{\text{J}} = 5$  so that  $E_N^{\text{J}}(q) = \mathcal{O}\left(q^{\frac{11}{8}}\right)$ . Consequently as  $\frac{1}{4} < \frac{4}{9} < \frac{1}{2} < \frac{11}{8}$ , we should observe that  $E_N^{\text{J}}(c_{\text{J}}(q)) < E_N^{\text{He}}(c_{\text{He}}(q)) < E_N^{\text{Le}}(c_{\text{Le}}(q))$ . For large values of q, we take  $q \in (1 - 10^{-3}, 1 - 10^{-4})$ . Observe that both Hermite and Laguerre polynomials behave similarly up to some logarithmic factor. If we set  $\alpha_{\text{J}} = 5, \beta_{\text{J}} = 1$ ,  $E_N^{\text{J}}(q) = \mathcal{O}\left(q^{\frac{11}{8}}\right)$ , and we should this time observe that  $E_N^{\text{J}}(c_{\text{J}}(q)) < E_N^{\text{He}}(c_{\text{He}}(q)) \approx E_N^{\text{La}}(c_{\text{La}}(q)) < E_N^{\text{Le}}(c_{\text{Le}}(q))$ . We take N = 20 and again  $M = 3 \times 10^5$  Monte Carlo samples.



Figure 4.5 –  $L_2$  error for the COPS w.r.t. small quantiles  $q \in (10^{-4}, 10^{-3})$  (left) and large quantiles  $q \in (1 - 10^{-3}, 1 - 10^{-4})$  (right).

# 4.4 Conclusion

To sum up, we have described a general framework for the meta-model of large sums of conditionally independent weighted Bernoulli random variables of the form  $\sum_{k=1}^{K} l_k \mathbf{1}_{Y_k \leq X}$ . When the common factor X is associated with the classical orthogonal polynomials, some tight  $L_2$ error estimates and a central limit theorem are proved which suggests an efficient meta-model, based on a polynomial chaos expansion on the indicator  $\mathbf{1}_{Y_k \leq X}$  along with a Gaussian-based approximation, depending on the values of  $Y_k$  with respect to X.

# 4.5 Proofs

### 4.5.1 Proof of Proposition 4.2.1

When working with the COPS, the first equality in (4.2.5) holds not only in  $L_2(\nu)$  but for every  $X \neq c$  (and  $|X| \neq 1$  for the Jacobi polynomials). When considering normal random variables (i.e. Hermite polynomials) see the discussion [34, Section 2.3]. For the Gamma random variables (i.e. Laguerre polynomials), this a direct consequence of Uspensky's criterion for pointwise convergence which holds both for Hermite and Laguerre series. Concerning Jacobi polynomials, up to our knowledge, there is no such result. However, in view of [157, Theorem
9.1.2], we simply have to show that, for every fixed  $\delta > 0$ , the Fourier cosine series of the function  $x \mapsto (1-x)^{\frac{2\alpha+1}{4}} (1+x)^{\frac{2\beta+1}{4}} \mathbf{1}_{[c,1]}(x)$  converges for every  $x \in [-1+\delta, c-\delta] \cup [c+\delta, 1+\delta]$ . Since this function is Hölder, this is a consequence of the Dini–Lipschitz criterion. Letting  $\delta$  tends to zero, this shows that the decomposition holds for the Jacobi polynomials as soon as  $X \in (-1, c) \cup (c, 1)$ . We now focus on establishing the announced formulas for  $\gamma_n(c)$  for every  $n \in \mathbb{N}$ .

 $\triangleright$  Coefficients  $\gamma_n(c)$  for the Hermite polynomials. From (4.2.5), we have first

$$\gamma_0(c) = \frac{1}{h_0} \int_c^\infty \operatorname{He}_0(x) \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} \mathrm{d}x = \Phi(-c), \quad \gamma_1(c) = \frac{1}{1!} \int_c^\infty x \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} \mathrm{d}x = \frac{e^{-\frac{c^2}{2}}}{\sqrt{2\pi}}$$

and for every  $n \in \mathbb{N}^*$ ,

$$\gamma_n(c) = \frac{(-1)^n}{n!\sqrt{2\pi}} \int_c^\infty \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left( e^{-\frac{x^2}{2}} \right) \mathrm{d}x = \frac{(-1)^{n-1}}{n!\sqrt{2\pi}} \left. \frac{\mathrm{d}^{n-1}}{\mathrm{d}x^{n-1}} \left( e^{-\frac{x^2}{2}} \right) \right|_{x=c} = \frac{e^{-\frac{c^2}{2}} \mathrm{He}_{n-1}(c)}{n!\sqrt{2\pi}}$$

 $\triangleright$  Coefficients  $\gamma_n(c)$  for the Laguerre polynomials. Again, one has by definition

$$\gamma_0(c) = \frac{1}{0!} \int_c^\infty 1 \times \frac{x^{\alpha} e^{-x}}{\Gamma_{\alpha+1}} \mathrm{d}x = \mathscr{G}_{\alpha+1}(c),$$

and a direct integration by parts gives

$$\gamma_1(c) = \frac{1}{\Gamma_{\alpha+2}} \int_c^\infty \left(1 + \alpha - x\right) x^\alpha e^{-x} \mathrm{d}x = -\frac{c^{1+\alpha} e^{-c}}{\Gamma_{\alpha+2}}.$$

Also combining both identities (see [146, 18.9.14, 18.9.24]),

$$\frac{\mathrm{d}}{\mathrm{d}x} \left( x^{\alpha} e^{-x} \mathrm{L}_{n}^{(\alpha)}(x) \right) = (n+1) x^{\alpha-1} e^{-x} \mathrm{L}_{n+1}^{(\alpha-1)}(x),$$

$$x \mathrm{L}_{n}^{(\alpha+1)}(x) = -(n+1) \mathrm{L}_{n+1}^{(\alpha)}(x) + (n+\alpha+1) \mathrm{L}_{n}^{(\alpha)}(x),$$
(4.5.1)

we have:

$$\gamma_n(c) = \frac{n!}{\Gamma_{n+\alpha+1}} \int_c^\infty \mathcal{L}_n^{(\alpha)}(x) x^\alpha e^{-x} dx$$
$$= -\frac{(n-1)!}{\Gamma_{n+\alpha+1}} c^{\alpha+1} e^{-c} \mathcal{L}_{n-1}^{(\alpha+1)}(c)$$
$$= \frac{(n-1)!}{\Gamma_{n+\alpha+1}} c^\alpha e^{-c} \left( n \mathcal{L}_n^{(\alpha)}(c) - (n+\alpha) \mathcal{L}_{n-1}^{(\alpha)}(c) \right)$$

 $\triangleright$  Coefficients  $\gamma_n(c)$  for the Jacobi polynomials. As  $P_0^{(\alpha,\beta)}(x) = 1$  and  $h_0 = 1$ , we have first:

$$\gamma_0(c) = \frac{2^{-\alpha-\beta-1}}{B_{\alpha+1,\beta+1}} \int_c^1 (1-x)^{\alpha} (1+x)^{\beta} dx \stackrel{(t=(1-x)/2)}{=} \mathscr{B}_{\alpha+1,\beta+1}\left(\frac{1-c}{2}\right)$$

Similarly, using this time that  $P_1^{(\alpha,\beta)}(x) = (\alpha+1) + (\alpha+\beta+2)\frac{(x-1)}{2}$  we get:

$$h_1 \gamma_1(c) = (\alpha + 1) \gamma_0(c) - \frac{2^{-\alpha - \beta - 2} (\alpha + \beta + 2)}{B_{\alpha + 1, \beta + 1}} \int_c^1 (1 - x)^{\alpha + 1} (1 + x)^{\beta} dx$$
$$= \frac{(\alpha + 1) B_{\alpha + 1, \beta + 1} \left(\frac{1 - c}{2}\right) - (\alpha + \beta + 2) B_{\alpha + 2, \beta + 1} \left(\frac{1 - c}{2}\right)}{B_{\alpha + 1, \beta + 1}},$$

hence the expression for  $\gamma_1(c)$  using that  $h_1 = \frac{\Gamma_{\alpha+2}\Gamma_{\beta+2}}{(\alpha+\beta+3)\Gamma_{\alpha+\beta+2}B_{\alpha+1,\beta+1}} = \frac{(\alpha+1)(\beta+1)}{\alpha+\beta+3}$ . From the identity (see [146, 18.9.16]),

$$\frac{\mathrm{d}}{\mathrm{d}x} \left[ (1-x)^{\alpha} (1+x)^{\beta} \operatorname{P}_{n}^{(\alpha,\beta)}(x) \right] = -2(n+1) (1-x)^{\alpha-1} (1+x)^{\beta-1} \operatorname{P}_{n+1}^{(\alpha-1,\beta-1)}(x), \quad (4.5.2)$$

we obtain:

$$\gamma_n(c,\alpha,\beta) = \frac{1}{h_n(\alpha,\beta)} \int_c^1 \mathbf{P}_n^{(\alpha,\beta)}(x) w(x) \mathrm{d}x = C(n,\alpha,\beta) (1-c)^{\alpha+1} (1+c)^{\beta+1} \mathbf{P}_{n-1}^{(\alpha+1,\beta+1)}(c).$$
(4.5.3)

 $\triangleright$  Coefficients  $\gamma_n(c)$  for the Legendre polynomials. Setting  $\alpha = \beta = 0$ , we easily get that

$$\gamma_n(c) = \frac{2n+1}{2(n+1)} \left( -c \mathbf{P}_n(c) + \mathbf{P}_{n-1}(c) \right),$$

and easy computation show that  $-cP_n(c) + P_{n-1}(c) = \frac{1-c^2}{n} \frac{d}{dc} P_n(c)$ . We conclude observing that from the three-term recurrence relation:

$$\frac{\mathrm{dP}_n(c)}{\mathrm{d}c} = \sum_{j=0}^{\lfloor \frac{n-1}{2} \rfloor} \left( 2\left(n-1-2j\right)+1 \right) \mathrm{P}_{n-1-2j}(c).$$

#### 4.5.2 Proof of Proposition 4.2.2

First notice that for any classical orthogonal polynomial, the following identity holds:

$$x \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left[ F(x)^{n+1} w(x) \right] \xrightarrow[x \to b]{} 0. \tag{4.5.4}$$

Indeed, in light of Table 4.1, (4.5.4) holds for the Hermite polynomials since

$$x\frac{\mathrm{d}^{n}}{\mathrm{d}x^{n}}\left[F(x)^{n+1}w(x)\right] = x\frac{\mathrm{d}^{n}}{\mathrm{d}x^{n}}\left[\frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}}\right] = (-1)^{n}x\mathrm{He}_{n}(x)\frac{e^{-\frac{x^{2}}{2}}}{\sqrt{2\pi}} \xrightarrow[x \to \infty]{} 0.$$

For the Laguerre polynomials, from the identity (4.5.1)

$$\frac{\mathrm{d}}{\mathrm{d}x} \left[ x^{\alpha+1} e^{-x} \mathcal{L}_{n+1}^{(\alpha+1)}(x) \right] = (n+1) x^{\alpha} e^{-x} \mathcal{L}_{n+1}^{(\alpha)}(x),$$

together with (4.2.3), we obtain:

$$\frac{\mathrm{d}^{n+1}}{\mathrm{d}x^{n+1}} \left[ x^{n+1} \frac{x^{\alpha} e^{-x}}{\Gamma_{\alpha+1}} \right] = (n+1)! \frac{x^{\alpha} e^{-x}}{\Gamma_{\alpha+1}} \mathcal{L}_{n+1}^{(\alpha)}(x) = n! \frac{\mathrm{d}}{\mathrm{d}x} \left[ \frac{x^{\alpha+1} e^{-x}}{\Gamma_{\alpha+1}} \mathcal{L}_{n+1}^{(\alpha+1)}(x) \right].$$

We then easily get that:

$$x\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left[F(x)^{n+1}w(x)\right] = x\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left[x^{n+1}\frac{x^{\alpha}e^{-x}}{\Gamma_{\alpha+1}}\right] = n!\frac{x^{\alpha+2}e^{-x}}{\Gamma_{\alpha+1}}\mathrm{L}_{n+1}^{(\alpha+1)}(x) \xrightarrow[x\to\infty]{} 0.$$

Similarly for the Jacobi polynomials, using both (4.2.3) and (4.5.2), we obtain:

$$\frac{\mathrm{d}}{\mathrm{d}x} \left[ (1-x)^{\alpha+1} \left(1+x\right)^{\beta+1} \mathrm{P}_n^{(\alpha+1,\beta+1)}(x) \right] = -2(n+1) \left(1-x\right)^{\alpha} (1+x)^{\beta} \mathrm{P}_{n+1}^{(\alpha,\beta)}(x),$$

and

$$\frac{\mathrm{d}^{n+1}}{\mathrm{d}x^{n+1}} \Big[ \left(1-x^2\right)^{n+1} \frac{\left(1-x\right)^{\alpha} \left(1+x\right)^{\beta}}{2^{\alpha+\beta+1} \mathrm{B}_{\alpha+1,\beta+1}} \Big] = \frac{\left(-2\right)^{n+1} \left(n+1\right)!}{2^{\alpha+\beta+1} \mathrm{B}_{\alpha+1,\beta+1}} \left(1-x\right)^{\alpha} \left(1+x\right)^{\beta} \mathrm{P}_{n+1}^{(\alpha,\beta)}(x)$$

$$= \frac{(-2)^{n+2} n!}{2^{\alpha+\beta+1} \mathbf{B}_{\alpha+1,\beta+1}} \frac{\mathrm{d}}{\mathrm{d}x} \Big[ (1-x)^{\alpha+1} (1+x)^{\beta+1} \mathbf{P}_n^{(\alpha+1,\beta+1)}(x) \Big],$$

We then conclude that:

$$\begin{aligned} x \frac{\mathrm{d}^{n}}{\mathrm{d}x^{n}} \left[ F(x)^{n+1} w(x) \right] &= x \frac{\mathrm{d}^{n}}{\mathrm{d}x^{n}} \left[ \left( 1 - x^{2} \right)^{n+1} \frac{(1-x)^{\alpha} (1+x)^{\beta}}{2^{\alpha+\beta+1} \mathrm{B}_{\alpha+1,\beta+1}} \right] \\ &= \frac{(-2)^{n+2} n!}{2^{\alpha+\beta+1} \mathrm{B}_{\alpha+1,\beta+1}} x \left( 1 - x \right)^{\alpha+1} (1+x)^{\beta+1} \mathrm{P}_{n}^{(\alpha+1,\beta+1)}(x) \xrightarrow[x \to 1]{} 0. \end{aligned}$$

Consequently, from Rodrigues' formula (4.2.3), (4.5.4) and the three-term recurrence relation (4.2.2), we have:

$$h_{n+2}\gamma_{n+2}(c) = \mathbb{E}\left[\mathbf{1}_{c \le X} p_{n+2}(X)\right]$$
  
=  $\mathbb{E}\left[\mathbf{1}_{c \le X}\left((A_{n+1}X + B_{n+1})p_{n+1}(X) - C_{n+1}p_n(X)\right)\right]$   
=  $B_{n+1}h_{n+1}\gamma_{n+1}(c) - C_{n+1}h_n\gamma_n(c) + A_{n+1}\mathbb{E}\left[\mathbf{1}_{c \le X} X p_{n+1}(X)\right].$ 

Besides, an integration by parts together with (4.5.4) give:

$$\mathbb{E}\left[\mathbf{1}_{c\leq X}Xp_{n+1}(X)\right] = \int_{c}^{b} xp_{n+1}(x)w(x)dx$$
  

$$= \frac{1}{\kappa_{n+1}}\int_{c}^{b} x\frac{d^{n+1}}{dx^{n+1}}\left[F(x)^{n+1}w(x)\right]dx$$
  

$$= \frac{1}{\kappa_{n+1}}\left(\left[x\frac{d^{n}}{dx^{n}}\left[F(x)^{n+1}w(x)\right]\right]_{c}^{b} - \int_{c}^{b}\frac{d^{n}}{dx^{n}}\left[F(x)^{n+1}w(x)\right]dx\right)$$
  

$$= -\frac{1}{\kappa_{n+1}}c\frac{d^{n}}{dx^{n}}\left[F(x)^{n+1}w(x)\right]\Big|_{x=c} + h_{n+1}\int_{c}^{b}\gamma_{n+1}(x)dx$$
  

$$= h_{n+1}\left(c\gamma_{n+1}(c) + \int_{c}^{b}\gamma_{n+1}(x)dx\right),$$

where we have used in the penultimate equality that  $-\frac{1}{\kappa_{n+1}} \frac{d^n}{dx^n} \left[ F(x)^{n+1} w(x) \right] = h_{n+1} \gamma_{n+1}(x)$ which results from the identity  $\kappa_{n+1} p_{n+1}(x) w(x) = \frac{d^{n+1}}{dx^{n+1}} \left[ F(x)^{n+1} w(x) \right]$  and the limit condition  $\lim_{x \to b} w(x) p_{n+1}(x) = 0$ . The recurrence relation (4.2.11) is proved. To specify the relation for every classical orthogonal polynomial, one only needs  $\int_c^b \gamma_{n+1}(x) dx$  in terms of  $\gamma_n(\cdot)$  and  $\gamma_{n+1}(\cdot)$ .  $\triangleright$  Hermite polynomials. As  $b = \infty$ , we easily get that:

$$\int_{c}^{\infty} \gamma_{n+1}(x) dx = -\frac{1}{(n+1)!\sqrt{2\pi}} \int_{c}^{\infty} \frac{d}{dx} \left( e^{-\frac{x^2}{2}} \operatorname{He}_{n-1}(x) \right) dx = \frac{\gamma_n(c)}{n+1},$$

where we have used the identity  $\frac{\mathrm{d}}{\mathrm{d}x}\left(e^{-\frac{x^2}{2}}\mathrm{He}_n(x)\right) = -e^{-\frac{x^2}{2}}\mathrm{He}_{n+1}(x).$  $\triangleright$  Laguerre polynomials. Expliciting the dependence on  $\alpha$ , it holds:

$$\int_{c}^{\infty} \gamma_{n+1}(x,\alpha) \, \mathrm{d}x = -\frac{(n-1)!}{\Gamma_{n+\alpha+2}} \int_{c}^{\infty} \frac{\mathrm{d}}{\mathrm{d}x} \left( x^{\alpha+2} e^{-x}(x) \mathcal{L}_{n-1}^{(\alpha+2)} \right) \, \mathrm{d}x$$
  
=  $-\gamma_n \left( c, \alpha + 1 \right)$   
=  $\frac{(n-1)!}{\Gamma_{n+\alpha+2}} c^{\alpha+2} e^{-c} \mathcal{L}_{n-1}^{(\alpha+2)}(c)$   
=  $\frac{(n-1)!}{\Gamma_{n+\alpha+2}} c^{\alpha+1} e^{-c} \left( -n \mathcal{L}_n^{(\alpha+1)}(c) + (n+\alpha+1) \mathcal{L}_{n-1}^{(\alpha+1)}(c) \right)$ 

$$= \gamma_{n+1}(c,\alpha) - \frac{\Gamma_{n+\alpha+1}}{\Gamma_{n+\alpha+2}} (n+\alpha+1) \gamma_n(c,\alpha)$$
$$= \gamma_{n+1}(c,\alpha) - \gamma_n(c,\alpha),$$

using that  $\Gamma_{x+1} = x\Gamma_x$  for x > 0. Whence from the identities,

$$B_{n+1} + A_{n+1}c = \frac{2n + \alpha + 3 - c}{n+2}, \quad \frac{h_{n+1}(\alpha)}{h_{n+2}(\alpha)} = (n+2)\frac{\Gamma_{n+\alpha+2}}{\Gamma_{n+\alpha+3}} = \frac{n+2}{n+\alpha+2},$$
$$\frac{h_n(\alpha)}{h_{n+2}(\alpha)} = \frac{(n+2)(n+1)}{(n+\alpha+2)(n+\alpha+1)},$$

we infer that:

,

$$\gamma_{n+2}(c,\alpha) = (B_{n+1} + A_{n+1}c) \frac{h_{n+1}(\alpha)}{h_{n+2}(\alpha)} \gamma_{n+1}(c,\alpha) - C_{n+1} \frac{h_n(\alpha)}{h_{n+2}(\alpha)} \gamma_n(c,\alpha) + \frac{h_{n+1}(\alpha)}{h_{n+2}(\alpha)} A_{n+1} \int_c^b \gamma_{n+1}(x,\alpha) \, \mathrm{d}x = \frac{2n + \alpha + 3 - c}{n + \alpha + 2} \gamma_{n+1}(c,\alpha) - \frac{n+1}{n + \alpha + 2} \gamma_n(c,\alpha) + \frac{1}{n + \alpha + 2} \gamma_n(c,\alpha + 1) = \frac{2n + \alpha + 2 - c}{n + \alpha + 2} \gamma_{n+1}(c,\alpha) - \frac{n}{n + \alpha + 2} \gamma_n(c,\alpha).$$

 $\triangleright$  Jacobi polynomials. We explicit the dependence in both  $\alpha$  and  $\beta$ . From [146, (18.9.3-4-6)], we have first:

$$P_n^{(\alpha+1,\beta)}(x) - P_n^{(\alpha,\beta+1)}(x) = P_{n-1}^{(\alpha+1,\beta+1)}(x),$$
(4.5.5)

$$(1-x) P_n^{(\alpha+1,\beta)}(x) + (1+x) P_n^{(\alpha,\beta+1)}(x) = 2P_n^{(\alpha,\beta)}(x),$$
(4.5.6)

$$\left(n + \frac{\alpha}{2} + \frac{\beta}{2} + 1\right)\left(1 + x\right) P_n^{(\alpha,\beta+1)}(x) = (n+1)P_{n+1}^{(\alpha,\beta)}(x) + (n+\beta+1)P_n^{(\alpha,\beta)}(x).$$
(4.5.7)

Whence, combining both (4.5.5) and (4.5.6), we first get:

$$2P_n^{(\alpha,\beta+1)}(x) = 2P_n^{(\alpha,\beta)}(x) + (x-1)P_{n-1}^{(\alpha+1,\beta)}(x).$$
(4.5.8)

Reinjecting (4.5.7) in (4.5.8) gives (after some direct simplification):

$$(x^{2} - 1) (2 + 2n + \alpha + \beta) P_{n-1}^{(\alpha+1,\beta+1)}(x) = 4(n+1) P_{n+1}^{(\alpha,\beta)}(x) - 2(\alpha - \beta + (2 + 2n + \alpha + \beta)x) P_{n}^{(\alpha,\beta)}(x).$$
(4.5.9)

We can derive another identity by combining [146, 18.9.15, 18.9.17],

$$(2n + \alpha + \beta) (1 - x^2) \frac{1}{2} (n + \alpha + \beta + 1) P_{n-1}^{(\alpha + 1, \beta + 1)}(x)$$
  
=  $n (\alpha - \beta - (2n + \alpha + \beta) x) P_n^{(\alpha, \beta)}(x) + 2 (n + \alpha) (n + \beta) P_{n-1}^{(\alpha, \beta)}(x).$  (4.5.10)

We can thus rewrite  $\gamma_{n}(\cdot)$  as

$$\gamma_n(c,\alpha,\beta) = \frac{2C(n,\alpha,\beta)(1-c)^{\alpha}(1+c)^{\beta}}{(2n+\alpha+\beta)(n+\alpha+\beta+1)} \times \left(n(\alpha-\beta-(2n+\alpha+\beta)c)\operatorname{P}_n^{(\alpha,\beta)}(c) + 2(n+\alpha)(n+\beta)\operatorname{P}_{n-1}^{(\alpha,\beta)}(c)\right). \quad (4.5.11)$$

After some simplification, we obtain:

$$\gamma_{n+2}(c,\alpha,\beta) = \Gamma_1(n,\alpha,\beta) \gamma_{n+1}(c,\alpha,\beta) + \Gamma_2(n,\alpha,\beta) \gamma_n(c,\alpha,\beta) + \Gamma_3(n,\alpha,\beta) \gamma_n(c,\alpha+1,\beta+1),$$

where:

$$\Gamma_{1}(n,\alpha,\beta) = \frac{(\alpha+\beta+2n+5)((\alpha-\beta)(\alpha+\beta)+c(\alpha+\beta+2n+2)(\alpha+\beta+2n+4))}{2(\alpha+n+2)(\beta+n+2)(\alpha+\beta+2n+2)},$$

$$\Gamma_{2}(n,\alpha,\beta) = -\frac{(n+1)(\alpha+\beta+n+1)(\alpha+\beta+2n+4)(\alpha+\beta+2n+2)}{(\alpha+n+2)(\beta+n+2)(\alpha+\beta+2n+1)(\alpha+\beta+2n+2)},$$

$$\Gamma_{3}(n,\alpha,\beta) = \frac{(\alpha+\beta+2n+4)(\alpha+\beta+2n+5)}{(\alpha+n+2)(\beta+n+2)(\alpha+\beta+n+2)}.$$

We now want to rewrite the last term  $\gamma_{n+1}(\alpha+1,\beta+1,c)$  in terms of  $\gamma_n(c,\alpha,\beta)$  and  $\gamma_{n+1}(c,\alpha,\beta)$ . Whence using both (4.5.3) and (4.5.11), we obtain (after some simplifications):

$$\gamma_{n+1}(\alpha+1,\beta+1,c) = \Gamma_4(n,\alpha,\beta)\gamma_{n+1}(c,\alpha,\beta) + \Gamma_5(n,\alpha,\beta)\gamma_n(c,\alpha,\beta),$$

where

$$\Gamma_4(n,\alpha,\beta) = \frac{(\alpha-\beta-(2n+\alpha+\beta+2)c)(n+\alpha+\beta+2)}{2(2n+\alpha+\beta+2)(n+\alpha+\beta+3)},$$
  
$$\Gamma_5(n,\alpha,\beta) = \frac{(\alpha+\beta+n+1)(\alpha+\beta+n+2)(\alpha+\beta+2n+3)}{(\alpha+\beta+n+3)(\alpha+\beta+2n+1)(2n+\alpha+\beta+2)}.$$

Finally, we deduce that:

$$\gamma_{n+2}(c,\alpha,\beta) = \Gamma_6(n,\alpha,\beta) \gamma_{n+1}(c,\alpha,\beta) + \Gamma_7(n,\alpha,\beta) \gamma_n(c,\alpha,\beta)$$

where

$$\Gamma_{6}(n,\alpha,\beta) = \Gamma_{1}(n,\alpha,\beta) + \Gamma_{3}(n,\alpha,\beta)\Gamma_{4}(n,\alpha,\beta)$$

$$= \frac{(\alpha+\beta+n+2)(\alpha+\beta+2n+5)((\alpha-\beta)(\alpha+\beta+2)+c(\alpha+\beta+2n+2)(\alpha+\beta+2n+4))}{2(\alpha+n+2)(\beta+n+2)(\alpha+\beta+n+3)(\alpha+\beta+2n+2)}$$

$$\Gamma_7(n,\alpha,\beta) = \Gamma_2(n,\alpha,\beta) + \Gamma_3(n,\alpha,\beta)\Gamma_5(n,\alpha,\beta)$$
  
=  $-\frac{n(\alpha+\beta+n+1)(\alpha+\beta+n+2)(\alpha+\beta+2n+4)(\alpha+\beta+2n+5)}{(\alpha+n+2)(\beta+n+2)(\alpha+\beta+n+3)(\alpha+\beta+2n+1)(\alpha+\beta+2n+2)}$ .

#### 4.5.3 Proof of Proposition 4.2.3

Let  $p_n(\cdot)$  (resp.  $h_n$ ) denote either the Hermite or Laguerre polynomials (resp. second moment). We recall that from the chaos decomposition of  $l(X)\mathbf{1}_{c\leq X}$ , we have

$$\Gamma_{l,n}(c) = \sum_{m=0}^{\infty} \frac{\mathbb{E}\left[\mathbf{1}_{c \leq X} p_n(X) p_m(X)\right] l_m}{h_n h_m},$$

where  $l_m = \mathbb{E}[l(X)p_m(X)]$ . If  $X \stackrel{d}{=} \mathcal{N}(0,1)$  then as the product of two Hermite polynomials (see Carlitz [42]) writes as

$$\operatorname{He}_{m}(x)\operatorname{He}_{n}(x) = 2^{-(n+m)/2}\operatorname{H}_{m}\left(\frac{x}{\sqrt{2}}\right)\operatorname{H}_{n}\left(\frac{x}{\sqrt{2}}\right) = \sum_{r=0}^{m\wedge n} r! \binom{m}{r} \binom{n}{r} \operatorname{He}_{m+n-2r}(x),$$

we obtain

$$\mathbb{E}\left[\mathbf{1}_{c\leq X}\mathrm{He}_{n}(X)\mathrm{He}_{m}(X)\right] = \sum_{r=0}^{m\wedge n} r! \binom{m}{r} \binom{n}{r} \mathbb{E}\left[\mathbf{1}_{c\leq X}\mathrm{He}_{m+n-2r}(X)\right]$$

$$=\sum_{r=0}^{m\wedge n}h_{m+n-2r}r!\left(\begin{array}{c}m\\r\end{array}\right)\left(\begin{array}{c}n\\r\end{array}\right)\gamma_{m+n-2r}(c)$$

Reorganizing the terms yields,

$$\Gamma_{l,n}(c) = \sum_{m=0}^{\infty} \left( \sum_{r=0}^{m \wedge n} \frac{r!}{(m+n-2r)!} \begin{pmatrix} m \\ r \end{pmatrix} \begin{pmatrix} n \\ r \end{pmatrix} \gamma_{m+n-2r}(c) \right) \frac{l_m}{n!m!},$$

and simple simplification gives the first result.

Similarly let  $X \stackrel{d}{=} \text{Gamma}(\alpha + 1, 1)$ . From Watson [165], the product of two Laguerre polynomials can be expressed as

$$\mathbf{L}_{m}^{(\alpha)}(x)\mathbf{L}_{n}^{(\alpha)}(x) = \sum_{r=|m-n|}^{m+n} \frac{(-1)^{m+n-r} 2^{m+n-r} r!}{(r-m)! (r-n)! (m+n-r)!} {}_{3}F_{2} \left( \begin{array}{c} \alpha+r+1, \frac{1}{2} (r-m-n), \frac{1}{2} (r-m-n+1) \\ r-m+1, r-n+1 \end{array}; 1 \right) \mathbf{L}_{r}^{(\alpha)}(x),$$

and the expression follows. Finally, we deal with the Jacobi polynomials. From [45, 12], the product of two Jacobi polynomials is given by

$$P_n^{(\alpha,\beta)}(x)P_m^{(\alpha,\beta)}(x) = \sum_{l=0}^{n+m} \kappa_{n,m}(l) P_l^{(\alpha,\beta)}(x) = \sum_{r=0}^{n+m} \kappa_{n,m}(n+m-r) P_{n+m-r}^{(\alpha,\beta)}(x),$$

where the linearization coefficient is equal to

$$\begin{split} \kappa_{n,m} \left( n+m-r \right) &= \frac{(\alpha+\beta+1)_{n+m-r} \left( \alpha+1 \right)_{n+m} \left( 2 \left( n+m-r \right) + \alpha+\beta+1 \right)}{(\alpha+1)_{n+m-r} \left( \alpha+\beta+1 \right)_{2(n+m)-r+1}} \\ &\times \frac{(-1)^r \left( n+m \right)! \left( \alpha+\beta+1 \right)_{2n} \left( \alpha+\beta+1 \right)_{2m}}{n!m!r! \left( \alpha+\beta+1 \right)_n \left( \alpha+\beta+1 \right)_m} \\ &\times F_{2:1}^{2:2} \left( \begin{array}{c} -r, -\alpha-\beta-1-2 \left( n+m \right) +r: -n, -\alpha-n; -m; -\alpha-m; \\ -\left( n+m \right), -\alpha-\left( n+m \right): -2n-\alpha-\beta; -2j-\alpha-\beta \end{array} \right), \end{split}$$

and the expression for  $\Gamma_{l,n}(c)$  follows.

#### 4.5.4 Proof of Theorem 4.2.4

 $\triangleright$  L<sub>2</sub> error for the Hermite polynomials. In light of (4.2.7), the L<sub>2</sub> error for the Hermite polynomials writes as

$$\mathcal{E}_{N}^{\mathrm{He}}(c) = \left(\sum_{n=N}^{\infty} h_{n+1}\gamma_{n+1}(c)^{2}\right)^{\frac{1}{2}} = e^{-\frac{c^{2}}{4}} \left(\sum_{n=N}^{\infty} \frac{e^{-\frac{c^{2}}{2}}\mathrm{He}_{n}^{2}(c)}{2\pi(n+1)!}\right)^{\frac{1}{2}}$$

We recall the following estimates for the Hermite polynomials.

**Lemma 4.5.1** (Estimates for the Hermite polynomials). For every  $n \in \mathbb{N}^*$ , there exist positive constants A, B, C, D such that (see [32, Theorem 1, Lemma 1]),

$$\begin{aligned} \frac{\operatorname{He}_{n}^{2}\left(c\right)e^{-\frac{c^{2}}{2}}}{n!} &\leq \frac{A}{\sqrt{4n+2-c^{2}}}, \quad if \ |c| < \sqrt{4n+2}, \quad (oscillatory \ region), \\ Bn^{-\frac{1}{6}} &\leq \sup_{c \in \mathbb{R}} \left(\frac{\operatorname{He}_{n}^{2}\left(c\right)e^{-\frac{c^{2}}{2}}}{n!}\right) \leq Cn^{-\frac{1}{6}}, \end{aligned}$$

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$$\frac{\operatorname{He}_{n}^{2}(c) e^{-\frac{c^{2}}{2}}}{n!} \leq \frac{Dn^{-\frac{5}{6}}}{\left(c - \sqrt{4n+2}\right)^{4}}, \quad if \ |c| > \sqrt{4n+2}, \quad (monotonic \ region).$$

When  $|c| \approx \sqrt{4n+2}$  (transition region), the function  $c \to \operatorname{He}_n^2(c) e^{-\frac{c^2}{2}}$  attains its maximum (see e.g. Krasikov [127]). Furthermore, let  $k \in \mathbb{R}$ , a > 0 and  $0 < \eta < 2$ , then there exist positive constants  $B_1$  and  $B_2$  (which depend on a and k) such that ([157, Theorem 8.91.3]),

$$\max_{a \le x} \left( x^k \frac{e^{-\frac{x^2}{4}} |\operatorname{He}_n(x)|}{(n!)^{\frac{1}{2}}} \right) \le B_1(k, a) n^{S_1}, \quad S_1 = \max\left(\frac{k}{2} - \frac{1}{12}, -\frac{1}{4}\right), \tag{4.5.12}$$

$$\max_{a \le x \le \sqrt{(2-\eta)n}} \left( x^k \frac{e^{-\frac{x^2}{4}} |\operatorname{He}_n(x)|}{(n!)^{\frac{1}{2}}} \right) \le B_2(k,a) n^{S_2}, \quad S_2 = \max\left(\frac{k}{2} - \frac{1}{4}, -\frac{1}{4}\right).$$
(4.5.13)

In the current proof, C denotes an independent positive constant that can change from one line to another.

ightarrow Global estimate. As  $c \to \frac{e^{-\frac{c^2}{2}\operatorname{He}_n^2(c)}}{(n+1)!}$  is an even function, we can assume (without loss of generality) that  $c \ge 0$ . Let  $\varepsilon \in (0, 1)$  that will be fixed later and introduce the intervals:

$$\Omega_{1,n}(\varepsilon) = \left[ (1+\varepsilon)\sqrt{4n+2}, \infty \right), \quad \Omega_{2,n}(\varepsilon) = \left[ 0, \sqrt{4n+2}\left(1-\varepsilon\right) \right]$$

From Lemma 4.5.1, if  $c \in \Omega_{1,n}(\varepsilon)$ ,

$$\frac{e^{-\frac{c^2}{2}}\operatorname{He}_n^2(c)}{(n+1)!} \le \frac{Cn^{-\frac{5}{6}}}{\varepsilon^4 \left(4n+2\right)^2 n} \le \frac{C_3}{\varepsilon^4 n^{\frac{23}{6}}}$$

while if  $c \in \Omega_{2,n}(\varepsilon)$ ,

$$\frac{e^{-\frac{c^2}{2}}\operatorname{He}_n^2(c)}{(n+1)!} \le \frac{C}{(n+1)\sqrt{4n+2-c^2}} \le \frac{C}{n\left(4n+2\right)^{\frac{1}{2}}\left(2\varepsilon-\varepsilon^2\right)^{\frac{1}{2}}} \le \frac{C_1}{\left(2\varepsilon-\varepsilon^2\right)^{\frac{1}{2}}n^{\frac{3}{2}}}.$$

Moreover still by Lemma 4.5.1, if  $c \in \mathbb{R}$  the following global estimate holds

$$\frac{e^{-\frac{c^2}{2}}\operatorname{He}_n^2(c)}{(n+1)!} \le \frac{C_2}{n^{\frac{7}{6}}}$$

Let us now set:

$$n_1(c,\varepsilon) = \left\lfloor \frac{1}{4} \left( \left( \frac{c}{1+\varepsilon} \right)^2 - 2 \right) \right\rfloor, \quad n_2(c,\varepsilon) = \left\lfloor \frac{1}{4} \left( \left( \frac{c}{1-\varepsilon} \right)^2 - 2 \right) \right\rfloor,$$

and notice that for every c, we have  $n_1(c, \varepsilon) \leq n_2(c, \varepsilon)$ . Moreover, for every  $n \leq n_1(c, \varepsilon)$  (resp.  $n > n_2(c, \varepsilon)$ )), we have  $c \in \Omega_{1,n}(\varepsilon)$  (resp.  $c \in \Omega_{2,n}(\varepsilon)$ ).

First suppose that  $N \leq n_1(c, \varepsilon) \leq n_2(c, \varepsilon)$ ; in that case, the sum can be decomposed as:

$$\sum_{n=I}^{\infty} \frac{e^{-\frac{c^2}{2}} \left(\operatorname{He}_n\left(c\right)\right)^2}{(n+1)!} = \sum_{n=N}^{n_1(c,\varepsilon)} \frac{e^{-\frac{c^2}{2}} \left(\operatorname{He}_n\left(c\right)\right)^2}{(n+1)!} + \sum_{n=n_2(c,\varepsilon)+1}^{\infty} \frac{e^{-\frac{c^2}{2}} \left(\operatorname{He}_n\left(c\right)\right)^2}{(n+1)!} + \sum_{n=n_1(c,\varepsilon)+1}^{n_2(c,\varepsilon)} \frac{e^{-\frac{c^2}{2}} \left(\operatorname{He}_n\left(c\right)\right)^2}{(n+1)!} =: R_1\left(c,\varepsilon\right) + R_2\left(c,\varepsilon\right) + R_{1,2}\left(c,\varepsilon\right).$$

Combining the estimates resulting from Lemma 4.5.1 with (4.1.2), we obtain

$$R_{1}(c,\varepsilon) \leq \sum_{n=N}^{n_{1}(c,\varepsilon)} \frac{C_{1}}{\varepsilon^{4}n^{\frac{23}{6}}} \leq \frac{C}{\varepsilon^{4}N^{\frac{17}{6}}},$$

$$R_{2}(c,\varepsilon) \leq \sum_{n=n_{2}(c,\varepsilon)+1}^{\infty} \frac{C_{2}}{(2\varepsilon - \varepsilon^{2})^{\frac{1}{2}}n^{\frac{3}{2}}} \leq \frac{C}{(2\varepsilon - \varepsilon^{2})^{\frac{1}{2}}N^{\frac{1}{2}}},$$

$$R_{1,2}(c,\varepsilon) \leq \sum_{n=n_{1}(c,\varepsilon)+1}^{n_{2}(c,\varepsilon)} \frac{C_{3}}{n^{\frac{7}{6}}} \leq C\frac{n_{2}(c) - n_{1}(c)}{n_{1}(c)^{\frac{7}{6}}}.$$

We now choose to take  $\varepsilon = \varepsilon(c)$  such that  $\varepsilon(c) \to 0$  as  $c \to +\infty$ . As  $\left(2\varepsilon(c) - \varepsilon^2(c)\right)^{\frac{1}{2}} \sim 2\varepsilon^{\frac{1}{2}}(c)$ ,  $\left(\frac{c}{1-\varepsilon(c)}\right)^2 - \left(\frac{c}{1+\varepsilon(c)}\right)^2 \sim 2c^2\varepsilon(c)$  and  $\left(\frac{c}{1-\varepsilon(c)}\right)^2 \sim c^2$ , we deduce that there exists a positive constant C such that:

$$\sum_{n=N}^{\infty} \frac{e^{-\frac{c^2}{2}} \left(\operatorname{He}_n(c)\right)^2}{(n+1)!} \le C \left(\frac{1}{\varepsilon^4(c) N^{\frac{17}{6}}} + \frac{1}{\varepsilon^{\frac{1}{2}}(c) N^{\frac{1}{2}}} + \frac{\varepsilon(c)}{c^{\frac{1}{3}}}\right).$$

Optimizing in  $\varepsilon$  for the r.h.s. of the previous inequality, we see that it is optimal (up to a positive constant) to choose  $\varepsilon(c) = \frac{1}{2} \wedge c^{-\frac{2}{3}}$ . Thus remembering that since  $n_1(c,\varepsilon) \ge N$ ,  $c \ge (4N+2)^{\frac{1}{2}}(1+\varepsilon(c)) \ge (4N+2)^{\frac{1}{2}}$  and then  $\varepsilon(c) c^{-\frac{1}{3}} \le CN^{-\frac{1}{2}}$ , we infer that

$$\sum_{n=N}^{\infty} \frac{e^{-\frac{c^2}{2}} \left(\operatorname{He}_n\left(c\right)\right)^2}{(n+1)!} \le C \left(\frac{1 \lor c^{\frac{8}{3}}}{N^{\frac{17}{6}}} + \frac{1 \lor c^{\frac{1}{3}}}{N^{\frac{1}{2}}} + \frac{1}{N^{\frac{1}{2}}}\right) \le C \frac{1 \lor c^{\frac{1}{3}} \lor c^{\frac{8}{3}} N^{-\frac{14}{3}}}{N^{\frac{1}{2}}}$$

If  $n_1(c) + 1 \le N \le n_2(c)$  then,  $c \ge (4N+2)^{\frac{1}{2}} (1-\varepsilon(c)) \ge \frac{(4N+2)^{\frac{1}{2}}}{2}$  and

$$\sum_{n=N}^{\infty} \frac{e^{-\frac{c^2}{2}} \left(\operatorname{He}_n(c)\right)^2}{(n+1)!} \le R_2 \left(c, \varepsilon\left(c\right)\right) + R_{1,2} \left(c, \varepsilon\left(c\right)\right) \le C \frac{1 \lor c^{\frac{1}{3}}}{N^{\frac{1}{2}}} + \frac{C}{N^{\frac{1}{2}}} \le C \frac{1 \lor c^{\frac{1}{3}}}{N^{\frac{1}{2}}}$$

Finally, if  $N \ge n_2(c) + 1$  then,  $\sum_{n=N}^{\infty} \frac{e^{-\frac{c^2}{2}}(\operatorname{He}_n(c))^2}{(n+1)!} \le R_2(c,\varepsilon(c)) \le C \frac{1\vee c^{\frac{1}{3}}}{N^{\frac{1}{2}}}$  and the estimate (4.2.17) is proved.

 $\triangleright$  Localized estimates for the Hermite polynomials. Let a > 0 and  $0 < \eta < 2$ . If  $|c| \ge a$  (resp.  $a \le |c| \le (2 - \eta)^{\frac{1}{2}} N^{\frac{1}{2}}$ ), the localized estimate (4.2.21) (resp. (4.2.22)) is a direct consequence of (4.5.12) (resp. (4.5.15)) with  $k = -\frac{1}{3}$  (resp. k = 0) together with (4.1.2).

 $\succ L_2$  error for the Laguerre polynomials. Recalling the expression for the second-moment  $h_n = \frac{\Gamma_{n+\alpha+1}}{n!\Gamma_{\alpha+1}}$  along with (4.2.8),

$$\gamma_n(c) = -\frac{(n-1)!}{\Gamma_{n+\alpha+1}} c^{\alpha+1} e^{-c} \mathcal{L}_{n-1}^{(\alpha+1)}(c),$$

the  $L_2$  error for the Laguerre polynomials writes as

$$\begin{split} \mathcal{E}_{N}^{\mathrm{La}}(c) &= \left(\sum_{n=N}^{\infty} \frac{\Gamma_{n+\alpha+2}}{(n+1)!\Gamma_{\alpha+1}} \left(\frac{n!}{\Gamma_{n+\alpha+2}} c^{\alpha+1} e^{-c} \mathcal{L}_{n}^{(\alpha+1)}(c)\right)^{2}\right)^{\frac{1}{2}} \\ &= \frac{1}{\Gamma_{\alpha+1}^{\frac{1}{2}}} \left(\sum_{n=N}^{\infty} \frac{n!}{(n+1)\Gamma_{n+\alpha+2}} \left(c^{\alpha+1} e^{-c} \mathcal{L}_{n}^{(\alpha+1)}(c)\right)^{2}\right)^{\frac{1}{2}}, \end{split}$$

Again, we start with some estimates on the maximum of Laguerre polynomials.

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**Lemma 4.5.2.** Let  $k \in \mathbb{R}$ ,  $\alpha > -1$ , a > 0 and  $0 < \eta < 4$ . Then, there exist positive constants  $C_1$  and  $C_2$  (which depend on  $a, \eta, \alpha$  and k) such that ([157, Theorem 8.91.2])

$$\sup_{a \le c} \left| c^k e^{-\frac{c}{2}} \mathcal{L}_n^{(\alpha)}(c) \right| \le C_1(k, a, \alpha) n^{Q_1}, \quad Q_1 = \max\left(k - \frac{1}{3}, \frac{\alpha}{2} - \frac{1}{4}\right).$$
(4.5.14)

$$\sup_{\leq c \leq (4-\eta)n} \left| c^k e^{-\frac{c}{2}} \mathcal{L}_n^{(\alpha)}(c) \right| \leq C_2(k, a, \eta, \alpha) n^{Q_2}, \quad Q_2 = \max\left(k - \frac{1}{2}, \frac{\alpha}{2} - \frac{1}{4}\right).$$
(4.5.15)

Moreover, the estimate (4.5.14) cannot be extended to  $(0, \infty)$  without increasing the order in n (see Duran [59]). More precisely, in this particular case the order in n becomes  $\max(k, \alpha)$  instead of  $\max\left(k-\frac{1}{3}, \frac{\alpha}{2}-\frac{1}{4}\right)$ . For every  $n \in \mathbb{N}^*$ , let  $\alpha \geq 0$  and  $\alpha \notin \mathbb{N}$ . We have (Rafalson [149, Lemma 3])

$$\left| c^{\frac{\alpha}{2} + \frac{1}{4}} e^{-\frac{c}{2}} \left| \mathcal{L}_{n}^{(\alpha)}(c) \right| \leq \begin{cases} (\alpha + 1)n^{\frac{\alpha}{2} - \frac{1}{4}} & \text{if } 0 \leq x \leq \frac{1}{n + \frac{\alpha + 1}{2}}, \\ n^{\frac{\alpha}{2} - \frac{1}{4}} \varphi_{1}(\alpha) + n^{\frac{\alpha}{2} - \frac{1}{2}} c^{\frac{5}{4}} \varphi_{2}(\alpha) & \text{if } c \geq \frac{1}{n + \frac{\alpha + 1}{2}}, \end{cases}$$
(4.5.16)

where  $\varphi_1, \varphi_2$  are positive functions which depend only on  $\alpha$ .

Observing that

$$\frac{n!}{(n+1)\Gamma_{n+\alpha+2}} \underset{n \to \infty}{\sim} \frac{1}{n^{2+\alpha}},$$

and from (4.5.16), there exists a function  $\Lambda(\cdot)$  depending only on  $\alpha$  such that

$$c^{\frac{\alpha+1}{2}+\frac{1}{4}}e^{-\frac{c}{2}}\left|\mathcal{L}_{n}^{(\alpha+1)}(c)\right| \leq \Lambda(\alpha)\left(n^{\frac{\alpha}{2}+\frac{1}{4}} \vee n^{\frac{\alpha}{2}}c^{\frac{5}{4}}\right),$$

and we conclude as for the Hermite polynomials. For the first localized estimate (4.2.23), apply (4.5.14) with  $k = \frac{\alpha+1}{2} + \frac{1}{4}$ ,  $\alpha + 1$  instead of  $\alpha$ , and as  $\max\left(\frac{\alpha}{2} + \frac{7}{12} - \frac{1}{3}, \frac{\alpha+1}{2} - \frac{1}{4}\right) = \frac{\alpha}{2} + \frac{1}{4}$ , we infer the existence of a positive constant C(a) such that

$$\begin{aligned} \mathcal{E}_{N}^{\mathrm{La}}(c) &\leq C(a) c^{\frac{\alpha}{2} + \frac{5}{12}} e^{-\frac{c}{2}} \left( \sum_{n=N}^{\infty} \frac{1}{n^{\alpha+2}} \left( c^{\frac{\alpha}{2} + \frac{7}{12}} e^{-\frac{c}{2}} \mathcal{L}_{n}^{(\alpha+1)}(c) \right)^{2} \right)^{\frac{1}{2}} \\ &\leq C(a) c^{\frac{\alpha}{2} + \frac{5}{12}} e^{-\frac{c}{2}} N^{-\frac{1}{4}}, \end{aligned}$$

and we conclude again with (4.1.2). The last estimate being similar, we skip details.  $\triangleright L_2$  error for the Jacobi polynomials. From (4.2.9), we have this time:

$$\mathcal{E}_{N}^{\mathbf{J}}(c) = \frac{2^{-\alpha-\beta-2}}{\mathbf{B}_{\alpha+1,\beta+1}} \left( \sum_{n=N}^{\infty} \frac{(1-c)^{2\alpha+2} \left(1+c\right)^{2\beta+2} \left(\mathbf{P}_{n}^{(\alpha+1,\beta+1)}(c)\right)^{2}}{(n+1)^{2} h_{n+1}} \right)^{\frac{1}{2}}$$

We consider the following preliminary result.

**Lemma 4.5.3.** For every  $c \in [-1, 1]$  and  $\alpha, \beta \geq 0$ , there exist a positive constant D such that,

$$\sum_{n=N}^{\infty} \frac{1}{n} \left( (1-c)^{\alpha+1} \left(1+c\right)^{\beta+1} \mathcal{P}_n^{(\alpha+1,\beta+1)}(c) \right)^2 \le D \frac{(1-c)^{\alpha+\frac{1}{2}} \left(1+c\right)^{\beta+\frac{1}{2}}}{N^{\frac{1}{2}}}.$$
 (4.5.17)

Proof of Lemma 4.5.3. Let us introduce the function

$$g_n^{(\alpha,\beta)}(c) = \Xi_{n,\alpha,\beta}(1-c)^{\frac{\alpha}{2}} (1+c)^{\frac{\beta}{2}} \mathbf{P}_n^{(\alpha,\beta)}(c),$$

with 
$$\Xi_{n,\alpha,\beta} = \left(2^{-\alpha-\beta} \frac{\Gamma_{n+1}\Gamma_{n+\alpha+1}\Gamma_{n+\beta+1}}{\Gamma_{n+\alpha+1}\Gamma_{n+\beta+1}}\right)^{\frac{1}{2}}$$
. Observe that the sum rewrites as  

$$\sum_{n=N}^{\infty} \frac{1}{n} \left( (1-c)^{\alpha+1} (1+c)^{\beta+1} P_n^{(\alpha+1,\beta+1)}(c) \right)^2$$

$$= \sum_{n=N}^{\infty} \frac{1}{n} \left( \frac{(1-c)^{\alpha+1} (1+c)^{\beta+1} (1-c)^{-\frac{\alpha+1}{2}} (1+c)^{-\frac{\beta+1}{2}} g_n^{(\alpha+1,\beta+1)}(c)}{\Xi_{n,\alpha,\beta}} \right)^2$$

$$= \sum_{n=N}^{\infty} \frac{1}{n} \left( \frac{(1-c)^{\frac{\alpha+1}{2}} (1+c)^{\frac{\beta+1}{2}} g_n^{(\alpha+1,\beta+1)}(c)}{\Xi_{n,\alpha,\beta}} \right)^2$$

$$= (1-c)^{\alpha+\frac{1}{2}} (1+c)^{\beta+\frac{1}{2}} \sum_{n=N}^{\infty} \frac{1}{n} \left( \frac{(1-c^2)^{\frac{1}{4}} g_n^{(\alpha+1,\beta+1)}(c)}{\Xi_{n,\alpha,\beta}} \right)^2.$$

As  $\alpha + 1, \beta + 1 > 0$ , applying Haagerup and Schlichtkrull [97, Theorem 1.1] we have the existence of a positive constant C such that,

$$\left| \left( 1 - c^2 \right)^{\frac{1}{4}} g_n^{(\alpha+1,\beta+1)}(c) \right| \le C \left( 2n + \alpha + \beta + 3 \right)^{-\frac{1}{4}}.$$

We obtain (4.5.17) noticing that

/

$$\Xi_{n,\alpha,\beta} \underset{n \to \infty}{\sim} 2^{-\frac{\alpha}{2} - \frac{\beta}{2}}, n \left(2n + \alpha + \beta + 3\right)^{\frac{1}{2}} \underset{n \to \infty}{\sim} n^{\frac{3}{2}}, \sum_{n=N}^{\infty} n^{-\frac{3}{2}} \underset{N \to \infty}{\sim} 2N^{-\frac{1}{2}}.$$

Observing that

$$\frac{1}{(n+1)^2 h_{n+1}} \underset{n \to \infty}{\sim} \frac{2\mathbf{B}_{\alpha+1,\beta+1}}{n},$$

and applying Lemma 4.5.3, we obtain the announced  $L_2$  error estimates for the Jacobi polynomials.

 $\triangleright$  L<sub>2</sub> error for the Legendre polynomials. Recall from (4.2.10) that

$$\gamma_{n+1}(c) = \frac{2n+3}{2n+4} \frac{1-c^2}{n+1} \frac{\mathrm{dP}_{n+1}(c)}{\mathrm{d}c}$$

From Antonov, Kholshevnikov, and Shaidulin [9], there exists an independent positive constant A > 0 such that for every  $n \in \mathbb{N}$ ,

$$\left| \left( 1 - c^2 \right)^{\frac{3}{4}} \frac{\mathrm{dP}_{n+1}(c)}{\mathrm{d}c} \right| \le A \left( n + \frac{5}{3} \right)^{\frac{1}{2}}.$$

and since  $\frac{2n+3}{2n+4} \frac{\left(n+\frac{5}{3}\right)^{\frac{1}{2}}}{n+1} \underset{n \to \infty}{\sim} n^{-\frac{1}{2}}$ , we have the existence of a positive constant C such that

$$|\gamma_{n+1}(c)|^2 \le C \frac{(1-c^2)^{\frac{1}{2}}}{n}.$$

We conclude remembering that  $h_{n+1} = \frac{2}{2n+3} \underset{n \to \infty}{\sim} n^{-1}$  and by use of (4.1.2).

#### 4.5.5 Proof of Lemma 4.3.1

For the Legendre polynomials, this is direct from the identity

$$\mathbf{E}_{N}^{\mathrm{Le}}\left(c_{\mathrm{Le}}(q)\right) = \left(1 - \left(2q - 1\right)^{2}\right)^{\frac{1}{4}} N^{-\frac{1}{2}} = \left(4q(1-q)\right)^{\frac{1}{4}} N^{-\frac{1}{2}}.$$

For the Hermite polynomials, recall that  $c_{\text{He}}(q) = \Phi^{-1}(q)$  and

$$\mathbf{E}_{N}^{\mathrm{He}}(c_{\mathrm{He}}(q)) = \left(1 \vee |\Phi^{-1}(q)|^{\frac{1}{6}} \vee |\Phi^{-1}(q)|^{\frac{4}{3}} N^{-\frac{7}{3}}\right) e^{-\frac{\Phi^{-1}(q)^{2}}{4}} N^{-\frac{1}{4}}.$$

From the expansion  $-\sqrt{2\pi}x\Phi(x) \underset{x\to-\infty}{\sim} e^{-\frac{x^2}{2}}$ , we infer that

$$\Phi^{-1}(q) \underset{q \to 0^+}{\sim} -\sqrt{-2\ln(q)}, \quad e^{-\frac{\Phi^{-1}(q)^2}{4}} \underset{q \to 0^+}{\sim} (2\pi)^{\frac{1}{4}} q^{\frac{1}{2}} (-2\ln(q))^{\frac{1}{4}}$$

and we obtain the announced asymptotic observing that

$$1 \vee |\Phi^{-1}(q)|^{\frac{1}{6}} \vee |\Phi^{-1}(q)|^{\frac{4}{3}} N^{-\frac{7}{3}} \underset{q \to 0^{+}}{\sim} |\Phi^{-1}(q)|^{\frac{1}{6}} \underset{q \to 0^{+}}{\sim} 2^{\frac{1}{12}} |\ln(q)|^{\frac{1}{12}}.$$

For the case  $q \to 1^-$ , we proceed as before evoking the identity  $\Phi^{-1}(1-q) = -\Phi^{-1}(q)$  and observing that

$$1 \vee |\Phi^{-1}(q)|^{\frac{1}{6}} \vee |\Phi^{-1}(q)|^{\frac{4}{3}} N^{-\frac{7}{3}} \underset{q \to 1^{-}}{\sim} |\Phi^{-1}(q)|^{\frac{4}{3}} N^{-\frac{7}{3}} \underset{q \to 1^{-}}{\sim} 2^{\frac{2}{3}} |\ln(1-q)|^{\frac{2}{3}} N^{-\frac{7}{3}}.$$

For the Laguerre polynomials, first observe:

$$\mathbf{E}_{N}^{\mathrm{La}}\left(c_{\mathrm{La}}(q)\right) = \mathscr{G}_{\alpha+1}^{-1}(q)^{\frac{\alpha}{2}+\frac{1}{4}} e^{-\frac{\mathscr{G}_{\alpha+1}^{-1}(q)}{2}} N^{-\frac{1}{4}} \left(1 \vee \mathscr{G}_{\alpha+1}^{-1}(q)^{\frac{5}{4}} N^{-\frac{1}{4}}\right),$$

where we have dropped the dependence on  $\alpha$ . For  $q \to 0^+$ ,  $\mathscr{G}_{\alpha+1}^{-1}(q)^{\frac{5}{4}}N^{-\frac{1}{4}} \to 0$  and from the asymptotic expansion ([146, 8.7.1])  $\mathscr{G}_{\alpha+1}(x) \underset{x\to 0^+}{\sim} \frac{x^{\alpha+1}}{\Gamma_{\alpha+2}}$ , we easily obtain

$$\mathscr{G}_{\alpha+1}^{-1}(q) \underset{q \to 0^+}{\sim} (q\Gamma_{\alpha+2})^{\frac{1}{\alpha+1}}$$

Similarly, starting from the well-known asymptotic expansion ([146, 8.11.2])  $\frac{\Gamma_{\alpha+1}(x)}{\Gamma_{\alpha+1}} \sim \frac{x^{\alpha}e^{-x}}{\Gamma_{\alpha+1}}$ , we infer that

$$\mathscr{G}_{\alpha+1}^{-1}(q)^{\alpha} e^{-\mathscr{G}_{\alpha+1}^{-1}(q)} = \Gamma_{\alpha+1}(1-q),$$

and consequently

$$\mathcal{G}_{\alpha+1}^{-1}(q) \approx_{q \to 1^{-}} -\alpha W_{-1} \left( -\frac{\Gamma_{\alpha+1}(1-q)^{\frac{1}{\alpha}}}{\alpha} \right)$$
$$\approx_{q \to 1^{-}} -\alpha \ln \left( -\frac{\Gamma_{\alpha+1}(1-q)^{\frac{1}{\alpha}}}{\alpha} \right)$$
$$\approx_{q \to 1^{-}} -\ln(1-q),$$

where  $W_{-1}(\cdot)$  denotes the lower branch of Lambert function and we have used that  $W_{-1}(-x) \underset{x \to 0^+}{\sim} \ln(x)$  (see Corless et al. [50] for a review of the Lambert function  $W(\cdot)$ ). All in all, we deduce that,

$$\mathbf{E}_{N}^{\mathrm{La}}\left(c_{\mathrm{La}}(q)\right) \underset{q \to 1^{-}}{\sim} \Gamma_{\alpha+1}^{\frac{1}{2}} (1-q)^{\frac{1}{2}} \mathscr{G}_{\alpha+1}^{-1}(q)^{\frac{1}{4}} N^{-\frac{1}{4}} \left(1 \vee |\ln(1-q)|^{\frac{5}{4}} N^{-\frac{1}{4}}\right)$$

$$\underset{q \to 1^{-}}{\sim} \Gamma_{\alpha+1}^{\frac{1}{2}} (1-q)^{\frac{1}{2}} \left| \ln(1-q) \right|^{\frac{1}{4}} N^{-\frac{1}{4}} \left( 1 \vee \left| \ln(1-q) \right|^{\frac{5}{4}} N^{-\frac{1}{4}} \right).$$

Finally, for the Jacobi polynomials, we have this time:

$$\mathbf{E}_{N}^{\mathbf{J}}(c_{\mathbf{J}}(q)) = 2^{\frac{\alpha+\beta+1}{2}} \left(1 - \mathscr{B}_{\alpha+1,\beta+1}^{-1}(q)\right)^{\frac{\alpha}{2}+\frac{1}{4}} \left(\mathscr{B}_{\alpha+1,\beta+1}^{-1}(q)\right)^{\frac{\beta}{2}+\frac{1}{4}} N^{-\frac{1}{4}}.$$

Now, from the equality  $B_{\alpha+1,\beta+1}x^{-(\alpha+1)}\mathscr{B}_{\alpha+1,\beta+1}(x) = \int_0^1 y^{\alpha} (1-xy)^{\beta} dy$ , we have

$$\mathscr{B}_{\alpha+1,\beta+1}(x) \underset{x \to 0^+}{\sim} \frac{x^{\alpha+1}}{(\alpha+1)B_{\alpha+1,\beta+1}},$$

and the identity  $\mathscr{B}_{\alpha+1,\beta+1}(x) = 1 - \mathscr{B}_{\beta+1,\alpha+1}(1-x)$ . We then deduce that

$$\mathscr{B}_{\alpha+1,\beta+1}^{-1}(q) \underset{q \to 0^{+}}{\sim} ((\alpha+1) \mathbf{B}_{\alpha+1,\beta+1})^{\frac{1}{\alpha+1}} q^{\frac{1}{\alpha+1}},$$
$$1 - \mathscr{B}_{\alpha+1,\beta+1}^{-1}(q) \underset{q \to 1^{-}}{\sim} ((\beta+1) \mathbf{B}_{\beta+1,\alpha+1})^{\frac{1}{\beta+1}} (1-q)^{\frac{1}{\beta+1}},$$

and this concludes the proof.

# Part III

Weak approximations, option price expansions, and small-time asymptotics

# CHAPTER 5

# SMALL-TIME ASYMPTOTICS FOR AMERICAN OPTIONS IN LOCAL VOLATILITY MODELS

Note. Working paper with Stefano De Marco.

Abstract. We derive short-maturity expansions for American put prices in local volatility models. The main building blocks of our results are a refined asymptotic expansion of the option exercise boundary close to maturity, the well-known small-time behavior for the transition density of a diffusion process, and the application of Laplace's method. Our main contribution is an efficient expansion of the at-the-money American put price, which reveals a non-trivial combination of time scales in the aymptotics of the option's premium (a combination of powers of  $\tau$  and iterated logarithmic functions of  $\tau$ ,  $\tau$  being the option's time to maturity). We also derive expansions for the out-of-the-money case, and deduce an asymptotic estimate for the difference between the European and the American implied volatility. Our results are illustrated by several numerical experiments.

## 5.1 Introduction

Call and put options written on individual stocks are generally of American nature while only a few American-style options exist for broad-based indices. As opposed to European vanillas, for which the calibration of Dupire's local volatility model [58] is fast and exact (as long as the implied volatility surface is arbitrage-free), and because the American and the European implied volatility have no reason to match, the calibration of the local volatility model on American Vanillas poses a delicate challenge. Actually, this is often disregarded in the industry by assuming that both the American and the European implied volatility match. More precisely, the calibration of a model to American options generally consists of the following three steps:

- 1. Compute the implied volatility from American options.
- 2. Input this smile as it was European.
- 3. Calibrate a model with standard methods (e.g. local volatility from Dupire's formula or other desired models).

Needless to say that such a procedure leads to a calibration error that (to our knowledge) has not been investigated in the financial literature. To overcome this industrial mispractice, De Marco and Henry-Labordère [53] recently described an efficient algorithm for the calibration of Dupire's local volatility on American options when starting from an arbitrage-free parametrization of a European implied volatility.

In this work, using that the maturity of the most liquid American options are less than two years, we aim at giving short-time estimates of the difference between American and European implied volatility in a time-homogeneous local volatility model.

Based on the methodology of Gatheral et al. [71], we provide short-time expansions for the American put prices along with upper–lower bounds for the American implied volatility.

#### 5.1.1 The model

We consider the following time-homogeneous local volatility (LV) model for the stock price S

$$\mathrm{d}S_t = rS_t \mathrm{d}t + S_t \sigma\left(S_t\right) \mathrm{d}W_t,\tag{5.1.1}$$

and we assume the following conditions on the local volatility function:  $\sigma$  is  $\mathcal{C}^2(\mathbb{R}_+)$  and there exists a positive constant C > 0 such that

$$\forall s > 0, \quad C^{-1} \le \sigma(s) \le C, \quad \left| s\sigma'(s) \right| \le C, \quad \left| s^2 \sigma''(s) \right| \le C. \tag{5.1.2}$$

Under the assumption (5.1.2), the function  $s \mapsto s\sigma(s)$  is globally Lipschitz and is worth zero at s = 0, therefore (5.1.1) has a unique strictly positive solution  $(S_t)_{t \ge 0}$ .

The price at time t < T of a put option with strike price K > 0 and maturity T > 0 under the model (5.1.1) is given by:

$$P(t, T, s, K) = \mathbb{E}\left[e^{-r(T-t)}(K - S_T)_+ \middle| S_t = s\right] =: \mathbb{E}_{t,s}\left[e^{-r(T-t)}(K - S_T)_+\right]$$

It is that, for every fixed (T, K), the price function  $(t, s) \mapsto P(t, T, s, K)$  solves the following backward parabolic partial differential equation (PDE):

$$\partial_t P + \frac{\sigma^2(s)s^2}{2}\partial_{ss}P + rs\partial_s P - rP = 0, \quad P(T, T, s, K) = (K - s)_+.$$

Unlike European options, American options give their owner the right to exercise the option at any time before the maturity T. It can be shown (see [139]) that the price A(t, T, s, K) of an American put option with maturity T and strike price K is the solution to the following backward parabolic PDE with obstacle:

$$\begin{cases} \partial_t A + \frac{\sigma^2(s)s^2}{2} \partial_{ss} A + rs \partial_s A - rA = 0, & t < T, \quad s > s^T(t) \\ A(t, T, s, K) > (K - s)_+, & t < T, \quad s > s^T(t) \\ A(t, T, s, K) = (K - s)_+, & t < T, \quad s \le s^T(t) \\ A(T, T, s, K) = (K - s)_+, & t = T, \quad s > 0. \end{cases}$$
(5.1.3)

The function  $t \mapsto s^T(t)$ , which is one of the unknowns of (5.1.3), is referred to as the exercise boundary and will be of significant importance in our study. For a recent survey on numerical approaches to American options, we refer to [4] and references therein.

Remark 3. Assumption (5.1.2) is considered in Gatheral et al. [71], where a proof of a smalltime expansion for the transition density of the process X is given, relying on the Lamperti transformation for the underlying SDE. As usual, in terms of the log-price process  $X_t = \ln S_t$ the model (5.1.1) reads

$$dX_t = \left(r - \frac{1}{2}\sigma^2\left(e^{X_t}\right)\right)dt + \sigma\left(e^{X_t}\right)dW_t.$$
(5.1.4)

It is immediate to check that assumption (5.1.2) amounts to asking that the diffusion coefficient  $x \mapsto \sigma(e^x)$  for the log-price process is in  $C_b^2(\mathbb{R})$ . The Black–Scholes model of course satisfies assumption (5.1.2), but otherwise this assumption is not really harmless: it is not fulfilled, for example, by a simple "academic" local volatility model such as the CEV model, for which the volatility function  $\sigma(s) = \delta s^{\beta/2-1}$ ,  $\delta > 0$  and  $\beta > 0$ , is unbounded and such that  $s\sigma'(s)$  blows up when  $s \to 0$  or  $s \to \infty$  (according to the value of  $\beta$ ). Strictly speaking, the asymptotic results we present in this work are therefore not justified for the CEV model; nevertheless, we can (and will) numerically check the expansions we obtain for American options in this modeling framework as well. In our numerical tests in Section 5.2.3, our relevant asymptotic formulas prove to be as accurate for a CEV model as for Black–Scholes; as in Gatheral et al. [71], we can argue that the unboundedness and the singularity at s = 0 of the volatility function in practice do not affect our asymptotic expansions for sufficiently small maturities (up to T = 2 years in our tests, as it is typically the case on most American options markets) and for values of the parameters  $S_0, r, \delta, \beta$  typical of Equity markets.

Finally, it is worth to notice that, even if (5.1.1) is a homogeneous local volatility model and therefore does not encompass Dupire's local volatility framework, the local volatilities  $\sigma_{\rm loc}(t, S)$ obtained from European option prices on Equity markets typically do satisfy assumption (5.1.2) for every fixed time t. A common market practice is indeed to apply smoothing procedures to the local (or implied) volatility surface when calibrating to European options via Dupire's formula (or via least-square calibration); the resulting local volatilities are designed to be smooth ( $C^2$  in the space direction at least) and bounded away from zero on a bounded region containing the traded maturities and strikes, and are often extrapolated to asymptotically constant values for very small or very large values of s and t. A function  $\sigma_{\rm loc}(t, S)$  constructed in such a way of course satisfies condition (5.1.2) for fixed t.

#### 5.1.2 Notations

- $\forall x \in \mathbb{R}, \quad x_{+} = \max(x, 0), \quad x_{-} = -\min(x, 0).$
- Throughout this chapter, we denote  $\tau := T t$  the time to maturity.
- We define a strike-dependent function  $\gamma = \gamma(K) := \frac{\sigma^2(K)}{8\pi r^2}$ . Whenever the strike price K is clear from the context, we will omit the explicit dependence with respect to K. Note that  $\gamma$  is homogeneous to time.
- We denote  $l(\tau) := \ln\left(\frac{\gamma}{\tau}\right) = \ln\left(\frac{\sigma^2(K)}{8\pi r^2 \tau}\right)$ , for every  $\tau \in (0,\infty)$ .
- For  $x \in \mathbb{R}$ , we denote  $\operatorname{Erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$ , resp.  $\operatorname{Erfc}(x) := \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt$ , the error resp. complementary error functions.
- For a local volatility function  $s \in (0, \infty) \mapsto \sigma(s)$  satisfying Assumption 5.1.2, the squared geodesic distance between the points  $(x, y) \in \mathbb{R}^2$  is defined by

$$d(x,y)^{2} := \left(\int_{x}^{y} \frac{dp}{\sigma(e^{p})}\right)^{2} = \left(\int_{e^{x}}^{e^{y}} \frac{ds}{s\sigma(s)}\right)^{2}$$

#### 5.1.3 Some classical results

We recall some well-known asymptotic expansions for the special functions. For the expansion (5.1.5) for the complementary error function, see [146, 7.12.1]; for (5.1.6), simply use the identity  $\operatorname{Erf}(x) = 1 - \operatorname{Erfc}(x)$  and the symmetry of  $\operatorname{Erf}$  around x = 0; for (5.1.7) see [146, 8.11.12].

$$\operatorname{Erfc}(x) = \frac{e^{-x^2}}{\sqrt{\pi}} \left( \frac{1}{x} - \frac{1}{2x^3} + \frac{3}{4x^5} + \mathcal{O}\left(\frac{1}{x^6}\right) \right), \quad (x \to \infty).$$
(5.1.5)

$$\operatorname{Erf}(x) = -1 + \frac{e^{-x^2}}{\sqrt{\pi}} \left( -\frac{1}{x} + \frac{1}{2x^3} - \frac{3}{4x^5} + \mathcal{O}\left(\frac{1}{x^6}\right) \right), \quad (x \to -\infty).$$
(5.1.6)

$$\Gamma_a(x) = x^{a-1} e^{-x} \left( \sum_{k=0}^{n-1} \frac{(a-1)\dots(a-k)}{x^k} + \mathcal{O}\left(x^{-n}\right) \right), \quad (n \in \mathbb{N}^*, a > 0, \ x \to \infty).$$
(5.1.7)

From now on, let  $f_S(u, y | x)$  (resp.  $f_X(u, y | x)$ ) denote the transition density of  $S_u$  (resp.  $X_u$ ) at time u > 0 starting at  $S_0 = s$  (resp.  $X_0 = x = \ln s$ ). We recall below the well-known smalltime expansions for the transition densities  $f_S$  and  $f_X$ , which were proven by Gatheral et al. [71] for the homogeneous local volatility model (5.1.2) under assumption (5.1.1), relying on the Lamperti transformation. (In the stochastic analysis literature, such expansions can be dated back to classical works of Yosida [170] and Varadhan [161, 162]; see also Henry-Labordère [107] for an extensive review of heat-kernel expansions and their applications in quantitative finance).

**Lemma 5.1.1** (Uniform small-time expansion for the transition density). As  $u \to 0^+$ ,

$$f_X(u, y | x) = \frac{e^{-\frac{d^2(x, y)}{2u}}}{\sqrt{2\pi u}} \left( u_0(x, y) + u_1(x, y) u + \mathcal{O}\left(u^2; x, y\right) \right),$$
(5.1.8)

$$f_S(u, e^y | e^x) = e^{-y} f_X(u, y | x), \qquad (5.1.9)$$

where

$$u_0(x,y) := \sigma \left(e^x\right)^{\frac{1}{2}} \sigma \left(e^y\right)^{-\frac{3}{2}} e^{-\frac{1}{2}(y-x) + r \int_x^y \frac{\mathrm{d}p}{\sigma^2(e^p)}},\tag{5.1.10}$$

$$u_{1}(x,y) := \frac{u_{0}(x,y)}{d(y,x)} \int_{e^{y}}^{e^{x}} \frac{\sigma(p)^{2} \left[ 2p^{2}\sigma''(p) \sigma(p) - (\sigma(p) - p\sigma'(p))^{2} \right] + 4r \left( 2p\sigma(p)\sigma'(p) + \sigma(p)^{2} - r \right)}{8p\sigma(p)^{3}} dp,$$
(5.1.11)

and the following uniform estimate holds

$$\exists C > 0, \forall (x, y) \in \mathbb{R}^2, \forall u \in (0, \tau], \quad \left| \mathcal{O} \left( u^2; x, y \right) \right| \le C u^2.$$

Furthermore, the following limits hold for both  $u_0(\cdot, \cdot)$  and  $u_1(\cdot, \cdot)$ ,

$$u_0(x,y) \xrightarrow[x \to y]{} \frac{1}{\sigma(e^y)},$$
 (5.1.12)

$$u_{1}(x,y) \xrightarrow[x \to y]{} \frac{2e^{2y}\sigma''(e^{y})\sigma(e^{y}) - (\sigma(e^{y}) - e^{y}\sigma'(e^{y}))^{2}}{8\sigma(e^{y})} + \frac{r\left(2e^{y}\sigma(e^{y})\sigma'(e^{y}) + \sigma(e^{y})^{2} - r\right)}{2e^{y}\sigma(e^{y})^{3}},$$
(5.1.13)

$$\frac{\partial u_0}{\partial y}\left(x,y\right) = u_0\left(x,y\right) \left(-\frac{3}{2}\frac{\sigma'\left(e^y\right)e^y}{\sigma\left(e^y\right)} - \frac{1}{2} + \frac{r}{\sigma^2\left(e^y\right)}\right).$$
(5.1.14)

*Proof of Lemma 5.1.1.* From [71], we already know that the following uniform short-time asymptotic expansion holds for the transition density of S,

$$f_{S}(u,K|s) = \frac{e^{-\frac{d^{2}(\ln K,\ln s)}{2u}}}{\sqrt{2\pi u}K} \left(u_{0}(\ln s,\ln K) + u_{1}(\ln s,\ln K)u + \mathcal{O}\left(u^{2};s,K\right)\right) \quad (u \to 0^{+}),$$

with  $u_1$  defined recursively as

$$u_{1}(\ln s, \ln K) = \frac{u_{0}(\ln s, \ln K)}{d(\ln K, \ln s)} \int_{K}^{s} \frac{\frac{1}{2}p^{2}\sigma^{2}(p)\partial_{pp}u_{0}(p, K) + rp\partial_{p}u_{0}(p, K)}{u_{0}(p, K)} \frac{dp}{p\sigma(p)}.$$

After some easy simplification, we obtain the announced expression for  $u_1(\cdot, \cdot)$ . Using that  $X_u = \ln S_u$ , a direct change of variable gives:

$$f_X(u, y | x) = e^y \times f_S(u, e^y | e^x) = \frac{e^{-\frac{d^2(y, x)}{2u}}}{\sqrt{2\pi u}} \left( u_0(x, y) + u_1(x, y) u + \mathcal{O}\left(u^2; e^x, e^y\right) \right).$$

Standard computations lead to (5.1.12), (5.1.13), and (5.1.14).

#### 5.1.4 The exercise boundary and the early premium formula

Using the fact that  $S_t$  is a time-homogeneous Markov process, there exists a function  $\overline{s}$  such that:

$$s^{T}(t) =: \overline{s}(T-t) = \overline{s}(\tau).$$

$$(5.1.15)$$

Equivalently, we will also work with the logarithmic exercise boundary defined as:

$$\overline{x}(\tau) := \ln \overline{s}(\tau) \,. \tag{5.1.16}$$

The main difference between a European and American option lies in the fact that the latter can be exercised anytime prior to expiration (exercise privilege). The difference between the two is given by the so-called early premium formula (see e.g. Carr et al. [44]) which provides an integral representation of the relation between both the American and European prices:

$$A(\tau, s, K) = P(\tau, s, K) + p(\tau, s, K) = P(\tau, s, K) + rK \int_0^\tau e^{-ru} \mathbb{P}_{0,s} \left( S_u \le \overline{s} \left( \tau - u \right) \right) \mathrm{d}u \quad (5.1.17)$$

where p is referred to as the American premium. Economically, it quantifies the right of exercising the option earlier than expiration. Note that in the Black–Scholes model, (5.1.17) rewrites as

$$A_{\rm BS}(\tau, s, K) = P_{\rm BS}(\tau, s, K) + rK \int_0^\tau e^{-ru} \Phi\left(-d_2\left(u, s, \overline{s}\left(\tau - u\right)\right)\right) du.$$
(5.1.18)

The exercise boundary has been extensively studied in the literature, and we just recall its main properties (see e.g. Karatzas and Shreve [122]): the map  $\tau \mapsto \overline{s}(\tau)$  is continuous, decreasing on  $\mathbb{R}_+$ , continuously differentiable on every interval  $[\alpha, \infty)$  for  $\alpha > 0$ ,  $\overline{s}(0) = K$ , and  $\lim_{\tau \to 0} \overline{s}'(\tau) = -\infty$ . In Figure 5.1, we plot the Black–Scholes exercise boundary when K = 100, r = 0.04,  $\sigma = 0.2$ , T = 1.0 along with its upper bound  $\overline{s}(0) = s^T(T) = K$  and lower bound  $\overline{s}(T) = s^T(0)$ as functions of the time to maturity  $\tau = T - t$ . For a detailed explanation of its numerical simulation, see Remark 13.



Figure 5.1 – Exercise boundary for a Black–Scholes put  $\tau \to \overline{s}(\tau)$  (blue) and its associated upper bound  $\tau \to \overline{s}(0) = K$  (green) and lower bound  $\tau \to \overline{s}(T)$  (red).

Upper and lower bounds for the American put price. Since the exercise boundary is decreasing on  $[0, \infty)$ , the following identity holds; for every  $\tau > 0$ ,

$$\forall u \in [0, \tau], \quad \overline{s}(\tau) \le \overline{s}(\tau - u) \le \overline{s}(0) = K.$$

Consequently, introducing the following lower–upper premiums, respectively defined as p and  $\overline{p}$ 

$$\underline{p}\left(\tau,s,K\right) := rK \int_{0}^{\tau} e^{-ru} \mathbb{P}_{0,s}\left(S_{u} \leq \overline{s}\left(\tau\right)\right) \mathrm{d}u, \quad \overline{p}\left(\tau,s,K\right) := rK \int_{0}^{\tau} e^{-ru} \mathbb{P}_{0,s}\left(S_{u} \leq K\right) \mathrm{d}u, \tag{5.1.19}$$

it holds that

$$\underline{p}(\tau, s, K) \le p(\tau, s, K) \le \overline{p}(\tau, s, K).$$
(5.1.20)

Similarly, we introduce the associated upper bound  $\overline{A}$  (resp. lower bound  $\underline{A}$ ) for the American put price defined as:

$$\overline{A}(\tau, s, K) := P(\tau, s, K) + \overline{p}(\tau, s, K), \quad \underline{A}(\tau, s, K) := P(\tau, s, K) + p(\tau, s, K).$$
(5.1.21)

# 5.2 Small-time asymptotics for the European and American put price

#### 5.2.1 At-the-money case

We start our analysis by recalling the short-time asymptotic expansion for at-the-money (hereafter ATM), i.e. s = K, European put prices when the underlying follows a time-homogeneous LV model (5.1.1).

**Proposition 5.2.1** (ATM European put). We have as  $\tau \to 0^+$ :

$$P(\tau, s) = P_0(s)\tau^{\frac{1}{2}} + P_1(s)\tau + P_2(s)\tau^{\frac{3}{2}} + \mathcal{O}(\tau^2), \qquad (5.2.1)$$

where  $P_0(s) := \frac{s\sigma(s)}{\sqrt{2\pi}}$ ,  $P_1(s) := -\frac{rs}{2}$  and

$$P_{2}(s) := \frac{s}{\sqrt{2\pi}} \left( \frac{r^{2}}{2\sigma(s)} - \frac{r\sigma(s)}{2} + \frac{s^{2}\sigma^{2}(s)\sigma''(s)}{12} - \frac{\sigma(s)}{24} \left( \sigma(s) - s\sigma'(s) \right)^{2} \right).$$

Observe that the small-time asymptotic of the ATM put price (5.2.1) is expressed as the sum of a combination of powers of the form  $\tau^{\frac{n}{2}}$  with  $n \in \mathbb{N}^*$ . This is specific to the ATM case, and this will be different when  $s \neq K$  (see Section 5.2.2). The proof of Proposition 5.2.1 (see Proof 5.5.3) combines both the small-time expansion for the transition density (5.1.8) and Laplace's method (see Section 5.5.1). Adding the well-known small-time expansion of the exercise boundary (see Ahn et al. [4, Section 7.1] and Lemma 5.5.2), a similar approach leads to the following small-time expansions for the American (resp. American lower-upper) premium defined in (5.1.17) (resp. (5.1.20)).

**Proposition 5.2.2** (Upper–lower bounds for the ATM premium). We have as  $\tau \to 0^+$ ,

$$\overline{p}(\tau,s) = \overline{p}_0(s)\tau + \overline{p}_1(s)\tau^{\frac{3}{2}} + \mathcal{O}(\tau^2), \qquad (5.2.2)$$

where

$$\overline{p}_{0}\left(s\right) = \frac{rs}{2}, \quad \overline{p}_{1}\left(s\right) = \frac{s}{\sqrt{2\pi}} \left(-\frac{2r^{2}}{3\sigma\left(s\right)} + \frac{r\sigma\left(s\right)}{3} + \frac{rs\sigma'\left(s\right)}{3}\right).$$

**Proposition 5.2.3** (Lower bound for the ATM premium). We have as  $\tau \to 0^+$ ,

$$\underline{p}(\tau,s) = \frac{4r^2s}{\sigma(s)} \frac{\tau^{\frac{3}{2}}}{l^{\frac{3}{2}}(\tau)} \left(1 + o(1)\right).$$
(5.2.3)

**Theorem 5.2.4** (ATM premium). We have as  $\tau \to 0^+$ ,

$$p(\tau,s) = p_0(s)\frac{\tau}{l(\tau)} + p_1(s)\frac{\tau \ln^2(l(\tau))}{l^2(\tau)} + p_2(s)\frac{\tau \ln(l(\tau))}{l^2(\tau)} + p_3(s)\frac{\tau}{l^2(\tau)} + \mathcal{O}\left(\frac{\tau \ln^2(l(\tau))}{l^3(\tau)}\right),$$
(5.2.4)

where

$$p_0(s) = \frac{rs}{2}, \quad p_1(s) = -\frac{rs}{16}, \quad p_2(s) = -\frac{rs(2+a+\ln 2)}{8},$$
$$p_3(s) = rs\frac{32-\pi^2-2\ln^2(2)-2a(4+a+2\ln 2)-8\ln 2}{64},$$

and  $a \approx 0.5772$  is the Euler-Mascheroni constant.

As a direct consequence, combining (5.1.17) along with (5.2.4) and (5.2.1), we have the following asymptotic expansion for the ATM American put.

Corollary 5.2.5 (ATM American put). We have as  $\tau \to 0^+$ ,

$$A(\tau, s) = P_0(s) \tau^{\frac{1}{2}} + P_1(s) \tau + p_0(s) \frac{\tau}{l(\tau)} + p_1(s) \frac{\tau \ln^2(l(\tau))}{l^2(\tau)} + p_2(s) \frac{\tau \ln(l(\tau))}{l^2(\tau)} + p_3(s) \frac{\tau}{l^2(\tau)} + \mathcal{O}\left(\frac{\tau \ln^2(l(\tau))}{l^3(\tau)}\right). \quad (5.2.5)$$

#### 5.2.2 Out-the-money and in-the-money cases

In this section, we proceed as for the ATM case though the expansions we are going to obtain will exhibit an exponential factor. We start our analysis for the out-the-money (OTM) case i.e. s > K.

**Proposition 5.2.6** (OTM European put). We have as  $\tau \to 0^+$ ,

$$P(\tau, s, K) = \left(P_0(s, K)\tau^{\frac{3}{2}} + P_1(s, K)\tau^{\frac{5}{2}} + \mathcal{O}\left(\tau^{\frac{7}{2}}\right)\right)e^{-\frac{d^2(\ln K, \ln s)}{2\tau}},$$
(5.2.6)

where

$$P_0(s,K) := \frac{u_0(\ln s, \ln K) K \sigma(K)^2}{\sqrt{2\pi} \mathrm{d}^2(\ln K, \ln s)},$$

$$P_{1}(s,K) := P_{0}(s,K) \left( -\frac{3}{d^{2}(\ln K,\ln s)} + \frac{u_{1}(\ln s,\ln K)}{u_{0}(\ln s,\ln K)} - \frac{2r}{d(\ln K,\ln s)\sigma} - r \right).$$

The first term  $P_0(s, K)$  was already found in [71, Theorem 2.3]. Before treating the American case, let us introduce the following function

$$p_0(s,K) := \frac{2rKu_0(\ln s,\ln K)\sigma(K)}{\sqrt{2\pi}d^3(\ln K,\ln s)}.$$

**Proposition 5.2.7** (Upper bound for the OTM premium). We have as  $\tau \to 0^+$ ,

$$\overline{p}\left(\tau, s, K\right) = p_0\left(s, K\right) \tau^{\frac{5}{2}} e^{-\frac{d^2(\ln K, \ln s)}{2\tau}} \left(1 + \mathcal{O}\left(\tau\right)\right).$$
(5.2.7)

**Proposition 5.2.8** (Lower bound for the OTM premium). We have as  $\tau \to 0^+$ ,

$$\underline{p}(\tau, s, K) = p_0(s, K) \tau^{\frac{5}{2}} e^{-\frac{d^2(\overline{x}(\tau), \ln s)}{2\tau}} (1 + o(1)), \qquad (5.2.8)$$

where

$$e^{-\frac{\mathrm{d}^2(\overline{x}(\tau),\ln s)}{2\tau}} = e^{-\frac{\mathrm{d}^2(\ln K,\ln s)}{2\tau}} e^{-\mathrm{d}(\ln K,\ln s)\sqrt{\frac{l(\tau)}{\tau}} \left(1 + \mathcal{O}\left(\frac{1}{l(\tau)^2}\right)\right)}.$$

Before stating our asymptotic expansion for the American premium, we give the following large-deviation estimates for the premium.

**Proposition 5.2.9** (Large-deviation estimates for the premium). The following asymptotic expansion holds for the risk premium p in the local volatility model (5.1.1) as  $\tau \to 0^+$ ,

$$\begin{aligned} \tau \ln\left(p\left(\tau, s, K\right)\right) &\to -\frac{\mathrm{d}^2\left(\ln K, \ln s\right)}{2} \quad \text{if } s > K, \\ \tau \ln\left(K\left(1 - e^{-r\tau}\right) - p\left(\tau, s, K\right)\right) &\to -\frac{\mathrm{d}^2\left(\ln K, \ln s\right)}{2} \quad \text{if } s < K. \end{aligned}$$

**Theorem 5.2.10** (OTM premium). We have as  $\tau \to 0^+$ ,

$$p(\tau, s, K) = p_0(s, K) \frac{\tau^{\frac{5}{2}}}{l(\tau)} e^{-\frac{d^2(\ln K, \ln s)}{2\tau}} (1 + o(1)).$$
(5.2.9)

Remark 12 (Discontinuity in S for the European put price expansions). Starting from the putcall parity, one can easily derive the European put price asymptotic expansions when K > s(ITM case) from the OTM expansion (5.2.6) (see [71, Section 2.4]), and show that when K > s,

$$P(\tau, s, K) \sim K e^{-r\tau} - s - P_0(s, K) \tau^{\frac{3}{2}} e^{-\frac{d^2(\ln K, \ln s)}{2\tau}}, \qquad (\tau \to 0^+).$$
(5.2.10)

For any fixed  $s, \tau$ , we then notice that from (5.2.1), (5.2.6), and (5.2.10), the asymptotic expansions found above for the three different regimes s > K, s < K, s = K are not continuous as  $s \to K$ . More precisely, if s < K (resp. K > s), the asymptotic expansion (5.2.10) (resp. (5.2.6)) goes to  $+\infty$  (resp.  $-\infty$ ) as  $s \to K$  (see Figure 5.2). Consequently, the expansions for both the ITM and OTM cases are of no use for approximating the put price around s = K.



Figure 5.2 – European Black–Scholes put prices and associated asymptotic expansions.

#### 5.2.3 Numerical results

To test our expansion formulas, we consider both a Black–Scholes model where  $\sigma(s) \equiv \sigma$  is a constant, and the constant elasticity of variance (hereafter CEV) model – introduced by Cox [51] – for which  $\sigma(s) = \delta s^{\frac{\beta}{2}-1}$  with  $\delta > 0$ ,  $\beta > 0$ . The resulting SDE for the asset price in the CEV model is

$$dS_t = rS_t dt + \delta S_t^{\frac{\beta}{2}} dW_t, \qquad S_0 > 0.$$
 (5.2.11)

Note that in the special case  $\beta = 2$ , the CEV model reduces to the Black–Scholes model. When  $\beta > 2$ , the solution to (5.2.11) (whose uniqueness follows from the local Lipschitz property of  $s^{\frac{\beta}{2}}$ ) remains strictly positive for all positive times. Otherwise, let us briefly discuss the well-posedness of Equation (5.2.11) on the domain  $[0, \infty)$ : when  $\beta \in [1, 2]$ , pathwise uniqueness follows from Yamada and Watanabe's uniqueness theorem for one-dimensional SDEs with 1/2–Hölder diffusion coefficient (see e.g. Karatzas and Shreve [122, p. 291]), the trajectories of the process hit zero in finite time with positive probability, and stick to zero afterwards. When  $\beta \in (0, 1)$ , uniqueness is granted (by the local Lipschitz property of  $s^{\frac{\beta}{2}}$  on  $(0, \infty)$ ) until the first hitting time of zero, but global uniqueness can be lost if no boundary condition is given: we assume that zero is an absorbing boundary, that is:  $S_u = 0$  for  $u \ge \inf\{t \ge 0 : S_t = 0\}$ . Under such conditions, the cumulative distribution function of the process S was evaluated by Cox [51], and subsequently simplified by Schroder [154], who provides the expression

$$\mathbb{P}_{0,s}\left[S_{\tau} \leq K\right] = \begin{cases} \mathcal{Q}\left(2ks^{2-\beta}e^{r(2-\beta)\tau}; \frac{2}{2-\beta}, 2kK^{2-\beta}\right) & \text{if } \beta < 2\\ \mathcal{Q}\left(2kK^{2-\beta}; 2+\frac{2}{\beta-2}, 2ks^{2-\beta}e^{r(2-\beta)\tau}\right) & \text{if } \beta > 2 \end{cases}$$

where

$$k := \frac{2r}{\delta^2 \left(2 - \beta\right) \left[e^{r(2 - \beta)\tau} - 1\right]}$$

and  $\mathcal{Q}(z;\nu,\varepsilon)$  is the complementary c.d.f. of a non-central chi-square distribution evaluated at z, with  $\nu$  degrees of freedom and non-central parameter  $\varepsilon$ . The knowledge of the c.d.f. of S allows us to obtain a closed-form expression for the call price under a CEV model (see Schroder [154, Section III]). Evoking the put–call parity, we can then easily derive the associated put price that we recall in the following lemma.

**Lemma 5.2.11** (Put price in the CEV model, see for the call price and use ). In a CEV model, the price of a put option with strike K is given by

$$P_{\text{CEV}}(\tau, s, K) = \begin{cases} Ke^{-r\tau} \mathcal{Q}(2ks^{2-\beta}e^{r(2-\beta)\tau}; \frac{2}{2-\beta}, 2kK^{2-\beta}) - s\left[(1 - \mathcal{Q}(2kK^{2-\beta}; 2 + \frac{2}{2-\beta}, 2ks^{2-\beta}e^{r(2-\beta)\tau})\right] & \text{if }\beta < 2, \\ Ke^{-r\tau} \mathcal{Q}\left(2kK^{2-\beta}; 2 + \frac{2}{\beta-2}, 2ks^{2-\beta}e^{r(2-\beta)\tau}\right) - s\left[1 - \mathcal{Q}(2ks^{2-\beta}e^{r(2-\beta)\tau}; \frac{2}{\beta-2}, 2kK^{2-\beta})\right] & \text{if }\beta > 2. \end{cases}$$

We need a benchmark value to check the accuracy of our expansions. Recall that (see (5.1.17)) under a time-homogeneous LV model, the early premium formula reads

$$A(\tau, s, K) = P(\tau, s, K) + rK \int_0^\tau e^{-ru} \mathbb{P}_{0,s} \left[ S_u \le \overline{s} \left( \tau - u \right) \right] \mathrm{d}u,$$

where for both models (Black–Scholes and CEV) the c.d.f. of S has a closed-form expression.

*Remark* 13 (On the evaluation of the exercise boundary and American option prices). Setting  $s = \overline{s}(\tau)$  in (5.1.17) and using the continuity condition (5.1.3),  $A(\tau, \overline{s}(\tau), K) = K - \overline{s}(\tau)$ , provide the following convolution-type integral equation (nonlinear Volterra integral equation of the second kind):

$$K - \overline{s}(\tau) = P(\tau, \overline{s}(\tau), K) + rK \int_0^\tau e^{-ru} \mathbb{P}_{0,\overline{s}(\tau)} \left( S_u \le \overline{s}(\tau - u) \right) du.$$
(5.2.12)

The exercise boundary  $\overline{s}(\tau)$  can then be recursively approximated starting at  $\overline{s}(0) = K$  and by discretizing the integral (see e.g. Kallast and Kivinukk [119] for a detailed algorithm).

More precisely, let us consider a Black–Scholes model, though (see below) as long as the c.d.f.  $\mathbb{P}_{0,s}(x,y)$  is known in closed-form, the procedure can applied to any model. Recall that s(T) = 0 (for the ease of notation, we drop the dependence on T for  $s^T(\cdot)$ ). We divide the interval of integration  $[t_0 = t, t_M = T]$  into  $M \in \mathbb{N}^*$  subintervals  $[t_{i-1}, t_i]$  with length  $\Delta t_i = t_i - t_{i-1}$  for  $i = 1, \ldots, M$  and we write  $s(t_i) = s_i$  for every  $i = 0, \ldots, M$ . We further recall that:

$$d_1(\tau, x, y) = \frac{\ln\left(\frac{x}{y}\right) + \left(r + \frac{\sigma^2}{2}\right)\tau}{\sigma\sqrt{\tau}}, \quad d_2(\tau, x, y) = \frac{\ln\left(\frac{x}{y}\right) + \left(r - \frac{\sigma^2}{2}\right)\tau}{\sigma\sqrt{\tau}},$$

and set

$$f(\tau, x, y) = rKe^{-r\tau}\Phi\left(-d_2\left(\tau, x, y\right)\right),$$
  

$$P\left(\tau, x, y\right) = Ke^{-r\tau}\Phi\left(-d_2\left(\tau, x, y\right)\right) - x\Phi\left(-d_1\left(\tau, x, y\right)\right), \quad \text{(Black-Scholes European put price)}.$$

With our notations, we have  $s_M = K$  and evoking (5.2.12),  $s_{M-1}$  is solution to:

$$K - s_{M-1} = P\left(\Delta t_M, s_{M-1}, K\right) + \int_{t_{M-1}}^{t_M} f\left(u - t_{M-1}, s_{M-1}, s\left(u\right)\right) du$$
  
$$\approx P\left(\Delta t_M, s_{M-1}, K\right) + \frac{\Delta t_M}{2} \left[f\left(0, s_{M-1}, s_{M-1}\right) + f\left(\Delta t_M, s_{M-1}, s_M\right)\right],$$

where we have used the trapezoidal rule to approximate the integral. Similarly for i = 0, ..., M - 2, the exercise boundary  $s_i$  at time  $t_i$  is solution to:

$$\begin{split} K - s_i &= P\left(t_M - t_i, s_i, K\right) + \sum_{j=i}^{M-1} \int_{t_j}^{t_{j+1}} f\left(u - t_i, s_i, s\left(u\right)\right) \mathrm{d}u \\ &\approx P\left(t_M - t_i, s_i, K\right) + \sum_{j=i}^{M-1} \frac{t_{j+1} - t_j}{2} \left[f\left(t_{j+1} - t_i, s_i, s_{j+1}\right) + f\left(t_j - t_i, s_i, s_j\right)\right] \\ &= P\left(\sum_{l=i+1}^M \Delta t_l, s_i, K\right) + \frac{\Delta t_M}{2} f\left(\sum_{l=i+1}^M \Delta t_l, s_i, s_M\right) + \frac{\Delta t_{i+1}}{4} r K \\ &+ \sum_{j=i+1}^{M-1} \frac{\Delta t_{j+1} + \Delta t_j}{2} f\left(\sum_{l=i+1}^j \Delta t_l, s_i, s_j\right), \end{split}$$

where we have used that  $f(0, s_i, s_i) = \frac{1}{2}rK$  since for every positive x,

$$f(0,x,x) = \lim_{\tau \to 0^+} f(\tau,x,x) = \frac{1}{2}rK.$$
(5.2.13)

 $\triangleright$  Approximating the exercise boundary. We now approximate each  $s_i$  (i = M - 1, ..., 0) using Newton-Raphson iteration algorithm. More precisely, setting a parameter  $L \in \mathbb{N}$ , we obtain an approximation of order L for the exercise boundary at time  $t_i$  i.e.

• 
$$s_i^{(0)} \leftarrow s_{i+1}$$

• For every  $l = 0, \ldots, L$  do:

$$-s_i^{(l+1)} \leftarrow s_i^{(l)} - \frac{F(s_i^{(l)})}{F'(s_i^{(l)})},$$

where we have set:

$$\begin{split} F\left(x\right) &= x - K + P\left(\sum_{l=i+1}^{M} \Delta t_{l}, x, K\right) + \frac{\Delta t_{M}}{2} f\left(\sum_{l=i+1}^{M} \Delta t_{l}, x, s_{M}\right) \\ &\quad + \frac{\Delta t_{i+1}}{4} rK + \sum_{j=i+1}^{M-1} \frac{\Delta t_{j+1} + \Delta t_{j}}{2} \left(\sum_{l=i+1}^{j} \Delta t_{l}, x, s_{j}\right), \\ F'\left(x\right) &= 1 + \frac{\partial P}{\partial x} \left(\sum_{l=i+1}^{M} \Delta t_{l}, x, K\right) + \frac{\Delta t_{M}}{2} \frac{\partial f}{\partial x} \left(\sum_{l=i+1}^{M} \Delta t_{l}, x, s_{M}\right) + \sum_{j=i+1}^{M-1} \frac{\Delta t_{j+1} + \Delta t_{j}}{2} \frac{\partial f}{\partial x} \left(\sum_{l=i+1}^{j} \Delta t_{l}, x, s_{j}\right) \\ &\quad \frac{\partial P}{\partial x} \left(\tau, x, y\right) = -\Phi \left(-d_{1} \left(\tau, x, y\right)\right), \quad \frac{\partial f}{\partial x} \left(\tau, x, y\right) = -\frac{rK}{y} \frac{e^{-\frac{d_{1}\left(\tau, x, y\right)^{2}}{2}}}{\sigma \sqrt{\tau} \sqrt{2\pi}}. \end{split}$$

 $\triangleright$  American put price approximation. Using the procedure above, we have now an approximation of the exercise boundary  $\{s_0, \ldots, s_M\}$ . Evoking once again the trapezoidal rule, we can now replug our boundary approximation in order to get the approximated American put price at time  $t = t_0 = 0$  (i = 0) i.e.

$$\begin{split} A\left(T, s, K\right) &= P\left(T, s, K\right) + \int_{0}^{T} f\left(u, s, s\left(u\right)\right) \mathrm{d}u. \\ &\approx P\left(T, s, K\right) + \frac{\Delta t_{1} f\left(0, s, s_{0}\right) + \Delta t_{M} f\left(T, s, s_{M}\right)}{2} + \sum_{j=1}^{M-1} \frac{\Delta t_{j+1} + \Delta t_{j}}{2} f\left(t_{j}, s, s_{j}\right), \end{split}$$

recalling that  $t_M = T$ . Note that the quantity  $f(0, s, s_0)$  is not uniquely defined and its value depends on the sign of the difference  $s - s_0$ . More precisely, one has

$$f(0, s, s_0) = \begin{cases} rK, & \text{if } s < s_0, \\ \frac{1}{2}rK & \text{if } s = s_0, \\ 0 & \text{if } s > s_0, \end{cases}$$

where we have used (5.2.13) for the case  $s = s_0$ . However, we know that for  $s \le s_0$  the American put price equals K - s (as it is optimal to exercise), and we deduce that for  $s > s_0$ ,

$$A(T, s, K) \approx P(T, s, K) + \frac{\Delta t_M f(T, s, s_M)}{2} + \sum_{j=1}^{M-1} \frac{\Delta t_{j+1} + \Delta t_j}{2} f(t_j, s, s_j).$$

**Corollary 5.2.12** (ATM prices in a Black–Scholes and CEV model). If s = K, we have as  $\tau \to 0^+$ ,

1. Put price:

$$\begin{split} P_{\text{CEV}}\left(\tau,s\right) &= \frac{\delta s^{\frac{\beta}{2}}}{\sqrt{2\pi}} \sqrt{\tau} - \frac{rs}{2} \tau \\ &+ \frac{s^{-\frac{\beta}{2}-2} \left(48r^2s^4 - 48\delta^2rs^{\beta+2} + (\beta-4)\beta\delta^4s^{2\beta}\right)}{96\delta\sqrt{2\pi}} \tau \sqrt{\tau} + \mathcal{O}\left(\tau^2\right) \\ P_{\text{BS}}\left(\tau,s\right) &= \frac{s\sigma}{\sqrt{2\pi}} \sqrt{\tau} - \frac{rs}{2} \tau + \frac{s}{\sqrt{2\pi}} \left(\frac{r^2}{2\sigma} - \frac{r\sigma}{2} - \frac{\sigma^3}{24}\right) \tau \sqrt{\tau} + \mathcal{O}\left(\tau^2\right). \end{split}$$

#### 2. American price:

$$A_{\rm BS}\left(\tau,s\right) = \frac{s\sigma}{\sqrt{2\pi}}\sqrt{\tau} - \frac{rs}{2}\tau + \frac{rs}{2}\tau\Sigma\left(\tau,\sigma\right)\left(1+o\left(1\right)\right),$$

$$A_{\text{CEV}}\left(\tau,s\right) = \frac{\delta s^{\frac{\beta}{2}}}{\sqrt{2\pi}}\sqrt{\tau} - \frac{rs}{2}\tau + \frac{rs}{2}\tau\Sigma\left(\tau,\delta s^{\frac{\beta}{2}-1}\right)\left(1+o\left(1\right)\right).$$

where  $l(\tau, \sigma(s)) = \ln\left(\frac{\sigma(s)^2}{8\pi r^2}\frac{1}{\tau}\right)$  and

$$\Sigma\left(\tau,\sigma\left(s\right)\right) = \frac{1}{l\left(\tau,\sigma\left(s\right)\right)} \left(1 + \frac{C_0 \ln^2\left(l\left(\tau,\sigma\left(s\right)\right)\right) + C_1 \ln\left(l\left(\tau,\sigma\left(s\right)\right)\right) + C_2}{l\left(\tau,\sigma\left(s\right)\right)}\right).$$

3. Upper bound for the American price:

$$\begin{split} \overline{A}_{\text{CEV}}\left(\tau,s\right) &= \frac{\delta s^{\frac{\beta}{2}}}{\sqrt{2\pi}}\sqrt{\tau} \\ &+ \frac{s^{-\frac{\beta}{2}-2}\left(-16r^2s^4 + 16(\beta-3)\delta^2rs^{\beta+2} + (\beta-4)\beta\delta^4s^{2\beta}\right)}{96\delta\sqrt{2\pi}}\tau\sqrt{\tau} + \mathcal{O}\left(\tau^2\right), \\ \overline{A}_{\text{BS}}\left(\tau,s\right) &= \frac{s\sigma}{\sqrt{2\pi}}\sqrt{\tau} + \frac{s}{\sqrt{2\pi}}\left(-\frac{r^2}{6\sigma} - \frac{r\sigma}{6} - \frac{\sigma^3}{24}\right)\tau\sqrt{\tau} + \mathcal{O}\left(\tau^2\right). \end{split}$$

4. Lower bound for the American price:

$$\underline{A}_{\text{CEV}}(\tau,s) = \frac{\delta s^{\frac{\beta}{2}}}{\sqrt{2\pi}} \sqrt{\tau} - \frac{rs}{2} \tau + \frac{s^{-\frac{\beta}{2}-2} \left(48r^2s^4 - 48\delta^2 rs^{\beta+2} + (\beta-4)\beta\delta^4 s^{2\beta}\right)}{96\delta\sqrt{2\pi}} \tau \sqrt{\tau} \\ + \frac{4r^2s^2}{\delta s^{\frac{\beta}{2}}} \frac{\tau\sqrt{\tau}}{\left(\ln\left(\frac{\delta^2s^{\beta-2}}{8\pi r^2}\frac{1}{\tau}\right)\right)^{\frac{3}{2}}} + \mathcal{O}\left(\frac{\tau\sqrt{\tau}}{\ln\left(\frac{1}{\tau}\right)^{\frac{5}{2}}}\right), \\ \underline{A}_{\text{BS}}(\tau,s) = \frac{s\sigma}{\sqrt{2\pi}} \sqrt{\tau} - \frac{rs}{2}\tau + \frac{s}{\sqrt{2\pi}} \left(\frac{r^2}{2\sigma} - \frac{r\sigma}{2} - \frac{\sigma^3}{24}\right)\tau\sqrt{\tau} \\ + \frac{4r^2s}{\sigma\left(s\right)}\frac{\tau\sqrt{\tau}}{l^{\frac{3}{2}}\left(\tau,\sigma\left(s\right)\right)} \left(1 + \mathcal{O}\left(\frac{1}{l\left(\tau,\sigma\left(s\right)\right)}\right)\right).$$

Remark 14 (On the parameter  $\gamma(K)$ ). As already observed in [53, Remark 3.3], the parameter  $\gamma(K)$  is homogeneous to time and plays the role of a time-scale. The quality of the American asymptotic expansions depends on the ratio  $\frac{\tau}{\gamma(K)}$ : the smaller the ratio, the more accurate the expansion.

To assess the accuracy of our approximation formulas, we consider a Black–Scholes model with parameters r = 0.02,  $\sigma = 0.5$ , s = K = 50,  $\gamma_{\rm BS} = \frac{\sigma^2}{8\pi r^2} \approx 24.9$  and a CEV model with parameters r = 0.03,  $\delta = 0.7$ ,  $\beta = 1.6$ , s = K = 1,  $\gamma_{\rm CEV} \approx \frac{\sigma(s)^2}{8\pi r^2} \approx 21.7$ . We first test the expansion (5.2.1) for the ATM European put price in Figures 5.3 and 5.5, and compare the different orders i.e. from the expansion up to the order  $\tau^{\frac{1}{2}}$  to  $\tau^2$ . We observe that from the order  $\tau^{\frac{3}{2}}$ , the expansion is extremely accurate (less than 0.1% on relative error). We then test in Figures 5.4 and 5.6 our American expansion formulas (5.2.2), (5.2.3), and (5.2.4). They too provide satisfactory results for both cases (less than -1% in relative error for the American put).



Figure 5.3 – At-the-money European put price and asymptotic expansions expressed in European implied volatility in the Black–Scholes model at different orders w.r.t.  $\tau$  (left) and corresponding relative errors in % (right).



Figure 5.4 – At-the-money American put price and asymptotic expansions expressed in European implied volatility in the Black–Scholes model at different orders w.r.t.  $\tau$  (left) and corresponding relative errors in % (right).



Figure 5.5 – At-the-money European put price and asymptotic expansions expressed in European implied volatility in the CEV model at different orders w.r.t.  $\tau$  (left) and corresponding relative errors in % (right).



Figure 5.6 – At-the-money American put price and asymptotic expansions expressed in European implied volatility in the CEV model at different orders w.r.t.  $\tau$  (left) and corresponding relative errors in % (right).

### 5.3 American implied volatility

#### 5.3.1 Definition

In this section, for more clarity we make explicit the dependence with respect to the Black–Scholes volatility parameter  $\sigma$  and write  $P_{\text{BS}}(\tau, s, K, \sigma) := P_{\text{BS}}(\tau, s, K)$ ,  $A_{\text{BS}}(\tau, s, K, \sigma) := A_{\text{BS}}(\tau, s, K)$ , and  $\overline{s}(\tau, \sigma) := \overline{s}(\tau)$ .

It is well-known that the following no-arbitrage bounds hold for European and American put options (see e.g. Kwok [128, Chapter 1]):

$$(Ke^{-r\tau} - s)_{+} \le P(\tau, s, K) < Ke^{-r\tau}, \quad (K - s)_{+} \le A(\tau, s, K) \le K$$

for every  $\tau, K \in \mathbb{R}^*_+$ . The definition of the European implied volatility  $\sigma_{\rm E}(\tau, s, K)$  is standard: using the fact that the map  $\sigma \mapsto P_{\rm BS}(\tau, s, K, \sigma)$  is strictly increasing, along with the limiting values  $P_{\rm BS}(\tau, s, K, \sigma) |_{\sigma=0} = (Ke^{-r\tau} - s)_+$  and  $P_{\rm BS}(\tau, s, K, \sigma) \xrightarrow[\sigma \to \infty]{} Ke^{-r\tau}$ , the implied volatility  $\sigma_{\rm E}(\tau, s, K)$  of the put price  $P(\tau, s, K)$  is well-defined as the unique solution  $\sigma_{\rm E}$  to:

$$P_{\rm BS}\left(\tau, s, K, \sigma_{\rm E}\right) = P\left(\tau, s, K\right).$$

For the American put price, the situation is slightly different. As for the European case, we aim to define the American implied volatility  $\sigma_{\rm A}(\tau, s, K)$  as the unique solution  $\sigma_{\rm A}$  to the equation

$$A_{\rm BS}\left(\tau, s, K, \sigma_{\rm A}\right) = A\left(\tau, s, K\right). \tag{5.3.1}$$

Let us define

$$K^* := \inf \left\{ K > 0 \, | \, A(\tau, s, K) = (K - s)_+ \right\}, \tag{5.3.2}$$

and note that  $K^* > s$  for every  $s, \tau > 0$ . This critical strike  $K^*$  depends on the local volatility model (and also on s and  $\tau$ , which we consider to be fixed and we therefore omit from the notation for simplicity); when the underlying model is Black–Scholes, the value of  $K^*$  can be seen in Figure 5.8. The situation is different according to whether  $K < K^*$  or  $K \ge K^*$ .

Let us first recall some basic properties of the American Black–Scholes price. We know from Hobson [110] and El Karoui et al. [60] that the map  $\sigma \mapsto A_{\rm BS}(\tau, s, K, \sigma)$  is non-decreasing for every fixed  $\tau, s, K$ . This map is also strictly increasing for  $K \leq s$ ; conversely, when K > s, there is a non-empty interval of values of  $\sigma$  for which  $A_{\rm BS}(\tau, s, K, \sigma)$  remains constant. More precisely, specifying the definition (5.3.2) in the Black–Scholes case to

$$K_{\rm BS}^*(\sigma) := \inf \left\{ K > 0 \, | \, A_{\rm BS}(\tau, s, K, \sigma) = (K - s)_+ \right\},\tag{5.3.3}$$

and identifying the value  $\sigma^*(K)$  of the volatility parameter such that  $K_{BS}^*(\sigma^*(K)) = K$ , then for every  $\sigma \in [0, \sigma^*(K)]$  we have  $A_{BS}(\tau, s, K, \sigma) = (K - s)_+$ , while  $A_{BS}(\tau, s, K, \sigma)$  is strictly increasing with respect to  $\sigma$  for  $\sigma > \sigma^*(K)$ , see Figure 5.7. Observe also that  $A_{BS}(\tau, s, K, \sigma)|_{\sigma=0} = (K - s)_+$  (when  $\sigma = 0$ , it is optimal to exercise straight away); on the other hand, we have

$$A_{\rm BS}\left(\tau, s, K, \sigma\right) \xrightarrow[\sigma \to \infty]{} K, \tag{5.3.4}$$

as we recall below. Overall, we have the following two situations:

Case  $K < K^*$ : by definition of  $K^*$ , the American option price  $A(\tau, s, K)$  in the local volatility model is strictly greater than the payoff function  $(K - s)_+$ . According to the behavior of the price function  $A_{BS}$  discussed above, Equation (5.3.1) has a unique solution  $\sigma > \sigma^*(K)$ , which allows to define the American implied volatility of the option price A for K in this region.

Case  $K \ge K^*$ : in this region,  $A(\tau, s, K) = (K - s)_+$ . As discussed above, all the values of  $\sigma$  in the interval  $[0, \sigma^*(K)]$  satisfy  $A_{BS}(\tau, s, K, \sigma) = (K - s)_+ = A(\tau, s, K)$ , meaning that Equation (5.3.1) has infinitely many solutions. For a strike K in this region, the American implied volatility of the option price A is not well-defined.



Figure 5.7 – ITM American put prices in the Black–Scholes model in terms of the volatility. The other parameters are s = 10.0, K = 11.0, r = 0.05, T = 2.0. Observe that  $A_{\text{BS}}(\tau, s, K, \sigma) = (K - s)_{+} = 1$  for  $\sigma \in [0, \sigma^{*}(K)]$  where  $\sigma^{*}(K) \approx 0.105$ .

As addressed above, let us recall an argument allowing to show (5.3.4). From the monotonicity of the exercise boundary  $\overline{s}(\tau, \sigma)$  with respect to time-to-maturity  $\tau$ , we deduce that  $\overline{s}(\tau, \sigma) \geq \lim_{\tau' \to \infty} \overline{s}(\tau', \sigma) = s_{\infty}(\sigma)$ , where  $s_{\infty}(\sigma)$  is the constant exercise boundary for a Black–Scholes perpetual American put option. It is well-known (see e.g. Lamberton and Lapeyre [129, Chapter 4, Section 4]) that

$$s_{\infty}(\sigma) = \frac{K}{1 + 2r/\sigma^2}.$$
(5.3.5)

Consequently, since  $s_{\infty}(\sigma) \xrightarrow[\sigma \to \infty]{\sigma \to \infty} K$  and  $s_{\infty}(\sigma) \leq \overline{s}(\tau, \sigma) \leq K$ , we deduce that  $\overline{s}(\tau, \sigma) \xrightarrow[\sigma \to \infty]{\sigma \to \infty} K^-$  for every  $\tau$ . Using the early premium formula (5.1.18), we infer that:

$$A_{\rm BS}(\tau, s, K, \sigma) \xrightarrow[\sigma \to \infty]{} Ke^{-r\tau} + rK \int_0^\tau e^{-ru} du = K$$

as expected.

Small-time regime. Since  $A(\tau, s, K, \sigma)$  and  $A_{BS}(\tau, s, K, \sigma)$  tend to  $(K - s)_+$  as  $\tau \to 0^+$ (see (5.1.3)), we infer that  $K^*(\tau, s) \searrow s$  as  $\tau \to 0^+$ . Therefore, the strike domain on which the American implied volatility  $\sigma_A(\tau, s, K)$  is well-defined for every strictly positive time-to-maturity is  $\cap_{\tau>0}(0, K^*(\tau, s)) = (0, s]$ : eventually, we can consider small-time asymptotic expansions of  $\sigma_A$  only for OTM or ATM put options, that is when  $K \leq s$ .



Figure 5.8 – American and European put prices in the Black–Scholes model in terms of the strike price K. The other parameters are s = 1.0, r = 0.05,  $\sigma = 0.3$ , T = 3.0. The point  $K_{BS}^*$  defined in (5.3.3) can be seen in the right part of the figure (approximately at K = 1.4).

For comparison, for every  $K \leq s$  we also define an upper bound  $\overline{\sigma}_{A}(\tau, s, K)$  and a lower bound  $\underline{\sigma}_{A}(\tau, s, K)$  for the American implied volatility, setting

$$A_{\rm BS}\left(\tau, s, K, \overline{\sigma}_{\rm A}\left(\tau, s, K\right)\right) = \overline{A}\left(\tau, s, K\right), \quad A_{\rm BS}\left(\tau, s, K, \underline{\sigma}_{\rm A}\left(\tau, s, K\right)\right) = \underline{A}\left(\tau, s, K\right)$$

#### 5.3.2 Asymptotics of the European implied volatility

**Proposition 5.3.1.** If  $s \neq K$ , we have as  $\tau \to 0^+$ ,

$$\sigma_{\rm E}\left(\tau, s, K\right) = \sigma_0\left(s, K\right) + \sigma_1\left(s, K\right)\tau + \sigma_2\left(s, K\right)\tau^2 + \mathcal{O}\left(\tau^3\right),\tag{5.3.6}$$

where

 $\sigma_2(s,$ 

$$\begin{aligned} \sigma_0\left(s,K\right) &= \frac{\ln\left(\frac{s}{K}\right)}{d\left(\ln K,\ln s\right)},\\ \sigma_1\left(s,K\right) &= \frac{\sigma_0^3\left(s,K\right)}{\ln\left(\frac{s}{K}\right)^2} \ln\left(\frac{u_0\left(\ln s,\ln K\right)\sigma^2\left(K\right)}{\sigma_0\left(s,K\right)}\right) - \frac{\sigma_0^3\left(s,K\right)}{2\ln\left(\frac{s}{K}\right)} + \frac{r\sigma_0\left(s,K\right)}{\ln\left(\frac{s}{K}\right)},\\ K) &= \frac{\sigma_0^3\left(s,K\right)}{\ln\left(\frac{s}{K}\right)^2} \frac{u_1\left(\ln s,\ln K\right)}{u_0\left(\ln s,\ln K\right)} + \frac{\sigma_0^5\left(s,K\right)}{8\ln\left(\frac{s}{K}\right)^2} - \frac{3\sigma_0^2\left(s,K\right)\sigma_1\left(s,K\right)}{\ln\left(\frac{s}{K}\right)^2} + \frac{3}{2}\frac{\sigma_1^2\left(s,K\right)}{\sigma_0\left(s,K\right)} \\ &+ r\left(-\frac{\sigma_0^3\left(s,K\right)}{2\ln\left(\frac{s}{K}\right)^2} - \frac{2\sigma_0^4\left(s,K\right)}{\ln\left(\frac{s}{K}\right)^3\sigma\left(K\right)} + \frac{2\sigma_0^3\left(s,K\right)}{\ln\left(\frac{s}{K}\right)^3} + \frac{r\sigma_0\left(s,K\right)}{2\ln\left(\frac{s}{K}\right)^2} - \frac{2\sigma_1\left(s,K\right)}{\ln\left(\frac{s}{K}\right)}\right). \end{aligned}$$

Furthermore, the following limits hold:

$$\sigma_0(s,K) \xrightarrow[K \to s]{} \sigma(s) =: \sigma_0(s), \tag{5.3.7}$$

$$\sigma_{1}(s,K) \xrightarrow[K \to s]{} \xrightarrow{(-)}{24} \left( -s\sigma^{-}(s)^{2} + 2\sigma(s) \left( \sigma^{-}(s) + s\sigma^{-}(s) \right) \right) =: \sigma_{1}(s), \qquad (5.3.8)$$

$$\sigma_{2}(s,K) \xrightarrow[K \to s]{} \frac{1}{1920\sigma(s)} \left[ s \left( 3s^{3}\sigma(s)^{2}\sigma'(s)^{4} - 12s^{2}\sigma(s)^{3}\sigma'(s)^{2} \left( s\sigma''(s) + \sigma'(s) \right) + 4s\sigma(s)^{4} \left( 3s^{2}\sigma''(s)^{2} + 2\sigma'(s)^{2} + 2s\sigma'(s) \left( 2s\sigma^{(3)}(s) + 9\sigma''(s) \right) \right) \right)$$

$$+8\sigma(s)^{5}\left(s\left(s^{2}\sigma^{(4)}(s)+6s\sigma^{(3)}(s)+7\sigma^{\prime\prime}(s)\right)+\sigma^{\prime}(s)\right)+80sr^{2}\sigma^{\prime}(s)^{2}\right]$$
  
=:  $\sigma_{2}(s).$  (5.3.9)

**Proposition 5.3.2** (ATM European implied volatility expansion). If s = K, we have as  $\tau \to 0^+$ ,

$$\sigma_{\rm E}\left(\tau,s\right) = \sigma_0\left(s\right) + \sigma_1\left(s\right)\tau + \mathcal{O}\left(\tau^2\right). \tag{5.3.10}$$

Remark 15 (On the continuity of the European implied volatility expansion). As opposed to the European put price expansions which were discontinuous when  $K \to s$  (see Remark 12 and Figure 5.2), Propositions 5.3.1 and 5.3.2 show that the European implied volatility expansion is continuous in s and/or K, at least for the first two correction terms  $\sigma_0$  and  $\sigma_1$ . It should be noted that if we sought to obtain an expansion up to order  $\tau^2$  for  $\sigma_{\rm E}(\tau, s)$ , we would need a more refined expansion for the ATM put price expansion (5.2.1).

In Figure 5.9, we compare the (second-order) implied volatility expansion (5.3.6) and (5.3.10) and the true smile generated by a CEV model with parameters s = 1.0, r = 0.04,  $\delta = 0.5$ ,  $\beta = 1.5$  and T = 1.0, and observe that it is extremely accurate.



Figure 5.9 – European CEV smile and its asymptotic expansion.

#### 5.3.3 Asymptotics of the American implied volatility

**Proposition 5.3.3** (Upper–lower bounds for the American implied volatility). If s = K, we have as  $\tau \to 0^+$ ,

$$\begin{split} \overline{\sigma}_{\mathcal{A}}\left(\tau,s\right) &= \sigma\left(s\right) + \sqrt{\frac{\pi}{2}} r \sqrt{\tau} \left(1 + \frac{1}{l\left(\tau\right)} \left(1 + \frac{C_0 \ln^2\left(l\left(\tau\right)\right) + C_1 \ln\left(l\left(\tau\right)\right) + C_2}{l\left(\tau\right)}\right) \left(1 + o\left(1\right)\right)\right),\\ \underline{\sigma}_{\mathcal{A}}\left(\tau,s\right) &= \sigma\left(s\right) - \sqrt{\frac{\pi}{2}} \frac{r \sqrt{\tau}}{l\left(\tau\right)} \left(1 + \frac{C_0 \ln^2\left(l\left(\tau\right)\right) + C_1 \ln\left(l\left(\tau\right)\right) + C_2}{l\left(\tau\right)}\right) \left(1 + o\left(1\right)\right), \end{split}$$

where  $C_0 = -\frac{1}{8}$ ,  $C_1 = -\frac{(2+a+\ln 2)}{4}$ ,  $C_2 = \frac{32-\pi^2-2\ln^2(2)-2a(4+a+2\ln 2)-8\ln 2}{32}$ , and  $a \approx 0.5772$  is the Euler-Mascheroni constant.

If s > K, we have as  $\tau \to 0^+$ ,

$$\overline{\sigma}_{\mathcal{A}}\left(\tau, s, K\right) = \sigma_{0}\left(s, K\right) + \sigma_{1}\left(s, K\right)\tau + \left(\sigma_{2}\left(s, K\right) - \frac{2\sigma_{0}\left(s, K\right)r}{d^{3}\left(\ln K, \ln s\right)\sigma\left(K\right)}\right)\tau^{2}\left(1 + o\left(1\right)\right) + \underline{\sigma}_{\mathcal{A}}\left(\tau, s, K\right) = \sigma_{0}\left(s, K\right) + \sigma_{1}\left(s, K\right)\tau + \sigma_{2}\left(s, K\right)\tau^{2}\left(1 + o\left(1\right)\right).$$

**Theorem 5.3.4** (Error estimate between the American and European implied volatility). We have as  $\tau \to 0^+$ ,

$$\begin{split} \sigma_{\mathrm{A}}\left(\tau,s\right) &= \sigma_{\mathrm{E}}\left(\tau,s\right) + \mathcal{O}\left(\frac{\tau}{l\left(\tau\right)}\right), \qquad \textit{if } s = K, \\ \sigma_{\mathrm{A}}\left(\tau,s,K\right) &= \sigma_{\mathrm{E}}\left(\tau,s,K\right) + \mathcal{O}\left(\frac{\tau^{2}}{l\left(\tau\right)}\right), \qquad \textit{if } s > K \end{split}$$

#### Numerical test 5.3.4

,

**Proposition 5.3.5.** For the CEV model, the coefficients  $\sigma_i(s, K)$  and  $\sigma_i(s)$  for i = 1, 2, 3 simplify to

$$\begin{aligned} \sigma_0\left(s,K\right) &= \frac{\ln\left(\frac{s}{K}\right)\delta\left(1-\frac{\beta}{2}\right)}{s^{1-\frac{\beta}{2}}-K^{1-\frac{\beta}{2}}}, \quad \sigma_0\left(s\right) = \delta s^{\frac{\beta}{2}-1}, \\ \sigma_1\left(s,K\right) &= \frac{\sigma_0^3\left(s,K\right)}{\rho^2} \left[\ln\left(\frac{\delta\left(sK\right)^{\frac{\beta}{4}-\frac{1}{2}}}{\sigma_0}\right) + r\left(\frac{K^{2-\beta}-s^{2-\beta}}{\delta^2\left(2-\beta\right)} + \frac{\rho}{\sigma_0^2\left(s,K\right)}\right)\right], \\ \sigma_1\left(s\right) &= \frac{1}{96}\left(\beta-2\right)^2 \delta^3 s^{\frac{3\beta}{2}-3} \\ \sigma_2\left(s,K\right) &= -\frac{3\sigma_1(s,K)\sigma_0(s,K)}{\rho^2} + \frac{3\sigma_1^2(s,K)}{2\sigma_0} + \frac{\sigma_0^5(s,K)}{8\rho^2} + \frac{\sigma_0^3}{\rho^2}\frac{\delta\beta}{4d}\left(\frac{1}{2} - \frac{\beta}{4\beta-8}\right)\left(s^{\frac{\beta}{2}-1} - K^{\frac{\beta}{2}-1}\right). \\ \sigma_2\left(s\right) &= \frac{\left(\beta-2\right)^2 \delta s^{\frac{\beta}{2}-5}\left(\delta^4 s^{2\beta}\left(28+27\left(-4+\beta\right)\beta\right) + 320s^4r^2\right)}{30720}. \end{aligned}$$

In Figure 5.10, we show that for three different sets of CEV parameters, the European and American smiles are extremely close (less than 10 basis points in absolute difference). In addition, in Figure 5.11, we plot the American and European implied volatility as a function to the time to maturity  $\tau$ . We also plot the upper-lower bounds for the American implied volatility and their associated asymptotic expansions (see Proposition 5.3.3).

*Remark* 16 (On the computation of the American implied volatility). By definition, the American implied volatility is computed solving for  $\sigma$  Equation (5.3.1) for which we use the bisection method as our root-finding algorithm. The Black–Scholes American put price is computed using the procedure exposed in Remark 13, that is we use the early premium formula as our American Black-Scholes pricer which was previously benchmarked with a binomial tree.



Figure 5.10 – American and European CEV smiles for different sets of parameters (left) and difference (in basis point) between the American and the European implied volatilities (right). The circles "○" correspond to the European asymptotic expansion. In the left pane, the dashed lines "- -" correspond to the American smile; some dotted lines "·" show the European smile, but in the figure, they are indistinguishable from the American smile.



Figure 5.11 – ATM European and American implied volatility, and American upper–lower bounds w.r.t.  $\tau$  along with their associated asymptotic expansions.

### 5.4 Conclusion

In this work, we have provided small-time expansions for the American put price in a timehomogeneous local volatility model, and deduce an error estimate for the difference between the American and European implied volatility. Asymptotics of some upper-lower bounds for both the put price and the American implied volatility were also given. In future research, we plan on expanding our results for a dividend-paying stock in an inhomogeneous local volatility model.

### 5.5 Proofs

#### 5.5.1 Reminders on Laplace's method

Before giving the main proofs, we recall the philosophy behind Laplace's method. This powerful asymptotic tool will be extensively used throughout the present section.

Suppose that we are interested in finding the leading behavior of Laplace-type integrals of the form:

$$I(\lambda) = \int_{c}^{d} g(z) e^{-\lambda f(z)} \mathrm{d}z, \qquad (5.5.1)$$

where  $\lambda$  is a large positive parameter, (c, d) a real (finite or infinite) interval and f, g some functions whose regularity will be specified later. The main idea behind Laplace's method is to observe that the main contribution of (5.5.1) comes from the neighborhood of the point where f attains its minimum. More precisely, suppose that f admits a unique minimum at  $x_0 \in (c, d)$ i.e.  $f'(x_0) = 0, f''(x_0) > 0$  and  $g(x_0) \neq 0$ . Then one can show that:

$$I(\lambda) \sim e^{-\lambda f(x_0)} g(x_0) \sqrt{\frac{2\pi}{\lambda f''(x_0)}}, \quad (\lambda \to \infty).$$

Let us try to provide a heuristic proof of this asymptotic.

1. Since the main contribution of  $I(\lambda)$  comes from a neighborhood  $(x_0 - \varepsilon, x_0 + \varepsilon)$  with  $\varepsilon > 0$ , the integration can be performed on this neighborhood instead of (c, d), namely

$$I(\lambda) = \int_{c}^{d} g(z) e^{-\lambda f(z)} dz \approx \int_{x_{0}-\varepsilon}^{x_{0}+\varepsilon} g(z) e^{-\lambda f(z)} dz.$$

2. On  $(x_0 - \varepsilon, x_0 + \varepsilon)$ , we approximate f(z) (resp. g(z)) by its second-order (resp. first-order) Taylor expansion in z to obtain:

$$I(\lambda) \approx \int_{x_0-\varepsilon}^{x_0+\varepsilon} g(z_0) e^{-\lambda \left(f(x_0) + \underbrace{f'(x_0)}_{=0}^{(z-x_0) + f''(x_0)\frac{(z-x_0)^2}{2}}\right)} dz$$
$$= e^{-\lambda f(x_0)} \int_{x_0-\varepsilon}^{x_0+\varepsilon} g(z_0) e^{-\lambda f''(x_0)\frac{(z-x_0)^2}{2}} dz.$$

3. Expanding the integration on  $(-\infty, \infty)$  boils down to the following Gaussian integral:

$$I(\lambda) \approx e^{-\lambda f(x_0)} \int_{-\infty}^{+\infty} g(z_0) \, e^{-\lambda f''(x_0)\frac{(z-x_0)^2}{2}} \mathrm{d}z = e^{-\lambda f(x_0)} g(x_0) \sqrt{\frac{2\pi}{\lambda f''(x_0)}}.$$

Each approximation step can be rigorously justified to obtain the following theorem.

**Theorem 5.5.1.** (Wong [168, Theorem 1], Nemes [143, Theorem 1.1])Let a be finite and b > a be finite or infinite and consider the Laplace-type integral:

$$I(\lambda) = \int_{a}^{b} g(z) e^{-\lambda f(z)} dz.$$

Suppose,

- 1. f(z) > f(a) for all  $z \in (a,b)$ , and for every  $\delta > 0$  the infimum of f(z) f(a) in  $[a + \delta, b)$  is positive.
- 2. f'(z) and g(z) are continuous in a neighborhood of z = a, expect possibly at z = a.

3. The following expansions hold; as  $z \to a^+$ :

$$f(z) \sim f(a) + \sum_{k=0}^{\infty} a_k (z-a)^{k+\alpha},$$
 (5.5.2)

$$g(z) \sim \sum_{k=0}^{\infty} b_k (z-a)^{k+\beta-1},$$
 (5.5.3)

where  $\alpha, \beta > 0$  and without loss of generality assume that  $a_0 \neq 0$  and  $b_0 \neq 0$ . Assume also that the expansion for f can be term-wise differentiated i.e.

$$f'(z) \sim \sum_{k=0}^{\infty} a_k (k+\alpha) (z-a)^{k+\alpha-1}$$
. (5.5.4)

4. The integral converges absolutely for all sufficiently large  $\lambda$ .

Then as  $\lambda \to \infty$ ,

$$I(\lambda) \sim e^{-\lambda f(a)} \sum_{k=0}^{\infty} \Gamma\left(\frac{k+\beta}{\alpha}\right) \frac{c_k}{\lambda^{\frac{k+\beta}{\alpha}}},$$
(5.5.5)

where the coefficients  $c_k$  are defined as (see [143, Equation 2.2]):

$$c_k = \frac{1}{\alpha a_0^{\frac{k+\beta}{\alpha}}} \sum_{m=0}^k \frac{b_{k-m}}{m!} \left[ \frac{\mathrm{d}^m}{\mathrm{d}x^m} \left( 1 + \sum_{l=1}^\infty \frac{a_l}{a_0} x^l \right)^{-\frac{k+\beta}{\alpha}} \right]_{x=0}$$

The first three terms are given by:

$$c_0 = \frac{b_0}{a_0^{\frac{\beta}{\alpha}}\alpha}, \quad c_1 = \frac{1}{a_0^{\frac{\beta+1}{\alpha}}} \left(\frac{b_1}{\alpha} - \frac{(\beta+1)a_1b_0}{\alpha^2 a_0}\right),$$

$$c_{2} = \frac{1}{a_{0}^{\frac{\beta+2}{\alpha}}} \left( \frac{b_{2}}{\alpha} - \frac{(\beta+2)a_{1}b_{1}}{\alpha^{2}a_{0}} + \left( (\beta+\alpha+2)a_{1}^{2} - 2\alpha a_{0}a_{2} \right) \frac{(\beta+2)b_{0}}{2\alpha^{3}a_{0}^{2}} \right).$$

### 5.5.2 Proofs of the technical Lemmas

In this section, we state some technical proofs that will be essential for our asymptotic expansions. We start with some small-time expansions regarding the exercise boundary.

Lemma 5.5.2. We have as  $\tau \to 0^+$ ,

$$\overline{x}(\tau) = \ln(K) - \sigma(K)\sqrt{\tau l(\tau)} \left(1 + \frac{1}{l(\tau)^2} + \frac{1}{2l(\tau)^3} + \mathcal{O}\left(\frac{1}{l(\tau)^4}\right)\right), \quad (5.5.6)$$

$$d(\bar{x}(\tau), \ln K)^{2} = \tau l(\tau) \left( 1 + \frac{2}{l(\tau)^{2}} + \frac{1}{l(\tau)^{3}} + \mathcal{O}\left(\frac{1}{l(\tau)^{4}}\right) \right),$$
(5.5.7)

$$e^{-\frac{\mathbf{d}(\overline{x}(\tau),\ln K)^2}{2\tau}} = \frac{\sqrt{\tau}}{\sqrt{\gamma}} \left( 1 - \frac{1}{l(\tau)} + \mathcal{O}\left(\frac{1}{l(\tau)^3}\right) \right), \tag{5.5.8}$$

$$\int_{0}^{\tau} \frac{e^{-\frac{d(\overline{u}(\tau),\ln K)^{2}}{2u}}}{\sqrt{u}} du = \frac{\tau}{\sqrt{\gamma}} \left(\frac{2}{l(\tau)} - \frac{8}{l(\tau)^{2}} + \frac{32}{l(\tau)^{3}} + \mathcal{O}\left(\frac{1}{l(\tau)^{4}}\right)\right),$$
(5.5.9)

$$\int_{0}^{\tau} \sqrt{u} e^{-\frac{\mathrm{d}(\bar{x}(\tau),\ln K)^{2}}{2u}} \mathrm{d}u = \frac{\tau^{2}}{\sqrt{\gamma}} \left( \frac{2}{l(\tau)} - \frac{12}{l(\tau)^{2}} + \frac{76}{l(\tau)^{3}} + \mathcal{O}\left(\frac{1}{l(\tau)^{4}}\right) \right),$$
(5.5.10)
Proof of Lemma 5.5.2. Both (5.5.6) and (5.5.7) are direct consequences of [53, Theorem 3.1]. Multiplying (5.5.7) by  $-\frac{\tau}{2}$  and exponentiating yields (5.5.8). For the other integrals, introducing  $u = \frac{d(\overline{x}(\tau), \ln K)^2}{2t^2}$  and integrating successively by parts,

$$\begin{split} \int_{0}^{\tau} e^{-\frac{\mathrm{d}(\overline{x}(\tau),\ln K)^{2}}{2u}} \sqrt{u} \mathrm{d}u &= \frac{\mathrm{d}\left(\overline{x}\left(\tau\right),\ln K\right)^{4}}{\sqrt{2}} \int_{\frac{\mathrm{d}(\overline{x}(\tau),\ln K)}{\sqrt{2\tau}}}^{\infty} \frac{e^{-t^{2}}}{t^{4}} \mathrm{d}t \\ &= \frac{1}{3} \left( \sqrt{2\pi} \mathrm{d}(\overline{x}\left(\tau\right),\ln K)^{3} \mathrm{Erfc}\left(\frac{\mathrm{d}(\overline{x}\left(\tau\right),\ln K)}{\sqrt{2}\sqrt{\tau}}\right) \right. \\ &\left. + 2\sqrt{\tau} e^{-\frac{\mathrm{d}(\overline{x}(\tau),\ln K)}{2\tau}} \left(\tau - \mathrm{d}(\overline{x}\left(\tau\right),\ln K)^{2}\right) \right). \end{split}$$

A similar study gives the following identity:

$$\int_{0}^{\tau} \frac{e^{-\frac{\mathrm{d}(\overline{x}(\tau),\ln K)^{2}}{2u}}}{\sqrt{u}} \mathrm{d}u = 2\sqrt{\tau}e^{-\frac{\mathrm{d}(\overline{x}(\tau),\ln K)^{2}}{2\tau}} - \sqrt{2\pi}\mathrm{d}\left(\overline{x}\left(\tau\right),\ln K\right)\mathrm{Erfc}\left(\frac{\mathrm{d}\left(\overline{x}\left(\tau\right),\ln K\right)}{\sqrt{2}\sqrt{\tau}}\right),$$

and using (5.5.8), we obtain (5.5.9) and (5.5.10).

**Lemma 5.5.3.** For every  $v \in (0,1)$  and  $\alpha \in \mathbb{R}$ , we have as  $\tau \to 0^+$ ,

$$l(v\tau)^{\alpha} = l(\tau)^{\alpha} \left( 1 - \frac{\alpha \ln(v)}{l(\tau)} + \frac{\alpha (\alpha - 1) \ln(v)^2}{2l(\tau)^2} + \mathcal{O}\left(\frac{\ln(v)^3}{l(\tau)^3}\right) \right).$$
(5.5.11)

$$\ln K - \overline{x} \left( v\tau \right) = \sigma \left( K \right) \sqrt{v} \sqrt{\tau l \left( \tau \right)} \left( 1 - \frac{\ln v}{2l \left( \tau \right)} + \mathcal{O} \left( \frac{1 - \frac{\ln(v)^2}{8}}{l \left( \tau \right)^2} \right) \right).$$
(5.5.12)

$$e^{-\frac{d^2(\overline{x}(v\tau),\ln K)}{2(1-v)\tau}} = e^{-\frac{v}{2(1-v)}l(\tau) + \frac{v\ln(v)}{2(1-v)}} \left(1 - \frac{v}{(1-v)l(\tau)} + \mathcal{O}\left(\frac{\frac{v^2}{(1-v)^2} + \frac{v\ln(v)}{1-v}}{l(\tau)^2}\right)\right).$$
(5.5.13)

$$e^{-\frac{d^2(\overline{x}(v\tau),\ln s)}{2(1-v)\tau}} = e^{-\frac{d^2(\ln K,\ln s)}{2(1-v)\tau}} e^{-\frac{d(\ln K,\ln s)}{\sqrt{\tau}}\frac{\sqrt{v}}{1-v}\left(l(\tau)^{\frac{1}{2}} - \frac{\ln(v)}{2l(\tau)^{\frac{1}{2}}} + \left(1 - \frac{\ln(v)^2}{8}\right)\frac{1}{l(\tau)^{\frac{3}{2}}} + \mathcal{O}\left(\frac{|\ln(v)|}{l(\tau)^2}\right)\right)}.$$
(5.5.14)

$$\overline{x}'(v\tau) = -\frac{\sigma(K)}{2} \frac{\sqrt{l(\tau)}}{\sqrt{v\tau}} \left( 1 - \left(1 + \frac{\ln(v)}{2}\right) \frac{1}{l(\tau)} + \mathcal{O}\left(\frac{1 - \frac{\ln(v)^2}{8}}{l^2(\tau)}\right) \right).$$
(5.5.15)

$$u_{0}(x, \overline{x}(v\tau)) = u_{0}(x, \ln K)$$

$$+ u_{0}(x, \ln K) \left( -\frac{3}{2}K\sigma'(K) + \frac{r}{\sigma(K)} - \frac{\sigma(K)}{2} \right) \sqrt{v}\sqrt{\tau l(\tau)} \left( 1 - \frac{\ln v}{2l(\tau)} + \mathcal{O}\left(\frac{1 - \frac{\ln(v)^{2}}{8}}{l(\tau)^{\frac{3}{2}}} \right) \right)$$

$$(5.5.16)$$

$$(5.5.17)$$

Remark 17 (On the expansion for the derivative of the exercise boundary (5.5.15)). To obtain the small-time asymptotic of  $\overline{x}'(\tau)$ , we differentiate w.r.t.  $\tau$  the expansion of the exercise boundary  $\overline{x}(\tau)$  in (5.5.12). We leave the rigorous justification for future research.

Proof of Lemma 5.5.3. From the identity  $l(v\tau)^{\alpha} = \ln\left(\frac{\gamma}{v\tau}\right)^{\alpha} = l(\tau)^{\alpha}\left(1 - \frac{\ln v}{l(\tau)}\right)^{\alpha}$  and using  $l(\tau) \xrightarrow[\tau \to 0^+]{} \infty$ , we get (5.5.11). Owing to (5.5.6) and (5.5.11), we obtain (5.5.12). Combining (5.5.7) and (5.5.11), we have first:

$$d\left(\overline{x}\left(v\tau\right),\ln K\right)^{2} = v\tau\left(l\left(v\tau\right) + 2l\left(v\tau\right)^{-1} + \mathcal{O}\left(l\left(v\tau\right)^{-2}\right)\right)$$

$$= v\tau \left( l\left(\tau\right) - \ln\left(v\right) + \frac{2}{l\left(\tau\right)} + \mathcal{O}\left(\frac{\left|\ln\left(v\right)\right|}{l\left(\tau\right)^{2}}\right) \right), \qquad (5.5.18)$$

and we obtain

$$\frac{\mathrm{d}\left(\overline{x}\left(v\tau\right),\ln K\right)^{2}}{2\left(1-v\right)\tau} = \frac{vl\left(\tau\right)}{2\left(1-v\right)} - \frac{v\ln\left(v\right)}{2\left(1-v\right)} + \frac{v}{\left(1-v\right)l\left(\tau\right)} + \mathcal{O}\left(\frac{\frac{v|\ln\left(v\right)|}{1-v}}{l^{2}\left(\tau\right)}\right).$$
(5.5.19)

Exponentiating (5.5.19) yields

$$e^{-\frac{d^2(\overline{x}(v\tau),\ln K)}{2(1-v)\tau}} = e^{-\frac{vl(\tau)}{2(1-v)} + \frac{v\ln(v)}{2(1-v)} - \frac{v}{(1-v)l(\tau)} + \mathcal{O}\left(\frac{\frac{v|\ln(v)|}{1-v}}{l(\tau)^2}\right)}$$

and we deduce the expansion (5.5.13). Similarly, from (5.5.18) and the identity:

$$d^{2}(\overline{x}(v\tau),\ln s) = d^{2}(\overline{x}(v\tau),\ln K) + 2d(\overline{x}(v\tau),\ln K)d(\ln K,\ln s) + d^{2}(\ln K,\ln s),$$

we obtain:

$$d(\overline{x}(v\tau), \ln K) = (v\tau)^{\frac{1}{2}} \left( l(\tau)^{\frac{1}{2}} - \frac{\ln(v)}{2l(\tau)^{\frac{1}{2}}} + \left( 1 - \frac{\ln(v)^2}{8} \right) \frac{1}{l(\tau)^{\frac{3}{2}}} + \mathcal{O}\left(\frac{|\ln(v)|}{l(\tau)^2}\right) \right)$$

Consequently,

$$\frac{2\mathrm{d}\left(\overline{x}\left(v\tau\right),\ln K\right)\mathrm{d}\left(\ln K,\ln s\right)}{2\left(1-v\right)\tau} = \frac{\mathrm{d}\left(\ln K,\ln s\right)}{\sqrt{\tau}}\frac{\sqrt{v}}{1-v}\left(l\left(\tau\right)^{\frac{1}{2}} - \frac{\ln\left(v\right)}{2l\left(\tau\right)^{\frac{1}{2}}}, +\left(1-\frac{\ln\left(v\right)^{2}}{8}\right)\frac{1}{l\left(\tau\right)^{\frac{3}{2}}} + \mathcal{O}\left(\frac{\left|\ln\left(v\right)\right|}{l\left(\tau\right)^{2}}\right)\right),$$

and using that  $d^{2}(\overline{x}(v\tau), \ln K) = \mathcal{O}(d(\overline{x}(v\tau), \ln K))$  as  $\tau \to 0^{+}$  (still by (5.5.18)), we infer:

$$e^{-\frac{d^2(\bar{x}(v\tau),\ln s)}{2(1-v)\tau}} = e^{-\frac{d^2(\ln K,\ln s)}{2(1-v)\tau}} e^{-\frac{d(\ln K,\ln s)}{\sqrt{\tau}}\frac{\sqrt{v}}{1-v}\left(l(\tau)^{\frac{1}{2}} - \frac{\ln(v)}{2l(\tau)^{\frac{1}{2}}} + \left(1 - \frac{\ln(v)^2}{8}\right)\frac{1}{l(\tau)^{\frac{3}{2}}} + \mathcal{O}\left(\frac{|\ln(v)|}{l(\tau)^2}\right)\right).$$

For (5.5.15), assuming that we can take the derivative w.r.t.  $\tau$  in (5.5.12) and from the identities  $\frac{\mathrm{d}}{\mathrm{d}\tau} \left( l\left(\tau\right) \right) = -\frac{1}{\tau}, \frac{\mathrm{d}}{\mathrm{d}\tau} \left( \sqrt{\tau l\left(\tau\right)} \right) = \frac{l(\tau) - 1}{2\sqrt{\tau l(\tau)}}, \frac{\mathrm{d}}{\mathrm{d}\tau} \left( \frac{\sqrt{\tau}}{\sqrt{l(\tau)}} \right) = \frac{1}{2\sqrt{\tau l(\tau)}} \left( 1 + \frac{1}{l(\tau)} \right)$  we infer:  $\overline{x}' \left( v\tau \right) = -\frac{\sigma\left(K\right)}{2} \frac{\sqrt{l\left(\tau\right)}}{\sqrt{v\tau}} \left( 1 - \left( 1 + \frac{\ln\left(v\right)}{2} \right) \frac{1}{l\left(\tau\right)} + \mathcal{O}\left( \frac{1 - \frac{\ln\left(v\right)^2}{8}}{l^{\frac{3}{2}}\left(\tau\right)} \right) \right).$ 

Finally, Taylor expanding  $u_0(x, \overline{x}(v\tau))$  around  $\ln K$  gives:

$$u_0(x,\overline{x}(v\tau)) = u_0(x,\ln K) + \partial_y u_0(x,\ln K) \times (\overline{x}(v\tau) - \ln K) + \mathcal{O}\left(\left(\overline{x}(v\tau) - \ln K\right)^2\right).$$

We then conclude using  $\partial_y u_0(x, \ln K) \stackrel{(5.1.14)}{=} u_0(x, \ln K) \left( -\frac{3}{2} \frac{K\sigma'(K)}{\sigma(K)} + \frac{r}{\sigma^2(K)} - \frac{1}{2} \right)$  and (5.5.12) to get (5.5.17).

**Lemma 5.5.4.** For every  $n \in \mathbb{N}$ , we have as  $\tau \to 0^+$ ,

$$\int_0^\tau \frac{\mathrm{d}t}{\ln^n(t)} \sim \frac{\tau}{\ln^n \tau},\tag{5.5.20}$$

$$\int_{0}^{\tau} \frac{\ln\left(-\ln\left(t\right)\right)}{\ln^{2}\left(t\right)} dt \sim \frac{\tau \ln\left(-\ln\left(\tau\right)\right)}{\ln^{2}\left(\tau\right)},$$
(5.5.21)

$$\int_{0}^{\tau} \frac{\ln^{2} \left(-\ln \left(t\right)\right)}{\ln^{2} \left(t\right)} dt \sim \frac{\tau \ln^{2} \left(-\ln \left(\tau\right)\right)}{\ln^{2} \left(\tau\right)}.$$
(5.5.22)

Proof of Lemma 5.5.4. Let  $F_n : \tau \in (0,1) \to \int_0^\tau \frac{dt}{\ln^n(t)}$ . Introducing  $y = -\ln t \iff t = e^{-y}$ , we have:

$$F_n(\tau) = (-1)^n \int_{-\ln \tau}^{\infty} y^{-n} e^{-y} dy = (-1)^n \Gamma_{1-n}(-\ln(\tau)).$$

We then obtain the desired asymptotic expansion owing to (5.1.7) with a = 1 - n and  $z = -\ln \tau \xrightarrow[\tau \to 0^+]{} \infty$ .

Let us now deal with (5.5.21); noticing that  $\frac{d}{dt} (\ln(-\ln(t))) = \frac{1}{t \ln t}$ , an integration by parts gives:

$$\int_0^\tau \frac{\ln(-\ln(t))}{\ln^2(t)} dt = [F_2(t)\ln(-\ln(t))]_0^\tau - \int_0^\tau \frac{F_2(t)}{t\ln t} dt.$$

Now thanks to (5.5.20) with n = 2, we have first:

$$F_2(t)\ln\left(-\ln t\right) \underset{t\to 0^+}{\sim} \frac{t\ln\left(-\ln t\right)}{\ln^2(t)} \xrightarrow[t\to 0^+]{} 0.$$

Similarly  $\frac{F_2(t)}{t \ln t} \sim_{t \to 0^+} \frac{1}{\ln^3(t)}$  and integrating from 0 to  $\tau$ , we get:

$$\int_0^\tau \frac{F_2(t)}{t \ln t} \mathrm{d}t \underset{\tau \to 0^+}{\sim} \int_0^\tau \frac{\mathrm{d}t}{\ln^3(t)} = F_3(\tau) \underset{\tau \to 0^+}{\sim} \frac{\tau}{\ln^3(\tau)}$$

using this time (5.5.20) with n = 3. We conclude using that  $\frac{\tau}{\ln^3(\tau)} = o\left(\frac{\tau \ln(-\ln \tau)}{\ln^2(\tau)}\right)$  as  $\tau \to 0^+$ . Considering the map  $\tau \mapsto \int_0^{\tau} \frac{\ln(-\ln(t))}{\ln^2(t)} dt$  instead of  $F_2(t)$  and conducting the same analysis yields the expansion (5.5.22).

**Lemma 5.5.5.** Let  $v \in (0,1)$  and suppose  $x \ge \ln K$ . Then, we have as  $\tau \to 0^+$ ,

$$\int_{0}^{\infty} u_{0}\left(x,\overline{x}\left(\tau\right)-z\right) \exp\left[-\frac{\mathrm{d}^{2}\left(\overline{x}\left(\tau\right)-z,x\right)}{2\tau v}\right] \mathrm{d}z$$
$$=\frac{u_{0}\left(x,\ln K\right)\sigma\left(e^{\overline{x}\left(\tau\right)}\right)}{\mathrm{d}\left(\overline{x}\left(\tau\right),x\right)}\tau v \exp\left[-\frac{\mathrm{d}^{2}\left(\overline{x}\left(\tau\right),x\right)}{2\tau v}\right]\left(1+\mathcal{O}\left(v\tau\right)\right).$$

Proof of Lemma 5.5.5. For every  $\tau > 0$ , define:

$$f_{\tau}: z \in [0,\infty) \to \frac{\mathrm{d}^2\left(\overline{x}\left(\tau\right) - z, x\right)}{2} - \frac{\mathrm{d}^2\left(\overline{x}\left(\tau\right), x\right)}{2},$$

such that:

$$f_{\tau}(0) = 0, \quad f_{\tau}'(z) = \frac{\mathrm{d}\left(\overline{x}\left(\tau\right) - z, x\right)}{\sigma\left(e^{\overline{x}(\tau) - z}\right)}, \quad f_{\tau}'(0) = \frac{\mathrm{d}\left(\overline{x}\left(\tau\right), x\right)}{\sigma\left(e^{\overline{x}(\tau)}\right)} > 0,$$

and

$$\int_{0}^{\infty} u_{0}\left(x,\overline{x}\left(\tau\right)-z\right) \exp\left[-\frac{\mathrm{d}^{2}\left(\overline{x}\left(\tau\right)-z,x\right)}{2\tau v}\right] \mathrm{d}z$$
$$= \exp\left[-\frac{\mathrm{d}^{2}\left(\overline{x}\left(\tau\right),x\right)}{2\tau v}\right] \int_{0}^{\infty} u_{0}\left(x,\overline{x}\left(\tau\right)-z\right) e^{-\frac{f\tau(z)}{\tau v}} \mathrm{d}z.$$

We first investigate the last integral. The key idea of the proof is to split the integral on two intervals  $(\delta, \infty)$  and  $(0, \delta)$  for a fixed  $\delta > 0$ , and show that the contribution of the first one is

exponentially small compared to that of the second. Hence let us fix  $\delta > 0$  and notice that for every z > 0,

$$f_{\tau}\left(z\right) = \frac{1}{2} \left( \int_{\overline{x}(\tau)-z}^{x} \frac{\mathrm{d}u}{\sigma\left(e^{u}\right)} + \int_{\overline{x}(\tau)}^{x} \frac{\mathrm{d}u}{\sigma\left(e^{u}\right)} \right) \int_{\overline{x}(\tau)-z}^{\overline{x}(\tau)} \frac{\mathrm{d}u}{\sigma\left(e^{u}\right)} \ge \frac{1}{2C^{2}} \left(2x - 2\overline{x}\left(\tau\right) + z\right) z \ge \frac{1}{2C^{2}} z^{2},$$

$$(5.5.23)$$

using Assumption 5.1.2 on the volatility  $\sigma(\cdot)$  and  $\overline{x}(\tau) < \ln K < x$  for every  $\tau > 0$ . Also, from (5.1.10) and still by (5.1.2), we have:

$$u_0\left(x,\overline{x}\left(\tau\right)-z\right) \le C^{-1}e^{\left(\frac{1}{2}+rC^2\right)\left(z+x-\overline{x}\left(\tau\right)\right)}$$

Consequently, we obtain (for every  $0 < \tau < 1$ ):

$$0 < \int_{\delta}^{\infty} u_0 \left( x, \overline{x} \left( \tau \right) - z \right) e^{-\frac{f_{\tau}(z)}{\tau v}} \mathrm{d}z = \int_{\delta}^{\infty} u_0 \left( x, \overline{x} \left( \tau \right) - z \right) e^{-f_{\tau}(z) \left( \frac{1}{\tau v} - 1 \right) - f_{\tau}(z)} \mathrm{d}z < C^{-1} e^{-\frac{\delta^2}{2C^2} \left( \frac{1}{\tau v} - 1 \right)} e^{\left( \frac{1}{2} + rC^2 \right) \left( x - \overline{x}(\tau) \right)} \int_0^{\infty} e^{\left( \frac{1}{2} + rC^2 \right) z} e^{-\frac{z^2}{2C^2}} \mathrm{d}z.$$

The last integral in z being finite and since  $\overline{x}(\tau) \to \ln K \leq x$  as  $\tau \to 0^+$ , we infer that:

$$\int_{\delta}^{\infty} u_0\left(x, \overline{x}\left(\tau\right) - z\right) e^{-\frac{f_{\tau}(z)}{\tau_v}} \mathrm{d}z = \mathcal{O}\left(e^{-\frac{\delta^2}{2C^2}\frac{1}{\tau_v}}\right).$$
(5.5.24)

Let us now deal with the interval  $(0, \delta)$ . Set  $\varepsilon, \nu > 0$ . Using that  $\frac{f_{\tau}(z) - f_{\tau}(0)}{z-0} = \frac{f_{\tau}(z)}{z} \xrightarrow[z \to 0^+]{} f'_{\tau}(0)$ , we deduce that there exists  $z_0(\varepsilon) < 0$  such that:

$$0 < z < z_0(\varepsilon) \Longrightarrow \left| \frac{f_\tau(z)}{z} - f'_\tau(0) \right| \le \varepsilon$$

Choosing  $\delta > z_0(\varepsilon)$ , we infer that on  $(0, \delta)$ :

$$(f'_{\tau}(0) - \varepsilon) z \le f_{\tau}(z) \le (f'_{\tau}(0) + \varepsilon) z.$$

Similarly as  $u_0(x, z + \overline{x}(\tau)) \xrightarrow[\tau \to 0^+]{} u_0(x, z + \ln K)$ , we have that for every z and sufficiently small values of  $\tau$ :

$$(1-\nu) u_0(x, \ln K - z) < u_0(x, \overline{x}(\tau) - z) < (1+\nu) u_0(x, \ln K - z),$$

getting that:

$$\int_{0}^{\delta} u_{0}\left(x,\ln K-z\right) e^{-\frac{f_{\tau}'(0)+\varepsilon}{\tau v}z} \mathrm{d}z < \int_{0}^{\delta} u_{0}\left(x,z+\overline{x}\left(\tau\right)\right) e^{-\frac{f_{\tau}(z)}{\tau v}} \mathrm{d}z < (1+\nu) \int_{0}^{\delta} u_{0}\left(x,\ln K-z\right) e^{-\frac{f_{\tau}'(0)-\varepsilon}{\tau v}z} \mathrm{d}z.$$
(5.5.25)

By a direct application of Theorem 5.5.1 with  $\lambda = \frac{f'_{\tau}(0) - \varepsilon}{\tau v} \xrightarrow[\tau \to 0^+]{} \infty$ , we get that:

$$(1+\nu)\int_0^\delta u_0\left(x,\ln K-z\right)e^{-\frac{f_{\tau}'(0)-\varepsilon}{\tau v}z}\mathrm{d}z = (1+\nu)\frac{u_0\left(x,\ln K\right)}{f_{\tau}'\left(0\right)-\varepsilon}\tau v + \mathcal{O}\left(\tau^2 v^2\right)$$

Needless to say that a similar estimate can be found for the l.h.s. of (5.5.25). Using the fact that  $\nu$  and  $\varepsilon$  are arbitrary small along with the estimate (5.5.24), and the equality  $f'_{\tau}(0) = \frac{\mathrm{d}(\overline{x}(\tau),x)}{\sigma(e^{\overline{x}(\tau)})}$ , we get the desired asymptotic.

#### 5.5.3 Proofs of Section 5.2.1

Recall that for the ATM case  $x = \ln K = \ln s$ .

Proof of Proposition 5.2.1. Introducing z = x - y, the European put price rewrites as

$$P(\tau, e^{x}) = \mathbb{E}_{0,x} \left[ e^{-r\tau} \left( e^{x} - e^{X_{\tau}} \right)_{+} \right]$$
$$= e^{x - r\tau} \int_{-\infty}^{x} \left( 1 - e^{y - x} \right) f_{X}(\tau, y \mid x) \, \mathrm{d}y$$
$$= e^{x - r\tau} \int_{0}^{\infty} \left( 1 - e^{-z} \right) f_{X}(\tau, x - z \mid x) \, \mathrm{d}z$$

From Lemma 5.1.1, we can replace  $f_X$  by its short-time asymptotic expansion to get:

$$P(\tau, e^{x}) = \frac{e^{x-r\tau}}{\sqrt{2\pi\tau}} \left( I_{0}(\tau) + I_{1}(\tau) + \mathcal{O}(\tau^{2}) \int_{0}^{\infty} (1 - e^{-z}) e^{-\frac{d^{2}(x-z,x)}{2\tau}} dz \right),$$

where we have introduced:

$$I_0(\tau) = \int_0^\infty (1 - e^{-z}) u_0(x, x - z) e^{-\frac{d^2(x - z, x)}{2\tau}} dz,$$
  
$$I_1(\tau) = \tau \int_0^\infty (1 - e^{-z}) u_1(x, x - z) e^{-\frac{d^2(x - z, x)}{2\tau}} dz$$

First note that from Assumption 5.1.2, we have  $-\frac{d^2(x-z,x)}{2\tau} \leq -\frac{z^2}{2C^2\tau}$  so that:

$$\int_0^\infty \left(1 - e^{-z}\right) e^{-\frac{\mathrm{d}^2(x - z, x)}{2\tau}} \mathrm{d}z \le \int_0^\infty e^{-\frac{\mathrm{d}^2(x - z, x)}{2\tau}} \mathrm{d}z \le \int_0^\infty e^{-\frac{z^2}{2C^2\tau}} \mathrm{d}z = \sqrt{\frac{\pi}{2}} C\sqrt{\tau},$$

which gives that  $\mathcal{O}\left(\tau^2\right) \int_0^\infty (1-e^{-z}) e^{-\frac{d^2(x-z,x)}{2\tau}} dz = \mathcal{O}\left(\tau^{\frac{5}{2}}\right)$ . We now deal with both integrals  $I_0, I_1$ . To keep on with the notations of Theorem 5.5.1, let  $f(z) = \frac{d^2(x-z,x)}{2}, g_0(z) = (1-e^{-z}) u_0(x,x-z), g_1(z) = (1-e^{-z}) u_1(x,x-z), \lambda = \frac{1}{\tau} \xrightarrow[\tau \to 0^+]{} \infty, a = 0, b = \infty.$ 

 $\triangleright$  Expansion for  $I_0(\tau)$ . First note that  $I_0(\tau)$  is a Laplace-type integral and that we need to go up to k = 2 in Theorem 5.5.1 in order to derive an expansion of order  $\tau^2$ . As f is nonnegative and f(0) = 0, we have that f admits a unique minimum at z = 0. Also, since  $f'(z) = \frac{d(x-z,x)}{\sigma(e^{x-z})}$ , we infer that both  $f', g_0$  are continuous on  $[0, \infty)$ , and thus Assumptions 1, 2, and 4 hold true. Note also that (5.5.2), (5.5.3), and (5.5.4) are satisfied with:

$$\alpha = 2, \quad \beta = 2, \quad a_0 = \frac{1}{2\sigma (e^x)^2}, \quad a_1 = \frac{e^x \sigma' (e^x)}{2\sigma (e^x)^3}, \quad b_0 = \frac{1}{\sigma (e^x)}, \quad b_1 = -\frac{r}{\sigma (e^x)^3},$$
$$a_2 = -\frac{e^x \left(4e^x \sigma (e^x) \sigma'' (e^x) - 11e^x \sigma' (e^x)^2 + 4\sigma (e^x) \sigma' (e^x)\right)}{24\sigma (e^x)^4},$$

$$b_{2} = \frac{1}{24\sigma (e^{x})^{5}} \Big( 12r^{2} - 60re^{x}\sigma (e^{x})\sigma' (e^{x}) - 18e^{2x}\sigma (e^{x})^{3}\sigma'' (e^{x}) - 18e^{x}\sigma (e^{x})^{3}\sigma' (e^{x}) + 45e^{2x}\sigma (e^{x})^{2}\sigma' (e^{x})^{2} + \sigma (e^{x})^{4} \Big).$$

By (5.5.5), we deduce that as  $\lambda \to \infty$ ,

$$I_0\left(\lambda\right) \sim \Gamma\left(1\right)\frac{c_0}{\lambda} + \Gamma\left(\frac{3}{2}\right)\frac{c_1}{\lambda^{\frac{3}{2}}} + \Gamma\left(2\right)\frac{c_2}{\lambda^2},$$

where the coefficients  $c_k$  simplify to:

$$c_0 = \sigma\left(e^x\right), \quad c_1 = -\sqrt{2}r,$$

$$c_{2} = \frac{r^{2}}{\sigma(e^{x})} - \frac{e^{x}}{6} \left( 6r + \sigma(e^{x})^{2} \right) \sigma'(e^{x}) - \frac{e^{2x}}{12} \sigma(e^{x}) \left( 2\sigma(e^{x}) \sigma''(e^{x}) - \sigma'(e^{x})^{2} \right) + \frac{\sigma(e^{x})^{3}}{12}.$$

 $\triangleright$  Expansion for  $I_1(\tau)$ . We proceed as before, considering this time  $g_1(z) \sim u_1(x, x) z$  as  $z \to 0^+$ . We then get (remembering the factor  $\frac{1}{\lambda}$ ):

$$I_1(\lambda) \sim \Gamma(1) \frac{c'_0}{\lambda^2},$$

with

$$\begin{split} c_{0}^{'} &= u_{1}\left(x,x\right)\sigma\left(e^{x}\right)^{2} \\ &\stackrel{(5.1.13)}{=} \frac{\sigma\left(e^{x}\right)}{8} \left(4r - \frac{4r^{2} + \sigma(e^{x})\left(\sigma(e^{x})\left(\left(\sigma(e^{x}) - e^{x}\sigma'(e^{x})\right)^{2} - 2e^{2x}\sigma(e^{x})\sigma''(e^{x})\right) - 8re^{x}\sigma'(e^{x})\right)}{\sigma(e^{x})^{2}}\right) \\ &= \frac{r\sigma\left(e^{x}\right)}{2} - \frac{r^{2}}{2\sigma\left(e^{x}\right)} - \frac{\sigma\left(e^{x}\right)}{8}\left(\sigma(e^{x}) - e^{x}\sigma'(e^{x})\right)^{2} + \frac{e^{2x}}{4}\sigma''(e^{x})\sigma\left(e^{x}\right)^{2} + re^{x}\sigma'\left(e^{x}\right). \end{split}$$

 $\triangleright$  Expansion for  $P(\tau, s)$ . Finally, using the special values  $\Gamma(1) = \Gamma(2) = 1$ ,  $\Gamma(\frac{3}{2}) = \frac{\sqrt{\pi}}{2}$  for the Gamma function and going back to  $\tau = \frac{1}{\lambda}$  along with the expansion  $e^{-r\tau} \sim 1 - r\tau$  as  $\tau \to 0^+$ , we obtain

$$P(\tau, e^{x}) = \frac{e^{x}}{\sqrt{2\pi}} \left( c_{0} \tau^{\frac{1}{2}} + \frac{\sqrt{\pi}}{2} c_{1} \tau + \left( c_{2} + c_{0}^{'} - c_{0} \right) \tau^{\frac{3}{2}} + \mathcal{O}(\tau^{2}) \right),$$

where a direct simplification gives the announced result:

$$c_{2} + c_{0}^{'} - rc_{0} = -\frac{r\sigma\left(e^{x}\right)}{2} + \frac{r^{2}}{2\sigma\left(e^{x}\right)} + \frac{e^{2x}}{12}\sigma^{\prime\prime}(e^{x})\sigma\left(e^{x}\right)^{2} - \frac{\sigma\left(e^{x}\right)}{24}\left(\sigma(e^{x}) - e^{x}\sigma^{\prime}(e^{x})\right)^{2}.$$

*Proof of Proposition* 5.2.2. By definition, the upper premium (5.1.19) rewrites as

$$\overline{p}(\tau, e^x) = re^x \int_0^\tau e^{-ru} \left( \int_{-\infty}^x f_X(u, y | x) \, \mathrm{d}y \right) \mathrm{d}u = re^x \int_0^\tau e^{-ru} \left( \int_0^\infty f_X(u, x - z | x) \, \mathrm{d}z \right) \mathrm{d}u,$$

where we have introduced the new variable y = x - z, and taking the derivative of  $\overline{p}(\tau, e^x)$  w.r.t.  $\tau$  yields

$$\partial_{\tau}\overline{p}\left(\tau,e^{x}\right) = re^{x-r\tau} \int_{0}^{\infty} f_{X}\left(\tau,x-z|x\right) \mathrm{d}z$$

Note that as we seek an asymptotic expansion up to  $\tau\sqrt{\tau}$  for the upper premium, we only need an expansion up to  $\sqrt{\tau}$  for its derivative. Hence, we proceed exactly as in the proof of Proposition 5.2.1. The only difference here is that the function g is now:

$$g(z) = u_0(x, x-z) \underset{z \to 0^+}{\sim} b_0 + b_1 z_2$$

with  $b_0 = u_0(x,x) = \frac{1}{\sigma(s)}$  and  $b_1 = \partial_y u_0(x,x) \stackrel{(5.1.14)}{=} \frac{1}{\sigma(s)} \left( -\frac{3}{2} \frac{s\sigma'(s)}{\sigma(s)} + \frac{r}{\sigma^2(s)} - \frac{1}{2} \right)$ . A direct application of Theorem 5.5.1 then gives that as  $\tau \to 0^+$ ,

$$\int_0^\infty f_X\left(\tau, x - z | x\right) \mathrm{d}y = \frac{1}{2} + \left(\frac{s\sigma'(s)}{2} - \frac{r}{\sigma(s)} + \frac{\sigma(s)}{2}\right) \frac{\sqrt{\tau}}{\sqrt{2\pi}} + \mathcal{O}\left(\tau\right).$$

We then conclude using that  $e^{-r\tau} = 1 + \mathcal{O}(\tau)$  and reintegrating the asymptotic in  $\tau$ .

*Remark* 18. The proof of Proposition 5.2.3 is postponed to Section 5.5.4.

Proof of Theorem 5.2.4. By definition,

$$p(\tau, e^x) = rK \int_0^\tau e^{-ru} \mathbb{E}_{0,x} \left[ \mathbf{1}_{X_u \le \overline{x}(\tau-u)} \right] \mathrm{d}u = rK \int_0^\tau e^{-ru} \int_{-\infty}^{\overline{x}(\tau-u)} f_X(u, y | x) \,\mathrm{d}y \mathrm{d}u$$

Taking the derivative w.r.t.  $\tau$  gives:

$$\partial_{\tau} p\left(\tau, e^{x}\right) = r K e^{-r\tau} \mathbb{E}_{0,x} \left[\mathbf{1}_{X_{u} \le \ln K}\right] \mathrm{d}u + I\left(\tau\right) = \partial_{\tau} \overline{p}\left(\tau, e^{x}\right) + I\left(\tau\right),$$

where  $I(\tau) := rK \int_0^{\tau} e^{-ru} f_X(u, \overline{x}(\tau - u) | x) \overline{x}'(\tau - u) du$  and  $\overline{p}(\tau, e^x)$  refers to the American upper premium (see (5.1.19)). Reintegrating in  $\tau$  and using  $p(0, e^x) = \overline{p}(0, e^x) = 0$  (since both American and European put price match at maturity) lead to the identity:

$$p(\tau, e^x) = \overline{p}(\tau, e^x) + \int_0^\tau I(u) \,\mathrm{d}u.$$

Hence we only need the asymptotic expansion of  $I(\tau)$  as  $\tau \to 0^+$ . Introducing the new variable  $v = 1 - \frac{u}{\tau} \iff u = \tau (1 - v)$  and owing to Lemma 5.1.1,  $I(\tau)$  rewrites as:

$$I(\tau) = rK\tau \int_{0}^{1} e^{-r(1-v)\tau} f_X((1-v)\tau, \overline{x}(v\tau)|x) \overline{x}'(v\tau) dv$$
  
=  $\frac{rK\sqrt{\tau}}{\sqrt{2\pi}} \int_{0}^{1} \frac{1}{\sqrt{1-v}} \{u_0(x, \overline{x}(v\tau)) + \mathcal{O}((1-v)\tau)\} e^{-\frac{d^2(\overline{x}(v\tau),x)}{2(1-v)\tau}} \overline{x}'(v\tau) dv$ 

where we have used that  $e^{-r(1-v)\tau} = 1 + \mathcal{O}((1-v)\tau)$ . Using (5.5.13), (5.5.15), (5.5.17), we then get

$$I(\tau) = -\frac{re^x \sqrt{l(\tau)}}{2\sqrt{2\pi}} \int_0^1 g(v) e^{-f(v)l(\tau)} \left(1 - \frac{h(v)}{l(\tau)} + \mathcal{O}\left(\frac{\Psi(v)}{l^2(\tau)}\right)\right) dv$$

,

with

$$g(v) := \frac{e^{\frac{v}{2(1-v)}\ln(v)}}{\sqrt{v(1-v)}}, \ h(v) := 1 + \frac{1}{2}\ln(v) + \frac{v}{1-v}, \ f(v) := \frac{v}{2(1-v)}$$
$$\Psi(v) := \frac{v^2}{(1-v)^2} + \frac{v\left|\ln(v)\right|}{1-v} + \left|1 - \frac{\ln(v)^2}{8}\right| + \left|1 + \frac{\ln(v)}{2}\right| \frac{v}{1-v}.$$

As  $v \to 0^+$ ,

$$g(v) \sim \frac{1}{\sqrt{v}} + (\ln(v) + 1)\frac{\sqrt{v}}{2} + (\ln^2(v) + 6\ln(v) + 3)\frac{v\sqrt{v}}{8}$$
$$h(v) \sim 1 + \frac{1}{2}\ln(v) + v + v^2 + v^3.$$

$$e^{-f(v)l(\tau)} \sim e^{-\frac{v}{2}l(\tau) - \frac{v^2}{2}l(\tau) - \frac{v^3}{2}l(\tau) - \frac{v^4}{2}l(\tau)}$$
$$\sim e^{-\frac{v}{2}l(\tau)} \left(1 - \frac{v^2}{2}l(\tau) - \frac{v^3}{2}l(\tau) + \frac{1}{8}(-4l(\tau) + l^2(\tau))v^4\right).$$

And we obtain (thanks to Mathematica) that, as  $\tau \to 0^+$ ,  $I(\tau)$  is asymptotic to:

$$C_{0} + C_{1} \frac{1}{l(\tau)} + C_{2} \frac{\ln^{2} (l(\tau))}{l(\tau)^{2}} + C_{3} \frac{\ln (l(\tau))}{l(\tau)^{2}} + C_{4} \frac{1}{l(\tau)^{2}},$$

where

$$C_0 = -\frac{rs}{2}, \quad C_1 = \frac{rs}{2}, \quad C_2 = -\frac{rs}{16}, \quad C_3 = -\frac{rs}{8}(2+a+\ln 2),$$

$$C_4 = -\frac{rs}{32} \left( -16 + \pi^2 + 2\ln^2(2) + 2\gamma \left(4 + a + 2\ln 2\right) + 8\ln 2 \right),$$

and a is Euler–Mascheroni constant. Now, integrating from 0 to  $\tau$  and introducing  $t=\frac{u}{\gamma}$  we have:

$$\int_0^\tau \frac{\mathrm{d}u}{l\left(u\right)} = \int_0^\tau \frac{\mathrm{d}u}{\ln\left(\frac{\gamma}{u}\right)} = -\gamma \int_0^{\frac{\tau}{\gamma}} \frac{\mathrm{d}t}{\ln\left(t\right)} \underset{\tau \to 0^+}{\sim} \frac{\tau}{l\left(\tau\right)},$$

where we have used (5.5.20) with n = 1. Owing to (5.5.21) and (5.5.22), a similar analysis gives:

$$\int_{0}^{\tau} I(u) \, \mathrm{d}u \sim_{\tau \to 0^{+}} \tau \left( C_{0} + C_{1} \frac{1}{l(\tau)} + C_{2} \frac{\ln^{2}(l(\tau))}{l(\tau)^{2}} + C_{3} \frac{\ln(l(\tau))}{l(\tau)^{2}} + (C_{1} + C_{4}) \frac{1}{l(\tau)^{2}} \right).$$

We conclude using the expansion of  $\overline{p}(\tau, s)$  in Proposition 5.2.2.

#### 5.5.4 Proofs of Section 5.2.2

Proof of Proposition 5.2.6. We proceed as in the proof of Proposition 5.2.1. Introducing  $z = \ln K - y$  and recalling s > K i.e.  $x > \ln K$  and from Lemma 5.1.1, we have:

$$P(\tau, e^{x}, K) = \frac{Ke^{-r\tau}}{\sqrt{2\pi\tau}} \int_{0}^{\infty} \left(1 - e^{-z}\right) \left(u_{0}(x, \ln K - z) + u_{1}(x, \ln K - z)\tau + \mathcal{O}(\tau^{2})\right) e^{-\frac{d^{2}(\ln K - z, x)}{2\tau}} dz.$$

The only difference here is that the function f is now  $f(z) = \frac{d^2(\ln K - z, x)}{2}$  and as  $z \to 0^+$ ,

$$f(z) = f(0) + a_0 z + a_1 z^2 + \mathcal{O}(z^3),$$

with

$$f(0) = \frac{d^2(\ln K, x)}{2}, \quad a_0 = \frac{d(\ln K, x)}{\sigma(K)}, \quad a_1 = \frac{1 + Kd(\ln K, x)\sigma'(K)}{2\sigma(K)^2}$$

Note that for the ATM case, we had  $a_0 = \frac{d(\ln K, x)}{\sigma(K)} = 0$ . A direct application of Theorem 5.5.1 then gives the desired asymptotic.

*Proof of Proposition 5.2.7.* The upper premium is equal to:

$$\overline{p}(\tau, e^x, K) = re^x \int_0^\tau e^{-ru} \left( \int_0^\infty f_X(u, \ln K - z | x) \, \mathrm{d}z \right) \mathrm{d}u.$$

Taking the derivative w.r.t.  $\tau$  gives:

$$\partial_{\tau}\overline{p}\left(\tau, e^{x}, K\right) = re^{x-r\tau} \int_{0}^{\infty} f_{X}\left(\tau, \ln K - z | x\right) \mathrm{d}z.$$

Proceeding exactly as in the proof of Proposition 5.2.2, we get by application of Theorem 5.5.1 that as  $\tau \to 0^+$ ,

$$\overline{p}(\tau, e^x, K) = \frac{u_0(x, \ln K) \sigma(K) rK}{\mathrm{d}(\ln K, x) \sqrt{2\pi}} \int_0^\tau \sqrt{u} \exp\left[-\frac{\mathrm{d}^2(\ln K, x)}{2u}\right] \mathrm{d}u$$
$$= \frac{u_0(x, \ln K) \tau^{\frac{3}{2}} \sigma(K) rK}{\mathrm{d}(\ln K, x) \sqrt{2\pi}} \int_0^1 \sqrt{v} \exp\left[-\frac{\mathrm{d}^2(\ln K, x)}{2\tau v}\right] \mathrm{d}v.$$

Introducing the new variable  $y^2 = \frac{d^2(\ln K, x)}{2\tau v}$  such that  $dv = -d^2(\ln K, x) y^{-3} dy$ , a direct computation yields:

$$\int_{0}^{1} \sqrt{v} \exp\left[-\frac{\mathrm{d}^{2}\left(\ln K, x\right)}{2\tau v}\right] \mathrm{d}v = \frac{\sqrt{2\pi} \mathrm{d}^{3}\left(\ln K, x\right) \operatorname{Erfc}\left(\frac{\mathrm{d}(\ln K, x)}{\sqrt{2\tau}}\right)}{3\tau^{\frac{3}{2}}} + \frac{2e^{-\frac{\mathrm{d}^{2}(\ln K, x)}{2\tau}}\left(\tau - \mathrm{d}^{2}\left(\ln K, x\right)\right)}{3\tau}$$

Since  $\frac{d(\ln K,x)}{\sqrt{2\tau}} \xrightarrow[\tau \to 0^+]{\infty}$ , by application of (5.1.5) we get

$$\operatorname{Erfc}\left[\frac{\mathrm{d}\left(\ln K,x\right)}{\sqrt{2\tau}}\right] = \sqrt{\tau}\sqrt{\frac{2}{\pi}}e^{-\frac{\mathrm{d}\left(\ln K,x\right)^{2}}{2\tau}}\left(\frac{1}{\mathrm{d}\left(\ln K,x\right)} - \frac{\tau}{\mathrm{d}\left(\ln K,x\right)^{3}} + \frac{3\tau^{2}}{\mathrm{d}\left(\ln K,x\right)^{5}} + \mathcal{O}\left(\tau^{3}\right)\right).$$

Finally, as  $\tau \to 0^+$ ,

$$\int_{0}^{1} \sqrt{v} \exp\left[-\frac{\mathrm{d}^{2}\left(\ln K, x\right)}{2\tau v}\right] \mathrm{d}v = \frac{2\tau}{\mathrm{d}^{2}\left(\ln K, x\right)} \exp\left[-\frac{\mathrm{d}^{2}\left(\ln K, x\right)}{2\tau}\right] \left(1 + \mathcal{O}\left(\tau\right)\right),$$

and we infer the desired asymptotic for the upper premium.

Proof of Propositions 5.2.3 and 5.2.8. Suppose that  $x \ge \ln K$ . By definition (see (5.1.19)),

$$\underline{p}(\tau, e^x, K) = rK \int_0^\tau e^{-ru} \mathbb{E}_{0,x} \left[ \mathbf{1}_{X_u \le \overline{x}(\tau)} \right] \mathrm{d}u = rK \int_0^\tau e^{-ru} \left( \int_{-\infty}^{\overline{x}(\tau)} f_X(u, y | x) \, \mathrm{d}y \right) \mathrm{d}u.$$

Introducing the new variables  $v = \frac{u}{\tau}$ ,  $z = \overline{x}(\tau) - y$  and by application of Lemma 5.1.1, the upper premium rewrites as:

$$\underline{p}(\tau, e^x, K) = rK\tau \int_0^1 e^{-r\tau v} I(\tau, v) \,\mathrm{d}v,$$

where we have defined for every  $v \in (0, 1), \tau \in (0, \infty)$ ,

$$I(\tau, v) = \int_0^\infty u_0\left(x, \overline{x}(\tau) - z\right) \frac{e^{-\frac{\mathrm{d}^2(\overline{x}(\tau) - z, x)}{2\tau v}}}{\sqrt{2\pi\tau v}} \mathrm{d}z + \mathcal{O}\left(\tau v\right) \int_0^\infty \frac{e^{-\frac{\mathrm{d}^2(\overline{x}(\tau) - z, x)}{2\tau v}}}{\sqrt{2\pi\tau v}} \mathrm{d}z.$$

Proceeding as in Lemma 5.5.5, we easily get that:

$$\int_{0}^{\infty} e^{-\frac{\mathrm{d}^{2}(\overline{x}(\tau)-z,x)}{2\tau v}} \mathrm{d}z = \frac{\tau v \sigma\left(e^{\overline{x}(\tau)}\right)}{\mathrm{d}\left(\overline{x}\left(\tau\right),x\right)} e^{-\frac{\mathrm{d}^{2}(\overline{x}(\tau),x)}{2\tau v}} \left(1 + \mathcal{O}\left(\tau v\right)\right),$$

and invoking Lemma 5.5.5, we deduce:

$$I(\tau, v) = \frac{u_0(x, \ln K) \sigma\left(e^{\overline{x}(\tau)}\right) \sqrt{\tau v} e^{-\frac{d^2(\overline{x}(\tau), x)}{2\tau v}}}{d(\overline{x}(\tau), x) \sqrt{2\pi}} \left(1 + \mathcal{O}(\tau v)\right)$$

Going back to  $p(\tau, e^x, K)$ , it holds:

$$\underline{p}\left(\tau, e^{x}, K\right) = \frac{rK\tau u_{0}\left(x, \ln K\right)\sigma\left(e^{\overline{x}(\tau)}\right)}{\mathrm{d}\left(\overline{x}\left(\tau\right), x\right)\sqrt{2\pi}} \int_{0}^{1} \sqrt{\tau v} e^{-\frac{\mathrm{d}^{2}\left(\overline{x}(\tau), x\right)}{2\tau v}} \left(1 + \mathcal{O}\left(\tau v\right)\right) \mathrm{d}v$$
$$\underset{\tau \to 0^{+}}{\sim} \frac{rKu_{0}\left(x, \ln K\right)\sigma\left(K\right)}{\mathrm{d}\left(\overline{x}\left(\tau\right), x\right)\sqrt{2\pi}} \int_{0}^{\tau} \sqrt{u} e^{-\frac{\mathrm{d}^{2}\left(\overline{x}(\tau), x\right)}{2u}} \mathrm{d}u,$$

using that  $e^{-rv\tau} \sim 1 + \mathcal{O}(\tau v)$ ,  $\overline{x}(\tau) \sim \ln K$  as  $\tau \to 0^+$  and where we have introduced the new variable  $u = \tau v$ .

If  $x = \ln K$ , from (5.5.10) and (5.5.7), we obtain:

$$\underline{p}\left(\tau, e^{x}, K\right) \underset{\tau \to 0^{+}}{\sim} 2 \frac{rK}{\sqrt{\gamma 2\pi}} \frac{\tau^{\frac{3}{2}}}{l^{\frac{3}{2}}\left(\tau\right)},$$

and we get the desired asymptotic recalling that  $\gamma = \frac{\sigma^2(K)}{8\pi r^2}$ . Proposition 5.2.3 is now proved. If  $x > \ln K$ , a direct computation gives:

$$\begin{split} \int_{0}^{\tau} \sqrt{u} \exp\left[-\frac{\mathrm{d}^{2}\left(\overline{x}\left(\tau\right),x\right)}{2u}\right] \mathrm{d}u \\ &= \frac{1}{3} \left(\sqrt{2\pi} \mathrm{d}^{3}(\overline{x}\left(\tau\right),x) \mathrm{Erfc}\left(\frac{\mathrm{d}(\overline{x}\left(\tau\right),x)}{\sqrt{2\tau}}\right) + 2\sqrt{\tau} e^{-\frac{\mathrm{d}(\overline{x}\left(\tau\right),x)}{2\tau}}\left(\tau - \mathrm{d}^{2}(\overline{x}\left(\tau\right),x)\right)\right) \right) \\ & \sim \\ & \sim \\ & \sim \\ & \tau \to 0^{+} \frac{2\tau^{\frac{5}{2}}}{\mathrm{d}^{2}\left(\ln K,x\right)} e^{-\frac{\mathrm{d}^{2}(\overline{x}\left(\tau\right),x)}{2\tau}}, \end{split}$$

using (5.1.5) and  $d(\overline{x}(\tau), x) \to d(\ln K, x)$  as  $\tau \to 0^+$ , and this concludes the proof.

Proof of Proposition 5.2.9. Suppose  $x > \ln K$  and denote  $C = \sqrt{\frac{2}{\pi}} \frac{rKu_0(\ln s, \ln K)\sigma(K)}{d^3(\ln K, x)}$ . By definition, the following identity holds for the American premium,

$$\tau \ln\left(\frac{\underline{p}\left(\tau, s, K\right)}{C\tau^{\frac{5}{2}}}\right) \le \tau \ln\left(\frac{p\left(\tau, s, K\right)}{C\tau^{\frac{5}{2}}}\right) \le \tau \ln\left(\frac{\overline{p}\left(\tau, s, K\right)}{C\tau^{\frac{5}{2}}}\right).$$
(5.5.26)

From Proposition 5.2.7, we know that  $p(\tau, s, K) = C\tau^{\frac{5}{2}}e^{-\frac{d^2(\ln K, x)}{2\tau}}(1 + \mathcal{O}(\tau))$ , and consequently for the r.h.s. of (5.5.26):

$$\tau \ln\left(\frac{\overline{p}\left(\tau, s, K\right)}{C\tau^{\frac{5}{2}}}\right) = -\frac{\mathrm{d}^{2}\left(\ln K, \ln s\right)}{2} + \ln\left(1 + \mathcal{O}\left(\tau\right)\right) \xrightarrow[\tau \to 0^{+}]{} - \frac{\mathrm{d}^{2}\left(\ln K, \ln s\right)}{2}.$$

Similarly for the l.h.s. of (5.5.26) (evoking this time Proposition 5.2.8), we get

$$\tau \ln\left(\frac{\underline{p}\left(\tau, s, K\right)}{C\tau^{\frac{5}{2}}}\right) = -\frac{\mathrm{d}^{2}\left(\overline{x}\left(\tau\right), \ln s\right)}{2} + \ln\left(1 + \mathcal{O}\left(\tau\right)\right) \xrightarrow[\tau \to 0^{+}]{} - \frac{\mathrm{d}^{2}\left(\ln K, \ln s\right)}{2}.$$

Hence, it holds for the premium

$$\frac{2\tau}{\mathrm{d}^2\left(\ln K,x\right)}\ln\left(\frac{C\tau^{\frac{5}{2}}}{p\left(\tau,s,K\right)}\right)\xrightarrow[\tau\to 0^+]{}1,$$

and we obtain the desired limit using that  $\tau \ln \left(\tau^{\frac{5}{2}}\right) \xrightarrow[\tau \to 0^+]{} 0$ . The proof being similar for the ITM case i.e.  $x < \ln K$ , we skip details.

Proof of Theorem 5.2.10. Recall first that we have:

$$p(\tau, e^x, K) = \frac{rK}{\sqrt{2\pi}} \sqrt{\tau} \int_0^1 \frac{e^{-r\tau v}}{\sqrt{v}} \left(1 + \mathcal{O}(\tau v)\right) \left\{ \int_{-\infty}^{\overline{x}(\tau(1-v))} u_0(x, y) \exp\left[-\frac{\mathrm{d}^2(x, y)}{2\tau v}\right] \mathrm{d}y \right\} \mathrm{d}v.$$

Since  $x > \ln K \Leftrightarrow s > K$ , we have  $\forall v \in (0, 1), \overline{x} (\tau (1 - v)) < \ln K < x$ . Thus the leading term of the integral in y is determined by the values of the integrand near the point  $y = \overline{x} (\tau (1 - v))$  as  $y \to d^2 (x, y)$  has its minimum attained at y = x. Hence introducing  $z = y - \overline{x} (\tau (1 - v))$ , we have:

$$\begin{split} \int_{-\infty}^{\overline{x}(\tau(1-v))} u_0\left(x,y\right) \exp\left[-\frac{\mathrm{d}^2\left(x,y\right)}{2\tau v}\right] \mathrm{d}y \\ &= \int_{-\infty}^{0} u_0\left(x,z+\overline{x}\left(\tau\left(1-v\right)\right)\right) \exp\left[-\frac{\mathrm{d}^2\left(z+\overline{x}\left(\tau\left(1-v\right)\right),x\right)}{2\tau v}\right] \mathrm{d}z \\ &\sim \\ &\sim \\ &\sim \\ & \tau \to 0^+ \frac{u_0\left(x,\ln K\right)\tau v\sigma\left(e^{\overline{x}((1-v)\tau)}\right)}{\mathrm{d}\left(\overline{x}\left((1-v)\tau\right),x\right)} \exp\left[-\frac{\mathrm{d}^2\left(\overline{x}\left(\tau\left(1-v\right)\right),x\right)}{2\tau v}\right], \end{split}$$

using the same ideas of Lemma 5.5.5. Thus we have for the premium,

$$p(\tau, e^x, K) \underset{\tau \to 0^+}{\sim} \frac{r K u_0(x, \ln K) \sigma(K) \tau^{\frac{3}{2}}}{\sqrt{2\pi} \mathrm{d}(\ln K, x)} \int_0^1 \sqrt{v} \exp\left[-\frac{\mathrm{d}^2\left(\overline{x}\left(\tau\left(1-v\right)\right), x\right)}{2\tau v}\right] \mathrm{d}v.$$

Let us introduce,

$$I(\tau) := \int_0^1 \sqrt{v} \exp\left[-\frac{\mathrm{d}^2\left(\overline{x}\left(\tau\left(1-v\right)\right), x\right)}{2\tau v}\right] \mathrm{d}v = \int_0^1 \sqrt{1-u} \exp\left[-\frac{\mathrm{d}^2\left(\overline{x}\left(\tau u\right), x\right)}{2\tau\left(1-u\right)}\right] \mathrm{d}u.$$

For every  $\tau > 0$ , let  $\varphi_{\tau} : u \in [0,1] \to \frac{d^2(\overline{x}(\tau u),x)}{2\tau(1-u)}$  which is a non-decreasing function (product of two non-decreasing functions) such that  $\varphi_{\tau}(0) = \frac{d^2(\ln K,x)}{2\tau}$  and  $\varphi_{\tau}(u) \xrightarrow[u \to 1^-]{} \infty$ . Whence denoting d for d (ln K, x), we can rewrite I as:

$$I(\tau) = e^{-\frac{d^2}{2\tau}} \int_0^1 \sqrt{1-u} e^{-(\varphi_{\tau}(u) - \varphi_{\tau}(0))} du.$$

From (5.5.18) along with

$$d^{2} (\overline{x} (\tau u), x) - d^{2} = d^{2} (\overline{x} (\tau u), \ln K) + 2d \times d (\overline{x} (\tau u), \ln K)$$
$$\sim_{\tau \to 0^{+}} 2d \times d (\overline{x} (\tau u), \ln K)$$

and observing that the main contribution is around u = 0, we infer that

$$e^{\frac{d^2}{2\tau}}I(\tau) \underset{\tau \to 0^+}{\sim} \int_0^1 e^{\frac{2d\sqrt{u\tau l(\tau)}}{2\tau(1-u)}du} \\ \underset{\tau \to 0^+}{\sim} \int_0^1 e^{\frac{d\sqrt{ul(\tau)}}{\sqrt{\tau}}du} \\ = \frac{\tau}{d^2l(\tau)} \int_0^{d^2\sqrt{\frac{l(\tau)}{\tau}}} e^{-\sqrt{s}}ds \\ \underset{\tau \to 0^+}{\sim} \frac{\tau}{d^2l(\tau)} \int_0^\infty e^{-\sqrt{s}}ds \\ = \frac{2\tau}{d^2l(\tau)}.$$

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#### 5.5.5 Proofs of Section 5.3

*Proof of Proposition 5.3.1.* We mimic the proof of [71, Theorem 2.4] and look for an implied volatility expansion of the form:

$$\sigma_{\rm E}(\tau) = \sigma_0 + \sigma_1 \tau + \sigma_2 \tau^2 + \mathcal{O}(\tau^3),$$

where we omit the dependence on both variables s, K in the coefficients  $(\sigma_i)_{i=1,2,3}$ . In [71, Theorem 2.4], only  $\sigma_0$  and  $\sigma_1$  were given though a more general approach (see [71, Section 3]), based on Yoshida's heat kernel expansion (see Yosida [170]), was proposed to derive an implied volatility expansion of the form  $\sigma_{\rm E}(\tau) \sim \sum_{i=0}^{n} \sigma_i \tau^i$  with  $n \in \mathbb{N}$ . Suppose that  $x > \ln K$  and set

$$\rho = x - \ln K > 0, \ d = d \left( \ln K, \ln s \right) > 0, \ u_0 \left( x, \ln K \right) = u_0,$$

such that:

$$\exp\left[-\frac{\left(x-\ln K\right)^2}{2\tau\sigma_{\rm E}^2\left(\tau\right)}\right] = \exp\left[-\frac{\rho^2}{2\tau\sigma_0^2} + \frac{\rho^2\sigma_1}{\sigma_0^3} + \frac{\rho^2\left(-3\sigma_1^2 + 2\sigma_0\sigma_2\right)}{2\sigma_0^4}\tau + \mathcal{O}\left(\tau^2\right)\right]$$

$$= \exp\left[-\frac{\rho^2}{2\tau\sigma_0^2} + \frac{\rho^2\sigma_1}{\sigma_0^3}\right] \left(1 + \rho^2\left(\frac{-3\sigma_1^2}{2\sigma_0^4} + \frac{\sigma_2}{\sigma_0^3}\right)\tau + \mathcal{O}\left(\tau^2\right)\right).$$

Similarly:

$$\begin{split} \sigma_{\rm E}^3\left(\tau\right) \exp\left[-\frac{r\rho}{\sigma_{\rm E}^2\left(\tau\right)}\right] &= \left(\sigma_0^3 + 3\sigma_0^2\sigma_1\tau + \mathcal{O}\left(\tau^2\right)\right) \exp\left[-\frac{r\rho}{\sigma_0^2}\right] \left(1 + \frac{2r\rho\sigma_1}{\sigma_0^3}\tau + \mathcal{O}\left(\tau^2\right)\right) \\ &= \sigma_0^3 \exp\left[-\frac{r\rho}{\sigma_0^2}\right] \left(1 + \frac{\left(2r\rho + 3\sigma_0^2\right)\sigma_1}{\sigma_0^3}\tau + \mathcal{O}\left(\tau^2\right)\right). \end{split}$$

And also:

$$\left(-\frac{2r}{\rho} - \frac{3\sigma_{\rm E}^2\left(\tau\right)}{\rho^2} - \frac{r^2}{2\sigma_{\rm E}^2\left(\tau\right)} - \frac{r}{2} - \frac{\sigma_{\rm E}^2\left(\tau\right)}{8}\right)\tau = \left(-\frac{2r}{\rho} - \frac{r}{2} - \frac{\sigma_0^2}{8} - \frac{3\sigma_0^2}{\rho^2} - \frac{r^2}{2\sigma_0^2}\right)\tau + \mathcal{O}\left(\tau^2\right).$$

0

Hence, we obtain (see (5.2.6)),

$$\begin{split} P_{\rm BS}\left(\tau, s, K, \sigma_{\rm E}\left(\tau\right)\right) &= e^{-\frac{\rho^2}{2\tau\sigma_{\rm E}^2(\tau)}} \frac{K\sigma_{\rm E}^3\left(\tau\right)\tau^{\frac{3}{2}}e^{\frac{\rho}{2}-\frac{r\rho}{\sigma_{\rm E}^2(\tau)}}}{\sqrt{2\pi}\rho^2} \\ &\qquad \times \left(1 + \left(-\frac{2r}{\rho} - \frac{3\sigma_{\rm E}^2\left(\tau\right)}{\rho^2} - \frac{r^2}{2\sigma_{\rm E}^2\left(\tau\right)} - \frac{r}{2} - \frac{\sigma_{\rm E}^2\left(\tau\right)}{8}\right)\tau + \mathcal{O}\left(\tau^2\right)\right) \\ &= \frac{\tau^{\frac{3}{2}}K\sigma_0^3 e^{-\frac{\rho^2}{2\tau\sigma_0^2}}e^{\frac{\rho}{2}-\frac{r\rho}{\sigma_0^2} + \frac{\rho^2\sigma_1}{\sigma_0^3}}}{\sqrt{2\pi}\rho^2} \times \left(1 + \left[\rho^2\left(\frac{-3\sigma_1^2}{2\sigma_0^4} + \frac{\sigma_2}{\sigma_0^3}\right)\right. \right. \right. \\ &\qquad + \frac{\left(2r\rho + 3\sigma_0^2\right)\sigma_1}{\sigma_0^3} - \frac{2r}{\rho} - \frac{r}{2} - \frac{\sigma_0^2}{8} - \frac{3\sigma_0^2}{\rho^2} - \frac{r^2}{2\sigma_0^2}\right]\tau + \mathcal{O}\left(\tau^2\right)\right). \end{split}$$

From (5.2.6), recall also that

$$P(\tau, s, K) = \frac{\tau^{\frac{3}{2}} K u_0 \sigma(K)^2}{\sqrt{2\pi} d^2} e^{-\frac{d^2}{2\tau}} \left( 1 + \left( \frac{u_1(x, \ln K)}{u_0(x, \ln K)} - r - \frac{2r}{\sigma(K) d} - \frac{3}{d^2} \right) \tau + \mathcal{O}\left(\tau^2\right) \right).$$

Whence, by comparing both the exponential factors  $e^{-\frac{d^2}{2\tau}}$  and  $e^{-\frac{\rho^2}{2\tau\sigma_0^2}}$ , we have first for  $\sigma_0$ :

$$\sigma_0 = \frac{\rho}{d} = (\ln s - \ln K) \times \left(\int_K^s \frac{\mathrm{d}u}{u\sigma(u)}\right)^{-1}.$$

Similarly, we get for  $\sigma_1$ :

$$\sigma_1 = \frac{\sigma_0^3}{\rho^2} \ln\left(\frac{u_0 \sigma \left(K\right)^2}{\sigma_0}\right) - \frac{\sigma_0^3}{2\rho} + \frac{r\sigma_0}{\rho}$$

Looking now at the factors of order  $\tau$ , we obtain that  $\sigma_2$  is solution of:

$$\rho^{2} \left( \frac{-3\sigma_{1}^{2}}{2\sigma_{0}^{4}} + \frac{\sigma_{2}}{\sigma_{0}^{3}} \right) + \frac{\left(2r\rho + 3\sigma_{0}^{2}\right)\sigma_{1}}{\sigma_{0}^{3}} - \frac{2r}{\rho} - \frac{r}{2} - \frac{\sigma_{0}^{2}}{8} - \frac{3\sigma_{0}^{2}}{\rho^{2}} - \frac{r^{2}}{2\sigma_{0}^{2}} = \frac{u_{1}\left(x, \ln K\right)}{u_{0}\left(x, \ln K\right)} - r - \frac{2r}{\sigma\left(K\right)d} - \frac{3\sigma_{0}^{2}}{d^{2}} + \frac{3\sigma_{0}^{2}}{\sigma_{0}^{2}} + \frac{3\sigma_{0}^{2}}{\sigma_{$$

After some simplification, we have:

$$\sigma_2 = \frac{\sigma_0^3 u_1(x, \ln K)}{\rho^2 u_0(x, \ln K)} + \frac{\sigma_0^5}{8\rho^2} - \frac{3\sigma_0^2 \sigma_1}{\rho^2} + \frac{3\sigma_1^2}{2\sigma_0} + r\left(-\frac{\sigma_0^3}{2\rho^2} - \frac{2\sigma_0^4}{\rho^3 \sigma(K)} + \frac{2\sigma_0^3}{\rho^3} + \frac{r\sigma_0}{2\rho^2} - \frac{2\sigma_1}{\rho}\right).$$

We now deal with the limits. Let s = K + h with h > 0. The second-order Taylor expansion in h gives first:

$$\sigma_0 \left( K + h, K \right) = \frac{\ln \left( K + h \right) - \ln \left( K \right)}{\int_{\ln(K)}^{\ln(K+h)} \frac{\mathrm{d}u}{\sigma(e^u)}}$$

$$= \sigma(K) + \frac{1}{2}\sigma'(K)h + \left(-\frac{\sigma'(K)}{12K} - \frac{\sigma'(K)^2}{12\sigma(K)} + \frac{\sigma''(K)}{6}\right)h^2 + \mathcal{O}(h^3),$$

and we infer that

$$\sigma_0\left(K+h,K\right) \xrightarrow[h \to 0]{} \sigma_0\left(K\right) = \sigma\left(K\right).$$

Similarly:

$$\begin{aligned} \sigma_{1}\left(s,K\right) &= \frac{\sigma_{0}^{3}\left(s,K\right)}{\ln\left(\frac{s}{K}\right)^{2}} \ln\left(\frac{\sigma\left(s\right)^{\frac{1}{2}}\sigma\left(K\right)^{\frac{1}{2}}}{\sigma_{0}\left(s,K\right)} \exp\left[\frac{\ln\left(\frac{s}{K}\right)}{2} + r\int_{\ln s}^{\ln K} \frac{\mathrm{d}u}{\sigma^{2}\left(e^{u}\right)}\right]\right) - \frac{\sigma_{0}^{3}\left(s,K\right)}{2\ln\left(\frac{s}{K}\right)} + \frac{r\sigma_{0}\left(s,K\right)}{\ln\left(\frac{s}{K}\right)} \\ &= \frac{\sigma_{0}^{3}\left(s,K\right)}{\ln\left(\frac{s}{K}\right)^{2}} \ln\left(\frac{\sigma\left(s\right)^{\frac{1}{2}}\sigma\left(K\right)^{\frac{1}{2}}}{\sigma_{0}\left(s,K\right)}\right) + r\left(\frac{\sigma_{0}\left(s,K\right)}{\ln\left(\frac{s}{K}\right)} - \frac{\sigma_{0}^{3}\left(s,K\right)}{\ln\left(\frac{s}{K}\right)^{2}}\int_{\ln K}^{\ln s} \frac{\mathrm{d}u}{\sigma^{2}\left(e^{u}\right)}\right). \end{aligned}$$

After some simplification, we have:

$$\sigma_1\left(K+h,K\right) = \frac{K\sigma\left(K\right)}{24} \left(-K\sigma'\left(K\right)^2 + 2\sigma\left(K\right)\left(\sigma'\left(K\right) + K\sigma''\left(K\right)\right)\right) + \mathcal{O}\left(h\right) \xrightarrow[h \to 0]{} \sigma_1\left(K\right).$$

The proof being similar for  $\sigma_2(s, K)$ , we skip details.

Proof of Proposition 5.3.2. We proceed as in the proof of Proposition 5.3.1 and look for an expansion of the form  $\sigma_{\rm E}(\tau,s) = \sigma_0 + \sigma_1 \tau + \mathcal{O}(\tau^2)$ . Using Proposition 5.2.1, we then have:

$$\frac{s\sigma\left(s\right)}{\sqrt{2\pi}} + \left[\frac{s}{\sqrt{2\pi}} \frac{12r^2 - \sigma(s)^2 \left(12r - 2s^2\sigma(s)\sigma''(s) + (\sigma(s) - s\sigma'(s))^2\right)}{24\sigma(s)}\right]\tau + \mathcal{O}\left(\tau^2\right)$$
$$= \frac{s\sigma_{\rm E}\left(\tau,s\right)}{\sqrt{2\pi}} + \left[\frac{s}{2\sqrt{2\pi}} \left(\frac{r^2}{\sigma_{\rm E}\left(\tau,s\right)} - r\sigma_{\rm E}\left(\tau,s\right) - \frac{\sigma_{\rm E}\left(\tau,s\right)^3}{12}\right)\right]\tau + \mathcal{O}\left(\tau^2\right).$$

Letting  $\tau \to 0^+$ , we see that  $\sigma_0 = \sigma(s)$ . Similarly, we get for  $\sigma_1$  (after some simplification):

$$\sigma_1 = \frac{s\sigma_0}{12} \left( s\sigma_0 \sigma^{''}(s) + \sigma_0 \sigma^{'}(s) - \frac{s\left(\sigma^{'}(s)\right)^2}{2} \right).$$

Proof of Proposition 5.3.3. We only deal with the upper American implied volatility  $\overline{\sigma}_{A}(\tau, s, K)$  expansion for s > K, the proofs being similar for the other cases. Suppose s > K and note that from the equality

$$\overline{A}\left(\tau,s,K\right) = A_{\mathrm{BS}}\left(\tau,s,K;\overline{\sigma}_{\mathrm{A}}\left(\tau,s,K\right)\right),$$

we see that the first two terms will be the same as for the European implied volatility expansion i.e.

$$\overline{\sigma}_{\mathrm{A}}\left(\tau,s,K\right)=\sigma_{0}\left(s,K\right)+\sigma_{1}\left(s,K\right)\tau\left(1+o\left(1\right)\right).$$

For the second term, let  $\overline{\sigma}_{A}(\tau, s, K) = \sigma_{0}(s, K) + \sigma_{1}(s, K)\tau + \overline{\sigma}_{2}^{AM}(s, K)\tau^{2}(1 + o(1))$ . Proceeding as in the proof of Proposition 5.3.1 gives (omitting the dependence in s, K):

$$\rho^2 \left( \frac{-3\sigma_1^2}{2\sigma_0^4} + \frac{\overline{\sigma}_2^{\text{AM}}}{\sigma_0^3} \right) + \frac{\left(2r\rho + 3\sigma_0^2\right)\sigma_1}{\sigma_0^3} - \frac{2r}{\rho} - \frac{r}{2} - \frac{\sigma_0^2}{8} - \frac{3\sigma_0^2}{\rho^2} - \frac{r^2}{2\sigma_0^2} = \frac{u_1\left(x,\ln K\right)}{u_0\left(x,\ln K\right)} - r - \frac{3}{d^2}.$$

Whence we get that  $\overline{\sigma}_{2}^{\text{AM}}(s, K) = \sigma_{2}(s, K) - \frac{2\sigma_{0}^{4}r}{\rho^{3}\sigma(K)}$ .

Proof of Theorem 5.3.4. We only prove the ATM case i.e. s = K, the OTM case being similar. We look for an asymptotic expansion

$$\sigma_{\mathcal{A}}(\tau, s) = \sigma_0 + \sigma_1 \tau + \eta(s, \tau), \quad \eta(s, \tau) \xrightarrow{\tau \to 0} 0.$$

From the equality  $A(\tau, s) = A_{BS}(\tau, s, \sigma_A(\tau, s))$  along with Corollary 5.2.5, and following the same strategy as in the proof of Proposition 5.3.2, the following identity holds

$$p_0\left(s\right)\frac{\tau}{\ln\left(\frac{\sigma(s)^2}{8\pi r^2\tau}\right)}\left(1+o\left(1\right)\right) = \frac{s\eta\left(s,\tau\right)}{\sqrt{2\pi}} + p_0\left(s\right)\frac{\tau}{\ln\left(\frac{\sigma_{\rm A}(\tau,s)^2}{8\pi r^2\tau}\right)}$$

Whence, this provides only an error term of order  $\mathcal{O}(\frac{\tau}{l(\tau)})$  for the difference between the American and the European implied volatility.

## CHAPTER 6

# WEAK APPROXIMATIONS AND VIX OPTION PRICES EXPANSIONS IN ROUGH FORWARD VARIANCES MODELS

Note. Working paper with Stefano De Marco and Emmanuel Gobet.

Abstract. We provide approximation formulas for VIX derivatives in forward variance models, with particular emphasis on the family of so-called Bergomi models: the rough Bergomi model of Bayer, Friz, and Gatheral [18], and an enhanced version that is able to generate realistic positive skew for VIX smiles – introduced simultaneously by De Marco [52] and Guyon [95] mimicking the ideas of Bergomi [28], that we refer to as "mixed rough Bergomi model". Following the methodology of Gobet and Miri [85], we derive weak approximations for the VIX random variable, leading to option price approximations under the form of explicit combinations of Black–Scholes prices and greeks. We stress that our approach does not rely on small-time asymptotics and can, therefore, be applied to any option maturity. Our results are illustrated by several numerical experiments and calibrations to VIX market data.

## 6.1 Introduction

Since the recent work from Gatheral, Jaisson, and Rosenbaum [72], rough fractional stochastic volatility (RFSV) models – in which the log-volatility is modeled as a fractional Brownian motion (see Mandelbrot and Van Ness [137]) with Hurst parameter H less than  $\frac{1}{2}$  instead of a standard Brownian motion as it is usually assumed in traditional stochastic volatility models – are generating much attention in the financial community. From recent high-frequency data, the authors in [72] statistically demonstrated that for any realistic time scale, the logarithm of realized variance essentially behaves as a fractional Brownian motion with  $H \approx 0.1$ . Starting from the fractional stochastic volatility model of Comte and Renault [49], they showed that RFSV models were able to reproduce extremely well stylized-facts of financial markets. Later, Bayer, Friz, and Gatheral [18] examined a simple example of RFSV models, namely the rough Bergomi model – a non-Markovian generalization of the variance curve model of Bergomi [27] – for the pricing of both the underlying and integrated variance. They showed that the rough Bergomi model outperforms conventional Markovian stochastic volatility models, and requires only three parameters for an efficient and reliable calibration of the S&P500 smile.

From its non-Markovian nature or its lack of affine structure, the pricing of options under RFSV models remains a delicate challenge. As PDE-based schemes or Fourier transform techniques cannot be used, Monte Carlo methods, though computationally intensive, have been proposed in Bennedsen, Lunde, and Pakkanen [23], Horvath, Jacquier, and Muguruza [111], Mc-Crickerd and Pakkanen [138], Horvath, Jacquier, and Tankov [112]. A new promising hierarchical approach, that combines adaptive sparse grids and quasi-Monte Carlo techniques, has also been recently introduced by Bayer, Ben Hammouda, and Tempone [19].

In this work, we bypass any time-consuming schemes and rather examine analytical approximation methods. More precisely, we focus on the pricing of VIX derivatives in the (plain and mixed) rough Bergomi model, though our methodology could be extended to a vast range of rough forward variance models.

The literature on weak approximations techniques applied to finance-related problems is vast and we refer to the introduction of Gobet and Miri [85] for a detailed discussion on the different approaches. For many works, the main motivation was the study of Asian options which is linked to the average in time of a stock process (see Kemna and Vorst [124], Geman and Yor [73], Lapeyre and Temam [130], Foschi, Pagliarani, and Pascucci [67], Cai, Li, and Shi [41], Pirjol and Zhu [148]), and is very close in spirit to the pricing of VIX derivatives (see also 2 for a detailed discussion).

In [83], Gobet and Miri derived expansion results for the weak approximation of the average of the marginal of diffusion processes. Following a similar approach, we express the VIX index as a combination of lognormal random variables (see also the moment-matching method of Turnbull and Wakeman [158]). This enables us to provide VIX calls, puts, and futures expansion formulas as a combination of a Black–Scholes price (zeroth-order or proxy's approximation) along with Black–Scholes Greeks (correction terms) – see Theorem 6.2.6. We illustrate our resulting formulas with many numerical tests, and we show that they provide satisfactory results (less than 2% in relative error) for a wide range of model parameters (in the rough Bergomi) such as the Hurst parameter H, the integration time interval  $\Delta$  or yet the vol-of-vol  $\eta$  (see Section 6.2.6).

The paper is organized as follows. In Section 6.3, we start our analysis with the plain rough Bergomi model and derive expansion results for VIX calls, puts, and futures. In Section 6.3, in order to cope with the inconsistent VIX smile generated by the plain rough Bergomi model, we introduce its mixed one-factor extension and provide similar expansion formulas, and numerically show that they can be used for a fast and efficient calibration of the market VIX smile.

#### Notations and special functions.

• Throughout the paper we make extensive use of the following integral (see Gradshteyn and Ryzhik [92, 3.197.8]):

$$\int_{0}^{u} x^{\nu-1} (x+\alpha)^{\lambda} (u-x)^{\mu-1} dx$$
  
=  $B_{\mu,\nu} \alpha^{\lambda} u^{\mu+\nu-1} {}_{2}F_{1} \left(-\lambda, \nu, \mu+\nu, -\frac{u}{\alpha}\right), \qquad (\mu, \nu > 0, u, \alpha, \lambda \in \mathbb{R}), \quad (6.1.1)$ 

where  $_2F_1$  denotes the hypergeometric function (see e.g. [146]).

### 6.2 Lognormal forward variance models

#### 6.2.1 The rough Bergomi model

We refer to Section 0.1.4 for a detailed discussion on rough forward variance models. In the rough Bergomi model (see Bayer, Friz, and Gatheral [18]), the instantaneous forward variance

 $(\xi_t^{\alpha})_{\alpha > t}$  solves the following SDE:

$$d\xi_t^{\alpha} = \xi_t^{\alpha} K^{\alpha}(t) \, dW_t, \quad \text{for all } \alpha \ge t, \tag{6.2.1}$$

or equivalently the instantaneous log-forward variance  $X_t^{\alpha} := \ln(\xi_t^{\alpha})$  solves

$$dX_t^{\alpha} = -\frac{1}{2} K^{\alpha} (t)^2 dt + K^{\alpha} (t) dW_t, \qquad (6.2.2)$$

where the kernel  $K^{\cdot}(\cdot)$  is given for  $t \in [0, \alpha)$ ,

$$K^{\alpha}(t) = \eta \left(\alpha - t\right)^{H - \frac{1}{2}},$$
(6.2.3)

where  $\eta > 0$  and  $H \in (0,1)$  is the so-called Hurst parameter. Let us fix  $T, \Delta > 0$ . We want to price an option on the

$$\operatorname{VIX}_{T}^{2} := \frac{1}{\Delta} \int_{T}^{T+\Delta} \xi_{T}^{\alpha} \mathrm{d}\alpha = \frac{1}{\Delta} \int_{T}^{T+\Delta} e^{X_{T}^{\alpha}} \mathrm{d}\alpha, \qquad (6.2.4)$$

with payoff  $\varphi$  and whose price at time 0 is given by

$$p_0 = \mathbb{E}\left[\varphi\left(\mathrm{VIX}_T^2\right)\right] = \mathbb{E}\left[\varphi\left(\frac{1}{\Delta}\int_T^{T+\Delta} e^{X_0^\alpha - \frac{1}{2}\int_0^T K^\alpha(t)^2 \mathrm{d}t + \int_0^T K^\alpha(t)\mathrm{d}W_t}\mathrm{d}\alpha\right)\right].$$
(6.2.5)

We stress that the  $VIX_T^2$  is an integral over a family lognormal random variables whose distribution is not explicit.

The time horizon  $\Delta$  is taken to be 30 days i.e.  $\Delta = \frac{1}{12}$ . Denote  $\mathcal{A} = [T, T + \Delta]$  and introduce the following integral operators for the arithmetic mean

$$\nu(X_T^{\cdot}) := \int_{\mathcal{A}} X_T^{\alpha} \nu(\mathrm{d}\alpha), \quad \nu_0(X_T^{\cdot}) := \int_{\mathcal{A}} X_T^{\alpha} \nu_0(\mathrm{d}\alpha),$$

and the mean of exponentials

$$\nu^{\exp}\left(X_{T}^{\cdot}\right) := \int_{\mathcal{A}} e^{X_{T}^{\alpha}} \nu\left(\mathrm{d}\alpha\right), \quad \nu_{0}^{\exp}\left(X_{T}^{\cdot}\right) := \int_{\mathcal{A}} e^{X_{T}^{\alpha}} \nu_{0}\left(\mathrm{d}\alpha\right).$$

Note that when the market initial instantaneous forward variance  $\alpha \to \xi_0^{\alpha}$  is flat, we have  $\nu = \nu_0$ . We further consider the probability measures

$$\nu \left( \mathrm{d} \alpha \right) = \frac{\mathrm{d} \alpha}{\Delta}, \quad \nu_0 \left( \mathrm{d} \alpha \right) = \frac{e^{X_0^{\alpha}}}{\nu^{\mathrm{exp}} \left( X_0^{\cdot} \right)} \nu \left( \mathrm{d} \alpha \right),$$

and introduce the following centered auxiliary variable

$$Y_T^{\alpha} := X_T^{\alpha} - X_0^{\alpha} = -\frac{1}{2} \int_0^T K^{\alpha} (t)^2 dt + \int_0^T K^{\alpha} (t) dW_t.$$
 (6.2.6)

#### 6.2.2 Proxy for the mean of exponentials

Armed with the notations above, observe that the desired quantity, that is the mean of exponentials, writes as

$$\operatorname{VIX}_{T}^{2} = \nu^{\exp}\left(X_{T}^{\cdot}\right) = \int_{\mathcal{A}} e^{X_{T}^{\alpha}} \nu\left(\mathrm{d}\alpha\right)$$
$$= \nu^{\exp}\left(X_{0}^{\cdot}\right) \int_{\mathcal{A}} e^{X_{T}^{\alpha} - X_{0}^{\alpha}} \nu_{0}\left(\mathrm{d}\alpha\right)$$
$$= \nu^{\exp}\left(X_{0}^{\cdot}\right) \int_{\mathcal{A}} e^{Y_{T}^{\alpha}} \nu_{0}\left(\mathrm{d}\alpha\right)$$
$$= \nu^{\exp}\left(X_{0}^{\cdot}\right) \nu_{0}^{\exp}\left(Y_{T}^{\cdot}\right).$$
(6.2.7)

We approximate  $\nu^{\exp}(X_T)$  with the exponential of the arithmetic mean, that is

$$\nu^{\exp, \mathcal{P}}(X_T^{\cdot}) := \nu^{\exp}(X_0^{\cdot}) e^{\int_{\mathcal{A}} (X_T^{\alpha} - X_0^{\alpha}) \nu_0(\mathrm{d}\alpha)} = \nu^{\exp}(X_0^{\cdot}) e^{\nu_0(Y_T^{\cdot})}, \qquad (6.2.8)$$

where the subscript P stands for proxy. The connection between  $\nu^{\exp}(X_T)$  and  $\nu^{\exp,P}(X_T)$  is made through the parametrization (or interpolation) ( $\varepsilon \in [0,1]$ ),

$$I(\varepsilon) := \nu^{\exp}\left(X_{0}^{\cdot}\right) \int_{\mathcal{A}} e^{\nu_{0}\left(Y_{T}^{\cdot}\right) + \varepsilon\left(Y_{T}^{\alpha} - \nu_{0}\left(Y_{T}^{\cdot}\right)\right)} \nu_{0}\left(\mathrm{d}\alpha\right), \qquad (6.2.9)$$

for which  $I(1) = \nu^{\exp}(X_T)$  and  $I(0) = \nu^{\exp,P}(X_T)$ . As  $\varepsilon \to I(\varepsilon)$  is smooth almost surely, the *n*th derivative of  $I(\varepsilon)$  is given by:

$$I^{(n)}\left(\varepsilon\right) = \nu^{\exp}\left(X_{0}^{\cdot}\right) \int_{\mathcal{A}} \left(Y_{T}^{\alpha} - \nu_{0}\left(Y_{T}^{\cdot}\right)\right)^{n} e^{\nu_{0}\left(Y_{T}^{\cdot}\right) + \varepsilon\left(Y_{T}^{\alpha} - \nu_{0}\left(Y_{T}^{\cdot}\right)\right)} \nu_{0}\left(\mathrm{d}\alpha\right).$$

$$(6.2.10)$$

Note also that as

$$I^{(1)}(0) = \nu^{\exp}(X_{0}^{\cdot}) e^{\nu_{0}(Y_{T}^{\cdot})} \int_{\mathcal{A}} (Y_{T}^{\alpha} - \nu_{0}(Y_{T}^{\cdot})) \nu_{0}(\mathrm{d}\alpha) = 0,$$

a direct application of Taylor's theorem with integral remainder gives

$$\nu^{\exp}\left(X_{T}^{\cdot}\right) - \nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right) = I\left(1\right) - I\left(0\right) = \int_{0}^{1} \left(1 - \varepsilon\right) I^{(2)}\left(\varepsilon\right) \mathrm{d}\varepsilon.$$
(6.2.11)

Consequently as  $I^{(2)}(\varepsilon) \geq 0$ , we infer that  $\nu^{\exp}(X_T) \geq \nu^{\exp,P}(X_T)$ , and the zeroth-order approximation  $\nu^{\exp,P}(X_T)$  always underestimates the desired quantity  $\nu^{\exp}(X_T)$ . This motivates the need to add other correction terms to get a more precise approximation in the limit  $\Delta \to 0$ . Finally, let us mention that the chosen proxy is a lognormal random variable whose characteristics are given in the following proposition.

**Proposition 6.2.1.** The proxy  $\nu^{\exp, P}(X_T)$  is lognormal

$$\ln\left(\nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right)\right) \stackrel{d}{=} \mathcal{N}\left(\mu_{\mathrm{P}},\sigma_{\mathrm{P}}^{2}\right)$$

with mean and variance equal to

$$\mu_{\mathrm{P}} := \ln\left(\nu^{\mathrm{exp}}\left(X_{0}^{\cdot}\right)\right) - \frac{1}{2} \int_{0}^{T} \nu_{0}\left(K^{\cdot}\left(t\right)^{2}\right) \mathrm{d}t, \quad \sigma_{\mathrm{P}}^{2} := \int_{0}^{T} \nu_{0}\left(K^{\cdot}\left(t\right)\right)^{2} \mathrm{d}t.$$
(6.2.12)

Proof of Proposition 6.2.1. From (6.2.8), a direct computation gives

$$\ln\left(\nu^{\exp, \mathcal{P}}\left(X_{T}^{\cdot}\right)\right) - \ln\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)\right)$$
$$= -\frac{1}{2}\int_{\mathcal{A}}\left(\int_{0}^{T}K^{\alpha}\left(t\right)^{2}\mathrm{d}t\right)\nu_{0}\left(\mathrm{d}\alpha\right) + \int_{\mathcal{A}}\left(\int_{0}^{T}K^{\alpha}\left(t\right)\mathrm{d}W_{t}\right)\nu_{0}\left(\mathrm{d}\alpha\right).$$

Evoking Fubini's theorem (see [83, Lemma 1.1]) and using that  $\int_{\mathcal{A}} \left( \int_0^T K^{\alpha}(t)^2 dt \right) \nu_0(d\alpha) < \infty$ , we can interchange integrals for both terms at the r.h.s. of the equality, and the proxy's mean and variance follow.

#### 6.2.3 Error estimates

In this section, we provide some error estimates between the  $VIX_T^2$  and its proxy. Their proofs are postponed to Section 6.5. To derive error estimates for  $\nu$  instead of  $\nu_0$ , the following assumption will be in force throughout this section. Note that when the initial instantaneous forward variance is flat i.e.  $X_0^{\alpha} = X_0$  for all  $\alpha \in [T, T + \Delta]$ , then  $\nu = \nu_0$  and the assumption trivially holds.

 $H, \eta, T, p.$ 

Assumption  $\mathcal{A}$ . There exist positive constants  $C_1, C_2$  such that for every p > 0,

$$\left( \int_{\mathcal{A}} \left| \int_{0}^{T} \left[ K^{\alpha} \left( t \right)^{2} - \nu_{0} \left( K^{\cdot} \left( t \right)^{2} \right) \right] dt \right|^{p} \nu_{0} \left( d\alpha \right) \right)^{\frac{1}{p}} \leq C_{1} \left( \int_{\mathcal{A}} \left| \int_{0}^{T} \left[ K^{\alpha} \left( t \right)^{2} - \nu \left( K^{\cdot} \left( t \right)^{2} \right) \right] dt \right|^{p} \nu \left( d\alpha \right) \right)^{\frac{1}{p}},$$

$$\left( \int_{\mathcal{A}} \left| \int_{0}^{T} \left[ K^{\alpha} \left( t \right) - \nu_{0} \left( K^{\cdot} \left( t \right) \right) \right]^{2} dt \right|^{p} \nu_{0} \left( d\alpha \right) \right)^{\frac{1}{p}} \leq C_{2} \left( \int_{\mathcal{A}} \left| \int_{0}^{T} \left[ K^{\alpha} \left( t \right) - \nu \left( K^{\cdot} \left( t \right) \right) \right]^{2} dt \right|^{p} \nu \left( d\alpha \right) \right)^{\frac{1}{p}}.$$

**Proposition 6.2.2** (Estimate for the drift coefficient). For every p > 0,

$$\left( \int_{\mathcal{A}} \left| \int_{0}^{T} \left[ K^{\alpha} \left( t \right)^{2} - \nu \left( K^{\cdot} \left( t \right)^{2} \right) \right] dt \right|^{p} \nu \left( d\alpha \right) \right)^{\frac{1}{p}} = \eta^{2} \begin{cases} f_{\text{drift}} \left( H, p \right) \Delta^{2H} \left( 1 + \mathcal{O}_{\Delta \to 0} \left( \Delta^{1-2H} \right) \right) & \text{if } H \in \left( 0, \frac{1}{2} \right) \\ 0 & \text{if } H = \frac{1}{2} \\ \frac{T^{2H-1}}{2(1+p)^{\frac{1}{p}}} \Delta \left( 1 + \mathcal{O}_{\Delta \to 0} \left( \Delta^{2H-1} \right) \right) & \text{if } H \in \left( \frac{1}{2}, 1 \right) \end{cases}, \quad (6.2.13)$$

where  $f_{\text{drift}}(H,p) := \frac{\left(\int_{0}^{1} \left|1 - (2H+1)y^{2H}\right|^{p} \mathrm{d}y\right)^{\frac{1}{p}}}{2H(2H+1)} = \frac{1}{2H(2H+1)} \left(\frac{\mathrm{B}_{1,p+1}(2H)^{p+1} {}_{2}F_{1}\left(1 - \frac{1}{2H}, p+1, p+2, -2H\right) + \mathrm{B}_{p+1,\frac{1}{2H}}}{2H(2H+1)^{\frac{1}{2H}}}\right)^{\frac{1}{p}}.$ 

**Proposition 6.2.3** (Estimate for the diffusion coefficient). For every p > 0,

$$\left( \int_{\mathcal{A}} \left| \int_{0}^{T} \left[ K^{\alpha} \left( t \right) - \nu \left( K^{\cdot} \left( t \right) \right) \right]^{2} \mathrm{d}t \right|^{p} \nu \left( \mathrm{d}\alpha \right) \right)^{\frac{1}{p}}$$

$$= \eta^{2} \begin{cases} f_{\mathrm{diff}} \left( H, p \right) \Delta^{2H} \left( 1 + o\left( 1 \right) \right) & \text{if } H \in (0, 1) \setminus \left\{ \frac{1}{2} \right\} \\ 0 & \text{if } H = \frac{1}{2} \end{cases} ,$$

where  $f_{\text{diff}}(H,p) := \frac{1}{(H+\frac{1}{2})^2} \left( \int_{\alpha=0}^1 \left| \int_{s=0}^\infty \left( (1+s)^{H+\frac{1}{2}} - s^{H+\frac{1}{2}} - \left(H+\frac{1}{2}\right) (\alpha+s)^{H-\frac{1}{2}} \right)^2 \mathrm{d}s \right|^{-1} \mathrm{d}\alpha \right)^{\nu}$ . To illustrate Propositions 6.2.2 and 6.2.3, we plot in Figure 6.1 the log  $L_p$  errors for both the drift and diffusion coefficients (evaluated by numerical quadrature) together with their asymptotic expansions w.r.t.  $\ln(\Delta)$  for  $\Delta \in [10^{-4}, 10^{-3}]$  and consider different sets of parameters of



Figure 6.1 – Log-log plot of the drift and diffusion estimate (circle " $\circ$ ") and their asymptotic expansion (cross "+") for different sets of parameters.

**Proposition 6.2.4.** For any  $p, q \ge 1$ , there exists a positive constant  $C_{(6.2.14)}$  (depending only on p, q, T, H) such that

$$\int_{\mathcal{A}} \|Y_T^{\alpha} - \nu_0 (Y_T^{\cdot})\|_p^q \nu_0 (\mathrm{d}\alpha) \le C_{(6.2.14)} \eta^q \Delta^{qH}.$$
(6.2.14)

**Theorem 6.2.5.** For any  $p \ge 1, n \in \mathbb{N}, \varepsilon \in [0, 1]$ , there exists a constant  $C_{(6.2.15)}$  (depending only on  $p, T, H, \eta$ ) such that

$$\|I^{(n)}(\varepsilon)\|_{p} \leq C_{(6.2.15)}\nu^{\exp}(X_{0})\Delta^{nH},$$
 (6.2.15)

and as a direct consequence

$$\left\|\nu^{\exp}\left(X_{T}^{\cdot}\right) - \nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right)\right\|_{p} \leq C_{(6.2.15)}\nu^{\exp}\left(X_{0}^{\cdot}\right)\Delta^{2H}.$$
(6.2.16)

*Proof of Theorem 6.2.5.* Evoking (6.2.10) and by successive applications of the generalized Minkowski and Hölder inequality, we have

$$\begin{aligned} \frac{\left\|I^{(n)}\left(\varepsilon\right)\right\|_{p}}{\nu^{\exp}\left(X_{0}^{\cdot}\right)} &\leq \int_{\mathcal{A}} \left\|\left(Y_{T}^{\alpha}-\nu_{0}\left(Y_{T}^{\cdot}\right)\right)^{n}e^{\varepsilon\left(Y_{T}^{\alpha}-\nu_{0}\left(Y_{T}^{\cdot}\right)\right)+\nu_{0}\left(Y_{T}^{\cdot}\right)}\right\|_{p}\nu_{0}\left(\mathrm{d}\alpha\right) \\ &\leq \int_{\mathcal{A}} \left\|Y_{T}^{\alpha}-\nu_{0}\left(Y_{T}^{\cdot}\right)\right\|_{3np}^{n}\times\left\|e^{\varepsilon\left(Y_{T}^{\alpha}-\nu_{0}\left(Y_{T}^{\cdot}\right)\right)}\right\|_{3p}\times\left\|e^{\nu_{0}\left(Y_{T}^{\cdot}\right)}\right\|_{3p}\nu_{0}\left(\mathrm{d}\alpha\right) \\ &\leq \left\|e^{\nu_{0}\left(Y_{T}^{\cdot}\right)}\right\|_{3p}\times\left(\int_{\mathcal{A}} \left\|Y_{T}^{\alpha}-\nu_{0}\left(Y_{T}^{\cdot}\right)\right\|_{3np}^{2n}\nu_{0}\left(\mathrm{d}\alpha\right)\right)^{\frac{1}{2}}\times\left(\int_{\mathcal{A}} \left\|e^{\varepsilon\left(Y_{T}^{\alpha}-\nu_{0}\left(Y_{T}^{\cdot}\right)\right)}\right\|_{3p}^{2}\nu_{0}\left(\mathrm{d}\alpha\right)\right)^{\frac{1}{2}}.\end{aligned}$$

Evoking Fubini's theorem, a direct computation first gives that for any p > 0,

$$\mathbb{E}\left[e^{p\nu_{0}\left(Y_{T}^{\cdot}\right)}\right] = \mathbb{E}\left[e^{p\int_{\mathcal{A}}\left(-\frac{1}{2}\int_{0}^{T}K^{\alpha}(t)^{2}\mathrm{d}t + \int_{0}^{T}K^{\alpha}(t)\mathrm{d}W_{t}\right)\nu_{0}(\mathrm{d}\alpha)}\right]$$
$$= e^{-\frac{p}{2}\int_{0}^{T}\nu_{0}\left(K^{\cdot}(t)^{2}\right)\mathrm{d}t} \times \mathbb{E}\left[e^{p\int_{0}^{T}\nu_{0}\left(K^{\cdot}(t)\right)\mathrm{d}W_{t}}\right]$$
$$= e^{-\frac{p}{2}\int_{0}^{T}\nu_{0}\left(K^{\cdot}(t)^{2}\right)\mathrm{d}t}e^{\frac{p^{2}}{2}\int_{0}^{T}\left(\nu_{0}(K^{\cdot}(t))\right)^{2}\mathrm{d}t}$$
$$= e^{\frac{1}{2}\int_{0}^{T}\left[\left(p\nu_{0}(K^{\cdot}(t))\right)^{2} - \nu_{0}\left(pK^{\cdot}(t)^{2}\right)\right]\mathrm{d}t},$$

where we have used that  $p \int_0^T \nu_0 (K^{\cdot}(t)) dW_t \stackrel{d}{=} \mathcal{N}\left(0, p^2 \int_0^T \nu_0 (K^{\cdot}(t))^2 dt\right)$  and for every t,  $\mathbb{E}\left[e^{tN}\right] = e^{t\mu + \frac{(t\sigma)^2}{2}}$  where  $N \stackrel{d}{=} \mathcal{N}\left(\mu, \sigma^2\right)$ . Observe also that as  $\Delta \to 0$ ,  $\int_0^T \nu_0 (K^{\cdot}(t))^2 dt \to \int_0^T K^T(t)^2 dt = \eta^2 \frac{T^{2H}}{2H}$ , the following limit holds:

$$\mathbb{E}\left[e^{p\nu_0\left(Y_T^{\cdot}\right)}\right] \xrightarrow[\Delta \to 0]{} e^{\frac{p(p-1)}{2}\int_0^T K^T(t)^2 \mathrm{d}t} = e^{\frac{p(p-1)\eta^2 T^{2H}}{4H}},$$

and consequently,

$$\left\| e^{\nu_0\left(Y_T^{\cdot}\right)} \right\|_{3p} \xrightarrow{\Delta \to 0} e^{\frac{(3p-1)\eta^2 T^{2H}}{4H}}.$$

Second, we have similarly

$$\mathbb{E}\left[e^{p\varepsilon\left(Y_{T}^{\alpha}-\nu_{0}\left(Y_{T}^{\cdot}\right)\right)}\right] = e^{-\frac{p\varepsilon}{2}\int_{0}^{T}\left(K^{\alpha}(t)^{2}-\nu_{0}\left(K^{\cdot}(t)^{2}\right)\right)\mathrm{d}t} \times \mathbb{E}\left[e^{p\varepsilon\int_{0}^{T}\left(K^{\alpha}(t)-\nu_{0}(K^{\cdot}(t))\right)\mathrm{d}W_{t}}\right]$$
$$= e^{-\frac{p\varepsilon}{2}\int_{0}^{T}\left(K^{\alpha}(t)^{2}-\nu_{0}\left(K^{\cdot}(t)^{2}\right)\right)\mathrm{d}t}e^{\frac{p^{2}\varepsilon^{2}}{2}\int_{0}^{T}\left(K^{\alpha}(t)-\nu_{0}(K^{\cdot}(t))\right)^{2}\mathrm{d}t}$$
$$\leq e^{\frac{p}{2}\int_{0}^{T}\left|K^{\alpha}(t)^{2}-\nu_{0}\left(K^{\cdot}(t)^{2}\right)\right|\mathrm{d}t}e^{\frac{p^{2}}{2}\int_{0}^{T}\left|K^{\alpha}(t)-\nu_{0}(K^{\cdot}(t))\right|^{2}\mathrm{d}t} < \infty,$$

and consequently,

$$\begin{split} \left( \int_{\mathcal{A}} \left\| e^{\varepsilon \left(Y_T^{\alpha} - \nu_0\left(Y_T^{\cdot}\right)\right)} \right\|_{3p}^2 \nu_0\left(\mathrm{d}\alpha\right) \right)^{\frac{1}{2}} \\ & \leq \left( \int_{\mathcal{A}} e^{\int_0^T \left|K^{\alpha}(t)^2 - \nu_0\left(K^{\cdot}(t)^2\right)\right| \mathrm{d}t} e^{3p \int_0^T \left|K^{\alpha}(t) - \nu_0\left(K^{\cdot}(t)\right)\right|^2 \mathrm{d}t} \nu_0\left(\mathrm{d}\alpha\right) \right)^{\frac{1}{2}} \xrightarrow{\Delta \to 0} 1. \end{split}$$

Finally, evoking Proposition 6.2.4, we have the existence of a positive constant  $C_{p,q,T,H,\eta}$  such that

$$\left(\int_{\mathcal{A}} \|Y_T^{\alpha} - \nu_0\left(Y_T^{\cdot}\right)\|_{3np}^{2n} \nu_0\left(\mathrm{d}\alpha\right)\right)^{\frac{1}{2}} \leq C_{p,q,T,H,\eta} \Delta^{nH},$$

and we obtain the first estimate. For the second estimate, in view of (6.2.11) and applying the generalized Minkowski inequality, we obtain

$$\left\|\nu^{\exp}\left(X_{T}^{\cdot}\right)-\nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right)\right\|_{p} \leq \int_{0}^{1}\left(1-\varepsilon\right)\left\|I^{(2)}\left(\varepsilon\right)\right\|_{p} \mathrm{d}\varepsilon$$

and we conclude with the first estimate setting n = 2.

## 6.2.4 General price expansion

Before stating our main result, we introduce the following coefficients  $(\gamma_i)_{i=1,2,3}$ 

$$\begin{split} \gamma_{1} &:= \frac{1}{8} \int_{\mathcal{A}} \left( \int_{0}^{T} \left[ K^{\alpha} \left( t \right)^{2} - \nu_{0} \left( K^{\cdot} \left( t \right)^{2} \right) \right] \mathrm{d}t \right)^{2} \nu_{0} \left( \mathrm{d}\alpha \right) + \frac{1}{2} \int_{\mathcal{A}} \left( \int_{0}^{T} \left[ K^{\alpha} \left( t \right) - \nu_{0} \left( K^{\cdot} \left( t \right) \right) \right]^{2} \mathrm{d}t \right) \nu_{0} \left( \mathrm{d}\alpha \right), \\ \gamma_{2} &:= \int_{\mathcal{A}} \left( \int_{0}^{T} \nu_{0} \left( K^{\cdot} \left( t \right) \right) \left[ K^{\alpha} \left( t \right) - \nu_{0} \left( K^{\cdot} \left( t \right) \right) \right] \mathrm{d}t \right) \times \left( \int_{0}^{T} \left[ -\frac{1}{2} K^{\alpha} \left( t \right)^{2} + \frac{1}{2} \nu_{0} \left( K^{\cdot} \left( t \right)^{2} \right) \right] \mathrm{d}t \right) \nu_{0} \left( \mathrm{d}\alpha \right), \\ \gamma_{3} &:= \frac{1}{2} \int_{\mathcal{A}} \left( \int_{0}^{T} \nu_{0} \left( K^{\cdot} \left( t \right) \right) \left[ K^{\alpha} \left( t \right) - \nu_{0} \left( K^{\cdot} \left( t \right) \right) \right] \mathrm{d}t \right)^{2} \nu_{0} \left( \mathrm{d}\alpha \right). \end{split}$$

The effective computations of those coefficients are discussed later in Section 6.2.5. In some cases, we can rely on analytical closed-form expressions (see Proposition 6.2.9). Note that we can always apply numerical integration techniques to evaluate the multiple integrals though care should be taken because of the singularity of the kernel.

**Theorem 6.2.6** (Option price approximation). Let  $\varphi$  be a function three times continuously differentiable with bounded derivatives. The price at time 0 of an option on the VIX<sup>2</sup><sub>T</sub> with payoff  $\varphi$  equals

$$\mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{T}^{\cdot}\right)\right)\right] = \mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)e^{\nu_{0}\left(Y_{T}^{\cdot}\right)}\right)\right] + \sum_{i=1}^{3}\gamma_{i}\,\partial_{\varepsilon}^{i}\mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)e^{\nu_{0}\left(Y_{T}^{\cdot}\right)+\varepsilon}\right)\right]\Big|_{\varepsilon=0} + \mathscr{E}_{(6.2.17)},\quad(6.2.17)$$

where  $\mathscr{E}_{(6.2.17)}$  is an error term such that  $|\mathscr{E}_{(6.2.17)}| \leq C_{(6.2.17)}\Delta^{3H}$  for a positive constant  $C_{(6.2.17)}$  depending only on  $T, \eta, H, X_0^{\cdot}$ .

Proof of Theorem 6.2.6. Recall that  $X_T^{\alpha} = \ln(\xi_T^{\alpha}), Y_T^{\alpha} = X_T^{\alpha} - X_0^{\alpha}$  and

$$\mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{T}^{\cdot}\right)\right)\right] = \mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)\nu_{0}^{\exp}\left(Y_{T}^{\cdot}\right)\right)\right].$$

As  $\varphi$  is three times differentiable, applying a second-order Taylor's formula with integral remainder to  $\varphi$  at  $\nu^{\exp, P}(X_T)$  gives

$$\mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{T}^{\cdot}\right)\right)\right] = \mathbb{E}\left[\varphi\left(\nu^{\exp,P}\left(X_{T}^{\cdot}\right)\right)\right] + \mathbb{E}\left[\varphi^{'}\left(\nu^{\exp,P}\left(X_{T}^{\cdot}\right)\right)\left(\nu^{\exp}\left(X_{T}^{\cdot}\right) - \nu^{\exp,P}\left(X_{T}^{\cdot}\right)\right)\right] + E_{0}\left(\varphi^{''}\right), \quad (6.2.18)$$

where  $E_0\left(\varphi''\right)$  is an error term given by

$$E_0\left(\varphi''\right) := \int_0^1 (1-\lambda) \mathbb{E}\left[\varphi''\left(\lambda\nu^{\exp}\left(X_T\right) + (1-\lambda)\nu^{\exp,P}\left(X_T\right)\right)\left(\nu^{\exp}\left(X_T\right) - \nu^{\exp,P}\left(X_T\right)\right)^2\right].$$

From the parametrization (6.2.11), we have also

$$\nu^{\exp}(X_T^{\cdot}) - \nu^{\exp,P}(X_T^{\cdot}) = \frac{I^{(2)}(0)}{2} + \int_0^1 \frac{(1-\varepsilon)^2}{2} I^{(3)}(\varepsilon) \,\mathrm{d}\varepsilon$$
$$= \nu^{\exp,P}(X_T^{\cdot}) \left[ \frac{1}{2} \int_{\mathcal{A}} (Y_T^{\alpha} - \nu_0(Y_T^{\cdot}))^2 \nu_0(\mathrm{d}\alpha) \right] + \int_0^1 \frac{(1-\varepsilon)^2}{2} I^{(3)}(\varepsilon) \,\mathrm{d}\varepsilon.$$

Then, introducing the error term

$$E_1\left(\varphi'\right) := \mathbb{E}\left[\varphi'\left(\nu^{\exp, \mathcal{P}}\left(X_T^{\cdot}\right)\right) \int_0^1 \frac{(1-\varepsilon)^2}{2} I^{(3)}\left(\varepsilon\right) \mathrm{d}\varepsilon\right],$$

together with the new function

$$\Psi\left(x\right) := \varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)e^{x}\right),$$

we have

$$\nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right)\varphi^{'}\left(\nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right)\right) = \nu^{\exp}\left(X_{0}^{\cdot}\right)e^{\nu_{0}\left(Y_{T}^{\cdot}\right)}\varphi^{'}\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)e^{\nu_{0}\left(Y_{T}^{\cdot}\right)}\right)$$
$$= \Psi^{'}\left(\nu_{0}\left(Y_{T}^{\cdot}\right)\right),$$

and the second term rewrites as

$$\mathbb{E}\left[\varphi^{'}\left(\nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right)\right)\left(\nu^{\exp}\left(X_{T}^{\cdot}\right)-\nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right)\right)\right]$$
$$=\mathbb{E}\left[\Psi^{'}\left(\nu_{0}\left(Y_{T}^{\cdot}\right)\right)\int_{\mathcal{A}}\frac{1}{2}\left(Y_{T}^{\alpha}-\nu_{0}\left(Y_{T}^{\cdot}\right)\right)^{2}\nu_{0}\left(\mathrm{d}\alpha\right)\right]+E_{1}\left(\varphi^{'}\right).$$
(6.2.19)

Now recalling that

$$Y_T^{\alpha} - \nu_0 \left( Y_T^{\cdot} \right) = -\frac{1}{2} \int_0^T \left[ K^{\alpha} \left( t \right)^2 - \nu_0 \left( K^{\cdot} \left( t \right)^2 \right) \right] \mathrm{d}t + \int_0^T \left[ K^{\alpha} \left( t \right) - \nu_0 \left( K^{\cdot} \left( t \right) \right) \right] \mathrm{d}W_t,$$

a direct application of Itô's formula readily implies

$$\frac{1}{2} \left(Y_T^{\alpha} - \nu_0 \left(Y_T^{\cdot}\right)\right)^2 = \int_0^T \left[ \int_0^t \left( -\frac{1}{2} K^{\alpha} \left(s\right)^2 + \frac{1}{2} \nu_0 \left(K^{\cdot} \left(s\right)^2\right) \right) \mathrm{d}s + \left(K^{\alpha} \left(s\right) - \nu_0 \left(K^{\cdot} \left(s\right)\right)\right) \mathrm{d}W_s \right] \right] \\ \times \left( \left[ -\frac{1}{2} K^{\alpha} \left(t\right)^2 + \frac{1}{2} \nu_0 \left(K^{\cdot} \left(t\right)^2\right) \right] \mathrm{d}t + \left[K^{\alpha} \left(t\right) - \nu_0 \left(K^{\cdot} \left(t\right)\right)\right] \mathrm{d}W_t \right) \right] \\ + \int_0^T \frac{1}{2} \left[K^{\alpha} \left(t\right) - \nu_0 \left(K^{\cdot} \left(t\right)\right)\right]^2 \mathrm{d}t.$$

We now recall the following integration by parts formula for stochastic processes.

**Lemma 6.2.7** ([85, Lemma A.2.]). Let  $a_t, e_t, f_t, g_t, h_t : [0,T] \to \mathbb{R}$  be square-integrable and deterministic processes, and l a bounded smooth function with bounded derivatives. Then,

$$\mathbb{E}\left[l\left(\int_{0}^{T}a_{t}\mathrm{d}W_{t}\right)\left(\int_{0}^{T}\left[\int_{0}^{t}g_{s}\mathrm{d}s+h_{s}\mathrm{d}W_{s}\right]\left(e_{t}\mathrm{d}t+f_{t}\mathrm{d}W_{t}\right)\right)\right]$$
$$=\sum_{i=0}^{2}\lambda_{i}\partial_{\varepsilon}^{i}\mathbb{E}\left[l\left(\int_{0}^{T}a_{t}\mathrm{d}W_{t}+\varepsilon\right)\right]\Big|_{\varepsilon=0}$$

where

$$\lambda_0 = \int_0^T \int_0^t e_t g_s \mathrm{d}s \mathrm{d}t, \quad \lambda_1 = \int_0^T \int_0^t \left(g_s a_t f_t + e_t a_s h_s\right) \mathrm{d}s \mathrm{d}t, \quad \lambda_2 = \int_0^T \int_0^t a_t f_t a_s h_s \mathrm{d}s \mathrm{d}t.$$

Setting

$$l(x) = \Psi'\left(x - \frac{1}{2}\int_0^T \nu_0\left(K^{\cdot}(t)^2\right) dt\right), \quad a_t = \nu_0\left(K^{\cdot}(t)\right),$$
  
$$f_t = h_t = K^{\alpha}(t) - \nu_0\left(K^{\cdot}(t)\right), \quad e_t = g_t = -\frac{1}{2}K^{\alpha}(t)^2 + \frac{1}{2}\nu_0\left(K^{\cdot}(t)^2\right),$$

and by symmetry, we have

$$\mathbb{E}\left[\nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right)\varphi^{'}\left(\nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right)\right)\int_{\mathcal{A}}\frac{1}{2}\left(Y_{T}^{\alpha}-\nu_{0}\left(Y_{T}^{\cdot}\right)\right)^{2}\nu_{0}\left(\mathrm{d}\alpha\right)\right]$$
$$=\sum_{i=1}^{3}\gamma_{i}\,\partial_{\varepsilon}^{i}\mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)e^{\nu_{0}\left(Y_{T}^{\cdot}\right)+\varepsilon\right)\right]\Big|_{\varepsilon=0}.$$

All in all, we have shown that

$$\mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{T}^{\cdot}\right)\right)\right] = \mathbb{E}\left[\varphi\left(\nu^{\exp,P}\left(X_{T}^{\cdot}\right)\right)\right] + \sum_{i=1}^{3}\gamma_{i} \,\partial_{\varepsilon}^{i}\mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)e^{\nu_{0}\left(Y_{T}^{\cdot}\right)+\varepsilon}\right)\right]\Big|_{\varepsilon=0} \qquad (6.2.20)$$
$$+ E_{1}\left(\varphi'\right) + E_{0}\left(\varphi''\right).$$

For the error terms, using that  $\varphi'$  and  $\varphi''$  are bounded along with Theorem 6.2.5, we infer the existence of two positive independent constants  $C_1, C_2$  (depending only on  $p, q, T, H, \eta, X_0$ ) such that

$$\left|E_0\left(\varphi''\right)\right| \le C_2 \Delta^{4H}, \qquad \left|E_1\left(\varphi'\right)\right| \le C_1 \Delta^{3H},$$

and this concludes the proof.

#### 6.2.5 Flat initial instantaneous forward variance

In this subsection, we assume that the initial instantaneous forward variance is flat, that is for all  $\alpha \in [T, T + \Delta]$ ,  $X_0^{\alpha} = X_0$  and thus  $\nu_0 = \nu$ . Consequently, we will show that the proxy's characteristics, the coefficients  $(\gamma_i)_{i=1,2,3}$ , and the correction terms in Theorem 6.2.6 have closed-form expressions.

**Corollary 6.2.8** (Characteristics of the proxy  $\nu^{\exp,P}(X_T)$ ). The mean and variance reduce to

$$\mu_{\rm P} = X_0 - \frac{\eta^2 \left[ (T+\Delta)^{2H+1} - \Delta^{2H+1} - T^{2H+1} \right]}{4H \left( 2H+1 \right) \Delta},$$

$$\sigma_{\rm P}^2 = \frac{\eta^2}{\Delta^2 \left(H + \frac{1}{2}\right)^2} \left(\frac{(T+\Delta)^{2H+2} + T^{2H+2} - \Delta^{2H+2}}{2H+2} - 2B_{1,H+\frac{3}{2}} \Delta^{H+\frac{1}{2}} T^{H+\frac{3}{2}} {}_2F_1\left(-H - \frac{1}{2}, H + \frac{3}{2}, H + \frac{5}{2}, -\frac{T}{\Delta}\right)\right).$$

Proof of Corollary 6.2.8. From (6.2.12), we have for the mean:

$$\mu_{\rm P} = X_0 - \frac{\eta^2}{2\Delta} \int_{t=0}^T \left( \int_{\alpha=T}^{T+\Delta} (\alpha - t)^{2H-1} \,\mathrm{d}\alpha \right) \mathrm{d}t = X_0 - \frac{\eta^2 \left[ (T+\Delta)^{2H+1} - \Delta^{2H+1} - T^{2H+1} \right]}{4\Delta H \left( 2H+1 \right)}.$$

Similarly, for the variance:

$$\begin{split} \sigma_{\rm P}^2 &= \frac{\eta^2}{\Delta^2 \left(H + \frac{1}{2}\right)^2} \int_0^T \left( (t+\Delta)^{2H+1} + t^{2H+1} - 2 \left(t+\Delta\right)^{H+\frac{1}{2}} t^{H+\frac{1}{2}} \right) \mathrm{d}t \\ &= \frac{\eta^2}{\Delta^2 \left(H + \frac{1}{2}\right)^2} \left( \frac{(T+\Delta)^{2H+2} + T^{2H+2} - \Delta^{2H+2}}{2H+2} \right. \\ &- 2\mathrm{B}_{1,H+\frac{3}{2}} \Delta^{H+\frac{1}{2}} T^{H+\frac{3}{2}} {}_2F_1 \left( -H - \frac{1}{2}, H + \frac{3}{2}, H + \frac{5}{2}, -\frac{T}{\Delta} \right) \right). \end{split}$$

The coefficients  $(\gamma_i)_{i=1,2,3}$  can also be explicitly derived as follows (the proof is postponed to Section 6.5).

**Proposition 6.2.9.** The coefficients  $(\gamma_i)_{i=1,2,3}$  reduce to

$$\begin{split} \gamma_1 &= \frac{\eta^4}{32H^2} \Big[ \frac{\left(T+\Delta\right)^{4H+1} + \Delta^{4H+1} - T^{4H+1}}{\Delta \left(4H+1\right)} - \Big( \frac{T^{2H+1} + \Delta^{2H+1} - \left(T+\Delta\right)^{2H+1}}{\Delta \left(2H+1\right)} \Big)^2 \\ &- 2\mathbf{B}_{1,2H+1} \Delta^{2H} T^{2H} {}_2F_1 \left( -2H, 1+2H, 2(1+H), -\frac{\Delta}{T} \right) \Big] + \frac{\eta^2 \left( \left(T+\Delta\right)^{2H+1} - T^{2H+1} - \Delta^{2H+1} \right)}{4H \left(2H+1\right) \Delta} - \frac{\sigma_{\mathrm{P}}^2}{2}, \end{split}$$

and

$$\begin{split} \gamma_{2} &= -\frac{T\eta^{4}}{4\Delta\left(H + \frac{1}{2}\right)H} \int_{0}^{1} \int_{0}^{1} \left[ \left(Tt^{'} + \Delta\right)^{H + \frac{1}{2}} - \left(Tt^{'}\right)^{H + \frac{1}{2}} \right] \\ & \times \left[ \left(T + \alpha^{'}\Delta\right)^{2H} - \left(\alpha^{'}\Delta\right)^{2H} \right] \left(Tt^{'} + \alpha^{'}\Delta\right)^{H - \frac{1}{2}} dt^{'} d\alpha^{'} \\ & + \frac{\eta^{2}}{2} \frac{(T + \Delta)^{2H + 1} - T^{2H + 1} - \Delta^{2H + 1}}{\Delta 2H \left(2H + 1\right)} \sigma_{\mathrm{P}}^{2}, \end{split}$$

and

$$\gamma_{3} = \frac{\eta^{4} T^{2} T^{4H}}{2\Delta^{2} \left(H + \frac{1}{2}\right)^{2}} \int_{0}^{1} \int_{0}^{1} \left[ \left(t + \frac{T}{\Delta}\right)^{H + \frac{1}{2}} - t^{H + \frac{1}{2}} \right] \left(t + \alpha \frac{T}{\Delta}\right)^{H - \frac{1}{2}} \Omega\left(\alpha\right) dt d\alpha,$$

where

$$\begin{split} \Omega\left(\alpha\right) &= (1-\alpha)^{H+\frac{1}{2}} \Delta^{H+\frac{1}{2}} \mathbf{B}_{1,H+\frac{1}{2}} \left[ (1+\alpha\Delta)^{H+\frac{1}{2}} {}_{2}F_{1} \left( -H - \frac{1}{2}, H + \frac{1}{2}, H + \frac{3}{2}, -\frac{1+\alpha\Delta}{(1-\alpha)\Delta} \right) \right. \\ &+ (\alpha\Delta)^{H+\frac{1}{2}} {}_{2}F_{1} \left( -H - \frac{1}{2}, H + \frac{1}{2}, H + \frac{3}{2}, -\frac{\alpha\Delta}{(1-\alpha)\Delta} \right) \right] \\ &- \mathbf{B}_{1,H+\frac{3}{2}} \left( \alpha\delta \right)^{H-\frac{1}{2}} {}_{2}F_{1} \left( -H + \frac{1}{2}, H + \frac{3}{2}, H + \frac{5}{2}, -\frac{1}{\alpha\Delta} \right). \end{split}$$

We now provide our expansion formula for the price of options on the  $VIX_T^2$  assuming an initial flat instantaneous forward variance. It is expressed as a combination of a Black–Scholes price (zeroth-order correction) along with Black–Scholes Greeks (higher-order corrections) which are given by, for all  $x, y, \sigma > 0$ ,

$$C_{\rm BS}(x,y,\sigma) := \mathbb{E}_{Z \sim \mathcal{N}(0,1)} \left[ \left( x e^{-\frac{\sigma^2}{2} + \sigma Z} - y \right)_+ \right] = x \Phi \left( \frac{\ln\left(\frac{x}{y}\right)}{\sigma} + \frac{\sigma}{2} \right) - y \Phi \left( \frac{\ln\left(\frac{x}{y}\right)}{\sigma} - \frac{\sigma}{2} \right),$$

$$P_{\rm BS}(x,y,\sigma) := \mathbb{E}_{Z \sim \mathcal{N}(0,1)} \left[ \left( y - x e^{-\frac{\sigma^2}{2} + \sigma Z} \right)_+ \right] = y \Phi \left( -\frac{\ln\left(\frac{x}{y}\right)}{\sigma} + \frac{\sigma}{2} \right) - x \Phi \left( -\frac{\ln\left(\frac{x}{y}\right)}{\sigma} - \frac{\sigma}{2} \right),$$

$$\Delta_{\rm BS}^{\rm call}(x,y,\sigma) := \partial_x C_{\rm BS}(x,y,\sigma) = \Phi \left( \frac{\ln\left(\frac{x}{y}\right)}{\sigma} + \frac{\sigma}{2} \right),$$

$$\Delta_{\rm BS}^{\rm put}(x,y,\sigma) := \partial_x P_{\rm BS}(x,y,\sigma) = -\Phi \left( -\frac{\ln\left(\frac{x}{y}\right)}{\sigma} - \frac{\sigma}{2} \right) = \Delta_{\rm BS}^{\rm call}(x,y,\sigma) - 1,$$

$$\Gamma_{\rm BS}(x,y,\sigma) := \partial_x^2 C_{\rm BS}(x,y,\sigma) = \partial_x^2 P_{\rm BS}(x,y,\sigma) = \frac{\Phi' \left( \frac{\ln\left(\frac{x}{y}\right)}{\sigma} + \frac{\sigma}{2} \right)}{x\sigma},$$
Speed\_{\rm BS}(x,y,\sigma) := \partial\_x^3 C\_{\rm BS}(x,y,\sigma) = \partial\_x^3 P\_{\rm BS}(x,y,\sigma) = -\frac{\Gamma\_{\rm BS}(x,y,\sigma)}{x} \left( \frac{\ln\left(\frac{x}{y}\right)}{\sigma^2} + \frac{3}{2} \right).

*Remark* 19. Although Theorem 6.2.6 is stated for smooth payoffs, we conjecture it remains valid for any Hölder continuous exponentially growing payoffs (like in [83]), which can presumably be justified by the heavy use of Malliavin calculus taking advantage of the smoothing properties of the non-degenerate lognormal distribution  $\nu^{\exp, P}(X_T)$ .

**Corollary 6.2.10.** For an initial flat instantaneous forward variance  $\xi_0^{\alpha} = \xi_0$  for all  $\alpha \in [T, T + \Delta]$ , the prices at time t = 0 of a call, put with strike  $\kappa > 0$ , and future on the VIX<sub>T</sub><sup>2</sup> can be approximated by

$$\mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T}^{2}\right)\right] = \sum_{i=0}^{3} \gamma_{i} P_{i} + \mathscr{E}_{(6.2.21)}, \qquad (6.2.21)$$

with the convention  $\gamma_0 = 1$  and where  $\mathscr{E}_{(6.2.21)}$  is an error term of order 3H if the payoff  $\varphi$  is smooth (see Theorem 6.2.6 and Remark 19). More precisely, for a call option i.e.  $\varphi(x) = (\sqrt{x} - \kappa)_+$ ,

$$\begin{split} P_0^{\text{call}} &= C_{\text{BS}} \left( e^{\frac{\mu_{\text{P}}}{2} + \frac{\sigma_{\text{P}}^2}{8}}, \kappa, \frac{\sigma_{\text{P}}}{2} \right), \\ P_1^{\text{call}} &= \frac{1}{2} e^{\frac{\mu_{\text{P}}}{2} + \frac{\sigma_{\text{P}}^2}{8}} \Delta_{\text{BS}}^{\text{call}} \left( e^{\frac{\mu_{\text{P}}}{2} + \frac{\sigma_{\text{P}}^2}{8}}, \kappa, \frac{\sigma_{\text{P}}}{2} \right), \\ P_2^{\text{call}} &= \frac{P_1^{\text{call}}}{2} + \frac{e^{\mu_{\text{P}} + \frac{\sigma_{\text{P}}^2}{4}}}{4} \Gamma_{\text{BS}} \left( e^{\frac{\mu_{\text{P}}}{2} + \frac{\sigma_{\text{P}}^2}{8}}, \kappa, \frac{\sigma_{\text{P}}}{2} \right), \\ P_3^{\text{call}} &= -\frac{P_1^{\text{call}}}{2} + \frac{3P_2^{\text{call}}}{2} + \frac{1}{8} e^{\frac{3\mu_{\text{P}}}{2} + \frac{3\sigma_{\text{P}}^2}{8}} \text{Speed}_{\text{BS}} \left( e^{\frac{\mu_{\text{P}}}{2} + \frac{\sigma_{\text{P}}^2}{8}}, \kappa, \frac{\sigma_{\text{P}}}{2} \right). \end{split}$$

For a future i.e.  $\varphi(x) = \sqrt{x}$ ,

$$P_0^{\rm F} = e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}}, \quad P_i^{\rm F} = 2^{-i} P_0^{\rm F} \text{ for } i = 1, 2, 3.$$

For a put option i.e.  $\varphi(x) = (\kappa - \sqrt{x})_+$ ,

$$P_0^{\text{put}} = P_{\text{BS}}\left(e^{\frac{\mu_{\text{P}}}{2} + \frac{\sigma_{\text{P}}^2}{8}}, \kappa, \frac{\sigma_{\text{P}}}{2}\right) = P_0^{\text{call}} - P_0^{\text{F}} + \kappa,$$

$$\begin{split} P_1^{\text{put}} &= \frac{1}{2} e^{\frac{\mu_{\text{P}}}{2} + \frac{\sigma_{\text{P}}^2}{8}} \Delta_{\text{BS}}^{\text{put}} \left( e^{\frac{\mu_{\text{P}}}{2} + \frac{\sigma_{\text{P}}^2}{8}}, \kappa, \frac{\sigma_{\text{P}}}{2} \right) = P_1^{\text{call}} - P_1^{\text{F}}, \\ P_2^{\text{put}} &= \frac{P_1^{\text{put}}}{2} + \frac{e^{\mu_{\text{P}} + \frac{\sigma_{\text{P}}^2}{4}}}{4} \Gamma_{\text{BS}} \left( e^{\frac{\mu_{\text{P}}}{2} + \frac{\sigma_{\text{P}}^2}{8}}, \kappa, \frac{\sigma_{\text{P}}}{2} \right) = P_2^{\text{call}} - P_2^{\text{F}}, \\ P_3^{\text{put}} &= -\frac{P_1^{\text{put}}}{2} + \frac{3P_2^{\text{put}}}{2} + \frac{1}{8} e^{\frac{3\mu_{\text{P}}}{2} + \frac{3\sigma_{\text{P}}^2}{8}} \text{Speed}_{\text{BS}} \left( e^{\frac{\mu_{\text{P}}}{2} + \frac{\sigma_{\text{P}}^2}{8}}, \kappa, \frac{\sigma_{\text{P}}}{2} \right) = P_3^{\text{call}} - P_3^{\text{F}}. \end{split}$$

Consequently, the expansion formula satisfies the put-call parity, that is for all  $n \in \{0, 1, 2, 3\}$ ,

$$\sum_{i=0}^{3} \gamma_i \left( P_i^{\text{call}} - P_i^{\text{put}} \right) = \gamma_i \sum_{i=0}^{3} P_i^{\text{F}} - \kappa.$$

*Proof of Corollary* 6.2.10. We start with the call option. From Theorem 6.2.6 and Proposition 6.2.8 the first correction is given by

$$P_0^{\text{call}} = \mathbb{E}\left[\varphi\left(\nu^{\exp, \mathcal{P}}\left(X_T^{\cdot}\right)\right)\right] = \mathbb{E}_{Z \sim \mathcal{N}(0, 1)}\left[\left(e^{\frac{\mu_{\mathcal{P}}}{2} + \frac{\sigma_{\mathcal{P}}^2}{8}}e^{-\frac{\sigma_{\mathcal{P}}^2}{8} + \frac{\sigma_{\mathcal{P}}}{2}Z} - \kappa\right)_+\right] = C_{\text{BS}}\left(e^{\frac{\mu_{\mathcal{P}}}{2} + \frac{\sigma_{\mathcal{P}}^2}{8}}, \kappa, \frac{\sigma_{\mathcal{P}}}{2}\right).$$

Introducing the new function,

$$\Psi: \varepsilon \in (0,\infty) \to \mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)e^{\nu_{0}\left(Y_{T}^{\cdot}\right)+\varepsilon}\right)\right] = C_{\mathrm{BS}}\left(e^{\frac{\varepsilon}{2}+\frac{\mu_{\mathrm{P}}}{2}+\frac{\sigma_{\mathrm{P}}^{2}}{8}}, \kappa, \frac{\sigma_{\mathrm{P}}}{2}\right)$$

we have

$$\begin{split} \Psi'(0) &= \frac{1}{2} e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}} \Delta_{\rm BS} \left( e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}}, \kappa, \frac{\sigma_{\rm P}}{2} \right), \\ \Psi''(0) &= \frac{1}{4} e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}} \left[ \Delta_{\rm BS} \left( e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}}, \kappa, \frac{\sigma_{\rm P}}{2} \right) + e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}} \Gamma_{\rm BS} \left( e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}}, \kappa, \frac{\sigma_{\rm P}}{2} \right) \right] \\ &= \frac{\Psi'(0)}{2} + \frac{e^{\mu_{\rm P} + \frac{\sigma_{\rm P}^2}{4}}}{4} \Gamma_{\rm BS} \left( e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}}, \kappa, \frac{\sigma_{\rm P}}{2} \right), \\ \Psi^{(3)}(0) &= \frac{1}{8} e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}} \left[ \Delta_{\rm BS}^{\rm call} \left( e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}}, \kappa, \frac{\sigma_{\rm P}}{2} \right) + 3 e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}} \Gamma_{\rm BS} \left( e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}}, \kappa, \frac{\sigma_{\rm P}}{2} \right) \right) \\ &\quad + e^{\mu_{\rm P} + \frac{\sigma_{\rm P}^2}{4}} \operatorname{Speed}_{\rm BS} \left( e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}}, \kappa, \frac{\sigma_{\rm P}}{2} \right) \right] \\ &= -\frac{\Psi'(0)}{2} + \frac{3\Psi''(0)}{2} + \frac{1}{8} e^{\frac{3\mu_{\rm P}}{2} + \frac{3\sigma_{\rm P}^2}{8}} \operatorname{Speed}_{\rm BS} \left( e^{\frac{\mu_{\rm P}}{2} + \frac{\sigma_{\rm P}^2}{8}}, \kappa, \frac{\sigma_{\rm P}}{2} \right), \end{split}$$

hence the announced expansion for the call price. For a future, it suffices to set  $\kappa = 0$  in the correction terms for the call option. For a put option, proceed as before using the identity  $\Delta^{\text{put}}(x, y, \sigma) = -1 + \Delta^{\text{call}}(x, y, \sigma)$ . The put–call parity directly follows.

#### 6.2.6 Numerical tests

In this section, we test our approximation formulas for the future, call and put options on the VIX. We refer to Horvath, Jacquier, and Tankov [112, Section 3.2] and Chapter 2 for a detailed study of VIX options pricing by discretization and Monte Carlo simulation (in rough forward variance models). We quickly recall that in order to estimate quantities of the form

$$\mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T}^{2}\right)\right] = \mathbb{E}\left[\varphi\left(\frac{1}{\Delta}\int_{T}^{T+\Delta}e^{X_{T}^{\alpha}}\mathrm{d}\alpha\right)\right],$$

we choose to first discretize the integral and then run a Monte Carlo simulation. More precisely, we divide the interval  $[T, T + \Delta]$  into  $n \in \mathbb{N}^*$  steps i.e. we consider a discretization grid  $\mathcal{D}_n =$ 

 $\{t_0 = T + ih, i = 0, ..., n\}$  where  $h = \frac{\Delta}{n}$  is the (uniform) time-step. We then approximate the VIX<sub>T</sub><sup>2</sup> with the following right-point rectangle scheme (but any discretization scheme is possible):

$$\operatorname{VIX}_{T}^{2,\mathcal{R}_{n}} = \frac{1}{n} \sum_{i=1}^{n} e^{X_{T}^{t_{i}}}.$$
(6.2.22)

Notice that such procedure amounts to the computation of a functional over a family of correlated lognormal random variables. Indeed the random variables  $(X_T^{t_i})_{i=0,...n}$  forms a Gaussian random vector with mean  $\mu = (\mu(t_i))_{i=0,...n}$  (see (2.2.2)) where

$$\mu(t_i) = X_0^{\alpha} - \frac{\eta^2}{4H} \left( t_i^{2H} - (t_i - T)^{2H} \right),$$

and covariance  $C = (C(t_i, t_j))_{0 \le i,j \le n}$  (see (2.2.3)) where for i = j,

$$C(t_i, t_i) = \frac{\eta^2}{2H} \left( t_i^{2H} - (t_i - T)^{2H} \right),$$

while if i < j,

$$C(t_i, t_j) = \frac{\eta^2 (t_j - t_i)^{H - \frac{1}{2}}}{H + \frac{1}{2}} \left[ t_i^{2H} {}_2F_1 \left( \frac{1}{2} - H, \frac{1}{2} + H, \frac{3}{2} + H, -\frac{t_i}{t_j - t_i} \right) \right] - (t_i - T)^{2H} {}_2F_1 \left( \frac{1}{2} - H, \frac{1}{2} + H, \frac{3}{2} + H, -\frac{t_i - T}{t_j - t_i} \right) \right].$$

Remark 20 (Control variate (see Section 2.2.2)). Observing that

$$\mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T}^{2,\mathcal{R}_{n}}\right)\right] = \mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T}^{2,\mathcal{R}_{n}}\right) - \varphi\left(\nu^{\mathrm{exp},\mathrm{P}}\left(X_{T}^{\cdot}\right)\right)\right] + P_{0},$$

we naturally use our proxy as a control variate for the right-point rectangle scheme. This was already proposed by Horvath, Jacquier, and Tankov [112, Section 3.2.2] which is close in spirit to Kemna and Vorst's control variate trick for Asian options (see Kemna and Vorst [124]). This is exactly what motivated our approximation, namely approaching the integral over a family of lognormal random variables with the exponential of the integral of the associated family of normal random variables. It should be noted that in practice, we approximate options on the  $VIX_T^2$  with

$$\mathbb{E}\left[\varphi\left(\mathrm{VIX}_{T}^{2,\mathcal{R}_{n}}\right)\right] \approx \frac{1}{M}\left[\varphi\left(\frac{1}{n}\sum_{i=1}^{n}e^{X_{T}^{t_{i},m}}\right) - \varphi\left(e^{\frac{1}{n}\sum_{i=1}^{n}X_{T}^{t_{i},m}}\right)\right] + P_{0}^{n},$$

where M is the number of Monte Carlo samples,  $(X_T^{t_1,m}, \ldots, X_T^{t_n,m})_{1 \le m \le M}$  are independent copies of the Gaussian vector  $(X_T^{t_1}, \ldots, X_T^{t_n})$  and  $P_0^n$  corresponds to the zeroth-order approximation for which we replace the proxy's mean  $\mu_{\rm P}$  and standard deviation  $\sigma_{\rm P}$  with their right-point rectangle approximation in the variable  $\alpha$  (see (6.2.8)) i.e.  $\mu_{\rm P}^n$  and  $\sigma_{\rm P}^n$  (see (2.2.6))

In what follows, we consider VIX futures, calls, and puts with strike  $\kappa = 0.2$  with maturity 1,3, and 6 months i.e.  $T = \frac{1}{12}, \frac{3}{12}, \frac{6}{12}$ . The initial flat instantaneous forward variance is fixed at  $\xi_0 = 0.235^2$  so that  $X_0 = \ln(\xi_0) \approx -2.896$ . We choose  $M = 10^6$  Monte Carlo samples and n = 300 discretization points. We wish to compare our expansions w.r.t.  $\eta, \Delta$  and H. For every type of option, we plot the "true" price (computed with the right-point rectangle scheme (6.2.22) and a Monte Carlo simulation with its 95% confidence interval) along with the relative error (expressed in %) for the four approximations of Corollary 6.2.10 with the greek of order 0 (v0), the greeks of order 0, 1 (v1), the greeks of order 0, 1, 2 (v2), or the greeks of order 0, 1, 2, 3 (v3). To keep track of the error sign, the relative error is computed as  $\frac{\text{Rectangle Price} - \text{Approximation Price}}{\text{Rectangle Price}} \times 100$ . Note that from (6.2.11) and since  $x \to (\sqrt{x} - \kappa)_+$  (resp.  $x \to (\kappa - \sqrt{x})_+$ ) is nondecreasing (resp. nonincreasing) for all  $\kappa$ , we already know that the relative error for v0 is nonnegative (resp. nonpositive) for the call and future (resp. put).

#### Approximations w.r.t. $\eta$

In Figures 6.2 and 6.3, we set the Hurst parameter at H = 0.1,  $\Delta = \frac{1}{12}$  (1 month) and choose 10 evenly-spaced  $\eta$  ranging from 0.1 to 1.5. We observe that the smaller  $\eta$ , the more accurate is our expansion formulas. Even for high values of  $\eta$  (as it is observed in practice), our approximations are extremely accurate: less than 2% for the put option, -1% for the future, and negligible for the call option when focusing on v3. Further, when  $\eta$  tends to 0, we retrieve the expected order from worst (v0) to the finest (v3) approximation.



Figure 6.2 – VIX future price and relative error in % for the price expansion w.r.t.  $\eta$ .



1

0

-1

-2

-3

0.2



Figure 6.3 – VIX call and put prices and relative error in % for the price expansion w.r.t.  $\eta$ .

1.4

1.4

1.2

1.2

0.8

0.8

η

VIX Put 1M

1.0

η

1.0

#### Approximations w.r.t. $\Delta$

For both Figures 6.4 and 6.5, we set  $\eta = 1.0$ , H = 0.1 and choose 10 evenly-spaced  $\Delta$  ranging from 0.05 to 0.6. Even though  $\Delta = \frac{1}{12} \approx 0.083$  for the VIX, we want to check that as for  $\eta$ , the smaller the  $\Delta$ , the more accurate the approximation. Again, Figures 6.4 and 6.5 are self-explanatory and yield excellent results: less than -0.25% for the future, negligible for the call, and less than 2.5% for the put in terms of relative error.



Figure 6.4 – VIX future price and relative error in % for the price expansion w.r.t.  $\Delta$ .



Call on forward volatility approximation 3M





-8

0.1

0.2

0.3

Δ

0.4

0.5

0.6

Call on forward volatility approximation 1M 2 0 -<u>∓</u>- v0 -<u>+</u>- v1  $^{-1}$ -<u>+</u>- v3 -2 -3 0.1 0.2 0.3 0.4 0.5 0.6

Δ



Put on forward volatility approximation 1M

2 0 -2 -4 -<u>+</u>- v0 -<u>+</u>- v1 -6 -----v3 -8 -10 -12 0.1 0.2 0.3 0.4 0.5 0.6 Δ



Figure 6.5 – VIX call and put prices and relative error in % for the price expansion w.r.t.  $\Delta$ . To check the order  $\mathcal{O}(\Delta^{3H})$  for the error (see Theorem 6.2.5), we also plot the log absolute

error between the true price and our approximation formulas v0 (with the points ".") and v3 (with the crosses "+") keeping the same parameters but with  $\Delta \in [0.05, 0.2]$  for the VIX future.



Figure 6.6 – Absolute error between the VIX future and the approximations (v0 and v3) w.r.t.  $\Delta$  for T = 1 month (blue), 3 months (green), and 6 months (orange).

#### Approximations w.r.t. H

Finally, for both Figures 6.7 and 6.8, we set  $\eta = 1$ ,  $\Delta = \frac{1}{12}$ , and choose 10 evenly-spaced H ranging from 0.05 to 0.4. As the closer H is to 0 the more singular the kernel, we expect the relative error to be a decreasing function of the Hurst parameter H, and this is what is observed in both Figures 6.7 and 6.8.



Figure 6.7 – VIX future price and relative error in % for the price expansion w.r.t. H.







1

0

-2

-3

-4

0.05

0.10

0.15

0.20

0.25

Н

0.30







Н



Н



Figure 6.8 – VIX call and put prices and relative error in % for the price expansion w.r.t. H.

v0

v1

v2

vЗ

0.40

Ŧ

0.35

#### Implied volatility

The implied volatility of VIX options is computed matching the forward (here spot as we assume zero interest rate, repo, and dividend) and the model-generated VIX future (computed by Monte Carlo simulation) in the Black–Scholes price. As the averaging time interval  $\Delta = 1$  month is rather short, and because in this particular model the forward variance is lognormal, the VIX itself is close to a lognormal random variable and we expect the VIX smile to be almost flat (see also Horvath, Jacquier, and Tankov [112, Section 3.3] for a detailed discussion). In practice, the market VIX smile exhibits a pronounced positive skew which motivates the need for a more general model.

In Figure 6.9, we plot the "true" VIX smile (the parameters being specified in the legend) along with its zeroth-order (v0) and third-order (v3) approximation for 1, 3 and 6 months (left figure) and its associated signed relative error (right figure). We first observe that the v3 approximation, which is almost indistinguishable from the "true" VIX smile, yields more accurate results (less than -2%) compare to the v0 approximation (less than 3.5%). Finally, as our chosen proxy is lognormal, the zeroth-order approximated VIX smile is flat.



Figure 6.9 – VIX smiles in the rough Bergomi model (left) for T = 1, 3, 6 months and relative error approximations in % (right) for  $X_0 = \ln(0.235^2)$ ,  $\eta = 1, H = 0.1, \Delta = \frac{1}{12}$ . The "+" (resp. "\*") corresponds to the zeroth-order (resp. third-order) approximation.

## 6.3 Mixed one-factor rough Bergomi model

To alleviate the inconsistent VIX smile generated by the plain rough Bergomi model (see Section 6.2.6), we consider the mixed (or skewed) one-factor rough Bergomi model, introduced simultaneously by De Marco [52] and Guyon [95]. Recall that in the mixed one-factor Bergomi model Bergomi [28] (originally with two factors), the instantaneous forward variance takes the form:

$$\xi_T^{\alpha} = \xi_0^{\alpha} \left[ \lambda \mathcal{E} \left( \omega_1 \int_0^T e^{-k(\alpha-t)} \mathrm{d}W_t \right) + (1-\lambda) \mathcal{E} \left( \omega_2 \int_0^T e^{-k(\alpha-t)} \mathrm{d}W_t \right) \right]$$

for some positive parameters  $k, \omega_1, \omega_2$  and where  $\mathcal{E}(X)$  is a shorthand notation for  $e^{X - \frac{1}{2} \operatorname{Var}(X)}$ . Its rough extension is then naturally defined as:

$$\xi_T^{\alpha} = \xi_0^{\alpha} \left[ \lambda \mathcal{E} \left( \eta_1 \int_0^T (\alpha - t)^{H - \frac{1}{2}} \, \mathrm{d}W_t \right) + (1 - \lambda) \, \mathcal{E} \left( \eta_2 \int_0^T (\alpha - t)^{H - \frac{1}{2}} \, \mathrm{d}W_t \right) \right],$$

where  $\eta_1, \eta_2 > 0$  can be different vol-of-vol parameters and  $\lambda \in [0, 1]$  is a mixing parameter. For simplicity, we introduce for i = 1, 2,

$$K_i^{\alpha}(t) = \eta_i K_0^{\alpha}(t), \quad K_0^{\alpha}(t) = (\alpha - t)^{H - \frac{1}{2}}.$$

The instantaneous forward variance is now modeled by the exponential mean of a convex combination of lognormal random variables. We choose to approximate  $\nu^{\exp}(X_T)$  with the following proxy

$$\nu^{\exp, \mathcal{P}} \left( X_{T}^{\cdot} \right) = \nu^{\exp} \left( X_{0}^{\cdot} \right) \left[ \lambda e^{\nu_{0} \left( Y_{T,1}^{\cdot} \right)} + (1 - \lambda) e^{\nu_{0} \left( Y_{T,2}^{\cdot} \right)} \right],$$

where for i = 1, 2,

$$Y_{T,i}^{\alpha} = -\frac{1}{2} \int_{0}^{T} K_{i}^{\alpha}(t)^{2} dt + \int_{0}^{T} K_{i}^{\alpha}(t) dW_{t}.$$

Observe that  $\nu^{\exp, P}(X_T)$  is given by a convex combination of lognormal random variables. Indeed for i = 1, 2, we have

$$\ln\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)e^{\nu_{0}\left(Y_{T,i}^{\cdot}\right)}\right) \stackrel{d}{=} \ln\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)\right) + \mathcal{N}\left(\mu_{i},\sigma_{i}^{2}\right),\tag{6.3.1}$$

with

$$\mu_i = -\frac{1}{2} \int_0^T \nu_0 \left( K_i^{\cdot}(t)^2 \right) \mathrm{d}t, \quad \sigma_i^2 = \int_0^T \nu_0 \left( K_i^{\cdot}(t) \right)^2 \mathrm{d}t.$$
(6.3.2)

Further as

$$\operatorname{Corr}\left(Y_{T,1}^{\alpha}, Y_{T,2}^{\alpha}\right) = \frac{\eta_{1}\eta_{2}\int_{0}^{T}\nu_{0}\left(K_{0}^{\cdot}\left(t\right)\right)^{2}\mathrm{d}t}{\sqrt{\eta_{1}^{2}\int_{0}^{T}\nu_{0}\left(K_{0}^{\cdot}\left(t\right)\right)^{2}\mathrm{d}t}\sqrt{\eta_{2}^{2}\int_{0}^{T}\nu_{0}\left(K_{0}^{\cdot}\left(t\right)\right)^{2}\mathrm{d}t}} = 1$$

we have that

$$\lambda e^{\nu_0 (Y_{T,1})} + (1-\lambda) e^{\nu_0 (Y_{T,2})} \stackrel{d}{=} \lambda e^{\mu_1 + \sigma_1 N} + (1-\lambda) e^{\mu_2 + \sigma_2 N}, \qquad N \stackrel{d}{=} \mathcal{N}(0,1).$$

The connection between  $\nu^{\exp}(X_T)$  and  $\nu^{\exp,P}(X_T)$  is made through the parametrization (or interpolation) ( $\varepsilon \in [0,1]$ ),

$$J(\varepsilon) = \nu^{\exp}(X_{0}) \int_{\mathcal{A}} \left[ \lambda e^{\nu_{0}(Y_{T,1}^{\cdot}) + \varepsilon(Y_{T,1}^{\alpha} - \nu_{0}(Y_{T,1}^{\cdot}))} + (1-\lambda) e^{\nu_{0}(Y_{T,2}^{\cdot}) + \varepsilon(Y_{T,2}^{\alpha} - \nu_{0}(Y_{T,2}^{\cdot}))} \right] \nu_{0}(\mathrm{d}\alpha),$$
(6.3.3)

for which  $J(1) = \nu^{\exp}(X_T)$  and  $J(0) = \nu^{\exp,P}(X_T)$  and we have almost surely,

$$J^{(n)}(\varepsilon) = \nu^{\exp}(X_{0}^{\cdot}) \int_{\mathcal{A}} \left[ \lambda \left( Y_{T,1}^{\alpha} - \nu_{0} \left( Y_{T,1}^{\cdot} \right) \right)^{n} e^{\nu_{0} \left( Y_{T,1}^{\cdot} \right) + \varepsilon \left( Y_{T,1}^{\alpha} - \nu_{0} \left( Y_{T,1}^{\cdot} \right) \right)} + (1 - \lambda) \left( Y_{T,2}^{\alpha} - \nu_{0} \left( Y_{T,2}^{\cdot} \right) \right)^{n} e^{\nu_{0} \left( Y_{T,2}^{\cdot} \right) + \varepsilon \left( Y_{T,2}^{\alpha} - \nu_{0} \left( Y_{T,2}^{\cdot} \right) \right)} \right] \nu_{0}(\mathrm{d}\alpha) \,.$$

Observing that as in the first part  $J^{(1)}(0) = 0$ , we infer that the zeroth-order approximation  $\nu^{\exp, P}(X_T)$  again always underestimates the desired quantity  $\nu^{\exp}(X_T)$ .

#### 6.3.1 Price expansion

For i = 1, 2, let

$$\begin{split} \gamma_{1}(\eta_{i}) &:= \frac{\eta_{i}^{4}}{8} \int_{\mathcal{A}} \left( \int_{0}^{T} \left[ K_{0}^{\alpha}(t)^{2} - \nu_{0} \left( K_{0}^{\cdot}(t)^{2} \right) \right] \mathrm{d}t \right)^{2} \nu_{0}(\mathrm{d}\alpha) \\ &+ \frac{\eta_{i}^{2}}{2} \int_{\mathcal{A}} \left( \int_{0}^{T} \left[ K_{0}^{\alpha}(t) - \nu_{0} \left( K_{0}^{\cdot}(t) \right) \right]^{2} \mathrm{d}t \right) \nu_{0}(\mathrm{d}\alpha) \,. \end{split}$$

$$\gamma_{2}(\eta_{i}) := \eta_{i}^{4} \int_{\mathcal{A}} \left( \int_{0}^{T} \nu_{0} \left( K_{0}^{\cdot}(t) \right) \left[ K_{0}^{\alpha}(t) - \nu_{0} \left( K_{0}^{\cdot}(t) \right) \right] dt \right)$$
$$\times \left( \int_0^T \left[ -\frac{1}{2} K_0^{\alpha} (t)^2 + \frac{1}{2} \nu_0 \left( K_0^{\cdot} (t)^2 \right) \right] dt \right) \nu_0 (d\alpha)$$
  
$$\gamma_3 (\eta_i) := \frac{\eta_i^4}{2} \int_{\mathcal{A}} \left( \int_0^T \nu_0 \left( K_0^{\cdot} (t) \right) \left[ K_0^{\alpha} (t) - \nu_0 \left( K_0^{\cdot} (t) \right) \right] dt \right)^2 \nu_0 (d\alpha).$$

**Theorem 6.3.1.** Let  $\varphi$  be a function three times continuously differentiable with bounded derivatives. The price at time 0 of an option on the VIX<sub>T</sub><sup>2</sup> with payoff  $\varphi$  equals

$$\mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{T}^{\cdot}\right)\right)\right] = P_{0} + \sum_{i=1}^{3} \gamma_{i}(\eta_{1})P_{i,1} + \gamma_{i}(\eta_{2})P_{i,2} + \mathscr{E}_{(6.3.4)}, \tag{6.3.4}$$

where  $\mathscr{E}_{(6.3.4)}$  is an error term satisfying  $|\mathscr{E}_{(6.3.4)}| \leq C_{(6.3.4)}\Delta^{3H}$  for an independent positive constant  $C_{(6.3.4)}$  and

$$P_{0} = \mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)\left[\lambda e^{\mu_{1}+\sigma_{1}Z}+\left(1-\lambda\right)e^{\mu_{2}+\sigma_{2}Z}\right]\right)\right]$$

where  $Z \stackrel{d}{=} \mathcal{N}(0,1)$ , and for all i = 1, 2, 3,

$$P_{i,1} = \partial_{\varepsilon}^{i-1} \mathbb{E} \left[ \Psi_1 \left( \mu_1 + \sigma_1 + Z + \varepsilon \right) \right] \Big|_{\varepsilon=0}, \qquad P_{i,2} = \partial_{\varepsilon}^{i-1} \mathbb{E} \left[ \Psi_2 \left( \mu_2 + \sigma_2 + Z + \varepsilon \right) \right] \Big|_{\varepsilon=0},$$

and

$$\Psi_{1}(x) = \partial_{\omega} \varphi \left( \nu^{\exp}(X_{0}) \left[ \lambda e^{x+\omega} + (1-\lambda) e^{\frac{\eta_{2}}{2}(\eta_{1}-\eta_{2})\int_{0}^{T} \nu_{0} \left(K_{0}(t)^{2}\right) dt + \frac{\eta_{2}}{\eta_{1}}x} \right] \right) \Big|_{\omega=0}, \qquad (6.3.5)$$

$$\Psi_{2}(x) = \partial_{\omega} \varphi \left( \nu^{\exp}(X_{0}^{\cdot}) \left[ \lambda e^{\frac{\eta_{1}}{2}(\eta_{2}-\eta_{1})\int_{0}^{T}\nu_{0}\left(K_{0}^{\cdot}(t)^{2}\right) dt + \frac{\eta_{1}}{\eta_{2}}x} + (1-\lambda) e^{x+\omega} \right] \right) \Big|_{\omega=0}.$$
 (6.3.6)

*Proof of Theorem 6.3.1.* We proceed as in the proof of Theorem 6.3.3. Applying a second-order Taylor formula with integral remainder to  $\varphi$  at  $\nu^{\exp, P}(X_T)$  gives

$$\mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{T}^{\cdot}\right)\right)\right] = \mathbb{E}\left[\varphi\left(\nu^{\exp,P}\left(X_{T}^{\cdot}\right)\right)\right] + \mathbb{E}\left[\varphi^{'}\left(\nu^{\exp,P}\left(X_{T}^{\cdot}\right)\right)\left(\nu^{\exp}\left(X_{T}^{\cdot}\right) - \nu^{\exp,P}\left(X_{T}^{\cdot}\right)\right)\right] + E_{0}\left(\varphi^{''}\right), \quad (6.3.7)$$

where  $E_0\left(\varphi''\right)$  is an error term given by

$$E_0\left(\varphi^{''}\right) := \int_0^1 \left(1-\lambda\right) \mathbb{E}\left[\varphi^{''}\left(\lambda\nu^{\exp}\left(X_T\right) + \left(1-\lambda\right)\nu^{\exp,\mathrm{P}}\left(X_T\right)\right)\left(\nu^{\exp}\left(X_T\right) - \nu^{\exp,\mathrm{P}}\left(X_T\right)\right)^2\right],$$

and

$$\mathbb{E}\left[\varphi\left(\nu^{\exp,\mathrm{P}}\left(X_{T}^{\cdot}\right)\right)\right] = \mathbb{E}\left[\varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)\left[\lambda e^{\nu_{0}\left(Y_{T,1}^{\cdot}\right)} + (1-\lambda)e^{\nu_{0}\left(Y_{T,2}^{\cdot}\right)}\right]\right)\right] =: P_{0},$$

where for i = 1, 2, we have  $\nu^{\exp}(X_0) e^{\nu_0(Y_{T,i})} \stackrel{d}{=} \nu^{\exp}(X_0) e^{\mu_i + \sigma_i Z}$  with  $Z \stackrel{d}{=} \mathcal{N}(0, 1)$ . From the parametrization (6.3.3), we have also

$$\nu^{\exp}(X_{T}^{\cdot}) - \nu^{\exp,P}(X_{T}^{\cdot}) = \frac{J^{(2)}(0)}{2} + \int_{0}^{1} \frac{(1-\varepsilon)^{2}}{2} J^{(3)}(\varepsilon) d\varepsilon$$
$$= \lambda \nu^{\exp}(X_{0}^{\cdot}) e^{\nu_{0}(Y_{T,1}^{\cdot})} \int_{\mathcal{A}} \frac{1}{2} \left(Y_{T,1}^{\alpha} - \nu_{0}\left(Y_{T,1}^{\cdot}\right)\right)^{2} \nu_{0}(d\alpha)$$
$$+ (1-\lambda) \nu^{\exp}(X_{0}^{\cdot}) e^{\nu_{0}(Y_{T,2}^{\cdot})} \int_{\mathcal{A}} \frac{1}{2} \left(Y_{T,2}^{\alpha} - \nu_{0}\left(Y_{T,2}^{\cdot}\right)\right)^{2} \nu_{0}(d\alpha)$$

$$+\int_0^1 \frac{(1-\varepsilon)^2}{2} J^{(3)}(\varepsilon) \,\mathrm{d}\varepsilon.$$

Introducing the error term

$$E_1\left(\varphi'\right) := \mathbb{E}\left[\varphi'\left(\nu^{\exp, \mathcal{P}}\left(X_T^{\cdot}\right)\right) \int_0^1 \frac{(1-\varepsilon)^2}{2} J^{(3)}\left(\varepsilon\right) \mathrm{d}\varepsilon\right],$$

and the new functions

$$\Psi_{1}(x) = \partial_{\omega}\varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)\left[\lambda e^{x+\omega} + (1-\lambda)e^{\frac{\eta_{2}}{2}(\eta_{1}-\eta_{2})\int_{0}^{T}\nu_{0}\left(K_{0}^{\cdot}(t)^{2}\right)dt + \frac{\eta_{2}}{\eta_{1}}x}\right]\right)\Big|_{\omega=0},$$

$$\Psi_{2}(x) = \partial_{\omega}\varphi\left(\nu^{\exp}\left(X_{0}^{\cdot}\right)\left[\lambda e^{\frac{\eta_{1}}{2}(\eta_{2}-\eta_{1})\int_{0}^{T}\nu_{0}\left(K_{0}^{\cdot}(t)^{2}\right)dt + \frac{\eta_{1}}{\eta_{2}}x} + (1-\lambda)e^{x+\omega}\right]\right)\Big|_{\omega=0}.$$

Observing that

$$\begin{split} \nu_0 \left( Y_{T,1}^{\cdot} \right) &= -\frac{\eta_1^2}{2} \int_0^T \nu_0 \left( K_0^{\cdot}(t)^2 \right) \mathrm{d}t + \eta_1 \int_0^T \nu_0 \left( K_0^{\cdot}(t) \right) \mathrm{d}W_t \\ &= -\frac{\eta_1^2}{2} \int_0^T \nu_0 \left( K_0^{\cdot}(t)^2 \right) \mathrm{d}t + \frac{\eta_1}{\eta_2} \left( \nu_0 \left( Y_{T,2}^{\cdot} \right) + \frac{\eta_2^2}{2} \int_0^T \nu_0 \left( K_0^{\cdot}(t)^2 \right) \mathrm{d}t \right) \\ &= \frac{\eta_1}{2} \left( \eta_2 - \eta_1 \right) \int_0^T \nu_0 \left( K_0^{\cdot}(t)^2 \right) \mathrm{d}t + \frac{\eta_1}{\eta_2} \nu_0 \left( Y_{T,2}^{\cdot} \right), \end{split}$$

and by symmetry,

$$\nu_0\left(Y_{T,2}^{\cdot}\right) = \frac{\eta_2}{2} \left(\eta_1 - \eta_2\right) \int_0^T \nu_0\left(K_0^{\cdot}(t)^2\right) \mathrm{d}t + \frac{\eta_2}{\eta_1} \nu_0\left(Y_{T,1}^{\cdot}\right),$$

we have that the second term at the r.h.s. of (6.3.7), rewrites as

$$\begin{split} \mathbb{E}\Big[\varphi'\Big(\nu^{\exp,P}(X_{T}^{\cdot})\Big)\Big(\nu^{\exp}(X_{T}^{\cdot})-\nu^{\exp,P}(X_{T}^{\cdot})\Big)\Big] \\ &= \mathbb{E}\Big[\varphi'\Big(\nu^{\exp}(X_{0}^{\cdot})\left[\lambda e^{\nu_{0}\left(Y_{T,1}^{\cdot}\right)}+(1-\lambda)\,e^{\nu_{0}\left(Y_{T,2}^{\cdot}\right)}\right]\Big) \\ &\times\left(\lambda\nu^{\exp}\left(X_{0}^{\cdot}\right)e^{\nu_{0}\left(Y_{T,1}^{\cdot}\right)}\int_{\mathcal{A}}\frac{1}{2}\left(Y_{T,1}^{\alpha}-\nu_{0}\left(Y_{T,2}^{\cdot}\right)\right)^{2}\nu_{0}\left(\mathrm{d}\alpha\right) \\ &+(1-\lambda)\,\nu^{\exp}\left(X_{0}^{\cdot}\right)e^{\nu_{0}\left(Y_{T,2}^{\cdot}\right)}\int_{\mathcal{A}}\frac{1}{2}\left(Y_{T,2}^{\alpha}-\nu_{0}\left(Y_{T,2}^{\cdot}\right)\right)^{2}\nu_{0}\left(\mathrm{d}\alpha\right)\Big)\Big]+E_{1}\left(\varphi'\right) \\ &=\mathbb{E}\Big[\Psi_{1}\left(\nu_{0}\left(Y_{T,1}^{\cdot}\right)\right)\times\int_{\mathcal{A}}\frac{1}{2}\left(Y_{T,1}^{\alpha}-\nu_{0}\left(Y_{T,2}^{\cdot}\right)\right)^{2}\nu_{0}\left(\mathrm{d}\alpha\right) \\ &+\Psi_{2}\left(\nu_{0}\left(Y_{T,2}^{\cdot}\right)\right)\times\int_{\mathcal{A}}\frac{1}{2}\left(Y_{T,2}^{\alpha}-\nu_{0}\left(Y_{T,2}^{\cdot}\right)\right)^{2}\nu_{0}\left(\mathrm{d}\alpha\right)\Big]+E_{1}\left(\varphi'\right). \end{split}$$

This is similar to the setting of (6.2.19) with  $\eta_1$  for  $\Psi_1$  and  $\eta_2$  for  $\Psi_2$  instead of  $\eta$  for  $\Psi'$ . Hence applying twice Lemma 6.2.7 with i = 1, 2 for both terms of the r.h.s. of the last equality with

$$l(x) = \Psi_i \left( x - \frac{1}{2} \int_0^T \nu_0 \left( K_i^{\cdot}(t)^2 \right) dt \right), \quad a_t = \nu_0 \left( K_i^{\cdot}(t) \right),$$
  
$$f_t = h_t = K_i^{\alpha}(t) - \nu_0 \left( K_i^{\cdot}(t) \right), \quad e_t = g_t = -\frac{1}{2} K_i^{\alpha}(t)^2 + \frac{1}{2} \nu_0 \left( K_i^{\cdot}(t)^2 \right),$$

we obtain the desired expansion.

For the error terms, observing that  $J^{(n)}(\varepsilon) = I^{(n)}(\varepsilon, \gamma_1) + I^{(n)}(\varepsilon, \gamma_2)$  (where we explicit the dependence on  $\gamma$  i.e.  $I^{(n)}(\varepsilon, \gamma) := I^{(n)}(\varepsilon)$ , see (6.2.10)), and conducting the same error analysis as in the proof of Theorem 6.2.6, we retrieve the error estimate of order  $\mathcal{O}(\Delta^{3H})$ .

**Corollary 6.3.2.** Suppose an initial flat instantaneous forward variance. Let  $F : x \in \mathbb{R} \to e^{X_0} \left[ \lambda e^{\mu_1 + \sigma_1 x} + (1 - \lambda) e^{\mu_2 + \sigma_2 x} \right]$  and set the constant  $A = F^{-1}(\kappa^2)$  where  $F^{-1}$  denote the inverse function of F. For a call option, it holds:

$$P_0^{\text{call}}\left(\mu_1,\mu_2,\sigma_1,\sigma_2\right) = \lambda^{\frac{1}{2}} e^{\frac{\mu_1+X_0}{2} + \frac{\sigma_1^2}{8}} \int_A^\infty \left(1 + \frac{1-\lambda}{\lambda} e^{\mu_2 - \mu_1 + (\sigma_2 - \sigma_1)\frac{\sigma_1}{2}} e^{(\sigma_2 - \sigma_1)y}\right)^{\frac{1}{2}} \frac{e^{-\frac{y^2}{2}}}{\sqrt{2\pi}} \mathrm{d}y$$
$$- \kappa \Phi\left(-A\right).$$

For a put option, it holds:

 $P_0^{\text{put}}\left(\mu_1, \mu_2, \sigma_1, \sigma_2\right) = \kappa \Phi\left(A\right)$ 

$$-\lambda^{\frac{1}{2}}e^{\frac{\mu_{1}+X_{0}}{2}+\frac{\sigma_{1}^{2}}{8}}\int_{-\infty}^{A}\left(1+\frac{1-\lambda}{\lambda}e^{\mu_{2}-\mu_{1}+(\sigma_{2}-\sigma_{1})\frac{\sigma_{1}}{2}}e^{(\sigma_{2}-\sigma_{1})y}\right)^{\frac{1}{2}}\frac{e^{-\frac{y^{2}}{2}}}{\sqrt{2\pi}}\mathrm{d}y.$$

Finally, for a future it holds:

$$P_0^{\rm F}(\mu_1,\mu_2,\sigma_1,\sigma_2) = \lambda^{\frac{1}{2}} e^{\frac{\mu_1 + X_0}{2} + \frac{\sigma_1^2}{8}} \int_{\mathbb{R}} \left( 1 + \frac{1 - \lambda}{\lambda} e^{\mu_2 - \mu_1 + (\sigma_2 - \sigma_1)\frac{\sigma_1}{2}} e^{(\sigma_2 - \sigma_1)y} \right)^{\frac{1}{2}} \frac{e^{-\frac{y^2}{2}}}{\sqrt{2\pi}} \mathrm{d}y.$$

Proof of Corollary 6.3.2. For the future, it holds that

$$\begin{split} P_0^{\rm F} &= \mathbb{E}\left[\varphi\left(\lambda e^{X_0+\mu_1+\sigma_1 Z} + (1-\lambda) e^{X_0+\mu_2+\sigma_2 Z}\right)\right] \\ &= \int_{\mathbb{R}} \lambda^{\frac{1}{2}} e^{\frac{\mu_1+X_0}{2} + \frac{\sigma_1}{2} z} \left(1 + \frac{1-\lambda}{\lambda} e^{\mu_2-\mu_1+(\sigma_2-\sigma_1)z}\right)^{\frac{1}{2}} \frac{e^{-\frac{z^2}{2}}}{\sqrt{2\pi}} \mathrm{d}z \\ &= \lambda^{\frac{1}{2}} e^{\frac{\mu_1+X_0}{2} + \frac{\sigma_1^2}{8}} \int_{\mathbb{R}} \left(1 + \frac{1-\lambda}{\lambda} e^{\mu_2-\mu_1+(\sigma_2-\sigma_1)z}\right)^{\frac{1}{2}} \frac{e^{-\frac{1}{2}\left(z-\frac{\sigma_1}{2}\right)^2}}{\sqrt{2\pi}} \mathrm{d}z \\ &= \lambda^{\frac{1}{2}} e^{\frac{\mu_1+X_0}{2} + \frac{\sigma_1^2}{8}} \int_{\mathbb{R}} \left(1 + \frac{1-\lambda}{\lambda} e^{\mu_2-\mu_1+(\sigma_2-\sigma_1)\left(y+\frac{\sigma_1}{2}\right)}\right)^{\frac{1}{2}} \frac{e^{-\frac{y^2}{2}}}{\sqrt{2\pi}} \mathrm{d}y \\ &= a \int_{\mathbb{R}} (1 + b e^{cy})^{\frac{1}{2}} \frac{e^{-\frac{y^2}{2}}}{\sqrt{2\pi}} \mathrm{d}y, \end{split}$$

where we have made the change of variables  $y = z - \frac{\sigma_1}{2}$  and set

$$a = \lambda^{\frac{1}{2}} e^{\frac{\mu_1 + X_0}{2} + \frac{\sigma_1^2}{8}} > 0, \ b = \frac{1 - \lambda}{\lambda} e^{\mu_2 - \mu_1 + (\sigma_2 - \sigma_1)\frac{\sigma_1}{2}} > 0, \ c = \sigma_2 - \sigma_1 \in \mathbb{R}.$$

For a call option i.e.  $\varphi(x) = (\sqrt{x} - \kappa)_+$ , as the map  $F: x \in \mathbb{R} \to e^{X_0} \left[ \lambda e^{\mu_1 + \sigma_1 x} + (1 - \lambda) e^{\mu_2 + \sigma_2 x} \right]$  is increasing, we can define its inverse  $F^{-1}(y)$  for all  $y \in (0, \infty)$ . We then obtain that

$$\mathbb{E}\left[\varphi\left(F\left(Z\right)\right)\right] = \mathbb{E}\left[F\left(Z\right)\mathbf{1}_{Z\geq F^{-1}(\kappa^{2})}\right] - \kappa\left[\mathbf{1}_{Z\geq F^{-1}(\kappa^{2})}\right]$$
$$= \int_{F^{-1}(\kappa^{2})}^{\infty} a\left(1 + be^{cy}\right)^{\frac{1}{2}} \frac{e^{-\frac{y^{2}}{2}}}{\sqrt{2\pi}} \mathrm{d}y - \kappa\Phi\left(-F^{-1}\left(\kappa^{2}\right)\right)$$

and the derivatives follow. The proof for the put option being similar, we skip details.  $\Box$ 

#### 6.3.2 Numerical tests

For every  $\alpha \in [T, T + \Delta]$  recall that  $\xi_T^{\alpha} = \xi_0^{\alpha} \left[ \lambda e^{Y_{T,1}^{\alpha}} + (1 - \lambda) e^{Y_{T,2}^{\alpha}} \right]$  and for i = 1, 2,

$$Y_{T,i}^{\alpha} = -\frac{\eta_i^2}{2} \int_0^T (\alpha - t)^{2H-1} \,\mathrm{d}t + \eta_i \int_0^T (\alpha - t)^{H-\frac{1}{2}} \,\mathrm{d}W_t,$$

and

$$\operatorname{Corr}\left(Y_{T,1}^{\alpha}, Y_{T,2}^{\alpha}\right) = \frac{\eta_{1}\eta_{2}\int_{0}^{T} (\alpha - t)^{2H-1} \,\mathrm{d}t}{\sqrt{\eta_{1}^{2}\int_{0}^{T} (\alpha - t)^{2H-1} \,\mathrm{d}t} \sqrt{\eta_{2}^{2}\int_{0}^{T} (\alpha - t)^{2H-1} \,\mathrm{d}t}} = 1$$

We proceed as in the rough Bergomi model. Let  $\mathcal{D}_n$  denote a discretization grid

$$\mathcal{D}_n = \left\{ t_0 = T < \dots < t_n = T + \Delta \right\},\,$$

and introduce the Gaussian vector  $(Z_i)_{i=1,...,n}$  with mean and covariance matrix given for all i, j = 1, ..., n,

$$\mathbb{E}[Z_i] = -\frac{1}{2} \int_0^T K_0^{t_i}(s) \,\mathrm{d}s, \qquad \mathbb{C}\mathrm{ov}(Z_i, Z_j) = \int_0^T K_0^{t_i}(s) \,K_0^{t_j}(s) \,\mathrm{d}s$$

Observe that this corresponds to the particular case  $\eta = 1$  for the plain rough Bergomi. We then approximate VIX option prices with the following rectangle scheme:

$$\mathbb{E}\left[\varphi\left(\frac{1}{n}\sum_{i=1}^{n}\xi_{T}^{t_{i}}\right)\right] = \mathbb{E}\left[\varphi\left(\frac{1}{n}\sum_{i=1}^{n}\xi_{0}^{t_{i}}\left[\lambda e^{Y_{T,1}^{t_{i}}} + (1-\lambda)e^{Y_{T,2}^{t_{i}}}\right]\right)\right]$$
$$= \mathbb{E}\left[\varphi\left(\frac{1}{n}\sum_{i=1}^{n}\xi_{0}^{t_{i}}\left[\lambda e^{\eta_{1}Z_{i}} + (1-\lambda)e^{\eta_{2}Z_{i}}\right]\right)\right].$$

As the two normal random variables in  $(Y_{T,1}^{t_i}, Y_{T,2}^{t_i})$  exhibit a correlation of 1, it is sufficient to consider a Gaussian vector of size n instead of 2n.

Remark 21 (Approximation prices). Observe that we have no closed-formulas for the prices  $P_{i,1}, P_{i,2}$  for i = 1, ..., 3. From Corollary 6.3.2, we compute  $P_0$  by numerical integration (quadrature) and evaluate the first/second (resp. third) derivative with a sixth-order (resp. fourth-order) accuracy central finite difference scheme (see Fornberg [66, Table 1] for the exact weights).

Implied volatility. As before, we compare the "true" VIX implied smile (computed with both the rectangle scheme and a Monte Carlo simulation) along with the approximated VIX implied smile (computed with our expansions). To test our approximation formulas and generate different VIX smiles, we consider 2 scenarios representing different sets of parameters. In all computations, we consider options with maturity 1, 3, and 6 months and we set  $X_0 = \ln (0.235^2) \approx -2.896$ ,  $H = 0.1, 10^6$  Monte Carlo samples and 300 discretization points. The signed relative error (expressed in %) is also given.

- Scenario 1:  $\eta_1 = 1.4, \ \eta_2 = 0.7, \ \lambda = 0.3, \ \kappa \in [0.1, 0.4].$
- Scenario 2:  $\eta_1 = 0.9, \eta_2 = 0, \lambda = 0.6, \kappa \in [0.17, 0.35]$  (displaced model).

Scenario	1M	3M	6M
1	$0.218650 \pm 5 \times 10^{-6}$	$0.206308 \pm 5 \times 10^{-6}$	$0.196890 \pm 5 \times 10^{-6}$
2	$0.229001 \pm 3 \times 10^{-6}$	$0.224244 \pm 3 \times 10^{-6}$	$0.220472 \pm 3 \times 10^{-6}$

Table 6.1 – VIX futures with maturity 1, 3, and 6 months for Scenario 1–2.



Figure 6.10 – VIX smiles in the mixed one-factor rough Bergomi model (left) for T = 1, 3, 6 months, and relative error approximations in % (right) for Scenario 1. The + (resp. \*) corresponds to the zeroth-order (resp. third-order) approximation.



Figure 6.11 – VIX smiles in the mixed one-factor rough Bergomi model (left) for T = 1, 3, 6 months and relative error approximations in % (right) for Scenario 2.

Here, the third-order approximation (v3) is slightly more accurate than the proxy's approximation (v0) which provides already quite satisfactory results as it is nearly indistinguishable from the VIX smile (approximately less than 2% of relative error). With this feature in mind, we are going to use our zeroth-order (which is even faster to evaluate compare to v3) approximation to calibrate our mixed model to real market data.

#### 6.3.3 Calibration

In this section, we calibrate the mixed one-factor rough Bergomi model to market VIX smiles on November 22, 2017, using our zeroth-order approximation. We set from now on the Hurst parameter to H = 0.1. As explained above, we have 4 different free parameters that can be used for the calibration, that is  $(\xi_0^T, \eta_1^T, \eta_2^T, \lambda^T)$  which depend on the maturity T. We have n = 4different future prices  $(F_i)_{i=1,...,n}$  each associated to a maturity  $(T_i)_{i=1,...,n}$ . The procedure (least squares optimization) to calibrate our model for  $T \in [T_i, T_{i+1}]$  is twofold:

1. For every  $(\eta_1^T, \eta_2^T, \lambda^T)$ , we set  $\xi_0^T$  as the unique solution to  $F_i = P_0^F(T_i, \xi_0^T, \eta_1^T, \eta_2^T, \lambda^T)$ where  $P_0^F$  corresponds to the zeroth-order approximation price for the future (see Theorem 6.3.1). 2. We then compute the VIX implied volatility surface using the value found for  $\xi_0^T$  in the previous step. We compare it (in terms of  $L_2$  error) to the "true" VIX smile. Until we find a minimum, we go back to step 1.



Figure 6.12 – Term structure of VIX futures (left) and market VIX smiles calibrated with the mixed one-factor rough Bergomi zeroth-order approximation (right).

The calibration to real market VIX smiles using our mixed model seems to provide efficient and reliable results even though we only used our zeroth-order approximation, and the procedure required only a few seconds.

	$T \in [\frac{1}{12}, \frac{2}{12}[$	$T \in [\frac{2}{12}, \frac{3}{12}[$	$T \in [\frac{3}{12}, \frac{4}{12}[$	$T \in [\frac{4}{12}, \frac{5}{12}[$
$\xi_0^T$	$1.474 \times 10^{-2}$	$2.130 \times 10^{-2}$	$2.629 \times 10^{-2}$	$2.927 \times 10^{-2}$
$\eta_1^T$	1.897	1.858	1.746	1.407
$\eta_2^T$	0.197	0.1527	0.167	0.124
$\lambda^T$	0.324	0.4917	0.550	0.650

Table 6.2 – Term structure for the free parameters  $(\xi_0^T, \eta_1^T, \eta_2^T, \lambda^T)$ .

### 6.4 Conclusion

We have derived weak approximations of the VIX index expressed as a combination of lognormal random variables in two different rough forward variance models i.e. the plain and mixed one-factor rough Bergomi model, and we have provided expansion results for VIX derivatives which have shown to be accurate. We have also demonstrated that our approximation formulas could be used for a fast and efficient calibration of real market VIX smile. We are now in the process of extending our approximation formulas for any Hölder continuous exponentially growing payoffs (see Remark 19).

### 6.5 Proofs of technical results

**Lemma 6.5.1.** For every  $n \in \mathbb{N}^*$  and sequence  $\boldsymbol{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$ , the following power inequality for the sum of n reals holds

$$\left|\sum_{i=1}^{n} x_{i}\right|^{p} \leq \begin{cases} \sum_{i=1}^{n} |x_{i}|^{p} & \text{if } p \in (0,1], \\ n^{p-1} \sum_{i=1}^{n} |x_{i}|^{p} & \text{if } p > 1. \end{cases}$$

Proof of Lemma 6.5.1. We start by proving that for every sequence  $\boldsymbol{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$ , the map  $p \in (0, \infty) \to \|\boldsymbol{x}\|_p = (\sum_{i=1}^n |x_i|^p)^{\frac{1}{p}}$  is non-increasing. Let  $0 and suppose that <math>\|\boldsymbol{x}\|_p = 1$ , then as each term  $x_i$  is less than or equal to 1,  $|x_i|^q \le |x_i|^p$ , and we infer that  $\|\boldsymbol{x}\|_q^q \le \|\boldsymbol{x}\|_p = 1$  and so  $\|\boldsymbol{x}\|_q \le \|\boldsymbol{x}\|_p$ . For the general case, proceed as before considering  $\frac{\boldsymbol{x}}{\|\boldsymbol{x}\|}$  which has unit  $\ell_p$  norm. If we now suppose that  $p \in (0, 1]$ , then we obtain

$$\left|\sum_{i=1}^{n} x_{i}\right| \leq \sum_{i=1}^{n} |x_{i}| = \|\boldsymbol{x}\|_{1} \leq \|\boldsymbol{x}\|_{p} = \left(\sum_{i=1}^{n} |x_{i}|^{p}\right)^{\frac{1}{p}},$$

and raising to the *p*-th power the quantity above gives the first inequality. Now if p > 1, a direct application of Hölder inequality gives

$$\left|\sum_{i=1}^{n} x_{i}\right| \leq \sum_{i=1}^{n} 1 \times |x_{i}| \leq \left(\sum_{i=1}^{n} 1\right)^{\frac{p-1}{p}} \left(\sum_{i=1}^{n} |x_{i}|^{p}\right)^{\frac{1}{p}},$$

and once again raise to the p-th power.

**Lemma 6.5.2.** For every  $C \in \mathbb{R}$ , H > 0, p > 0, we have

$$\begin{split} \int_{0}^{1} \left| C - y^{2H} \right|^{p} \mathrm{d}y &= \begin{cases} \left( -C \right)^{p} {}_{2}F_{1} \left( \frac{1}{2H}, -p, 1 + \frac{1}{2H}, \frac{1}{C} \right) & \text{if } C < 0, \\ \frac{1}{2Hp+1} & \text{if } C = 0, \\ \frac{C^{p+\frac{1}{2H}}}{2H} B_{p+1,\frac{1}{2H}} + \frac{B_{(1,p+1)}}{2H} C^{\frac{1}{2H}-1} \left( 1 - C \right)^{p+1} {}_{2}F_{1} \left( 1 - \frac{1}{2H}, p+1, p+2, -\frac{1-C}{C} \right) & \text{if } 0 < C \leq 1, \\ C^{p} {}_{2}F_{1} \left( \frac{1}{2H}, -p, 1 + \frac{1}{2H}, \frac{1}{C} \right) & \text{if } C > 1. \end{cases}$$

Proof of Lemma 6.5.2. If C = 0, it holds that  $\int_0^1 |-y^{2H}|^p dy = \int_0^1 y^{2Hp} dy = \frac{1}{2Hp+1}$ . Suppose now  $0 < C \le 1$  and observe,

$$\int_0^1 |C - y^{2H}|^p \, \mathrm{d}y = \int_0^{C^{\frac{1}{2H}}} \left(C - y^{2H}\right)^p \, \mathrm{d}y + \int_{C^{\frac{1}{2H}}}^1 \left(y^{2H} - C\right)^p \, \mathrm{d}y.$$

Introducing successively  $z = C - y^{2H}$  i.e.  $y = (C - z)^{\frac{1}{2H}}$ ,  $dy = -\frac{1}{2H}(C - z)^{\frac{1}{2H}-1} dz$  and  $t = \frac{z}{C}$  we have:

$$\int_{0}^{C^{\frac{1}{2H}}} \left(C - y^{2H}\right)^{p} \mathrm{d}y = \frac{1}{2H} \int_{0}^{C} z^{p} \left(C - z\right)^{\frac{1}{2H} - 1} \mathrm{d}z = \frac{C^{p + \frac{1}{2H}}}{2H} \int_{0}^{1} t^{p} \left(1 - t\right)^{\frac{1}{2H} - 1} \mathrm{d}t$$
$$= \frac{C^{p + \frac{1}{2H}}}{2H} B_{p+1,\frac{1}{2H}}.$$

For the second integral, let  $z = y^{2H} - C$ ,  $y = (C+z)^{\frac{1}{2H}}$ ,  $dy = \frac{1}{2H} (C+z)^{\frac{1}{2H}-1} dz$ ,

$$\int_{C^{\frac{1}{2H}}}^{1} (y^{2H} - C)^{p} dy = \frac{1}{2H} \int_{0}^{1-C} z^{p} (z + C)^{\frac{1}{2H}-1} dz$$
$$= \frac{1}{2H} B_{1,p+1} C^{\frac{1}{2H}-1} (1 - C)^{p+1} {}_{2}F_{1} \left(1 - \frac{1}{2H}, p+1, p+2, -\frac{1-C}{C}\right)$$

A similar analysis gives for C > 1,

$$\int_0^1 |C - y^{2H}|^p \, \mathrm{d}y = C^p {}_2F_1\left(\frac{1}{2H}, -p, 1 + \frac{1}{2H}, \frac{1}{C}\right),$$

and if C < 0,

$$\int_0^1 |C - y^{2H}|^p \, \mathrm{d}y = (-C)^p \,_2 F_1\left(\frac{1}{2H}, -p, 1 + \frac{1}{2H}, \frac{1}{C}\right).$$

Proof of Proposition 6.2.2. A direct computation gives

$$\nu\left(K^{\cdot}(t)^{2}\right) = \frac{1}{\Delta} \int_{T}^{T+\Delta} K^{\alpha}(t)^{2} \nu(d\alpha) = \frac{\eta^{2}}{2H\Delta} \left[ (T+\Delta-t)^{2H} - (T-t)^{2H} \right]$$

and consequently

$$\int_0^T \left( K^{\alpha} (t)^2 - \nu \left( K^{\cdot} (t)^2 \right) \right) dt = \eta^2 \int_0^T \left( (\alpha - t)^{2H-1} - \frac{(T + \Delta - t)^{2H} - (T - t)^{2H}}{2H\Delta} \right) dt$$
$$= \frac{\eta^2}{2H} \left( \alpha^{2H} - (\alpha - T)^{2H} + \frac{T^{2H+1} + \Delta^{2H+1} - (T + \Delta)^{2H+1}}{\Delta (2H + 1)} \right).$$

Observe that if  $H = \frac{1}{2}$ ,  $\alpha^{2H} - (\alpha - T)^{2H} + \frac{T^{2H+1} + \Delta^{2H+1} - (T+\Delta)^{2H+1}}{\Delta(2H+1)} = \alpha - (\alpha - T) - \frac{2\Delta T}{2\Delta} = 0$ and  $\int_{0}^{T} \left( K^{\alpha}(t)^{2} - \nu \left( K^{\cdot}(t)^{2} \right) \right) dt = 0.$ 

$$\int_0^1 \left( K^{\alpha} \left( t \right)^2 - \nu \left( K^{\cdot} \left( t \right)^2 \right) \right) \mathrm{d}t = 0$$

To lighten notations, we introduce the auxiliary function

$$\Lambda(T, \Delta, H) = \frac{T^{2H+1} + \Delta^{2H+1} - (T + \Delta)^{2H+1}}{\Delta(2H+1)},$$

such that the  $L_p$  norm (after having introduced the new variable  $y = \frac{\alpha - T}{\Delta}$ ) rewrites as

$$\left( \int_{\mathcal{A}} \left| \int_{0}^{T} \left[ K^{\alpha} \left( t \right)^{2} - \nu \left( K^{\cdot} \left( t \right)^{2} \right) \right] \mathrm{d}t \right|^{p} \nu \left( \mathrm{d}\alpha \right) \right)^{\frac{1}{p}}$$
$$= \frac{\eta^{2}}{2H} \left( \int_{0}^{1} \left| (T + \Delta y)^{2H} - \Delta^{2H} y^{2H} + \Lambda \left( T, \Delta, H \right) \right|^{p} \mathrm{d}y \right)^{\frac{1}{p}},$$

As  $\Delta \rightarrow 0$ ,

$$(T + \Delta y)^{2H} - \Delta^{2H} y^{2H} + \Lambda (T, \Delta, H) \underset{\Delta \to 0}{\sim} HT^{2H-1} \Delta (2y-1) + \Delta^{2H} \left(\frac{1}{2H+1} - y^{2H}\right),$$

uniformly on  $y \in [0, 1]$ . Consequently (see Bender and Orszag [22, 6.2.2]),

$$\left( \int_{\mathcal{A}} \left| \int_{0}^{T} \left[ K^{\alpha} \left( t \right)^{2} - \nu \left( K^{\cdot} \left( t \right)^{2} \right) \right] \mathrm{d}t \right|^{p} \nu \left( \mathrm{d}\alpha \right) \right)^{\frac{1}{p}}$$
  
$$\underset{\Delta \to 0}{\sim} \frac{\eta^{2} T^{2H-1}}{2} \Delta \left( \int_{0}^{1} |1 - 2y|^{p} \mathrm{d}y \right)^{\frac{1}{p}} + \frac{\eta^{2}}{2H} \Delta^{2H} \left( \int_{0}^{1} \left| 2H + 1 - y^{2H} \right|^{p} \mathrm{d}y \right)^{\frac{1}{p}}.$$

We conclude observing that  $\Delta = \mathcal{O}\left(\Delta^{2H}\right)$  if  $H \in \left(0, \frac{1}{2}\right)$  (resp.  $\Delta^{2H} = \mathcal{O}\left(\Delta\right)$  if  $H \in \left(\frac{1}{2}, 1\right)$ ) and  $\int_{0}^{1} |1 - 2y|^{p} dy = \frac{1}{p+1}$  and evoking Lemma 6.5.2 with C = 2H + 1 for the second integral.  $\Box$ 

Proof of Proposition 6.2.3. Introducing the new variables  $\beta' = \frac{\beta - T}{\Delta}, \alpha' = \frac{\alpha - T}{\Delta}, t' = \frac{T - t}{T}$ , the  $L_p$  norm rewrites as

$$\begin{split} &\left(\frac{1}{\Delta}\int_{\alpha=T}^{T+\Delta}\left|\int_{t=0}^{T}\left[\frac{1}{\Delta}\int_{\beta=T}^{T+\Delta}\left\{K^{\alpha}\left(t\right)-K^{\beta}\left(t\right)\right\}\mathrm{d}\beta\right]^{2}\mathrm{d}t\right|^{p}\mathrm{d}\alpha\right)^{\frac{1}{p}} \\ &= \left(\int_{\alpha'=0}^{1}\left|T\int_{t'=0}^{1}\left[\int_{\beta'=0}^{1}\left\{K^{\Delta\alpha'+T}\left(T-Tt'\right)-K^{\Delta\beta'+T}\left(T-Tt'\right)\right\}\mathrm{d}\beta'\right]^{2}\mathrm{d}t'\right|^{p}\mathrm{d}\alpha'\right)^{\frac{1}{p}} \\ &= \eta^{2}T\left(\int_{\alpha'=0}^{1}\left|\int_{t'=0}^{1}\left[\int_{\beta'=0}^{1}\left\{\left(\Delta\alpha'+Tt'\right)^{H-\frac{1}{2}}-\left(\Delta\beta'+Tt'\right)^{H-\frac{1}{2}}\right\}\mathrm{d}\beta'\right]^{2}\mathrm{d}t'\right|^{p}\mathrm{d}\alpha'\right)^{\frac{1}{p}} \\ &= \eta^{2}T^{2H}\left(\int_{\alpha=0}^{1}\left|\int_{t=0}^{1}\left[\int_{\beta=0}^{1}\left\{\left(\frac{\Delta}{T}\alpha+t\right)^{H-\frac{1}{2}}-\left(\frac{\Delta}{T}\beta+t\right)^{H-\frac{1}{2}}\right\}\mathrm{d}\beta\right]^{2}\mathrm{d}t}\right|^{p}\mathrm{d}\alpha\right)^{\frac{1}{p}} \end{split}$$

Writing  $\Delta$  instead of  $\frac{\Delta}{T}$ , let us introduce the function

$$I(\Delta, p) = \left( \int_{\alpha=0}^{1} \left| \int_{t=0}^{1} \left[ \int_{\beta=0}^{1} \left\{ (\Delta \alpha + t)^{H-\frac{1}{2}} - (\Delta \beta + t)^{H-\frac{1}{2}} \right\} \mathrm{d}\beta \right]^{2} \mathrm{d}t \right|^{p} \mathrm{d}\alpha \right)^{\frac{1}{p}}.$$

First observe

$$\begin{split} \left( \int_{\beta=0}^{1} \left[ (\Delta \alpha + t)^{H - \frac{1}{2}} - (\Delta \beta + t)^{H - \frac{1}{2}} \right] \mathrm{d}\beta \right)^2 \\ &= \frac{\left( t^{H + \frac{1}{2}} - (\Delta + t)^{H + \frac{1}{2}} + \Delta \left( H + \frac{1}{2} \right) (\alpha \Delta + t)^{H - \frac{1}{2}} \right)^2}{\Delta^2 \left( H + \frac{1}{2} \right)^2}, \end{split}$$

which gives

$$\begin{split} \frac{\Delta^2 \left(H + \frac{1}{2}\right)^2 I\left(\Delta, p\right)}{\Delta^{2H+2}} &= \left(\int_{\alpha=0}^1 \left|\int_{t=0}^1 \left(\frac{t^{H+\frac{1}{2}} - (\Delta+t)^{H+\frac{1}{2}}}{\Delta^{H+1}} + \left(H + \frac{1}{2}\right) \frac{(\alpha\Delta+t)^{H-\frac{1}{2}}}{\Delta^H}\right)^2 \mathrm{d}t\right|^p \mathrm{d}\alpha \right)^{\frac{1}{p}} \\ &= \left(\int_{\alpha=0}^1 \left|\int_{t=0}^1 \left(\left(\frac{t}{\Delta}\right)^{H+\frac{1}{2}} - (1 + \frac{t}{\Delta})^{H+\frac{1}{2}} + \left(H + \frac{1}{2}\right) (\alpha + \frac{t}{\Delta})^{H-\frac{1}{2}}\right)^2 \frac{\mathrm{d}t}{\Delta}\right|^p \mathrm{d}\alpha \right)^{\frac{1}{p}} \\ &= \left(\int_{\alpha=0}^1 \left|\int_{s=0}^{\frac{1}{\Delta}} \left((1 + s)^{H+\frac{1}{2}} - s^{H+\frac{1}{2}} - \left(H + \frac{1}{2}\right) (\alpha + s)^{H-\frac{1}{2}}\right)^2 \mathrm{d}s\right|^p \mathrm{d}\alpha \right)^{\frac{1}{p}}. \end{split}$$

Now for every  $\alpha \in [0, 1]$ , we have that as  $s \to \infty$ ,

$$\left((1+s)^{H+\frac{1}{2}} - s^{H+\frac{1}{2}} - \left(H + \frac{1}{2}\right)(\alpha+s)^{H-\frac{1}{2}}\right)^2 \underset{s \to \infty}{\sim} (H^2 - 1)^2 \alpha^2 s^{2H-3},$$

and for every A > 0,

$$\int_{A}^{\infty} s^{2H-3} \mathrm{d}s = \frac{1}{2-2H} \frac{1}{A^{2-2H}} < \infty$$

Consequently,

$$I(\Delta, p) \underset{\Delta \to 0}{\sim} \frac{\Delta^{2H}}{\left(H + \frac{1}{2}\right)^2} \left( \int_{\alpha=0}^1 \left| \int_{s=0}^\infty \left( (1+s)^{H + \frac{1}{2}} - s^{H + \frac{1}{2}} - \left(H + \frac{1}{2}\right) (\alpha+s)^{H - \frac{1}{2}} \right)^2 \mathrm{d}s \right|^p \mathrm{d}\alpha \right)^{\frac{1}{p}}$$

and going back to the  $L_p$  norm and writing  $\frac{\Delta}{T}$  instead of  $\Delta$ , we finally get the announced asymptotic.

Proof of Proposition 6.2.4. By definition,

$$Y_T^{\alpha} - \nu_0 \left( Y_T^{\cdot} \right) = -\frac{1}{2} \int_0^T \left( K^{\alpha} \left( t \right)^2 - \nu_0 \left( K^{\cdot} \left( t \right)^2 \right) \right) \mathrm{d}t + \int_0^T \left( K^{\alpha} \left( t \right) - \nu_0 \left( K^{\cdot} \left( t \right) \right) \right) \mathrm{d}W_t.$$

Hence, by application of both Minkowski and Burkholder–Davis–Gundy inequalities, there exists a constant  $c_p$  such that

$$\|Y_T^{\alpha} - \nu_0(Y_T^{\cdot})\|_p \le \frac{1}{2} \left| \int_0^T \left( K^{\alpha}(t)^2 - \nu_0 \left( K^{\cdot}(t)^2 \right) \right) dt \right| + c_p \left| \int_0^T \left( K^{\alpha}(t) - \nu_0 \left( K^{\cdot}(t) \right) \right)^2 dt \right|^{\frac{1}{2}}.$$

Raising to the q-th power and applying Lemma 6.5.1 readily implies that

$$\|Y_T^{\alpha} - \nu_0(Y_T^{\cdot})\|_p^q \le \frac{1}{2} \left| \int_0^T \left( K^{\alpha}(t)^2 - \nu_0 \left( (K^{\cdot}(t))^2 \right) \right) dt \right|^q + 2^{q-1} c_p^q \left| \int_0^T \left( K^{\alpha}(t) - \nu_0 \left( K^{\cdot}(t) \right) \right)^2 dt \right|^{\frac{q}{2}}$$

From Propositions 6.2.2 and 6.2.3 along with Assumption  $\mathcal{A}$  6.2.3, we have the existence of two positive constants  $\tilde{c}_{T,p,q,H}$  and  $\bar{c}_{T,p,q,H}$  such that,

$$\int_{\mathcal{A}} \left| \int_{0}^{T} \left( K^{\alpha} \left( t \right)^{2} - \nu_{0} \left( \left( K^{\cdot} \left( t \right) \right)^{2} \right) \right) \mathrm{d}t \right|^{q} \nu_{0} \left( \mathrm{d}\alpha \right) \leq \tilde{c}_{T,p,q,H} \eta^{2q} \Delta^{q(2H\wedge1)},$$
$$\int_{\mathcal{A}} \left| \int_{0}^{T} \left( K^{\alpha} \left( t \right) - \nu_{0} \left( K^{\cdot} \left( t \right) \right) \right)^{2} \mathrm{d}t \right|^{\frac{q}{2}} \nu_{0} \left( \mathrm{d}\alpha \right) \leq \bar{c}_{T,p,q,H} \eta^{q} \Delta^{qH},$$

and observing that  $\Delta^{q(2H\wedge 1)} = \mathcal{O}(\Delta^{qH})$ , this concludes the proof.

Proof of Proposition 6.2.9. Recall that  $\nu_0 = \nu$ . To lighten notations, introduce

$$\Lambda\left(T,\Delta,H\right):=\frac{T^{2H+1}+\Delta^{2H+1}-\left(T+\Delta\right)^{2H+1}}{\Delta\left(2H+1\right)}$$

 $\triangleright$  Coefficient  $\gamma_1$ . Let  $\gamma_1 = \gamma_{10} + \gamma_{11}$  with

$$\gamma_{10} = \frac{1}{8} \int_{\mathcal{A}} \left( \int_{0}^{T} \left( K^{\alpha} (t)^{2} - \nu_{0} \left( K^{\cdot} (t)^{2} \right) \right) dt \right)^{2} \nu_{0} (d\alpha),$$
  
$$\gamma_{11} = \frac{1}{2} \int_{\mathcal{A}} \left( \int_{0}^{T} |K^{\alpha} (t) - \nu_{0} (K^{\cdot} (t))|^{2} dt \right) \nu_{0} (d\alpha).$$

It holds first that

$$\gamma_{10} = \frac{1}{8} \int_{\mathcal{A}} \left( \int_{0}^{T} \left( K^{\alpha} (t)^{2} - \nu_{0} \left( K^{\cdot} (t)^{2} \right) \right) dt \right)^{2} \nu_{0} (d\alpha)$$
$$= \frac{\eta^{4}}{32H^{2}\Delta} \int_{0}^{\Delta} \left| (T+x)^{2H} - x^{2H} + \Lambda (T, \Delta, H) \right|^{2} dx,$$

and  $\int_0^{\Delta} \left| (T+x)^{2H} - x^{2H} + \Lambda (T, \Delta, H) \right|^2 dx$  equals

$$\begin{split} &\int_{0}^{\Delta} \left( (T+x)^{4H} + x^{4H} + \Lambda \left(T, \Delta, H\right)^2 \right) \mathrm{d}x + 2\Lambda \left(T, \Delta, H\right) \int_{0}^{\Delta} (T+x)^{2H} \, \mathrm{d}x \\ &\quad -2\Lambda \left(T, \Delta, H\right) \int_{0}^{\Delta} x^{2H} \mathrm{d}x - 2\int_{0}^{\Delta} (T+x)^{2H} \, x^{2H} \mathrm{d}x \\ &= \frac{(T+\Delta)^{4H+1} + \Delta^{4H+1} - T^{4H+1}}{4H+1} + \Delta\Lambda \left(T, \Delta, H\right)^2 \end{split}$$

$$+ 2\Lambda (T, \Delta, H) \frac{(T + \Delta)^{2H+1} - T^{2H+1} - \Delta^{2H+1}}{2H + 1} - 2B_{1,2H+1} \Delta^{2H+1} T^{2H} {}_{2}F_{1} \left( -2H, 1 + 2H, 2(1 + H), -\frac{\Delta}{T} \right) = \frac{(T + \Delta)^{4H+1} + \Delta^{4H+1} - T^{4H+1}}{4H + 1} - \Delta\Lambda (T, \Delta, H)^{2} - 2B_{1,2H+1} \Delta^{2H+1} T^{2H} {}_{2}F_{1} \left( -2H, 1 + 2H, 2(1 + H), -\frac{\Delta}{T} \right).$$

For  $\gamma_{11}$ , evoke Tonelli's theorem to obtain

$$\begin{split} \gamma_{11} &= \frac{1}{2} \int_{0}^{T} \left( \nu_{0} \left( K^{\cdot} \left( t \right)^{2} \right) - \left( \nu_{0} \left( K^{\cdot} \left( t \right) \right) \right)^{2} \right) \mathrm{d}t \\ &= \frac{1}{2} \left( \frac{\eta^{2}}{\Delta} \int_{t=0}^{T} \int_{\alpha=T}^{T+\Delta} \left( \alpha - t \right)^{2H-1} \mathrm{d}\alpha \mathrm{d}t - \sigma_{\mathrm{P}}^{2} \right) \\ &= \frac{1}{2} \left( \frac{\eta^{2} \left( (T+\Delta)^{2H+1} - T^{2H+1} - \Delta^{2H+1} \right)}{2H \left( 2H+1 \right) \Delta} - \sigma_{\mathrm{P}}^{2} \right). \end{split}$$

 $\triangleright$  Coefficient  $\gamma_2$ . By definition,

$$\begin{split} \gamma_2 &= -\frac{1}{2} \int_{\mathcal{A}} \int_0^T \int_0^T \left( \nu_0 \left( K^{\cdot} \left( t \right) \right) K^{\alpha} \left( t \right) - \nu_0 \left( K^{\cdot} \left( t \right) \right)^2 \right) \left( K^{\alpha} \left( s \right)^2 - \nu_0 \left( K^{\cdot} \left( s \right)^2 \right) \right) \mathrm{d}t \mathrm{d}s \nu_0 \left( \mathrm{d}\alpha \right) \\ &= -\frac{1}{2} \int_{\mathcal{A}} \int_0^T \int_0^T \left( \nu_0 \left( K^{\cdot} \left( t \right) \right) K^{\alpha} \left( t \right) K^{\alpha} \left( s \right)^2 - \nu_0 \left( K^{\cdot} \left( t \right) \right) K^{\alpha} \left( t \right) \nu_0 \left( K^{\cdot} \left( s \right)^2 \right) \\ &- \nu_0 \left( K^{\cdot} \left( t \right) \right)^2 K^{\alpha} \left( s \right)^2 + \nu_0 \left( K^{\cdot} \left( t \right) \right)^2 \nu_0 \left( K^{\cdot} \left( s \right)^2 \right) \right) \mathrm{d}t \mathrm{d}s \nu_0 \left( \mathrm{d}\alpha \right) \\ &= -\frac{1}{2} \int_0^T \int_0^T \nu_0 \left( K^{\cdot} \left( t \right) \right) \nu_0 \left( K^{\cdot} \left( t \right) K^{\cdot} \left( s \right)^2 \right) \mathrm{d}t \mathrm{d}s + \frac{1}{2} \int_0^T \nu_0 \left( K^{\cdot} \left( t \right) \right)^2 \mathrm{d}t \int_0^T \nu_0 \left( K^{\cdot} \left( s \right)^2 \right) \mathrm{d}s \end{split}$$

The second term at the r.h.s. is given by

$$\frac{1}{2} \int_0^T \nu_0 \left( K^{\cdot}(t) \right)^2 \mathrm{d}t \int_0^T \nu_0 \left( K^{\cdot}(s)^2 \right) \mathrm{d}s = \frac{1}{2} \sigma_{\mathrm{P}}^2 \eta^2 \frac{(T+\Delta)^{2H+1} - T^{2H+1} - \Delta^{2H+1}}{2H \left(2H+1\right) \Delta}.$$

For the first term at the r.h.s. , observe first that

$$\nu_0 \left( K^{\cdot}(t) K^{\cdot}(s)^2 \right) = \frac{\eta^3}{\Delta} \int_T^{T+\Delta} (\alpha - t)^{H-\frac{1}{2}} (\alpha - s)^{2H-1} d\alpha$$
$$= \eta^3 \int_0^1 \left( T - t + \alpha' \Delta \right)^{H-\frac{1}{2}} \left( T - s + \alpha' \Delta \right)^{2H-1} d\alpha',$$

so that  $-\frac{1}{2}\int_0^T\int_0^T\nu_0\left(K^{\cdot}\left(t\right)\right)\nu_0\left(K^{\cdot}\left(t\right)K^{\cdot}\left(s\right)^2\right)\mathrm{d}t\mathrm{d}s$  is equal to

$$\begin{split} &-\frac{T^2\eta^4}{2\Delta\left(H+\frac{1}{2}\right)}\int_0^1\int_0^1\int_0^1\left(\left[\left(Tt'+\Delta\right)^{H+\frac{1}{2}}-\left(Tt'\right)^{H+\frac{1}{2}}\right]\right)\\ &\times\left(Tt'+\alpha'\Delta\right)^{H-\frac{1}{2}}\left(Ts'+\alpha'\Delta\right)^{2H-1}\right)\mathrm{d}t'\mathrm{d}s'\mathrm{d}\alpha'\\ &=-\frac{T\eta^4}{4\Delta H\left(H+\frac{1}{2}\right)}\int_0^1\int_0^1\left(\left[\left(Tt'+\Delta\right)^{H+\frac{1}{2}}-\left(Tt'\right)^{H+\frac{1}{2}}\right]\left(Tt'+\alpha'\Delta\right)^{H-\frac{1}{2}}\right)\\ &\times\left[\left(T+\alpha'\Delta\right)^{2H}-\left(\alpha'\Delta\right)^{2H}\right]\right)\mathrm{d}t'\mathrm{d}\alpha', \end{split}$$

and we get the announced claim for  $\gamma_2$ .  $\triangleright$  *Coefficient*  $\gamma_3$ . We have:

$$\gamma_{3} = \frac{1}{2} \int_{0}^{T} \int_{0}^{T} \nu_{0} \left( K^{\cdot}(t) \right) \nu_{0} \left( K^{\cdot}(s) \right) \int_{\mathcal{A}} \left( K^{\alpha}(t) - \nu_{0} \left( K^{\cdot}(t) \right) \right) \left( K^{\alpha}(s) - \nu_{0} \left( K^{\cdot}(s) \right) \right) d\alpha dt ds$$
$$= \frac{1}{2} \int_{0}^{T} \int_{0}^{T} \nu_{0} \left( K^{\cdot}(t) \right) \nu_{0} \left( K^{\cdot}(s) \right) \left[ \nu_{0} \left( K^{\cdot}(t) K^{\cdot}(s) \right) - \nu_{0} \left( K^{\cdot}(t) \right) \nu_{0} \left( K^{\cdot}(s) \right) \right] dt ds$$
$$= \frac{1}{2} \int_{0}^{T} \int_{0}^{T} \nu_{0} \left( K^{\cdot}(t) \right) \nu_{0} \left( K^{\cdot}(s) \right) \nu_{0} \left( K^{\cdot}(t) K^{\cdot}(s) \right) dt ds - \frac{\sigma_{P}^{4}}{2}.$$

Notice also

$$\nu_0 \left( K^{\cdot}(t) \, K^{\cdot}(s) \right) = \frac{\eta^2}{\Delta} \int_T^{T+\Delta} (\alpha - t)^{H-\frac{1}{2}} (\alpha - s)^{H-\frac{1}{2}} \, \mathrm{d}\alpha$$
$$= \eta^2 \int_0^1 \left( \alpha' \Delta + T - t \right)^{H-\frac{1}{2}} \left( \alpha' \Delta + T - s \right)^{H-\frac{1}{2}} \, \mathrm{d}\alpha',$$

so that

$$\begin{split} \gamma_{3} &= \frac{\eta^{4}T^{2}}{2\Delta^{2}\left(H + \frac{1}{2}\right)^{2}} \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \left[ \left(t'T + \Delta\right)^{H + \frac{1}{2}} - \left(t'T\right)^{H + \frac{1}{2}} \right] \left[ \left(s'T + \Delta\right)^{H + \frac{1}{2}} - \left(s'T\right)^{H + \frac{1}{2}} \right] \\ &\times \left(t'T + \alpha'\Delta\right)^{H - \frac{1}{2}} \left(s'T + \alpha'\Delta\right)^{H - \frac{1}{2}} dt' ds' d\alpha' - \frac{\sigma_{P}^{4}}{2} \\ &= \frac{\eta^{4}T^{2}T^{4H}}{2\Delta^{2}\left(H + \frac{1}{2}\right)^{2}} \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \left[ (t + \delta)^{H + \frac{1}{2}} - t^{H + \frac{1}{2}} \right] \left[ (s + \delta)^{H + \frac{1}{2}} - s^{H + \frac{1}{2}} \right] \\ &\times (t + \alpha\delta)^{H - \frac{1}{2}} (s + \alpha\delta)^{H - \frac{1}{2}} dt ds d\alpha - \frac{\sigma_{P}^{4}}{2}, \end{split}$$

where we have introduced  $\delta = \frac{\Delta}{T}$ . We have also,

$$\gamma_{31}(\alpha) := \int_0^1 s^{H+\frac{1}{2}} \left(s + \alpha\delta\right)^{H-\frac{1}{2}} \mathrm{d}s = \mathrm{B}_{1,H+\frac{3}{2}}\left(\alpha\delta\right)^{H-\frac{1}{2}} {}_2F_1\left(-H + \frac{1}{2}, H + \frac{3}{2}, H + \frac{5}{2}, -\frac{1}{\alpha\delta}\right) + \frac{1}{2} \mathrm{d}s$$

and introducing  $x = s + \alpha \delta$ ,

$$\begin{split} \gamma_{32}\left(\alpha\right) &:= \int_{0}^{1} (s+\delta)^{H+\frac{1}{2}} (s+\alpha\delta)^{H-\frac{1}{2}} \,\mathrm{d}s, \\ &= \int_{0}^{1+\alpha\delta} (x+(1-\alpha)\,\delta)^{H+\frac{1}{2}} \,x^{H-\frac{1}{2}} \,\mathrm{d}x - \int_{0}^{\alpha\delta} (x+(1-\alpha)\,\delta)^{H+\frac{1}{2}} \,x^{H-\frac{1}{2}} \,\mathrm{d}x \\ &= (1-\alpha)^{H+\frac{1}{2}} \,\delta^{H+\frac{1}{2}} \mathrm{B}_{1,H+\frac{1}{2}} \left[ (1+\alpha\delta)^{H+\frac{1}{2}} \,_{2}F_{1}\left(-H-\frac{1}{2},H+\frac{1}{2},H+\frac{3}{2},-\frac{1+\alpha\delta}{(1-\alpha)\,\delta}\right) \right. \\ &+ (\alpha\delta)^{H+\frac{1}{2}} \,_{2}F_{1}\left(-H-\frac{1}{2},H+\frac{1}{2},H+\frac{3}{2},-\frac{\alpha\delta}{(1-\alpha)\,\delta}\right) \right]. \end{split}$$

Finally, we get

$$\gamma_{3} = \frac{\eta^{4} T^{2} T^{4H}}{2\Delta^{2} \left(H + \frac{1}{2}\right)^{2}} \int_{0}^{1} \int_{0}^{1} \left[ \left(t + \frac{T}{\Delta}\right)^{H + \frac{1}{2}} - t^{H + \frac{1}{2}} \right] \left(t + \alpha \frac{T}{\Delta}\right)^{H - \frac{1}{2}} \left(\gamma_{32} \left(\alpha\right) - \gamma_{31} \left(\alpha\right)\right) \mathrm{d}t \mathrm{d}\alpha.$$

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ECOLE DOCTORALE DE MATHEMATIQUES HADAMARD

Titre : Approximations stochastiques pour les calculs de risques financiers

**Mots clés :** Monte Carlo multi-niveaux, Marge Initiale, Risk management, Mesures de risque de crédit, Métamodélisation, Décomposition en polynômes du chaos, Polynômes orthogonaux, Options américaines, VIX, Approximation faibles, Variance Forward.

**Résumé :** Dans cette thèse, nous examinons plusieurs méthodes d'approximations stochastiques à la fois pour le calcul de mesures de risques financiers et pour le pricing de produits dérivés. Comme les formules explicites sont rarement disponibles pour de telles quantités, le besoin d'approximations analytiques rapides, efficaces et fiables est d'une importance capitale pour les institutions financières. Nous visons ainsi à donner un large aperçu de ces méthodes d'approximation et nous nous concentrons sur trois approches distinctes.

Dans la première partie, nous étudions plusieurs méthodes d'approximation Monte Carlo multi-niveaux et les appliquons à deux problèmes pratiques : l'estimation de quantités impliquant des espérances imbriquées (comme la marge initiale) ainsi que la discrétisation des intégrales apparaissant dans les modèles rough pour la variance forward pour le pricing d'options sur le VIX. Dans les deux cas, nous analysons les propriétés d'optimalité asymptotique des estimateurs multi-niveaux correspondants et démontrons numériquement leur supériorité par

rapport à une méthode de Monte Carlo classique.

Dans la deuxième partie, motivés par les nombreux exemples issus de la modélisation en risque de crédit, nous proposons un cadre général de métamodélisation pour de grandes sommes de variables aléatoires de Bernoulli pondérées, qui sont conditionnellement indépendantes par rapport à un facteur commun X. Notre approche générique est basée sur la décomposition en polynômes du chaos du facteur commun et sur une approximation gaussienne. Les estimations d'erreur  $L_2$  sont données lorsque le facteur X est associé à des polynômes orthogonaux classiques.

Enfin, dans la dernière partie de cette thèse, nous nous intéressons aux asymptotiques en temps court de la volatilité implicite américaine et les prix d'options américaines dans les modèles à volatilité locale. Nous proposons également une approximation en loi de l'indice VIX dans des modèles rough pour la variance forward, exprimée en termes de proxys log-normaux et dérivons des résultats d'expansion pour les options sur le VIX dont les coefficients sont explicites.

**Title :** Stochastic approximations for financial risk computations

**Keywords :** Multilevel Monte Carlo, Initial Margin, Risk management, Credit risk measures, Meta-modeling, Polynomial Chaos Expansion, Orthogonal polynomials, American options, VIX, Weak approximations, Forward Variance.

**Abstract :** In this thesis, we investigate several stochastic approximation methods for both the computation of financial risk measures and the pricing of derivatives. As closed-form expressions are scarcely available for such quantities, the need for fast, efficient, and reliable analytic approximation formulas is of primal importance to financial institutions. We aim at giving a broad overview of such approximation methods and we focus on three distinct approaches.

In the first part, we study some Multilevel Monte Carlo approximation methods and apply them for two practical problems: the estimation of quantities involving nested expectations (such as the initial margin) along with the discretization of integrals arising in rough forward variance models for the pricing of VIX derivatives. For both cases, we analyze the properties of the corresponding asymptotically-optimal multilevel estimators and numerically demonstrate the superiority of multilevel methods compared to a standard Monte

Carlo.

In the second part, motivated by the numerous examples arising in credit risk modeling, we propose a general framework for meta-modeling large sums of weighted Bernoulli random variables which are conditionally independent of a common factor X. Our generic approach is based on a Polynomial Chaos Expansion on the common factor together with some Gaussian approximation.  $L_2$  error estimates are given when the factor X is associated with classical orthogonal polynomials.

Finally, in the last part of this dissertation, we deal with small-time asymptotics and provide asymptotic expansions for both American implied volatility and American option prices in local volatility models. We also investigate weak approximations for the VIX index in rough forward variance models expressed in terms of lognormal proxies and derive expansion results for VIX derivatives with explicit coefficients.