Heuristic Algorithms for Graph Coloring Problems

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Contents

General Introduction

Context

Graph vertex coloring problems are known to be very general and useful models to formulate numerous practical problems [Lewis, 2015]. Given an undirected graph $G = (V, E)$ with the vertex set $V = \{1, 2, \ldots, n\}$, the edge set $E \in V \times V$, graph vertex coloring problems typically involve assigning a color to each vertex of V such that two vertices linked by an edge must receive different colors while optimizing a given optimization objective.

This thesis focuses on four generalized graph coloring problems, namely the graph coloring problem (GCP), the equitable coloring problem (ECP), the weighted vertex coloring problem (WVCP) and the k-vertex critical subgraphs (k-VCS). The first one is the most basic graph coloring problem. The ECP requires that the sizes of two arbitrary color classes differ in at most one unit while the WVCP aims to minimize the sum of the largest weights of the vertices of each color class. The k-VCS is to find a subgraph H of G with minimum vertices such that removing any vertex from the subgraph H decreases its chromatic number.

These four problems are practically relevant since they have wide applications in real world such as garbage collection, load balancing, timetabling, scheduling, operating system, manufacturing, etc.

From the perspective of computational theory, graph coloring problems belong to the class of the NP-hard problems, meaning that optimal solutions cannot be found in polynomial time in the general case. For solving large and challenging problem instances, heuristic and metaheuristic approaches are commonly used with the purpose of finding sub-optimal solutions in reasonable time. In this thesis, we investigate hybrid metaheuristic approaches to effectively solve the four problems of interest aforementioned. Each proposed algorithm will be thoroughly documented with extensive computational experiments.

Objectives

One of the main objectives of this thesis is to develop high-performance hybrid metaheuristic algorithms that improve the state-of-the-art solutions for each problem considered. The main objective can be further divided into several specific objectives:

— Develop an effective reduction approach based on a backbone coarsening operator.
— Devise feasible and infeasible search algorithms that allow search process to cross the feasibility boundaries to explore the enlarged search space.
— Develop an adaptive mechanism to further control feasible and infeasible searches.
— Extend the removal strategy with backtracking mechanism to reconsider some removed vertices and investigate a perturbation strategy to escape local optima traps.
— Evaluate the proposed algorithms on a wide range of benchmark instance and perform a comprehensive comparison with the state-of-the-art algorithm.

Contributions

The main contributions of this thesis are summarized below:

— For the graph coloring problem, we proposed a reduction-based memetic algorithm (RMA) which integrates several original ingredients. First, we devise a backbone-based crossover operator to merge certain vertices. This operator aims to reduce the current graph and preserve common contributive objects that are shared by parent solutions. Second, to explore efficiently the search space around an offspring solution generated by the crossover operator, we propose a weighted tabu search algorithm, Finally, we apply a perturbation strategy to escape from the region of the local optimum. Experiment results on 39 popular DIMACS and COLOR02-04 benchmark instances, which are commonly used to test graph coloring algorithms in the literature, showed that RMA is competitive in terms of solution quality and run-time efficiency compared with state-of-the-art algorithms in the literature.

— For the equitable coloring problem, we propose a feasible and infeasible search algorithm (FISA). FISA combines an equity-feasible search phase where only equitable colorings are considered and an equity-infeasible search phase where the search is enlarged to include non-equitable solutions. To guide the equity-infeasible search phase (which is based on tabu search), we devise an extended fitness function that uses a penalty to discourage candidate solutions which violate the equity constraint. A perturbation procedure is adopted as a diversification method to help the algorithm explore new search regions. We assess the performance of the FISA algorithm on the set of 73 benchmark instances from DIMACS and COLOR competitions and present comparative results with respect to state-of-the-art algorithms. Computational results showed that FISA performs very well by finding 9 new upper bounds and matching the best-known results for the remaining instances except one case. This study demonstrates the benefit of examining both equity-feasible and equity-infeasible solutions for solving the ECP by using the mixed search strategy.

— For the weighted vertex coloring problem, we develop an adaptive feasible and infeasible search algorithm (AFISA). Like FISA, the proposed algorithm relies on a mixed search strategy exploring both feasible and infeasible solutions. To prevent the search from going too far away from the feasible boundary, we design an adaptive penalty-based evaluation function that is used to guide the search for an effective examination of candidate solutions, by enabling the search to oscillate between feasible and infeasible regions. To explore a given search zone, we rely on the popular tabu search meta heuristic [Glover, 1989; Glover, 1990]. We assess the proposed algorithm on 111 benchmark instances from literatures (one set of 46 instances from the DIMACS and COLOR competitions and two sets of 65 instances from matrix-decomposition problems). We report especially 5 improved best solutions (new upper bounds). We also present new results on an additional set of 50 larger instances.

— For the k-VCS problem, we propose an iterated backtrack-based removal (IBR) algorithm to solve it. IBR adopts the popular removal strategy that reduces current graph by tentatively moving vertices to the set of uncritical vertices. Although such an idea has been proved to be very effective for finding a k-VCS for a given graph G, the status of some vertices are sometimes irreversibly misclassified, leading to meaningless result. A backtracking mechanism is proposed to expand the current subgraph by adding back some vertices. We also devise a perturbation strategy to reconsider some vertices that would have been incorrectly identified as critical ones. Experiment results on 80 popular DIMACS and COLOR02-04 benchmark instances, which are commonly used to test k-VCS algorithms in the literature, show that IBR is very competitive in terms of solution quality and run-time efficiency compared with state-of-the-art algorithms in the literature. Specifically, the proposed algorithm improves the best-known solution for 9 graphs (improves the lower bound for 6 instances,

at the same k, IBR obtains a better solution (smaller size of k-VCS) for 8 instances), matches the best results for other 70 instances, and obtains a slightly worse result only in one case.

Organization

The manuscript is organized in the following way:

— In the first chapter, we introduce the four graph coloring problems considered in this thesis, i.e., graph coloring, equitable coloring, weighted vertex coloring and k-vertex-critical subgraphs. For each problem, we also provide a brief overview of solution methods, including approximation algorithms, exact algorithms and heuristic/metaheuristic algorithms.

— In the second chapter, we present the RMA algorithm for the graph coloring problem. We first describe in detail the main components of the proposed approach that integrates a greedy initial procedure, a backbone-based coarsening operator, a weight-based tabu search algorithm, an uncoarsening phase and the pool updating rule. Then, we present experimental results and comparisons with the state-of-the-art algorithms to show the efficacy of the proposed algorithm and discuss the impacts of some key components.

— In the third chapter, we study the equitable coloring problem. This chapter begins with a short introduction. After a detailed description of each component of the proposed FISA algorithm, we show experimental studies on a set of 73 benchmark instances to assess the effectiveness of the proposed FISA algorithm by comparing it with other best performing algorithms. An analysis of the key ingredients is presented allowing us to understand the behavior of all components in the proposed algorithm.

— In the fourth chapter, we consider the weighted vertex coloring problem and present the adaptive feasible and infeasible search algorithm (AFISA) to solve it. After introducing the main scheme of the proposed algorithm, we explain each of its internal components. Computational comparisons with other algorithms and analysis of different components are presented.

— In the last chapter, we present an iterated backtrack-based removal (IBR) heuristic to find k-VCS for a given graph. We firstly describe in detail the main components of the proposed approach including the removal strategy, a backtracking mechanism and a perturbation strategy. Then, we provide an experimental study of the new algorithms, as well as comparisons with state-of-the-art algorithms. Finally, we study some key ingredients of the proposed approach.

1

Introduction

Graph coloring problems are a class of well-known NP-hard combinatorial optimization problems with a wide range of applications. In this chapter, four graph coloring problems that are studied in this thesis are introduced: classic graph coloring, equitable coloring, weighted vertex coloring and k-vertex-critical subgraphs. A brief introduction for each problem is given first and then state-of-the-art approaches for solving these problems in the literature are reviewed.

Contents

1.1 Graph coloring problem

1.1.1 Problem Introduction

Given a simple undirected graph $G = (V, E)$ with vertex set $V = \{1, 2, \ldots, n\}$ and edge set $E \subset V \times V$, a legal k-coloring of G is a mapping $c : V \to \{1, \ldots, k\}$, such that $c(i) \neq c(j)$ for all edges (i, j) in E. The graph k-coloring problem (k-GCP) is to determine if a legal k-coloring of G exists for a given k. The classical graph coloring problem (GCP) is to find the minimum integer k (chromatic number $\chi(G)$) for which a legal k-coloring of G exists. k-GCP is known to be NP-complete while the optimization problem GCP is NP-hard [Garey and Johnson, 1979].

(a) A graph $G = (V, E)$ (b) A 3-coloring solution for graph G

Figure 1.1 – A graph and its a 3-coloring solution

The leftmost of Figure 1.1 shows an undirected graph G with five vertices $V = \{1, 2, \ldots, 5\}$ and a legal 3-coloring solution is shown in the rightmost. A graph coloring is to assign one color to each vertex. In this example, vertices 1 and 4 are colored grey, 3 and 5 are colored green, and 2 is colored orange. This 3-coloring is the optimal coloring of G and the chromatic number for this graph is 3.

The GCP can also be viewed as a grouping problem, in which a k-coloring corresponding to a grouping of the set of vertices into k groups such that no adjacent vertices i and j belong to the same group. For instance, the 3-coloring showing in the rightmost of Figure 1.1 can be represented as a grouping, i.e.,$\{1, 4\}$,$\{2\}$,$\{3, 5\}$.

k-GCP is a very popular NP-complete problem in graph theory [Garey and Johnson, 1979] and has attracted much attention from scholars. As one of the three target problems of several international competitions including the well-known Second DIMACS Implementation Challenge on Maximum Clique, Graph Coloring, and Satisfiability, GCP also arises naturally in a wide variety of real-world applications, such as register allocation [Chaitin, 1982], timetabling [Burke *et al.*, 1994; de Werra, 1985], frequency assignment [Gamst, 1986; Hale, 1980], scheduling [Leighton, 1979; Zufferey *et al.*, 2008]. Comprehensive reviews on graph coloring algorithms can be found in [Galinier *et al.*, 2013; Galinier and Hertz, 2006; Malaguti and Toth, 2010].

1.1.2 Exact algorithm

Exact algorithms for the graph coloring are often based on branch and bound/cut or branch and price procedures with linear programming relaxations. There is a wide variety of such approaches for graph coloring. Table 1.1 summarizes eight encodings of graph coloring, together with the corresponding integer programming formulations. Specifically, Coll et al. [Coll *et al.*, 2002], Zabala et al. [Méndez-Díaz and Zabala, 2006], and Méndez-Díaz et al.[Méndez-Díaz and Zabala, 2008] used a natural assignment-type formulation. Lee [Lee, 2002] and Lee and Margot [Lee and Margot, 2007] studied a binary encoded formulation. [Mehrotra and Trick, 1996] and [Schindl, 2004; Hansen *et al.*, 2009] have used formulations based on independent sets. [Williams and Yan, 2001] studied a formulation with precedence constraints. Barbosa et al. [Barbosa *et al.*, 2004] experimented with encodings based on acyclic orientations. Campêlo et al. [Campêlo *et al.*,

Table 1.1 – Integer programming formulations of graph coloring

Based on	Variables	Constraints	references
Vertices (Standard)	$k\|V\|$	$\|V\|+k\|E\|$	Méndez-Díaz and Zabala [Méndez-Díaz and Zabala, 2008] Zabala and Méndez-Díaz [Méndez-Díaz and Zabala, 2006] Coll et al. [Coll *et al.*, 2002]
Binary encoding	$\lceil log_2 k \rceil \|V\|$	Exp. many	Lee [Lee, 2002]
Max. independent sets	Exp. many	$\|V\|+1$	Mehrotra and Trick [Mehrotra and Trick, 1996]
Any independent sets	Exp. many	$\|V\|+1$	Hansen et al. [Hansen *et al.*, 2009]
Precedencies	$O(\|V\|2)$	$\|E\|$	Williams and Yan [Williams and Yan, 2001]
Acyclic orientations	$\|E\|$	Exp. many	Barbosa et al. [Barbosa *et al.*, 2004]
Asymmetric represent.	$O(\|E\|)$	$O(\|V\|\|E\|)$	Campêlo et al. [Campêlo *et al.*, 2008]
Supernodes	$k\|Q\|$	$\|Q\|+k\|E\|$	Edmund K. Burke et al.[Burke *et al.*, 2010]

2008; Campêlo *et al.*, 2009] proposed a formulation based on asymmetric representatives. [Burke *et al.*, 2010] introduced a new approach using "supernodes". [Malaguti *et al.*, 2011] proposed an exact algorithm based on the well-known set covering formulation of the problem. Zhou et al. [Zhou *et al.*, 2014] investigated an exact algorithm with learning which exploits the implicit constraints using propositional logic and presented very good computational results on DIMACS benchmark instances.

There have also been some studies on graph coloring by analyzing the graph structure or by decomposing the graph. For instance, [Rao, 2004] investigated the GCP by using a split decomposition tree, in which a graph is recursively partitioned into smaller graphs until they cannot be split anymore. Then, after coloring the prime graphs that cannot be split, solutions are combined gradually to get the solutions for the graph. [Bhasker and Samad, 1991] researched clique-partitioning for a graph based on the principle that graph coloring and clique partitioning are equivalent to some extent and presented two methods to partition cliques, which perform more effectively than some efficient graph coloring algorithms. [Lucet *et al.*, 2006] presented an exact graph coloring algorithm by linearly decomposing a graph, which can run faster than other exact algorithms when the linear width is small.

Moreover, there are many studies on the chromatic polynomial and the number of best solutions. [Read, 1968] got the chromatic polynomial by applying the traditional method "deletion contraction" that utilizes characteristics of chromatic polynomial to do the operations to the graph. [Lin, 1993] investigated an approximation algorithm to calculate the chromatic polynomial after obtaining its upper bound and lower bound, and had good performance in time complexity. [Martin, 2010] proposed Total solutions Exact graph Coloring algorithm (TexaCol), which can get all graph coloring solutions as well as the chromatic polynomial. TexaCol algorithm is realized by the way that the graph is decomposed into maximal cliques and the relationship between these maximal cliques is analyzed to get all coloring solutions. [Guo *et al.*, 2018] improved TexaCol by proposing two exact graph coloring algorithms, Partial best solutions Exact graph Coloring algorithm (PexaCol) and All best solutions Exact graph Coloring algorithm (AexaCol), which are able to obtain a best solution subset and all best solutions respectively. Based on TexaCol, these two algorithms adopt the backtracking method, in which only the best solution subset at each step is chosen to continue the coloring until partial or all best solutions are obtained.

1.1.3 Heuristic algorithm

Exact algorithms can encounter difficulties in many situations, for which the use of heuristic and metaheuristic techniques is necessary.

In what follows, we focus on some representative heuristic-based coloring algorithms.

Two well-known greedy algorithms DSATUR [Brélaz, 1979] and RLF [Leighton, 1979] employ refined rules to dynamically determine the next vertex to color. These greedy heuristic algorithms are usually fast. Consequently, they are often used as initialization procedures in hybrid

algorithms.

[Hertz and de Werra, 1987] proposed tabu search which is one of the most popular local search method for the GCP. The principle of the tabu search is to start from an initial solution and tries to improve the coloring by operating local changes. However, local search algorithms are often substantially limited by the fact that they do not exploit enough global information, and cannot compete with hybrid population-based algorithms. [Galinier and Hertz, 2006] summarized the local search algorithms for graph coloring. Thus, the tabu search is often used as a subroutine in hybrid algorithms, such as hybrid evolutionary algorithms [Fleurent and Ferland, 1996; Lü and Hao, 2010; Moalic and Gondran, 2015; Porumbel *et al.*, 2010].

Population-based hybrid algorithms [Galinier and Hao, 1999; Lü and Hao, 2010; Moalic and Gondran, 2015; Porumbel *et al.*, 2010; Titiloye and Crispin, 2011] are among the most effective approaches for graph coloring, which have reported the best solutions on most of the difficult DIMACS instances. Population-based hybrid approaches operate with multiple solutions by using operators called recombination or crossover or modification operators. Besides, to maintain the population diversity which is critical to avoid a premature convergence, population-based algorithms usually integrate dedicated diversity preservation mechanisms which require the computation of a suitable distance metric between solutions [Lü and Hao, 2010; Porumbel *et al.*, 2010]. Moreover, the success of hybrid algorithms mostly relies on the combination of a meaningful recombination operator, an effective local optimization procedure and a mechanism for maintaining population diversity.

[Hao and Wu, 2012; Wu and Hao, 2013] proposed "Reduce and solve" approaches. The general "Reduce and solve" framework typically combines a preprocessing phase and a coloring phase. The pre-processing phase identifies and extracts some vertices (typically independent sets) from the original graph and obtains a reduced graph. The coloring phase is then applied to determine a proper coloring for the reduced graph. Empirical results showed that "reduce and solve" approaches achieve a remarkable performance on some large and very large graphs. Though "Reduce and solve" approaches perform well for solving large graphs, it is less suitable for small and medium-scale graphs. Additionally, the success of those methods heavily depends on the vertices extraction process and the underlying coloring algorithm.

Other approaches include a method that encodes the GCP as a boolean satisfiability problem [Bouhmala and Granmo, 2008], a modified cuckoo algorithm [Mahmoudi and Lotfi, 2015], a grouping hyper-heuristic algorithm [Elhag and Özcan, 2015] a multi-agent based distributed algorithm [Sghir *et al.*, 2015] and a learning-based heuristic algorithm [Zhou *et al.*, 2018], etc.

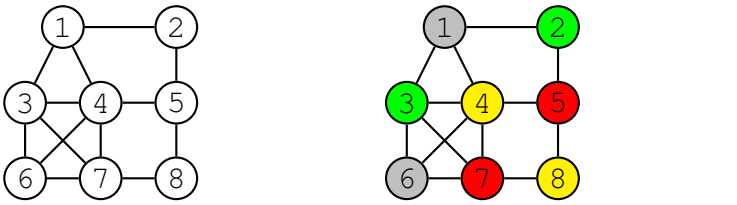
1.1.4 Summary

Given the NP-hardness of the GCP, exact algorithms are usually effective only for solving small or easy graphs. In fact, some graphs with as few as 150 vertices cannot be solved optimally by any exact algorithm [Malaguti *et al.*, 2011; Zhou *et al.*, 2014]. To deal with large and difficult graphs, heuristic algorithms are preferred to solve the problem approximately. The first work of this thesis is dedicated to developing an effective heuristic for handling the graph coloring problem. For this purpose, we propose a reduction-based memetic algorithm which integrates a greedy initial procedure, a backbone coarsening operator, a weighted tabu search algorithm, an uncoarsening phase and a pool updating mechanism. Although the evolutionary framework has been proved to be very useful for designing effective heuristics for the graph coloring problem, it is adopted for the first time in the context of the reduction approach based on the backbone-based coarsening operator.

1.2 Equitable coloring problem

Given an undirected graph $G = (V, E)$ with the vertex set V and the edge set $E \subset V \times V$, an independent set of G is a subset of V such that any pair of its vertices is not linked by an edge of E. An equitable legal k-coloring of G is a partition of the vertex set V into k disjoint independent sets (or stables) $\{V_1, V_2, \cdots, V_k\}$ such that $||V_i| - |V_j|| \leq 1, i \neq j, 1 \leq i, j \leq k$. This last constraint is called the equity constraint of a coloring. The equitable coloring problem (ECP) in graphs involves finding an equitable legal k-coloring with k minimum for general graphs. This minimum k is called the equitable chromatic number of G and denoted by $\chi_e(G)$.

As a variant of the conventional graph coloring problem (GCP), the decision version of the ECP is NP-complete. This can be proved by a straightforward reduction from graph coloring to equitable coloring by adding sufficiently many isolated vertices to a graph and testing whether the graph has an equitable coloring with a given number of colors [Furmanczyk and Kubale, 2004]. The ECP model has a number of practical applications related to garbage collection [Tucker, 1973], load balancing [Blazewicz *et al.*, 1997], timetabling [Kitagawa and Ikeda, 1988], scheduling [Meyer, 1973; Irani and Leung, 1996; Ding *et al.*, 2015] and so on.



(a) A graph G (b) An equitable coloring of a graph

Figure 1.2 – An example of equitable coloring of a graph

1.2.1 Theoretical Studies

Much effort has been devoted to theoretical studies of the ECP. For example, Meyer conjectured that $\chi_e(G) \leq \Delta(G)$ for any connected graph except the complete graphs and the odd circuits, where $\Delta(G)$ is the maximum vertex degree of G [Meyer, 1973]. This conjecture has been proved to be true for trees and graphs with $\Delta(G) = 3$ [Chen *et al.*, 1994], connected bipartite graphs [Lih and Wu, 1996], graphs with the average degree at most $\Delta/5$ [Kostochka and Nakprasit, 2005] and outerplanar graphs [Kostochka, 2002]. Bodlaender and Fomin [Bodlaender and Fomin, 2004] identified that the ECP can be solved in polynomial time for graphs with bounded treewidth. Furmańczyk and Kubale investigated the computational complexity of the ECP for some special graphs [Furmańczyk and Kubale, 2005]. Yan and Wang discussed the ECP for kronecker products of the complete multipartite graphs and complete graphs [Yan and Wang, 2014].

1.2.2 Exact approaches

From a perspective of solution methods for the ECP in the general case, several exact algorithms have been proposed.

[Diaza *et al.*, 2008] gave an integer programming formulation for the equitable coloring problem based on its polyhedral structure and developed a cutting plane algorithm. Experimental results indicate that the performance on 234 randomly generated graphs (with 35 nodes) has been improved compared to a pure Branch-and-Bound algorithm.

[Bahiense *et al.*, 2014] presented two new integer programming formulations based on representatives to derive a Branch-and-Cut algorithm for the equitable coloring problem. The computational experiments were carried out on randomly generated graphs, DIMACS graphs and other graphs from the literature. This algorithm outperforms the previously existing Branch-and-Cut approach by finding optimum solutions for random graphs with up to 70 nodes and obtaining a smaller average relative gap (UB-LB)/LB over all test instances.

[Méndez-Díaz *et al.*, 2014] studied the polytope associated with a 0/1-integer programming formulation for the equitable coloring problem, which found several families of valid inequalities and derives sufficient conditions in order to be facet-defining inequalities. Computational results show the efficacy of these inequalities used in a cutting-plane algorithm.

[Méndez-Díaz *et al.*, 2015] proposed a Dsatur-based algorithm and presented computational results for a subset of benchmark instances from the DIMACS and COLOR competitions. The Dsatur-based algorithm uses a pruning rule based on arithmetical properties related to equitable partitions, which has shown to be very effective. Experimental results show the effectiveness of the proposed algorithm by obtaining better solutions than other algorithms in the literature.

1.2.3 Heuristic approaches

Given the computational challenge of the ECP, exact algorithms suffer from an exponential time complexity and thus are only applicable to graphs of limited sizes (typically with less than 150 vertices). To handle larger graphs, heuristic algorithms are used to find sub-optimal solutions in a reasonable time frame.

Two constructive heuristics called Naive and SubGraph are given in [Furmanczyk and Kubale, 2004] to generate greedily an equitable coloring of a graph.

The TabuEqCol algorithm [Díaz *et al.*, 2014] is an adaptation of the well-known TabuCol algorithm for the classical graph coloring problem [Hertz and de Werra, 1987; Galinier and Hao, 1999]. Computational experiments show good performances of TabuEqCol on the benchmark instances.

The BITS algorithm [Lai *et al.*, 2015] improves TabuEqCol by embedding a backtracking scheme under the iterated local search framework. BITS uses a backtracking scheme to define different k-ECP instances, an iterated tabu search approach to solve each particular k-ECP instance for a fixed k and a binary search approach to find a suitable initial value of k. Computational results show that BITS is very competitive in terms of solution quality and computing efficiency compared to the TabuEqCol algorithm. Specifically, BITS obtains new upper bounds for 21 benchmark instances and matches the previous best upper bounds for the remaining instances.

The HTS algorithm [Wang *et al.*, 2018] relaxes the equity constraint step by step and repairs the infeasible result in the end. Based on three complementary neighborhoods, the algorithm alternates between a feasible local search phase where the search focuses on the most relevant feasible solutions and an infeasible local search phase where a controlled exploration of infeasible solutions is allowed by relaxing the equity constraint. A novel cyclic exchange neighborhood is also proposed in order to enhance the search ability of the hybrid tabu search algorithm. Evaluated on graphs, the proposed algorithm is demonstrated to be highly effective. Additional analysis shows the importance of the cyclic exchange operator and the feasible and infeasible local search to the success of the proposed algorithm.

1.2.4 Summary

One can observe that unlike the popular graph coloring problem for which many heuristic algorithms have been proposed, research on heuristics for the ECP is quite limited and is still in its infancy. In particular, one important feature of the problem identified by its equity constraint is little explored by the existing algorithms. On the other hand, it is well known that for constrained

optimization problems (like the ECP), allowing a controlled exploration of infeasible solutions may facilitate transitions between structurally different solutions and help discover high-quality solutions that are difficult to locate if the search is confined to the feasible region [Glover and Hao, 2011]. Thus, in this thesis, we investigate a feasible and infeasible search algorithm for the ECP which enlarges the search to include equity-infeasible solutions. Furthermore, to prevent the search from going too far away from the feasible boundary, we devise an extended penalty-based fitness function to guide the search for an effective examination of candidate solutions.

1.3 Weighted vertex coloring problem

Graph vertex coloring problems can also concern weighted graphs where a weight (typically a positive value) is associated to each vertex. The Weighted Vertex Coloring Problem (WVCP) considered in this work is a typical example of this class of coloring problems. Informally, the WVCP aims to find a legal coloring such that the sum of the costs of its stables is minimized, where the cost of each stable is given by the maximum weight of a vertex (representative) in that stable.

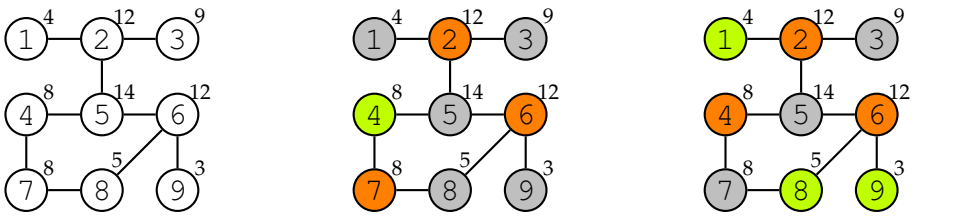
Given an undirected graph $G = (V, E)$ with the vertex set $V = \{1, 2, \ldots, n\}$, the edge set $E \in V \times V$, let $W = \{w_1, w_2, \ldots, w_n\}$ be the set of positive weights associated to the vertices of V. Recall that an independent set (a stable or a color class) of G is a subset of V such that any pair of its vertices is not linked by an edge of E. A legal or feasible k-coloring of G is a partition of the vertex set V into k disjoint independent sets $\{V_1, V_2, \ldots, V_k\}$. Let $s = \{V_1, V_2, \ldots, V_k\}$ be a partition of the vertex set V, the Weighted Vertex Coloring Problem can be stated as follows.

$$(WVCP) minimize \quad f(s) = \sum_{i=1}^{k} max_{j \in V_i}\{w_j\} \tag{1.1}$$

$$subject\ to\ \forall u, v \in V_i, \{u, v\} \notin E, i = 1, 2, \ldots, k \tag{1.2}$$

where the constraints (1.2) ensure that partition $\{V_1, V_2, \ldots, V_k\}$ is a legal k-coloring (i.e., each V_i $(i = 1, 2, \ldots, k)$ is a stable) and the objective (1.1) is to minimize the maximum weight of a vertex (representative) in each of the k stables V_i $(i = 1, 2, \ldots, k)$. Notice that for a given graph, the number of colors k is unknown before the optimal solution is discovered.

Figure 1.3(a) shows a graph $G = (V, E)$ with 9 vertices whose weights are indicated next to the vertices. Figure 1.3(b) shows a coloring with three stables, leading to an objective value of 14 + 12 + 8 = 34, since the three stables have respectively a maximum weight of 14 (gray stable), 12 (orange stable) and 8 (green stable). Figure 1.3(c) illustrates an optimal solution with a minimum objective value of 14 + 12 + 5 = 31.



(a) A graph $G = (V, E)$ (b) A feasible coloring (c) An optimal solution

Figure 1.3 – A graph, a feasible solution, an optimal solution

One notices that an instance of the NP-hard vertex coloring problem can be conveniently reduced to an instance of the WVCP by defining a weight of 1 for each vertex. As a result, the WVCP is NP-hard [Malaguti, 2009; Michael and David, 1979], and thus computationally challenging in the general case. From a practical perspective, the WVCP has a number of practical applications in different fields and arises naturally in the context of buffer management in operating systems [Prais and Ribeiro, 2000; Ribeiro *et al.*, 1989], batch scheduling [Gavranovic and Finke, 2000] and manufacturing [Hochbaum and Landy, 1997]. As a result, effective solution methods for the WVCP can help to solve these practical problems.

1.3.1 Exact approaches

From a perspective of solution methods for the WVCP in the general case, several exact algorithms have been proposed.

Specifically, a column generation approach combined with the general branch-and-bound method was investigated in [Ribeiro *et al.*, 1989]. Extensive computational experiments were reported for the matrix decomposition problem encountered in satellite switching systems, showing the effectiveness of this approach.

A branch-and-price approach based on column generation was presented in [Furini and Malaguti, 2012] and computational results were shown on a subset of benchmark instances from the DIMACS and COLOR competitions and two sets of instances from matrix-decomposition problems, which shows excellent performances when compared with the best heuristic algorithms from the literature.

In [Cornaz *et al.*, 2017], the WVCP was solved as Maximum Weight Stable Set Problems on an associated graph and this approach showed excellent results on the tested benchmark graphs.

The above review indicates that despite the theoretical and practical significance of the WVCP, solution methods for the problem are quite limited and the WVCP benchmark instances are of small sizes in comparison with those used for other graph coloring problems.

1.3.2 Heuristic approaches

Given that the WVCP is a NP-hard problem, several heuristic algorithms have also been investigated, which aim to provide high-quality solutions in acceptable computation time, but without provable optimal guarantee of the attained solutions.

For example, a Greedy Randomized Adaptive Search Procedure (GRASP) was introduced in [Prais and Ribeiro, 2000] in the context of a practical problem called TDMA traffic assignment (an application of the WVCP). This algorithm iterates a mixed search strategy combining a randomized greedy construction procedure followed by a local optimization procedure. Extensive computational experiments indicate that the Reactive GRASP heuristic matches the optimal solution found by an exact column generation based branch-and-bound algorithm.

In [Malaguti *et al.*, 2009], an effective 2_*Phase* algorithm was proposed, where in the first phase a large number of independent sets is heuristically produced, and in the second phase the set covering problem associated with these sets is solved by the Lagrangian heuristic algorithm introduced previously in [Caprara *et al.*, 1999]. These heuristics have reported interesting results on a number of benchmark instances. However, one notices that these methods only examine feasible solutions.

1.3.3 Summary

Our literature review given in Section 1.3.1 and 1.3.2 indicates that unlike the popular vertex coloring problem for which numerous solution methods are available (see the reviews [Galinier

and Hertz, 2006; Malaguti and Toth, 2010; Galinier *et al.*, 2013]), research on algorithms for the WVCP is still in its infancy with very few advanced methods.

In this work, we aim to fill the gap by investigating effective heuristics that can be used to find high-quality approximate solutions for problem instances that cannot be solved exactly.

Our interest on heuristics for the WVCP is fully motivated by the hardness of the considered problem. Indeed, unless P =NP , exact algorithms for the WVCP will inevitably have an exponential time complexity and can only be applied to solve problem instances of limited sizes or with particular features.

Our work focuses on investigating a feasible and infeasible search procedure and is driven by the following consideration. The WVCP is a constrained combinatorial optimization problem where a feasible solution must satisfy the coloring constraint (i.e., two adjacent vertices must receive different colors). Due to the presence of the coloring constraint, the feasible region can be broken into several zones which are separated from each other by infeasible regions in the search space. In this case, an algorithm searching only feasible solutions could be blocked in a particular feasible zone, thus miss the global optima or high quality solutions located in other feasible zones. On the other hand, as illustrated in numerous studies on constrained optimization, e.g., [Chen *et al.*, 2016b; Glover and Hao, 2011; Jin and Hao, 2016; Lai *et al.*, 2018; Lin, 2013; Martinez-Gavara *et al.*, 2017; Sun *et al.*, 2017; Wang *et al.*, 2018], methods that are allowed to oscillate between feasible and infeasible regions constitute an appropriate means to cope with such a situation. Indeed, allowing a controlled exploration of infeasible solutions may facilitate transitions between structurally different solutions and help discover high-quality solutions that are difficult to locate if the search is limited to the feasible region. Based on previous studies of examining feasible and infeasible solutions for solving other constrained optimization problems, we present in this thesis the first study that mixes both feasible and infeasible searches with the context of the WVCP.

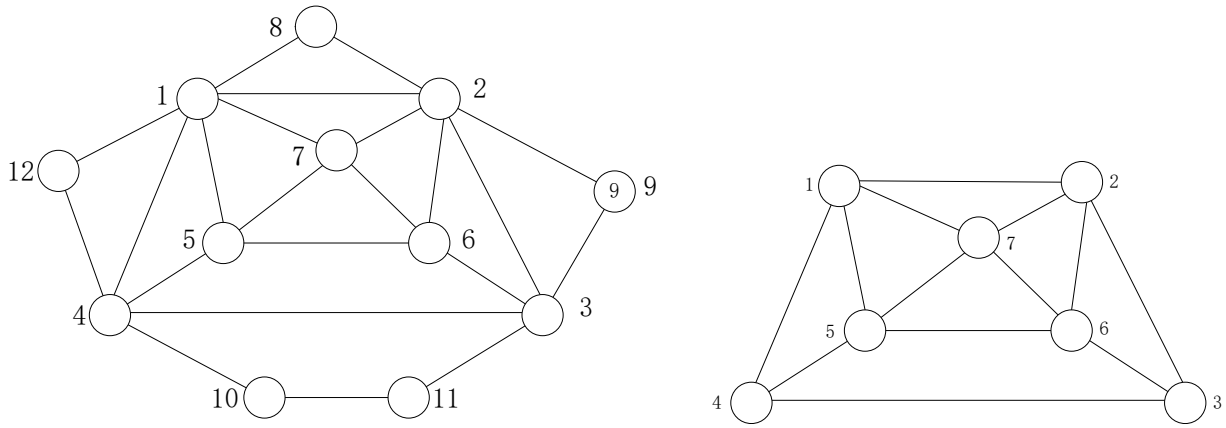
1.4 k-vertex critical subgraphs problem

1.4.1 Problem Introduction

A graph is a vertex-critical graph if removing any vertex from the graph decreases its chromatic number [Desrosiers *et al.*, 2008]. Given an integer k, a k-vertex-critical subgraph (k-VCS) of G is a vertex-critical subgraph H such that $\chi(H) = k$. Note that each graph G contains at least one k-VCS for $1 \leq k \leq \chi(G)$. Finally, a subgraph H^* is a minimum k-VCS if no other k-vertex-critical subgraph with fewer vertices than in H^* exists in G. The k-VCS problem (k-VCSP) is to find a minimum k-vertex-critical subgraph of G. The k-VCSP is a NP-hard problem and thus computationally challenging [Desrosiers *et al.*, 2008]. For simplicity, if $H = (A, E_A)$ is a k-VCS, we also use its vertex set A to denote the k-VCS.

The k-VCS problem has important theoretical significance and large application potential. For instance, The k-VCS problem helps to find lower bounds on the chromatic number of these graphs and identify hard or unsolvable subproblems that help the tractability of satisfiability testing of the real world applications [Herrmann and Hertz, 2002; Hu *et al.*, 2011].

As an example, consider the graph G of Figure 1.4(a) with $\chi(G) = 4$. Figure 1.4(b) shows a 4-vertex-critical subgraph of G since removing any vertex decreases its chromatic number to 3. Moreover, this 4-VCS is also minimum since no other 4-critical subgraph can be found in G. Note that k-VCS of G provides a means of determining lower bounds of $\chi(G)$, and a k-VCS with a larger k thus leads to a better (tighter) bound (eg., the 4-VCS of Figure 1.4(b) corresponds to a better lower bound with respect to any 3-VCS formed by a clique of size 3 like {1,2,7}).



(a) A graph with chromatic number of 4 (b) A 4-vertex-critical subgraph

Figure 1.4 – An example for the 4-vertex-critical subgraph.

1.4.2 Exact approaches

In [Herrmann and Hertz, 2002], Herrmann and Hertz suggested a vertex removal algorithm combined with an insertion algorithm to find the chromatic number of a graph. Computational experiments on random graphs and on DIMACS benchmark problems demonstrate that the proposed algorithm can solve larger problems than previous known exact methods.

1.4.3 Heuristic approaches

In the context of graph coloring, some approaches have been proposed to extract k-VCS in a graph.

[Eisenberg and Faltings, 2003] presented two breakout algorithms to identify hard and unsolvable subgraph in a graph. The first approach uses the breakout with backtracking (BOBT) algorithm to solve constraint satisfaction problems or identify an unsolvable subproblem if it exists, the second algorithm is the breakout with backtracking for a smallest unsolvable subproblem (BOBT-SUSP) that identifies a k-VCS. Evaluated on randomly generated graph 3-coloring problems, the proposed algorithm is demonstrated to be highly effective in discovering high quality solutions.

[Desrosiers *et al.*, 2008] proposed the neighborhood weight heuristic algorithm that is combined with classical critical subgraph detection algorithms, leading to several effective k-VCS detection heuristics including the $Ins + h$ algorithm. Computational experiments are reported on random and DIMACS benchmark graphs to compare the proposed algorithms, as well as to find lower bounds on the chromatic number of these graphs. Computational testing shows that this algorithm improves the best known lower bound for some of these graphs and is even able to determine the chromatic number of some graphs for which only bounds were known previously.

1.4.4 Summary

Although many exact algorithms have been devised for the graph coloring, they can only be used to solve small instances. Heuristics coloring algorithms can be used on much larger instances, but only to get an upper bound on the chromatic number $\chi(G)$. Given that the removal strategy is quite effective for this problem, the last work of this thesis is to design a removal strategy with a backtracking mechanism and a perturbation procedure to solve the k-VCS in an efficient way.

2

A reduction-based memetic algorithm for GCP

In this chapter, we investigate a reduction-based memetic algorithm (RMA) to find a graph coloring solution for a given graph G. Graph coloring is one of the most studied NP-complete problems. Given a graph $G = (V, E)$, the task is to partition the vertex set V into k disjoint subsets, such that no edge has endpoints in the same subsets. In this work, we present a memetic algorithm, which integrates a backbone-based coarsening operator (to preserve common information and reduce the size of graph), a weighted tabu search procedure (to improves the quality of the solution of the reduced graph) and a perturbation procedure (to escape from the region of the local optimum). Extensive experimental studies on numerous benchmark instances from the graph coloring problem show that the proposed approach, performs equally well as some best existing graph algorithms in terms of solution quality.

Contents

2.1 Introduction

Given a simple undirected graph $G = (V, E)$ with vertex set $V = \{1, 2, \ldots, n\}$ and edge set $E \subset V \times V$, a legal k-coloring of G is a mapping $c : V \rightarrow \{1, \ldots, k\}$, such that $c(i) \neq c(j)$ for all edges (i, j) in E. The graph k-coloring problem (k-GCP) is to determine if a legal k-coloring of G exists for a given k. The classical graph coloring problem (GCP) is to find the minimum integer k (chromatic number $\chi(G)$) for which a legal k-coloring of G exists. k-GCP is known to be NP-complete while the optimization problem GCP is NP-hard [Garey and Johnson, 1979].

Since memetic algorithms have been proved to be very effective for solving coloring problems [Galinier and Hao, 1999; Porumbel *et al.*, 2010; Lü and Hao, 2010; Malaguti *et al.*, 2008; Moalic and Gondran, 2015], in this chapter, we introduce the Reduction-based Memetic Algorithm that integrates the idea of multilevel optimization [Benlic and Hao, 2011; Walshaw, 2004] within the memetic search framework.

In this work, we adopt for the first time the idea of reduction in a memetic algorithm for the GCP. For this purpose, we address three relevant issues which are critical to make our approach successful. First, we need to identify the previous common information of the parents which is contained in high quality solutions. Second, we want to reduce the original graph to a smaller graph through the common information, i.e., common fragment showed in the parents can be merged into one vertex. Third, we wish to search effectively the reduced graph. RMA uses a backbone-based group matching mechanism for identifying common information of the parents. By incorporating this mechanism, RMA merges identical information fragment (with at least two vertices) to form one vertex. The weighted tabu search algorithm examines the reduced graph to further improve the solution.

Computational results on 39 benchmark graphs from the DIMACS and COLOR competitions show that RMA competes favorably with state-of-the-art algorithms in the literature in terms of solution quality. Specifically, RMA obtains the best-know results for 19 easy instances with an improvement of the computation time and matches the best-known results for 13 difficult instances.

The rest of the chapter is organized as follows. Section 2.2 describes the proposed algorithm in detail. Section 2.3 presents computational results and comparisons with state of the art algorithms. Section 2.4 analyzes the impact of some key components of the proposed algorithm. Conclusions and future work are discussed in the last section.

2.2 Memetic algorithm for the GCP

The conventional GCP can be approximated by finding a series of legal k-colorings for decreasing k values[Galinier and Hertz, 2006; Galinier *et al.*, 2013]. This process is repeated until no legal k-coloring can be found. Therefore, we will only consider the k-coloring problem in the rest of this section. To seek a legal k-coloring for a given k, we adopt the memetic search which is a powerful framework that promotes the idea of combining evolutionary computing and local optimization.

In this section, we propose a way of collapsing vertices based on common information and the resulting RMA algorithm for solving k-GCP.

2.2.1 General approach

As shown in Algorithm 2.1, RMA starts from an initial solution S_i generated by the greedy procedure and further ameliorated by the iterated tabu search procedure described in Section 2.2.2. The initialization process repeats p times in order to generate the parent solutions (lines

Algorithm 2.1: The RMA algorithm for solving the k-GCP

1: **Input**: Graph $G = (V, E)$, number of colors k, population size p.
2: **Output**: the best k-coloring S^* found so far
3: **for** $i = 1, 2, \ldots, N$ **do**
4: $w_i \leftarrow 1$/ * Initialize the weight of each edge */
5: **end for**
6: **for** $i = 1, 2, \ldots, p$ **do**
7: $S_0 \leftarrow Greedy\_Initial(G, k)$ /*Greedy Initialization, Section 2.2.2 */
8: $S_i \leftarrow Tabu\_Search(G, S_0, k)$ /* Tabu search, Section 2.2.2 */
9: $S_{best} \leftarrow S_i$ /*Record the best legal solution at each loop */
10: **end for**
11: $S^* \leftarrow arg\,minF(S_i), i = 1, 2, \ldots, p$ /* Record the best solution S^* found so far*/
12: **while** stop condition met **do**
13: $S_0 \leftarrow Adaptive\_MultiParent\_Crossover$ /*Initialize offspring solution S_0, Section 2.2.3*/
14: $Randomly\ choose\ 2\ individuals\ solution\ S_m, S_n\ from\ parents\ set\ P$
15: $(G', S_0', w) \leftarrow Backbone\_Coarsening\_Operator(S_m, S_n, G, S_0)$ /* Section 2.2.4*/
16: $S_{best}' \leftarrow Weighted\_Tabu\_Search(G', S_0', k, w)$ /*Section 2.2.5*/
17: $(G, S_c) \leftarrow Uncoarsening\_Perturbation(G', S_{best}')$ /* Section 2.2.6*/
18: $S_{best} \leftarrow Tabu\_Search(G, S_c, k)$ /* Future improve the solution, Section 2.2.6*/
19: **if** $f(S_{best}) < f(S^*)$ **then**
20: $S^* \leftarrow S_{best}$
21: **end if**
22: $\{S_1, S_2, \ldots, S_p\} \leftarrow Pool\_Updating(S_{best}, S_1, \ldots, S_p)$ /*Section 2.2.7*/
23: **end while**

6-10). After initializing the global variable best solution S^* found so far (line 11), the search enters into the evolution loop. It repeats an evolution process to improve the population until a predefined stopping condition (typically a fixed number of generations) is verified or a legal coloring is found. At each generation, the algorithm randomly selects two parent solutions S_m, S_n from the population. Then, we obtain a coarsening graph G' from G with its corresponding coloring S_0' and the weight set w by using a backbone coarsening operator (line 15, Section 2.2.4). This coarsening phase is followed by a weighted tabu search in order to improve the solution (line 16, Section 2.2.5). The uncorsening phase, which recovers the initial graph G from G' with its corresponding coloring, uses a slight perturbation of the corresponding coloring to escape from the local optimal solution (line 17, Section 2.2.6). This newly generated coloring is further improved by the iterated tabu search process (line 18, Section 2.2.6). Finally, a quality-and-distance based rule is applied to decide if the improved solution can be inserted into the population (line 22, Section 2.2.7).

In the remainder of this section, we explain the main components of the proposed RMA algorithm: the initial population generator, the iterated tabu search procedure, the backbone-based coarsening operator, the weighted tabu search process and the population updating strategy.

2.2.2 Population initialization

The purpose of the initialization step is to generate an initial coloring with as few conflicts as possible for the given k-GCP problem. This is achieved by two steps: the greedy algorithm proposed in [Glover *et al.*, 1996] and the tabu search in [Galinier and Hao, 1999].

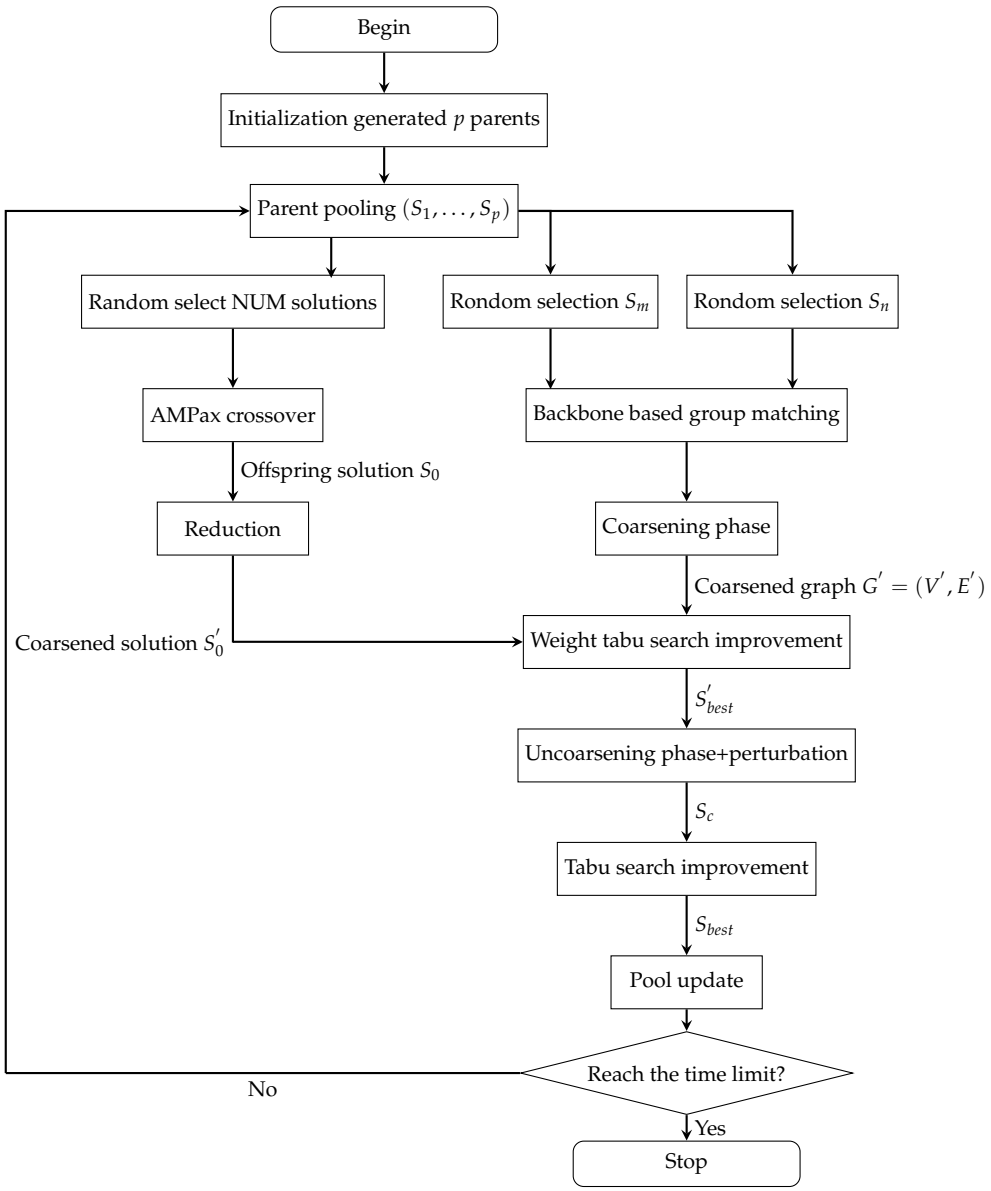


Figure 2.1 – Flow chart of RMA algorithm for solving the k-GCP.

Greedy initialization

RMA constructs an initial solution according to the greedy constructive heuristic (called DANGER), which was first proposed in [Glover *et al.*, 1996], and subsequently was used in several studies [Lü and Hao, 2010].

To create each individual of the initial population, we assign a vertex from the set of unassigned vertices a color class at one time. Specifically, we firstly use a scoring function according to the dynamic vertex danger measure to score the unassigned vertices. Given these scores, an unallocated vertex with the highest score is probabilistically selected. Next, the scores of the colors for the selected vertex are calculated according to the possibility that this colors are required by neighboring vertices. Finally, a color is choosen probabilistically. This process is repeated until all vertices are assigned a color.

Afterwards, in order to further optimize the solution constructed by the DANGER procedure, we apply an iterated tabu search (Section 2.2.2), previously presented in [Galinier and Hao, 1999]. The refinement step is essential for our approach to improve progressively the quality of the initial solution, which also helps the memetic algorithm to save some computational efforts during the first generations of its search. This initialization procedure is iterated until the population is filled

with p (population size) individuals (Algorithm 2.1, lines 6-10).

The iterated tabu search

(1) Search space and fitness function

Before presenting the ingredients of the tabu search process, we first define the search space Ω_k explored by the algorithm, the evaluation function $f(s)$ to measure the quality of a candidate solution and the solution representation used by the RMA algorithm.

For a given graph $G = (V, E)$ with k available colors, the search space Ω_k visited by RMA is composed of all allocations of vertices to the k color class. In other words, the RMA algorithm visits all the k-colorings. Then the search space is given by:

$$\Omega_k = \{\{V_1, V_2, \cdots, V_k\} : \cup_{i=1}^{k} V_i = V, V_i \cap V_j = \emptyset\} \tag{2.1}$$

where $i \neq j, 1 \leq i, j \leq k$.

A candidate solution in Ω_k can be represented by $s = \{V_1, V_2, \ldots, V_k\}$ such that V_i is the group of vertices receiving the same color i. For any candidate solution $s \in \Omega_k$, its quality is evaluated directly by the fitness function $f(s)$, which is used to count the conflicting edges induced by s.

$$f(s) = \sum_{i=1}^{k} |C(V_i)| \tag{2.2}$$

where $C(V_i)$ is the set of conflicting edges in color class V_i. Accordingly, a coloring s with $f(s) = 0$ corresponds to a legal k-coloring. The objective of RMA is to minimize f, i.e., the number of conflicting edges to find a legal k-coloring in the search space.

(2) Move operators to explore the space Ω_k

One of the most critical features of local search is the definition of its neighborhood. Typically, a neighborhoods is defined by a move operator which transforms a current solution $s = \{V_1, V_2, \ldots, V_k\}$ to generate a neighboring solution by some local changes of s. To explore the search space Ω_k, the search phase employs one basic move operator to generate neighboring solutions which displaces a conflicting vertex v from its current color class V_i to another color class V_j. The neighborhood $N(s)$ induced by this operator is given by:

$$N(s) = \{s \oplus < v, V_i, V_j >: v \in V_i \cap C(s), 1 \leq i, j \leq k, i \neq j\} \tag{2.3}$$

where $C(s)$ denotes the set of conflicting vertices of s, i.e., the vertices involved in a conflicting edge.

Clearly $N(s)$ is bounded by $O(|C(s)| \times k)$ in size. To effectively calculate the move gain that identifies the change in the fitness function f (Equation (2.2)), we adopt the fast incremental evaluation technique of [Dorne and Hao, 1999; Fleurent and Ferland, 1996; Galinier and Hao, 1999]. The main idea is to maintain a matrix A of size $n \times k$ with elements $A[v][q]$ recording the number of vertices adjacent to v in color class V_q $(1 \leq q \leq k)$. Then, the gain of each one-move in terms of fitness variation can be efficiently calculated as

$$\Delta f = A[v][j] - A[v][i] \tag{2.4}$$

Each time a one-move operation involving the vertex v is performed, we just need to update a subset of values affected by this move as follows. For each vertex u adjacent to vertex v, $A[u][i] \leftarrow A[u][i] - 1$, and $A[u][j] \leftarrow A[u][j] + 1$.

2.2.3 The adaptive multi-parent crossover procedure

The AMPaX operator is proposed in [Lü and Hao, 2010] which builds one by one the color classes of the offspring. Firstly, we chose $NUM = 2 + rand()\%4$ parents for the population pool. Each time the color class with the maximal cardinality in all NUM parent individuals is chosen, in order to transmit as more vertices as possible such that the number of unassigned vertices after k transmitting steps is as small as possible. After one color class has been assigned, all the vertices in this color class are removed from all parents. This process is repeated until all k color classes are built. At the end of these k steps, some vertices may remain unallocated. These vertices are randomly assigned to a color class. Thus, offspring solution S_0 is constructed.

This crossover step of creating an offspring solution S_0 is essential for our approach, which helps the weight coloring algorithm to improve progressively the quality of the initial solution and saves some computational efforts during its search (Section 2.2.5).

2.2.4 Backbone-based group matching

Algorithm 2.2: The backbone-based collapsing algorithm

Input: two parent solutions $S_m = \{V_1^m, V_2^m, \ldots, V_k^m\}$ and $S_n = \{V_1^n, V_2^n, \ldots, V_k^n\}$.
Output: a matching scheme J
$J \leftarrow \emptyset$
/*Match the set of the vertices*/
Let $H = \{(V_i^m, V_j^n) \mid i \in k, j \in k\}$ *denote the set of all* $k \times k$ *group combinations of* S_m *and* S_n.
Compute the number of common vertices for each group combination $(V_i^m, V_j^n) \in H$
repeat
  Choose the combination $\{(V_i^m, V_j^n)\}$ *with the largest* $\omega_{V_i^m, V_j^n}$ *from* H
  $J \leftarrow J \cup \{(V_i^m, V_j^n)\}$
  $H \leftarrow H \setminus \{(V_i^m, V_j^n)\}$
  Remove from E all combinations associated with V_i^m *and* V_j^n
until $H = \emptyset$

Our backbone-based coarsening operator is composed of two steps: backbone-based group matching and coarsening phase, whose components are detailed in the following sections.

We introduce the following basic definitions which are helpful for the description of the proposed approach. Let $S_m = \{V_0^m, V_1^m, ..., V_k^m\}$ and $S_n = \{V_0^n, V_1^n, ..., V_k^n\}$ be two parent solutions respectively.

Definition 2.2.1. The *set of common objects* H denotes tthe set of common objects that has identical object grouping of S_m and S_n , i.e., $H = \{(V_i^m, V_j^n) | i \in k, j \in k\}$ denote the set of all $k * k$ group combinations o f S_m and S_n.

Definition 2.2.2. The *Backbone matching set* $J = \{(V_i^m, V_j^n), 1 \leq i, j \leq k\}$ denotes the largest set of common objects for each color of two parents S_m and S_n. We apply a fast greedy algorithm to seek a near-optimal backbone matching.

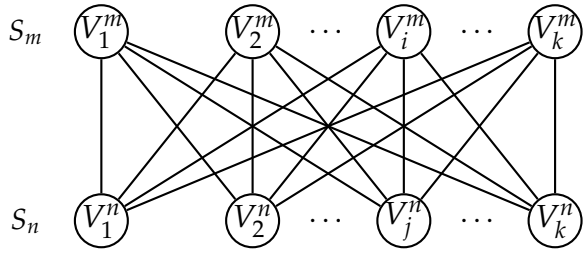
At the first step, the algorithm randomly selects two parent solutions S_m, S_n from the population and matches them by using a backbone-based group matching operator, thus gets the matching scheme J. According to the identical information set, we merge each identical information fragment $I_i = V_i \cap V_j, (V_i^m, V_j^n) \in J, 1 \leq i, j \leq k$ to one coarsened vertex which ends up with the coarsening graph $G^{'}$ (see Figure 2.4 for an illustrative example).

Backbone-based group matching

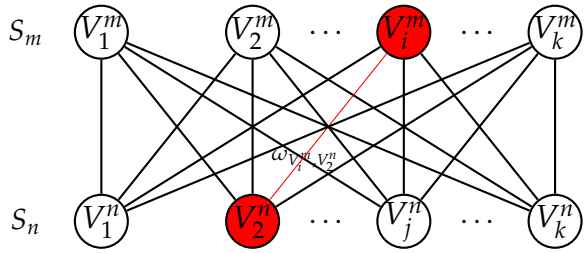
Apart from the local optimization procedure, group matching is another key component for our RMA algorithm. A successful group matching operator should be able to transmit the meaningful features from parents to offspring and offer some diversity.

As described in Section 2.1, a solution can be regarded as a partition of N vertices into k classes. It is more significant to manipulate classes of vertices than individual vertex when transmitting useful information.

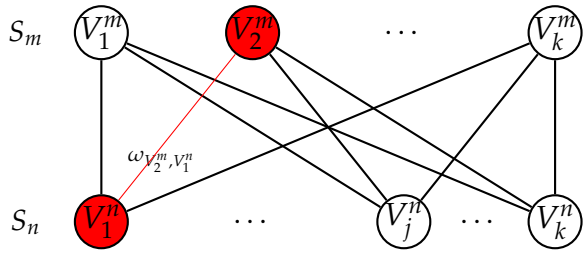
Preliminary experiments show that high quality local optimal solutions share many grouping vertices. It is thus expected that vertices that always share the same color are very likely to be part of a global optimum or a high quality solution. Following this observation, the general idea of our proposed collapsing operator is to preserve the vertices groupings (backbone) of maximal size from parent solutions and color the rest vertices randomly.



(a) A complete bipartite graph H with an edge weight ω



(b) Choose an edge with the largest ω and delete all edges incident to vertices



(c) Repeat the last step until $H = \emptyset$

Figure 2.2 – The classes matching procedure by a complete bipartite graph H

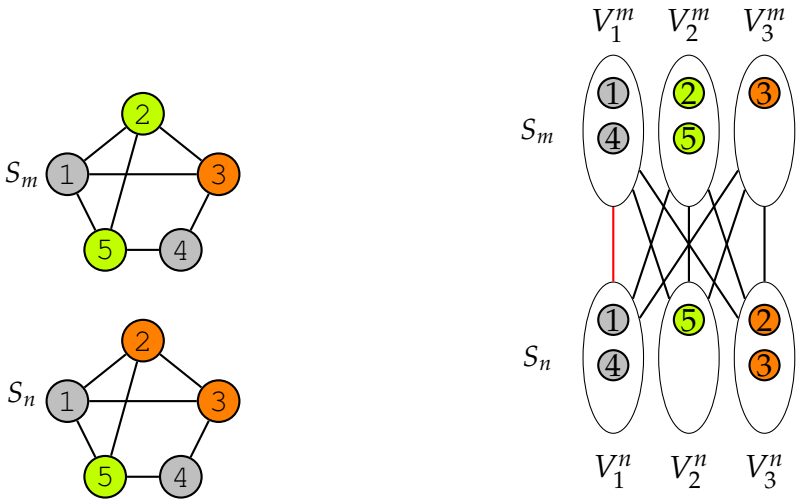
Each vertex set (or color class) V_i^m from parent solution S_m that shares the most common vertices typically corresponds to another set V_j^n of parent solution S_n. Therefore, in order to find out the largest number of common vertices of two parent solutions, the first step is to match each set in two parents.

This is achieved by finding a maximum weight matching in a complete bipartite graph $H = (V_H, E_H)$ (Figure 2.2(a)) where V_H consists of k upside vertices and k downside vertices that correspond respectively to the vertex sets of parent solutions S_m and S_n; each edge $(V_i^m, V_j^n) \in H$ is associated with a weight $\omega_{V_i^m,V_j^n}$, which is defined as the number of identical vertices in V_i^m of

solution S_m and V_j^n of solution S_n.

The maximum weight matching problem can be solved by using the classical Hungarian algorithm [Kuhn, 1955]. However, invoking this algorithm for each iteration would be too computationally expensive ($O(k^3)$). We apply a fast greedy algorithm [Chen and Hao, 2016] to seek a near-optimal weight matching for the maximum weight matching problem. The main idea is that at each step our greedy algorithm chooses an edge $(V_i^m, V_j^n) \in H$ with the largest $\omega_{V_i^m, V_j^n}$, keep this set (V_i^m, V_j^n) in the group matching set J, i.e., $J \leftarrow J \cup \{(V_i^m, V_j^n)\}$ and delete it from the graph H ($H \leftarrow H \setminus \{(V_i^m, V_j^n)\}$). All edges incident to vertex V_i^m and to vertex V_j^n are also deleted in order to make it easier to identify the next match set, as showed in the Figure 2.2(b)-(c). This procedure is repeated until H becomes empty (lines 4-11 of Algorithm 2.2), which occurs when all vertex sets are matched.

To illustrate the main steps of the backbone-based matching operator, we use the case of Figure 2.3 as a working example. The example involves an instance of 5 vertices and 3 colors and operates with two parent solutions S_m and S_n. In the first step, as showed in Figure 2.3, S_m and S_n are matched using the fast greedy algorithm and the results are: S_m-V_1^m matches S_n-V_1^n, S_m-V_2^m matches S_n-V_3^n (randomly choice between S_m-V_3^m and S_n-V_2^n for equal weight) and the matching set $J = \{(V_1^m, V_1^n), (V_2^m, V_3^n), (V_4^m, V_2^n)\}$.



(a) S_m and S_n for a graph $G = (V, E)$ (b) An example of classes matching

Figure 2.3 – two solutions for a graph coloring and its graph matching G'

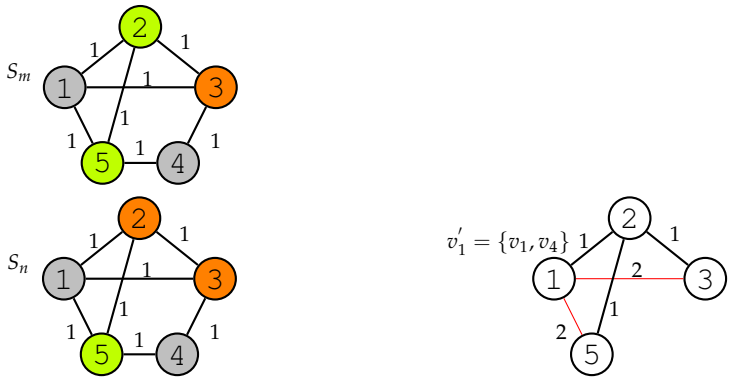
Algorithm 2.3: The coarsening phase

1: **Input**: Matching set J.
2: **Output**: the coarsener graph G'
3: $G' \leftarrow G$/* Initial the coarsener graph G'*/
4: **for** each set $(V_i, V_j) \in J$ **do**
5: $I_i \leftarrow V_i \cap V_j$ /*I_i is the ith identical information fragment*/
6: Collapse all vertices in the set I_i to form one vertex in the graph G'
7: Update the weight of the edges in the graph G'
8: **end for**

Coarsening phase

Let $G = (V, E)$ be the initial graph. Creating a coarsened graph $G' = (V', E')$ from G consists of finding an identical information set, merging each identical information fragment and then collapsing those sets to one vertex to form a new vertex in G'. Any vertex that dose not belong to any fragment is simply copied to G'.

The proposed coarsening phase is illustrated in Algorithm 2.3. Firstly, let the initial graph G' as G and the edge weight of G be initialized to 1 (line 3, Algorithm 2.3). Then, we collapse the identical vertices from parent solutions which are recorded in the backbone matching set J to form one vertex (line 5-6, Algorithm 2.3). Finally, we update the weight of each edge of G' (line 7, Algorithm 2.3). To be specific, the weight of each edge of a coarsened graph G' equals the sum of weights of the edges of the initial graph whose endpoints respectively belong to the vertices of this edge of the coarsened graph. Therefore, the sum of the weights of the edges of the coarsened graph equals the number of the edges of the initial graph G. Repeat this process until all the identical vertices are collapsed.



(a) S_m and S_n for a graph $G = (V, E)$ (b) A coarsened graph G'

Figure 2.4 – two solution for a graph coloring and its coarsened graph G'

An example of the coarsened graph G' of an initial graph G with 5 vertices is provided in Figure 2.4. Let v'_1 of G' be vertex formed by collapsing $\{v_1, v_4\}$ of G. These edges between $\{v_1, v_4\}$ and the vertices incident to vertices and $\{v_1, v_4\}$ in the initial graph G are merged to form a new edge with a weight that is set equal to the sum of the weights of the edges whose endpoints are incident to v_1 or v_4, .i.e., $W'_{1,5} = W_{1,5} + W_{4,5} = 2$, $W'_{1,3} = W_{1,3} + W_{4,3} = 2$.

After coarsening the original graph G to G', we apply a weighted tabu search to improve the solution in the graph G'(see the Section 2.2.5). Normally, the quality of a solution for the graph G' is worse than that of G because there is a less degree of freedom for refinement. However, this phase helps the search quickly attain a promising search area.

2.2.5 Weight tabu search improvement

Recall that the purpose of the backbone based group matching phase is to obtain a coarsened graph G'. In order to find a good initial solution S'_0 for the graph G', we simplify the solution S_0 (which is generated by the adaptive multi-parent crossover procedure), which means that if a vertex is merged with another vertex, the color of this vertex is deleted; otherwise, we keep the color of the vertex.

We apply a weighted iterated tabu search algorithm whose basic components are briefly described in this section. We first define the search space and the evaluation function. For a given

graph $G^{'} = (V^{'}, E^{'})$ with k available colors, the search space contains all possible k-colorings (candidate solutions). A candidate solution in $\Omega_k^{'}$ can be represented by $s = \{V_1, V_2, \ldots, V_k\}$ such that V_i is the set of vertices receiving the same color i.

$$\Omega_k^{'} = \{\{V_1, V_2, \cdots, V_k\} : \cup_{i=1}^{k} V_i = V^{'}, V_i \cap V_j = \emptyset\} \tag{2.5}$$

where $i \neq j, 1 \leq i, j \leq k$.

The evaluation function $f^{'}(s)$ is used to count the sum of the weight of conflicting edges induced by a coloring s.

$$f^{'}(s) = \sum_{i=1}^{k} |w(V_i)| \tag{2.6}$$

where $|w(V_i)|$ is the weight of conflicting edges in color class V_i. Accordingly, a coloring s with $f^{'}(s) = 0$ corresponds to a legal k-coloring.

Weighted graph coloring

The used optimization procedure is a version based on the weight of edge of the tabu coloring procedure (TabuCol) proposed in [Dorne and Hao, 1998; Galinier and Hao, 1999].

Given a conflicting k-coloring solution $s = \{V_1, V_2, \ldots, V_k\}$, the basic idea of the one move neighborhood $N(s)$ is to move a conflicting vertex v from its original vertices set V_i to another subset V_j.

The move gain, which represents the change in the optimization objective, which is expressed as follows

$$\Delta f^{'} = B[v][j] - B[v][i] \tag{2.7}$$

According to incremental technique, each time a one-move operation involving vertex v is performed, we just need to update a subset of values affected by this move as follows. For each vertex u adjacent to vertex v, $B[u][i] \leftarrow B[u][i] - w_{v,u}$, and $B[u][j] \leftarrow B[u][j] + w_{v,u}$.

Weight TabuCol selects a best neighbor $s_{Nbest} \in N(s)$ according to the move gain given by Equation 2.7 and the tabu tenure such that either the move gain for the s_{Nbest} is the minimum (s_{Nbest} is the best solution) not forbidden by the tabu list or is better than the best solution found so far. If there is more than one vertex with the same move gain, we will choose one vertex randomly.

2.2.6 Uncoarsening phase

The uncoarsening phase carries out the inverse of the coarsening phase and further improves the solution. The details of the underlying steps are described as follows.

(1) Recover the initial graph G from the collapsed graph $G^{'}$ with its corresponding coloring. As we mentioned, the quality of a solution for the graph $G^{'}$ is worse than that of G because there is a less degree of freedom for refinement. Thus, The first step of the uncoarsening phase is to recover from the collapsed graph $G^{'}$ the original graph G in order to explore the search space further.

(2) Perturbation process. Since our tabu search procedure focuses its search only around conflicting vertices, it can get trapped in a local optimum. Therefore, we periodically apply a simple

perturbation before the tabu search process. The perturbation consists of moving a fixed number of vertices (is set in this chapter to $0.3 * N$) in the following way.

This perturbation adopts the one-move operator. To avoid a too strong deterioration of the perturbed solution, a directed perturbation move takes into consideration the fitness value and cannot move back to the original color. While a decent perturbation performs a one-move without considering the tabu tenure. To combine these two types of perturbations, each type of perturbation is determined probabilistically. The resulting solution from the perturbation procedure is then used as the new starting solution of the next round of the search phase.

After the uncoarsening phase, we run the tabu search (see Section 2.2.2) to further improve the solution.

2.2.7 Pool updating strategy

Maintaining a healthy diversity of the population is another key issue for population-based al- gorithms. To decide whether the newly generated solution should be inserted into the population or be discarded, we consider not only the solution quality but also the distance between individuals in population. Our algorithm adopts the idea presented in [Lü and Hao, 2010].

Distance measure: Given two k-colorings S_m and S_n, according to the well-known set-theoretic partition distance [Gusfield, 2002], the distance between S_m and S_n is defined as the minimum number of one-move steps needed to transform S_m to S_n, i.e., $d(S_m, S_n) = |V| - sim(S_m, S_n)$, where $sim(S_m, S_n)$ represents the maximum number of elements of S_m that do not need to be displaced to obtain the solution S_n.

$$D_{i,POP} = min\{d_{i,j} : S_j \in POP, j \neq i\} \tag{2.8}$$

We use the $sim(S_m, S_n)$ identify the similarity (S_m, S_n) in Section 2.2.4.

$$Q_{i,POP} = f(S_i) + e^{\beta / D_{i,POP}} \tag{2.9}$$

where f represents its fitness in the equation 2.2. and β a parameter set to $\beta = 0.08 * |V|$.

The pool updating strategy consists thus of three steps: for each individual S_i, $i \in POP$, calculating $D_{i,POP}$ and the corresponding $Q_{i,POP}$ score (lines 5 of Algorithm 2.4); identifying the maximum score Q_{max} (lines 6 of Algorithm 2.4); and updating the pool (lines 10-15 of Algorithm 2.4). This pool updating strategy contributes to avoid premature convergence for population-based algorithms. The pool updating procedure is described in Algorithm 2.4.

2.3 Experimental results and comparisons

This section is dedicated to an experimental assessment of the proposed RMA algorithm for solving the GCP and comparisons with other state of the art methods. The study is based on 39 conventional benchmark instances which are commonly used in the literature and initially proposed for the DIMCAS and COLOR competitions for graph coloring problems [1, 2].

1. http://www.dimacs.rutgers.edu/
2. http://www.cs.hbg.psu.edu/txn131/graphcoloring.html/

Algorithm 2.4: Pool updating strategy

Input: Population $POP = \{S_1, S_2, \ldots, S_p\}$ and new solution S_0.
Output: Updated population $POP = \{S_1, S_2, \ldots, S_p\}$
/*Evaluate each solution*/
Tentatively add S_0 to population $POP = POP \cup S_0$
for i =0,1,...,p **do**
    Calculate the distance $D_{i,POP}$ between any individual in POP according to the Equation 2.8
    Calculate the goodness score $Q_{i,POP}$ according to the Equation 2.9
end for
/*Select the worst solution*/
Choose the $k-$coloring with the largest Q value
$S_w \leftarrow arg\,max Q(S_i), i = 0, 1, \ldots, p$
/*Update the pool population*/
if $S_w \neq S_0$ **then**
    Replace S_w with S_0 /*Replace the worst solution*/
else if $rand(0,1) < 0.2$ **then**
    $S_{sw} \leftarrow arg\,max Q(S_i), i = 1, \ldots, p$
    Replace the orignal pop worst solution S_{sw} with S_0 /*Replace the second worst solution*/
end if

2.3.1 Benchmark instances

The 33 benchmark instances are classified into two categories: easy graphs and difficult graphs according to [Galinier *et al.*, 2013; Galinier *et al.*, 2008]. Let BKV (the best-known value) represents $\chi(G)$ (if known) or the best-known value in the literature.

1. The first category, easy graphs, contains 19 instances that can be colored with BKV colors by a basic coloring algorithm like DSATUR [Brélaz, 1979] (thus by numerous algorithms).
2. The second category contains 20 instances that are hard graphs that can only only be achieved by a few advanced coloring algorithms.

2.3.2 Experiment settings

The proposed algorithm was programmed in C++ and compiled by GNU g++ 4.1.2 with -O3 flag (option). The experiments were conducted on a computer with an Intel Xeon E5-2670 processor (2.5 GHz and 2 GB RAM) running Ubuntu 12.04. Without using a compiler optimization flag, it requires respectively 0.46, 2.68 and 10.70 seconds to solve the well-known DIMACS machine benchmark graphs r300.5, r400.5 and r500.5 on our machine.

Parameters

Since our algorithm is built up on the memetic algorithm proposed in [Lü and Hao, 2010], we adopt the parameters in [Lü and Hao, 2010], as the default setting of the RMA algorithm, as shown in Table 2.1. We use the default setting of Table 2.1 to report the experimental results shown in the rest of this chapter.

Table 2.1 – Settings of important parameters

Parameters	Description	Value
p	size of population	20
β	maximum number of iterations for the tabu search methods	10000
P_0	probability for accepting worse solution	0.2

Reference algorithms

To evaluate the performance of the proposed algorithm, ten state-of-the-art heuristic algorithms in the literature are used as the main reference algorithms, including (1) Iterated local search algorithm (IGrAl) [Caramia and Dell Olmo, 2008] (a 2.8 GHz Pentium 4 processor and a cut off time of 1 hour); (2) Variable space search algorithm (VSS) [Hertz *et al.*, 2008] (a 2.0 GHz Pentium 4 processor and a cut off time of 10 hours); (3) Local search algorithm using partial solutions (Partial) [Blöchliger and Zufferey, 2008] (a 2.0 GHz Pentium 4 and a time limit of 10 hours together with a limit of $2 * 10^9$ iterations without improvement); (4) Probability learning based local search (PLSCOL) [Zhou *et al.*, 2018] (Intel Xeon E5-2760 2.8 GHz processor and 2 GB RAM with a cutoff of 5 hours); (5) Hybrid evolutionary algorithm (HEA) [Galinier and Hao, 1999] (the processor used is not available for this oldest algorithm and the results were obtained with different parameter settings); (6) Adaptive memory algorithm (AMA) [Galinier *et al.*, 2008] (the processor applied is not available and the results were obtained with different parameter settings); (7) Two-phase evolutionary algorithm (MMT) [Malaguti *et al.*, 2008] (a 2.4 GHz Pentium processor and a cut off time of 6000 or 40000 seconds); (8) Evolutionary algorithm with diversity guarantee (Evo-Div) [Porumbel *et al.*, 2010] (a 2.8 GHz Xeon processor and a cut off time of 12 hours); (9) Memetic algorithm (MACOL or MA) [Lü and Hao, 2010] (a 3.4 GHz processor and a cutoff time of 5 hours); (10) Distributed quantum annealing algorithm (QACOL or QA) [Titiloye and Crispin, 2011; Titiloye and Crispin, 2012] (a 3.0 GHz Intel processor with 12 cores and a cut off time of 5 hours); (11) The newest parallel memetic algorithm (HEAD) [Moalic and Gondran, 2015] (a 3.1 GHz Intel Xeon processor with 4 cores used to run in parallel the search processes with a cut off time of at least 3 hours).

Stopping condition

Despite the extremely vast literature on graph coloring, there is no uniform experimental stopping criteria to assess a coloring algorithm. This is mainly because the difficult DIMACS instances are really challenging, the best-known solutions for these instances can be found only by few most powerful algorithms which were implemented with different programming languages and executed under various computing platforms and different stopping conditions (maximum allowed generations, maximum allowed fitness evaluations, maximum allowed iterations or maximum allowed time limit).

On the other hand, these reference algorithm were tested on different CPU frequency, it would be quite difficult to compare CPU times of the compared algorithms.

To make a relatively fair comparison of the runtime, we use the best solution (i.e., the smallest number of used colors) for this comparative study. This experimental conditions of the compared algorithms are not equivalent, since the computing time of each algorithm is not only influenced by the processor, but also by some inaccessible factors such as the operating systems, compliers, the comparison is just intended to show the relative performance of the proposed algorithm.

One can observe that the majority of the reference algorithms allowed large run time limits of at least 5 hours (the cut off limit for our experiments). Additionally, our Intel Xeon E5-2670 2.5 GHz processor is almost the same with those used by the reference algorithms. Thus, we use the stopping criterion of 5 hours to investigate the ehavior of our RMA algorithm on the set of 39 instances. For each instance, our algorithm was executed 20 times independently. As a result, our adopted stopping conditions can be considered as reasonable with respect to those used by the reference algorithms.

2.3.3 Comparison with state-of-the-art algorithms

2.3.4 Comparative results on easy instances

Table 2 reports the results of our RMA algorithm on the first set of 19 DIMACS/COLOR instances commonly used in the literature, together with the results of 10 state-of-the-art coloring algorithms in the literature. We focus on the criterion of solution quality in terms of the smallest number of colors used to find a legal coloring. The first column indicates the name of each instance. The second column shows the best-known value (BKV) reported in the literature [Caramia and Dell Olmo, 2008; Hertz *et al.*, 2008; Blöchliger and Zufferey, 2008; Galinier and Hao, 1999; Galinier *et al.*, 2008; Malaguti *et al.*, 2008; Porumbel *et al.*, 2010; Lü and Hao, 2010; Titiloye and Crispin, 2011; Titiloye and Crispin, 2012; Moalic and Gondran, 2015]. The following three columns report the best results (Best), the success rate (SR) to achieve the best result over 10 runs and the computation time obtained by the reference algorithms. The next four columns show the results of RMA for each instance: the best result (i.e., the smallest number of colors used) over 20 independent runs (Best), the success rate (SR) to achieve the best result over 20 runs, the minimal computation time ($t(s)_{Min}$) and the average computation time (in seconds) of the successful runs to obtain the best result ($t(s)_{Avg}$).

Additionally, the rows #Better, #Equal and #Worse indicate respectively the number of instances for which an algorithm performs better, equally well or worse compared to the best-known values (BKV). Finally, an entry with * indicates the optimal objective value.

Table 2.2 – Comparative results of RMA with state-of-the-art algorithms MACOL and PLSCOL on 19 easy benchmark instances. Improved upper bounds are indicated in bold.

		MACOL			PLSCOL			RMA			
Instance	*BKV*	*Best*	*SR*	$t(m)_{Avg}$	*Best*	*SR*	$t(m)_{Avg}$	*Best*	*SR*	$t(s)_{Min}$	$t(s)_{Avg}$
DSJC125.1.col	5	5*	10/10	1	5*	10/10	< 1	5*	20	0	0.014
DSJC125.5.col	17	17	10/10	3	17	10/10	< 1	17	20	0.03	0.263
DSJC125.9.col	44	44	10/10	4	44	10/10	< 1	44	20	0.01	0.027
DSJC250.1.col	8	8	10/10	2	8	10/10	< 1	8	20	0.01	0.0615
DSJC250.9.col	72	72	10/10	3	72	10/10	< 1	72	20	0.28	2.911
R125.1.col	5	5	10/10	2	5	10/10	< 1	5	20	0	0.002
R125.1c.col	46	46	10/10	5	46	10/10	< 1	46	20	3.11	6.147
R125.5.col	36	36	10/10	1	36	10/10	< 1	36	20	0.05	1.7565
R250.1.col	8	8	10/10	5	8	10/10	< 1	8	20	0	0.0075
R250.1c.col	64	64	10/10	4	64	10/10	1	64	20	0.06	**19.9475**
DSJR500.1.col	12	12	10/10	4	12	10/10	< 1	12	20	0.04	0.1385
R1000.1.col	20	20	10/10	2	20	10/10	< 1	20	20	0.25	0.2735
le450_15a.col	15*	15*	10/10	2	15*	10/10	< 1	15*	20	0.12	0.3605
le450_15b.col	15*	15*	10/10	2	15*	10/10	< 1	15*	20	0.09	0.2195
le450_25a.col	25*	25*	10/10	4	25*	10/10	< 1	25*	20	0.04	0.0475
le450_25b.col	25*	25*	10/10	3	25*	10/10	< 1	25*	20	0.04	0.0475
school1.col	14	14	10/10	6	14	10/10	< 1	14	20	0.03	0.043
school1_nsh.col	14	14	10/10	1	14	10/10	< 1	14	20	0.03	0.0425
flat300_20_0.col	20*	20*	10/10	4	20*	10/10	< 1	20*	20	0.05	0.0855
#Better		0/19			0/19			0/19			
#Equal		19/19			19/19			19/19			
#Worse		0/19			0/19			0/19			

Table 2.2 reports the comparative results with MACOL [Lü and Hao, 2010] which is respectively one of the most powerful population-based coloring algorithms in the literature and PLSCOL, which is the most recent heuristic algorithm [Zhou *et al.*, 2018]. We can observe that for these 19 easy instances, the MACOL algorithm was run on a PC with 3.4 GHz CPU and 2G RAM and the results of the PLSCOL is obtained on a computer equipped with 2.8 GHz and 2G RAM (against 2.5 GHz and 2 GB RAM for our computer). Table 2.2 indicates that all MACOL, PLSCOL and RMA can easily find the best-known results with a 100% success rate. However, RMA can attain the best-known solutions more quickly, i.e., RMA uses less time (at most 20s) to find its best results while MACOL needs 1 to 5 minutes to achieve the same results and the PLSCOL uses less than60s.

2.3.5 Comparative results on difficult instances

Table 2.3 presents the comparative results of RMA with state-of-the-art algorithms on the 20 difficult instances. In this table, column 2 recalls the chromatic number or best-known value (BKV) in the literature. The next four columns show the results of the local search algorithm for each instance. The following 10 columns report the best results obtained by the 4 reference local search algorithm and 7 reference population-based algorithms. The last column is the best result obtained by RMA.

Additionally, in order to show the performance of RMA, we use the rows #Better_compareRMA, #Equal_compareRMA and #Worse_compareRMA to indicate respectively the number of instances for which an algorithm performs better, equally well or worse compared to the best-known values of RMA (Best). As we observe from Table 2.3, RMA competes favorably with the reference algo-

Table 2.3 – Comparative results of RMA with state-of-the-art algorithms MACOL and PLSCOL on 20 difficult benchmark instances. The best results are in bold.

Instance	*BKV*	Local search algorithms				Population-based algorithms							
		IGrAI 2008	VSS 2008	Partial 2008	PLSCOL 2018	HEA 1999	AMA 2008	MMT 2008	Evo-Div 2010	MA 2010	QA 2011	HEAD 2015	RMA Best
DSJC250.5.col	28	29	-	-	**28**	-	**28**	**28**	-	**28**	**28**	**28**	**28**
DSJC500.1.col	12	**12**	**12**	**12**	**12**	**12**	**12**	**12**	**12**	**12**	**12**	**12**	**12**
DSJC500.5.col	47	50	48	48	48	48	48	48	48	48	48	**47**	48
DSJC500.9.col	126	129	**126**	127	**126**	**126**	**126**	127	**126**	**126**	**126**	**126**	**126**
DSJC1000.1.col	20	22	**20**	**20**	**20**	**20**	**20**	**20**	**20**	**20**	**20**	**20**	**20**
DSJC1000.5.col	82	94	86	89	87	83	84	84	83	83	83	**82**	83
DSJC1000.9.col	222	239	224	226	223	224	224	225	223	223	**222**	**222**	223
DSJR500.1c.col	85	**85**	**85**	**85**	**85**	-	86	**85**	**85**	**85**	**85**	**85**	**85**
DSJR500.5.col	122	126	125	125	126	-	127	**122**	**122**	**122**	**122**	-	**122**
le450_15c.col	15*	16	**15***	**15***	**15***	**15***	**15***	**15***	-	**15***	**15***	-	**15***
le450_15d.col	15*	16	**15***	**15***	**15***	**15***	**15***	**15***	-	**15***	**15***	-	**15***
le450_25c.col	25*	27	**25***	**25***	**25***	26	26	**25***	**25***	**25***	**25***	**25***	**25***
le450_25d.col	25*	27	**25***	**25***	**25***	26	26	**25***	**25***	**25***	**25***	**25***	**25***
flat300_26_0.col	26*	-	-	-	**26***	-	**26***	**26***	-	**26***	-	-	**26***
flat300 28 0.col	28*	-	**28***	**28***	30	31	31	31	31	29	31	31	29
flat1000_76_0.col	81	-	85	87	86	83	84	83	82	82	82	**81**	83
R250.5.col	65*	-	-	66	66	-	-	**65**	**65***	**65***	**65***	**65***	**65***
R1000.1c.col	98	-	-	-	**98**	-	-	**98**	**98**	**98**	**98**	**98**	**98**
R1000.5.col	234	238	245	238	254	255	-	**234**	238	245	238	245	254
latin_square_10.col	97	100	-	-	99	-	104	101	100	99	98	-	98
#Better		0/14	0/14	0/16	0/20	0/12	0/17	0/20	0/16	0/20	0/19	0/15	0/20
#Equal		2/14	9/14	8/16	11/20	5/12	7/17	13/20	9/16	13/20	13/19	13/15	13/20
#Worse		12/14	5/14	8/16	9/20	7/12	10/17	7/20	7/16	7/20	6/19	2/15	7/20
#Better_compareRMA		0/14	1/14	2/16	1/20	0/12	0/17	1/20	2/16	2/20	3/19	4/15	-
#Equal_compareRMA		2/14	9/14	8/16	13/20	8/12	8/17	14/20	12/16	17/20	15/19	9/15	-
#Worse_compareRMA		12/14	4/14	6/16	7/20	4/12	9/17	5/20	2/16	1/20	1/19	1/15	-

rithms. In order to facilitate comparisons, we divide these reference algorithms into three groups. The first group contains 3 algorithm, MA, PLSCOL and MMT, which has the complete experimental results for the 20 difficult instances. Observes that RMA attains 13 best known values while PLSCOL, MA and MMT obtains 11, 13 and 13 respectively. RMA, MA and MMT perform similarly, while the differnce between RMA and PLSCOL is significant.

The second category contains algorithms IGrAI, Partial, HEA, AMA and Evo-Div, which does not contain all 20 corresponding resluts. However, RMA competes favorably with those algorithm since it can obtain less values in the row of #Worse, which means RMA at least can dominate those algorithms. In detail, RMA is worse than BKV for 7 instances out of 20 instances, while IGrAI, Partial, HEA, AMA, Evo-Div are worse than BKV for 12, 8, 7, 10 and 7 respectively.

The third category cantains the last three algorithms (VSS, QA and HEAD), whose values of the row of #Worse are smaller than the value of the row of #Worse of RMA. which also misses some corresponding resluts in the 20 difficulty instances. When comparing RMA with VSS, one observes that RMA also performs very well. Specifically, RMA improves the best results of VSS for 4 instances while matching the best results of RMA for other 9 instances. Only in one case, $flat$300_28_0, RMA obtains a slightly worse results. Additionally, when comparing to the best results obtained by QA, RMA obtains 3 worse results, 1 better results and matches the remaining instances. Finally, RMA obtains 5 worse results and 1 better result compared with the results of HEAD.

2.4 Analysis

This section performs additional experiments to gain understanding of some important ingredients of the proposed RMA approach: the number of parents for RMA, the strategy of the group matching and the perturbation strategy.

2.4.1 Effectiveness of the number of parents for RMA

To assess the influence of the number of parents in the proposed algorithm, we create a algorithmic variant (called RMAmutiparents) in which multi-parents are used in the backbone matching process (Section 2.2.4) when collapsing vertices. In detail, those vertices whose colors are identical should also be allocated to the same color in all chosen parents. For this experiment, we select 16 instances which are relatively difficult according to the results reported in Tables 2.3.

We ran 10 times both algorithms to solve each selected instance with a cutoff time of 9000 seconds (2.5 hour). The comparative results of this experiment are presented in Table 2.4 with the same information as before.

The rows *#Better*/*#Equal*/*#Worse* indicate the number of instances for which each algorithm attain a better, equal and worse results compared to the other algorithm in terms of the best objective value found by RMA.

Table 2.4 reports that RMA dominates the RMAmutiparents algorithm on the 16 instances tested by both algorithm, by obtaining better results for 12 instances and the same results for the remaining 4 instances.

Table 2.4 – Assessment of different number of the parents. The better results are in bold.

		RMA				RMAmutiparents			
Instance	*BKV*	*Best*	*SR*	$t(s)_{Min}$	$t(s)_{Avg}$	*Best*	*SR*	$t(s)_{Min}$	$t(s)_{Avg}$
DSJC1000.1.col	20	**20**	8	1456.91	2919.92	21	10	1.23	8.177
DSJC1000.5.col	84	**84**	4	3140.62	6015.84	88	848.9	4703.63	9
DSJC1000.9.col	224	**224**	9	3073.77	5248.5	226	4937.8	5406.56	2
DSJC500.5.col	48	**48**	10	568	952.641	>48	-	-	-
DSJC500.9.col	126	**126**	9	356.77	831.989	>126	-	-	-
DSJR500.1c.col	85	**85**	9	51.52	1439.14	>85	-	-	-
DSJR500.5.col	123	**123**	4	2568.1	5904.71	127	555.21	3787.49	5
flat300_28_0.col	29	**29**	2	915.63	1109.07	30	3	2382.55	3375.8
latin_square_10.col	99	**99**	6	1818.46	4148.19	>99	-	-	-
le450_15c.col	15	**15**	10	1471.31	2386.74	**15**	5	0	2826.1
le450_15d.col	15	**15**	9	1885.01	3457.61	16	10	0.29	6.986
le450_25c.col	25	**25**	4	252.26	4844.03	**25**	7	1984.45	4842.53
le450_25d.col	25	**25**	5	2106.12	4861.31	**25**	3	3004.16	6340.4
r1000.1c.col	98	**98**	10	137.6	275.987	**98**	10	225.45	1767.97
R1000.5.col	256	**256**	3	6672.23	7708.9	>256	-	-	-
R250.5.col	65	**65**	10	374.91	2273.22	>65	-	-	-
#Better		12/16				0/16			
#Equals		4/16				4/16			
#Worse		0/16				12/16			

2.4.2 Effectiveness of the different matching strategies for RMA

The group matching procedure (Section 2.2.4) allows the information of the parents to be preserved during the coarsening process. In this section, we discuss how those group matching coarsening processes contribute to the overall performance of our RMA algorithm.

For this study, we create *RMA_maxmatch*, which is a RMA variant where we replace line 15 of Algorithm 2.1 with the group comparison procedure of MACOL. We ran *RMA_maxmatch* under the same stopping condition as before in Section 2.4.1 if a legal k-coloring is found or the maximum allowed run time of 2.5 CPU hours is reached. Each tested instance was solved 10 times.

Table 2.5 displays the comparative results between RMA and *RMA_maxmatch*, based on the same indicators adopted in Table 2.4. From this table, we observe that RMA outperforms *RMA_maxmatch*, achieving better values for 5 out of 16 instances and equal results for the remaining 11 instances. Moreover, for the 11 instances where both algorithms achieve the same

Table 2.5 – Assessment of different strategies. The better results are in bold.

		RMA				RMA MAXmatch			
Instance	*BKV*	*Best*	*SR*	$t(s)_{Min}$	$t(s)_{Avg}$	*Best*	*SR*	$t(s)_{Min}$	$t(s)_{Avg}$
DSJC1000.1.col	20	**20**	8	1456.91	2919.92	21	10	2.46	14.068
DSJC1000.5.col	84	**84**	4	3140.62	6015.84	88	9	848.9	4703.63
DSJC1000.9.col	224	**224**	9	3073.77	5248.5	**224**	2	4084.86	4715.52
DSJC500.5.col	48	**48**	10	568	952.641	**48**	9	1363.79	2810.19
DSJC500.9.col	126	**126**	9	356.77	831.989	**126**	10	1240.1	2592.08
DSJR500.1c.col	85	**85**	9	51.52	1439.14	**85**	8	2.07	54.64
DSJR500.5.col	123	**123**	4	2568.1	5904.71	**123**	4	2670.3	6493.06
flat300_28_0.col	29	**29**	2	915.63	1109.07	30	7	844.3	3754.1
latin_square_10.col	99	**99**	6	1818.46	4148.19	>99	-	-	-
le450_15c.col	15	**15**	10	1471.31	2386.74	**15**	9	291.87	1370.87
le450_15d.col	15	**15**	9	1885.01	3457.61	**15**	9	1997.77	3779.21
le450_25c.col	25	**25**	4	252.26	4844.03	**25**	4	1569.42	1912.22
le450_25d.col	25	**25**	5	2106.12	4861.31	**25**	1	7432.84	7432.84
r1000.1c.col	98	**98**	10	137.6	275.987	**98**	10	115.79	193.373
R1000.5.col	256	**256**	3	6672.23	7708.9	257	5	2355.7	7083.36
R250.5.col	65	**65**	10	374.91	2273.22	**65**	9	449.22	1642.08
#Better		5/16				0/16			
#Equal		11/16				11/16			
#Worse		0/16				5/16			

best objective values, RMA obtains a high successful rate than *RMA_maxmatch* for 6 instances and equal successful rate for 4 instances. These observations confirm the usefulness of the group matching procedure for the RMA algorithm.

2.4.3 Effectiveness of the perturbation operation

As shown in Section 2.2.6, the proposed algorithm uses a perturbation strategy as an additional means of diversification. To assess this strategy, we compare RMA with a RMA variant (denoted as $RMA^{'}$) where the perturbation strategy is disabled. We ran 10 times both algorithms to solve each selected instance with a cutoff time of 9000s. Table 2.6 presented the results of

Table 2.6 – Analysis of the influence of the perturbation on the performance of the RMA algorithm. The better results are in bold.

		RMA				$RMA^{'}$			
Instance	*BKV*	*Best*	*SR*	$t(s)_{Min}$	$t(s)_{Avg}$	*Best*	*SR*	$t(s)_{Min}$	$t(s)_{Avg}$
DSJC1000.1.col	20	**20**	8	1456.91	2919.92	**20**	1	4844.62	4844.62
DSJC1000.5.col	84	**84**	4	3140.62	6015.84	**84**	4	2673.52	4360.01
DSJC1000.9.col	224	**224**	9	3073.77	5248.5	**224**	3	4904.07	5699.28
DSJC500.5.col	48	**48**	10	568	952.641	**48**	10	357.43	658.692
DSJC500.9.col	126	**126**	9	356.77	831.989	**126**	10	199.17	1085.46
DSJR500.1c.col	85	**85**	9	51.52	1439.14	**85**	6	41.24	346.385
DSJR500.5.col	123	**123**	4	2568.1	5904.71	**123**	5	2885.95	5967.13
flat300_28_0.col	29	**29**	2	915.63	1109.07	30	4	2143.44	4007.43
latin_square_10.col	99	**99**	6	1818.46	4148.19	**99**	2	4489.02	5026.55
le450_15c.col	15	**15**	10	1471.31	2386.74	**15**	10	1271.21	2255.93
le450_15d.col	15	**15**	9	1885.01	3457.61	**15**	9	1877.32	3262.46
le450_25c.col	25	**25**	4	252.26	4844.03	**25**	2	4396.54	4906.53
le450_25d.col	25	**25**	5	2106.12	4861.31	**25**	2	4079.44	5885
r1000.1c.col	98	**98**	10	137.6	275.987	**98**	10	94.2	244.228
R1000.5.col	256	**256**	3	6672.23	7708.9	**256**	5	4657.43	6093.6
R250.5.col	65	**65**	10	374.91	2273.22	**65**	10	215.27	1632.82
#Better		1/16	6/15			0/16	3/16		
#Equal		15/16	6/15			15/16	6/15		
#Worse		0/16	3/15			1/16	6/15		

this experiment with the same statistics as before. One can observe that RMA dominates the RMA variant ($RMA^{'}$) just in one instances (flat300_28_0) and achieves the same values for other instances. For these same results, the SR of RMA is higher than $RMA^{'}$. This experiment demonstrates the interest of the perturbation strategy, which enables the algorithm to get rid of local optimal traps in certain instances.

2.5 Conclusions

The graph coloring problem (GCP) is an NP-hard problem with a number of practical applications. In this Chapter, we presented RMA for this well-known problem.

The proposed algorithm uses the evolutionary framework that integrates several procedures such as greedy initialization and backbone-based collapsing operator to generate a coarsened graph G', the weighted iterated tabu search to explore the search region, an uncoarsening process to recover the original graph, a perturbation to escape local optima traps, a tabu search to explore the search region when the solution is near the optimal solution and a diversity-based population updating rule to maintain a healthy population.

We assessed the performance of the RMA algorithm on popular DIMACS challenge benchmark graph instances that are commonly used in the literature and the experiment results showed that the proposed algorithm competes favorably with the state of the art coloring algorithms.

For future work, several directions could be followed. First, it would be interesting to investigate whether using a more powerful coloring algorithm instead of the TabuCol algorithm leads to even better results.

Second, it would be interesting to adopt other approaches for collapsing vertices with the feature of graphs.

Third, the way of collapsing vertex could be promising in solving a number of grouping problems such as bin packing [Nicholson, 1998], quadratic multiple knapsack problem [Chen and Hao, 2016] and graph partitioning [Benlic and Hao, 2011; Galinier *et al.*, 2011].

3

On feasible and infeasible search for ECP

In this chapter, we propose a feasible and infeasible search algorithm for the ECP which enlarges the search to include equity-infeasible solutions. The resulting algorithm relies on a mixed search strategy exploring both equitable and inequitable colorings unlike existing algorithms where the search is limited to equitable colorings only. We present experimental results on 73 DIMACS and COLOR benchmark graphs and demonstrate the competitiveness of this search strategy by showing 9 improved best-known results (new upper bounds). The content of this chapter is based on an article published in the In Proceedings of the Genetic and Evolutionary Computation Conference 2017 [Sun *et al.*, 2017].

Contents

3.1 Introduction

In this chapter, we present a feasible and infeasible search algorithm (FISA) for the equitable graph coloring problem which enlarges the search to include equity-infeasible solutions. Recall that an equitable legal k-coloring of an undirected graph $G = (V, E)$ is a partition of the vertex set V into k disjoint independent sets, such that the cardinalities of any two independent sets differ by at most one (this is called the equity constraint). As a variant of the popular graph coloring problem (GCP), the equitable coloring problem (ECP) involves finding a minimum k for which an equitable legal k-coloring exists.

The proposed FISA algorithm relies on two search phases (see Sections 3.3.2 and 3.3.3) to ensure a rapid and effective examination of the search space. The first phase examines only the space of equity-feasible colorings to seek a legal (i.e., conflict-free) k-coloring, which is based on the basic tabu search procedure of the BITS algorithm [Lai *et al.*, 2015] which is the most effective equity-feasible algorithm for the ECP. The first phase is repeated until legal k-coloring is found is found or the best solution found so far cannot be improved after a number of consecutive iterations. If a legal k-coloring is found, the k-ECP problem is solved with the current k value and we continue with the new k-ECP problem by setting $k = k - 1$. If the first phase fails to find a legal k-coloring in the equity-feasible space, the second phase is called to search the enlarged space include equity-infeasible colorings by using an extended fitness function to guide the search process. If the search is trapped in a deep local optimum, the perturbation phase applies a operator to definitively lead the search process to a distant region from which a new round of the search procedure starts. The second phase is repeated until the stopping condition met.

The proposed FISA algorithm includes the following original features. First, before the infeasible search, the proposed FISA algorithm adopts a feasible tabu procedure to quickly attain a promising search area. This combination prevents the search procedure from running the more expensive infeasible tabu search procedure in an unpromising area and thus helps to increase the search efficiency of the algorithm. Second, to prevent the search from going too far away from the feasible boundary, we devise an extended penalty-based fitness function which is used to guide the search for an effective examination of candidate solutions.

We show computational results on a set of 73 benchmark graphs from the DIMACS and COLOR competitions to assess the interest of the proposed approach. These results include especially 9 improved best solutions (new upper bounds) which can be used to assess other algorithms for the ECP.

The chapter is organized as follows. Section 3.2 introduces some preliminary definitions. Section 3.3 is dedicated to the description of the proposed algorithm. Section 3.4 presents computational results and comparisons with state of the art algorithms. Section 3.5 analyzes the impact of some key components of the proposed algorithm. Conclusions and future work are discussed in the last section.

3.2 Basic definitions

We introduce the following basic definitions which are useful for the description of the proposed approach. Let $G = (V, E)$ be a given graph.

Definition 3.2.1. A *candidate coloring* of G is any partition of the vertex set V into k subsets $V_1, V_2, \ldots, V_k$, where each V_i is called a color class.

Definition 3.2.2. A *legal coloring* is a conflict-free coloring composed of independent sets, i.e., any pair of vertices of any color class are not linked by an edge in E. Otherwise, it is an illegal or conflicting coloring.

Definition 3.2.3. An *equitable coloring* or *equity-feasible solution* is any candidate coloring satisfying the equity constraint, i.e., the cardinalities of any two color classes differ by at most one. Otherwise, it is an *equity-infeasible solution*.

3.3 Feasible and infeasible search algorithm for ECP

3.3.1 General approach

The equitable coloring problem (ECP) involves finding the smallest number of colors k such that an equitable legal k-coloring exists for a given graph G. Like for the conventional GCP [Galinier *et al.*, 2013], the ECP can be approximated by finding a series of equitable legal k-colorings for decreasing k values. To seek an equitable legal k-coloring for a given k, one typically explores the space of equity-feasible colorings while minimizing a fitness function f which counts the number of conflicting edges [Díaz *et al.*, 2014; Lai *et al.*, 2015]. The ECP problem with a given k is called the k-ECP problem.

This study follows this general approach of solving a series of k-ECP problems. However for each fixed k, our algorithm explores candidate solutions which include both equity-feasible and equity-infeasible colorings. For this, our feasible and infeasible search algorithm (FISA) introduces an extended fitness function F which is employed to measure the quality of any candidate solution.

The proposed FISA algorithm is composed of two search phases (see Sections 3.3.2 and 3.3.3). The first phase examines only the space of equity-feasible colorings to seek a legal (i.e., conflict-free) k-coloring. If a legal k-coloring is found, the k-ECP problem is solved with the current k value and we continue with the new k-ECP problem by setting $k = k - 1$. To be effective, the first phase is based on the basic tabu search procedure of the BITS algorithm [Lai *et al.*, 2015]. If the first phase fails to find a legal k-coloring with the equity-feasible space, the second phase is invoked to enlarge the search to include equity-infeasible colorings. To explore the enlarged search space, this second phase relies on the extended fitness function F to guide the search process. The infeasible search terminates if an equitable coloring is found or if the best solution found so far cannot be improved after a number of consecutive iterations. The pseudo-code of the FISA algorithm is given in Algorithm 3.1. The algorithm starts with an initial equity-feasible solution which is generated with a simple greedy heuristic presented in [Lai *et al.*, 2015]. In the next sections, we explain the search strategies of both phases of the FISA algorithm.

Algorithm 3.1: Main Scheme of the FISA algorithm for the ECP

```
1: Input: Graph G; k colors
2: Output: An equitable legal k-coloring if found
3: s_0 ← greedy_initial(G, k) /* Generate an initial equity-feasible k-coloring */
4: s_1 ← feasiable_search(s_0) /* Section 3.3.2 */
5: if f(s_1) = 0 then
6:    return(s_1) and stop
7: end if
8: while stopping condition is not met do
9:    s_2 ← infeasiable_search(s_1) /* Section 3.3.3 */
10:   if F(s_2) = 0 then
11:      return(s_2) and stop
12:   end if
13:   s_1 ← perturbation(s_2)
14: end while
```

3.3.2 Searching equity-feasible solutions

The first phase of the proposed FISA algorithm searches the space of candidate solutions which verifies the equity constraint and tries to find a legal k-coloring. This is achieved by minimization of the number of conflicting edges of candidate equitable k-colorings, an edge is conflicting if its endpoints belong to the same color class.

Equity-feasible space and fitness function

We define the equity-feasible space Ω_k to be the set of all candidate colorings verifying the equity constraint. Formally, Ω_k is given by

$$\Omega_k = \{\{V_1, V_2, \cdots, V_k\} : ||V_i| - |V_j|| \leq 1, \cup_{i=1}^{k} V_i = V, V_i \cap V_j = \emptyset\} \tag{3.1}$$

where $i \neq j, 1 \leq i, j \leq k$.

To assess the quality of a candidate solution s in Ω_k, the evaluation or fitness function counts the number of conflicting edges in the color classes of s. Specifically, let $s = \{V_1, V_2, \ldots, V_k\} \in \Omega_k$ be a candidate solution, let $C(V_i)$ denote the set of conflicting edges with both endpoints in V_i. The fitness function f (which is to be minimized) is given by

$$f(s) = \sum_{i=1}^{k} |C(V_i)| \tag{3.2}$$

Therefore, a solution s with $f(s) = 0$ is an equitable legal k-coloring satisfying both the equity and coloring constraints. When such a solution is found, the associated k-ECP problem is solved.

The feasible search phase of the FISA algorithm uses this fitness function to guide its search process to visit solutions of Ω_k in order to obtain a solution s with $f(s) = 0$.

Move operators to explore space Ω_k

To explore the space Ω_k, the feasible search phase applies two move operators to generate neighboring solutions from the current solution. Let $s = \{V_1, V_2, \ldots, V_k\}$ be the current solution. Let $C(s)$ denote the set of conflicting vertices involved in the conflicting edges of s.

1. One-move operator: It transfers a conflicting vertex v from its current color class V_i to a different color class V_j ensuring that the equity constraint is always respected, i.e., $|V_i| > \lfloor \frac{n}{k} \rfloor, |V_j| < \lceil \frac{n}{k} \rceil$. Let $< v, V_i, V_j >$ denote such a move. We use $s \oplus < v, V_i, V_j >$ to denote the neighboring solution generated by applying the move to s. Then the neighborhood N_1 induced by this move operator contains all possible solutions obtained by applying "one-move" to s, i.e.,

$$N_1(s) = \{s \oplus < v, V_i, V_j > : v \in V_i \cap C(s)\} \tag{3.3}$$

where $1 \leq i, j, \leq k, i \neq j, |V_i| > \lfloor \frac{n}{k} \rfloor, |V_j| < \lceil \frac{n}{k} \rceil$.

Note that the one-move operator is not applicable if $\lfloor \frac{n}{k} \rfloor = \lceil \frac{n}{k} \rceil$. In this case, the neighborhood N_1 is empty.

2. Swap operator: It exchanges a conflicting vertex v of color class V_i with another vertex u of color class V_j ($i \neq j$). Let $swap(v,u)$ denote such a move. The neighborhood N_2 induced by the swap operator is composed of all possible solutions obtained by applying "swap" to s (recall that $C(s)$ is the set of conflicting vertices of s).

$$N_2(s) = \{s \oplus swap(v,u) : v \in V_i, u \in V_j, i \neq j, \{v,u\} \cap C(s) \neq \emptyset\} \tag{3.4}$$

Since this operator does not change the cardinality of any color class, a neighboring solution generated by this operator is always equity-feasible (given that the current solution is an equitable k-coloring).

Exploration of the space Ω_k

Starting from an equitable (conflicting) k-coloring of Ω_k, the first phase of FISA iteratively improves the solution according to the tabu search method [Glover and Laguna, 2013]. Specifically, the basic tabu search procedure (TS^0) described in [Lai *et al.*, 2015] is applied to find a conflict-free k-coloring. At each iteration, a best admissible candidate solution is taken among the neighboring solutions of N_1 and N_2 to replace the current solution. The underlying move ($< v, V_i, V_j >$ for one-move or $swap(v,u)$) is recorded in the so-called tabu list in order to forbid the reverse move for a fixed number of next iterations. This tabu search process continues until either a solution s with $f(s) = 0$ is found in which case, the current k-ECP problem is solved, or the current solution is not improved during a fixed number of consecutive iterations in which case the FISA algorithm moves to the second search phase.

3.3.3 Searching equity-infeasible solutions

When the first phase fails to identify an equitable legal k-coloring within the equity-feasible space Ω_k, the FISA algorithm invokes the second phase to explore an enlarged space Ω_k^+ including both equity-feasible and equity-infeasible solutions.

Equity-infeasible space and extended fitness function

The enlarged search space Ω_k^+ explored by the second phase contains all possible partitions of the vertex set V into k disjoint subsets as follows.

$$\Omega_k^+ = \{\{V_1, V_2 : \cdots, V_k\} : \cup_{i=1}^{k} V_i = V, V_i \cap V_j = \emptyset\} \tag{3.5}$$

where $i \neq j, 1 \leq i, j \leq k$.

We note that this enlarged search subsumes the equity-feasible space Ω_k and additionally includes the equity-infeasible solutions.

To evaluate the quality of the solutions of Ω_k^+, we devise an extended penalty-based fitness function F. For this purpose, we first introduce some notations.

Let $W^+ = \lceil n/k \rceil$ and $W^- = \lfloor n/k \rfloor$, which represent respectively the theoretical cardinality of the largest and smallest color classes in an equitable k-coloring. Then for an equitable k-coloring $s = \{V_1, V_2, \cdots, V_k\}$, $W^- \leq |V_i| \leq W^+$ $(i = 1, \cdots, k)$ holds. Let $s = \{V_1, V_2, \cdots, V_k\}$ be a candidate solution in Ω_k^+, we define the penalty ρ_i $(i = 1, \cdots, k)$ for each color class V_i of the solution s to be the gap between $|V_i|$ and the theoretical cardinalities as follows.

$$\rho_i = \begin{cases} |V_i| - W^+, if\ |V_i| \geq W^+ \\ W^- - |V_i|, if\ |V_i| \leq W^- \end{cases} \tag{3.6}$$

Following the general idea of penalty function for constrained optimization [Michalewicz and Schoenauer, 1996], we introduce an extended evaluation function F to asses both feasible and infeasible solutions of Ω_k^+, which enriches the objective function f (Equation (3.2)) with a penalty function $P = \varphi \sum_{i=1}^{k} \rho_i$.

$$F(s) = \sum_{i=1}^{k} |C(V_i)| + \varphi \sum_{i=1}^{k} \rho_i \tag{3.7}$$

where $C(V_i)$ is the set of conflicting edges in color class V_i and φ (a parameter with $\varphi \geq 1$) is the penalty coefficient which is used to control the importance given to the penalty function (see Section 3.5.1 for an analysis of φ). According to this definition, a candidate solution violating strongly (weakly) the equity constraint will be penalized more harshly (slightly). Since in general the number of conflicting edges (the first term) of F decreases quickly when the search progresses, the penalty term has the desirable property of helping the search process to avoid infeasible solutions which are too far from the feasibility boundaries. Note that the penalty term of an equitable coloring equals 0.

Therefore, a partition $s \in \Omega_k^+$ with $F(s) = 0$ corresponds to a equitable and legal k-coloring, i.e., satisfying both the equity and coloring constraints and is thus a solution to the k-ECP problem.

Move operators to explore the space Ω_k^+

To explore the search space Ω_k^+, the infeasible search phase also applies two move operators to generate neighboring solutions. Let $s = \{V_1, V_2, \ldots, V_k\}$ be the current solution. Let $C(s)$ denote the set of conflicting vertices of s, i.e., the vertices involved in a conflicting edge.

1. One-move operator: Like for the first search phase, this operator displaces a conflicting vertex v from its current color class V_i to another color class V_j. However, the equity constraint is no more considered. This leads to the following enlarged neighborhood.

$$N_1^+(s) = \{s \oplus < v, V_i, V_j > : v \in V_i \cap C(s), 1 \leq i, j \leq k, i \neq j\} \tag{3.8}$$

Clearly N_1^+ is bounded by $O(|C(s)| \times k)$ in size. To effectively calculate the move gain which identifies the change in the fitness function F (Equation (3.7)), we adopt the fast incremental evaluation technique of [Lai *et al.*, 2015]. The main idea is to maintain a matrix A of size $n \times k$ with elements $A[v][q]$ recording the number of vertices adjacent to v in color class V_q $(1 \leq q \leq k)$. Another $n \times k$ matrix B is maintained with elements $B[v][q]$ representing the penalty value of vertex v assigned to color class q in the current solution. Then, the move gain of each one-move in terms of extended fitness variation can be conveniently computed by

$$\Delta F = A[v][j] - A[v][i] + \varphi(B[v][j] - B[v][i]) \tag{3.9}$$

where φ is the penalty coefficient used in the extended fitness function F.

Each time a one-move operation involving vertex v is performed, we just need to update a subset of values affected by this move as follows. For each vertex u adjacent to vertex v, $A[u][i] \leftarrow A[u][i] - 1$, and $A[u][j] \leftarrow A[u][j] + 1$. For any vertex w, $B[w][j] \leftarrow \sum_{i=1}^{k} \rho_i, 1 \leq j \leq k$. $B[w][j] = B[u][j]$, if w and u belong to the same color class.

2. Swap operator: The same swap operator as for the first phase is applied to exchange a pair of vertices (u, v) from different color classes where at least one of them is a conflicting vertex. However, there is an important difference. Since the second search phase operates in the enlarged space Ω_k^+ instead of Ω_k, the equity-feasibility of a neighboring solution fully depends on the current solution. That is, if the current solution is equity-infeasible (equity-feasible), application of swap leads to an equity-infeasible (equity-feasible) solution. The resulting swap-based neighborhood is thus given as follows.

$$N_2^+(s) = \{s \oplus swap(v, u) : v \in V_i, u \in V_j, i \neq j, \{v, u\} \cap C(s) \neq \emptyset\} \tag{3.10}$$

where $C(s)$ is the set of conflicting vertices of s. Notice that the swap operation has no impact on the penalty value of the neighboring solution and can only change the number of conflicting edges. Then the fitness gain of a swap operation can be computed by

$$\Delta F = A[u][i] - A[u][j] + A[v][j] - A[v][i] - 2e_{v,u} \tag{3.11}$$

where $e_{v,u} = 1$ if v and u are adjacent vertices, otherwise $e_{v,u} = 0$.

Exploration of the enlarged space Ω_k^+

To explore the enlarged space Ω_k^+, we apply again the tabu search method. Specifically, each iteration of tabu search selects the best admissible solutions among the neighboring solution of N_1^+ and N_2^+. The procedure makes transitions between various k-coloring while minimizing the extended fitness function F with the purpose of attaining a solution s with $F(s) = 0$.

3.3.4 Perturbation of infeasible search

The tabu list used by the equity-infeasible exploration phase helps the search process to go beyond some local optima. Yet, this mechanism may not be sufficient to escape deep traps. To overcome this problem, we apply a perturbation procedure inspired by the procedure of [Lai *et al.*, 2015]. This operator follows the perturbation scheme of breakout local search [Benlic and Hao, 2013] and combines directed and random applications of the one-move and swap operators. To avoid a too strong deterioration of the perturbed solution, a directed perturbation move takes into consideration the fitness variation and performs the most favorable move (i.e., deteriorating the solution the least). In contrary, a random perturbation performs a one-move or swap operation without considering the fitness deterioration. To combine these two types of perturbations, the number of performed moves dynamically varies in an adaptive way while the application of each type of perturbation is determined probabilistically. The random and directed perturbations are applied with a probability of $p \in [0, 1]$ and $1 - p$, respectively. In this paper, we take the $p = 0.3$, The length of the perturbations $L = 500 * F$ (F is the objective function as shown in equitation 3.7)). The resulting solution from the perturbation procedure is then used as the new starting solution of the next round of the infeasible search phase.

3.4 Experimental results and comparisons

In this section, we assess the performance of the proposed FISA algorithm on the set of 73 benchmark instances which are commonly used in the literature and were initially proposed for the DIMCAS and COLOR competitions for graph coloring problems [1, 2].

3.4.1 Experiment settings

The proposed algorithm was coded in C++ and compiled by GNU g++ 4.1.2 with -O3 flag (option). The experiments were conducted on a computer with an Intel Xeon E5-2670 processor (2.5 GHz and 2 GB RAM) running Ubuntu 12.04. When solving the DIMACS machine benchmark procedure 'dfmax.c' [3] without compilation optimization flag, the run time on the computer is 0.46, 2.68 and 10.70 seconds for graphs r300.5, r400.5 and r500.5, respectively.

For our comparative study, we use the most recent heuristic algorithms [Díaz *et al.*, 2014; Lai *et al.*, 2015] as our references. The TabuEqCol algorithm (2014) [Díaz *et al.*, 2014] was run on an Intel i5 CPU with 750 2.67 GHz and tested under a time limit of 1 hour. The BITS algorithm (2015) [Lai *et al.*, 2015] was run on an Intel Xeon E5440 CPU with 2.83 GHz and 2 GB RAM and tested under a time limit of 1 hour and a relaxed limit (10^4 seconds for the instances with up to 500 vertices and 2×10^4 seconds for larger instances with more than 500 vertices). As shown in [Lai *et al.*, 2015], the computational results of the more recent BITS algorithm dominate those of TabuEqCol. We also include the lower and upper bounds reported in [Méndez-Díaz *et al.*, 2014; Méndez-Díaz *et al.*, 2015] which were obtained by exact methods under various test conditions. These bounds provide useful information when they are contrasted with the results (upper bounds) obtained by the compared heuristic algorithms (TabuEqCol, BITS and FISA).

The FISA algorithm requires the tuning of some parameters related to tabu search and the extended fitness function F. Since our tabu search procedures are adaptations of the basic tabu search procedure of [Lai *et al.*, 2015], we adopted the parameter settings used in the original paper. As to the penalty coefficient φ of the extended fitness function F, we provide an analysis in Section 3.5.

Following [Díaz *et al.*, 2014; Lai *et al.*, 2015], we present a first experiment where we ran our FISA algorithm only once per instance with a cutoff time of 3,600 seconds (1 hour). Like [Lai *et al.*, 2015], we carried out a second experiment where we ran FISA 20 times to solve each instance under the extended stopping condition – 10^4 seconds for the instances with up to 500 vertices and 2×10^4 seconds for larger instances with more than 500 vertices. We note that, our Intel Xeon E5-2670 2.5 GHz processor is slightly slower than those used by the reference algorithms. As a result, our adopted stopping conditions can be considered as reasonable with respect to those used by the reference algorithms. Finally, as shown in [Lai *et al.*, 2015], the more recent BITS algorithm fully dominates the TabuEqCol algorithm. So the results of BITS have the most significant reference value.

3.4.2 Comparison with state-of-the-art algorithms

From Table 3.1, we can see that FISA shows a remarkable performance compared to the TabuEqCol and BITS algorithms under both stopping conditions. Under the 1 hour condition, FISA dominates TabuEqCol (Columns 5 and 8) on the 50 instances tested by both algorithms, by obtaining better results for 30 instances and the same results for the remaining 20 instances. Compared

1. http://www.dimacs.rutgers.edu/
2. http://www.cs.hbg.psu.edu/txn131/graphcoloring.html/
3. dfmax: ftp://dimacs.rutgers.edu/pub/dsj/clique/

to the most recent BITS algorithm, FISA obtains better solutions for 14 instances (see negative entries in Column $\Delta(k_1)$), the same best results for other 58 instances and one worse result.

When comparing FISA with BITS under the long time condition (the results of TabuEqCol under this condition are unavailable), one observes that FISA also performs very well. Specifically, FISA improves the best results of BITS for 9 instances (see negative entries in Column $\Delta(k_{best})$ while matching the best results of BITS for other 63 instances. Only in one case, FISA obtains a slightly worse result.

Finally, when comparing to the upper bounds obtained by exact algorithms (Column 4), it is clear that the bounds of FISA (Column 9) are much better. Contrasting the current best lower bounds (Column 3) obtained by exact approaches of [Méndez-Díaz *et al.*, 2014; Méndez-Díaz *et al.*, 2015] and the best upper bounds of FISA (Column 9), we observe there is still potential for further improvement.

3.5 Analysis

This section performs additional experiments to analyze the proposed FISA algorithm: the penalty coefficient φ and the perturbation strategy. These experiments were performed on a selection of 26 instances which are computationally relatively difficult to solve.

3.5.1 Analysis of the penalty coefficient φ

This section investigates the influence of the penalty coefficient φ on the performance of the proposed algorithm. For this purpose, we tested FISA with 3 different values of $\varphi = 1, 2, 3$ (larger values lead to worse results). We ran 20 times the algorithm with each φ value to solve each selected instance with a cutoff time of 1 hour.

The experimental results are presented in Table 3.2. The first column shows the names of instances, and the second column indicates the best results (k_1^*) obtained in this experiment. The results of FISA with different φ values are respectively listed in columns 3 to 5. The rows #Equal and #Worse respectively indicate the number of instances for which each φ values attains an equal and worse result compared to k_1^*. We note that the best results were obtained with $\varphi = 1$. This justifies the setting of this parameter used in our previous experiments.

3.5.2 Impact of the perturbation operation

As shown in Section 3.3.4, the proposed algorithm uses a perturbation strategy to ensure a global diversification within the enlarged search space Ω_k^+. In order to assess this strategy, we compare it with a traditional restart strategy (denoted as REST), where each restart begins its search with a new equitable k-coloring generated by the greedy procedure mentioned in Section 3.3. The two algorithms were run 20 times on the 26 selected instances with a time limit of 1 hour per run.

The results of this experiment are shown in Table 3.3. Column 1 lists the names of instances. Column 2 indicates the best results (k_{best}^*) obtained in this experiment. The best results (k_{best}) and the average results (k_{avg}) of FISA and REST are respectively listed in columns 3 to 6. The rows #Equal and #Worse respectively indicate the number of instances for which FISA and REST attain an equal and worse result compared to k_{best}^*. It is clear that FISA dominates the REST variant by obtaining 12 better results out of the 26 tested instances and no worse result. This experiment confirms thus the interest of the adopted perturbation strategy.

Table 3.1 – Comparative results of FISA with state-of-the-art algorithms on the 73 benchmark instances.

				TabuEqCol	BITS		FISA						
Instance	$\|V\|$	LB	UB	k_1	$k_1(pre)$	$k_{best}(pre)$	k_1	k_{best}	k_{avg}	SR	t_{avg}	$\Delta(k_1)$	$\Delta(k_{best})$
DSJC125.1.col	125	5	5	5*	5*	5*	5*	5*	5	20/20	0.617	0	0
DSJC125.5.col	125	9	18	18	17	17	17	17	17	20/20	428.281	0	0
DSJC125.9.col	125	43	45	45	44	44	44	44	44	20/20	0.094	0	0
DSJC250.1.col	250	5	8	8	8	8	8	8	8	20/20	3.619	0	0
DSJC250.5.col	250	12	32	32	32	29	**29**	29	29.35	13/20	5235.95	-3	0
DSJC250.9.col	250	63	83	83	72	72	72	72	72	20/20	892.236	0	0
DSJC500.1.col	500	5	13	13	13	13	13	13	13	20/20	3.569	0	0
DSJC500.5.col	500	13	62	63	57	56	**53**	**52**	53.25	1/20	8197.02	-4	-4
DSJC500.9.col	500	101	148	182	130	129	131	130	131	3/20	6269.63	1	1
DSJR500.1.col	500	12	12	12*	12*	12*	12*	12*	12	20 /20	0.38	0	0
DSJR500.5.col	500	120	131	133	126	126	126	126	126.5	10/20	4459.5	0	0
DSJC1000.1.col	1000	5	22	22	22	21	**21**	21	21	20/20	1866.63	-1	0
DSJC1000.5.col	1000	15	112	112	112	101	**98**	**95**	96.1	2/20	15698.6	-14	-6
DSJC1000.9.col	1000	126	268	329	254	252	**253**	252	252.2	16/20	2240.02	-1	0
R125.1.col	125	-	-	-	5	5	5	5	5	20/20	0.0025	0	0
R125.5.col	125	-	-	-	36	36	36	36	36	20/20	0.6745	0	0
R250.1.col	250	-	-	-	8	8	8	8	8	20/20	0.0045	0	0
R250.5.col	250	-	-	-	67	66	67	66	66.9	2/20	3041.22	0	0
R1000.1.col	1000	-	-	-	20	20	20	20	20	20/20	2.244	0	0
R1000.5.col	1000	-	-	-	269	250	**251**	250	250.45	11/20	11564.2	-18	0
le450_5a.col	450	5	5	-	5*	5*	5*	5*	5	20/20	30.1971	0	0
le450_5b.col	450	5	5	7	5*	5*	5*	5*	5	20/20	44.2914	0	0
le450_5c.col	450	-	-	-	5	5	5	5	5	20/20	16.391	0	0
le450_5d.col	450	5	8	8	5*	5*	5*	5*	5	20/20	14.0655	0	0
le450_15a.col	450	15	15	-	15*	15*	15*	15*	15	20/20	2.993	0	0
le450_15b.col	450	15	15	15*	15*	15*	15*	15*	15	20/20	2.4125	0	0
le450_15c.col	450	-	-	-	15	15	15	15	15.2	16/20	553.786	0	0
le450_15d.col	450	15	16	16	15*	15*	15*	15*	15.85	3/20	638.127	0	0
le450_25a.col	450	25	25	-	25*	25*	25*	25*	25	20/20	0.41	0	0
le450_25b.col	450	25	25	25*	25*	25*	25*	25*	25	20/20	0.46	0	0
le450_25c.col	450	-	-	-	26	26	26	26	26	20/20	86.9035	0	0
le450_25d.col	450	25	27	27	26	26	26	26	26	20/20	95.845	0	0
wap01a.col	2368	41	46	46	43	42	**42**	42	42.95	1/20	4544.77	-1	0
wap02a.col	2464	40	44	44	42	41	42	41	41	2/20	2538.33	0	0
wap03a.col	4730	40	50	50	46	45	46	45	45.7	6/20	20201.8	0	0
wap04a.col	5231	-	-	-	46	44	46	44	44.45	11/20	15614.2	0	0
wap05a.col	905	-	-	-	50	50	50	50	50	20/20	99.2625	0	0
wap06a.col	947	-	-	-	42	41	42	41	41.9	2/20	9340.42	0	0
wap07a.col	1809	-	-	-	43	43	43	43	43.05	19/20	4077.71	0	0
wap08a.col	1870	-	-	-	43	43	43	43	43.1	10/20	4872.74	0	0
flat300_28_0.col	300	11	36	36	35	34	**33**	**32**	33.6	1/20	4910.48	-2	-2
flat1000_50_0.col	1000	-	-	-	112	101	**96**	**94**	94.7	6/20	17321.4	-16	-7
flat1000_60_0.col	1000	-	-	-	112	101	**97**	**94**	94.8	5/20	10488.8	-15	-7
flat1000_76_0.col	1000	14	112	112	112	102	**98**	**94**	95.15	2/20	15246.4	-14	-8
latin_square_10.col	900	90	130	130	129	113	**105**	**104**	104.55	10/20	12666.2	-24	-9
C2000.5.col	2000	-	-	-	202	201	**198**	**183**	183.4	13/20	19702.3	-4	-18
C2000.9.col	2000	-	-	-	504	502	**503**	**493**	495.21	2/20	21163.9	-1	-9
mulsol.i.1.col	197	49	49	50	49*	49*	49*	49*	49	20/20	44.3365	0	0
mulsol.i.2.col	188	34	39	48	36	36	36	36	36.95	2/20	1914.22	0	0
fpsol2.i.1.col	496	65	65	78	65*	65*	65*	65*	65	20/20	1723.52	0	0
fpsol2.i.2.col	451	47	47	60	47*	47*	47*	47*	47.2	17/20	2357.15	0	0
fpsol2.i.3.col	425	55	55	79	55*	55*	55*	55*	55	20/20	1310.01	0	0
inithx.i.1.col	864	54	54	66	54*	54*	54*	54*	56.9	7/20	3356.31	0	0
inithx.i.2.col	645	30	93	93	36	36	36	36	38.8	5/20	3275.5	0	0
inithx.i.3.col	621	-	-	-	38	37	38	37	39.85	4/20	2891.78	0	0
zeroin.i.1.col	211	49	49	51	49*	49*	49*	49*	49.6	8/20	1088.94	0	0
zeroin.i.2.col	211	36	36	51	36*	36*	36*	36*	36	20/20	123.876	0	0
zeroin.i.3.col	206	36	36	49	36*	36*	36*	36*	36	20 /20	129.445	0	0
myciel6.col	95	7	7	7*	7*	7*	7*	7*	7	20/20	0.0035	0	0
myciel7.col	191	8	8	8*	8*	8*	8*	8*	8	20/20	0.0185	0	0
4_FullIns_3.col	114	7	7	-	7*	7*	7*	7*	7	20/20	0.0005	0	0
4_FullIns_4.col	690	6	8	8	8	8	8	8	8	20/20	0.12	0	0
4_FullIns_5.col	4146	6	9	9	9	9	9	9	9	20/20	0.12	0	0
1_Insertions_6.col	607	3	7	7	7	7	7	7	7	20/20	0.1655	0	0
2_Insertions_5.col	597	3	6	6	6	6	6	6	6	20/20	0.056	0	0
3_Insertions_5.col	1406	3	6	6	6	6	6	6	6	20/20	0.3525	0	0
school1.col	385	15	15	15*	15*	15*	15*	15*	15	20/20	0.932	0	0
school1_nsh.col	352	14	14	14*	14*	14*	14*	14*	14	20/20	1.774	0	0
qg.order40.col	1600	40	40	40*	40*	40*	40*	40*	40	20/20	3.437	0	0
qg.order60.col	3600	60	60	60*	60*	60*	60*	60*	60	20/20	14.534	0	0
ash331GPIA.col	662	4	4	4*	4*	4*	4*	4*	4	20/20	0.7755	0	0
ash608GPIA.col	1216	3	4	4	4	4	4	4	4	20/20	0.249	0	0
ash958GPIA.col	1916	3	4	4	4	4	4	4	4	20/20	10.887	0	0

Table 3.2 – Comparative results of the FISA algorithm with 3 different values of φ on the 26 instances. The best results are in bold.

Instance	k_1^*	$k_{1,\varphi=1}$ [1]	$k_{1,\varphi=2}$	$k_{1,\varphi=3}$
C2000.5.col	198	**198**	200	199
DSJC1000.1.col	21	**21**	**21**	**21**
DSJC1000.5.col	98	**98**	100	101
DSJC1000.9.col	253	**253**	254	254
DSJC125.5.col	17	**17**	**17**	**17**
DSJC250.1.col	8	**8**	**8**	**8**
DSJC250.5.col	29	**29**	**29**	**29**
DSJC250.9.col	72	**72**	**72**	**72**
DSJC500.5.col	53	**53**	**53**	**53**
DSJC500.9.col	130	131	131	**130**
DSJR500.5.col	126	**126**	**126**	**126**
flat1000_50_0.col	96	**96**	98	99
flat1000_60_0.col	97	**97**	98	99
flat1000_76_0.col	98	**98**	99	101
flat300_28_0.col	32	33	**32**	**32**
fpsol2.i.1.col	65	**65**	**65**	**65**
fpsol2.i.2.col	47	**47**	**47**	**47**
inithx.i.2.col	36	**36**	37	54
inithx.i.3.col	37	38	**37**	57
latin_square_10.col	105	**105**	114	115
mulsol.i.2.col	36	**36**	**36**	**36**
R1000.5.col	250	251	251	**250**
R250.5.col	66	67	**66**	67
zeroin.i.1.col	49	**49**	**49**	**49**
zeroin.i.2.col	36	**36**	**36**	**36**
zeroin.i.3.col	36	**36**	**36**	**36**
#Equal		21	16	16
#Worse		5	10	10

[1] $k_{1,\varphi=1}$,$k_{1,\varphi=2}$,$k_{1,\varphi=3}$ respectively indicates the best results of FISA with different φ values obtained under 1 hour condition in this experiment.

Table 3.3 – Analysis of the influence of the perturbation on the performance of the FISA algorithm.

		FISA		REST	
Instance	k_{best}^*	k_{best}	k_{avg}	k_{best}	k_{avg}
C2000.5.col	198	**198**	199.55	201	201
DSJC1000.1.col	21	**21**	21	21	21
DSJC1000.5.col	98	**98**	99.45	102	102.15
DSJC1000.9.col	253	**253**	254.35	253	254.3
DSJC125.5.col	17	**17**	17	17	17
DSJC250.1.col	8	**8**	8	8	8
DSJC250.5.col	29	**29**	29.8	29	29.95
DSJC250.9.col	72	**72**	72.1	72	72.1
DSJC500.5.col	53	**53**	53.35	54	55.15
DSJC500.9.col	131	**131**	131.6	131	131.7
DSJR500.5.col	126	**126**	126.85	126	127.05
flat1000_50_0.col	96	**96**	97.4	101	101.5
flat1000_60_0.col	97	**97**	97.9	101	101.75
flat1000_76_0.col	98	**98**	98.65	101	101.95
flat300_28_0.col	33	**33**	33.85	33	34.3
fpsol2.i.1.col	65	**65**	65	77	79.4
fpsol2.i.2.col	47	**47**	47.25	56	73.05
inithx.i.2.col	36	**36**	38.8	60	63.85
inithx.i.3.col	38	**38**	39.05	57	64.85
latin_square_10.col	105	**105**	106.1	105	106.5
mulsol.i.2.col	36	**36**	36.95	37	37.75
R1000.5.col	251	**251**	253.9	252	255.35
R250.5.col	67	**67**	67	67	67.05
zeroin.i.1.col	49	**49**	49.75	55	55.9
zeroin.i.2.col	36	**36**	36	39	42
zeroin.i.3.col	36	**36**	36	38	43.05
#Equal		26		14	
#Worse		0		12	

3.6 Conclusions

The equitable coloring problem (ECP) is an NP-hard problem with a number of practical applications. In addition to the conventional coloring constraint (i.e., adjacent vertices must receive different colors), a solution of the ECP must satisfy the equity constraint (the cardinalities of the color classes must differ by at most one). In this work, we investigated for the first time the benefit of examining both feasible and infeasible solutions with respect to the equity constraint. The resulting algorithm (called FISA) combines an equity-feasible search phase where only equitable colorings are considered and an equity-infeasible search phase where the search is enlarged to include non-equitable solutions. To guide the search procedure (which is based on tabu search), we devised an extended fitness function which uses a penalty to discourage candidate solutions which violates the equity constraint. A perturbation procedure was also used as a diversification means to help the algorithm to explore new search regions.

We assessed the performance of the FISA algorithm on the set of 73 benchmark instances from DIMACS and COLOR competitions and presented comparative results with respect to state of the art algorithms. The comparisons showed that FISA performs very well by discovering 9 improved best results (new upper bounds) and matching the best-known results for the remaining instances except one case. The new bounds can be used for assessment of other ECP algorithms. This study demonstrates the benefit of the mixed search strategy examining both equity-feasible and equity-infeasible solutions for solving the ECP.

For future work, several directions could be followed. First, the penalty term of the extended fitness function could be improved by introducing adaptive techniques like [Chen *et al.*, 2016a; Glover and Hao, 2011] to enable a strategic oscillation for transitioning between feasible and infeasible space. Second, other search operators (rather than those used in this work) can be sought to further improve the performance of the search algorithm. Finally, the proposed algorithm could be advantageously integrated into a hybrid population-based method (e.g., memetic search, path-linking) as a key intensification component.

4

Adaptive feasible and infeasible search for WVCP

This chapter presents the adaptive feasible and infeasible search for solving the NP-hard weighted vertex coloring. The proposed algorithm employs the heuristic algorithm that relies on a mixed search strategy exploring both feasible and infeasible solutions. We show extensive experimental results on a large number of benchmark instances and present new upper bounds that are useful for future studies. We assess the benefit of the key features of the proposed approach. The chapter is based on an journal article published in Information Sciences [Sun *et al.*, 2018b].

Contents

4.1 Introduction

The weighted vertex coloring problem of a vertex weighted graph is to partition the vertex set into k disjoint independent sets such that the sum of the costs of these sets is minimized, where the cost of each set is given by the largest weight of the vertices assigned to that set.

We summarize the main contributions of this work as follows.

First, the adaptive feasible and infeasible search algorithm (AFISA) presented in this work is the first heuristic method that explores both feasible and infeasible solutions for the WVCP. To prevent the search from going too far away from the feasible boundary, we design an adaptive penalty-based evaluation function that is used to guide the search for a fruitful examination of candidate solutions, by enabling the search to oscillate between feasible and infeasible regions. To ensure an effective exploration of both feasible and infeasible regions, we adopt the popular tabu search meta-heuristic [Glover, 1997] and design specific search components to cope with the particular features of the considered coloring problem.

Second, we assess the proposed algorithm on 111 conventional benchmark instances from the literature (one set of 46 instances from the DIMACS and COLOR competitions and two sets of 65 instances from matrix-decomposition problems). We report especially 5 improved best solutions (new upper bounds). We also present results on an additional set of 50 (larger) DIMACS instances. These results and the proposed algorithm can serve as a new reference to assess future WVCP algorithms and can be useful for the design of effective exact algorithms as well.

The remainder of the chapter is organized as follows. Section 4.2 presents the proposed algorithm. Section 4.3 is dedicated to the description of computational results and comparisons with state-of-the-art algorithms. Section 4.4 analyzes the impact of some key components of the proposed algorithm. Conclusions and future work are discussed in the last section.

4.2 Adaptive feasible and infeasible search for the WVCP

In this section, we present the adaptive feasible and infeasible search algorithm for solving the WVCP. We first show the general approach and then explain in detail the components of the proposed algorithm including the search space, the evaluation function, the neighborhood, the tabu search procedure, the adaptive mechanism to control feasible and infeasible searches and the perturbation strategy.

4.2.1 General approach

Unlike existing methods for the WVCP [Malaguti *et al.*, 2009; Prais and Ribeiro, 2000] that only consider feasible colorings, the adaptive feasible and infeasible search algorithm (AFISA) proposed in this work enlarges the search to include both feasible and infeasible colorings. Indeed, as explained in the introduction, methods that are allowed to oscillate between feasible and infeasible regions can help to attain solutions of high-quality that would not be discovered otherwise. Specifically, we first generate an initial feasible solution with a greedy procedure (Section 4.2.2). Then, we improve the solution by enlarging the search to include infeasible solutions. To enable the search to oscillate between feasible and infeasible regions, we devise an extended evaluation function F that combines the objective function of Eq. (1) with a penalty function (Section 4.2.3). To control the importance given to the penalty function, we introduce an adaptive parameter that is dynamically adjusted according to the search context (Section 4.2.4). To explore the search space, we use a tabu search procedure that relies on a neighborhood induced by the one-move operator and that is guided by the penalty-based evaluation function (Section 4.2.4). Finally, to escape local optimum traps, we introduce an adaptive perturbation strategy to gener-

ate a new starting solution for the next round of tabu search (Section 4.2.5). The pseudo-code of the proposed algorithm is presented in Algorithm 4.1.

Algorithm 4.1: Main scheme of the AFISA algorithm for the WVCP

1: **Input**: Graph G
2: **Output**: The best solution found
3: $s_0 \leftarrow greedy\_initial(G)$ /* Generate an initial feasible k-coloring, Section 4.2.2 */
4: $s_{best} \leftarrow s_0$ /* Record the best legal solution */
5: $\gamma \leftarrow 0$ /* γ is the counter for consecutive non-improving local optima */
6: $s_1 \leftarrow s_0$
7: $L \leftarrow L_0$/* Initialize the depth of perturbation, Section 4.2.5 */
8: $\varphi \leftarrow 1$ /* Initialize penalty coefficient of the extended evaluation function, Sections 4.2.3 and 4.2.4 */
9: **while** stopping condition is not met **do**
10: $s_2 \leftarrow tabu\_search(s_1)$ /* Section 4.2.4 */
11: **if** $F(s_2) < F(s_{best})$ *and* $F(s_2) = f(s_2)$ **then**
12: $s_{best} \leftarrow s_2$ /* Record the best legal solution */
13: $L \leftarrow L_0$ /* Reinitialize the depth of perturbation */
14: $\gamma \leftarrow 0$ /* Reset the counter for consecutive non-improving local optima */
15: **else**
16: $\gamma \leftarrow \gamma + 1$
17: **end if**
18: **if** $\gamma = T$ **then**
19: $L \leftarrow L_{max}$ /* Increase the depth of perturbation if the best solution is not updated during T consecutive tabu search runs */
20: **end if**
21: $\varphi \leftarrow adaptive\_parameter(s_2, \varphi)$ /* Adjust penalty coefficient, Section 4.2.4 */
22: $s_1 \leftarrow perturbation(s_2, L)$ /* Section 4.2.5 */
23: **end while**
24: **return** s_{best}

4.2.2 Initial solution

The purpose of the initialization step is to generate an initial feasible solution of acceptable quality. This is achieved by adopting the greedy procedure of [Prais and Ribeiro, 2000] that iteratively assigns the vertices to a suitable color class (Algorithm 4.2). Let $\{V_1, V_2, \ldots, V_k\}$ be the current partial solution with k color classes (initially k is set to 1, $V_1 = \emptyset$), we choose an unassigned vertex v (Algorithm 4.2, line 6) and assign it to the color class $V_i, 1 \leq i \leq k$ such that the objective function f is minimized while the coloring constraint is met. If no suitable color class $V_i, 1 \leq i \leq k$ exists for vertex v, we create a new color class V_k by setting $k \leftarrow k + 1$ and assign the vertex v to this new color class (Algorithm 4.2, line 15-16). This process is repeated until all vertices are assigned to a color class.

This initialization procedure provides thus the AFISA algorithm with a legal k-coloring of certain quality, which will be further improved during the tabu search phase of the algorithm.

4.2.3 Search space and penalty-based evaluation function

To further improve the initial solution provided by the above initialization procedure, the search phase of the AFISA algorithm explores an enlarged space Ω including both feasible and infeasible solutions. In other words, the space Ω is composed of the partitions of the vertex set V into k disjoint subsets.

Algorithm 4.2: Greedy initialization for the WVCP

```
1: Input: Graph G = (V, E)
2: Output: A legal k-coloring s
3: U ← V /* U is the set of unassigned vertices */
4: i = 1, k = 1, V_i = ∅
5: while U ≠ ∅ do
6:    choose a vertex v from U with maximum weight
7:    assign = 0 /* assign is a flag indicating if vertex v is assigned a color */
8:    for i = 1, 2, ..., k do
9:       if there is no edge between v and any vertex of V_i then
10:         V_i ← V_i ∪ {v} /* v is assigned to color class V_i */
11:         assign = 1 /* v is now assigned a color */
12:      end if
13:   end for
14:   if assign = 0 then
15:      k ← k + 1
16:      V_k ← V_k ∪ {v} /* Create a new color class V_k to hold v */
17:   end if
18:   U ← U \ {v}
19: end while
20: return s = {V_1, V_2, ..., V_k} /* s is a legal or feasible k-coloring */
```

$$\Omega = \{\{V_1, V_2, \ldots, V_k\} : \cup_{i=1}^{k} V_i = V, V_i \cap V_j = \emptyset, 1 \leq k \leq |V|\} \tag{4.1}$$

where $i \neq j, 1 \leq i, j \leq k$.

Then we define our extended fitness function F (to be minimized) as a linear combination of the basic fitness function f (Equation (1.1)) and a penalty function P as follows. Let $s = \{V_1, V_2, \ldots, V_k\}$ be a candidate solution in Ω, we define its penalty $P(s)$ as $P(s) = \sum_{i=1}^{k} |C(V_i)|$ where $C(V_i)$ counts the number of pair of conflicting vertices in color class V_i that are linked by an edge. In other words, $P(s)$ indicates the number of conflicts in the candidate solution s. Therefore, for the candidate solution s, if the penalty $P(s)$ equals 0, then s corresponds to a feasible k-coloring satisfying the coloring constraint. Otherwise (i.e., $P(s) > 0$), the solution includes at least two adjacent vertices violating the coloring constraint, i.e., belonging to a same color class.

Then the quality of the solution $s = \{V_1, V_2, \ldots, V_k\}$ is given by the following extended evaluation function:

$$F(s) = f(s) + \varphi P(s) \tag{4.2}$$

where $f(s)$ is the objective function value and $\varphi \geq 1$ is a parameter that is used to control the relative importance given to the penalty function.

Since F is to be minimized, increasing φ augments the value of F, making thus the infeasible solution under consideration less attractive. Inversely, decreasing φ lowers the evaluation value, making the solution more attractive. By varying φ, we can control the transition between feasible and infeasible regions. We explain in Section 4.2.4 the adaptive technique to dynamically tune φ according to the search situation. We investigate in Section 4.4.2 the impact of the φ parameter.

Using the extended evaluation function F, we assess the relative quality of two candidate solutions x and y as follows: x is better than y if $F(x) < F(y)$.

4.2.4 Searching feasible and infeasible solutions with tabu search

Neighborhood and its evaluation

The AFISA algorithm examines the search space Ω by making transitions from the current solution to one neighboring solution. A neighboring solution is generated by using the popular "one-move" operator. Give a solution $s = \{V_1, V_2, \ldots, V_k\}$, the one-move operator displaces a vertex v from its current color class V_i to a different color class V_j ($i \neq j$, $j \in \{1, 2, \ldots, |V|\}$), leading to a neighboring solution designated by $s \oplus < v, V_i, V_j >$. The one-move neighborhood is then given by:

$$N(s) = \{s \oplus < v, V_i, V_j > : v \in V_i, 1 \leq i \leq k, 1 \leq j \leq |V|, i \neq j\} \tag{4.3}$$

This neighborhood allows a vertex to be moved to a currently empty color class V_j with $j > k$ (thus the number of color classes can increase). Inversely, a color class can also become empty and thus be removed when its last vertex is transferred to another existing class (thus k is decreased). As a result, search algorithms using this neighborhood like the tabu search procedure presented in Section 4.2.4 typically visit solutions whose number of color classes varies during the search.

Notice that this neighborhood is different from the one-move neighborhood used for other coloring problems (e.g., conventional vertex coloring [Galinier and Hertz, 2006; Malaguti and Toth, 2010] and equitable coloring problem [Lai *et al.*, 2015; Sun *et al.*, 2017; Wang *et al.*, 2018], because 1) in these studies the vertex $v \in V_i$ to be displaced must be a conflicting vertex (i.e., there exists in V_i at least another vertex u such that v and u are adjacent in the graph), and 2) the number of color classes k remains fixed.

Finally, one important issue concerns the evaluation of the neighborhood that impacts significantly the computational efficiency of any local search algorithm. In our case, we employ an incremental evaluation technique that is similar to the evaluation technique designed for another graph coloring problem (i.e., equitable coloring) [Lai *et al.*, 2015; Sun *et al.*, 2017]. With this technique, the objective variation of each neighbor solution can be conveniently obtained in constant time. We refer the readers to [Lai *et al.*, 2015; Sun *et al.*, 2017] for more details of this evaluation technique.

Tabu search

To explore the above neighborhood, the proposed AFISA algorithm uses the well-known tabu search (TS) meta-heuristic [Glover, 1989; Glover, 1990] that has been applied to many difficult combinatorial optimization problems [Glover, 1997]. In particular, TS is known to be quite successful in solving several different graph coloring problems such as general graph coloring [Galinier and Hao, 1999; Hertz and de Werra, 1987], minimum sum coloring [Jin and Hao, 2016] and equitable coloring [Lai *et al.*, 2015]. As a general meta-heuristic, TS has some attractive features. First, it can be adapted to graph coloring problems rather easily. Moreover, TS offers simple strategies to promote a suitable and necessary search balance between intensification (with the best-improvement principle to explore a given neighbourhood) and diversification (with a tabu list).

In our case, the tabu search procedure make transitions between various k-colorings guided by the extended evaluation function F of Section 4.2.3. Our TS procedure is based on the popular TabuCol algorithm for the conventional Vertex Coloring Problem [Hertz and de Werra, 1987] and adopts the improvements presented in [Galinier and Hao, 1999]. For the sake of completeness, we show the pseudo-code of the tabu search procedure in Algorithm 4.3 and provide the following description.

The tabu search procedure iteratively replaces the current solution s by a neighboring solution s' taken from the one-move neighborhood $N(s)$ defined in Section 4.2.4 until a stopping condition is met. At each iteration, TS examines the neighborhood and selects a best admissible neighboring solution s' (see below) to substitute s. After each iteration, the associate one-move is recorded on the tabu list to prevent the search from revisiting s for the next tt iterations (tt is called the tabu tenure). To tune the tabu tenure, we use $tt = Random(A) + \alpha F$ where F stands for the extended evaluation function, the function $Random(A)$ returns a random number in $\{0, \ldots, A\text{-}1\}$ (A is set to 10 in this work) and α is a parameter set to 0.6. Meanwhile, the best solution found is updated if the new solution is better than all previous visited solutions. A neighboring solution s' is considered to be admissible if it is not forbidden by the tabu list or if it is better (according to the extended evaluation function F) than the best solution found. If the best solution is not updated during β consecutive iterations (β is called the depth of tabu search), then the current tabu search process is considered to be stagnating and stops.

Algorithm 4.3: Tabu search algorithm

Input: initial solution s, depth of tabu search β
Output: The best solution s_b found during the tabu search process
$s_c \leftarrow s$ /* s_c is the current solution */
$s_b \leftarrow s_c$ /* s_b is the best solution found */
$d \leftarrow 0$ /* d counts the consecutive iterations during which s_b is not updated */
repeat
  Choose a best admissible neighboring solution $s' \in N(s_c)$
  /* s' is admissible if it is not forbidden by the tabu list or better than s_b */
  $s_c \leftarrow s'$
  /* Update the best solution */
  if $F(s_c) < F(s_b)$ **then**
    $s_b \leftarrow s_c$
    $d \leftarrow 0$
  else
    $d \leftarrow d + 1$
  end if
until $d = \beta$
return s_b

Adaptive mechanism to control feasible and infeasible searches

The AFISA algorithm uses the extended evaluation function F (see Section 4.2.3) combining the objective function f and the penalty function P to assess the quality of candidate solutions and guide the search process. By varying the penalty coefficient φ of F, we can change the search trajectory according to the search situation. Basically, a large (small) φ value strongly (weakly) penalizes infeasible solutions and incites the search process to give more importance to feasible (infeasible) solutions. To allow the search process to go back and forth between feasible and infeasible zones, we devise an adaptive mechanism to dynamically adjust φ such that a suitable diversification-intensification balance can be reached. This adaptive mechanism relies on known ideas proposed for continuous optimization like those reviewed in [Hamida and Schoenauer, 2000].

The adaptive adjustment mechanism is shown in Algorithm 4.4. According to whether the solution s (obtained from the last round of tabu search) is a feasible k-coloring, we adjust φ to influence the search trajectory of the next round of tabu search. Specifically, if $P(s) \neq 0$ (i.e.,

$F(s) \neq f(s)$) (Algorithm 4.4, line 3), which means solution s is an infeasible k-coloring, we increase φ to penalize more strongly the infeasible solutions. As such, if the tabu search procedure always ends up with an infeasible solution during several consecutive runs, the search is considered to perform enough exploration in infeasible zones and thus encouraged to move towards feasible regions to intensify its search during the next round of tabu search. Inversely, if $P(s) = 0$ (i.e., $F(s) = f(s)$), the solution returned by the last round of tabu search is a feasible k-coloring, indicating that the search just examined a feasible region. In this case, we decrease φ to raise the chance of visiting infeasible regions during the next tabu search run and thus diversify the search. The computational results of Section 4.3 show that the AFISA algorithm equipped with this adaptive mechanism of exploring feasible and infeasible solutions reaches a high performance.

Algorithm 4.4: Adaptive adjustment mechanism for penalty coefficient φ

1: **Input**: Penalty coefficient φ, the best solution from the last round of tabu search s
2: **Output**: Adjusted penalty coefficient φ
3: **if** $F(s) \neq f(s)$ **then**
4: $\quad \varphi = \varphi + 1$ /* Increase the penalty term to guide the search toward feasible regions */
5: **else**
6: $\quad \varphi = \varphi - 1$ /* Decrease the penalty term to increase the chance of visiting infeasible solutions */
7: **end if**
8: **if** $\varphi \leq 0$ **then**
9: $\quad \varphi = 1$
10: **end if**

4.2.5 Perturbation strategy

As illustrated in Section 4.2.4, the tabu procedure ends up with a local optimal solution. To enable the search to move to new search zones, we apply a perturbation strategy to modify the last local optimum that is then used as the new starting solution of the next round of tabu search (line 22, Algorithm 4.1). To make the perturbation strategy as effective as possible, we borrow ideas from breakout local search [Benlic and Hao, 2013] whose perturbation strategy relies on two factors: the jump magnitude L (also called depth of perturbation) and the perturbation type.

The jump magnitude L indicates the number of perturbation moves to be applied and in our case, is set to a small value (L_0) in the beginning (line 7, Algorithm 4.1). If the search is observed to be stagnating (i.e., no better feasible solution can be found during T consecutive tabu search runs), L is increased to a large value (L_{max}) to enable a stronger diversification (line 19, Algorithm 4.1). Then each time the search moves to a new promising search zone by discovering a better feasible solution, L is switched to L_0 again (line 13, Algorithm 4.1).

To perform a perturbation, two types of moves, both being based on the one-move operator (see Section 4.2.4), are applied according to a probability P_0. The first type of perturbation, called tabu-based perturbation, relies on the tabu principle and selects a one-move $< v, V_i, V_j >$ that minimizes the objective degradation while considering the tabu list, as in Section 4.2.4. Starting from an empty tabu list, each time a perturbation move is performed, the move is recorded in the tabu list and will not be considered during the current perturbation procedure (this is achieved by setting the tabu tenure to ∞). The second type of perturbation, called direct perturbation, also chooses a one-move that leads to the least objective degradation, but without considering any tabu restriction (this is achieved by setting the tabu tenure to 0). Finally, during the perturbation procedure, if a feasible solution that is better than the best solution found from the start of the search is reached, the best recorded solution is updated accordingly.

4.2.6 Connections with existing studies

For the WVCP considered in this work, one notices that existing heuristic algorithms [Malaguti *et al.*, 2009; Prais and Ribeiro, 2000] visit only feasible solutions while ignoring infeasible solutions. As such, these algorithms could encounter difficulties when the feasible solutions are scattered in different zones that are separated by infeasible zones. In this work, we explore for the first time the idea of searching both feasible and infeasible solutions for solving the WVCP. Indeed, as illustrated in other settings, e.g., [Chen *et al.*, 2016b; Martinez-Gavara *et al.*, 2017; Sun *et al.*, 2017; Wang *et al.*, 2018], such a mixed search strategy is highly effective for solving several difficult problems (e.g., capacitated arc routing, capacitated clustering and equitable coloring). Among these studies, two of them [Sun *et al.*, 2017; Wang *et al.*, 2018] are worthy of a special mention, because they consider the related equitable coloring problem (ECP). Given that the WVCP studied in this work and the ECP considered in [Sun *et al.*, 2017; Wang *et al.*, 2018] are two different coloring problems, our work posses several particular features that distinguish itself from these studies.

First, the proposed AFISA algorithm incorporates search components (dedicated neighborhood, specific penalty-based evaluation function, perturbation technique...) that are customized to the WVCP. Second, unlike [Sun *et al.*, 2017; Wang *et al.*, 2018] where different algorithms are designed to search separately feasible and infeasible solutions, AFISA uses the same tabu search procedure to exploit both types of solutions, making the algorithm simpler in design and implementation. Third, AFISA integrates an adaptive mechanism to dynamically control the feasible and infeasible searches by the self-tuned parameter φ. Such a mechanism is missing in the studies mentioned above. Fourth, unlike [Sun *et al.*, 2017; Wang *et al.*, 2018], AFISA does not solve a series of k-coloring problems where each coloring problem is defined for a fixed number of colors k. Instead, the number of colors k varies during the search of our algorithm as explained in Section 4.2.4. Finally, as we show in Section 4.3, the proposed algorithm integrating these features competes very favorably with the state of the art methods for the WVCP in the literature.

4.3 Experimental results and comparisons

This section is dedicated to a large experimental assessment of the proposed AFISA algorithm for solving the WCVP and comparisons with other state of the art methods. The study is based on 111 conventional benchmark instances in the literature as well as 50 new (large) instances from the DIMACS and COLOR competitions.

4.3.1 Benchmark instances

Test instances. We consider 111 instances from the literature on the WCVP [Cornaz *et al.*, 2017; Malaguti *et al.*, 2009; Prais and Ribeiro, 2000] and 50 additional instances from the DIMACS and COLOR competitions initially proposed for the conventional graph coloring problems [1, 2]. We classify these instances into four sets.

1. The first set contains 46 (small) instances from the DIMCAS/COLOR competitions. Graphs of this set have $DSJC^*$, $GEOM^*$ or R^* in their name with up to 125 vertices. The exact algorithm ($MWSS$) [Cornaz *et al.*, 2017] is able to find the optimal solutions for 40 instances in this set. These instances are tested in [Cornaz *et al.*, 2017; Malaguti *et al.*, 2009], whose results will be used as our references.

1. http://www.dimacs.rutgers.edu/
2. http://www.cs.hbg.psu.edu/txn131/graphcoloring.html

2. The second set contains 35 instances from matrix-decomposition problems. These graphs named as pxx have up to 138 vertices and 1186 edges. The exact algorithm (*MWSS*) [Cornaz *et al.*, 2017] is able to find the optimal solutions for all graphs in this set. These instances are tested in [Cornaz *et al.*, 2017; Malaguti *et al.*, 2009; Prais and Ribeiro, 2000], whose results will be used as our references.
3. The third set contains 30 rxx instances proposed in [Prais and Ribeiro, 2000] from matrix-decomposition problems. These instances have the same structure as the pxx instances, but are larger, having up to 301 vertices and 4122 edges. These instances are tested in [Cornaz *et al.*, 2017; Prais and Ribeiro, 2000] and the exact algorithm (*MWSS*) [Cornaz *et al.*, 2017] is able to find the optimal solutions for all graphs in this set.
4. The fourth set contains 50 additional larger instances (with at least 120 vertices) [3]. These instances are created by adding random vertex weights between 1 to 20 to DIMACS/COLOR graphs.

4.3.2 Experimental settings

The proposed algorithm was coded in C++ and compiled by GNU g++ 4.1.2 with -O3 flag (option). The experiments were conducted on a computer with an Intel Xeon E5-2670 processor (2.5 GHz and 2 GB RAM) running Ubuntu 12.04. When solving the DIMACS machine benchmark procedure 'dfmax.c' [4] without compilation optimization flag, the run time on the computer is 0.46, 2.68 and 10.70 seconds for graphs r300.5, r400.5 and r500.5, respectively.

Parameters. The setting of the parameters is given in Table 4.1, which was determined by a preliminary experiment. For this, we first identify a rough range of values for each parameter. To identify the default value of a particular parameter, we test different values from the range while fixing the other parameters to their default values (typically those of Table 4.1). As to the penalty coefficient φ of the extended evaluation function F, it is tuned adaptively as explained in Section 4.2.4. We use the default setting of Table 4.1 to report the experimental results shown in the rest of this chapter, though fine-tuning some parameters could lead to improved results.

Table 4.1 – Settings of important parameters

Parameters	Description	Value
L_0, L_{max}	Small and large jump magnitude	0.05*N, 0.5*N
T	Max number of non-improving local optima visited before strong perturb	50
P_0	Probability for applying tabu-based or direct perturbation	0.7
β	Depth of tabu search	100,$N < 50$ 10000, $N \geqslant 50$

Reference algorithms. For our comparative study, we use the most recent heuristic algorithms [Malaguti *et al.*, 2009; Prais and Ribeiro, 2000] as our references. The *GRASP* algorithm [Prais and Ribeiro, 2000] was run on an IBM 9672 model R34 mainframe computer under a limit of 1000 iterations. The 2_*Phase* algorithm [Malaguti *et al.*, 2009] was run on a PIV 2.4 MHz with 512 MB RAM under Windows XP and tested by stopping phase 1 after 500 iterations and phase 2 after 75 seconds. When solving the DIMACS machine benchmark procedure 'dfmax.c', the run time on the instance r500.5 reported in [Malaguti *et al.*, 2009] for this machine is 7 seconds (against 10.7 seconds for our computer). We also include the lower and upper bounds reported by the exact algorithm *MWSS* in [Cornaz *et al.*, 2017]. The results of *MWSS* were obtained on a computer equipped with an Intel Xeon E3-1220 at 3.10 GHz with 8 GB RAM, which spent 4.5

3. These new instances are available at:
http://www.info.univ-angers.fr/~hao/wvcp.html
4. dfmax:ftp://dimacs.rutgers.edu/pub/dsj/clique/

seconds to solve the benchmark instance r500.5 (this computer is roughly 2 times faster than our computer). These bounds provide useful information when they are contrasted with the results (upper bounds) obtained by the compared heuristic algorithms (*GRASP*, 2_*Phase* and AFISA).

Following [Barr *et al.*, 1995], we show computational results in terms of solution quality and computation time. Since computation time can be greatly biased by many factors like computing platform, programming language, data structures and so on, solution quality is the primary criterion while timing information is provided only for indicative purposes.

Stopping condition. Following [Malaguti *et al.*, 2009; Prais and Ribeiro, 2000], we ran our AFISA algorithm 20 times for the instances from the first, second and fourth sets with a cutoff time of 1 hour per run. For the rxx instances of the third set, a cutoff time of 4 hours is used in [Cornaz *et al.*, 2017] used on their computer (Intel Xeon E3-1220 processor, 3.10 GHz and 8 GB RAM), which roughly corresponds to 8 hours on our computer. We set a cutoff time of 2 hours for the instances with up to 200 vertices and 4 hours for larger instances for our AFISA algorithm (longer times do not lead to significantly improved results). Finally, note that for 8 instances of the first set that cannot be solved by *MWSS* [Cornaz *et al.*, 2017] in 1 hour, a large time limit of 10 hours was allowed (marked with ⊛ in Table 4.2), leading to optimality proof of two instances (R100_1g and R100_1gb).

4.3.3 Computational results and comparisons with state-of-the-art algorithms

Table 4.2 – Comparative results of AFISA with state-of-the-art algorithms on the 46 DIMACS benchmark instances. Improved upper bounds are indicated in bold.

				AFISA				*MWSS*		2_*Phase*			
Instance	$\|V\|$	$\|E\|$	*BKV*	*Best*	*SR*	*Avg*	$t(s)$	*Best*	$t(s)$	*Best*	$t(s)$	Δ_1	Δ_2
DSJC125_1g.col⊛	125	736	24	**23**	2	24.0	3016.32	25	36000.0	24	152	-2	-1
DSJC125_1gb.col⊛	125	736	95	**90**	1	92.5	402.57	95	36000.0	95	170	-5	-5
DSJC125_5g.col⊛	125	3891	76	**71**	2	72.3	216.04	78	36000.0	76	180	-7	-5
DSJC125_5gb.col⊛	125	3891	251	**243**	1	250.2	369.34	263	36000.0	251	182	-20	-8
DSJC125_9g.col	125	6961	169*	169*	3	169.9	16.00	169*	0.3	169*	162	0	0
DSJC125_9gb.col	125	6961	604*	604*	3	605.5	443.96	604*	0.4	605	237	0	-1
GEOM100.col	100	547	65*	65*	20	65.0	0.81	65*	3.8	65*	131	0	0
GEOM100a.col	100	992	89*	89*	10	89.5	110.42	89*	2.4	89*	112	0	0
GEOM100b.col	100	1050	32*	32*	1	33.1	59.11	32*	3.8	32*	15	0	0
GEOM110.col	110	638	68*	68*	20	68.0	33.81	68*	59.5	69	172	0	-1
GEOM110a.col	110	1207	97*	97*	6	97.8	176.76	97*	12.9	97*	111	0	0
GEOM110b.col	110	1256	37*	37*	14	37.9	130.85	37*	5.0	37*	5	0	0
GEOM120.col	120	773	72*	72*	20	72.0	33.14	72*	157	72*	157	0	0
GEOM120a.col	120	1434	105*	105*	1	106.3	156.00	105*	7.0	105*	136	0	0
GEOM120b.col	120	1491	35*	35*	7	37.3	67.72	35*	16.5	35*	14	0	0
GEOM30b.col	30	81	12*	12*	20	12.0	0.02	12*	0.0	12*	0	0	0
GEOM40b.col	40	157	16*	16*	20	16.0	0.03	16*	0.1	16*	1	0	0
GEOM50b.col	50	249	18*	18*	20	18.0	0.02	18*	0.1	18*	0	0	0
GEOM60b.col	60	366	23*	23*	20	23.0	0.22	23*	0.5	23*	0	0	0
GEOM70.col	70	267	47*	47*	20	47.0	4.99	47*	0.3	47*	96	0	0
GEOM70a.col	70	459	73*	73*	20	73.0	4.42	73*	0.4	73*	3	0	0
GEOM70b.col	70	488	24*	24*	20	24.0	12.03	24*	0.9	24*	6	0	0
GEOM80.col	80	349	66*	66*	20	66.0	2.11	66*	1.1	66*	0	0	0
GEOM80a.col	80	612	76*	76*	19	76.1	137.1	76*	1.1	76*	102	0	0
GEOM80b.col	80	663	27*	27*	5	27.8	66.8	27*	2.5	27*	90	0	0
GEOM90.col	90	441	61*	61*	16	61.2	88.92	61*	2.0	61*	166	0	0
GEOM90a.col	90	789	73*	73*	3	74.0	512.41	73*	4.8	73*	157	0	0
GEOM90b.col	90	860	30*	30*	19	30.1	67.38	30*	1.7	30*	11	0	0
R100_1g.col⊛	100	509	21*	21*	1	22.0	113.77	21*	28788.5	22	155	0	-1
R100_1gb.col⊛	100	509	81*	81*	1	83.8	3.04	81*	9362.2	-	171	0	-
R100_5g.col⊛	100	2456	59	59	5	60.1	6.97	59	36000.0	-	179	0	-
R100_5gb.col⊛	100	2456	225	**221**	1	224.1	186.81	225	36000.0	-	179	-4	-
R100_9g.col	100	4438	141*	141*	15	141.3	21.36	141*	0.1	-	123	0	-
R100_9gb.col	100	4438	518*	518*	1	549.3	1152.83	518*	0.3	-	127	0	-
R50_1g.col	50	108	14*	14*	20	14.0	0.14	14*	0.8	14*	0	0	0
R50_1gb.col	50	108	53*	53*	20	53.0	0.24	53*	1.6	53*	95	0	0
R50_5g.col	50	612	37*	37*	20	37.0	0.95	37*	1.4	37*	167	0	0
R50_5gb.col	50	612	135*	135*	14	135.3	3.72	135*	1.5	137	145	0	-2
R50_9g.col	50	1092	74*	74*	20	74.0	0.74	74*	0.0	74*	36	0	0
R50_9gb.col	50	1092	262*	262*	20	262.0	12.61	262*	0.0	262*	33	0	0
R75_1g.col	70	251	18*	18*	12	18.4	10.96	18*	132.8	19	154	0	-1
R75_1gb.col	70	251	70*	70*	19	70.1	2.46	70*	192.2	72	166	0	-2
R75_5g.col	75	1407	51*	51*	12	51.4	0.08	51*	1056.0	53	172	0	-2
R75_5gb.col	75	1407	186*	186*	2	189.0	19.42	186*	989.3	190	173	0	-4
R75_9g.col	75	2513	110*	110*	20	110.0	2.65	110*	0.0	110*	79	0	0
R75_9gb.col	75	2513	396*	396*	12	396.4	145.89	396*	0.0	399	50	0	-3
#Better				5/46				0/46		0/41			
#Equal				41/46				43/46		32/41			
#Worse				0/46				3/46		9/41			
p_value				-				2.5e-2		3.1e-4			

Table 4.2 reports the results of our AFISA algorithm on the first set of 46 DIMACS/COLOR

instances commonly used in the literature, together with the results of the reference algorithms *MWSS* [Cornaz *et al.*, 2017] and 2_*Phase* [Malaguti *et al.*, 2009]. The first 3 columns indicate for each instance its name, the number of vertices and the number of edges. The fourth column shows the best-known value (BKV) reported in the literature [Cornaz *et al.*, 2017; Malaguti *et al.*, 2009; Prais and Ribeiro, 2000]. The next four columns show the results of the AFISA algorithm for each instance: the best result (i.e., the smallest objective function value) over 20 independent runs (*Best*), the success rate (*SR*) to achieve the best result over 20 runs, the average result (*Avg*) and the average computation time (in seconds) of the successful runs to obtain the best result ($t(s)$) (0 is given if the time is less than 0.009 second). The following four columns report the results and the computation time obtained by the reference algorithms (MWSS and 2_*Phase*). For MWSS, the indicated time corresponds to the time of 1000 iterations. For 2_*Phase*, the time is the sum of the time of 500 iterations of phase 1 and the time of phase 2. The last two columns (Δ_1,Δ_2) indicate the difference between our result (*Best*) and the result of *MWSS* and 2_*Phase*. To verify the statistical significance of the comparisons between AFISA and each reference algorithm, we show in the row "*p*-values" the results from the non-parametric Friedman test applied to the best values of AFISA and each compared algorithm, and a *p*-value smaller than 0.05 implies a significant difference between two compared results.

Additionally, the rows #Better, #Equal and #Worse indicate respectively the number of instances for which an algorithm performs better, equally well or worse compared to the best-known values (BKV).

Finally, an entry with * indicates the optimal objective value. A bold entry highlights an improved upper bound, i.e., an improved result over the current best-known value. Entries with "-" mean that the corresponding results are not available in the literature.

Table 4.3 – Comparative results of AFISA with state-of-the-art algorithms on the 35 p*xx* benchmark instances. Improved upper bounds are indicated in bold.

				AFISA				*MWSS*		2_*Phase*		*GRASP*				
Instance	$\|V\|$	$\|E\|$	*BKV*	*Best*	*SR*	*Avg*	$t(s)$	*Best*	$t(s)$	*Best*	$t(s)$	*Best*	$t(s)$	Δ_1	Δ_2	Δ_3
p06.col	16	38	565*	565*	20	565.0	0	565*	0.0	565*	0.4	565*	1.1	0	0	0
p07.col	24	92	3771*	3771*	20	3771.0	0.02	3771*	0.0	3771*	0.1	3771*	4.0	0	0	0
p08.col	24	92	4049*	4049*	20	4049.0	0.17	4049*	0.0	4049*	1.3	4049*	1.3	0	0	0
p09.col	25	100	3388*	3388*	16	3388.2	0.95	3388*	0.0	3388*	0.1	3388*	3.0	0	0	0
p10.col	16	32	3983*	3983*	20	3983.0	0.68	3983*	0.0	3983*	0.1	3983*	4.5	0	0	0
p11.col	18	48	3380*	3380*	20	3380.0	0.01	3380*	0.0	3380*	0.1	3380*	4.7	0	0	0
p12.col	26	90	657*	657*	20	657.0	0	657*	0.0	657*	0.1	657*	3.8	0	0	0
p13.col	34	160	3220*	3220*	17	3221.1	0.68	3220*	0.0	3225	2.3	3230	7.8	0	-5	-10
p14.col	31	110	3157*	3157*	20	3157.0	0	3157*	0.0	3157*	0.1	3157*	10.1	0	0	0
p15.col	34	136	341*	341*	20	341.0	1.81	341*	0.0	341*	0.1	341*	4.7	0	0	0
p16.col	34	134	2343*	2343*	20	2343.0	0.76	2343*	0.0	2343*	0.5	2343*	14.5	0	0	0
p17.col	37	161	3281*	3281*	7	3322.2	2.72	3281*	0.0	3281*	1.4	3281*	5.5	0	0	0
p18.col	35	143	3228*	3228*	20	3228.0	0.05	3228*	0.0	3228*	0.2	3228*	10.4	0	0	0
p19.col	36	156	3710*	3710*	20	3710.0	0.36	3710*	0.0	3710*	0.1	3710*	14.6	0	0	0
p20.col	37	142	1830*	1830*	13	1841.0	4.86	1830*	0.0	1830*	1.3	1860	20.0	0	0	-30
p21.col	38	155	3660*	3660*	19	3660.5	0.75	3660*	0.0	3660*	0.2	3660*	18.4	0	0	0
p22.col	38	154	1912*	1912*	18	1912.2	0.29	1912*	0.0	1912*	0.2	1912*	20.0	0	0	0
p23.col	44	204	3770*	3770*	3	3793.0	0.28	3770*	0.1	3770*	1.4	3810	21.4	0	0	-40
p24.col	34	104	661*	661*	20	661.0	0	661*	0.0	661*	0.1	661*	27.9	0	0	0
p25.col	36	120	504*	504*	20	504.0	0.28	504*	0.0	504*	0.1	504*	23.9	0	0	0
p26.col	37	131	520*	520*	20	520.0	0.11	520*	0.0	520*	0.1	520*	28.3	0	0	0
p27.col	44	174	216*	216*	20	216.0	0.08	216*	0.1	216*	0.2	216*	7.8	0	0	0
p28.col	44	174	1729*	1729*	14	1735.1	2.56	1729*	0.1	1729*	0.1	1729*	44.5	0	0	0
p29.col	53	254	3470*	3470*	20	3470.0	0.10	3470*	0.1	3470*	65.7	3470*	65.7	0	0	0
p30.col	60	317	4891*	4891*	20	4891.0	53.79	4891*	0.2	4891*	2.1	4891*	56.6	0	0	0
p31.col	47	179	620*	620*	20	620.0	3.69	620*	0.1	620*	0.1	620*	70.9	0	0	0
p32.col	51	221	2480*	2480*	20	2480.0	0.35	2480*	0.1	2480*	0.0	2480*	70.9	0	0	0
p33.col	56	258	3018*	3018*	7	3029.7	0.43	3018*	0.3	3018*	0.1	3018*	62.3	0	0	0
p34.col	74	421	1980*	1980*	19	1980.5	3.05	1980*	0.6	1980*	0.1	1980*	131.9	0	0	0
p35.col	86	566	2140*	2140*	15	2145.0	4.48	2140*	0.6	2140*	0.1	2140*	135.0	0	0	0
p36.col	101	798	7210*	7210*	12	7385.0	0.13	7210*	1.4	7210*	0.1	7210*	163.1	0	0	0
p38.col	87	537	2130*	2130*	1	2139.5	9.54	2130*	1.2	2130*	0.4	2130*	231.8	0	0	0
p40.col	86	497	4984*	4984*	1	5016.6	5.05	4984*	1.0	4984*	0.2	4984*	224.2	0	0	0
p41.col	116	900	2688*	2688*	2	2688.1	0.10	2688*	3.2	2688*	0.1	2688*	313.7	0	0	0
p42.col	138	1186	2466*	2466*	4	2671.2	930.96	2466*	3.2	2509	2.8	2480	405.8	0	-43	-14
#Better				0/35				0/35		0/35		0/35				
#Equal				35/35				35/35		33/35		31/35				
#Worse				0/35				0/35		2/35		4/35				
p-value				-				-		1.6e-1		4.6e-2				

From Table 4.2, we observe that AFISA reaches a remarkable performance on the first set of 46 DIMACS/COLOR instances. Compared to the most recent exact algorithm *MWSS*, AFISA attains all known optimal results (40 cases). For 5 out of the 6 remaining instances whose optimal

Table 4.4 – Comparative results of AFISA with state-of-the-art algorithms on the 30 rxx benchmark instances. Improved upper bounds are indicated in bold.

				AFISA				*MWSS*		*GRASP*			
Instance	$\|V\|$	$\|E\|$	*BKV*	*Best*	*SR*	*Avg*	$t(s)$	*Best*	$t(s)$	*Best*	$t(s)$	Δ_1	Δ_2
r01.col	144	1280	6724*	6724*	8	6727.8	49.57	6724*	17.6	6724*	887	0	0
r02.col	142	1246	6771*	6771*	3	6780.6	85.33	6771*	11.3	6771*	1041	0	0
r03.col	139	1188	6473*	6473*	10	6490.8	190.19	6473*	10.4	6475	966	0	-2
r04.col	151	1406	6342*	6342*	1	6403.2	467.37	6342*	11.4	6342*	989	0	0
r05.col	142	1266	6408*	6408*	1	6466.3	71.68	6408*	12.3	6409	904	0	-1
r06.col	148	1381	7550*	7550*	4	7555.9	29.24	7550*	10.3	7550*	899	0	0
r07.col	141	1253	6889*	6889*	3	7555.9	34.76	6889*	13.7	6889*	6889	0	0
r08.col	138	1191	6057*	6057*	1	6080.3	311.66	6057*	4.1	6076	810	0	-19
r09.col	129	1027	6358*	6358*	1	6393.8	395.24	6358*	9.5	6424	868	0	-66
r10.col	150	1409	6508*	6508*	1	6519.3	461.98	6508*	13.1	6525	1048	0	-17
r11.col	208	2247	7654*	7654*	1	7710.6	259.25	7654*	57.2	7669	2423	0	-15
r12.col	199	2055	7690*	7691	1	7710.4	9542.18	7690*	53.7	7691	2267	1	0
r13.col	217	2449	7500*	7521	1	7558.3	619.53	7500*	105.2	7524	2365	21	-3
r14.col	214	2387	8254*	8254*	1	8283.9	8044.07	8254*	65.3	8254*	2342	0	0
r15.col	198	2055	8021*	8021*	1	8126.8	2559.06	8021*	25.1	8021*	2395	0	0
r16.col	188	1861	7755*	7755*	2	7789.2	195.53	7755*	26.7	7755*	2696	0	0
r17.col	213	2392	7979*	7979*	2	8030.3	855.38	7979*	79.3	8025	3175	0	-46
r18.col	200	2079	7232*	7232*	1	7278.9	868.19	7232*	58.2	7232*	1902	0	0
r19.col	185	1803	6826*	6840	1	6868.1	395.5	6826*	32.7	6858	2082	14	-18
r20.col	217	2447	8023*	8023*	1	8102.0	1028.5	8023*	104.1	8027	3452	0	-4
r21.col	281	3554	9284*	9284*	1	9384.5	4588.72	9284*	390.0	9287	4948	0	-3
r22.col	285	3684	8887*	8887*	1	8959.3	12911	8887*	302.6	8887*	5603	0	0
r23.col	288	3732	9136*	9136*	1	9267.9	3251.96	9136*	375.3	9145	5887	0	-9
r24.col	269	3284	8464*	8464*	1	8572.9	13142.6	8464*	201.7	8464*	4997	0	0
r25.col	266	3177	8426*	8468	1	8560.8	874.75	8426*	225.6	8504	5139	42	-36
r26.col	284	3629	8819*	8819*	1	8927.9	14225.1	8819*	439.6	8819*	5462	0	0
r27.col	259	3019	7975*	7975*	1	8019.7	14074.9	7975*	248.1	7975*	5064	0	0
r28.col	288	3765	9407*	9407*	1	9599.4	8691.00	9407*	222.7	9407*	5874	0	0
r29.col	281	3553	8693*	8693*	1	8743.7	7613.14	8693*	388.0	8693*	4923	0	0
r30.col	301	4122	9816*	9816*	1	10003.2	8838.59	9816*	346.9	9816*	6145	0	0
#Better				0/30				0/30		0/30			
#Equal				26/30				30/30		16/30			
#Worse				4/30				0/30		14/30			
p-value				-				4.6e-2		3.2e-4			

Table 4.5 – Comparative results of FISA with CPLEX on the additional set of 50 larger DIMACS/COLOR instances. Improved upper bounds are indicated in bold.

			AFISA				*CPLEX*			
Instance	$\|V\|$	$\|E\|$	*Best*	*SR*	*Avg*	$t(s)$	*UB*	*LB*	*status*	Δ
miles250.col	128	387	102*	8	102.7	56.61	102*	102*	Optimal	0
miles500.col	128	1170	260	1	261.3	48.46	-	-	-	-
miles1000.col	128	3216	**432**	1	444.7	480.02	437	31.692	Feasible	-5
miles1500.col	128	5198	587	1	644.3	32.31	-	-	-	-
mulsol.i.5.col	186	3973	367.0	20	367.0	416.91	360	109.034	Feasible	7
queen10_10.col	100	2940	166	3	169.2	68.43	-	-	-	-
queen11_11.col	121	3960	178	1	182.3	55.24	-	-	-	-
queen12_12.col	144	5192	**194**	1	198.6	92.7	208	47.000	Feasible	-14
queen13_13.col	169	6656	204	2	207.5	199.85	-	-	-	-
queen14_14.col	196	8372	**224**	2	227.4	360.05	316	23.000	Feasible	-92
queen15_15.col	225	10360	237	1	241.2	183.44	-	-	-	-
queen16_16.col	256	12640	**253**	2	256.3	300.85	365	22.033	Feasible	-112
zeroin.i.1.col	211	4100	518	20	518.0	0	-	-	-	-
zeroin.i.2.col	211	3541	336	3	337.6	440.84	300	26.103	Feasible	36
zeroin.i.3.col	206	3540	299	2	301.7	139.64	-	-	-	-
DSJC250.1.col	250	3218	140	1	141.9	48.94	-	-	-	-
DSJC250.5.col	250	15668	415	1	428.1	269.23	-	-	-	-
DSJC250.9.col	250	55794	925	1	942.7	856.25	-	-	-	-
DSJC500.1.col	500	12458	210	1	215.6	426.64	-	-	-	-
DSJC500.5.col	500	125248	778	1	845.1	159.27	-	-	-	-
DSJC500.9.col	500	224874	1790	1	1854.5	831.07	-	-	-	-
DSJR500.1.col	500	3555	169	1	175.4	458.86	-	-	-	-
DSJC1000.1.col	1000	99258	359	4	362.9	430.54	-	-	-	-
DSJC1000.5.col	1000	499652	1357	1	1430.9	371.65	-	-	-	-
DSJC1000.9.col	1000	898898	3166	1	3231.0	490.2	-	-	-	-
inithx.i.1.col	864	18707	587	5	587.9	527.46	-	-	-	-
inithx.i.2.col	645	13979	341	8	341.6	0.03	-	-	-	-
inithx.i.3.col	621	13969	352	11	355.6	0.01	-	-	-	-
le450_15a.col	450	8168	241	1	247.1	288.37	-	-	-	-
le450_15b.col	450	8169	239	2	245.1	368.35	-	-	-	-
le450_15c.col	450	16680	313	1	320.8	432.95	-	-	-	-
le450_15d.col	450	16750	306	2	314.1	113.7	-	-	-	-
le450_25a.col	450	8260	317	1	329.9	362.26	-	-	-	-
le450_25b.col	450	8263	318	1	325.8	285.88	-	-	-	-
le450_25c.col	450	17343	378	1	387.9	359.37	-	-	-	-
le450_25d.col	450	17345	375	1	385.3	254.76	-	-	-	-
flat1000_50_0.col	1000	245000	1289	1	1315.7	981.77	-	-	-	-
flat1000_60_0.col	1000	245830	1338	1	1354	201.98	-	-	-	-
flat1000_76_0.col	1000	246708	1314	1	1337.6	2396.63	-	-	-	-
C2000.5.col	2000	999836	2400	1	2425.1	3133.97	-	-	-	-
C2000.9.col	2000	1799532	6228	1	6284.0	2798.3	-	-	-	-
latin_square_10.col	900	307350	1690	1	1900.0	780.26	-	-	-	-
wap01a.col	2368	110871	638	1	653.1	1133.51	-	-	-	-
wap02a.col	2464	111742	637	1	638.1	3270.46	-	-	-	-
wap03a.col	4730	286722	687	1	707.5	2901.51	-	-	-	-
wap04a.col	5231	294902	698	1	709.0	4.79	-	-	-	-
wap05a.col	905	43081	598	1	610.9	1574.52	-	-	-	-
wap06a.col	947	43571	599	1	607.6	65.32	-	-	-	-
wap07a.col	1809	103368	680	1	692.5	384.82	-	-	-	-
wap08a.col	1870	104176	663	1	673.4	2627.2	-	-	-	-
#Better			47/50				2/7			
#Equal			1/50				1/7			
#Worse			2/50				4/7			

values are still unknown, AFISA improves the current best upper bounds (see negative entries in column Δ_1). AFISA also dominates the 2_*Phase* algorithm on the 41 instances tested by both algorithms, by obtaining better results for 13 instances (see negative entries in column Δ_2) and the same results for the remaining 28 instances. The small p-values (< 0.05) indicates that there is a significant difference between our best results and those of the two reference algorithms *MWSS* (p-value=2.5e-2) and 2_*Phase* (p-value=3.1e-4).

Table 4.3 reports the comparative results on the first set of 35 pxx instances from matrix-decomposition problems with one more reference algorithm (*GRASP*) [Prais and Ribeiro, 2000]. One observes that AFISA performs very well on these pxx instances. AFISA attains always the known optimal values of *MWSS*, while 2_*Phase* and *GRASP* miss 2 and 4 instances respectively. The difference between AFISA and 2_*Phase* is however not statistically significant (p-value of 1.6e-1), while the difference between AFISA and *GRASP* is significant with a p-value of 4.6e-2.

Table 4.4 shows the results of AFISA on the second set of 30 rxx instances from matrix-decomposition problems, along with those of *MWSS* and *GRASP*. Table 4.4 indicates that AFISA finds the optimal solutions for 26 out of the 30 rxx instances, which were previously obtained by the exact algorithm *MWSS*. Among the four cases where AFISA misses the optimal solution, the gap to the optimal value is no more than 0.498% (instance $r25$). Compared to the reference heuristic algorithm *GRASP*, AFISA (Column 4) dominates *GRASP* by attaining 13 better and 17 equal results. The p-value of 4.6e-2 between AFISA and *MWSS* indicates that there is a slight difference and the p-value of 3.2e-4 between AFISA and *GRASP* indicates that there is significant difference between the results of AFISA and *GRASP*.

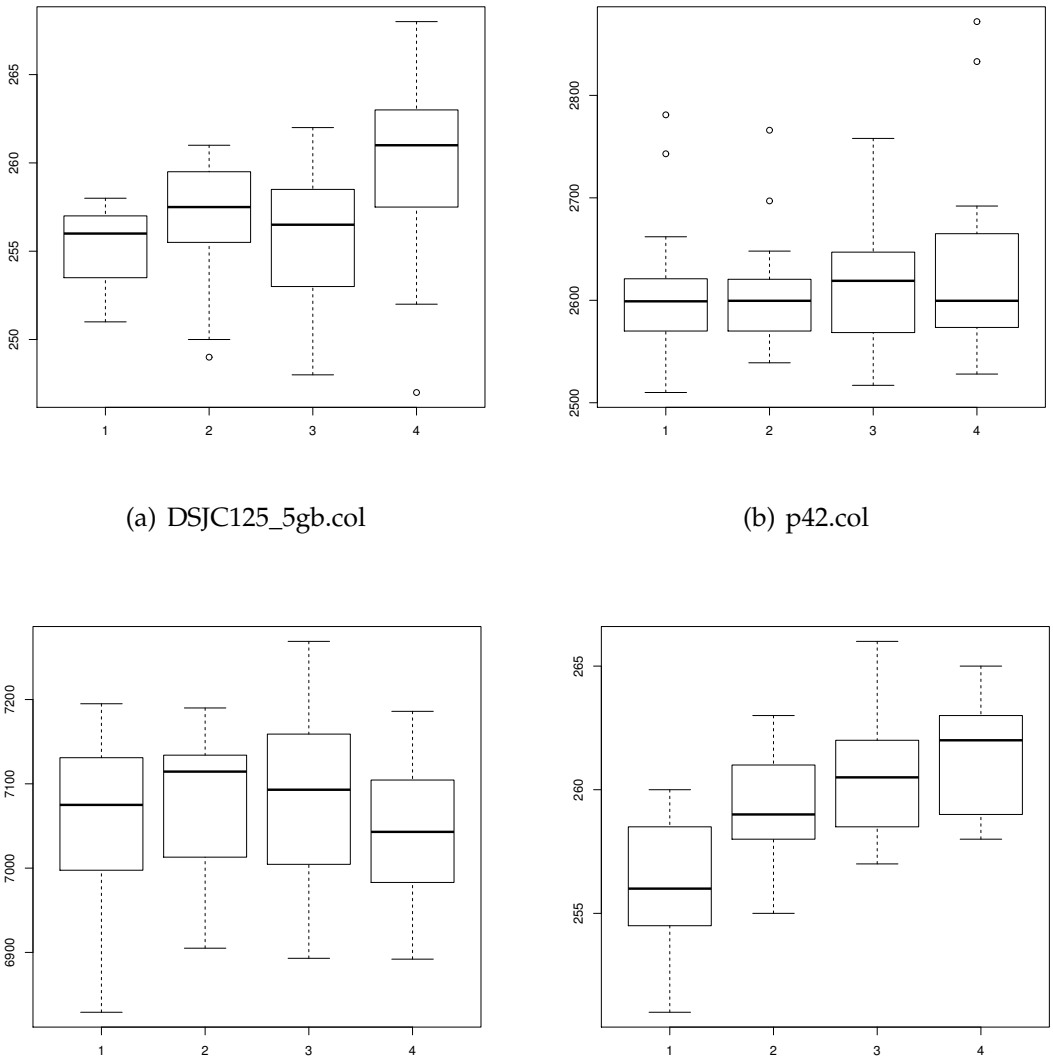
Notice that according to [Malaguti *et al.*, 2009], 2_*Phase* is able to find (in comparable computing times) 3 solutions better than those of *GRASP* reported in [Prais and Ribeiro, 2000], 9 solutions of equal quality and 18 worse solutions. However the detailed results of 2_*Phase* on the rxx instances are not available.

Finally, Table 4.5 summarizes our results on the set of 50 additional (larger) DIMACS/COLOR instances. Since these instances are not tested previously by any WVCP method, we use the general MIP solver CPLEX (version 12.6) as our reference method. We run CPLEX, with a cutoff limit of one hour, to solve the 0/1 ILP model shown in Appendix 5.6. Entries with $-$ in Table 4.5 indicate that no feasible solution is found by CPLEX within the time limit and this happens for 43 out of the 50 instances. The last column (Δ) indicates the difference between our best result and the upper bound of CPLEX (a negative value implies thus a better result). We observe that only one instance can be solved to optimality by CPLEX within the one hour time limit. For the six instances for which CPLEX reaches a feasible solution, but fails to find the optimal solution, its upper bounds are worse than the bounds of AFISA in four cases. Due to the small number of instances solved by CPLEX, we omit the statistical test.

To sum up, this computational assessment indicates that AFISA performs very well on the four sets of benchmark instances. The new upper bounds (5 for the first set and the results for the fourth set) established by AFISA can serve as valuable reference values to evaluate future algorithms for the WVCP. Meanwhile, AFISA failed to attain the optimal values for four instances of the third set, indicating there is room for further improvement. Finally, this experimental study confirms that like for many NP-hard problems, both exact and heuristic algorithms are complementary and can be used to solve problem instances of different sizes and different characteristics. These approaches can even be combined to create powerful hybrid algorithms.

4.4 Analysis

This section performs additional experiments to analyze the benefits of three important ingredients of the proposed AFISA algorithm: the penalty coefficient of the extended evaluation



(a) DSJC125_5gb.col (b) p42.col

(c) r05.col (d) queen16_16.col

Figure 4.1 – Influence of the increment/decrement value of the penalty efficient

function, the strategy of visiting both feasible and infeasible solutions and the perturbation strategy.

4.4.1 Impact of the penalty coefficient

AFISA uses the extended evaluation function F defined in Section 4.2.3 to explore both feasible and infeasible solutions. The oscillation between feasible and infeasible zones is adaptively controlled by increasing or decreasing the penalty coefficient φ (≥ 1). In this study, we analyze the impact of the increment/decrement value used to adjust φ and for this purpose, we test the following increment/decrement values: 1,2,3,4 (larger values make the search oscillate too much between feasible and infeasible zones).

Box and whisker plots of the results on 4 representative instances from the four benchmark sets (which are relatively difficult according to Tables 4.2-4.5) are shown in Figure 4.1, where the X-axis indicates the tested increment/decrement values and the Y-axis indicates the objective values. As a supplement, we also compute the p-value for each tested instance. The results are based on 20

independent runs for each instance with a cutoff time of 300 seconds per run. One observes that the performance of the AFISA algorithm is significantly influenced by the increment/decrement value on the instances DSJC125_5gb (p-value = 1.4e-2) and queen16_16 (p-value = 1.2e-4). This is less the case for the instances p42 (p-value = 2.0e-1) and r05 (p-value = 7.6e-1). Furthermore, the AFISA algorithm with the increment/decrement value of 1 gives the best performance compared to other values. This explains why we adopt 1 as the default increment/decrement value in this study. Finally, one notices that the outcome of this experiment remains coherent with the intuitive understanding that the search will go back and forth more frequently between feasible and infeasible regions with a large increment/decrement value than with a small value. This implies that a large increment/decrement value may make the search leave each newly discovered (feasible or infeasible) zone too early before the search zone is sufficiently exploited.

4.4.2 Benefit of searching both feasible and infeasible solutions

Table 4.6 – Assessment of searching both feasible and infeasible solutions. The better results are in bold.

Instance	$\|V\|$	$\|E\|$	AFISA				*Tabu_Feasible*				Δ
			Best	*SR*	*Avg*	$t(s)$	*Best*	*SR*	*Avg*	$t(s)$	
DSJC1000.1.col	1000	99258	359	4	362.9	430.54	**354**	1	**358.9**	450.15	5
DSJC1000.5.col	1000	499652	1357	1	1430.9	371.65	**1354**	1	**1371.3**	84.75	3
DSJC1000.9.col	1000	898898	3166	1	**3231.0**	490.2	3166	1	3231.1	490.2	0
DSJC125_1g.col	125	736	23	2	24.0	3016.32	23	4	**23.8**	1467.63	0
DSJC125_1gb.col	125	736	**90**	1	**92.5**	402.57	91	1	94.6	30.09	-1
DSJC125_5g.col	125	3891	71	2	**72.3**	216.04	71	1	72.5	199.14	0
DSJC125_5gb.col	125	3891	**243**	1	**250.2**	369.34	246	3	250.9	292.08	-3
DSJC125_9g.col	125	6961	169	3	**170.0**	16	169	4	170.2	42.1	0
DSJC125_9gb.col	125	6961	**604**	3	**605.0**	443.96	606	2	608.7	18.24	-2
DSJC250.1.col	250	3218	140	1	**141.9**	48.94	140	4	142.1	57.37	0
DSJC250.5.col	250	15668	**415**	1	**428.1**	269.23	421	1	431.2	318.86	-6
DSJC250.9.col	250	55794	**925**	1	**942.7**	856.25	948	1	965.8	365.4	-23
DSJC500.1.col	500	12458	**210**	1	215.6	426.64	212	1	**215.3**	84.83	-2
DSJC500.5.col	500	125248	**778**	1	845.1	159.27	780	1	**796.1**	450.89	-2
DSJC500.9.col	500	224874	**1790**	1	**1854.5**	831.07	1791	1	1869.2	345.13	-1
DSJR500.1.col	500	3555	**169**	1	175.4	458.86	170	2	**171.9**	272.89	-1
GEOM100.col	100	547	65	20	65.0	0.81	65	20	65.0	9.86	0
miles1500.col	128	5198	**587**	1	**644.3**	32.31	797	4	798.6	0.13	-210
p13.col	34	160	3220	17	**3221.1**	0.68	3220	16	3221.5	0.83	0
p20.col	37	142	1830	13	1841	4.86	1830	16	**1835.5**	0.76	0
p42.col	138	1186	**2466**	4	2671.2	930.96	2646	1	**2659.7**	12.51	-180
queen12_12.col	144	5192	**194**	1	**198.6**	92.7	196	2	199.0	96.04	-2
queen14_14.col	196	8372	**224**	2	**227.4**	360.05	225	1	227.7	129.47	-1
queen16_16.col	256	12640	253	2	256.3	300.85	**250**	1	**254.8**	14.15	3
r03.col	139	1188	**6473**	10	**6490.8**	190.19	6487	1	6536	119.3	-14
r05.col	142	1266	**6408**	1	**6466.3**	71.68	6495	1	6525.6	143.13	-87
R100_1g.col	100	509	21	1	22.0	113.77	21	3	**21.9**	533.65	0
R100_5g.col	100	2456	59	5	**60.1**	6.97	59	2	60.3	2.56	0
R100_5gb.col	100	2456	**221**	1	**224.1**	186.81	222	1	224.7	1362.52	-1
R100_9g.col	100	4438	141	15	**141.3**	21.36	141	11	141.5	2.43	0
R100_9gb.col	100	4438	518	1	549.3	1152.83	518	13	**518.5**	21.25	0
R50_5gb.col	50	612	135	14	135.3	3.72	135	18	135.3	0.11	0
R75_1g.col	70	251	18	12	**18.4**	10.96	18	10	18.5	32.89	0
R75_1gb.col	70	251	70	19	**70.1**	2.46	70	17	70.3	6.58	0
R75_5g.col	75	1407	51	12	**51.4**	0.08	51	7	51.7	5.11	0
R75_5gb.col	75	1407	186	2	**189.0**	19.42	186	2	189.2	31.93	0
R75_9gb.col	75	2513	396	12	**396.4**	145.89	396	9	396.7	4.35	0
zeroin.i.2.col	211	3541	336	3	337.6	440.84	336	13	**336.4**	0.91	0
#Better			16/38		24/38		3/38		12/38		
#Equal			19/38		2/38		19/38		2/38		
#Worse			3/38		12/38		16/38		24/38		
p_value			-		-		2.9e-3		4.6e-2		

To assess the strategy of oscillating between feasible and infeasible regions of the proposed algorithm, we create a algorithmic variant (called Tabu_Feasible) in which the search visits only feasible solutions. For this, we set the penalty coefficient φ of the extended evaluation function (Eq. (4.2), Section 4.2.3) to a large value in order to penalize strongly any infeasible solution. In our case, φ is set to the largest weight of vertices of the given graph. For this experiment, we select 38 instances that are relatively difficult according to the results reported in Tables 4.2-4.5, i.e., their best-known results cannot consistently be attained by all algorithms. We ran 20 times both algorithms to solve each selected instance with a cutoff time of 1 hour.

The comparative results of this experiment are presented in Table 4.6 with the same information as before. The rows #Better/#Equal/#Worse indicate the number of instances for which each

algorithm attain a better, equal and worse result compared to the other algorithm in terms of the best objective value found. The last column indicates the difference between the best results of AFISA and Tabu_Feasible. We observe that even if both algorithms obtain 19 equal results, AFISA achieves 16 better results (against 3 for Tabu_Feasible). The small p-values (< 0.05) in terms of *Best* and *Avg* confirm the statistical significance of the reported differences between AFISA and Tabu_Feasible. This experiment shows that searching both feasible and infeasible solutions enables the algorithm to reach a better performance.

4.4.3 Impact of the perturbation operation

Table 4.7 – Assessment of the perturbation strategy. The better results are in bold.

Instance	$\|V\|$	$\|E\|$	AFISA				AFISA$^-$				Δ
			Best	*SR*	*Avg*	*t*(*s*)	*Best*	*SR*	*Avg*	*t*(*s*)	
DSJC1000.1.col	1000	99258	**359**	4	**362.9**	430.54	384	10	385.5	0.08	-25
DSJC1000.5.col	1000	499652	**1357**	1	**1430.9**	371.65	1427	10	1434.5	0.07	-70
DSJC1000.9.col	1000	898898	**3166**	1	**3231.0**	490.2	3291	10	3302.5	0.04	-125
DSJC125_1g.col	125	736	23	2	**24.0**	3016.32	33	6	33.7	0	-10
DSJC125_1gb.col	125	736	**90**	1	**92.5**	402.57	120	13	122.8	0	-30
DSJC125_5g.col	125	3891	**71**	2	**72.3**	216.04	87	14	88.5	0	-16
DSJC125_5gb.col	125	3891	**243**	1	**250.2**	369.34	293	20	293.0	0.01	-50
DSJC125_9g.col	125	6961	**169**	3	**170.0**	16	186	12	188.8	0	-17
DSJC125_9gb.col	125	6961	**604**	3	**605.0**	443.96	652	10	668.0	0	-48
DSJC250.1.col	250	3218	**140**	1	**141.9**	48.94	168	10	170.5	0.01	-28
DSJC250.5.col	250	15668	**415**	1	**428.1**	269.23	472	8	476.5	0	-57
DSJC250.9.col	250	55794	**925**	1	**942.7**	856.25	1039	11	1060.0	0	-114
DSJC500.1.col	500	12458	**210**	1	**215.6**	426.64	242	10	243.0	0.02	-32
DSJC500.5.col	500	125248	**778**	1	**845.1**	159.27	853	8	856.0	0.03	-75
DSJC500.9.col	500	224874	**1790**	1	**1854.5**	831.07	1937	20	1937.0	0.01	-147
DSJR500.1.col	500	3555	**169**	1	**175.4**	458.86	184	10	191.5	0.01	-15
GEOM100.col	100	547	**65**	20	**65.0**	0.81	74	9	74.6	0.01	-9
miles1500.col	128	5198	**587**	1	**644.3**	32.31	799	8	809.8	0	-212
p13.col	34	160	**3220**	17	**3221.1**	0.68	3568	7	3764.3	0	-348
p20.col	37	142	**1830**	13	**1841.0**	4.86	2270	20	2270	0.01	-440
p42.col	138	1186	**2466**	4	**2671.2**	930.96	2880	12	2887.2	0	-414
queen12_12.col	144	5192	**194**	1	**198.6**	92.7	229	9	230.0	0	-35
queen14_14.col	196	8372	**224**	2	**227.4**	360.05	254	14	255.5	0	-30
queen16_16.col	256	12640	**253**	2	**256.3**	300.85	280	9	282.2	0	-27
r03.col	139	1188	**6473**	10	**6490.8**	190.19	6603	1	6687.3	376.19	-130
r05.col	142	1266	**6408**	1	**6466.3**	71.68	6495	2	6637.7	0	-87
R100_1g.col	100	509	**21**	1	**22.0**	113.77	30	8	30.6	0	-9
R100_5g.col	100	2456	**59**	5	**60.1**	6.97	72	10	73.5	0	-13
R100_5gb.col	100	2456	**221**	1	**224.1**	186.81	260	1	264	0	-39
R100_9g.col	100	4438	**141**	15	**141.3**	21.36	153	9	157.4	0	-12
R100_9gb.col	100	4438	**518**	1	**549.3**	1152.83	548	9	551.5	0	-30
R50_5gb.col	50	612	**135**	14	**135.3**	3.72	152	8	156.8	0	-17
R75_1g.col	70	251	**18**	12	**18.4**	10.96	24	7	25.2	0	-6
R75_1gb.col	70	251	**70**	19	**70.1**	2.46	88	11	89.4	0	-18
R75_5g.col	75	1407	**51**	12	**51.4**	0.08	63	20	63.0	0	-12
R75_5gb.col	75	1407	**186**	2	**189.0**	19.42	231	11	233.7	0	-45
R75_9gb.col	75	2513	**396**	12	**396.4**	145.89	425	12	428.2	0.01	-29
zeroin.i.2.col	211	3541	**336**	3	**337.6**	440.84	337	13	337.7	0	-1
#Better			38/38		38/38		0/38		0/38		
#Equal			0/38		0/38		0/38		0/38		
#Worse			0/38		0/38		38/38		38/38		
p-value			-		-		7.1e-10		7.1e-10		

As shown in Section 4.2.5, the proposed algorithm uses a perturbation strategy as an additional means of diversification. To assess this strategy, we compare AFISA with a AFISA variant (denoted as AFISA$^-$) where the perturbation strategy is disabled (i.e., by removing line 22 in Algorithm 4.1). This experiment is based on the 38 instances used in Section 4.4.2. We ran 20 times both algorithms to solve each selected instance with a cutoff time of 1 hour.

The results of this experiment are shown in Table 4.7 with the same statistics as before. We observe that AFISA dominates, in terms of *Best* and *Avg*, the AFISA$^-$ variant by obtaining a better result for each instance. The small p-values confirm the dominance of AFISA over AFISA$^-$. This experiment demonstrates the interest of the adopted perturbation strategy as a meaningful means of diversification that enables the algorithm to better explore the search space.

4.5 Conclusions

The weighted vertex coloring problem (WVCP) considered in this work is a generalization of the conventional vertex coloring problem with a number of practical applications. Motivated by the observation that existing methods limit their search to feasible solutions, we investigated for the first time the benefit of examining both feasible and infeasible solutions for solving the problem. The resulting AFISA algorithm oscillates between feasible and infeasible search zones guided by an extended evaluation function that combines the initial objective function and an adaptive penalty function. To explore feasible and infeasible spaces, we introduced a tabu search procedure enhanced by a dedicated perturbation strategy to escape local optima traps.

We assessed the performance of the AFISA algorithm on three sets of 111 instances commonly tested in the literature and an additional set of 50 (large) DIMACS and COLOR instances initially proposed for graph coloring problems. We presented 5 improved best results (new upper bounds) among the 111 instances of the literature and the first upper bounds for the new set of 50 instances. These new bounds can serve as valuable references to assess future WVCP algorithms and might be used by a branch-and-bound algorithm as high-quality initial bounds. This study demonstrates the benefit of the search strategy examining both feasible and infeasible solutions for solving the WVCP. The computational results on different types of benchmark instances also confirm that exact and heuristic algorithms are complementary solution approaches that can be advantageously employed to handle instances of different sizes with particular features.

For future work, several directions could be followed. First, other penalty-based evaluation functions could be devised to enable a better strategic oscillation between feasible and infeasible spaces. Second, other neighborhoods (rather than the one-move based neighborhood used in this work) can be sought to further improve the performance of the search algorithm. Third, the proposed algorithm could be advantageously integrated into a hybrid population-based method (e.g., memetic search, path-linking) as a key intensification component. Fourth, this work uses tabu search to explore candidate solutions. Other meta-heuristics can be investigated to ensure this task while reusing most algorithmic components of AFISA. Finally, few exact algorithms are available for the WVCP, there is thus much room for research in this direction. In this context, AFISA could be used to generate high-quality initial bounds or to obtain upper bound estimations of subproblems during the search process.

5

Iterated backtrack removal search for finding k-VCS

In this chapter, we propose an iterated backtrack-based removal (IBR) heuristic to find k-VCS for a given graph. IBR extends the popular removal strategy with two new search components – a backtracking mechanism to reconsider some removed vertices and a perturbation strategy to escape local optima traps. Computational results on 80 benchmark graphs show that IBR is very competitive in terms of solution quality and run-time efficiency compared with state-of-the-art algorithms in the literature. Specifically, IBR improves best-known solutions for 9 graphs and matches the best results for other 70 instances. An article describing IBR is published in Journal of Heuristics [Sun *et al.*, 2018a].

Contents

5.1 Introduction

This chapter is dedicated to the k-vertex-critical subgraphs problem which was introduced in Chapter 1. Recall that given an undirected graph $G = (V, E)$ and a positive integer k, a k-vertex-critical subgraph (k-VCS) of G is a subgraph H such that its chromatic number equals k (i.e., $\chi(H) = k$), and removing any vertex causes a decrease of $\chi(H)$. The k-VCS problem (k-VCSP) is to find the smallest k-vertex-critical subgraph H^* of G. We extend previous studies by proposing an Iterated Backtrack Removal Search (IBR) for finding k-VCS in a graph. IBR reinforces the classical removal procedure [Chinneck, 1997b; Chinneck and Dravnieks, 1991; Desrosiers *et al.*, 2008; Herrmann and Hertz, 2002] with a backtracking scheme and a perturbation strategy. The basic idea of our approach is as follows. The removal procedure reduces the current graph by tentatively moving vertices to the set of uncritical vertices (see Section 5.3.2). This process is repeated until the subgraph induced by set of critical vertices is such that its chromatic number equals k. If the current subgraph does contain a k-VCS (the chromatic number of the current subgraph less than k), which means some critical vertices were removed to the set of uncritical vertices in error, the backtracking procedure is invoked. The backtracking procedure expands the current subgraph by adding back some vertices which are in the set of the uncritical vertices until the chromatic number of the current subgraph increases to k again. The perturbation procedure provides a means of reconsidering some vertices which would have been incorrectly identified as critical ones (see Section 5.3.5). This phase terminates once the stop condition is met.

We assess the proposed IBR algorithm on 80 popular DIMACS and COLOR02-04 benchmark instances which are commonly used to test k-VCS algorithms in the literature . The experimental results show that our IBR algorithm competes favorably with the state-of-the-art results. Specifically, the proposed algorithm improves best-known solutions for 9 graphs (improves the lower bound for 6 instances, at the same k, IBR obtains a better solution (smaller size of k-VCS) for 8 instances) and matches the best results for other 70 instances. Only in one case, IBR obtains a slightly worse result.

The chapter is organized as follows. Section 5.2 introduces some useful notations. Section 5.3 presents the components of the IBR algorithm, including the basic removal algorithm, the backtrack-based removal algorithm and the perturbation procedure. Section 5.4 shows computational evaluation and comparisons with state-of-the-art results. Section 5.5 investigates the key components of the proposed algorithm, followed by conclusions in Section 5.6.

5.2 Notations

Let $G = (V, E)$ be an input graph, we introduce the following notations, which are useful for the description of the proposed approach.

We define three working sets of vertices A, B and C that are used by the algorithm. For each vertex of V, we first define its status (critical, unknown, uncritical).

A *critical vertex* is a vertex that belongs to a k-VCS. We use A to denote the *set of critical vertices* that have been detected. A is also called the critical set.

An *unknown or undetected vertex* is a vertex whose status is still unknown. We use B to denote the *set of unknown vertices*, which is also called the unknown set.

An *uncritical vertices* refers to a vertex that does not belong to a k-VCS. We use C to denote the *set of uncritical vertices*, which is also called the uncritical set.

Given the critical set A and the unknown set B, the subgraph induced by A, $H = G_A = (A, E_A)$ ($E_A = A \times A \cap E$), is called the *critical subgraph* of G. The subgraph induced by $A \cup B$, $G_{A \cup B} = (A \cup B, E_{A \cup B})$ ($E_{A \cup B} = ((A \cup B) \times (A \cup B)) \cap E$), is the *remaining subgraph* of G.

As explained in the next section, the proposed approach operates on these three sets of ver-

tices, which are initially set as $A = \emptyset$, $B = V$, $C = \emptyset$. Then the algorithm searches a k-VCS by moving vertices from one set to another according to the temporarily identified status of each vertex.

For any vertex i, we also associate a weight $w(i)$, which is defined as follows:

$$w(i) = \begin{cases} |E|, if\ i \in A. \\ 1, if\ i \in B; \\ 0, if\ i \in C; \end{cases} \tag{5.1}$$

At the beginning of the search, we set $w(i) = 1$ for each vertex i of V (since $A = \emptyset, B = V, C = \emptyset$). The weight of a vertex is updated each time the vertex changes its status (critical, unknown, uncritical) (see Section 5.3). The weight information is mainly used by the removal algorithm for vertex selection.

5.3 The Iterated Backtrack-based Removal Algorithm

In this section, we present the iterated backtrack-based removal algorithm (IBR) for detecting k-VCS in a graph. IBR extends the classical removal algorithm with a backtracking scheme and a perturbation procedure.

5.3.1 General structure of the IBR algorithm

Given a graph $G = (V, E)$ and an integer $k \leq K$ (K being $\chi(G)$ or the smallest number of colors for which a k-coloring exists), the proposed IBR algorithm (see Figure 5.1 and Algorithm 5.1) aims to find a small k-VCS, i.e., a small set of critical vertices $A \subseteq V$ such that the induced subgraph $H = (A, E_A)$ has a chromatic number of $\chi(H) = k$, and removing any vertex from H decreases $\chi(H)$.

The IBR algorithm operates with three working sets of vertices, initialized as $A = \emptyset, B = V, C = \emptyset$. Basically, according to the coloring results on the remaining graph provided by a heuristic coloring algorithm, IBR uses three main procedures to move vertices among these sets in order to find a k-VCS.

Recall that each graph G contains at least one k-VCS for $1 \leq k \leq \chi(G)$. Furthermore, a graph G is $(k-1)$-colorable if and only if G does not contain a k-VCS. Note that the problem of deciding whether a graph G is $(k-1)$-colorable is itself NP-hard. For this reason, we adopt a heuristic coloring algorithm *Color* (see Section 5.3.3) to judge whether G is $(k-1)$-colorable.

1. The *removal procedure* inspects, one by one, the vertices of set B of unknown vertices to determine their status (Algorithm 5.1, lines 7-16). Specifically, at each iteration, a vertex i from B is first moved to C (i.e., i is supposed to be uncritical, line 8). If the graph $G_{A \cup B}$ after removing i does not contains a k-VCS any longer, i.e., becomes $(k-1)$-colorable, (checked with a heuristic coloring algorithm, see Section 5.3.3), then vertex i is identified as critical and moved from C to A (lines 9-10, see Section 5.3.2). We check again with the heuristic coloring algorithm whether the graph $G_{A \cup B}$ contains a k-VCS (line 12). If the graph $G_{A \cup B}$ after adding i back still does not contain a k-VCS, then certain critical vertices were incorrectly classified into the uncritical set C, a *backtracking procedure* is invoked (line 12). This process is repeated until the subgraph induced by set A of critical vertices is such that its chromatic number equals k (line 7).
2. Since the algorithm used to judge whether the remaining graphs $G_{A \cup B}$ contains a k-VCS is not an exact algorithm (see Section 5.3.3), a critical vertex can be incorrectly classified into

Algorithm 5.1: The IBR algorithm for solving the k-VCSP

Input: Graph $G = (V, E)$, integer $k \leq K$ (K being $\chi(G)$ or the smallest number of colors for which a k-coloring exists), R maximum allowed perturbations.
Output: H the smallest k-colorable subgraph
/*Initialization*/
$H_1 = \emptyset, \cdots, H_R = \emptyset$ /* each H_r records a detected candidate k-VCS*/
$A = \emptyset, B = V, C = \emptyset, H = (A, E_A)$ /*A is set of critical vertices, B is set of unknown vertices, C is set of uncritical vertices*/
$r = 0$ /*r is the number of performed perturbations*/
while $r < R$ **do**
  while H does not contains a k-VCS **do**
    Choose a vertex $i \in B$, move i from B to C /*vertex removal, Section 5.3.2*/
    if $G_{A \cup B}$ does not contains a k-VCS **then**
      move i from C to A /*i is detected as a critical vertex*/
      $H = (A, E_A)$
      /*Backtracking, Section 5.3.4*/
      while $G_{A \cup B}$ does not contains a k-VCS **do**
        Choose a vertex $l \in C$, move l from C to B
      end while
    end if
  end while
  $r = r + 1$
  $H_r = H$
  /*Perturbation operator for the critical subgraph*/
  $H' \leftarrow Perturbation(H_r)$ /*Section 5.3.5*/
  /*Update the set A, B and C*/
  $\{A, B, C\} \leftarrow Update\_set(H')$ /*Section 5.3.6*/
  $H = (A, E_A)$
end while
$H \leftarrow$ the smallest k-colorable subgraph

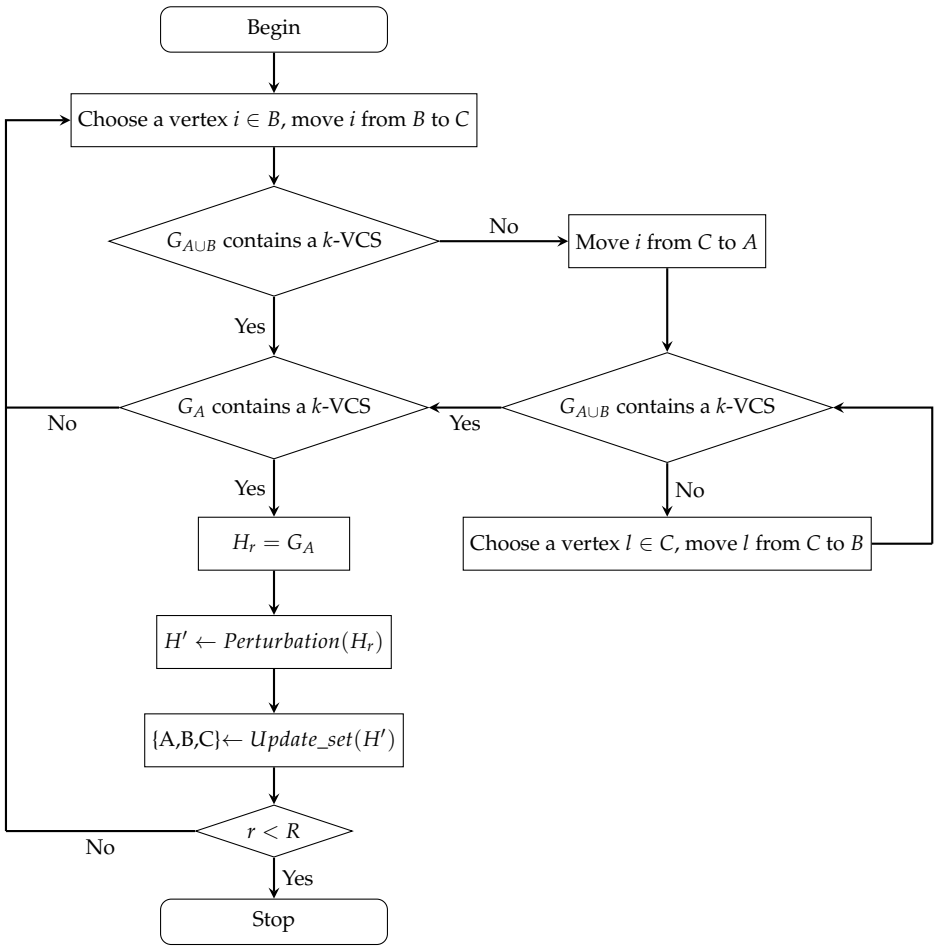


Figure 5.1 – Flow chart of the iterated backtrack-based removal algorithm for finding k-VCS in a graph.

the uncritical set C. To remedy this problem, we introduce a *backtracking procedure* which reconsiders the vertices of C (i.e., moving them back to the unknown set B, see Section 5.3.4). This procedure extends the removal procedure by continually moving uncritical vertices from C to B until the chromatic number of $G_{A\cup B}$ increases to k again (lines 12-14, see Section 5.3.4). Once $\chi(G_{A\cup B}) = k$ (which means the graph $G_{A\cup B}$ once again contains a k-VCS), the backtracking phase stops and returns to the removal phase. Otherwise, one repeats this backtracking phase.

3. The *perturbation procedure* is used to remedy the problem of some misclassified critical vertices moves vertices from set A to B (line 19, see Section 5.3.5) and updates the sets A, B and C and the subgraph H (lines 20-21, see Section 5.3.6). Then, the removal algorithm is applied on the graph G with the updated sets. This phase terminates once the allowed number of perturbations is reached (line 6).

We note that Algorithm 5.1 becomes the conventional removal algorithm of [Desrosiers *et al.*, 2008] when the backtrack procedure (lines 12-14) and perturbation procedure (lines 17-21) are disabled.

In the remainder of this section, we explain the main procedures of the IBR algorithm: the removal procedure, the heuristic coloring procedure, the backtracking procedure and the perturbation procedures.

5.3.2 The removal algorithm

Our removal procedure is based on the removal heuristic algorithm presented in [Desrosiers *et al.*, 2008], which can be conveniently described using the notion of critical, unknown and uncritical sets of vertices.

After initialization, $B = V$, $A = \emptyset$, $C = \emptyset$, $H = (A, E_A)$. We note that $G_{A \cup B} = G$ is not $(k-1)$-colorable, thus contains a k-VCS (see Section 5.3.1 and Algorithm 5.1). In each iteration, the removal algorithm tentatively moves one vertex i from the unknown set B to the uncritical set C. If $G_{A \cup B}$ without vertex i is always not $(k-1)$-colorable (i.e., $G_{A \cup B}$ contains a k-VCS), the removed vertex i is considered as an *uncritical* vertex and is kept in C. Otherwise, if $G_{A \cup B}$ without vertex i becomes $(k-1)$-coloring (i.e., $G_{A \cup B}$ does not contain a k-VCS), vertex i is considered as a *critical* vertex and thus transferred from set C to set A. In both cases, we update the sets A, B, C, the graphs H, $G_{A \cup B}$ and the weights of vertices accordingly. The removal algorithm repeats this process until $\chi(H)$ increases to k, which occurs when a k-VCS is detected.

In the removal algorithm, the rule used to select the next vertex from B impacts the critical subgraphs generated. In order to favor small critical subgraphs, the removal algorithm adopts the neighborhood weight heuristic strategy proposed in [Desrosiers *et al.*, 2008], which uses information contained in the weights of vertices.

Recall that when a vertex i is placed in the set A, B and C, its weight is set as $|E|$, 1 and 0 correspondingly. The neighborhood weight $W(i)$ of a vertex i is defined as the sum of the weights of the vertices that are adjacent to this vertex. When all weights of vertices are equal to 1 (e.g., after initialization), the neighborhood weight of a vertex equals its degree and can be considered as an indicator on the density of the region surrounding this vertex. The neighborhood weight heuristic strategy moves the vertices with the smallest neighborhood weight firstly, and preserves the denser ones. This strategy proved to be effective to detect a k-VCS with a small size [Desrosiers *et al.*, 2008].

5.3.3 Heuristic coloring algorithm

We adopt a heuristic coloring algorithm *Color* to judge whether a graph G is $(k-1)$-colorable (i.e., whether G contains a k-VCS). The removal algorithm can guarantee that the extracted subgraph $H = (A, E_A)$ is a k-VCS when the coloring algorithm *Color* is an *exact* algorithm (i.e., able to verify that the given remaining graph is colorable with a given k). However, given that the general k-coloring problem is itself NP-complete, exact methods can be too time consuming even for graphs of relatively small sizes (with several tens of vertices). For this reason and like [Desrosiers *et al.*, 2008], we adopt a heuristic coloring algorithm (i.e., TabuCol [Hertz and de Werra, 1987; Dorne and Hao, 1999; Galinier and Hao, 1999]). Contrary to an exact algorithm, the heuristic algorithm may fail to find a legal coloring with a given k, even if such a coloring exists.

Recall that at each iteration of the removal procedure, we move one unknown vertices i from B to C. Then, one needs to know whether there is a legal $(k-1)$-coloring on graph $H = (A, E_A)$ (the stopping condition is met or not) and on graph $G_{A \cup B} = (A \cup B, E_{A \cup B})$ (the last moved vertex is critical or not).

To solve the $(k-1)$-coloring problem, TabuCol iteratively explores partitions of V in $k-1$ classes. Each partition c is attributed to a fitness value $f(c)$ which is equal to the number of edges of the graph that have both endpoints in the class. Therefore, if $f(c) = 0$, the partition c corresponds to a proper $(k-1)$-coloring. The purpose of the tabu search coloring algorithm is then to minimize the fitness function f. The tabu coloring process stops when $f(c) = 0$ or the fitness function cannot be improved within a given number of iterations.

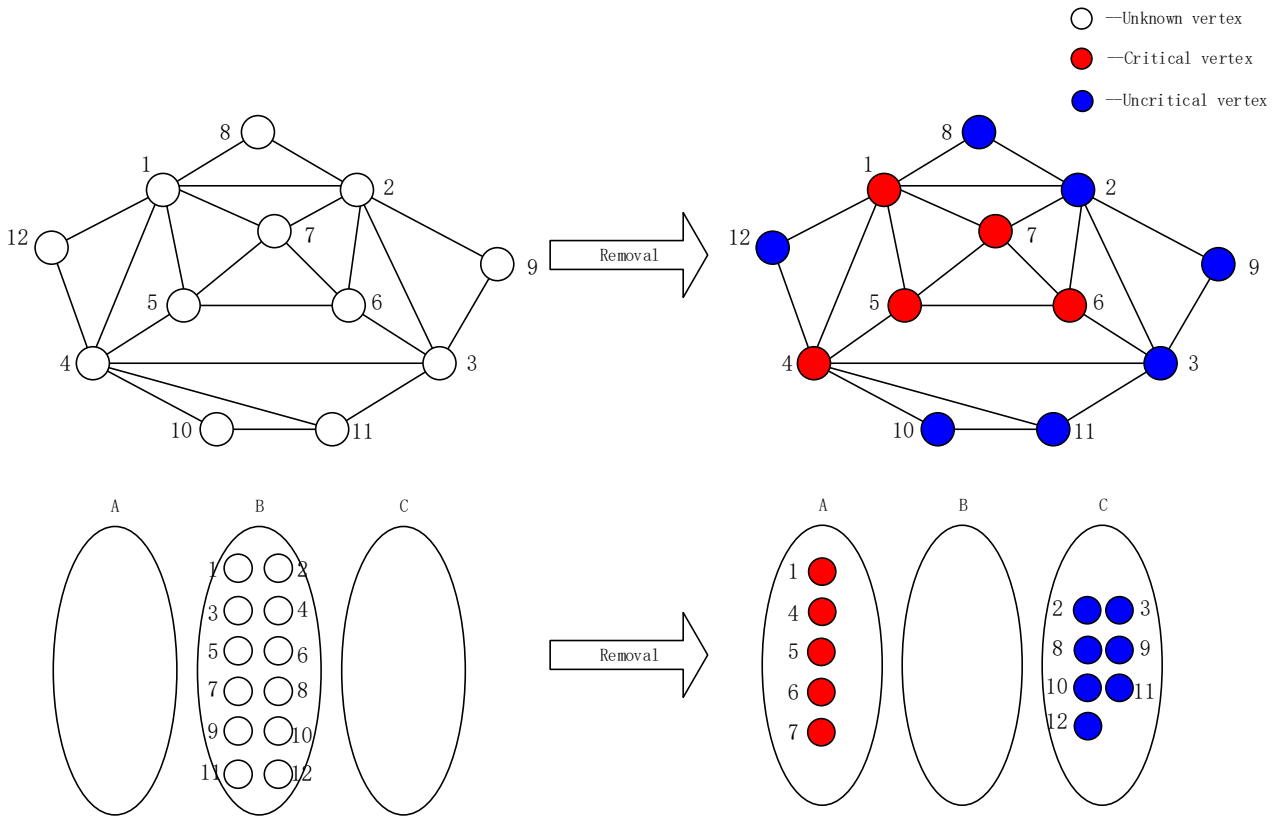


Figure 5.2 – Removal procedure.

5.3.4 Backtrack-based removal approach

The purpose of the backtracking phase is to cope with the problem caused by the heuristic coloring algorithm, that some critical vertices may be mistakenly moved to C. This situation happens as follows. When a *critical* vertex i is moved from B to C, *Color* should find a legal $(k-1)$-coloring in $G_{A\cup B}$ with $f_{A\cup B}=0$ (Algorithm 5.1, line 9), and the vertex i should be moved from C to A (Algorithm 5.1, line 10). However, since our coloring algorithm is not an exact method, it may fail to find a $(k-1)$-coloring in $G_{A\cup B}$. In this circumstance, the critical vertex is unexpectedly classified to set C and $\chi(G_{A\cup B})$ decreases to $k-1$. To alleviate this problem, we calls for a backtracking scheme. When we find a legal $(k-1)$-coloring for graph $G_{A\cup B}$, we invoke the backtrack procedure, i.e., we move vertices from C to set B, until $\chi(G_{A\cup B})$ increases to k again. The key issue concerns the way to select vertices of C that are moved back to the unknown set B.

To make the choice, we consider two strategies: (1) according to the reverse order by which the vertices have been moved from the set B to the set C; (2) according to the non-increasing order of neighborhood weights (see Section 5.3.2). Experiments indicated that the first strategy performs quite well and is thus used in this chapter (see Section 5.5.3 for a computational analysis). This can be explained by the removal heuristic algorithm which prefers vertices with a small neighborhood weight. Thus, the last moved vertex (with a larger sum of neighborhood weights) has more chance to be a critical vertex compared to a vertex that was moved since long time. While in rare cases, there are also erroneous movements such that some uncritical vertices are moved to the critical set A.

To illustrate the procedure, we consider the graph G of Figure 1.4(a) ($\chi(G)=4$) and a 4-VCS shown in Figure 1.4(b) (with vertices $\{1,2,3,4,5,6,7\}$). Figure 5.2 shows a possible situation in

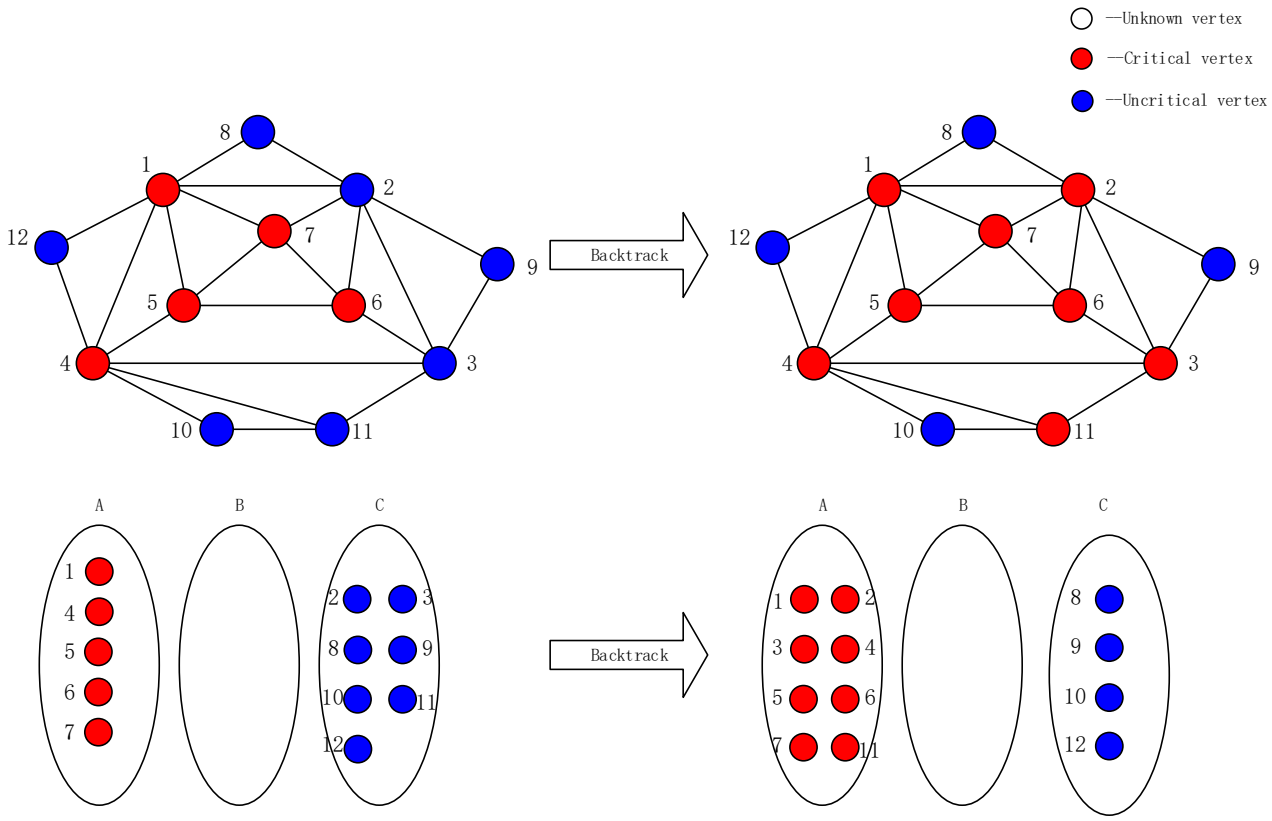


Figure 5.3 – Backtrack-based removal procedure.

the removal procedure: suppose that the coloring algorithm *Color* fails to find a legal 3-coloring for $G_{A\cup B}$ when the vertices 2, 3 were moved to the uncritical set C, then the vertices 2, 3 are retained in the set C. In this case, $A = \{1,4,5,6,7\}$, $B = \emptyset$, $C = \{2,3,8,9,10,11,12\}$. Suppose that after adding back the last removed vertex 6 to the graph $G_{A\cup B}$, we detected that $G_{A\cup B}$ becomes 3-colorable ($G_{A\cup B}$ does not contain a 4-VCS) using the heuristic coloring algorithm, the backtracking phase is invoked. This involves moving vertices from set C to set A according to the reverse order by which the vertices have been moved from set B to set C, until $\chi(G_{A\cup B})$ increases to 4 again ($G_{A\cup B}$ contains a 4-VCS again). Figure 5.3 illustrates this backtracking procedure for the given graph G. However, if the uncritical vertex 11 is moved before the last critical vertex was moved, the uncritical vertex 11 will also be moved into the critical set A. Thus $A = \{1,2,3,4,5,6,7,11\}$, $B = \emptyset$, $C = \{8,9,10,12\}$. We note that this backtracking procedure is effective for repairing the misjudgments that misclassify critical vertices as uncritical vertices. Meanwhile, this procedure may unfortunately classify uncritical vertices into the critical set A.

5.3.5 Perturbation operator of backtrack-based removal algorithm

As illustrated in Section 5.3, the backtrack-based removal procedure ends up with a k-VCS (Algorithm 5.1, lines 6-16). However, it may happens that some uncritical vertices are misclassified as critical vertices (always due to the use of a heuristic coloring algorithm). To overcome this problem, we introduce a perturbation procedure, which partially reconfigures A, B and C by moving some vertices from set A to set B. This procedure also provides new opportunities of finding k-VCS of smaller sizes.

The perturbation procedure (Algorithm 5.2) is inspired by the techniques proposed by [Lü and Hao, 2009; Glover *et al.*, 2010], which is decomposed into two parts:

Algorithm 5.2: Perturbation

```
1: Input: a k-critical-vertex-subgraph H, a probability threshold p
2: Output: a perturbed solution H' /*Score the vertices in the set A*/
3: for i ∈ A do
4:    calculate score(i) with Equation 5.2
5: end for
6: A'← η vertices with the highest scores
7: A'← sort A' in descending order of the scores /*Choose and move the perturbed vertices*/
8: for i ∈ A' do
9:    i is the jth element in A', calculate the possibility P_j using Equation 5.3
10:   if P_j > p then
11:      move i from A to B
12:   end if
13: end for
14: H' = (A, E_A)
```

(1) Scoring the vertices in set A. We define a function $score(i)$ to score each vertex i. Let $FlipFreq(i)$ be the number of times vertex i has been displaced among sets A, B and C, $EliteSol = [H_1, \cdots, H_R]$ a set of R critical subgraphs discovered so far (R is the size of $EliteSol$), $EliteFreq(i)$ the total number of times vertex i appears in $EliteSol$, the scoring function is then defined as:

$$sorce(i) = EliteFreq(i)(r - EliteFreq(i))/r^2 + (1 - FliteFreq(i)/Max\_Freq) \tag{5.2}$$

where $1 \leq r \leq R$ and $Max\_Freq = max_{i \in \{1\ldots,|V|\}}\{FlipFreq(i)\}$.

(2) Choosing and moving the perturbed vertices. We sort all vertices in non-increasing order according to their scores and then choose probabilistically certain vertices from set A. The possibility of the jth highly-scored vertex being selected is given by:

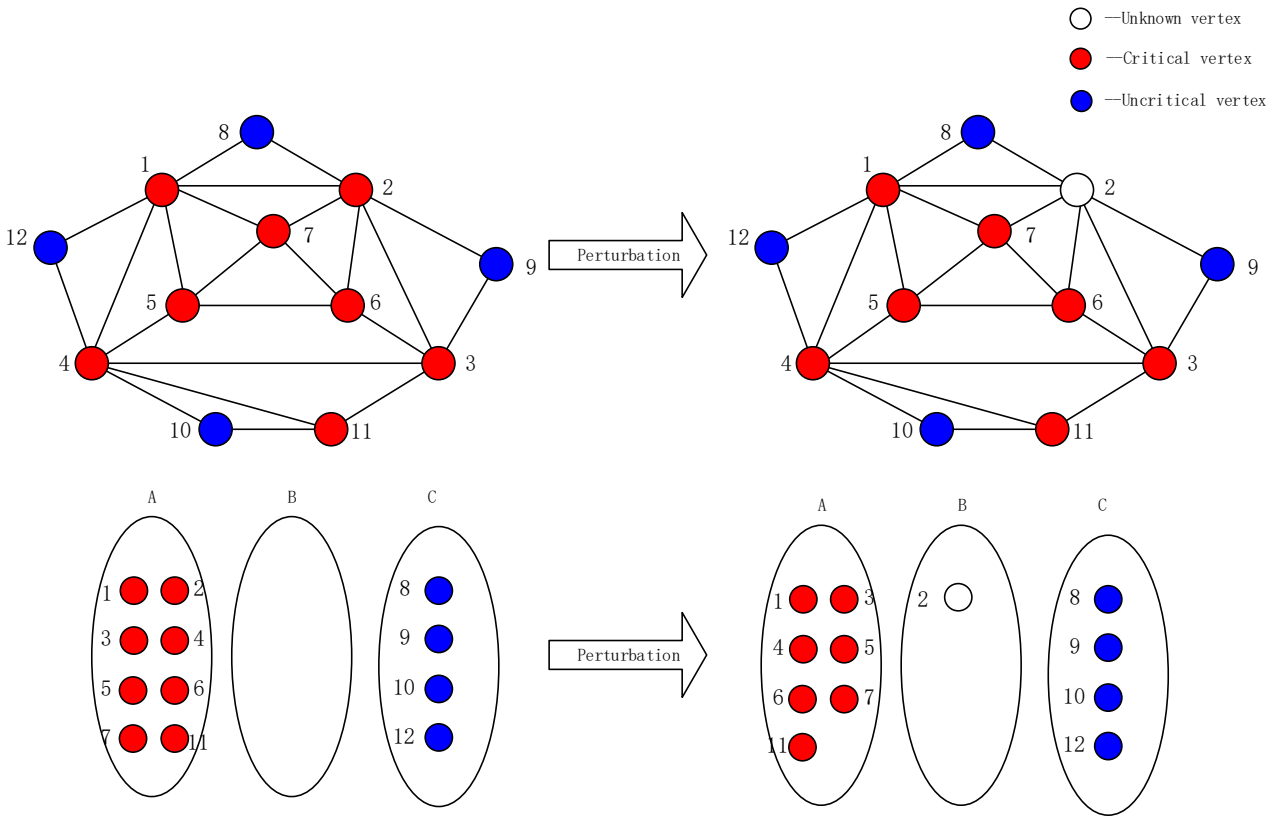
$$P_j = \frac{j^{-1}}{\sum_{z=1}^{\eta} z^{-1}} \tag{5.3}$$

where η is usually set as $|A|/2$. Then we move the chosen vertices from set A to set B and update the sets A, B and C (see Section 5.3).

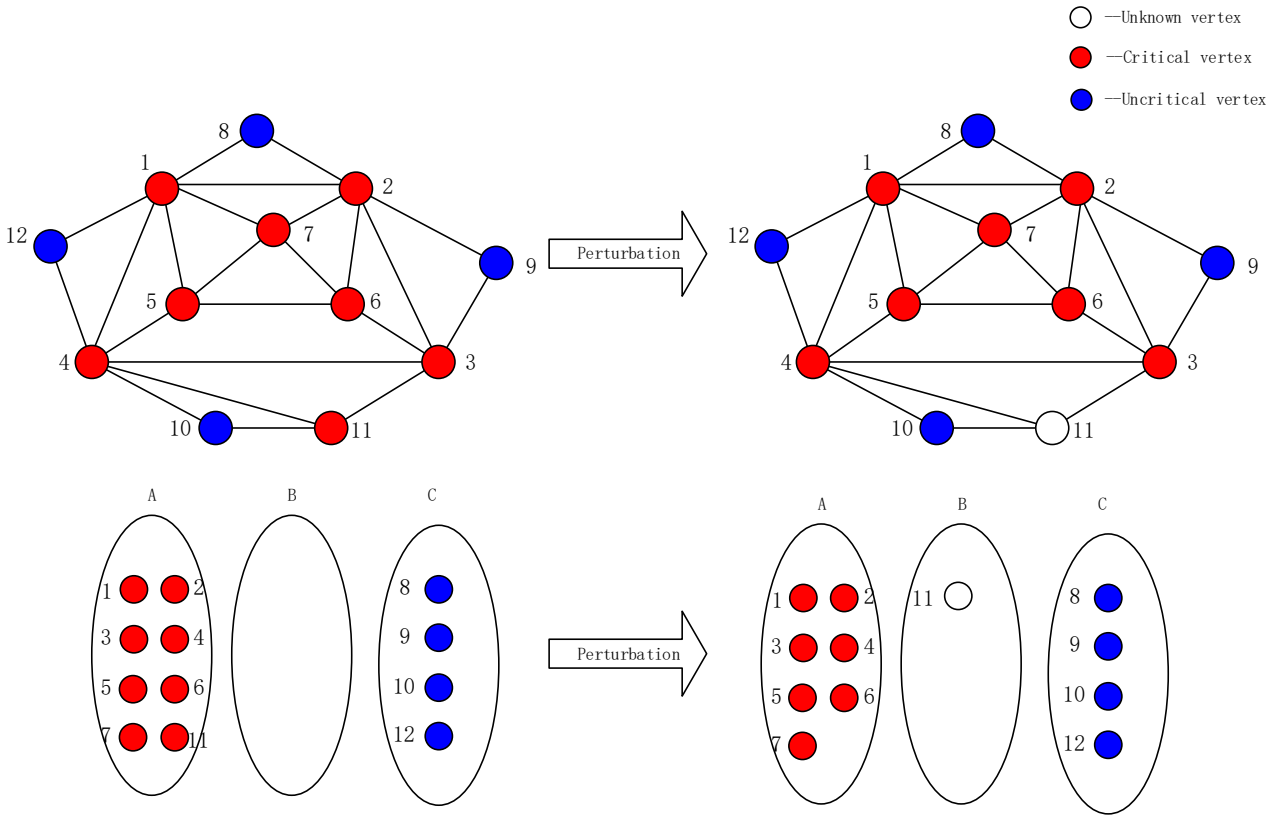
As an example, we consider the graph in Figure 5.4 with a chromatic number of 4 and one 4-VCS, i.e., $\{1, 2, 3, 4, 5, 6, 7\}$. Following Section 5.3.4, after the backtrack-based removal procedure, $A = \{1, 2, 3, 4, 5, 6, 7, 11\}$ as critical vertices and other ones are uncritical vertices ($C = \{8, 9, 10, 12\}$, $B = \emptyset$}), while the vertex 11 is mistaken for a critical vertex. The perturbation procedure moves certain vertices from set A to set B according to Algorithm 5.2. Figure 5.4(a) and Figure 5.4(b) respectively present two situations where uncritical vertex 2 and the uncritical vertex 11 are moved from the set A to the set B by the perturbation procedure.

5.3.6 Update procedure

Before invoking a next round of the backtrack-based removal procedure after the perturbation operation, an additional update operation is applied (Algorithm 5.3). According to whether the perturbed solution contains a k-VCS, we use different strategies to update sets A, B and C. If the subgraph $H' = (A, E_A)$ does not contain a k-VCS (see Algorithm 5.3, line 4), which means certain critical vertices are misclassified in set B or even in set C, we move all vertices of C to B in order to re-examine each vertex of $B \cup C$ in the next step. Otherwise, we come to the conclusion that



(a) Case 1 for the perturbation procedure.



(b) Case 2 for the perturbation procedure.

Figure 5.4 – Perturbation procedure.

Algorithm 5.3: Update_Set

```
Input: a perturbed graph H' ;
Output: a update set A, B, C
f_{H'} = Color(H', k − 1)
if f_{H'} = 0 then
    move all vertices from C to B /*in order to re-detect each vertex of (B ∪ C) is uncritical or not*/
else
    move all vertices from B to C   /*all the vertices in set B are uncritical vertices*/
    move all vertices from A to B /*in order to rejudge each vertex of A is critical or not*/
end if
```

all vertices in set B are uncritical and move all vertices from B to C. Then, in order to determine whether the vertices of set A are uncritical or not, we move all vertices of A to B.

Following Figure 5.4, after the backtracking procedure and the perturbation procedure, two cases are possible according to whether the subgraph $H' = (A, E_A)$ contains a 4-VCS. As shown in Figure 5.5(a), $H' = (A, E_A)$ does not contain a k-VCS. Then the update procedure moves all vertices from C to B in order to re-consider each vertex in $B \cup C$ in the next step. Accordingly, $A = \{1, 3, 4, 5, 6, 7, 11\}$, $B = \{2, 8, 9, 10, 12\}$ and $C = \emptyset$. Figure 5.5(b) shows a subgraph $H' = (A, E_A)$ that contains a 4-VCS. In this case, the update procedure moves all vertices from B to C and all vertices from A to B, leading to $A = \emptyset$, $B = \{1, 2, 3, 4, 5, 6, 7\}$ and $C = \{8, 9, 10, 11, 12\}$.

5.4 Experimental results and analysis

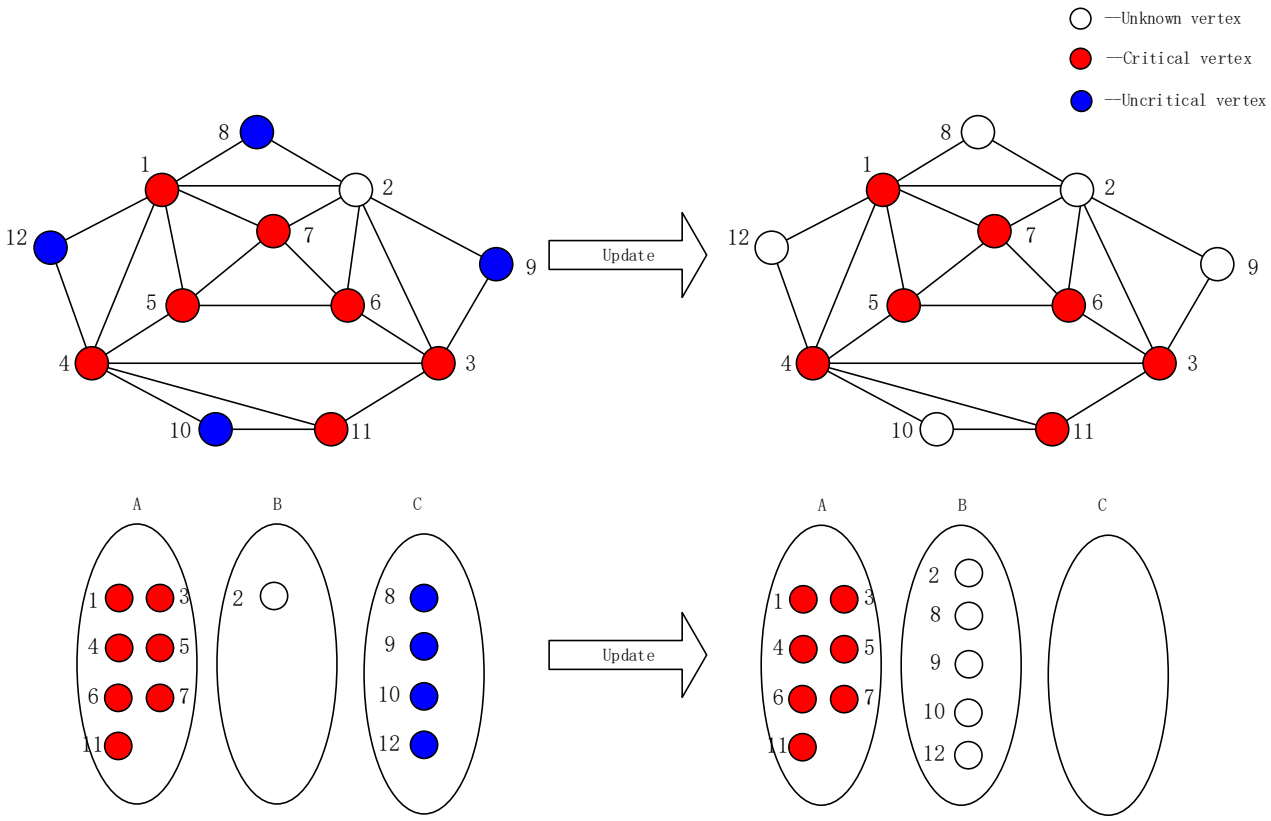
In this section, we assess the performance of the proposed IBR algorithm on a collection of benchmark graphs from the DIMACS [1] and COLOR02/03/04 competitions [2].

5.4.1 Experiment settings

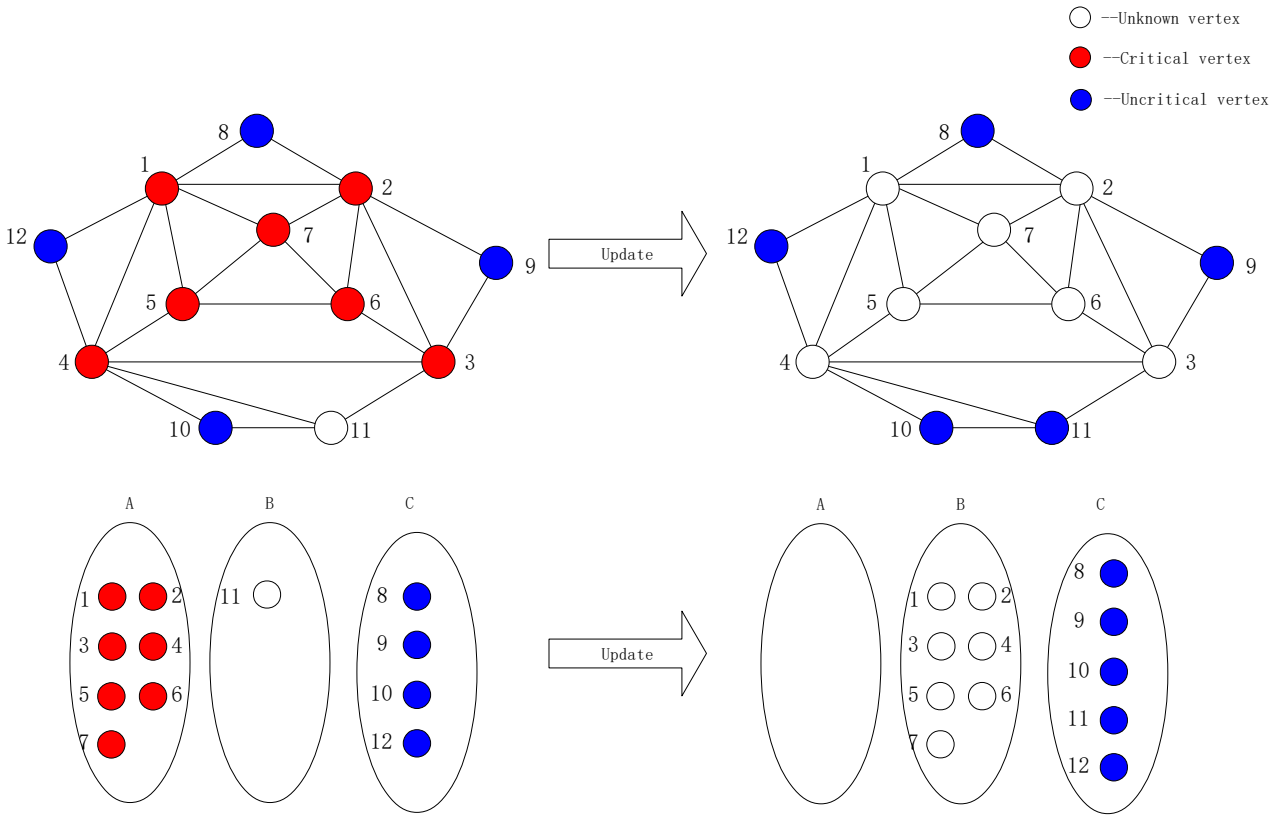
The proposed algorithm was programmed in C and compiled by GNU g++ with the '-O3' flag (option). The experiments were conducted on a computer with Xeon E5440 (2.83GHz CPU and 2GB RAM) and Ubuntu Linux system 12.04. Running the DIMACS machine benchmark program dfmax.c [3], our computer requires 0.23, 1.42 and 5.42 seconds to solve graphs r300.5, r400.5, and r500.5, respectively.

For our comparative study, we used the best performing heuristic algorithm $Ins + h$ [Desrosiers *et al.*, 2008] as our main reference. The $Ins + h$ algorithm was run on an Athlon processor (1.6 GHz and 512 Mb of RAM). The comparison was performed mainly by considering the quality criterion of the solutions found. We note that our processor is about 1.8 times faster than that used by the reference algorithm. Thus, in all the experiments, our recorded CPU times were multiplied by 2 in order to make a reasonable comparison. Given that the compared algorithms were tested on different computing platforms and the runtime of an algorithm depends also on other factors (programming language, data structures, etc), it is difficult to strictly compare the runtimes. Thus, timing information was just provided for indicative purposes.

1. http://www.dimacs.rutgers.edu/
2. http://www.cs.hbg.psu.edu/txn131/graphcoloring.html/
3. dfmax: ftp://dimacs.rutgers.edu/pub/dsj/clique/



(a) Case 1 of the update procedure.



(b) Case 2 of the update procedure.

Figure 5.5 – Update procedure.

5.4.2 Instances and experimental settings

Test instances. We considered the set of 80 popular benchamrk graphs which were tested in [Desrosiers *et al.*, 2008]. These graphs are divided into four categories.

1. The first category contains 17 instances that are probably critical themselves. Graphs having *myciel**, *mug** or *Insertions** in their name fall into this category. The reference algorithm ($Ins + h$) extracts the minimum k-VCS for all graphs in this category at $k = \chi(G)$.
2. The second category contains instances which have cliques as minimum k-VCS, for $k = \chi(G)$. This category of graphs includes *le*450*, *fpso**, *inithx**, *mulsol**, *zeroin**, *school*1*, *miles**, *anna*, *david*, *homer*, *huck*, *jean* graphs. The $Ins + h$ algorithm also detects the optimum k-VCS at $k = \chi(G)$ for all graphs in this category.
3. The third category contains the instances which have DSJC in their name. According to [Desrosiers *et al.*, 2008], these graphs are harder than other graphs for which a k-VCS is difficult to detect. In fact, the $Ins + h$ algorithm fails to find a k-VCS for most of graphs in this category.
4. The last category is composed of all the instances falling in none of the above three categories.

Parameters. Following [Desrosiers *et al.*, 2008], we ran our IBR algorithm 5 times to solve each instance, and reported the best values of the successful runs.

Stopping condition. The IBR algorithm stops once the number of the perturbation reaches the given limit $R = 20$.

Quality criteria. The experiments have two goals. The first one is to compare the quality of the detected k-VCS for the given k. In this case, a smaller k-VCS represents a better solution. The second goal concerns the quality of the lower bound of $\chi(G)$ that an algorithm can reach [Desrosiers *et al.*, 2008]. In this case, we try to find k-VCS with increasing k values (so a k-VCS with a larger k is better, which corresponds to a tighter lower bound of $\chi(G)$).

Finally, like [Desrosiers *et al.*, 2008], we verify the validity of a candidate k-VCS returned by the IBR algorithm with an exact coloring algorithm. Indeed, since the returned k-VCS is usually of small size, its chromatic number can be determined exactly by a modern exact coloring problem within a time frame of several hours. In our case, we used the recent algorithm presented in [Zhou *et al.*, 2014].

5.4.3 Comparison with state of the art algorithm

Tables 5.1, 5.2, 5.3 and 5.4 summarize the computational results of our IBR algorithm on the four categories of DIMACS benchmark graphs, respectively. In these tables, the first 4 columns show the name of each instance, the number of vertices V, the number of edges E and the best-known upper bound k_UB of the chromatic number reported in the literature. Values followed by an asterisk $*$ indicate that they correspond to $\chi(G)$. The following four columns indicate the results of the $Ins + h$ algorithm [Desrosiers *et al.*, 2008]: the k value for which a k-VCS is detected (i.e., lower bound of $\chi(G)$), the number of vertices and the number of edges of the detected k-VCS, and the CPU time in seconds needed to find the k-VCS. The last four columns show the results obtained by our IBR algorithm. In Table 5.3, we show some improved lower bounds obtained by the IBR algorithm compared to the lower bounds obtained by the $Ins + h$ algorithm. For each of these cases, we list the best lower bound that IBR can achieve and its corresponding k-VCS in an additional row.

Table 5.1 displays the results of $Ins + h$ and the results of IBR for the 17 instances of the first category, which are probably critical graphs themselves [Desrosiers *et al.*, 2008]. Both algorithms

Table 5.1 – Comparative results of IBR with state-of-the-art algorithm on the first category of instances.

Instance				*Ins* + *h* [Desrosiers *et al.*, 2008]				IBR			
name	$\|V\|$	$\|E\|$	*k_UB*	*k*	$\|V\|$	$\|E\|$	*time*(*s*)	*k*	$\|V\|$	$\|E\|$	*time*(*s*)
myciel5	47	236	6*	6*	47*	236*	0.1	6*	47*	236*	0.00
myciel6	95	755	7*	7*	95*	755*	0.2	7*	95*	755*	0.01
myciel7	191	2360	8*	8*	191*	2360*	30.65	8*	191*	2360*	11.46
mug88_1	88	146	4*	4*	88*	146*	0.05	4*	88*	146*	0.03
mug88_25	88	146	4*	4*	88*	146*	0.05	4*	88*	146*	0.02
mug100_1	100	166	4*	4*	100*	166*	0.05	4*	100*	166*	0.03
mug100_25	100	166	4*	4*	100*	166	0.05	4*	100*	166*	0.03
1_Insertion_4	67	232	5*	5*	67*	232*	0.05	5*	67*	232*	0.3
1_Insertion_5	202	1227	6	6	202	1227	0.05	6	202	1227	0.23
1_Insertion_6	607	6337	7	7	607	6337	49.85	7	607	6337	390.24
2_Insertion_4	149	541	5	5	149	541	0.15	5	149	541	0.04
2_Insertion_5	597	3936	6	6	597	3936	8.0	6	597	3936	14.67
3_Insertion_3	56	110	4*	4*	56*	110*	0.2	4*	56*	110*	0.02
3_Insertion_4	281	1046	5	5	281	1046	0.4	5	281	1046	0.58
3_Insertion_5	1406	96,957	6	6	1406	96, 957	257.4	6	1406	96, 957	1580.37
4_Insertion_3	79	156	4	4	79	156	0.3	4	79	156	0.02
4_Insertion_4	475	1795	5	5	475	1795	0.75	5	475	1795	0.95

can obtain the optimal subgraphs, but IBR is faster than $Ins + h$ for 10 graphs. The same observation can be made for the 39 instances of the second category which have maximum cliques as minimum k-VCS for $k = \chi(G)$.

Table 5.2 – Comparative results of IBR with state-of-the-art algorithm on the second category of instances.

Instance				*Ins* + *h* [Desrosiers *et al.*, 2008]				IBR			
name	$\|V\|$	$\|E\|$	*k_UB*	*k*	$\|V\|$	$\|E\|$	*time*(*s*)	*k*	$\|V\|$	$\|E\|$	*time*(*s*)
le450_5a	450	5714	5*	5*	5*	10*	5.35	5*	5*	10*	2.24
le450_5b	450	5734	5*	5*	5*	10*	7.7	5*	5*	10*	2.48
le450_5c	450	9803	5*	5*	5*	10*	8.9	5*	5*	10*	2.33
le450_5d	450	9757	5*	5*	5*	10*	8.35	5*	5*	10*	3.67
le450_15a	450	8168	15*	15*	15*	105*	5.4	15*	15*	105*	1.39
le450_15b	450	8169	15*	15*	15*	105*	3.0	15*	15*	105*	1.4
le450_15c	450	16680	15*	15*	15*	105*	22.25	15*	15*	105*	6.8
le450_15d	450	16750	15*	15*	15*	105*	14.65	15*	15*	105*	5.39
le450_25a	450	8260	25*	25*	25*	300*	7.2	25*	25*	300*	3.34
le450_25b	450	8263	25*	25*	25*	300*	6.6	25*	25*	300*	3.14
le450_25c	450	17343	25*	25*	25*	300*	9.1	25*	25*	300*	4.07
le450_25d	450	17425	25*	25*	25*	300*	8.95	25*	25*	300*	6.65
school1	385	19,095	14*	14*	14*	91*	6.25	14*	14*	91*	1.94
school1_nsh	385	19,095	14*	14*	14*	91*	15.1	14*	14*	91*	1.19
miles250	128	387	8*	8*	8*	28*	0.1	8*	8*	28*	0.04
miles500	128	1170	20*	20*	20*	190*	0.1	20*	20*	190*	0.09
miles750	128	2113	31*	31*	31*	465*	1.05	31*	31*	465*	0.41
miles1000	128	3216	42*	42*	42*	861*	1.5	42*	42*	861*	1.33
miles1500	128	5198	73*	73*	73*	2628*	1.6	73*	73*	2628*	0.64
anna	138	493	11*	11*	11*	55*	0.15	11*	11*	55*	0.07
david	87	406	11*	11*	11*	55*	0.15	11*	11*	55*	0.04
homer	561	1629	13*	13*	13	78*	0.4	13*	13*	78*	0.23
huck	74	301	11*	11*	11*	55*	0.1	11*	11*	55*	0.04
jean	80	254	10*	10*	10*	45*	7.1	10	10*	45*	0.09
games120	120	638	9*	9*	9*	36*	0.2	9*	9*	36*	0.07
fpsol2.i.1	496	11654	65*	65*	65*	2080*	104.95	65*	65*	2080*	21.93
fpsol2.i.2	451	8691	30*	30*	30*	435*	10.0	30*	30*	435*	3.33
fpsol2.i.3	451	8691	30*	30*	30*	435*	26.25	30*	30*	435*	4.34
mulsol.i.1	197	3925	49*	49*	49*	1176*	2.2	49*	49*	1176*	0.47
mulsol.i.2	188	3885	31*	31*	31*	465*	3.2	31*	31*	465*	0.5
mulsol.i.3	184	3916	31*	31*	31*	465*	3.25	31*	31*	465*	0.47
mulsol.i.4	185	3946	31*	31*	31*	465*	3.4	31*	31*	465*	0.37
mulsol.i.5	186	3973	31*	31*	31*	465*	3.45	31*	31*	465*	1.86
zeroin.i.1	211	4100	49*	49*	49*	1176*	2.2	49	49*	1176*	0.45
zeroin.i.2	211	3541	30*	30*	30*	435*	5.7	30*	30*	435*	1.69
zeroin.i.3	206	3540	30*	30*	30*	435*	2.8	30*	30*	435*	1.68
inithx.i.1	864	18707	54*	54*	54*	1431*	448.85	54*	54*	1431*	38.13
inithx.i.2	645	13979	31*	31*	31*	465*	5.1	31	31*	465*	0.99

inithx.i.3	621	13969	31*	31*	31*	465*	7.1	31*	31*	465*	1.9

Table 5.3 – Comparative results of IBR with state-of-the-art algorithm on the third category of instances. Improved results are indicated in bold.

Instance				*Ins* + *h* [Desrosiers *et al.*, 2008]				IBR			
name	$\|V\|$	$\|E\|$	*k_UB*	*k*	$\|V\|$	$\|E\|$	*time*(*s*)	*k*	$\|V\|$	$\|E\|$	*time*(*s*)
DSJC125.1	125	736	5*	5*	10	26	0.4	5*	10	26	2.29
DSJC125.5	125	3891	17*	14	70	1341	46.35	14	**66**	**1266**	11.69
								15	**82**	**1862**	35.4
DSJC250.1	250	3218	8	6	64	362	27.65	6	**51**	**290**	21.45
								7	**120**	**983**	134
DSJC250.5	250	15,668	28	14	74	1505	59.6	14	**50**	**836**	32.54
								16	**75**	**1742**	43.92
DSJC500.1	500	12,458	12*	6	65	369	73.15	6	**32**	**159**	48.23
								7	**79**	**617**	353.06
DSJR500.1	500	3555	12*	12*	12*	66*	1.9	12*	12*	66*	41.23
DSJR500.1C	500	121,275	85*	80	84	3477	710.75	80	**80**	**3160**	153.96
								83	**83**	**3403**	1280.19
DSJR500.5	500	58,862	122	90	90	4005	373.6	90	90	4005	15.78
								119	**119**	**7,021**	29.08

Table 5.4 – Comparative results of IBR with state-of-the-art algorithm on the fourth category of instances. Improved results are indicated in bold.

Instance				*Ins* + *h* [Desrosiers *et al.*, 2008]				IBR			
name	$\|V\|$	$\|E\|$	*k_UB*	*k*	$\|V\|$	$\|E\|$	*time*(*s*)	*k*	$\|V\|$	$\|E\|$	*time*(*s*)
queen6_6	36	290	7*	7*	**22**	**119**	0.8	7*	24	140	1.24
queen8_8	64	728	9*	9*	54	538	12.6	9*	**53**	**519**	2.6
queen9_9	81	2112	10*	10*	74	897	13.8	10*	**72**	**869**	920.45
ash331GPIA	662	4185	4	4	9	16	1.6	4	**7**	**12**	287.08
1-FullIns_3	30	100	4	4	7	12	0.1	4	7	12	0.09
1-FullIns_4	93	593	5	5	15	43	**0.25**	5	15	43	0.32
1-FullIns_5	282	3247	6	6	31	144	7.3	6	31	144	2.10
2-FullIns_3	52	201	5	5	9	22	0.1	5	9	22	0.09
2-FullIns_4	212	1621	6	6	19	75	**0.25**	6	19	75	0.58
2-FullIns_5	852	12,201	7	7	39	244	**13.3**	7	39	244	22.4
3-FullIns_3	80	346	6	6	11	35	0.15	6	11	35	0.15
3-FullIns_4	405	3524	7	7	23	116	**1.25**	7	23	116	3.38
3-FullIns_5	2030	33,751	8	8	47	371	**78.6**	8	47	371	396.26
4-FullIns_3	114	541	7	7	13	51	0.2	7	13	51	0.25
4-FullIns_4	690	6650	8	8	27	166	**12.3**	8	27	166	15.35
5-FullIns_3	154	792	8	8	15	70	1.2	8	15	70	0.47

The most interesting results concern the 8 random instances of the third category. When comparing IBR and *Ins* + *h* for this category, one observes that IBR improves the lower bound for 6 instances (DSJC125.5, DSJC250.1, DSJC250.5, DSJC500.1, DSJR500.1c, DSJR500.5). Moreover, at the same *k*, IBR obtains a better solution (smaller size of *k*-VCS) for 5 instances (DSJC125.5, DSJC250.1, DSJC250.5, DSJC500.1, DSJR500.1c). IBR is also faster than *Ins* + *h* on all instances when using the same *k*.

The results on the instances of the fourth category are shown in Table 5.4. One observes that IBR improves the best-known results for 3 instances while matching the best-known results for other 12 instances. Only in one case, IBR obtains a worse result.

5.5 Analysis and discussions

This section performs additional experiments to analyze the proposed IBR algorithm: the backtrack strategy and the perturbation operator. These experiments were performed on a selection of 13 representative instances.

5.5.1 Effectiveness of different backtrack strategies for k-VCS detection

This section compares the backtracking strategy adopted by IBR (i.e., using the reverse order by which the vertices were moved from the set B to the set C) and the backtracking rule according to the non-increase order of the sum of neighborhood weights of the vertices in the current graph. We use IBR1 to denote the IBR variant using the second backtracking strategy. We ran both IBR and IBR1 5 times to obtain the k-VCS of each instance.

Table 5.5 – Comparative results of the IBR algorithm with two different backtrack strategies. Improved results are indicated in bold.

Instance				IBR1					IBR				
name	$\|V\|$	$\|E\|$	k_UB	k	$\|V\|$	$\|E\|$	$time(s)$	SR	k	$\|V\|$	$\|E\|$	$time(s)$	SR
DSJC125.5	125	3891	17	15	83	1,898	1.3	2/5	15	**82**	**1854**	35.4	5/5
DSJC250.1	250	3218	8	7	**116**	995	30.57	1/5	7	120	**983**	133.56	1/5
DSJC250.5	250	15,668	28	16	77	1675	73.37	1/5	16	**75**	**1742**	43.92	1/5
DSJC500.1	500	12,458	12	7	83	671	276.58	1/5	7	**79**	**617**	353.06	1/5
DSJR500.1C	500	121,275	85	83	83	3403	1255.93	1/5	83	83	3403	1280.19	5/5
DSJR500.5	500	58,862	122	119	119	7,021	21.91	5/5	119	119	7,021	29.08	5/5
queen6_6	36	290	7	7	24	140	1.0	2/5	7	24	140	1.24	1/5
queen8_8	64	728	9	9	54	542	14.92	1/5	9	**53**	**519**	2.6	1/5
queen9_9	81	2112	10	9	9	36	0.35	2/5	9	9	36	0.35	5/5
									10	**72**	**869**	920.45	5/5
ash331GPIA	662	4185	4	4	7	12	132.55	3/5	4	7	12	287.08	2/5
1-FullIns_5	282	3247	6	6	31	144	3.07	1/5	6	31	144	2.10	2/5
2-FullIns_5	852	12,201	7	7	39	244	53.07	2/5	7	39	244	22.4	5/5
3-FullIns_5	2030	33,751	8	8	48	374	800.85	1/5	8	**47**	**371**	396.26	2/5

The experimental results are presented in Table 5.5, including the lower bound k, the number of vertices and edges of the k-VCS found, and the success rate (SR) to obtain the k-VCS over 5 runs. When comparing the k-VCS obtained by IBR and IBR1, one observes that IBR obtains better solutions for 5 instances at the same k and improves the lower bound for 1 instance. This justifies the backtracking strategy used in our previous experiments.

5.5.2 Effectiveness of perturbation for k-VCS detection

Table 5.6 – Analysis of the influence of the perturbation on the performance of the IBR algorithm. The BR algorithm is obtained by replacing the perturbation procedure of the IBR algorithm with a restart strategy. Improved results are indicated in bold.

Instance				BR					IBR				
name	$\|V\|$	$\|E\|$	k_UB	k	$\|V\|$	$\|E\|$	$time(s)$	SR	k	$\|V\|$	$\|E\|$	$time(s)$	SR
DSJC125.5	125	3891	17	15	82	1858	24.98	1/5	15	82	**1854**	35.4	2/5
DSJC250.1	250	3218	8	7	116	1010	51.2	1/5	7	**120**	**983**	133.56	3/5
DSJC250.5	250	15,668	28	16	75	1740	42.75	1/5	16	**75**	**1740**	42.75	1/5
DSJC500.1	500	12,458	12	7	91	767	318.41	1/5	7	**79**	**617**	353.06	1/5
DSJR500.1C	500	121,275	85	80	80	3160	153.96	1/5	**80**	**80**	**3160**	153.96	5/5
									83	**83**	**3403**	1280.19	5/5
DSJR500.5	500	58,862	122	119	119	7,021	46.56	5/5	119	119	7,021	57.1	5/5
queen6_6	36	290	7	7	24	140	1.03	2/5	7	24	140	1.24	3/5
queen8_8	64	728	9	9	54	542	14.92	1/5	9	**53**	**519**	2.6	1/5
queen9_9	81	2112	10	9	9	36	0.35	2/5	9	9	36	0.35	5/5
									10	**72**	**869**	920.45	5/5
ash331GPIA	662	4185	4	4	9	16	11.86	5/5	4	**7**	**12**	287.08	2/5
1-FullIns_5	282	3247	6	6	31	144	1.48	1/5	6	31	144	2.10	2/5
2-FullIns_5	852	12,201	7	7	39	244	27.89	1/5	7	39	244	22.4	5/5
3-FullIns_5	2030	33,751	8	8	47	371	833.14	1/5	8	47	371	396.26	2/5

As shown in Section 5.3.5, the proposed algorithm uses a perturbation strategy to reconfigure the sets A, B and C. In order to show the effect of the perturbation procedure, we compare IBR

Table 5.7 – Influence of the backtracking procedure on the performance of the IBR algorithm. IR is obtained by disabling the backtracking procedure. Improved results are indicated in bold.

Instance				IR					IBR				
name	$\|V\|$	$\|E\|$	*k_UB*	k	$\|V\|$	$\|E\|$	$time(s)$	SR	k	$\|V\|$	$\|E\|$	$time(s)$	SR
DSJC125.5	125	3891	17	14	67	1299	21.22	1/5	14	**66**	**1266**	11.69	5/5
									15	**82**	**1854**	35.4	5/5
DSJC250.1	250	3218	8	6	57	335	8.23	1/5	6	**51**	**290**	21.45	1/5
									7	**120**	**983**	133.56	3/5
DSJC250.5	250	15,668	28	13	38	478	1095.26	1/5	13	**35**	**434**	947.51	1/5
									16	**75**	**1742**	43.92	1/5
DSJC500.1	500	12,458	12	6	39	196	73.5	1/5	**6**	**32**	**159**	48.23	3/5
									7	**79**	**617**	353.06	1/5
DSJR500.1C	500	121,275	85	80	80	3160	153.96	1/5	80	**80**	**3160**	153.96	5/5
									83	**83**	**3403**	1280.19	5/5
DSJR500.5	500	58,862	122	119	119	7,021	31.71	5/5	119	119	7,021	57.1	5/5
queen6_6	36	290	7	7	26	163	0.05	5/5	7	**24**	**140**	1.24	1/5
queen8_8	64	728	9	9	54	542	14.92	1/5	9	**53**	**519**	2.6	1/5
queen9_9	81	2112	10	9	9	36	0.35	2/5	9	9	36	0.35	5/5
									10	**72**	**869**	920.45	5/5
ash331GPIA	662	4185	4	4	9	16	3.52	5/5	4	**7**	**12**	287.08	2/5
1-FullIns_5	282	3247	6	6	40	220	2.29	1/5	6	**31**	**144**	2.10	2/5
2-FullIns_5	852	12,201	7	7	39	244	46.31	1/5	7	39	244	22.4	5/5
3-FullIns_5	2030	33,751	8	8	47	371	275.60	1/5	8	47	371	396.26	2/5

with a traditional restart strategy (denoted as BR) where each restart begins its search with an initial configuration $A = \emptyset, B = V, C = \emptyset, H = (A, E_A)$. The two algorithms were run 5 times on the 13 selected instances and the results are provided in Table 5.6.

From Table 5.6, we observe that IBR significantly outperforms BR. IBR dominates BR by finding improved lower bounds for two instances, smaller k-VCS sizes for 6 instances at the same k and no worse result. This experiment confirms the interest of the adopted perturbation operator.

5.5.3 Effectiveness of backtrack for k-VCS detection

This section evaluates the influence of the backtracking scheme on the performance of the proposed algorithm. For this purpose, we compare it with an IBR variant without the backtracking strategy (named IR). We ran both algorithms 5 times on the 13 selected instances. The experimental results are presented in Table 5.7. Compared with IR, IBR obtains smaller k-VCS for 8 instances at the same given k, 6 better lower bounds, and no worse result. This experiment confirms the value of the backtracking strategy.

5.6 Conclusion

This chapter presented the iterated backtracking removal search for identifying small k-vertex-critical subgraph in a general graph. This method extends the previous removal algorithm by integrating a backtracking strategy and a perturbation procedure. These extensions provide two complementary ways to alleviate the problem of misclassifying vertices caused by the use of a heuristic coloring algorithm.

We assessed the performance of the IBR algorithm on the set of 80 benchmark instances from DIMACS and COLOR competitions and presented comparative results with respect to the state-of-the-art results. The comparisons showed that IBR performs very well by discovering several improved best results (8 smaller size of k-VCS for a given k and 6 new lower bounds for unfixed k) and matching the best-known results for the remaining instances except one case. This study demonstrates the benefit of the backtracking scheme and the perturbation procedure for solving the k-VCS. The idea of this work could be applied to other problems related to irreducibly inconsistent systems.

General Conclusion

Conclusions

This thesis concerns four NP-hard graph coloring problems, graph coloring, equitable coloring, weighted vertex coloring and k-vertex-critical subgraph. These problems are extensively studied in the literature not only for their theoretical intractability, but also for their real world applications in many domains. In this thesis, we adopted heuristic and meta-heuristic methods to find sub-optimal solutions in a reasonable time frame for large graphs.

In chapter 2, we treated the basic GCP model and proposed a reduction-based memetic algorithm to solve it. RMA reduces the current graph by tentatively merging vertices to one vertex if the vertices are always in the same color class of parent solutions. The weighted tabu search algorithm was proposed to improve the quality of the solution, Finally we devised a perturbation strategy to escape local optimum traps. We assessed the performance of the proposed RMA approach and compared our results with the state-of-the-art algorithms on 39 popular DIMACS and COLOR02-04 benchmark instances, which are commonly used to test graph coloring algorithms in the literature. The computational results showed that RMA is competitive in terms of solution quality and run-time efficiency compared with the state-of-the-art algorithms. Specially, RMA consistently attains the best-known solutions with a 100% success rate for all 20 small sized instances. For the set of 19 hard instances, RMA finds 13 best-known results, which dominates all 4 local search algorithms (IGrAL, VSS, partial, PLSCOL) and 4 population based algorithms (HEA, AMA MMT, Evo-Div). For the 3 recent algorithms, MA, QA and HEAD, RMA is slightly worse than them.

In chapter 3, we considered a feasible and infeasible search algorithm (FISA) for solving the equitable coloring problem (ECP). The proposed FISA algorithm is based on two different searches phases namely equity-feasible colorings (first phase) and the equity-infeasible colorings (second phase). The first phase adopts a feasible tabu procedure to examine only the space of equity-feasible colorings to seek a legal (i.e., conflict-free) k-coloring, which is based on the basic tabu search procedure of the BITS algorithm [Lai *et al.*, 2015]. If the first phase fails to find a legal k-coloring in the equity-feasible space, the second phase is invoked to search the enlarged space including equity-infeasible colorings by using an extended fitness function to guide the search process. The perturbation phase is applied as a means of strong diversification to get out of deep loal optimum traps. We conducted experiments on a set of 73 benchmark graphs from the DIMACS and COLOR competitions to assess the interest of the proposed FISA approach. Experimental results showed that the proposed approach obtains significantly better results including especially 9 improved best solutions (new upper bounds).

In chapter 4, we proposed an adaptive infeasible search algorithm (AFISA) for the weighted vertex coloring problem. The proposed algorithm again relies on a mixed search strategy exploring both feasible and infeasible solutions. First, AFISA is the first heuristic method that explores both feasible and infeasible solutions for the WVCP. To prevent the search from going too far away from the feasible boundary, we designed an adaptive penalty-based evaluation function that is used to guide the search for an effective examination of can- didate solutions, by enabling

the search to oscillate between feasible and infeasible regions. To explore a given search zone, we relied on the popular tabu search metaheuristic. We assessed the proposed algorithm on 111 benchmark instances from literatures (one set of 46 instances from the DIMACS and COLOR competitions and two sets of 65 instances from matrix-decomposition problems). We reported especially 5 improved best solutions (new upper bounds). We also presented new results on an additional set of 50 larger instances.

In the last chapter, we studied the k-VCS problem and proposed an iterated backtrack-based removal (IBR) algorithm to solve it. For the k-VCS, the classic removal strategy that reduces current graph by tentatively moving vertices to the set of uncritical vertices is not so effective since the status of some vertices is sometimes irreversibly misclassified. Therefore, we developed a repair mechanism for the misclassified status of vertices. For this purpose, we devised a backtracking mechanism to expand the current subgraph by adding back some vertices. Finally, we devised a perturbation strategy to reconsider some vertices that could have been incor- rectly identified as critical ones. Computational results on 80 popular DIMACS and COLOR02-04 benchmark instances, which are commonly used to test k-VCS algorithms in the literature, show that IBR is very competitive in terms of solution quality and run-time efficiency compared with state-of-the-art algorithms in the literature. Specifically, the proposed algorithm is able to discover improved best solutions for 9 graphs (improves the lower bound for 6 instances, at the same k, IBR obtains a better solution (smaller size of k-VCS) for 8 instances), matches the best results for other 70 instances, and obtains a slightly worse result only in one case.

Perspectives

In this thesis, we consider algorithms and experimental validations for four graph coloring problems. For future work, several directions could be followed.

— Extend to solve other problems. First, our proposed feasible and infeasible search methods are general-purpose, which could be applied to solve a wide family of constrained problem. For example, we adopted this method to the ECP (in the Chapter 3) and the WVCP (in the Chapter 4). It would be reasonable to apply FISA to solve other graph coloring problems, such as minimum sum coloring. Second, our k-VCS problem is also called the MUC (Minimal Unsatisfiable Core) in the SAT problem, or the IIS (irreducible infeasible subset) problem in the CSP, it would be interesting to adjust the IBR algorithm to these problems.

— Improve the performance of the proposed algorithms. First, the penalty term of the extended fitness function of the ECP could be improved by introducing adaptive techniques like [Chen *et al.*, 2016b; Glover and Hao, 2011] to enable a strategic oscillation for dynamically transitioning between feasible and infeasible spaces. Second, the evaluation function of the problem should be able to discriminate solutions of equal quality by taking into account all additional information. Third, the high and robust performance of the proposed algorithms depends critically on a set of good parameters, whose optimal settings are usually instance independent. However, parameter tuning is normally a hard task, especially when a number of sensitive parameters exist. Hence, developing an automatic parameter tuning method based on the characteristics of the current instance to be solved could be a very valuable.

— Improve the algorithm in order to solve still larger instances. The instances tested in this work are based on the conventional DIMACS coloring benchmark graphs. These graphs can be considered as being limited in size with respect to massive graphs obtained from a number of modern applications like complex networks and biological networks. Contrary to DIMACS graphs, these massive graphs are typically very sparse with very low edge density. It would be interesting to investigate the ideas of this work in the context of

coloring massive graphs.

Appendix

ILP formulation of the WVCP

In this section, we describe the 0-1 integer linear programming (ILP) model for the WVCP proposed in [Malaguti *et al.*, 2009], extended with a symmetry breaking constraint. This model is used for the computational experiment presented in Section 5.4.3. Firstly, we define the following decision variables:

— Let $s = \{V_1, V_2, \ldots, V_k\}$ be a candidate solution.
— $x_{vk} \in \{0, 1\}$ is a binary decision variable that is equal to 1 if and only if vertex v is part of set V_k, 0 otherwise for all $v \in V$ and for all $k \in \{1, \ldots, N\}$.
— W_k is a positive decision variable that is equal to the weight of stable V_k, for all $k \in \{1, \ldots, N\}$.

We obtain the following ILP model for the WVCP:

$$f(s) = min \sum_{k=1}^{N} W_k \tag{4}$$

$$\begin{cases} \sum_{k=1}^{N} x_{vk} = 1 & \forall v \in V \\ x_{vk} + x_{uk} \leq 1 & \forall (u, v) \in E, \forall k \in \{1, \ldots, N\} \\ x_{vk} w_v \leq W_k & \forall (v, k) \in V \times \{1, \ldots, N\} \\ W_k \geq W_{k+1} & \forall k \in \{1, \ldots, N-1\} \\ W_k \geq 0 & \forall k \in \{1, \ldots, N\} \\ x_{vk} \in \{0, 1\} & \forall (v, k) \in V \times \{1, \ldots, N\} \end{cases}$$

The objective function (4) is to minimize the sum of the weights of the stables used. The first constraints ensures that each vertex belongs to exactly one set. The second constraints enforces that the same color cannot be assigned to adjacent vertices. The third constraints sets W_k to the weight of the maximum weight vertex in the k-th set. The fourth constraint partially breaks symmetry by enforcing that the stables are ordered by decreasing order of their sizes.

List of Publications

Published/accepted journal papers

1. Wen Sun, Jin-Kao Hao, and Alexandre Caminada. Iterated backtrack removal search for finding *k*-vertex-critical subgraphs. Journal of Heuristics, pages 1-26, 2018.
2. Wen Sun, Jin-Kao Hao, Xiangjing Lai and Qinghua Wu. Adaptive feasible and infeasible tabu search for weighted vertex coloring. Information Sciences, 466: 203-219,2018.

Published/accepted conference papers

1. Wen Sun, Jin-Kao Hao, Xiangjing Lai, Qinghua Wu. On feasible and infeasible search for equitable graph coloring. In Proceedings of the Genetic and Evolutionary Computation Conference, pages 369-376. ACM, 2017.

List of Figures

List of Tables

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Titre : Algorithmes heuristiques pour des problèmes de coloration de graphes

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Mots clés : Optimisation combinatoire, Problèmes de coloration de graphes, Recherche mixte réalisable et irréalisable, Heuristiques et métaheuristiques.

Résumé : Cette thèse concerne quatre problèmes de coloration de graphes NP-difficiles, à savoir le problème de coloration (GCP), le problème de coloration équitable (ECP), le problème de coloration des sommets pondérés et le problème de sous-graphe critique (k-VCS). Ces problèmes sont largement étudiés dans la littérature, non seulement pour leur difficulté théorique, mais aussi pour leurs applications réelles dans de nombreux domaines. Étant donné qu'ils appartiennent à la classe de problèmes NP-difficiles, il est difficile de les résoudre dans le cas général de manière exacte.

Pour cette raison, cette thèse est consacrée au développement d'approches heuristiques pour aborder ces problèmes complexes. Plus précisément, nous développons un algorithme mémétique de réduction (RMA) pour la coloration des graphes, un algorithme de recherche réalisable et irréalisable (FISA) pour la coloration équitable et un réalisable et irréalisable (AFISA) pour le problème de coloration des sommets pondérés et un algorithme de suppression basé sur le retour en arrière (IBR) pour le problème k-VCS. Tous les algorithmes ont été expérimentalement évalués et comparés aux méthodes de l'état de l'art.

Title : Heuristic Algorithms for Graph Coloring Problems

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Keywords : Combinatorial optimization, Graph coloring problems, Feasible and infeasible search strategies, Heuristics and metaheuristics.

Abstract : This thesis concerns four NP-hard graph coloring problems, namely, graph coloring (GCP), equitable coloring (ECP), weighted vertex coloring (WVCP) and k-vertex-critical subgraphs (k-VCS). These problems are extensively studied in the literature not only for their theoretical intractability, but also for their real-world applications in many domains. Given that they belong to the class of NP-hard problems, it is computationally difficult to solve them exactly in the general case.

For this reason, this thesis is devoted to developing effective heuristic approaches to tackle these challenging problems. We develop a reduction memetic algorithm (RMA) for the graph coloring problem, a feasible and infeasible search algorithm (FISA) for the equitable coloring problem, an adaptive feasible and infeasible search algorithm (AFISA) for the weighted vertex coloring problem and an iterated backtrack-based removal (IBR) algorithm for the k-VCS problem. All these algorithms were experimentally evaluated and compared with state-of-the-art methods.