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Sébastien Kerleau

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THÈSE DE DOCTORAT

DE L'UNIVERSITÉ PSL

Préparée à Université Paris Dauphine-PSL

**Graphical and geometrical perspectives on positive
spanning sets with applications to derivative-free
optimization**

Soutenue par

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*“I don’t want to be quoted, and don’t quote me
that I don’t want to be quoted.”*

— WINSTON BURDETT

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Chapter 1

Introduction

The theory of linear programming gained an important exposure with the start of the second world war [56], leading to multiple discoveries such as that of the simplex algorithm [19, 20] and raising numerous mathematical questions. In particular, linear programming motivated researchers to study matrices $\mathbf{A} \in \mathbb{R}^{n \times m}$ for which the following linear feasibility problem

$$\mathbf{Ax} = \mathbf{b}, \quad \mathbf{x} \geq \mathbf{0}_m \tag{1.1}$$

possesses a solution. A first step in that direction was made in a seminal paper by Chandler Davis [21], introducing the important notion of positive spanning sets (PSSs), sets of columns of matrices for which equation (1.1) admits a solution independently of the value of $\mathbf{b} \in \mathbb{R}^n$.

Initially, research on PSSs and positive bases - inclusion-wise minimal positive spanning sets - allowed for the discovery of new results involving the convex hull of sets of vectors [61] or for the simplification of proofs in the field of convex analysis [62]. Nowadays, these sets play an important role in derivative-free optimization (DFO), a field concerned with solving optimization problems where gradient information is unavailable or unreliable [6, 15]. In that context, the directions induced by positive spanning sets provide a structured means of exploring the search space. Using PSSs allows for the identification of descent directions even without access to gradient evaluations, as such sets always contain at least one element that forms an acute angle with any given nonzero vector. In the case of direct-search algorithms, a subclass of DFO methods that relies solely on function evaluations, this property guarantees convergence toward a critical point of the function to be optimized. Moreover, worst-case complexity guarantees of direct-search algorithms depend heavily on the positive spanning sets used throughout the algorithm [77]. The quality of a positive spanning set is typically assessed using the *cosine measure* [75, 40], in that a large cosine measure implies a better coverage of the space and thus more effective search directions for optimization. As a result, derivative-free methods favor the use of

PSSs with high cosine measure while maintaining low cardinality [77, 25]. Algorithms for computing the cosine measure of positive spanning sets are non-polynomial time methods [31, 64]. In the case of positive bases, whose non-constant size illustrates their complex structure [68, 21], the challenge of finding a tight upper bound on their cosine measure was only successfully tackled for bases of size $n + 1$ and $2n$ [57, 65]. Recent research thus focused on computing the cosine measure of classes of positive bases with simpler structures [33].

Davis’s initial characterization of positive bases made use of *Gale diagrams*, an important tool in polyhedral theory which allows for the representation of certain polytopes in lower-dimensional spaces. Such diagrams can be used to characterize positive k -spanning sets (PkSSs), a class of resilient PSSs which remains positively spanning upon losing some elements [50, 79]. To this day however, the literature on PkSSs is sparse and their properties remain relatively unknown.

This manuscript explores the properties of positive spanning sets, positive bases and positive k -spanning sets, both through theoretical analysis and practical applications. It aims at identifying novel, simple structural results which characterize these sets, in order to simplify their use in optimization methods.

1.1 Contributions

The first contribution of this thesis can be found in Chapter 2, where the elementary properties of positive (k-)spanning sets are leveraged to obtain a novel characterization of inclusion-wise minimal positive 2-spanning sets of minimal size in \mathbb{R}^n in Theorem 2.3.2.

Further contributions are found in Chapter 3, which presents an extended version of an article published in the scientific journal *Discrete Applied Mathematics* [17]. The chapter takes interest in *network matrices*, a concept generalizing that of incidence matrix. We provide in Theorem 3.2.1 a characterization of strongly connected digraphs, in that these are directed graphs whose network matrices are positively spanning. Leveraging the relationship between strongly directed graphs and PSSs allows for the discovery of a decomposition result on the latter, given by Theorem 3.3.1. We exploit this result in Theorems 3.4.2, 3.4.3 and 3.4.4 to provide characterizations of positive bases of size $2n - 1$, $2n - 2$ and $n + 2$ in \mathbb{R}^n . In turn, the relationship between directed graphs and positive spanning sets allows us to derive characterizations of minimally strongly connected digraphs of near extreme sizes. Characterizations are provided for graphs on n vertices and m arcs where $m = 2n - 3$, $m = 2n - 4$ and $m = n + 1$ in Corollaries 3.4.1, 3.4.2 and 3.4.3 respectively.

The contributions of Chapter 4 involve a polynomial time algorithm (Al-

gorithm 1) for computing the cosine measure of orthogonally structured positive bases - a concept originally introduced by Hare, Jarry-Bolduc, and Planiden [31]. By applying this algorithm, we derive in Lemma 4.2.1 the cosine measure of the canonical positive basis $\{\mathbf{e}_1, \dots, \mathbf{e}_n, -\mathbf{1}_n\}$, which contains the canonical vectors in \mathbb{R}^n and their negative sum. We also introduce the k -cosine measure (Definition 4.3.1), a tool that allows for the characterization of positive k -spanning sets. We then provide simple methods for building inclusion-wise minimal PkSSs with guarantees on the value of their k -cosine measure - see Theorem 4.3.3 and Corollary 4.3.1. The results associated with this chapter were published in *Linear Algebra and Its Applications* [17].

Our last contribution is found in Chapter 5, where we introduce a derivative-free algorithm of direct-search type which exploits the properties of PkSSs to guarantee convergence in the presence of failed function evaluations (Algorithm 4). The method is endowed with complexity guarantees, that depend on both on the size of the PkSSs used within the algorithm and on their k -cosine measure.

1.2 Outline of the thesis

The remainder of this thesis is divided as follows. State of the art results on positive spanning sets, positive k -spanning sets and positive bases are summarized in Chapter 2 and exploited in Section 2.3.3 to derive new properties on the structure of PkSSs. Chapter 3 discusses a newfound relationship between strongly connected digraphs and positive spanning sets and shows how some key features of the latter can be deduced from those of the former. Next, Chapter 4 takes interest in the cosine measure of positive spanning sets. It demonstrates how this value can be easily computed for sets with specific structures, then shows how to build positive k -spanning sets with satisfying guarantees on the cosine measure of their subsets. Finally, Chapter 5 aims at applying the results of Chapter 4 to derivative-free optimization. It investigates the convergence rate of a newly built, derivative-free algorithm that exploits the resilient properties of positive k -spanning sets, and takes inspiration from articles by Dodangeh, Vicente and Zhang [77, 25].

1.3 Notations

In the remainder of this manuscript, we work in the Euclidean space \mathbb{R}^n with $n \geq 2$, or a linear subspace thereof, denoted by $\mathbb{L} \subset \mathbb{R}^n$. Unless explicitly stated otherwise, the dimension of such a subspace will always be assumed to be at least 1. The set of real matrices with n rows and m columns will be denoted as $\mathbb{R}^{n \times m}$. Those dimensions will always be assumed to be at least 1. Bold lowercase letters (e.g. \mathbf{v}, \mathbf{a}) will be used to designate

vectors and arcs in directed graphs, while bold uppercase letters (e.g. \mathbf{D}) will denote matrices. For a vector $\mathbf{x} \in \mathbb{R}^n$, the coordinate of index $i \leq n$ will be denoted by $[\mathbf{x}]_i \in \mathbb{R}$. In the absence of brackets, any notation of the form \mathbf{x}_i should be understood as denoting a vector. The notations $\mathbf{0}_n$ and $\mathbf{1}_n$ will respectively be used to designate the null vector and the all-ones vector in \mathbb{R}^n , while $\mathbf{I}_n = [\mathbf{e}_1 \ \dots \ \mathbf{e}_n]$ will denote the identity matrix in $\mathbb{R}^{n \times n}$. Given a matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$, its set of columns will be denoted $\text{col}(\mathbf{D})$ while its linear span (*i.e.* the set of linear combinations of its columns) will be denoted by $\text{span}(\mathbf{D})$. The associated nullspace will be denoted by $\text{Null}(\mathbf{D}) = \{\mathbf{x} \in \mathbb{R}^m, \mathbf{D}\mathbf{x} = \mathbf{0}_n\}$. The matrix whose entries are the signs of those of \mathbf{D} will be noted $\text{sgn}(\mathbf{D})$. Calligraphic letters such as \mathcal{D} and \mathcal{S} will be used for finite families of vectors or of indices. For any integers a and b in \mathbb{Z} , we let $\llbracket a, b \rrbracket := \{z : a \leq z \leq b, z \in \mathbb{Z}\}$. Finally, for a digraph $G = (V, A)$ the notations (u, v) and $u - v$ will respectively designate an arc and an oriented path in A going from u to v .

Chapter 2

Positive spanning sets

In this chapter we formally define the concept of positive spanning set, central to the thesis. The notion was introduced in a seminal paper by Chandler Davis [21]. Davis took a particular interest in the study of *frames* - inclusion-wise minimal PSSs, more commonly called positive bases - and characterized their structure through diagrams [21, Theorem 5.3]. The study of positive spanning sets and positive bases later allowed for the discovery or simplification of results in the field of convex analysis [61, 62]. Since the late 1990s, positive spanning sets have played a crucial role in continuous optimization, particularly in derivative-free methods [6, 15], as discussed at length in Chapter 5.

This chapter reviews the main results on positive spanning sets that are relevant for this thesis, following several reference works spanning decades of research on PSSs [63, 68, 64]. Section 2.1 is dedicated to listing the fundamental properties and definitions associated to PSSs. Next, important structural results are presented in Section 2.2, namely Romanowicz's characterization of positive bases through *criticality* [68], as well as Davis and Shephard's works on *Gale diagrams* [21, 71]. These results are simplified using the notion of *structural equivalence* [60], formally introduced in Section 2.2.1. Last, we conclude our analysis of positive spanning sets by taking interest in positive k -spanning sets (PkSSs) in Section 2.3, a particular subclass of PSSs which remain positively spanning upon removing some of their elements. After summarizing the main properties of such sets, we discuss in Section 2.3.2 an important connection between polytope theory, Gale diagrams and PkSSs, based on the works of Marcus and Wotzlaw [48, 50, 79].

2.1 Main definitions and properties

We start this section by formally defining positive spanning sets (PSSs). First introduced in a seminal paper by Chandler Davis [21], PSSs were initially described as families of vectors or, equivalently, as sets of columns of matrices. For both sake of simplicity and consistency of notations, this manuscript shall adopt a slightly different approach and introduce them as matrices.

Definition 2.1.1 (Positive span and positive spanning set) *Let \mathbb{L} be a linear subspace of \mathbb{R}^n and $m \geq 1$. The positive span of a matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$, denoted $\text{pspan}(\mathbf{D})$, is the set*

$$\text{pspan}(\mathbf{D}) := \{\mathbf{D}\mathbf{x}, \mathbf{x} \in \mathbb{R}^m, \mathbf{x} \geq \mathbf{0}_m\}.$$

A positive spanning set (PSS) of \mathbb{L} is a matrix \mathbf{D} such that $\text{pspan}(\mathbf{D}) = \mathbb{L}$. When $\mathbb{L} = \mathbb{R}^n$, the matrix \mathbf{D} will simply be called a positive spanning set.

As a relatively straightforward consequence of Definition 2.1.1, note that a matrix \mathbf{D} can only be a PSS for its linear span.

Example 2.1.1 *The matrix $\mathbf{D} = \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix} \in \mathbb{R}^{2 \times 4}$ is a PSS. Indeed, any vector $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in \mathbb{R}^2$ satisfies*

$$\mathbf{x} = \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} \max(x_1, 0) \\ \max(x_2, 0) \\ \max(-x_1, 0) \\ \max(-x_2, 0) \end{bmatrix}.$$

More generally, a matrix \mathbf{D} is a PSS for $\text{span}(\mathbf{D})$ whenever $\text{span}(\mathbf{D})$ is nonnegatively spanned by \mathbf{D} .

Example 2.1.2 *Let $\mathbf{D} = [\mathbf{d}_1 \ \mathbf{d}_2 \ \mathbf{d}_3] \in \mathbb{R}^{2 \times 3}$ be the matrix represented on Figure 2.1 below. Then \mathbf{D} is a PSS as any vector in \mathbb{R}^2 is a nonnegative linear combination of its columns: for instance, $\mathbf{v} = \mathbf{d}_1 + \mathbf{d}_2$. In the case of Figure 2.2, however, the matrix $\tilde{\mathbf{D}} = [\mathbf{d}'_1 \ \mathbf{d}'_2 \ \mathbf{d}'_3]$ is not positively spanning as \mathbf{v}' cannot be expressed as a nonnegative combination of $\mathbf{d}'_1, \mathbf{d}'_2$ and \mathbf{d}'_3 .*

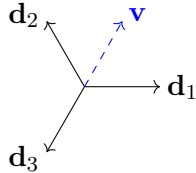


Figure 2.1. A PSS in \mathbb{R}^2 .

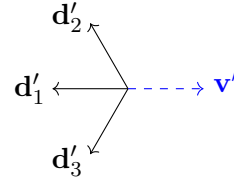


Figure 2.2. Not a PSS of \mathbb{R}^2 .

Numerous characterizations of positive spanning sets can be found in the literature. Proposition 2.1.1 summarizes the most elementary ones [21, Theorem 3.6], [64, Theorem 2.5].

Proposition 2.1.1 *Let $\mathbf{D} \in \mathbb{R}^{n \times m}$. The following statements are equivalent.*

- (i) \mathbf{D} is a PSS for some ℓ -dimensional linear space $\mathbb{L} \subset \mathbb{R}^n$, with $\ell \geq 0$.
- (ii) $\text{pspan}(\mathbf{D}) = \text{span}(\mathbf{D})$.
- (iii) There exists a positive vector $\mathbf{x} \in \mathbb{R}^m$ such that $\mathbf{D}\mathbf{x} = \mathbf{0}_n$.

Statement (iii) of Proposition 2.1.1 justifies the use of the expression *positive spanning set*, as it immediately entails that nonnegatively spanning a linear space is equivalent to positively spanning it. Moreover when the matrix \mathbf{D} has full rank, statement (iii) provides a certificate that \mathbf{D} is a PSS of \mathbb{R}^n . Conversely the next proposition - derived from Farkas's lemma [22] - can be used to obtain a certificate that a given matrix does *not* positively span \mathbb{R}^n .

Proposition 2.1.2 [21, Theorem 3.1] *A matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$ does not positively span \mathbb{R}^n if and only if there exists a vector $\mathbf{y} \in \mathbb{R}^n \setminus \{\mathbf{0}_n\}$ such that $\mathbf{y}^\top \mathbf{D} \geq \mathbf{0}_m^\top$.*

Taking a second glance at Figure 2.2 above and letting $\mathbf{y} = \mathbf{d}'_1$, it can easily be observed that $\mathbf{y}^\top \mathbf{d}'_i \geq 0$, for all $i \leq 3$, providing yet another proof that $\tilde{\mathbf{D}}$ is not positively spanning. Later in this chapter, we shall see that the result stated in Proposition 2.1.2 can be generalized to characterize PSSs of arbitrary linear spaces - see Corollary 2.2.3. Proposition 2.1.2 also bears a close connection with the concept of *cosine measure*, which will be the focus of Chapter 4.

As pointed out in Proposition 2.1.1, the linear span of a PSS must always be equal to its positive span. In fact, positive spanning sets have the property of being *resilient* spanning sets, in the following sense.

Proposition 2.1.3 [21, Theorem 3.7] *Let $\mathbf{D} \in \mathbb{R}^{n \times m}$ be a PSS of its linear span. Any matrix $\mathbf{D}_{\mathbf{d}_i} \in \mathbb{R}^{n \times (m-1)}$ obtained from \mathbf{D} by removing exactly one column satisfies $\text{span}(\mathbf{D}_{\mathbf{d}_i}) = \text{span}(\mathbf{D})$.*

Based on the previous result, it is clear that $\dim(\text{span}(\mathbf{D}))$ is a lower bound on the number of columns of a PSS \mathbf{D} . The next proposition provides a sharper bound.

Proposition 2.1.4 [21, Theorem 3.8] *Let $\mathbb{L} \subset \mathbb{R}^n$ be ℓ -dimensional. The smallest possible size for a PSS $\mathbf{D} \in \mathbb{R}^{n \times m}$ of \mathbb{L} is given by $m = \ell + 1$.*

Just as there is no upper bound on the size of a spanning set, one easily builds PSSs of \mathbb{L} with an arbitrarily large number of columns. A natural next step shall be to explore the largest possible size for *positively independent* matrices - a notion that generalizes that of linear independence.

Definition 2.1.2 (Positive independence) A matrix $\mathbf{D} = [\mathbf{d}_1 \ \cdots \ \mathbf{d}_m]$ is positively independent when $\mathbf{d}_i \notin \text{pspan}([\mathbf{d}_1 \ \cdots \ \mathbf{d}_{i-1} \ \mathbf{d}_{i+1} \ \cdots \ \mathbf{d}_m])$, for all $i \leq m$.

Alternatively, a positively independent matrix can be defined as one such that all submatrices $\tilde{\mathbf{D}}$ obtained by removing exactly one column from \mathbf{D} satisfy $\text{pspan}(\tilde{\mathbf{D}}) \neq \text{pspan}(\mathbf{D})$ [64, Theorem 3.2].

It is well established that the maximal size for a linearly independent set in \mathbb{R}^n is given by n [9]. In the case of positive independence however, a finite bound can only be obtained in dimension 2 or less.

Proposition 2.1.5 [64, Theorem 3.4] Let $n > r \geq 2$ and let $\{\mathbf{d}_1, \dots, \mathbf{d}_m\}$ be the set of vertices of a polytope in \mathbb{R}^r . Then $\mathbf{D} = \begin{bmatrix} \mathbf{d}_1 & \cdots & \mathbf{d}_m \\ \mathbf{1}_{n-r} & \cdots & \mathbf{1}_{n-r} \end{bmatrix}$ is positively independent in \mathbb{R}^n .

The connection between polytope theory and positive spanning sets will be studied at length in Section 2.2.3. For now, we simply note that Proposition 2.1.5 implies that the number of columns of a positively independent matrix in \mathbb{R}^n can be arbitrarily large, whenever $n \geq 3$. In the case of positively independent PSSs however, we shall see that an upper bound can be obtained.

Definition 2.1.3 (Positive basis) Let $\mathbb{L} \subset \mathbb{R}^n$ be ℓ -dimensional. A positive basis of \mathbb{L} of size $\ell + m$, denoted $\mathbf{D}_{\mathbb{L},m}$, is a positively independent PSS of \mathbb{L} with $\ell + m$ columns. When $\mathbb{L} = \mathbb{R}^n$, such a matrix will be denoted by $\mathbf{D}_{n,m}$.

In the case $\mathbb{L} = \mathbb{R}^n$, we simply say that $\mathbf{D}_{n,m}$ is a positive basis (of size $n + m$). Just as linear bases can be defined as inclusion-wise minimal spanning sets, positive bases can be characterized as inclusion-wise minimal positive spanning sets.

Proposition 2.1.6 [63] A matrix $\mathbf{D}_{\mathbb{L},m} \in \mathbb{R}^{n \times (\ell+m)}$ is a positive basis of \mathbb{L} if and only if $\text{pspan}(\mathbf{D}_{\mathbb{L},m}) = \mathbb{L}$ and no proper submatrix $\tilde{\mathbf{D}}$ of $\mathbf{D}_{\mathbb{L},m}$ satisfies $\text{pspan}(\tilde{\mathbf{D}}) = \mathbb{L}$.

The structure of positive bases in \mathbb{R}^n has been the topic of several articles. For now, we simply provide the most fundamental properties in relation with their cardinality. The next result, by Davis [21, Theorem 6.7], was initially derived from a theorem of distance geometry by Blumenthal [12, Theorem 120.2].

Theorem 2.1.1 Let $\mathbf{D}_{\mathbb{L},m} \in \mathbb{R}^{n \times (\ell+m)}$ be a positive basis for $\mathbb{L} \subset \mathbb{R}^n$, with $\dim(\mathbb{L}) = \ell$. Then $1 \leq m \leq \ell$.

The structure of positive bases of extremal sizes shall be described in details in Section 2.2.

Definition 2.1.4 (Maximal and minimal basis) *A positive basis $\mathbf{D}_{\mathbb{L},m}$ of the ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$ is called maximal whenever $m = \ell$. It is called minimal, noted $\mathbf{D}_{\mathbb{L}}$, whenever $m = 1$.*

Note that although the lower bound in Theorem 2.1.1 is trivially obtained, such is not the case of the upper bound. For the sake of completeness, we provide a short proof that the size of a positive basis of \mathbb{L} does not exceed $2\dim(\mathbb{L})$, inspired by Audet [3] - see also [50, page 50] - and based on the following result of linear programming.

Lemma 2.1.1 [53, Theorem 4.2.3] *Let $\mathbf{D} \in \mathbb{R}^{n \times m}$, $\mathbf{b} \in \mathbb{R}^n$ and $\mathbf{c} \in \mathbb{R}^m$. The linear program*

$$\text{maximize } \mathbf{c}^\top \mathbf{x} \quad \text{subject to } \mathbf{D}\mathbf{x} = \mathbf{b} \text{ and } \mathbf{x} \geq \mathbf{0}_m \quad (2.1)$$

possesses an optimal solution if and only if it possesses a basic feasible solution that is optimal. Basic feasible solutions denote feasible points with at most n nonzero entries associated with linearly independent columns of \mathbf{D} .

Lemma 2.1.1 implies that any vector contained in the positive span of an arbitrary matrix \mathbf{D} must also be contained in the positive span of a non-singular submatrix of \mathbf{D} . The partial proof of Theorem 2.1.1 then goes as follows.

Proof of the upper bound in Theorem 2.1.1. Let $\mathbf{D}_{\mathbb{L},m} \in \mathbb{R}^{n \times (\ell+m)}$ be a positive basis of \mathbb{L} and let $\mathbf{B} \in \mathbb{R}^{n \times \ell}$ be a submatrix of $\mathbf{D}_{\mathbb{L},m}$ satisfying $\text{span}(\mathbf{B}) = \mathbb{L}$. The negative sum $\mathbf{s}_{\mathbf{D}}$ of all columns of $\mathbf{D}_{\mathbb{L},m}$ is contained in $\mathbb{L} = \text{pspan}(\mathbf{D}_{\mathbb{L},m})$. By Lemma 2.1.1, there exists a submatrix $\tilde{\mathbf{D}} \in \mathbb{R}^{n \times \tilde{m}}$ of $\mathbf{D}_{\mathbb{L},m}$ satisfying $\mathbf{s}_{\mathbf{D}} \in \text{pspan}(\tilde{\mathbf{D}})$ and $\tilde{m} \leq \ell$. Let \mathbf{M} be a submatrix of $\mathbf{D}_{\mathbb{L},m}$ satisfying $\text{col}(\mathbf{M}) = \text{col}(\mathbf{B}) \cup \text{col}(\tilde{\mathbf{D}})$. As $\mathbf{0}_n \in \text{pspan}(\mathbf{M})$, by Proposition 2.1.1 \mathbf{M} must be a PSS of $\text{span}(\mathbf{M}) = \mathbb{L}$. Thus $\mathbf{M} = \mathbf{D}_{\mathbb{L},m}$ and so $\ell + m = |\text{col}(\mathbf{B}) \cup \text{col}(\tilde{\mathbf{D}})| \leq 2\ell$. \square

We conclude this section with an elegant procedure to build positive bases of arbitrary sizes.

Proposition 2.1.7 [64, Corollary 5.5] *Let $\mathbf{B} = [\mathbf{b}_1 \ \dots \ \mathbf{b}_\ell] \in \mathbb{R}^{n \times \ell}$ be a linear basis of the ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$, consider a partition of $\llbracket 1, \ell \rrbracket$ into $m \leq \ell$ distinct sets \mathcal{S}_i and for all $i \leq m$, let $\mathbf{d}_i = -\sum_{j \in \mathcal{S}_i} \mathbf{b}_j$. The matrix*

$\mathbf{D}_{\mathbb{L},m} = [\mathbf{B} \ \mathbf{d}_1 \ \dots \ \mathbf{d}_m] \in \mathbb{R}^{n \times (\ell+m)}$ *is a positive basis of \mathbb{L} .*

Note that the procedure described in Proposition 2.1.7 does *not* characterize all positive bases: counter examples are provided in Chapter 3.

Example 2.1.3 $\mathbf{D}_{3,2} = \begin{bmatrix} 1 & 5 & 2 & -6 & -2 \\ 4 & 6 & 5 & -10 & -5 \\ 7 & 9 & 8 & -16 & -8 \end{bmatrix}$ and $\tilde{\mathbf{D}}_{3,2} = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -1 \end{bmatrix}$
are positive bases associated to the partition $\llbracket 1, 3 \rrbracket = \{1, 2\} \cup \{3\}$.

Although the fact that matrix $\mathbf{D}_{3,2}$ from Example 2.1.3 is a positive basis should be clear at first glance, this property can initially seem harder to spot in the case of matrix $\tilde{\mathbf{D}}_{3,2}$. The notion of *structural equivalence*, described in the next section, is a handy tool to make positive spanning sets more noticeable.

2.2 Structural results

In this section, we present a structural perspective on the positive spanning set property. Section 2.2.1 describes an equivalence relation between matrices that characterizes certain transformations preserving the PSS nature of a matrix. Section 2.2.2 focuses on the notion of criticality, which is instrumental to the characterization of positive bases. Section 2.2.3 describes an alternate characterization of positive spanning sets and positive bases through the use of Gale diagrams.

2.2.1 Structural equivalence

We have defined positive spanning sets and positive bases as matrices, while the positive spanning property in its core applies to a set of vectors. As a result, we can identify certain matrix operations that preserve the positive spanning property. For instance, any permutation of the columns of a PSS yields a matrix that is also a PSS and positively spans the same linear space. More broadly, the positive spanning property is preserved by structural equivalence, in the sense of Definition 2.2.1.

Definition 2.2.1 (Structural equivalence) *Two matrices \mathbf{D} and $\tilde{\mathbf{D}}$ in $\mathbb{R}^{n \times m}$ are structurally equivalent if there exists a non-singular matrix $\mathbf{B} \in \mathbb{R}^{n \times n}$, a permutation matrix $\mathbf{P} \in \mathbb{R}^{m \times m}$ and a diagonal matrix $\mathbf{\Delta} \in \mathbb{R}^{m \times m}$ with positive diagonal entries such that*

$$\tilde{\mathbf{D}} = \mathbf{B}^{-1}\mathbf{D}\mathbf{P}\mathbf{\Delta}.$$

We then write $\mathbf{D} \equiv \tilde{\mathbf{D}}$.

Clearly the structural equivalence is an equivalence relation. An example of structurally equivalent matrices is provided below.

Example 2.2.1 *The two matrices $\mathbf{D}_{3,2}$ and $\tilde{\mathbf{D}}_{3,2}$ defined in Example 2.1.3 are structurally equivalent as $\tilde{\mathbf{D}}_{3,2} = \mathbf{B}^{-1}\mathbf{D}_{3,2}$, where $\mathbf{B} = \begin{bmatrix} 1 & 5 & 2 \\ 4 & 6 & 5 \\ 7 & 9 & 8 \end{bmatrix}$.*

Alternatively, we now consider the two matrices

$$\mathbf{D}'_{3,2} = \begin{bmatrix} 1 & 2 & 5 & -6 & -4 \\ 4 & 5 & 6 & -10 & -10 \\ 7 & 8 & 9 & -16 & -16 \end{bmatrix} \quad \text{and} \quad \tilde{\mathbf{D}}'_{3,2} = \begin{bmatrix} 1 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 & 0 \end{bmatrix}.$$

We have $\tilde{\mathbf{D}}'_{3,2} \equiv \mathbf{D}'_{3,2}$ since

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 & 0 \end{bmatrix}}_{\tilde{\mathbf{D}}'_{3,2}} = \underbrace{\begin{bmatrix} \frac{1}{2} & -\frac{11}{3} & \frac{13}{6} \\ \frac{1}{2} & -1 & \frac{1}{2} \\ -1 & \frac{13}{3} & -\frac{7}{3} \end{bmatrix}}_{\mathbf{B}^{-1}} \underbrace{\begin{bmatrix} 1 & 2 & 5 & -6 & -4 \\ 4 & 5 & 6 & -10 & -10 \\ 7 & 8 & 9 & -16 & -16 \end{bmatrix}}_{\mathbf{D}'_{3,2}} \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & \frac{1}{2} & 0 \end{bmatrix}}_{\mathbf{P}\Delta}.$$

The expression *structural equivalence* takes its origins in a research article from 2003 [60, Definition 2.3]. The following proposition is primarily a restatement of a result from a more recent work [64, Corollary 4.7].

Proposition 2.2.1 *Let $\mathbf{D} \in \mathbb{R}^{n \times m}$ be a PSS for $\mathbb{L} \subset \mathbb{R}^n$. Any matrix $\tilde{\mathbf{D}} \equiv \mathbf{D}$ is a PSS for some linear space $\tilde{\mathbb{L}}$ such that $\dim(\tilde{\mathbb{L}}) = \dim(\mathbb{L})$. Moreover $\tilde{\mathbf{D}}$ is a positive basis for $\tilde{\mathbb{L}}$ if and only if \mathbf{D} is a positive basis for \mathbb{L} .*

As a first and immediate corollary of Proposition 2.2.1, let us now describe the structure of minimal positive bases in simple terms.

Corollary 2.2.1 [21, Theorem 3.8] *Let $\mathbf{D}_{\mathbb{L}} \in \mathbb{R}^{n \times (\ell+1)}$ be a minimal positive basis of the ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$. Then*

$$\mathbf{D}_{\mathbb{L}} \equiv \begin{bmatrix} \mathbf{I}_{\ell} & -\mathbf{1}_{\ell} \\ \mathbf{0}_{n-\ell, \ell} & \mathbf{0}_{n-\ell} \end{bmatrix}.$$

In the case of maximal positive bases, although far from being trivial to obtain, the following result can be derived using tools presented in sections 2.2.2 and 2.2.3. While Davis does not state this result explicitly, it can also be deduced from his work [21, Theorem 6.7].

Proposition 2.2.2 [68, End of section 2] *Let $\mathbf{D}_{\mathbb{L}, \ell} \in \mathbb{R}^{n \times 2\ell}$ be a maximal positive basis of the ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$. Then*

$$\mathbf{D}_{\mathbb{L}, \ell} \equiv \begin{bmatrix} \mathbf{I}_{\ell} & -\mathbf{I}_{\ell} \\ \mathbf{0}_{n-\ell, \ell} & \mathbf{0}_{n-\ell} \end{bmatrix}.$$

More generally, the combination of Propositions 2.1.1 and 2.2.1 yields the following characterization of positive spanning sets.

Corollary 2.2.2 *Let $\mathbf{D} \in \mathbb{R}^{n \times (\ell+m)}$ satisfy $\text{span}(\mathbf{D}) = \mathbb{L}$, where $\mathbb{L} \subset \mathbb{R}^n$ is ℓ -dimensional. Then \mathbf{D} is a PSS of \mathbb{L} if and only if there exist m vectors $\mathbf{d}_1, \dots, \mathbf{d}_m$ in \mathbb{R}^ℓ such that*

$$\mathbf{D} \equiv \begin{bmatrix} \mathbf{I}_\ell & \mathbf{d}_1 & \cdots & \mathbf{d}_m \\ \mathbf{0}_{n-\ell, \ell} & \mathbf{0}_{n-\ell} & \cdots & \mathbf{0}_{n-\ell} \end{bmatrix} \quad \text{and} \quad \sum_{i=1}^m \mathbf{d}_i = -\mathbf{1}_\ell \quad (2.2)$$

2.2.2 Criticality and decomposition of positive bases

An important milestone in the study of positive spanning set was reached in 1987 with the publication of a research article by Zbigniew Romanowicz [68] introducing the concept of *criticality*, from which was derived a characterization of positive bases of intermediate size. In short, any positive basis of a finite-dimensional linear space \mathbb{L} can be expressed as the union of minimal bases to which affine transformations are applied. The main results leading to this decomposition are detailed thereafter.

Definition 2.2.2 (Critical set, critical vector) *A set $\mathcal{C} \subset \mathbb{L}$ is critical for the positive basis $\mathbf{D}_{\mathbb{L},m}$ of \mathbb{L} whenever no matrix $\tilde{\mathbf{D}}$ obtained by replacing an arbitrary column of $\mathbf{D}_{\mathbb{L},m}$ with an arbitrary element of \mathcal{C} satisfies $\text{pspan}(\tilde{\mathbf{D}}) = \mathbb{L}$. The elements of \mathcal{C} are called critical vectors for $\mathbf{D}_{\mathbb{L},m}$.*

The notion of criticality is only meaningful with respect to a positive basis: in the case of a non-minimal PSS \mathbf{D} , it should be clear that \mathbf{D} does not possess any critical vector.

Example 2.2.2 *The set $\mathcal{C} = \left\{ \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \end{bmatrix} \right\}$ is critical for $\mathbf{D}_2 = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix}$ as none of the six matrices $\begin{bmatrix} 1 & 0 & -1 \\ 1 & 1 & -1 \end{bmatrix}, \begin{bmatrix} -1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix}, \dots, \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$ obtained by replacing an arbitrary column of \mathbf{D}_2 with an arbitrary element of \mathcal{C} is a PSS. However \mathcal{C} is not critical for $\mathbf{D}_{2,2} = \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix}$ as it contains the third column of $\mathbf{D}_{2,2}$.*

Henceforth, we shall denote by $\mathcal{C}(\mathbf{D}_{\mathbb{L},m})$ the set of all critical vectors of the positive basis $\mathbf{D}_{\mathbb{L},m}$. The following proposition is a characterization of this set [68, Equation 7].

Proposition 2.2.3 *Let $\mathbf{D}_{\mathbb{L},m}$ be a positive basis of \mathbb{L} and for $i \leq m + \ell$, let $\mathbf{D}_{\mathbf{d}_i}$ be obtained from $\mathbf{D}_{\mathbb{L},m}$ by removing the columns of index i . Then*

$$\mathcal{C}(\mathbf{D}_{\mathbb{L},m}) = - \left(\mathbb{L} \setminus \left\{ \bigcup_{i \leq m+\ell} \text{int}(\text{pspan}(\mathbf{D}_{\mathbf{d}_i})) \right\} \right). \quad (2.3)$$

The notation $\text{int}(\text{pspan}(\mathbf{D}_{\mathbf{d}_i}))$ designates the interior set of $\text{pspan}(\mathbf{D}_{\mathbf{d}_i})$. Owing to the structure of $\mathbf{D}_{\mathbf{d}_i}$, this interior set is simply the set of *positive* linear combinations of the columns of $\mathbf{D}_{\mathbf{d}_i}$.

Example 2.2.3 Consider the positive basis $\mathbf{D}_2 = [\mathbf{d}_1 \ \mathbf{d}_2 \ \mathbf{d}_3]$, whose columns are represented in Figure 2.3. The set $\text{int}(\text{pspan}(\mathbf{D}_{\mathbf{d}_1}))$ is drawn in Figure 2.4 - note that it does not contain any of the two vectors \mathbf{d}_2 and \mathbf{d}_3 . Similarly, the set $\mathcal{S} = \bigcup_{i \leq 3} \text{int}(\text{pspan}(\mathbf{D}_{\mathbf{d}_i}))$ is represented in Figure 2.5, while critical vectors of \mathbf{D}_2 are shown in Figure 2.6. More precisely, $\mathcal{C}(\mathbf{D}_2) = -(\mathbb{R}^2 \setminus \mathcal{S})$ is the set of all nonnegative multiples of any of the three vectors given in Figure 2.6.

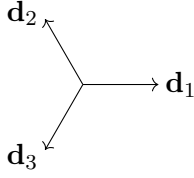


Figure 2.3

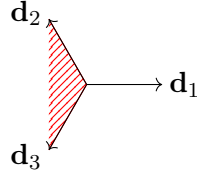


Figure 2.4

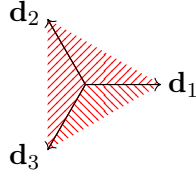


Figure 2.5

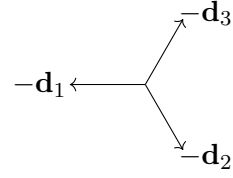


Figure 2.6

As illustrated by Example 2.2.3, in the case of minimal positive bases $\mathbf{D}_{\mathbb{L}}$, the characterization of $\mathcal{C}(\mathbf{D}_{\mathbb{L}})$ given by Equation (2.3) can be simplified. An even heavier simplification occurs for maximal positive bases.

Proposition 2.2.4 [68, Equation (8)] Let $\mathbf{D}_{\mathbb{L}} \in \mathbb{R}^{n \times (\ell+1)}$ be a minimal positive basis of the ℓ -dimensional linear space $\mathbb{L} \subset \mathbb{R}^n$. Whenever $1 \leq i < j \leq \ell + 1$, denote by $\mathbf{D}_{\mathbf{d}_i, \mathbf{d}_j}$ the matrix obtained from $\mathbf{D}_{\mathbb{L}}$ by removing its i^{th} and j^{th} column. Then $\mathcal{C}(\mathbf{D}_{\mathbb{L}}) = -\bigcup_{i < j} \text{pspan}(\mathbf{D}_{\mathbf{d}_i, \mathbf{d}_j})$.

Moreover $\mathcal{C}(\mathbf{D}_{\mathbb{L}, \ell}) = \{\mathbf{0}_n\}$, for each maximal positive basis $\mathbf{D}_{\mathbb{L}, \ell} \in \mathbb{R}^{n \times 2\ell}$ of \mathbb{L} .

From the definition and properties of critical vectors that precede, a complete characterization of positive bases can be derived: the next theorem shows how such PSSs are structurally equivalent to matrices obtained by stacking together altered minimal positive bases. It can be seen as an improved version of a decomposition result for positive bases by Reay [63, Lemma 6].

Theorem 2.2.1 [68, Theorem 1] A matrix $\mathbf{D}_{\mathbb{L}, m} \in \mathbb{R}^{n \times (\ell+m)}$ with $\text{span}(\mathbf{D}_{\mathbb{L}, m}) \subset \mathbb{L}$ is a positive basis of the ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$ if and only if there exist linear spaces $\mathbb{L}_1, \dots, \mathbb{L}_m$ and positive bases of minimal size $\mathbf{D}_{\mathbb{L}_1}, \dots, \mathbf{D}_{\mathbb{L}_m}$ associated to those spaces, such that

$$\mathbf{D}_{\mathbb{L}, m} \equiv [\mathbf{D}_{\mathbb{L}_1} \ \mathbf{D}_{\mathbb{L}_2} + \mathbf{c}_1 \ \dots \ \mathbf{D}_{\mathbb{L}_m} + \mathbf{c}_{m-1}] \quad (2.4)$$

with $\mathbb{L}_1 + \dots + \mathbb{L}_m = \mathbb{L}$, with $\mathbb{L}_i \cap \mathbb{L}_j = \{\mathbf{0}_n\}$ whenever $i \neq j$ and where \mathbf{c}_j denotes a critical vector of the positive basis $[\mathbf{D}_{\mathbb{L}_1} \quad \mathbf{D}_{\mathbb{L}_2} + \mathbf{c}_1 \quad \dots \quad \mathbf{D}_{\mathbb{L}_j} + \mathbf{c}_{j-1}]$ of the linear space $\mathbb{L}_1 + \dots + \mathbb{L}_j$.

A few remarks are to be made, regarding Theorem 2.2.1. First, note that the structural equivalence given in (2.4) only involves a permutation matrix, as the non-singular matrix \mathbf{B} and the diagonal matrix Δ can be assumed to be identity matrices. Moreover, in the case where $m = 1$, note that Theorem 2.2.1 yields the trivial decomposition $\mathbf{D}_{\mathbb{L}} = \mathbf{D}_{\mathbb{L}}$. Last and for the sake of clarity, note that the critical vector \mathbf{c}_1 is defined with respect to the positive basis $\mathbf{D}_{\mathbb{L}_1}$ and that the expression $\mathbf{D}_{\mathbb{L}_j} + \mathbf{c}_{j-1}$ should be understood as the Minkowski addition [44] of the two sets $\text{col}(\mathbf{D}_{\mathbb{L}_j})$ and $\{\mathbf{c}_{j-1}\}$.

Example 2.2.4 *The positive basis*

$$\mathbf{D}_{5,3} = [\mathbf{I}_5 \quad -(\mathbf{e}_1 + \mathbf{e}_2) \quad -(\mathbf{e}_3 + \mathbf{e}_4) \quad -(\mathbf{e}_2 + \mathbf{e}_5)]$$

can be decomposed as:

$$\mathbf{D}_{5,3} \equiv \underbrace{\begin{bmatrix} 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix}}_{\mathbf{D}_{\mathbb{L}_1}} \underbrace{\quad}_{\mathbf{D}_{\mathbb{L}_2} + \mathbf{c}_1} \underbrace{\quad}_{\mathbf{D}_{\mathbb{L}_3} + \mathbf{c}_2}$$

where $\mathbb{L}_1 = \text{span}([\mathbf{e}_1 \quad \mathbf{e}_2])$, $\mathbb{L}_2 = \text{span}([\mathbf{e}_3 \quad \mathbf{e}_4])$, $\mathbb{L}_3 = \text{span}(\frac{1}{2}\mathbf{e}_2 + \mathbf{e}_5)$, where $\mathbf{D}_{\mathbb{L}_2} = [\mathbf{e}_3 \quad \mathbf{e}_4 \quad -(\mathbf{e}_3 + \mathbf{e}_4)]$, $\mathbf{D}_{\mathbb{L}_3} = [\frac{1}{2}\mathbf{e}_2 + \mathbf{e}_5 \quad -(\frac{1}{2}\mathbf{e}_2 + \mathbf{e}_5)]$, where $\mathbf{c}_1 = \mathbf{0}_5$ and where $\mathbf{c}_2 = -\frac{1}{2}\mathbf{e}_2$ is critical for $[\mathbf{D}_{\mathbb{L}_1} \quad \mathbf{D}_{\mathbb{L}_2} + \mathbf{c}_1]$.

As highlighted by its original author, we mention that Theorem 2.2.1 provides an immediate proof to not only Theorem 2.1.1 - the maximal achievable size for \mathbf{D} is reached when $m = \ell$, that is when each subspace \mathbb{L}_i is uni-dimensional - but also to the structural result given in Proposition 2.2.2 - when $m = \ell$, each critical vector \mathbf{c}_j is zero while each positive basis $\mathbf{D}_{\mathbb{L}_j}$ consists of two vectors, each being a negative multiple of the other. For bases of intermediate size however, the decomposition (2.4) might prove difficult to determine owing to the potential presence of non trivial critical vectors. The case when each critical vector in the decomposition (2.4) of a positive basis $\mathbf{D}_{\mathbb{L},m}$ is $\mathbf{0}_n$ has been the subject of a recent work [33] whose details are discussed in Chapter 4.

2.2.3 Gale diagrams and positive bases

The first characterization of positive bases due to Davis [21] leveraged the concept of \oplus -canonical matrix. In the next definition, the notation \mathbb{R}_+^n designates the orthant $\{\mathbf{x} \in \mathbb{R}^n, \forall i, [\mathbf{x}]_i \geq 0\}$.

Definition 2.2.3 (\oplus -canonical matrix) *A positively independent matrix \mathbf{M} such that \mathbf{M}^\top is also positively independent and that some linear space $\mathbb{L} \subset \mathbb{R}^n$ satisfies $\mathbb{L} \cap \mathbb{R}_+^n = \text{pspan}(\mathbf{M})$ is called a \oplus -canonical matrix.*

For a trivial example of a \oplus -canonical matrix, one can think of the identity matrix $\mathbf{M} = \mathbf{I}_n$. The following theorem is a reformulation of Davis's characterization of positive bases.

Theorem 2.2.2 [21, Theorem 5.3] *A matrix $\mathbf{D} \in \mathbb{R}^{n \times (\ell+m)}$ is a positive basis for the ℓ -dimensional space $\text{span}(\mathbf{D})$ if and only if there exists $\mathbf{X} \in \mathbb{R}^{m \times (\ell+m)}$ such that $\text{col}(\mathbf{X}^\top)$ is a linear basis of $\text{Null}(\mathbf{D})$ satisfies $\mathbf{X} \equiv [\mathbf{M} \ \mathbf{M} \ \mathbf{N}]$, where \mathbf{M} is \oplus -canonical and $\text{col}(\mathbf{N}) \subset \text{pspan}(\mathbf{M}) \setminus \{\mathbf{0}\}$.*

We call the matrix \mathbf{X} a *diagram* for \mathbf{D} . Note that just as for Theorem 2.2.1, the structural equivalence in Theorem 2.2.2 only involves a permutation matrix. It should be highlighted that the matrix \mathbf{N} could be empty: in fact, when determining the size of maximal positive bases of \mathbb{R}^n , Davis showed how such PSSs were exclusively associated to diagrams in which \mathbf{M} is diagonal and \mathbf{N} is empty [21, Theorem 6.7].

Example 2.2.5 *The diagram $\mathbf{X}_1 = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 \end{bmatrix}$ attests that $\mathbf{D}_{3,2} =$*

$\begin{bmatrix} 1 & 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 1 & -1 \end{bmatrix}$ is a positive basis of \mathbb{R}^3 , as $\text{span}(\mathbf{X}_1^\top) = \text{Null}(\mathbf{D}_{3,2})$.

Similarly, the matrix $\mathbf{X}_2 = \begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \end{bmatrix}$ satisfying $\mathbf{X}_2 \equiv \mathbf{X}_1$ is a dia-

gram for $\tilde{\mathbf{D}}_{3,2} = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 & -1 \end{bmatrix}$, as $\text{span}(\mathbf{X}_2^\top) = \text{Null}(\tilde{\mathbf{D}}_{3,2})$.

Although not explicitly identified as such in Davis's seminal article, the diagrams used in Theorem 2.2.2 to characterize positive bases are examples of a key concept in polytope theory and affine geometry, namely *Gale diagrams* [30, Section 5.4]. We detail thereafter some important results related to this concept, reformulated to fit the chosen notations of this manuscript [71].

Definition 2.2.4 (Gale diagram) *Let $\mathbf{D} = [\mathbf{d}_1 \ \dots \ \mathbf{d}_{\ell+m}] \in \mathbb{R}^{n \times (\ell+m)}$ satisfy $\text{rank}(\mathbf{D}) = \ell$. A matrix $\mathbf{X}_\mathbf{D} \in \mathbb{R}^{m \times (\ell+m)}$ whose set of rows $\text{col}(\mathbf{X}_\mathbf{D}^\top)$ is a linear basis of $\text{Null}(\mathbf{D})$ is a Gale diagram of \mathbf{D} . We note $\mathbf{X}_\mathbf{D} = [\tilde{\mathbf{d}}_1 \ \dots \ \tilde{\mathbf{d}}_{\ell+m}]$.*

Just as there exist infinitely many linear bases of $\text{Null}(\mathbf{D})$, a matrix \mathbf{D} admits infinitely many Gale diagrams. Unless explicitly stated otherwise, the choice of the diagram $\mathbf{X}_{\mathbf{D}}$ will have no impact on the propositions and theorems listed in this section.

Theorem 2.2.2 showed how Gale diagrams can be used to characterize positive bases. More generally, they also provide a clear description of PSSs.

Proposition 2.2.5 [71, Corollary of theorem 1] *The matrix $\mathbf{D} \in \mathbb{R}^{n \times (\ell+m)}$ is a PSS of its linear span if and only if $\mathbf{0}_m \notin \text{conv}(\mathbf{X}_{\mathbf{D}})$, where $\mathbf{X}_{\mathbf{D}}$ is a Gale diagram of \mathbf{D} .*

A few notes on Proposition 2.2.5: first, the statement $\mathbf{0}_m \notin \text{conv}(\mathbf{X}_{\mathbf{D}})$ is equivalent to saying that the only nonnegative linear combination of columns of $\mathbf{X}_{\mathbf{D}}$ adding up to zero is the trivial combination. Second, using the well known property that the orthogonal complement of a matrix's null space is equal to its row space [72], the result of Proposition 2.2.5 can be used to improve that of Proposition 2.1.2. Indeed, saying that $\mathbf{0}_n$ is in $\text{conv}(\mathbf{X}_{\mathbf{D}})$ is equivalent to claiming the existence of a nonzero, nonnegative vector in $\text{Null}(\mathbf{D})^\perp = \text{span}(\mathbf{D}^\top)$. We obtain the following characterization.

Corollary 2.2.3 *A matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$ is not a PSS of $\text{span}(\mathbf{D})$ if and only if there exists a vector $\mathbf{y} \in \mathbb{R}^n \setminus \{\mathbf{0}_n\}$ satisfying $\mathbf{y}^\top \mathbf{D} \geq \mathbf{0}_m^\top$ and $\mathbf{y}^\top \mathbf{D} \neq \mathbf{0}_m^\top$.*

The following example highlights the connection between Proposition 2.2.5 and Corollary 2.2.3.

Example 2.2.6 *The matrix $\mathbf{D} = \begin{bmatrix} 0 & 1 & 1 & 0 & -1 \\ 1 & 0 & 1 & -1 & -2 \\ 1 & 1 & 0 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 \end{bmatrix}$, associated to the*

diagram $\mathbf{X}_{\mathbf{D}} = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ 0 & -1 & 2 & 0 & 1 \end{bmatrix}$ has a linear span given by $\text{span}(\mathbf{D}) = \left\{ \mathbf{x} \in \mathbb{R}^4, [\mathbf{x}]_4 = \frac{[\mathbf{x}]_1 + [\mathbf{x}]_2 + [\mathbf{x}]_3}{2} \right\}$. Letting $\mathbf{v}^\top = [0 \ \frac{1}{2} \ 0 \ 0 \ \frac{1}{2}]$, we find that $\mathbf{X}_{\mathbf{D}} \mathbf{v} = \mathbf{0}_2$, that is $\mathbf{0}_2 \in \text{conv}(\mathbf{X}_{\mathbf{D}})$ and so \mathbf{D} is not a PSS of its linear span, as per Proposition 2.2.5.

Alternatively, as $\text{Null}(\mathbf{X}_{\mathbf{D}}) = \text{span}(\mathbf{X}_{\mathbf{D}}^\top)^\perp = \text{Null}(\mathbf{D})^\perp = \text{span}(\mathbf{D}^\top)$, we observe that $\mathbf{v} \in \text{span}(\mathbf{D}^\top)$ thus there exists a vector $\mathbf{y} \in \mathbb{R}^4 \setminus \{\mathbf{0}_4\}$ satisfying $\mathbf{y}^\top \mathbf{D} = \mathbf{v}^\top \geq \mathbf{0}_5^\top$. By Corollary 2.2.3, \mathbf{D} is not a PSS of its linear span.

Building on Proposition 2.2.5, the following characterization of positive bases can be obtained. Note that is is a reformulation of a theorem by Shephard.

Theorem 2.2.3 [71, Theorem 3] *The matrix $\mathbf{D} \in \mathbb{R}^{n \times (\ell+m)}$ is a positive basis of its linear span if and only if $\mathbf{0}_m \notin \text{conv}(\mathbf{X}_{\mathbf{D}})$ and for all $\mathbf{y} \in \mathbb{R}^m$, the vector $\mathbf{X}_{\mathbf{D}}^\top \mathbf{y}$ does not admit a unique nonpositive coordinate.*

The characterization above is relatively straightforward to derive: it was previously shown that the condition $\mathbf{0}_m \notin \text{conv}(\mathbf{X}_{\mathbf{D}})$ was equivalent to \mathbf{D} being a PSS of its linear span. Moreover, since $\text{span}(\mathbf{X}_{\mathbf{D}}^{\top}) = \text{Null}(\mathbf{D})$, the second condition is equivalent to saying that no element of $\text{Null}(\mathbf{D})$ has a unique nonpositive coordinate, which simply translates into a condition of positive independence.

In Section 2.3.2, we will take a closer look at Gale diagrams through polytope theory.

2.3 Positive k -spanning sets

In this section, we take an interest in PSSs that retain their positively spanning ability when one or more of their elements are removed. Such PSSs were originally termed *positive k -spanning sets* (PkSSs) in the literature [48] and we adopt the same terminology. After recalling the key definitions and properties of positive k -spanning sets and positive k -bases [48, 50] we highlight their connections with Gale diagrams and neighborly polytopes.

2.3.1 From PSSs to PkSSs

As for PSSs, we define positive k -spanning sets as matrices.

Definition 2.3.1 (Positive k -span and positive k -spanning set) *Let \mathbb{L} be a linear subspace of \mathbb{R}^n and $k \geq 1$. The positive k -span of a matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$, denoted $\text{pspan}_k(\mathbf{D})$, is the set*

$$\text{pspan}_k(\mathbf{D}) := \bigcap_{\substack{\tilde{\mathbf{D}} \in \mathbb{R}^{n \times \tilde{m}} \\ \tilde{m} \geq m-k+1 \\ \tilde{\mathbf{D}} \text{ submatrix of } \mathbf{D}}} \text{pspan}(\tilde{\mathbf{D}}).$$

A positive k -spanning set (PkSS) of \mathbb{L} is a matrix \mathbf{D} such that $\text{pspan}_k(\mathbf{D}) = \mathbb{L}$.

As for PSSs, a PkSS for $\mathbb{L} = \mathbb{R}^n$ will simply be called a PkSS.

Equivalently to Definition 2.3.1, positive k -spanning sets of an ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$ are defined as matrices $\mathbf{D} \in \mathbb{R}^{n \times m}$, $m \geq k$, such that any matrix $\tilde{\mathbf{D}}$ obtained from \mathbf{D} by removing $k-1$ columns is a PSS of \mathbb{L} . As a result, any PkSS of \mathbb{L} is also a PSS for \mathbb{L} , and the two notions coincide when $k=1$ (as do the notions of positive k -span and positive span).

Example 2.3.1 *The matrix $\mathbf{D} = \begin{bmatrix} 1 & 0 & -1 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 & 1 & -1 \end{bmatrix} \in \mathbb{R}^{2 \times 6}$ is a P2SS. Indeed, any matrix $\tilde{\mathbf{D}}$ obtained from \mathbf{D} by removing one column ad-*

mits one of the two positive bases $\begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix}$ and $\begin{bmatrix} -1 & 0 & 1 \\ 0 & -1 & 1 \end{bmatrix}$ as a submatrix, thus $\text{pspan}(\tilde{\mathbf{D}}) = \mathbb{R}^2$.

The geometric characterization of PSSs based on Farkas's lemma can easily be generalized to positive k -spanning sets of \mathbb{R}^n . This is the object of Proposition 2.3.1, stating that the intersection of any open half-space with the set of columns of a PkSS must always be of size k or more.

Proposition 2.3.1 [48] *A matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$ is not a PkSS if and only if there exists a vector $\mathbf{y} \in \mathbb{R}^n \setminus \{\mathbf{0}_n\}$ such that $\mathbf{y}^\top \mathbf{D}$ possesses at most $k - 1$ positive coordinates.*

Equivalently, Proposition 2.3.1 states that any vector $\mathbf{y} \neq \mathbf{0}_n$ must make an acute angle with at least k columns of any PkSS.

Example 2.3.2 *The columns of matrix $\mathbf{D} \in \mathbb{R}^{2 \times 6}$ from Example 2.3.1 are represented in Figure 2.7 below. Any nonzero vector in \mathbb{R}^2 makes a positive dot product with at least two of these columns: for instance, the values $\mathbf{y}^\top \mathbf{d}_1, \mathbf{y}^\top \mathbf{d}_2$ and $\mathbf{y}^\top \mathbf{d}_5$ are positive. However and as illustrated by Figure 2.8, the matrix obtained from \mathbf{D} by removing \mathbf{d}_5 is not a P2SS: only one of the five vectors $\{\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3, \mathbf{d}_4, \mathbf{d}_6\}$ makes a positive dot product with $\mathbf{y}' = \mathbf{d}_2$.*

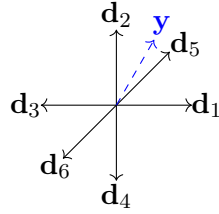


Figure 2.7. P2SS in \mathbb{R}^2

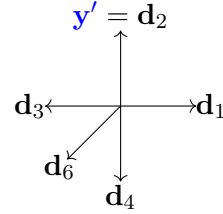


Figure 2.8. Not a P2SS of \mathbb{R}^2

We stated earlier that positive k -spanning sets are PSSs retaining this property when removing $k - 1$ of their columns. As so, PkSSs of ℓ -dimensional spaces must possess at least $\ell + k$ columns. Using Proposition 2.3.1 allows to derive a sharper bound.

Proposition 2.3.2 [50, based on Corollary 5] *Let $\mathbb{L} \subset \mathbb{R}^n$ be ℓ -dimensional. The smallest attainable size for a PkSS $\mathbf{D} \in \mathbb{R}^{n \times m}$ of \mathbb{L} is given by $m = (\ell - 1) + 2k$.*

Since the inequality $(\ell - 1) + 2k \geq \ell + k$ holds for all positive integers k and becomes strict when $k \geq 2$, the bound given in Proposition 2.3.2 is an improvement over that of $\ell + k$. Figure 2.9 below shows an example of a PkSS satisfying the bound for $k = \ell = n = 2$. Note that proofs of Proposition 2.3.2 are far from being trivial and usually require the use of

Gale diagrams of well chosen polytopes. We provide an alternative, algebraic proof which does not *explicitly* use any property of polytopes.

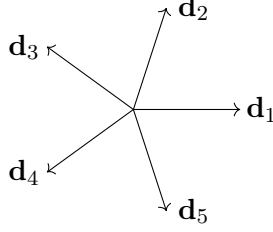


Figure 2.9. P2SS of minimal size in \mathbb{R}^2

Proof of Proposition 2.3.2. As always, we simply prove the result for $\ell = n$ as all other cases directly ensue. First, consider a positive k -spanning set $\mathbf{D} = [\mathbf{d}_1 \ \dots \ \mathbf{d}_m]$ of \mathbb{R}^n . Clearly $m \geq n$ and we let $\mathbf{y} \in \mathbb{R}^n \setminus \{\mathbf{0}_n\}$ be orthogonal to $\text{span}(\mathbf{d}_1, \dots, \mathbf{d}_{n-1})$. Then the first $n-1$ entries of $\mathbf{y}^\top \mathbf{D} \in \mathbb{R}^m$ are zero. As per Proposition 2.3.1, at least k other entries are positive. Moreover this vector also possesses at least k negative coordinates as the result of Proposition 2.3.2 also applies to $-\mathbf{y}^\top \mathbf{D}$. In total, we see that the number m of entries must satisfy $m \geq (n-1) + 2k$.

Now, consider a matrix $\mathbf{P} = [\mathbf{d}_1 \ \dots \ \mathbf{d}_{2k+n-1}] \in \mathbb{R}^{(2k-1) \times (2k+n-1)}$ satis-

fying $\mathbf{d}_i = \begin{bmatrix} i^0 \\ i^1 \\ \dots \\ i^{2k-2} \end{bmatrix}$, for all $i \leq 2k+n-1$. Clearly, \mathbf{P} is of full rank and we

let $\mathbf{X}_\mathbf{P} \in \mathbb{R}^{n \times (2k+n-1)}$ be one of its Gale diagrams. We show that $\mathbf{X}_\mathbf{P}$ is a positive k -spanning set in \mathbb{R}^n . Indeed, let $\mathcal{J} \subset \llbracket 1, 2k+n-1 \rrbracket$ be a set of cardinal $k-1$ or less and let $\mathbf{x} \in \mathbb{R}^{2k-1}$. The dot product $\mathbf{x}^\top \mathbf{d}_i = \sum_{j=0}^{2k-2} [\mathbf{x}]_{j+1} i^j$ is a polynomial of degree $2k-2$, with respect to i . Therefore \mathbf{x} can be chosen so that for all i , $\mathbf{x}^\top \mathbf{d}_i = i^{2k-2-2|\mathcal{J}|} \prod_{j \in \mathcal{J}} (i-j)^2$. By construction, each

column \mathbf{d}_i of \mathbf{P} satisfies $\mathbf{x}^\top \mathbf{d}_i \geq 0$ with an equality if and only if $i \in \mathcal{J}$. Now, letting $\mathbf{y}^\top = \mathbf{x}^\top \mathbf{P}$, we find that $\mathbf{y} \geq \mathbf{0}_{2k+n-1}$ and that $\mathbf{X}_\mathbf{P} \mathbf{y} = \mathbf{0}_n^\top$, as $\mathbf{P} \mathbf{X}_\mathbf{P}^\top = \mathbf{0}_{2k-1, n}$. Last, let $\tilde{\mathbf{y}}$ be the vector obtained from \mathbf{y} by removing the entries whose indices are in \mathcal{J} and similarly, let $\tilde{\mathbf{X}}_\mathbf{P}$ be obtained from $\mathbf{X}_\mathbf{P}$ by removing the columns of indices in \mathcal{J} . Then $\tilde{\mathbf{y}}$ is positive and satisfies $\tilde{\mathbf{X}}_\mathbf{P} \tilde{\mathbf{y}} = \mathbf{0}$, so by Proposition 2.1.1 $\tilde{\mathbf{X}}_\mathbf{P}$ is a PSS of its linear span. Since the result holds for any subset $|\mathcal{J}| \leq k-1$ and since $\text{span}(\mathbf{X}_\mathbf{P}) = \mathbb{R}^n$, a quick induction based on Proposition 2.1.3 allows us to conclude that $\mathbf{X}_\mathbf{P}$ is a positive k -spanning set. \square

Throughout Section 2.1, we highlighted positive bases as a special class

of positive spanning sets. We now define the counterpart notion for positive k -spanning sets, that are termed *positive k -bases*. Note that although PkSSs have been studied starting in the 1980s [48, 50, 79], the terminology *positive k -basis* was formally defined in the context of this thesis.

Definition 2.3.2 (Positive k -basis) *Let $\mathbb{L} \subset \mathbb{R}^n$ satisfy $\dim(\mathbb{L}) = \ell$, let $k \geq 1$ and let $m \geq \max(k, \ell)$. A matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$ is called a positive k -basis of \mathbb{L} if and only if $\text{pspan}_k(\mathbf{D}) = \mathbb{L}$ and no proper submatrix $\tilde{\mathbf{D}}$ of \mathbf{D} satisfies $\text{pspan}_k(\tilde{\mathbf{D}}) = \mathbb{L}$.*

Numerous properties of positive spanning sets and positive bases can be adapted to PkSSs and positive k -bases in a straightforward manner. In this chapter, we are primarily interested in cardinality results regarding both PkSSs and positive k -bases. The minimal possible size for a PkSS (and thus for a positive k -basis) was already established in Proposition 2.3.2. The maximum possible size, however, is still an open problem.

In specific cases with added restrictions on the values of k and the (sub)space dimension, Marcus [48] obtained the following bound on the size of a positive k -basis.

Proposition 2.3.3 [48, Theorem 1 and Corollary 1] *Let $\mathbf{D} \in \mathbb{R}^{n \times m}$ be a positive k -basis for the ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$. Suppose that $\ell = 2$, or that $k = 2$ and $\ell \leq 5$. Then $m \leq 2k\ell$.*

Note that the bound given in Proposition 2.3.3 is tight as stacking k copies of a maximal positive basis $\mathbf{D}_{\mathbb{L}, \ell}$ of a linear space \mathbb{L} together yields a positive k -basis of \mathbb{L} . In higher dimensions however, polytopes can be used to construct positive k -bases whose size greatly exceeds $2k\ell$ [80]. We describe this construction and the associated relationship between PkSSs and polytopes in the next section.

2.3.2 Positive k -spanning sets and polytopes

The notion of Gale diagram - see Definition 2.2.4 - was introduced in Section 2.2.3 where we showed how such matrices are used to characterize PSSs and positive bases. Gale diagrams are more commonly used in convex geometry to classify polytopes [55, 2, 74, 76], leading to an unexpected connection between PkSSs and a class of polytopes called *unneighborly polytopes*. To describe these results, we first provide background definitions from affine and polyhedral geometry. An ℓ -dimensional *affine space* $\tilde{\mathbb{L}}$ is defined as the translation of a linear space \mathbb{L} of similar dimension. Affine hyperplanes can be characterized as sets of solutions to equations of the form

$$\mathbf{x}^\top \mathbf{y} = a, \quad \mathbf{y} \in \mathbb{R}^n \setminus \{\mathbf{0}_n\}, \quad a \in \mathbb{R}. \quad (2.5)$$

Any affine hyperplane $\tilde{\mathbb{L}}$ is associated to two *half-spaces* of \mathbb{R}^n , defined by replacing the equality symbol in (2.5) with the symbol \geq or \leq . We say that

$\tilde{\mathbb{L}}$ is a *supporting hyperplane* for a set \mathcal{S} whenever \mathcal{S} is entirely contained within one of the two associated half-spaces. An example is provided in Figure 2.10 below.

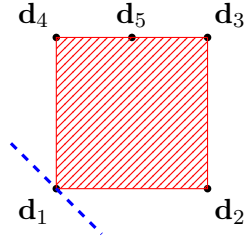


Figure 2.10. Supporting hyperplane of a square

The properties of supporting hyperplanes of convex polytopes will be a topic of interest.

Definition 2.3.3 (Convex polytope) A set $\mathcal{P} \subset \mathbb{R}^n$ is a convex polytope whenever it is the convex hull of a finite set $\{\mathbf{d}_1, \dots, \mathbf{d}_m\}$. In other words, \mathcal{P} is the set of nonnegative combinations of the \mathbf{d}_i whose coefficients add up to 1.

As illustrated by Figure 2.10, the set of vertices of the polytope $\mathcal{P} = \text{conv}(\{\mathbf{d}_1, \dots, \mathbf{d}_m\})$ cannot be defined as $\{\mathbf{d}_1, \dots, \mathbf{d}_m\}$. Instead, vertices are defined using supporting hyperplanes of \mathcal{P} .

Definition 2.3.4 (Face, vertex) The intersection of a supporting hyperplane with \mathcal{P} is called a face. By convention, \mathcal{P} is also considered as a face of itself. A vertex is a face composed of a single point. The set of vertices of \mathcal{P} is noted $\mathcal{V}_{\mathcal{P}}$.

It will often be useful to consider the complementary set of a vertex set associated with the face of a polytope.

Definition 2.3.5 (Coface) Let $\mathcal{P} \subset \mathbb{R}^n$ be a convex polytope. A set $\mathcal{C} \subset \mathcal{V}_{\mathcal{P}}$ is called a coface of \mathcal{P} if $\text{conv}(\mathcal{V}_{\mathcal{P}} \setminus \mathcal{C})$ is a face of \mathcal{P} .

Example 2.3.3 In the polytope \mathcal{P} from Figure 2.10, $\mathcal{V}_{\mathcal{P}} = \{\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3, \mathbf{d}_4\}$. The set $\{\mathbf{d}_1, \mathbf{d}_2\}$ is a coface of \mathcal{P} , associated to the face $\text{conv}(\{\mathbf{d}_3, \mathbf{d}_4\})$. Similarly, the coface $\{\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3\}$ is associated to the face $\{\mathbf{d}_4\}$.

Let us now highlight the key connections between Gale diagrams - see Definition 2.2.4 - and convex polytopes. In the remainder of this section, for a convex polytope $\mathcal{P} \subset \mathbb{R}^n$ on m vertices we denote by $\mathbf{P} \in \mathbb{R}^{n \times m}$ a matrix satisfying $\text{col}(\mathbf{P}) = \mathcal{V}_{\mathcal{P}}$. Any Gale diagram $\mathbf{X}_{\mathbf{P}}$ of the matrix \mathbf{P} is also called a Gale diagram of \mathcal{P} . We shall take a particular interest towards

convex polytopes whose *affine hull* - the smallest affine space in which they are contained - does not contain $\mathbf{0}_n$. To ensure that a polytope satisfies this property, one can consider a copy \mathcal{P} of this polytope in a space of higher dimension, where each vertex is lifted above ground.

Definition 2.3.6 (Lifted polytope) *A convex polytope $\mathcal{P} \subset \mathbb{R}^n$ on m vertices is said to be lifted whenever the last row of \mathbf{P} is equal to $\mathbf{1}_m^\top$.*

The *affine dimension* ℓ of a lifted polytope $\mathcal{P} \subset \mathbb{R}^n$, which is defined as the dimension of the smallest affine space in which \mathcal{P} is contained, must always satisfy $\ell \leq n-1$. Similarly, the number of vertices m must always be greater than ℓ .

Example 2.3.4 *By considering a lifted copy of the unit square represented in Figure 2.10, one obtains a new polytope $\mathcal{P} \subset \mathbb{R}^3$ whose associated matrix*

$$\text{is given by } \mathbf{P} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}.$$

We are now ready to state one of the main properties of Gale diagrams, connecting them to the cofaces of lifted polytopes. The following proposition is due to Marcus [48], and is adapted from a theorem by Shephard [71, Theorem 1].

Proposition 2.3.4 [48] *Let $\mathcal{P} \subset \mathbb{R}^n$ be an ℓ -dimensional lifted polytope on $\ell + m$ vertices. Let $\mathbf{X}_\mathbf{P} = [\bar{\mathbf{d}}_1 \ \dots \ \bar{\mathbf{d}}_{\ell+m}]$ be a Gale diagram of the associated matrix \mathbf{P} . A set of vertices $\{\mathbf{d}_{i_1}, \dots, \mathbf{d}_{i_j}\} \subset \mathcal{V}_\mathcal{P}$ is a coface of \mathcal{P} if and only if the associated matrix $[\bar{\mathbf{d}}_{i_1} \ \dots \ \bar{\mathbf{d}}_{i_j}]$ is a PSS of its linear span.*

Note that Shephard's alternative formulation of Proposition 2.3.4 was applied to convex cones in \mathbb{R}^n instead of polytopes, and used to derive Proposition 2.2.5. The reformulation given in this manuscript proves to be more practical for studying positive k -spanning sets.

Example 2.3.5 *Let $\mathbf{P} = [\mathbf{d}_1 \ \mathbf{d}_2 \ \mathbf{d}_3 \ \mathbf{d}_4]$ be the matrix from Example 2.3.4. A Gale diagram is given by $\mathbf{X}_\mathbf{P} = [\bar{\mathbf{d}}_1 \ \dots \ \bar{\mathbf{d}}_4] = [-1 \ 1 \ -1 \ 1]$. Clearly, the matrix $[\bar{\mathbf{d}}_1 \ \bar{\mathbf{d}}_2] = [-1 \ 1]$ is a PSS of \mathbb{R} . The associated set of vertices $\{\mathbf{d}_1, \mathbf{d}_2\}$ is a coface of \mathcal{P} as its complementary set $\{\mathbf{d}_3, \mathbf{d}_4\}$ generates an edge of the square \mathcal{P} . Conversely, the matrix $[\bar{\mathbf{d}}_1 \ \bar{\mathbf{d}}_3] = [-1 \ -1]$ is not a PSS of \mathbb{R} and $\{\mathbf{d}_1, \mathbf{d}_3\}$ is not a coface of \mathcal{P} as the complementary set $\{\mathbf{d}_2, \mathbf{d}_4\}$ generates a diagonal of the square instead of a face.*

Let $\mathcal{P} \subset \mathbb{R}^{\ell+p}$ be an ℓ -dimensional lifted polytope on $\ell + m$ vertices, with $m > p$. Which properties should \mathcal{P} satisfy in order to ensure that the associated Gale diagram $\mathbf{X}_\mathbf{P} \in \mathbb{R}^{(m-p) \times (\ell+m)}$ is a positive k -spanning set? First, by Proposition 2.3.4, the matrix $\mathbf{X}_\mathbf{P}$ is guaranteed to be a PSS. Indeed,

the set $\mathcal{V}_{\mathcal{P}}$ must be a coface of \mathcal{P} as the empty set is a face. In fact, since any vertex $\mathbf{d}_i \in \mathcal{V}_{\mathcal{P}}$ is a face, the matrix $\mathbf{X}_{\mathcal{P}, \mathbf{d}_i}$ obtained from $\mathbf{X}_{\mathcal{P}}$ by removing the column \mathbf{d}_i is a PSS of its linear span which by Proposition 2.1.3 is equal to $\text{span}(\mathbf{X}_{\mathcal{P}}) = \mathbb{R}^{m-1}$. Consequently, we obtain a first connection between P2SSs and convex polytopes.

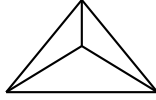
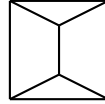
Proposition 2.3.5 [50, Corollary 1] *Let $\mathcal{P} \subset \mathbb{R}^{\ell+p}$ be an ℓ -dimensional lifted polytope on $\ell + m$ vertices, with $m > p$. Any Gale diagram $\mathbf{X}_{\mathcal{P}} \in \mathbb{R}^{(m-p) \times (\ell+m)}$ of \mathcal{P} is a P2SS of \mathbb{R}^{m-p} .*

The Gale diagram of an lifted square was given in Example 2.3.5 and we saw it was equal to $\mathbf{X}_{\mathcal{P}} = [-1 \ 1 \ -1 \ 1]$, which is indeed a P2SS of \mathbb{R} . In order to continue the induction that led us to Proposition 2.3.5, we now consider polytopes \mathcal{P} for which each set of k vertices or less is a face.

Definition 2.3.7 ((Un)neighborly polytope) *A polytope $\mathcal{P} \subset \mathbb{R}^n$ is called k -neighborly if each set of k -vertices or less generates a face. If, in addition, each vertex \mathbf{d}_i is contained in at least one set of $k + 1$ vertices which do not generate a face of \mathcal{P} , the polytope is called k -unneighborly.*

The expression *unneighborly polytope* originates from McMullen [54], and has been featured more recently in the polytope literature [80].

Example 2.3.6 *The tetrahedron $\mathcal{P}_1 \subset \mathbb{R}^3$ given in Figure 2.11 below is 4-neighborly as any set of 4 vertices or less forms a face. In fact, any simplex in \mathbb{R}^n is $(n + 1)$ -neighborly. The triangular prism $\mathcal{P}_2 \subset \mathbb{R}^3$ given in Figure 2.12 is 1-unneighborly as for each vertex u , there exists some other vertex v such that $[u, v]$ is not an edge of \mathcal{P}_2*

Figure 2.11. Tetrahedron \mathcal{P}_1 Figure 2.12. Triangular prism \mathcal{P}_2

When considering neighborly polytopes, the result of Proposition 2.3.5 can be generalized.

Theorem 2.3.1 [50, Corollary 5] *Let $\mathcal{P} \subset \mathbb{R}^{\ell+p}$ be an ℓ -dimensional lifted polytope on $\ell + m$ vertices, with $m > p$. A Gale diagram $\mathbf{X}_{\mathcal{P}} \in \mathbb{R}^{(m-p) \times (\ell+m)}$ of \mathcal{P} is a Pk SS of \mathbb{R}^{m-p} if and only if \mathcal{P} is $(k - 1)$ -neighborly. If moreover \mathcal{P} is $(k - 1)$ -unneighborly, any such diagram is a positive k -basis.*

Whenever $\ell \leq 3$, the only ℓ -dimensional, lifted, 2-neighborly polytopes are simplices [26]. An example of a 2-neighborly polytope of higher dimension is provided below.

Example 2.3.7 *The lifted polytope $\mathcal{P} \subset \mathbb{R}^6$ on 8 vertices associated to the matrix \mathbf{P} below is known to be 2-neighborly [45]. One can easily check that the associated Gale diagram $\mathbf{X}_{\mathbf{P}}$ is a positive 3-basis of \mathbb{R}^2 . It follows from Theorem 2.3.1 that \mathcal{P} is 2-unneighborly.*

$$\mathbf{P} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \quad \mathbf{X}_{\mathbf{P}} = \begin{bmatrix} 0 & -2 & 2 & 0 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & 1 & 0 & 0 \end{bmatrix}$$

As illustrated by the previous example, Theorem 2.3.1 can either be used to build positive k -spanning sets or as a tool to prove that a given polytope is (un)neighborly. Note that the relationship between a matrix \mathbf{P} and its diagram $\mathbf{X}_{\mathbf{P}}$ is symmetrical, in the sense that \mathbf{P} is a Gale diagram of $\mathbf{X}_{\mathbf{P}}$ [71]. In consequence, Theorem 2.3.1 can also be used to build k -neighborly polytopes from positive $(k - 1)$ -spanning sets.

The lower bound on the size of a PkSS given in Proposition 2.3.2 was derived from Theorem 2.3.1 by Marcus by considering the Gale diagram of a cyclic polytope - see for instance [16] for a definition - and exploiting the neighborliness of such polytopes. In the case of this manuscript, while the matrix \mathbf{P} introduced in the proof of Proposition 2.3.2 was also that of a cyclic polytope, we do not make use of this fact in our reasoning. In that sense, our proof of Proposition 2.3.2 can equivalently be considered as a proof on the neighborliness of cyclic polytopes.

We conclude this section with a quick summary of the results on the maximal size of positive k -bases of ℓ -dimensional spaces. Marcus initially believed this bound to be $2k\ell$ [50], a conjecture that he later dismissed. Explicit counterexamples were provided by Wotzlaw [79] after a thorough study of *illuminated* polytopes - a particular type of unneighborly polytopes [47, Definition 2], [80]. The next three propositions and corollary, by Wotzlaw, were initially stated for PkSSs in \mathbb{R}^n . We provide a straightforward generalization to all subspaces.

Proposition 2.3.6 [79, Theorem 10.3.1] *Let $k \geq 2$, $n \geq \ell \geq 1$ and let $\mathbb{L} \subset \mathbb{R}^n$ be an ℓ -dimensional linear subspace. There exists a positive k -basis of \mathbb{L} of size $f_{k,\ell}$ if k is even and of size $f_{k,\ell} + \lfloor \frac{\ell+1}{2} \rfloor + 1$ otherwise, where $f_{k,\ell} = \lfloor \frac{k}{2} \rfloor \left(\lfloor \frac{\ell}{2} \rfloor \lfloor \frac{\ell+1}{2} \rfloor + \ell + 1 \right)$.*

In short, Proposition 2.3.6 states the existence of positive k -bases of $\Theta(k\ell^2)$ columns, for ℓ -dimensional spaces. In particular, in sufficiently large dimensions, the size of positive k -bases can exceed $2k\ell$: the smallest known example is given by a positive 2-basis in \mathbb{R}^{12} of size $49 = 2kn + 1$. While the existence of large positive k -bases in spaces of dimension $\ell < 12$ remains possible, as per Proposition 2.3.3 any such basis would satisfy $\ell > 5$ or $k > 2$.

Corollary 2.3.1 [79, Corollary 10.3.2] *Suppose that $n \geq \ell \geq 12$ and that k is even, or that $n \geq \ell \geq 18$ and that k is odd. Then there exists a positive k -basis of the ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$ with strictly more than $2k\ell$ columns.*

An explicit formula for the maximal size of a positive k -bases is yet to be found. Note that this size is known to be finite.

Proposition 2.3.7 [79, Theorem 10.4.2] *Let $k \geq 2$. The size of a positive k -basis for an ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$ does not exceed $k\ell(\ell + 1)^{k-1}$.*

2.3.3 Structural results

The structure of minimal positive bases in \mathbb{R}^n was described in Corollary 2.2.1, where we showed that such matrices were all structurally equivalent to $[\mathbf{I}_n \quad -\mathbf{1}_n]$. Let us now investigate a generalization of this result for positive k -bases of minimal size. With that purpose in mind, the following two lemmas shall come as handy tools.

Lemma 2.3.1 *Each row of a $PkSS$ of \mathbb{R}^n must contain at least k positive entries and k negative entries.*

Proof. If a row of $\mathbf{D} \in \mathbb{R}^{n \times m}$ contains strictly less than k positive (resp. negative) entries, remove the columns associated to these entries and name $\tilde{\mathbf{D}}$ the resulting matrix. Then $\mathbf{1}_n \notin \text{pspan}(\tilde{\mathbf{D}})$ (resp. $-\mathbf{1}_n \notin \text{pspan}(\tilde{\mathbf{D}})$), therefore $\tilde{\mathbf{D}}$ is not a PSS and so \mathbf{D} is not a $PkSS$. \square

We emphasize that Lemma 2.3.1 does *not* characterize $PkSS$ s. It is a weaker formulation of Proposition 2.3.1. The next result states that at least two additional vectors are required to build a $PkSS$ from a positive $(k - 1)$ -basis.

Lemma 2.3.2 *Let $\mathbf{D} \in \mathbb{R}^{n \times m}$ be a positive k -basis for an ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$, let $\mathbf{d} \in \mathbb{R}^n$. The matrix $[\mathbf{d} \quad \mathbf{D}]$ is not a $P(k + 1)SS$ of \mathbb{L} .*

Proof. The matrix \mathbf{D} is a PSS and so $\mathbf{d} \in \text{pspan}(\mathbf{D})$. More precisely and as entailed by Lemma 2.1.1, there exist a nonsingular submatrix \mathbf{B} of \mathbf{D} such that $\mathbf{d} \in \text{pspan}(\mathbf{B})$. Thus up to structural equivalence we can assume that $\mathbf{D} = [\mathbf{I}_n \quad \mathbf{S}]$, $\mathbf{S} \in \mathbb{R}^{n \times (m-n)}$, with \mathbf{d} being nonnegative. Clearly, $(m - n) \geq k$ as \mathbf{D} is a positive k -basis. With the necessary setup complete, we now proceed with the proof.

To show that $[\mathbf{d} \quad \mathbf{D}]$ is not a $P(k + 1)SS$, we now remove its last k columns and show that the resulting matrix $\tilde{\mathbf{D}} = [\mathbf{d} \quad \mathbf{I}_n \quad \tilde{\mathbf{S}}]$ is not a PSS. As $\mathbf{D} = [\mathbf{I}_n \quad \mathbf{S}]$ is a positive k -basis, the matrices obtained from \mathbf{S} by removing k columns can never contain a negative vector in their positive span. In particular the cone $\text{pspan}(\tilde{\mathbf{S}})$ does not contain any negative vector. Trivially,

the result extends to any matrix obtained from $\tilde{\mathbf{S}}$ by adding nonnegative columns. Therefore $\tilde{\mathbf{D}}$ is not a PSS as $-\mathbf{1}_n \notin \text{pspan}(\tilde{\mathbf{D}})$. \square

At best, building a PkSS from a positive $(k-1)$ -basis can thus only be done by stacking of two more columns. Using Lemmas 2.3.1 and 2.3.2, we now investigate a generalization of Corollary 2.2.1, which characterized minimal positive bases.

Proposition 2.3.8 *Let $\mathbf{D} \in \mathbb{R}^{n \times (\ell+2k-1)}$ be a minimal positive k -basis of a ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$. Then*

$$\mathbf{D} \equiv \begin{bmatrix} \mathbf{I}_\ell & -\mathbf{1}_\ell & -\mathbf{X} & \mathbf{Y} \\ \mathbf{0}_{n-\ell,\ell} & \mathbf{0}_{n-\ell} & \mathbf{0}_{n-\ell,k-1} & \mathbf{0}_{n-\ell,k-1} \end{bmatrix}, \text{ } \mathbf{X} \text{ and } \mathbf{Y} \text{ positive in } \mathbb{R}^{\ell \times (k-1)}.$$

Proof. For the sake of simplicity, we assume that $\ell = n$ as the proof easily generalizes to all other cases. We proceed by induction; when $n = 1$, the result is trivially true for all values of k . Similarly, Corollary 2.2.1 shows that the result is true for all n , when $k = 1$.

Let $n \geq 2$ and $k \geq 2$. Suppose the result to hold for all minimal positive $(k-1)$ -bases in \mathbb{R}^n and for all values of \tilde{k} , in \mathbb{R}^{n-1} . Let $\mathbf{D} \in \mathbb{R}^{n \times (n+2k-1)}$ be a minimal positive k -basis. We easily deduce from Lemma 2.3.2 that $\mathbf{D} \equiv [\tilde{\mathbf{D}} \ \mathbf{d}_1 \ \mathbf{d}_2]$, where $\tilde{\mathbf{D}}$ is a minimal positive $(k-1)$ -basis in \mathbb{R}^n . The induction hypothesis applies and we have $\mathbf{D} \equiv \mathbf{D}_1 = [\mathbf{I}_n \ -\mathbf{1}_n \ -\tilde{\mathbf{X}} \ \tilde{\mathbf{Y}} \ \tilde{\mathbf{v}} \ \tilde{\mathbf{w}}]$, with $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}$ both positive in $\mathbb{R}^{n \times (k-2)}$. By removing the first row of \mathbf{D}_1 , we obtain a positive k -spanning set in \mathbb{R}^{n-1} whose first column is $\mathbf{0}_{n-1}$. Remove this column too to obtain a PkSS $\tilde{\mathbf{D}}_1 \in \mathbb{R}^{(n-1) \times (n+2k-2)}$, which must in fact necessarily be a minimal positive k -basis in \mathbb{R}^{n-1} . Applying once again the induction hypothesis, we can thus write $\mathbf{D} \equiv \mathbf{D}_2 = [\mathbf{I}_n \ -\mathbf{1}_n \ -\mathbf{X} \ \mathbf{Y} \ \mathbf{v} \ \mathbf{w}]$ with \mathbf{X} and \mathbf{Y} both positive in $\mathbb{R}^{n \times (k-1)}$ and with \mathbf{v} and \mathbf{w} both in \mathbb{R}^n , $[\mathbf{v}]_i < 0 < [\mathbf{w}]_i$ for all $i > 1$ and $-\mathbf{v}_1 = \mathbf{w}_1 \in \mathbb{R} \setminus \{0\}$. If $[\mathbf{v}]_1 < 0$ the result is immediately proved up to permuting columns. Otherwise, it suffices to change basis using $\mathbf{B} = [\mathbf{v} \ \mathbf{e}_2 \ \dots \ \mathbf{e}_n]$ to obtain the desired structure. \square

In its current form, the structural result of Proposition 2.3.8 does not characterize minimal positive k -bases: for instance, one easily checks that the matrix $[\mathbf{I}_2 \ -\mathbf{1}_2 \ -\mathbf{e}_1 - 2\mathbf{e}_2 \ \mathbf{e}_1 + 2\mathbf{e}_2]$ in \mathbb{R}^2 is not a P2SS. In order to attain such a result, additional restrictions should be applied to the two blocks $-\mathbf{X}$ and \mathbf{Y} contained in the minimal positive k -basis. In the case where $k = 2$, these constraints can be explicitly determined. The following characterization of minimal positive 2-bases ensues.

Theorem 2.3.2 *A matrix $\mathbf{D} \in \mathbb{R}^{n \times (\ell+3)}$ is a positive 2-basis for some ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$ if and only if there exist two positive vectors \mathbf{x}*

and \mathbf{y} in \mathbb{R}^n , with $[\mathbf{x}]_1 = [\mathbf{y}]_1 = 1$ and whose entries are in strictly increasing order, such that

$$\mathbf{D} \equiv \begin{bmatrix} \mathbf{I}_\ell & -\mathbf{1}_\ell & -\mathbf{x} & \mathbf{y} \\ \mathbf{0}_{n-\ell,\ell} & \mathbf{0}_{n-\ell} & \mathbf{0}_{n-\ell} & \mathbf{0}_{n-\ell} \end{bmatrix}, \text{ with } \max_{s \in [2,n]} \frac{[\mathbf{y}]_s}{[\mathbf{x}]_s} < 1 \text{ and } \forall i \in [2, n-1]$$

$$m_{i_+} < m_{i_-}, \text{ where } m_{i_+} = \max_{s \in [i+1,n]} \frac{[\mathbf{y}]_s - [\mathbf{y}]_i}{[\mathbf{x}]_s - [\mathbf{x}]_i} \text{ and } m_{i_-} = \min_{s \in [1,i-1]} \frac{[\mathbf{y}]_i - [\mathbf{y}]_s}{[\mathbf{x}]_i - [\mathbf{x}]_s}.$$

Proof. We only prove the result for $\ell = n$ as all other cases easily ensue. Suppose that $\mathbf{D} \equiv \mathbf{D}_0 = [\mathbf{I}_n \quad -\mathbf{1}_n \quad -\mathbf{x} \quad \mathbf{y}]$, where \mathbf{x} and \mathbf{y} satisfy the conditions listed above. Let us prove that \mathbf{D}_0 is a P2SS (and so, a positive 2-basis), as the same will then hold for \mathbf{D} . This amounts to proving that any matrix obtained from \mathbf{D}_0 by removing exactly one column is positively spanning. First, observe that by removing one of the three column $-\mathbf{1}_n$, $-\mathbf{x}$ and \mathbf{y} , we obtain a matrix in which one of the two positive bases $[\mathbf{I}_n \quad -\mathbf{1}_n]$ and $[\mathbf{I}_n \quad -\mathbf{x}]$ is contained. This matrix must thus be a PSS. Now, let $i \leq n$ and denote by $\mathbf{D}_{\mathbf{e}_i}$ the matrix obtained from \mathbf{D}_0 by removing its i^{th} column. In order to prove that $\mathbf{D}_{\mathbf{e}_i}$ is a PSS, it suffices to show that $\text{pspan}([-\mathbf{1}_n \quad -\mathbf{x} \quad \mathbf{y}])$ contains a vector \mathbf{z} with a unique positive coordinate, the i^{th} : indeed, this is equivalent to saying that $\mathbf{e}_i \in \text{pspan}(\mathbf{D}_{\mathbf{e}_i})$.

If $i = 1$ then $\mathbf{z} = \mathbf{y} - \max_{s \in [2,n]} \frac{[\mathbf{y}]_s}{[\mathbf{x}]_s} \mathbf{x}$ is a suitable choice as $\max_{s \in [2,\ell]} \frac{[\mathbf{y}]_s}{[\mathbf{x}]_s} < 1 = \frac{[\mathbf{y}]_1}{[\mathbf{x}]_1}$.

If $i = n$ we take $\mathbf{z} = \mathbf{y} - [\mathbf{y}]_{n-1} \mathbf{1}_n$.

If $i \in [2, n-1]$, since $[\mathbf{x}]_i > [\mathbf{y}]_i$ and $[\mathbf{x}]_i > [\mathbf{x}]_1 = 1$, we start by observing that $\frac{[\mathbf{y}]_i}{[\mathbf{x}]_i} - \frac{[\mathbf{y}]_i - [\mathbf{y}]_1}{[\mathbf{x}]_i - [\mathbf{x}]_1} > 0$, thus $m_{i_-} < \frac{[\mathbf{y}]_i}{[\mathbf{x}]_i}$. Now, let $\mathbf{w} = \mathbf{y} - \varepsilon \mathbf{x}$, where $\varepsilon \in]m_{i_+}, m_{i_-}[$. From what precedes, $[\mathbf{w}]_i > 0$. Moreover we find that $[\mathbf{w}]_s < [\mathbf{w}]_i$, for all $s \neq i$. Thus if $\max_{s \neq i} [\mathbf{w}]_s \leq 0$, we take $\mathbf{z} = \mathbf{w}$. Otherwise, we take

$$\mathbf{z} = \mathbf{w} - \max_{s \neq i, [\mathbf{w}]_s > 0} [\mathbf{w}]_s \mathbf{1}_n.$$

Conversely, let us show that all positive 2-bases $\mathbf{D} \in \mathbb{R}^{n \times (n+3)}$ satisfy the conditions listed above. Combining the result of Proposition 2.3.8 with some rescaling and permuting, we write $\mathbf{D} \equiv \mathbf{D}_0 = [\mathbf{I}_n \quad -\mathbf{1}_n \quad -\mathbf{x} \quad \mathbf{y}]$ with \mathbf{x} and \mathbf{y} both positive in \mathbb{R}^n and $1 = [\mathbf{x}]_1 = [\mathbf{y}]_1 < [\mathbf{y}]_2 < \dots < [\mathbf{y}]_n$. The proof is then done by contradiction.

First, suppose that $[\mathbf{x}]_{i+1} \leq [\mathbf{x}]_i$, for some index $i \leq n-1$. Then each vector $\mathbf{z} \in \text{pspan}([-\mathbf{1}_n \quad -\mathbf{x} \quad \mathbf{y}])$ satisfies $[\mathbf{z}]_i \leq [\mathbf{z}]_{i+1}$ and in particular, the i^{th} coordinate of any such vector \mathbf{z} is never uniquely positive. Therefore $\mathbf{e}_i \notin \text{pspan}(\mathbf{D}_{\mathbf{e}_i})$ and so $\mathbf{D}_{\mathbf{e}_i}$ is not a PSS.

Now, let $s \in [2, n]$ and suppose that $\frac{[\mathbf{y}]_s}{[\mathbf{x}]_s} \geq 1$. For all $\varepsilon > 0$, let $\mathbf{z}_\varepsilon = \mathbf{y} - \varepsilon \mathbf{x}$. In order to show that $\text{pspan}([-\mathbf{1}_n \quad -\mathbf{x} \quad \mathbf{y}])$ does not contain a vector \mathbf{z} whose first coordinate is uniquely positive, we prove that $[\mathbf{z}_\varepsilon]_1$ is either nonpositive or less than $[\mathbf{z}_\varepsilon]_s$. Indeed, if $\varepsilon \geq 1$, then $[\mathbf{z}_\varepsilon]_1 \leq 0$. Yet if $\varepsilon < 1$, we find that $[\mathbf{z}_\varepsilon]_s - [\mathbf{z}_\varepsilon]_1 = [\mathbf{y}]_s - [\mathbf{y}]_1 + \varepsilon([\mathbf{x}]_1 - [\mathbf{x}]_s) \geq ([\mathbf{x}]_s - 1)(1 - \varepsilon) > 0$. From what precedes we have $\mathbf{e}_1 \notin \text{pspan}(\mathbf{D}_{\mathbf{e}_1})$ and so $\mathbf{D}_{\mathbf{e}_1}$ is not a PSS.

Last, suppose that some index $i \in \llbracket 2, n-1 \rrbracket$ satisfies $m_{i+} \geq m_{i-}$. Once again we consider $\mathbf{z}_\varepsilon = \mathbf{y} - \varepsilon \mathbf{x}$, where $\varepsilon > 0$; we show that $[\mathbf{z}_\varepsilon]_i$ is either nonpositive, non-maximal or non-uniquely maximal. Indeed, if $\varepsilon < m_{i+}$ then let $s > i$ maximize the ratio $\frac{[\mathbf{y}]_i - [\mathbf{y}]_s}{[\mathbf{x}]_i - [\mathbf{x}]_s}$. If $\varepsilon \geq m_{i+}$, then $\varepsilon \geq m_{i-}$ and we let instead $s < i$ minimize this ratio. We find $[\mathbf{z}_\varepsilon]_i \leq [\mathbf{z}_\varepsilon]_s$, as $[\mathbf{z}_\varepsilon]_i - [\mathbf{z}_\varepsilon]_s = ([\mathbf{y}]_i - [\mathbf{y}]_s) + \varepsilon([\mathbf{x}]_s - [\mathbf{x}]_i) < 0$. \square

When building a positive 2-basis using Theorem 2.3.2, it is worth noting that the condition $m_{i+} < m_{i-}$ may be heavily simplified, depending on value of the vector $\mathbf{y} \in \mathbb{R}^n$ considered.

Example 2.3.8 Let $\mathbf{y} = [1 \ 2 \ \dots \ n]^\top$ and let $[\mathbf{x}] \in \mathbb{R}^n$ satisfy $[\mathbf{x}]_1 = 1$ and $\max_{i \in \llbracket 2, n \rrbracket} \frac{[\mathbf{y}]_i}{[\mathbf{x}]_i} < 1$. One easily checks that the inequality $m_{i+} < m_{i-}$ holds for all $i \in \llbracket 2, n-1 \rrbracket$ if and only if each such index i satisfies $[\mathbf{x}]_{i+1} - [\mathbf{x}]_i > [\mathbf{x}]_i - [\mathbf{x}]_{i-1}$. In consequence, the matrix $\mathbf{D} = [\mathbf{I}_n \ -\mathbf{1}_n \ -\mathbf{x} \ \mathbf{y}]$ is a positive 2-basis in \mathbb{R}^n , where $[\mathbf{x}]_i = \frac{i(i+1)}{2}$ for all $i \in \llbracket 1, n \rrbracket$.

2.4 Summary of Chapter 2

This chapter described the main results on *positive spanning sets* (PSSs), which span the whole Euclidean space with nonnegative linear combinations, and on *positive bases*, which are inclusion-wise minimal for this property. The two concepts were introduced in Section 2.1, a section dedicated to providing formal definitions based on matrix theory and to restating the main properties of PSSs from that angle.

In Section 2.2, an important emphasis was put on the structure of positive bases, a topic that will be of particular interest in Chapter 3. In that regard, the concept of *structural equivalence* - developed in Section 2.2.1 - was introduced and used as a powerful tool to reformulate some classical results characterizing positive bases: first, Romanowicz's important work on criticality - discussed in more depth in Chapter 3 - then Davis's and Shephard's works on Gale diagrams.

Last, *positive k-spanning sets* (PkSSs), a class of resilient PSSs, were examined in Section 2.3.2. The main properties of such sets were formalized in Section 2.3.1, where the expressions *positive k-basis* and *positive k-span* were coined. We provided a short, algebraic proof on the minimal cardinality of such bases, inspired by Marcus's geometrical proof of this result. In Section 2.3.2, an important connection between polytope theory and positive *k*-spanning sets was highlighted. We showed how this relationship could be enabled by considering *neighborly polytopes* and their Gale diagrams. We concluded the chapter by discussing the structure of positive *k*-bases,

with a particular emphasis on those of minimal size which we successfully characterized, in the case where $k = 2$.

Chapter 3

Ties between positive spanning sets and strongly edge-connected digraphs

This chapter presents important results on strongly edge-connected digraphs, a class of directed graphs sharing an interesting relationship with positive spanning sets. After listing the main properties of said graphs, the relationship is highlighted through the use of *network matrices* in Section 3.2. The main result of this chapter, generalizing the ear-decomposition of strongly edge-connected digraphs to positive spanning sets and positive bases, is derived in Sections 3.3 and 3.4. Building on this work, the last section of the chapter is dedicated to determining a similar relationship between strongly k -connected digraphs and PkSSs. The first four sections of this chapter correspond to an article published in **Discrete Applied Mathematics**.

3.1 Strongly edge-connected digraphs

3.1.1 Background on directed graphs

In this chapter, we recall classical results on the ear-decomposition of strongly edge-connected digraphs. We first define the main concepts and properties of digraphs to be used [10, 70]. We consider directed graphs of the form $G = (V, A)$, where V denotes a set of vertices and A denotes a set of arcs.

Definition 3.1.1 (Directed path, circuit) *A directed path in the digraph $G = (V, A)$ is a sequence of arcs of the form $\{(u_i, u_{i+1})\}_{i=1, \dots, k}$. Directed paths such that $u_1 = u_{k+1}$ with u_2, \dots, u_k all distinct are called circuits.*

When the set of arcs of a digraph $G = (V, A)$ does not contain any circuit, we say that G is *acyclic*.

Example 3.1.1 Figure 3.2 below gives an example of an acyclic digraph. The set of dashed arcs in Figure 3.1 represents an oriented path from u to v , while the three remaining arcs form a circuit.

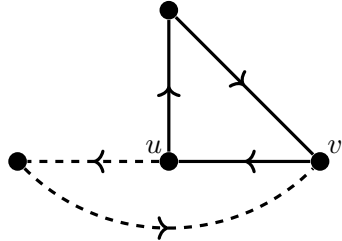


Figure 3.1. Oriented path and circuit

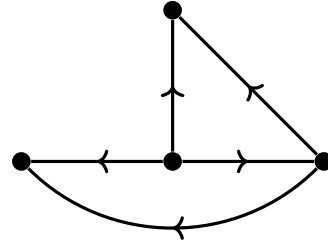


Figure 3.2. Acyclic digraph

We take a particular interest in *oriented spanning trees* contained in a digraph.

Definition 3.1.2 (Oriented spanning tree) We say that the digraph $T = (V, \hat{A})$ is an oriented spanning tree of $G = (V, A)$ (or simply a spanning tree of G) if the underlying undirected graph associated with T is a tree. We say that the oriented spanning tree T is contained in G when $\hat{A} \subset A$.

We focus on the properties of strongly edge-connected digraphs, defined thereafter.

Definition 3.1.3 (Strongly edge-connected digraph) A digraph G is strongly edge-connected whenever for any pair (u, v) of its vertices, it contains a directed path going from u to v .

As should immediately be clear, any circuit is strongly edge-connected. An alternative example of a strongly edge-connected digraph is found in the digraph G from Figure 3.1, which consists of two circuits stacked to one another. We shall see that any strongly edge-connected digraph can be built in a similar fashion. In fact, G is also an example of a *minimally* strongly edge-connected digraph.

Definition 3.1.4 (Minimally strongly edge-connected digraph) A digraph $G = (V, A)$ is minimally strongly edge-connected if it is strongly edge-connected and all digraphs obtained from G by removing exactly one arc are not strongly edge-connected.

The number of arcs in a minimally strongly edge-connected digraph on n vertices is not fixed. The next proposition provides exact bounds, along with structural results.

Proposition 3.1.1 [27, Lemma 3] Let $G = (V, A)$ be minimally strongly edge-connected on $n \geq 2$ vertices. Then

$$n \leq |A| \leq 2(n - 1). \quad (3.1)$$

Moreover $|A| = n$ if and only if G is a circuit and $|A| = 2(n - 1)$ if and only if G is a bi-directed tree.

The expression *bi-directed tree*, used in Proposition 3.1.1, denotes a directed graph formed by replacing each edge in a tree with two arcs in either direction.

Example 3.1.2 Figures 3.3 and 3.4 below are two examples of minimally strongly edge-connected digraphs of minimal and maximal size, on $n = 4$ vertices.

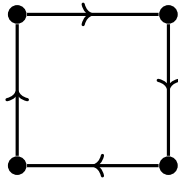


Figure 3.3. $|A| = n$

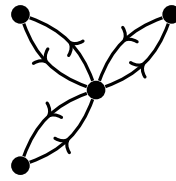


Figure 3.4. $|A| = 2(n - 1)$

We conclude this section with a characterization of strongly edge-connected digraphs based on cuts [28, page 7]. Although the next proposition is straightforward, we include a short proof for the sake of completeness.

Proposition 3.1.2 A digraph $G = (V, A)$ is not strongly edge-connected if and only if there exists an oriented cut of G , i.e. a set $\tilde{A} \subset A$ and two vertex-disjoint subgraphs $G_1 = (V_1, A_1)$ and $G_2 = (V_2, A_2)$ of G with $V_1 \neq \emptyset$, $V_2 \neq \emptyset$, such that

$$A = \tilde{A} \cup A_1 \cup A_2 \quad \text{and} \quad \forall (u, v) \in \tilde{A}, \quad u \in V_1 \text{ and } v \in V_2.$$

Proof. Suppose first that there exists an oriented cut of G given by $\tilde{A} \subset A$, $G_1 = (V_1, A_1)$ and $G_2 = (V_2, A_2)$. Let $v_1 \in V_1$ and $v_2 \in V_2$. By definition of an oriented cut, there does not exist a directed path in A joining v_2 to v_1 , proving that G is not strongly edge-connected.

Conversely, suppose that G is not strongly edge-connected and let v_1, v_2 be two vertices for which there is no $v_2 - v_1$ path in A . Let $V_2 \subset V$ be the set of vertices v such that A contains a $v_2 - v$ path and let $V_1 = V \setminus V_2$. If A_1 (resp. A_2) denotes the set of arcs between vertices of V_1 (resp. V_2), then $G_1 = (V_1, A_1)$, $G_2 = (V_2, A_2)$ and $\tilde{A} = A \setminus (A_1 \cup A_2)$ define an oriented cut for G as by construction, the arcs in \tilde{A} (if any) must be of the form (u_1, u_2) with $u_1 \in V_1$ and $u_2 \in V_2$. \square

Proposition 3.1.2 provides a negative certificate for strong connectivity. In the next section, we turn towards finding a positive certificate associated to such a property.

3.1.2 Ear-decomposition

Circuits were highlighted in Section 3.1.1 as a basic example of strongly edge-connected digraphs. In fact, it is easy to deduce from Definition 3.1.3 that any vertex of a strongly edge-connected digraph must be contained in a circuit. Based on this observation and on the concept of *ears* in digraphs, a decomposition result can be derived [10, Section 5.3].

Definition 3.1.5 (Ear and ear-decomposition) *An ear of the digraph $G = (V, A)$ is a directed path $\{(u_i, u_{i+1})\}_{i=1, \dots, k} \subset A$ such that for any $i \in \llbracket 2, k \rrbracket$, u_i is the head and the tail of exactly one arc in A .*

The digraph $G = (V, A)$ possesses an ear-decomposition if there exists a sequence of digraphs $\{G_i = (V_i, A_i)\}_{i \in \llbracket 1, s \rrbracket}$ such that

- (i) $V_1 \subseteq V_2 \subseteq \dots \subseteq V_s = V$,
- (ii) $A_1 \subseteq A_2 \subseteq \dots \subseteq A_s = A$,
- (iii) G_1 consists of one vertex and no arcs,
- (iv) For any $i \in \llbracket 2, s \rrbracket$, $A_i \setminus A_{i-1}$ defines an ear of G_i .

Figures 3.5 to 3.8 describe an ear-decomposition of a digraph which happens to be strongly edge-connected.

Example 3.1.3 *Each of the digraphs below is obtained from the previous one by adding an ear. Together, these graphs form a sequence corresponding to an ear-decomposition of Figure 3.8.*



Figure 3.5



Figure 3.6

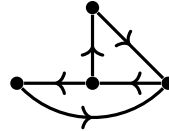


Figure 3.7

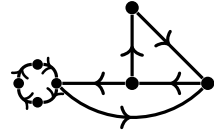


Figure 3.8

As announced, ear-decompositions are used as a tool to characterize strongly edge-connected digraphs.

Theorem 3.1.1 [70, Theorem 6.9] *A digraph $G = (V, A)$ is strongly edge-connected if and only if it possesses an ear-decomposition.*

Theorem 3.1.1 thus provides a positive certificate for the strongly edge-connected property. It is known that finding an ear-decomposition of a strongly edge-connected digraph can be done in linear time [10, Corollary 5.3.7]. On the other hand, determining the existence of an ear-decomposition with few non-trivial ears, or with ears of specific lengths is NP-complete [34, 10].

Let us now highlight a relationship between digraphs and PSSs based on network matrices. Using this relationship, we aim at creating an analog result to Theorem 3.1.1, adapted to PSSs.

3.2 Network matrices

This section outlines the main properties of a particular class of totally unimodular matrices constructed using directed graphs and oriented spanning trees [69, Section 13.3]. In particular, we show how such matrices can easily be made to be positively spanning.

3.2.1 Definition and examples

We take a particular interest in *network matrices*, a notion that generalizes that of incidence matrices.

Definition 3.2.1 (Network matrix) Let $G = (V, A)$ be a digraph with $A = \{(u_j, v_j)\}_{j=1}^m$ and let $T = (V, \hat{A})$ be an oriented spanning tree with $\hat{A} = \{(\hat{u}_i, \hat{v}_i)\}_{i=1}^n$. The network matrix associated with G and T is the matrix $\mathbf{M} \in \mathbb{R}^{n \times m}$ satisfying, for all $i \in \llbracket 1, n \rrbracket$ and all $j \in \llbracket 1, m \rrbracket$

$$\mathbf{M}_{i,j} = \begin{cases} 0 & \text{if the path } u_j - v_j \text{ in } T \text{ does not pass through } (\hat{u}_i, \hat{v}_i), \\ 1 & \text{if } u_j - v_j \text{ passes through } (\hat{u}_i, \hat{v}_i) \text{ in forward direction,} \\ -1 & \text{if } u_j - v_j \text{ passes through } (\hat{u}_i, \hat{v}_i) \text{ in backward direction.} \end{cases}$$

Note that there is no ambiguity in the definition as any path joining two vertices in T is unique. The incidence matrix of any digraph $G = (V, A)$ is a network matrix, as illustrated by the example below.

Example 3.2.1 The figure below represents a circuit $G = (V, A)$ on three vertices and its incidence matrix \mathbf{M} . After adding a new, isolated vertex in red, we obtain a new digraph $\hat{G} = (V \cup \{u\}, A)$. An oriented spanning tree T of \hat{G} is easily obtained by transforming u into a universal vertex. This tree is represented by the dashed, red arcs. Then \mathbf{M} is a network matrix associated to \hat{G} and T as for all i , the i^{th} column of \mathbf{M} represents the i^{th} arc of \hat{G} .



Figure 3.9. Incidence and network matrix

For simplicity, we focus on network matrices whose associated spanning tree T is contained in the associated digraph G - see Definition 3.1.2. An example is provided below

Example 3.2.2 The network matrix \mathbf{M} below is associated to the directed graph G on its left and to the spanning tree T contained in G and represented by the non-dashed arcs. The i^{th} column of \mathbf{M} represents the arc labeled i .

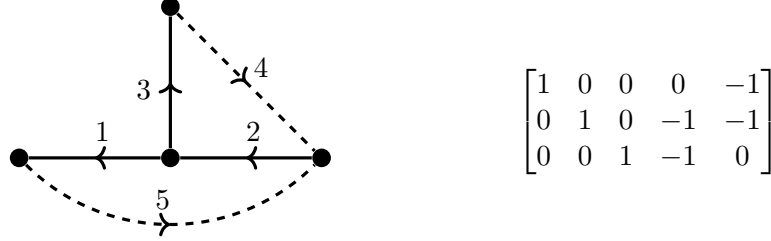


Figure 3.10. Digraph, spanning tree and network matrix

Network matrices play an important role in linear programming, as they are totally unimodular [70]. Moreover, two network matrices associated to the same graph and spanning tree but to a different ordering of the arcs are structurally equivalent, in the sense of Definition 2.2.1 [69, Section 19.3, page 277]. This is the object of Proposition 3.2.1, which we state and demonstrate below. Owing to this proposition, in the rest of this manuscript and unless otherwise needed, we will not specify the arc orderings anymore.

Proposition 3.2.1 Let $G = (V, A)$ be a strongly edge-connected digraph with $|V| = n + 1$ and $|A| = m$. Let $T = (V, \hat{A})$ with $\hat{A} \subset A$ be a spanning tree of G and let $\mathbf{M} \in \mathbb{R}^{n \times m}$ be the associated network matrix. Then, a matrix \mathbf{M}' is a network matrix for G and for a spanning tree T' contained in G if and only if $\mathbf{M}' = \mathbf{B}^{-1}\mathbf{M}\mathbf{P}$ where $\mathbf{B} \in \mathbb{R}^{n \times n}$ is nonsingular, $\text{col}(\mathbf{B}) \subset \text{col}(\mathbf{M})$ and $\mathbf{P} \in \mathbb{R}^{m \times m}$ is a permutation matrix.

Proof. Letting $A = \{a_1, \dots, a_m\}$ and $T = (V, \hat{A})$, we assume without loss of generality that $\hat{A} = \{a_1, \dots, a_n\}$ and that the columns of \mathbf{M} , denoted by $\mathbf{c}_1, \dots, \mathbf{c}_m$, correspond to the arcs a_1, \dots, a_m in that order. Since \mathbf{M} is a network matrix, we thus have $\mathbf{c}_i = \mathbf{e}_i$ for every $i \in \{1, \dots, n\}$, while any \mathbf{c}_i with $i \in \{m + 1, \dots, n\}$ has coefficients in $\{-1, 0, 1\}$. Suppose first that \mathbf{M}' is a network matrix associated with G and with a spanning tree $T' = (V, \hat{A}')$ such that $\hat{A}' \subset A$, and let a_{i_1}, \dots, a_{i_n} denote the arcs in \hat{A}' with $1 \leq i_1 < i_2 < \dots < i_n \leq m$. There exists a permutation matrix $\mathbf{P} \in \mathbb{R}^{m \times m}$ such that the columns of $\mathbf{P}_i = \mathbf{M}'\mathbf{P}^{-1}$, denoted by $\mathbf{c}'_1, \dots, \mathbf{c}'_m$, correspond to arcs a_1, \dots, a_m in that order. Then, for any $1 \leq j \leq n$, we have $\mathbf{c}'_{i_j} = \mathbf{e}_j$. Moreover, since \hat{A}' defines a tree on G , the columns $\mathbf{c}_{i_1}, \dots, \mathbf{c}_{i_n}$ of \mathbf{M} define a basis of \mathbb{R}^n . Letting $\mathbf{B} \in \mathbb{R}^{n \times n}$ be the matrix defined with those columns in order, it follows that \mathbf{B} is a nonsingular matrix defining the change of basis from $\{\mathbf{c}_i\}_{i=1, \dots, n}$ to $\text{col}(\mathbf{B}) = \{\mathbf{c}_{i_j}\}_{j=1, \dots, n}$. As a result, we have $\mathbf{B}\mathbf{c}'_{i_j} = \mathbf{B}\mathbf{e}_j = \mathbf{c}_{i_j}$ for any $1 \leq j \leq n$ and $\mathbf{B}\mathbf{c}'_i = \mathbf{e}_i$ for any $1 \leq i \leq n$, from which it follows that $\mathbf{B}\mathbf{P}_i = \mathbf{M}$. Overall, we have shown

that $\mathbf{B}\mathbf{M}'\mathbf{P}^{-1} = \mathbf{M}$ with \mathbf{B} nonsingular such that $\text{col}(\mathbf{B}) \subset \text{col}(\mathbf{M})$ and \mathbf{P} a permutation matrix.

Suppose now that $\mathbf{M}' = \mathbf{B}^{-1}\mathbf{M}\mathbf{P}$ with $\mathbf{B} \in \mathbb{R}^{n \times n}$ nonsingular such that $\text{col}(\mathbf{B}) \subset \text{col}(\mathbf{M})$ and \mathbf{P} a permutation matrix. Since \mathbf{B} is nonsingular, the columns of \mathbf{B} , which we denote by $\mathbf{c}_{i_1}, \dots, \mathbf{c}_{i_n}$ with $1 \leq i_1 < i_2 < \dots < i_n \leq m$, define a basis of \mathbb{R}^n . Consequently, those columns define a set of arcs $\hat{A}' = \{a_{i_j}\}_{j=1, \dots, n}$ such that $T' = (V, \hat{A}')$ is a spanning tree for G . Since \mathbf{B} represents the change of basis from $\mathbf{c}_1, \dots, \mathbf{c}_n$ to $\mathbf{c}_{i_1}, \dots, \mathbf{c}_{i_n}$, the columns of $\mathbf{B}^{-1}\mathbf{M}$ represent the expression of each path in the basis $\{\mathbf{c}_{i_j}\}_{j=1, \dots, n}$. It follows that $\mathbf{B}^{-1}\mathbf{M} = \mathbf{M}'\mathbf{P}^{-1}$ is a network matrix, hence \mathbf{M}' is also a network matrix associated with the same spanning tree. \square

3.2.2 Network matrices and positive spanning property

We now turn to the main result of this chapter, which establishes a direct connection between PSSs and strongly edge-connected digraphs. A similar result was stated without proof by Marcus [50]. However, to the best of our knowledge, Theorem 3.2.1 in its present form and its proof are new.

Theorem 3.2.1 *Let $T = (V, \hat{A})$ be an oriented spanning tree contained in a digraph $G = (V, A)$ with $|\hat{A}| = n$. Let $\mathbf{M} \in \mathbb{R}^{n \times m}$ be the associated network matrix. Then, the matrix \mathbf{M} is a PSS for \mathbb{R}^n if and only if the graph G is strongly edge-connected.*

Proof. Without loss of generality, we consider an ordering $A = \{a_i\}_{i=1}^m$ such that $\hat{A} = \{a_i\}_{i=1}^n$. As a result, the first n columns of \mathbf{M} form the identity matrix \mathbf{I}_n , thus ensuring that \mathbf{M} has full row rank. We now proceed with the proof.

Suppose first that G is strongly edge-connected and consider an ear-decomposition $\{G_i = (V_i, A_i)\}$ associated with G . Since G_1 consists of a single vertex without arcs, there exists no circuit within G_1 . Now, for any $i \in \llbracket 2, k \rrbracket$, consider the ear of G_i defined by $A_i \setminus A_{i-1}$. The arcs in this ear belong to a circuit of G that possibly contains other arcs in G_{i-1} . Let $\mathbf{x}_i \in \mathbb{R}^m$ be the characteristic vector of this circuit, i.e. $[\mathbf{x}_i]_j = 1$ if arc a_j is in the circuit, and $[\mathbf{x}_i]_j = 0$ otherwise. Then, we have $\mathbf{M}\mathbf{x}_i = \mathbf{0}_n$. Finally, consider the vector $\mathbf{x} = \sum_{i=2}^s \mathbf{x}_i$. This vector has positive coefficients, since every arc in G is contained in an ear of the decomposition. We have thus found a positive vector \mathbf{x} such that $\mathbf{M}\mathbf{x} = \mathbf{0}_n$, hence \mathbf{M} is a PSS by Proposition 2.1.1.

Conversely, suppose that G is *not* strongly edge-connected. We will show that there exists a vector $\mathbf{y} \in \mathbb{R}^n$ such that $\mathbf{y}^\top \mathbf{M} \geq \mathbf{0}_m$, thereby implying that \mathbf{M} is not a PSS thanks to Proposition 2.1.2. Since G is not strongly edge-connected, Proposition 3.1.2 ensures that there exists a set $\tilde{A} \subset A$ and two subgraphs $G_1 = (V_1, A_1)$, $G_2 = (V_2, A_2)$ that define an oriented cut of G . Then, since G is connected, we find that $\tilde{A} \cap \hat{A}$ is non-empty. Without

loss of generality, we assume that $\tilde{A} \cap \hat{A} = \{a_1, \dots, a_k\}$ for some $k \leq n$. Consider the vector $\mathbf{y} = \sum_{\ell=1}^k \mathbf{y}_\ell$, where \mathbf{y}_ℓ is the ℓ^{th} column of \mathbf{M} . Since the first n columns of \mathbf{M} correspond to the identity matrix, it follows that

$$\mathbf{y}^\top \mathbf{y}_i = \begin{cases} 1 & \text{if } i \in \llbracket 1, k \rrbracket \\ 0 & \text{if } i \in \llbracket k+1, n \rrbracket. \end{cases}$$

In addition, if $i \in \llbracket n+1, m \rrbracket$, then two situations can occur. If arc a_i belongs to either A_1 or A_2 , then the directed path in T linking the head and tail of a_i must thus contain an even number of arcs in \tilde{A} (possibly 0), with half of them used in the forward direction. As a result, one must have

$$\mathbf{y}^\top \mathbf{y}_i = \sum_{\ell=1}^k \mathbf{y}_\ell^\top \mathbf{y}_i = 0.$$

Otherwise a_i belongs to $A \setminus (A_1 \cup A_2)$, that is $a_i \in \tilde{A}$ therefore the tail of a_i is in V_1 and its head is in V_2 . As a result, the directed path in T linking the head and tail of a_i must use an odd number of arcs in $\tilde{A} \cap \hat{A}$, with one more arc in the forward direction. Thus,

$$\mathbf{y}^\top \mathbf{y}_i = \sum_{\ell=1}^k \mathbf{y}_\ell^\top \mathbf{y}_i = 1.$$

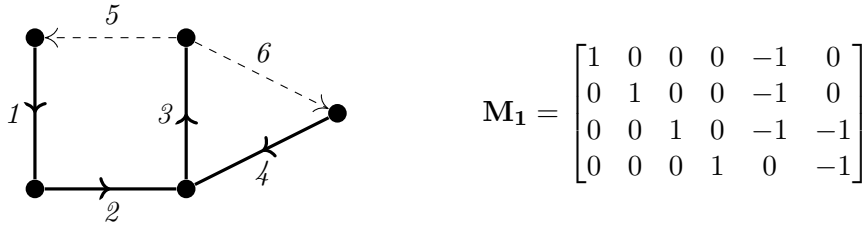
Overall, we have shown that $\mathbf{y}^\top \mathbf{M} \geq \mathbf{0}_m$, from which we conclude that \mathbf{M} cannot be a PSS. \square

Theorem 3.2.1 provides positive and negative certificates regarding the PSS (or non-PSS) nature of a network matrix based on those for strongly edge-connected digraphs. More generally, the theorem yields the following relationship between positive bases and minimally strongly edge-connected digraphs.

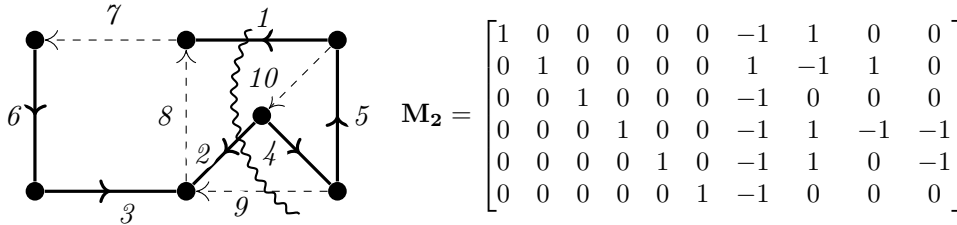
Corollary 3.2.1 *Let $G = (V, A)$ be a connected digraph with $|V| = n$ and $|A| = n - 1 + s$ and let $T = (V, \hat{A})$ be an oriented spanning tree contained in G . Let $\mathbf{D} \in \mathbb{R}^{(n-1) \times (n-1+s)}$ be a network matrix associated with $\{G, T\}$. Then, \mathbf{D} is a positive basis for \mathbb{R}^{n-1} if and only if G is minimally strongly edge-connected.*

We illustrate below the results of Theorem 3.2.1 and of its corollary.

Example 3.2.3 (A PSS network matrix) *The positive basis \mathbf{M}_1 is a network matrix associated to the minimally strongly edge-connected digraph below and to the spanning tree formed by the thick arcs.*



Example 3.2.4 (A non-PSS network matrix) Let $T = (V, \hat{A})$ be the spanning tree formed by the thick arcs in the digraph G below. The wavy cut \tilde{A} certifies that G is not strongly edge-connected. Similarly, the network matrix \mathbf{M}_2 is not a PSS as the characteristic vector $\mathbf{y}^\top = [1 \ 1 \ 0 \ 0 \ 0 \ 0]$ of $\tilde{A} \cap \hat{A}$ in T satisfies $\mathbf{y}^\top \mathbf{M}_2 \geq \mathbf{0}_{10}$.



In the next section, we will exploit the link between strongly edge-connected digraphs and PSSs by showing that the ear-decomposition can be extended to more general matrices.

3.3 Ear-decomposition for PSSs

Theorem 3.1.1 states that a digraph is strongly edge-connected if and only if it admits an ear-decomposition. Together with Theorem 3.2.1, it thus implies that a network matrix is a PSS if and only if its associated graph admits an ear-decomposition. We will now establish a similar result for positive spanning sets, thereby generalizing Theorem 3.1.1. To this end, we start this section by extending the notions of circuits and acyclic graphs to matrices.

3.3.1 Acyclic and circuit matrices

The ear-decomposition for strongly edge-connected digraphs relies on the fundamental notion of circuit. Our goal is to define an equivalent concept for matrices. To this end, we first introduce the companion notion of acyclic matrix, inspired by acyclic graphs.

Definition 3.3.1 (Acyclic matrix) A matrix $\mathbf{A} \in \mathbb{R}^{n \times m}$ is called acyclic if

$$[\mathbf{Ax} = \mathbf{0}_n \text{ and } \mathbf{x} \geq \mathbf{0}_m] \Leftrightarrow \mathbf{x} = \mathbf{0}_m.$$

Per Definition 3.3.1, any network matrix associated to an acyclic graph is acyclic. Alternative characterizations can be obtained from Gordan's Lemma [46].

Proposition 3.3.1 *For any $\mathbf{A} \in \mathbb{R}^{n \times m}$, the following statements are equivalent.*

- (i) *The matrix \mathbf{A} is acyclic.*
- (ii) *There exists a nonzero vector $\mathbf{y} \in \mathbb{R}^n$ such that $\mathbf{y}^\top \mathbf{A} > \mathbf{0}_m^\top$.*
- (iii) *For any $\bar{\mathbf{A}} \in \mathbb{R}^{n \times \bar{m}}$ with $\text{col}(\bar{\mathbf{A}}) \subset \text{col}(\mathbf{A})$ and $\bar{m} > 0$, $\text{pspan}(\bar{\mathbf{A}})$ is not a linear space.*

Proof. The equivalence between (i) and (ii) is a restatement of Gordan's lemma. The equivalence between (i) and (iii) follows from that between the first and last statements of Proposition 2.1.1. \square

From Proposition 3.3.1, we note that matrices with positive entries are necessarily acyclic. In fact, positive entries characterize acyclic matrices in the following sense.

Proposition 3.3.2 *A matrix $\mathbf{A} \in \mathbb{R}^{n \times m}$ is acyclic if and only if it is structurally equivalent to a matrix with positive entries.*

Proof. Suppose first that \mathbf{A} is acyclic. From Proposition 3.3.1(ii), there exists $\mathbf{y} \in \mathbb{R}^n$ such that $\mathbf{y}^\top \mathbf{A} > \mathbf{0}_m^\top$. Then, there exists $\eta > 0$ such that the

matrix $\mathbf{B} = \begin{bmatrix} \mathbf{y}^\top \\ \dots \\ \mathbf{y}^\top \end{bmatrix} + \eta \mathbf{I}_n \in \mathbb{R}^{n \times n}$ is invertible and $\mathbf{B}\mathbf{A}$ has positive entries,

proving the desired result.

Conversely, suppose that \mathbf{A} is not acyclic. Then, there must exist a nonzero vector $\mathbf{x} \geq \mathbf{0}_m$ such that $\mathbf{A}\mathbf{x} = \mathbf{0}_n$. For any invertible matrix \mathbf{B} , one then has $\mathbf{B}^{-1}\mathbf{A}\mathbf{x} = \mathbf{0}_n$, hence the matrix $\mathbf{B}^{-1}\mathbf{A}$ must have one non-positive entry.

\square

Proposition 3.3.2 provides a certificate for showing that a matrix is acyclic, by finding a basis defining a structurally equivalent matrix. A certificate for showing that a matrix is *not* acyclic is obtained by finding a nonzero vector with nonnegative entries in the null space of the matrix.

We are now ready to provide the definition of a circuit matrix.

Definition 3.3.2 (Circuit) *A matrix $\mathbf{C} \in \mathbb{R}^{n \times m}$ is called a circuit matrix if it is a PSS for some linear subspace \mathbb{L} of \mathbb{R}^n and if any matrix $\bar{\mathbf{C}} \in \mathbb{R}^{n \times \bar{m}}$ formed by $0 < \bar{m} < \dim(\mathbb{L}) + 1$ columns of \mathbf{C} is acyclic.*

The next proposition shows that circuit matrices can be identified with minimal positive bases. Those are instrumental in obtaining decompositions of PSSs, and we will use circuit matrices for a similar purpose in the next section. In particular, the following structural equivalence will be leveraged.

Proposition 3.3.3 *Let $\mathbf{C} \in \mathbb{R}^{n \times m}$ be a circuit matrix. Then \mathbf{C} is a positive basis for a linear subspace of dimension $\ell = m - 1$, therefore*

$$\mathbf{C} \equiv \begin{bmatrix} \mathbf{I}_\ell & -\mathbf{1}_\ell \\ \mathbf{0}_{n-\ell, \ell} & \mathbf{0}_{n-\ell} \end{bmatrix}. \quad (3.2)$$

Proof. By definition, \mathbf{C} is a PSS for some linear subspace \mathbb{L} of \mathbb{R}^n . For the purpose of contradiction, suppose that $m > \ell + 1$, where $\ell = \dim(\mathbb{L})$. Since \mathbf{C} is a PSS for \mathbb{L} , Proposition 2.1.1 ensures that there exists a positive vector $\mathbf{x} \in \mathbb{R}^n$ such that $\mathbf{C}\mathbf{x} = \mathbf{0}_n$. In addition, there also exists a matrix $\tilde{\mathbf{C}} \in \mathbb{R}^{n \times (m-1)}$ formed by columns of \mathbf{C} such that $\text{span}(\tilde{\mathbf{C}}) = \mathbb{L}$. Without loss of generality, suppose that $\tilde{\mathbf{C}}$ consists of the first $m - 1$ columns of \mathbf{C} . Since $m - 1 > \ell$, the matrix $\tilde{\mathbf{C}}$ has a nonzero null space, i.e. there exists a nonzero vector $\tilde{\mathbf{y}} \in \mathbb{R}^{m-1}$ such that $\tilde{\mathbf{C}}\tilde{\mathbf{y}} = \mathbf{0}_{m-1}$. Letting $\mathbf{y} = [\tilde{\mathbf{y}}^\top \ 0]^\top$, it follows that $\mathbf{C}\mathbf{y} = \mathbf{0}_n$.

Now, the vectors \mathbf{x} and \mathbf{y} are not colinear since $[\mathbf{x}]_m > 0 = [\mathbf{y}]_m$. Therefore, there exists $\sigma \geq 0$ such that $\mathbf{z} = \sigma\mathbf{x} + \mathbf{y} \geq \mathbf{0}_n$ with \mathbf{z} having at least one component equal to zero. Let $\tilde{\mathbf{C}}$ be the matrix formed by columns of \mathbf{C} corresponding to nonzero components of \mathbf{z} , and let $\tilde{\mathbf{z}}$ be the vector formed by those components. It follows from the construction of $(\tilde{\mathbf{C}}, \tilde{\mathbf{z}})$ that

$$\tilde{\mathbf{C}}\tilde{\mathbf{z}} = \mathbf{C}\mathbf{z} = \mathbf{C}(\sigma\mathbf{x} + \mathbf{y}) = \mathbf{0}_n.$$

As a result, we have shown that $\tilde{\mathbf{C}}$ satisfies Proposition 2.1.1, and thus it must be a PSS for some linear space of \mathbb{R}^n . Therefore, $\tilde{\mathbf{C}}$ is not acyclic, and this contradicts the fact that \mathbf{C} is a circuit, from which we conclude that $m = \ell + 1$.

The second part of the result then follows from Corollary 2.2.1. \square

Note that Proposition 3.3.3 justifies the terminology *circuit matrix*, as a circuit of $n + 1$ vertices admits $[\mathbf{I}_n \ -\mathbf{1}_n]$ as a network matrix. Using structural equivalence for circuits, we can obtain an improved certificate for non-acyclic matrices.

Lemma 3.3.1 *A matrix $\mathbf{M} \in \mathbb{R}^{n \times m}$ is not acyclic if and only if*

- (i) *One of the columns of \mathbf{M} is the zero vector $\mathbf{0}_n$, or*
- (ii) *There exists $\ell \in \llbracket 1, n \rrbracket$ such that*

$$\mathbf{M} \equiv \begin{bmatrix} \mathbf{I}_\ell & -\mathbf{1}_\ell & \mathbf{X} \\ \mathbf{0}_{n-\ell, \ell} & \mathbf{0}_{n-\ell} & \mathbf{Y} \end{bmatrix},$$

where the matrices $\mathbf{X} \in \mathbb{R}^{\ell \times (m-\ell-1)}$ and $\mathbf{Y} \in \mathbb{R}^{(n-\ell) \times (m-\ell-1)}$ can be empty.

Proof. If (i) holds, then the matrix \mathbf{M} is not acyclic as Proposition 3.3.1(ii) fails. If (ii) holds, then the first $\ell + 1$ columns of \mathbf{M} form a matrix $\bar{\mathbf{M}}$ such that $\text{pspan}(\bar{\mathbf{M}})$ is a linear space. Thus, Proposition 3.3.1(iii) fails to hold, hence \mathbf{M} is not acyclic. Conversely, suppose that \mathbf{M} is not acyclic. Then by Proposition 3.3.1(iii), there must exist a matrix \mathbf{C} formed by a subset of columns of \mathbf{M} such that $\text{pspan}(\mathbf{C})$ is a linear space. Without loss of generality, suppose that this matrix is minimal for that property, and that it consists of the first $\ell + 1$ columns of \mathbf{M} (thus the linear subspace spanned by \mathbf{C} is of dimension ℓ). Then the matrix \mathbf{C} is a circuit. Applying Proposition 3.3.3, we then know that there exists an invertible matrix \mathbf{B} , a permutation matrix \mathbf{P} and a diagonal matrix Δ with positive diagonal entries such that

$$\mathbf{B}^{-1}\mathbf{C}\mathbf{P}\Delta = \begin{bmatrix} \mathbf{I}_\ell & -\mathbf{1}_\ell \\ \mathbf{0}_{n-\ell,\ell}^\top & \mathbf{0}_{n-\ell} \end{bmatrix}.$$

Letting then $\mathbf{P}' = \begin{bmatrix} \mathbf{P}\Delta & \mathbf{0}_{\ell+1,m-\ell-1} \\ \mathbf{0}_{m-\ell-1,\ell+1} & \mathbf{I}_{m-\ell-1} \end{bmatrix} \in \mathbb{R}^{m \times m}$, it follows that $\mathbf{M} \equiv \mathbf{B}^{-1}\mathbf{M}\mathbf{P}'$, that has the desired structure. \square

A consequence of Lemma 3.3.1 is that the vector $\mathbf{x} = \begin{bmatrix} \mathbf{1}_{\ell+1} \\ \mathbf{0}_{m-\ell-1} \end{bmatrix}$ can be used to attest that \mathbf{M} is not acyclic by structural equivalence, thus improving over the certificate from Proposition 3.3.2.

3.3.2 A new certificate for positive spanning sets

Building on the results of the previous subsection, we now generalize the concept of ear-decomposition of digraphs to matrices. As a result, we will obtain a characterization of PSSs improving that of Corollary 2.2.2.

Definition 3.3.3 (Negative row echelon matrix) *A matrix $\mathbf{N} \in \mathbb{R}^{n \times s}$, with $1 \leq s \leq n$, is a negative row echelon matrix (NEM) if there exists a sequence $z_0 = 1 < z_1 < z_2 < \dots < z_{s-1} \leq n$ such that*

- (i) For all $j \in \llbracket 1, s-1 \rrbracket$, for all $i \in \llbracket z_j, n \rrbracket$, $\mathbf{N}_{i,j} = 0$.
- (ii) For all $j \in \llbracket 1, s-1 \rrbracket$, for all $i \in \llbracket z_{j-1}, z_j - 1 \rrbracket$, $\mathbf{N}_{i,j} = -1$.
- (iii) $\mathbf{N}_{i,s} = -1$, for all $i \geq z_{s-1}$.

An example of NEM is

$$\begin{bmatrix} -1 & \times & \times & \times \\ -1 & \times & \times & \times \\ 0 & -1 & \times & \times \\ 0 & -1 & \times & \times \\ 0 & 0 & -1 & \times \\ 0 & 0 & 0 & -1 \end{bmatrix},$$

where the crosses \times indicate arbitrary values. Matrices of that form can be used to create PSSs as follows.

Proposition 3.3.4 *Let $\mathbf{M} \in \mathbb{R}^{n \times (n+s)}$ with $s \in \llbracket 1, n \rrbracket$ such that $\mathbf{M} \equiv \begin{bmatrix} \mathbf{I}_n & \mathbf{N} \end{bmatrix}$ where \mathbf{N} is a NEM. Then, \mathbf{M} is a PSS.*

Proof. Let $\mathbf{N} = [\mathbf{u}_1 \ \cdots \ \mathbf{u}_s]$. Consider the vectors $\{\mathbf{w}_i\}_{i=1, \dots, s}$ defined by

$$\begin{aligned} \mathbf{w}_1 &= \mathbf{u}_s \\ \forall i = 1, \dots, s-1, \quad \mathbf{w}_{i+1} &= \mathbf{w}_i + 2\|\mathbf{w}_i\|_\infty \mathbf{u}_{s-i}. \end{aligned}$$

By construction, the vector \mathbf{w}_s is a positive linear combination of the columns of \mathbf{N} and all its components are negative. It follows that there exists a positive combination of columns of $\begin{bmatrix} \mathbf{I}_n & \mathbf{N} \end{bmatrix}$ adding to $\mathbf{0}_n$, i.e. a vector $\mathbf{x} \in \mathbb{R}^{n+s}$ with positive coefficients such that $\begin{bmatrix} \mathbf{I}_n & \mathbf{N} \end{bmatrix} \mathbf{x} = \mathbf{0}_n$. By Proposition 2.1.1(iii) and structural equivalence, this implies that \mathbf{M} is also a PSS. \square

Proposition 3.3.4 complements Corollary 2.2.2 in that it provides a sufficient condition for a matrix to be a PSS. Note that the result can be generalized to any matrix \mathbf{M} such that $\mathbf{M} \equiv \begin{bmatrix} \mathbf{I}_\ell & \mathbf{N} \\ \mathbf{0}_{n-\ell, \ell} & \mathbf{0}_{n-\ell, m-\ell} \end{bmatrix}$ where \mathbf{N} is NEM. Such a matrix \mathbf{M} is indeed a PSS for some ℓ -dimensional linear space.

We now aim at providing certificates for determining whether a matrix is a PSS using NEMs, based on identifying a desirable structure within the matrix. Recall from Gaussian elimination that any matrix in $\mathbb{R}^{n \times m}$ is structurally equivalent to a matrix of the form

$$\begin{bmatrix} \mathbf{I}_\ell & \mathbf{X} \\ \mathbf{0}_{n-\ell, \ell} & \mathbf{0}_{n-\ell, m-\ell} \end{bmatrix},$$

for some $\ell \in \llbracket 0, n \rrbracket$ and some matrix $\mathbf{X} \in \mathbb{R}^{\ell \times (m-\ell)}$. When $\ell = n$ and \mathbf{X} is a NEM, such a structure allows to conclude that the matrix is a spanning set of \mathbb{R}^n . Following Proposition 3.3.4, we now define structures of interest for positive spanning sets.

Definition 3.3.4 (IN and INA matrix) *Given dimensions n, m , let $\ell \in \llbracket 1, n \rrbracket$ and $k \in \llbracket 0, m - \ell \rrbracket$.*

(i) An IN matrix in $\mathbb{R}^{n \times m}$ is a matrix of the form

$$\begin{bmatrix} \mathbf{I}_{n,\ell} & \mathbf{N} & \mathbf{X} \end{bmatrix}, \quad (3.3)$$

where $\mathbf{I}_{n,\ell}$ represents the first ℓ columns of the identity matrix in $\mathbb{R}^{n \times n}$, $k \leq n$, $\mathbf{N} \in \mathbb{R}^{n \times k}$ is a NEM when $k > 0$ and $\mathbf{X} \in \mathbb{R}^{n \times (m-\ell-k)}$ is arbitrary.

(ii) An INA matrix in $\mathbb{R}^{n \times m}$ is a matrix of the form

$$\begin{bmatrix} \mathbf{I}_\ell & \mathbf{N} & \mathbf{X} \\ \mathbf{0}_{n-\ell,\ell} & \mathbf{0}_{n-\ell,k} & \mathbf{A} \end{bmatrix}, \quad (3.4)$$

where $k \leq \ell < n$, $\mathbf{N} \in \mathbb{R}^{\ell \times k}$ is a NEM when $k > 0$, $\mathbf{X} \in \mathbb{R}^{n \times (m-\ell-k)}$ is arbitrary and $\mathbf{A} \in \mathbb{R}^{(n-\ell) \times (m-\ell-k)}$ is an acyclic matrix.

Since the definition of IN and INA matrices allows for $k = 0$, any nonzero matrix is structurally equivalent to an IN matrix with $k = 0$, per the Gaussian elimination argument above. However, the NEM and acyclic components in IN and INA matrices, respectively, allow for identifying positive spanning properties (or lack thereof) of a matrix. This is the purpose of the following theorem, that forms the central result of this chapter.

Theorem 3.3.1 *Let $\mathbf{M} \in \mathbb{R}^{n \times m}$ be a nonzero matrix with $n \geq 2$.*

- (i) \mathbf{M} is a PSS of \mathbb{R}^n if and only if \mathbf{M} is structurally equivalent to an IN matrix with $\ell = n$ and $k > 0$.
- (ii) \mathbf{M} is not a PSS of \mathbb{R}^n if and only if \mathbf{M} is structurally equivalent to an INA matrix.

Proof. For both results, the reverse implication is immediate. Indeed, if \mathbf{M} is structurally equivalent to an IN matrix with $\ell = n$ and $k > 0$, Proposition 3.3.4 guarantees that this IN matrix contains a PSS of \mathbb{R}^n , thus both this IN matrix and \mathbf{M} are PSSs of \mathbb{R}^n . In addition, if \mathbf{M} is structurally equivalent to an INA matrix, Proposition 3.3.2 implies that \mathbf{M} is also structurally equivalent to a matrix whose last $n - \ell$ rows are nonnegative.

In the rest of the proof, we thus focus on establishing the forward implication for both (i) and (ii) through an induction argument on the dimension m . Note that $m < n + 1$ implies that \mathbf{M} cannot be a PSS and that it is structurally equivalent to an INA matrix with $k = 0$.

Suppose first that $m = n + 1$. On one hand, if \mathbf{M} is a PSS, then it is also a circuit matrix with $\ell = n$. Proposition 3.3.3 then ensures that \mathbf{M} is equivalent to an IN matrix with $\ell = n$ and $k = 1$. On the other hand, if \mathbf{M} is not a PSS it is either acyclic - and structurally equivalent to an INA matrix with $\ell = k = 0$ - or it contains a circuit, say of length ℓ . We choose

this circuit such that $\ell < n$ is as large as possible. From Proposition 3.3.3, it follows that $\mathbf{M} \equiv \begin{bmatrix} \mathbf{I}_\ell & -\mathbf{1}_\ell & \bar{\mathbf{X}} \\ \mathbf{0}_{n-\ell,\ell} & \mathbf{0}_{n-\ell} & \bar{\mathbf{A}} \end{bmatrix}$, where $\bar{\mathbf{X}} \in \mathbb{R}^{\ell \times (n-\ell)}$ is arbitrary and $\bar{\mathbf{A}} \in \mathbb{R}^{(n-\ell) \times (n-\ell)}$ is acyclic from the definition of ℓ . It follows that \mathbf{M} is equivalent to an INA matrix with $k = 1$, and we have thus shown that (i) and (ii) hold for $m = n + 1$ whenever $n \geq 2$.

Suppose now that $m > n + 1$, and that (i) and (ii) hold for any $n \geq 2$ and any $\tilde{m} \in \llbracket n + 1, m - 1 \rrbracket$. We will establish that (i) and (ii) hold as well.

On the one hand, suppose that \mathbf{M} is a PSS of \mathbb{R}^n . If there exists a strict subset of columns of \mathbf{M} that is a PSS of \mathbb{R}^n , let $\bar{\mathbf{M}} \in \mathbb{R}^{n \times \tilde{m}}$ be a matrix formed by these columns. Then, $\mathbf{M} \equiv [\bar{\mathbf{M}} \ \mathbf{X}_1]$ for some matrix $\mathbf{X}_1 \in \mathbb{R}^{n \times (m-\tilde{m})}$. Since $\tilde{m} < m$ by assumption, the induction argument applied to $\bar{\mathbf{M}}$ guarantees that $\bar{\mathbf{M}}$ is equivalent to an IN matrix, i.e.

$$\bar{\mathbf{M}} \equiv [\mathbf{I}_n \ \bar{\mathbf{N}} \ \bar{\mathbf{X}}],$$

where $\bar{\mathbf{N}} \in \mathbb{R}^{n \times k}$ is a NEM with $k > 0$. Letting $\mathbf{X} = [\bar{\mathbf{X}} \ \mathbf{X}_1]$, it follows that \mathbf{M} is equivalent to the IN matrix $[\mathbf{I}_n \ \bar{\mathbf{N}} \ \mathbf{X}]$.

If no strict subset of columns of \mathbf{M} is a PSS of \mathbb{R}^n , we use the fact that \mathbf{M} is a PSS, thus it is not acyclic. Lemma 3.3.1 then guarantees that there exists $\ell_1 \in \llbracket 1, n \rrbracket$ such that

$$\mathbf{M} \equiv \begin{bmatrix} \mathbf{I}_{\ell_1} & -\mathbf{1}_{\ell_1} & \mathbf{X}_1 \\ \mathbf{0}_{n-\ell_1,\ell_1} & \mathbf{0}_{n-\ell_1} & \bar{\mathbf{M}} \end{bmatrix}. \quad (3.5)$$

where $\bar{\mathbf{M}} \in \mathbb{R}^{(n-\ell_1) \times \tilde{m}}$ with $\tilde{m} := m - (\ell_1 + 1) \in \llbracket (n - \ell_1) + 1, m - 1 \rrbracket$. Since \mathbf{M} is a PSS of \mathbb{R}^n , it follows from (3.5) that $\bar{\mathbf{M}}$ must be a PSS of $\mathbb{R}^{n-\ell_1}$. Applying the induction argument to $\bar{\mathbf{M}}$ yields the structural equivalence

$$\bar{\mathbf{M}} \equiv [\mathbf{I}_{n-\ell_1} \ \bar{\mathbf{N}} \ \bar{\mathbf{X}}],$$

where $\bar{\mathbf{N}}$ is a NEM, and $\bar{\mathbf{X}}$ is arbitrary. With an appropriate change of basis, the following equivalence holds:

$$\begin{bmatrix} \mathbf{I}_{\ell_1} & \mathbf{X}_1 \\ \mathbf{0}_{n-\ell_1,\ell_1} & \bar{\mathbf{M}} \end{bmatrix} \equiv \begin{bmatrix} \mathbf{I}_{\ell_1} & \mathbf{0}_{\ell_1,n-\ell_1} & \mathbf{X}_2 & \mathbf{X}_3 \\ \mathbf{0}_{n-\ell_1,\ell_1} & \mathbf{I}_{n-\ell_1} & \mathbf{N}_1 & \mathbf{X}_4 \end{bmatrix}$$

where \mathbf{N}_1 is a NEM and $\mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_4$ are arbitrary. It follows that

$$\mathbf{M} \equiv [\mathbf{I}_n \ \mathbf{N} \ \mathbf{X}] \quad \text{where} \quad \mathbf{N} = \begin{bmatrix} -\mathbf{1}_{\ell_1} & \mathbf{X}_2 \\ \mathbf{0}_{n-\ell_1} & \mathbf{N}_1 \end{bmatrix} \quad \text{and} \quad \mathbf{X} = \begin{bmatrix} \mathbf{X}_3 \\ \mathbf{X}_4 \end{bmatrix}.$$

Since \mathbf{N} is a NEM by construction, we have shown that \mathbf{M} is equivalent to an IN matrix with $\ell = n$ and $k > 0$.

On the other hand, suppose that \mathbf{M} is not a PSS of \mathbb{R}^n . If \mathbf{M} is acyclic, then it is an INA matrix with $\ell = k = 0$. Otherwise, Lemma 3.3.1 guarantees that there exists $\ell_1 \in \llbracket 1, n \rrbracket$ such that $\mathbf{M} \equiv \begin{bmatrix} \mathbf{I}_{\ell_1} & -\mathbf{1}_{\ell_1} & \mathbf{M}_1 \\ \mathbf{0}_{n-\ell_1, \ell_1} & \mathbf{0}_{n-\ell_1} & \mathbf{M}_2 \end{bmatrix}$, where $\mathbf{M}_2 \in \mathbb{R}^{n-\ell_1 \times (m-\ell_1)}$ does not positively span $\mathbb{R}^{n-\ell}$ as \mathbf{M} is not a PSS of \mathbb{R}^n . Applying the induction argument, it follows that \mathbf{M}_2 is structurally equivalent to an INA matrix, i.e.

$$\mathbf{M}_2 \equiv \begin{bmatrix} \mathbf{I}_{\bar{\ell}} & \bar{\mathbf{N}} & \bar{\mathbf{X}} \\ \mathbf{0}_{\bar{\ell}, \bar{\ell}} & \mathbf{0}_{\bar{\ell}} & \mathbf{A} \end{bmatrix} \quad \text{and so} \quad \mathbf{M} \equiv \begin{bmatrix} \mathbf{I}_{\ell_1} & -\mathbf{1}_{\ell_1} & \mathbf{0}_{\ell_1, \bar{\ell}} & \mathbf{X}_1 & \mathbf{X}_2 \\ \mathbf{0}_{\bar{\ell}, \ell_1} & \mathbf{0}_{\bar{\ell}} & \mathbf{I}_{\bar{\ell}} & \bar{\mathbf{N}} & \bar{\mathbf{X}} \\ \mathbf{0}_{\bar{\ell}, \ell_1} & \mathbf{0}_{\bar{\ell}} & \mathbf{0}_{\bar{\ell}, \bar{\ell}} & \mathbf{0}_{\bar{\ell}, k} & \mathbf{A} \end{bmatrix}$$

with $\bar{\ell} < n - \ell_1$, $\bar{\ell} = n - \ell_1 - \bar{\ell}$, $\bar{\mathbf{N}} \in \mathbb{R}^{\bar{\ell} \times k}$ a NEM and \mathbf{A} an acyclic matrix. Letting $\mathbf{X} = \begin{bmatrix} \bar{\mathbf{X}}_2 \\ \bar{\mathbf{X}} \end{bmatrix}$ and $\mathbf{N} = \begin{bmatrix} -\mathbf{1}_{\ell_1} & \mathbf{X}_1 \\ \mathbf{0}_{\bar{\ell}} & \bar{\mathbf{N}} \end{bmatrix}$ we obtain $\mathbf{M} \equiv \begin{bmatrix} \mathbf{I}_{n-\bar{\ell}} & \mathbf{N} & \mathbf{X} \\ \mathbf{0}_{\bar{\ell}, \bar{\ell}} & \mathbf{0}_{\bar{\ell}} & \mathbf{A} \end{bmatrix}$, hence \mathbf{M} is equivalent to an INA matrix with $\ell = \bar{\ell} < n$. \square

Remark 3.3.1 *Although Theorem 3.3.1 assumes $n \geq 2$, a similar result can be stated when $n = 1$. Indeed, given any nonzero matrix $\mathbf{M} \in \mathbb{R}^{1 \times m}$, is it clear that \mathbf{M} is a PSS of \mathbb{R} if and only if $\mathbf{M} \equiv [1 \quad -1 \quad \mathbf{X}]$ for some arbitrary $\mathbf{X} \in \mathbb{R}^{1 \times (m-2)}$, while it is not a PSS if and only if $\mathbf{M} \equiv [1 \quad \mathbf{A}]$ for some matrix $\mathbf{A} \in \mathbb{R}^{1 \times (m-1)}$ with nonnegative coefficients.*

Akin to the proof of Theorem 3.1.1, the proof of Theorem 3.3.1 relies on an induction argument based on any column of a PSS being part of a circuit. The latter proof can thus be viewed as a generalization of the former. In the next section, we will study implications of Theorem 3.3.1 on the characterization of positive bases.

3.4 Consequences on positive bases

Positive bases can be succinctly defined as inclusion-wise minimal positive spanning sets [15, Chapter 2]. We begin this section by drawing connections with digraphs as in Section 3.2.2. We then provide a general characterization.

3.4.1 Positive bases and digraphs

Recall from Section 3.2.2 that the network matrix of a strongly edge-connected digraph is a PSS. In particular, as stated in Section 3.3.1, a circuit G on $n+1$ vertices admits the minimal positive basis $[\mathbf{I}_n \quad -\mathbf{1}_n]$ as a network matrix. Similarly, the maximal positive basis $[\mathbf{I}_n \quad -\mathbf{I}_n]$ is associated to a bi-directed tree on $n+1$ vertices. More generally, we stated in Corollary 3.2.1 that a

network matrix was a positive basis if and only if the associated digraph G was minimally strongly edge-connected.

Remark 3.4.1 *Using the bound on the size of positive bases, we note that Corollary 3.2.1 can be used to prove that the number of arcs in a minimally strongly edge-connected digraph on $n \geq 2$ vertices ranges from n to $2(n-1)$, as stated in Proposition 3.1.1. To the best of our knowledge, such a proof technique is novel.*

Given the link between positive bases and minimally strongly connected digraphs, we seek a characterization of positive bases. Adapting Theorem 3.3.1 to such matrices, one sees that any positive basis $\mathbf{D}_{n,s}$ satisfies the structural equivalence

$$\mathbf{D}_{n,s} \equiv \begin{bmatrix} \mathbf{I}_n & \mathbf{N} \end{bmatrix} \quad \text{where } \mathbf{N} \in \mathbb{R}^{n \times s} \text{ is a NEM.} \quad (3.6)$$

This structural characterization leads to the following result.

Lemma 3.4.1 *Let $G = (V, A)$ be minimally strongly edge-connected, let $T = (V, \hat{A})$ be a spanning tree contained in G , and let $\mathbf{D}_{n,s} \in \mathbb{R}^{n \times (n+s)}$ be the network matrix associated with (G, T) . Then, for any matrix $\begin{bmatrix} \mathbf{I}_n & \mathbf{N} \end{bmatrix}$ given by (3.6), the matrix $\text{sgn}(\begin{bmatrix} \mathbf{I}_n & \mathbf{N} \end{bmatrix})$ is also a network matrix associated with G and a spanning tree $T' = (V, \hat{A}')$ with $\hat{A}' \subset A$.*

Proof. By structural equivalence, the matrix $\mathbf{M} = \begin{bmatrix} \mathbf{I}_n & \mathbf{N} \end{bmatrix}$ can be written $\mathbf{M} = \mathbf{B}^{-1} \mathbf{D}_{n,s} \mathbf{P} \Delta$ where $\mathbf{B} \in \mathbb{R}^{n \times n}$ is nonsingular, $\mathbf{P} \in \mathbb{R}^{(n+s) \times (n+s)}$ is a permutation matrix and $\Delta = \text{diag}(\delta_1, \dots, \delta_{n+s})$ is a diagonal matrix with positive diagonal entries. Letting $\hat{\Delta} = \text{diag}(\delta_1, \dots, \delta_n) \in \mathbb{R}^{n \times n}$, we find that $\hat{\Delta} \mathbf{B}^{-1} \mathbf{D}_{n,s} \mathbf{P} = \begin{bmatrix} \mathbf{I}_n & \tilde{\mathbf{N}} \end{bmatrix}$, where $\text{sgn}(\tilde{\mathbf{N}}) = \text{sgn}(\mathbf{N})$. It then follows from Proposition 3.2.1 that $\hat{\Delta} \mathbf{B}^{-1} \mathbf{D}_{n,s} \mathbf{P}$ is a network matrix and thus $\hat{\Delta} \mathbf{B}^{-1} \mathbf{D}_{n,s} \mathbf{P} = \text{sgn}(\hat{\Delta} \mathbf{B}^{-1} \mathbf{D}_{n,s} \mathbf{P}) = \text{sgn}(\mathbf{M})$. \square

Unlike Theorem 3.3.1 however, property (3.6) does not provide a full characterization of positive bases. For instance, the PSS $\begin{bmatrix} \mathbf{I}_2 & -\mathbf{e}_1 & -\mathbf{1}_2 \end{bmatrix}$ satisfies (3.6) but is not minimal (the third column can be removed without losing the positive spanning property).

Deriving a characterization thus requires a more precise study of the IN matrices that correspond to positive bases, which is the purpose of the next sections.

3.4.2 Criticality

A characterization of positive bases was given by Zbigniew Romanowicz [68] based on the concept of critical vectors - see Section 2.2.2. Partly due to this concept, this decomposition has proven difficult to use for characterizing positive bases. We redefine the notion of criticality below, and show that it

simplifies in the case of NEMs and IN matrices. To this end, we will make use of special cones in \mathbb{R}^n .

Definition 3.4.1 (Critical cones $\mathcal{K}_{i,j}(\mathbb{R}^n)$ and $\mathcal{K}_i(\mathbb{R}^n)$) For all $i \in \llbracket 1, n \rrbracket$, we define $\mathcal{K}_i(\mathbb{R}^n) = \text{pspan} \left(\bigcup_{k \neq i} \{-\mathbf{e}_k\} \right)$. It is a cone that consists of vectors with non-positive coordinates with at least one coordinate equal to zero.

We also define $\mathcal{K}_{i,j}(\mathbb{R}^n) = \text{pspan} \left(\{\mathbf{1}_n\} \cup \bigcup_{k \notin \{i,j\}} \{-\mathbf{e}_k\} \right)$, for any pair $(i, j) \in \llbracket 1, n \rrbracket$ with $i < j$. This cone consists of vectors with a nonnegative, non-unique largest entry.

For the sake of clarity, we give a description of the critical cones $\mathcal{K}_{i,j}(\mathbb{R}^n)$ and $\mathcal{K}_i(\mathbb{R}^n)$ in low dimension.

Example 3.4.1 The critical cones in \mathbb{R}^2 are given by

$$\mathcal{K}_1(\mathbb{R}^2) = \text{pspan}(-\mathbf{e}_2) \quad \mathcal{K}_2(\mathbb{R}^2) = \text{pspan}(-\mathbf{e}_1) \quad \mathcal{K}_{1,2}(\mathbb{R}^2) = \text{pspan}(\mathbf{1}_2).$$

Considering all critical cones in \mathbb{R}^n leads to the definition of critical vectors.

Definition 3.4.2 (Critical vector and critical matrix) The set of critical vectors in \mathbb{R}^n , denoted by $\mathcal{K}(\mathbb{R}^n)$, is defined as the union of all $\{\mathcal{K}_i(\mathbb{R}^n)\}$ and $\{\mathcal{K}_{i,j}(\mathbb{R}^n)\}$. A matrix $\mathbf{X} \in \mathbb{R}^{n \times m}$ is called critical whenever $\text{pspan}(\mathbf{X}) \subset \mathcal{K}(\mathbb{R}^n)$.

We emphasize that the set $\mathcal{K}(\mathbb{R}^n)$ is not a cone, which partly explains that the notion of critical vector is difficult to manipulate. We now describe the link between our definition of critical vectors and that of Romanowicz [68] - see Definition 2.2.2. In the latter, a vector $\mathbf{x} \in \mathbb{R}^n$ is called critical *with respect to* a positive basis $\mathbf{D}_{n,s}$ whenever no PSS can be obtained by substituting a column of $\mathbf{D}_{n,s}$ with the vector \mathbf{x} . As explained in the proposition below, those definitions are equivalent.

Proposition 3.4.1 A vector $\mathbf{v} \in \mathbb{R}^n$ is critical in the sense of Definition 3.4.2 if and only if for all $k \in \llbracket 1, n+1 \rrbracket$, the matrix obtained by replacing the k^{th} column of $[\mathbf{I}_n \quad -\mathbf{1}_n]$ with \mathbf{v} is not positively spanning.

Proof. Let $\mathbf{v} \in \mathbb{R}^n$, $\mathbf{M}_0 = [\mathbf{I}_n \quad \mathbf{v}]$. For any $k \in \llbracket 1, n \rrbracket$, let \mathbf{M}_k be the matrix obtained from $[\mathbf{I}_n \quad -\mathbf{1}_n]$ by replacing its k^{th} column with \mathbf{v} .

Suppose that \mathbf{v} is a critical vector. On the one hand, if $\mathbf{v} \in \mathcal{K}_i(\mathbb{R}^n)$ for some $i \in \llbracket 1, n \rrbracket$, Proposition 2.1.2 entails that \mathbf{M}_0 and \mathbf{M}_k are not positively spanning, as certified by the vectors \mathbf{e}_i and $-\mathbf{e}_k$, respectively. On the other hand, if there exist $(i, j) \in \llbracket 1, n \rrbracket^2$ with $i < j$ such that $\mathbf{v} \in \mathcal{K}_{i,j}(\mathbb{R}^n) \setminus \mathcal{K}_i(\mathbb{R}^n)$, then \mathbf{v} satisfies $[\mathbf{v}]_i = [\mathbf{v}]_j = \max_{\ell \in \llbracket 1, n \rrbracket} [\mathbf{v}]_\ell > 0$. Without loss of generality,

suppose that $i \neq k$. Then, Proposition 2.1.2 certifies that \mathbf{M}_0 and \mathbf{M}_k are not positively spanning, using the vectors \mathbf{e}_i and $\mathbf{e}_i - \mathbf{e}_k$, respectively.

Conversely, suppose that \mathbf{v} is not a critical vector. If all coordinates of \mathbf{v} are negative, then \mathbf{M}_0 is a PSS. Otherwise, the maximal coordinate $[\mathbf{v}]_\ell$ of \mathbf{v} must be strictly positive and unique since $\mathbf{v} \notin \mathcal{K}(\mathbb{R}^n)$. As a result, we can write $\mathbf{0}_n = \mathbf{v} - [\mathbf{v}]_\ell \mathbf{1}_n + \sum_{k \neq \ell} ([\mathbf{v}]_\ell - [\mathbf{v}]_k) \mathbf{e}_k$, and thus the zero vector can be expressed as a positive linear combination of the columns of \mathbf{M}_ℓ . Using Proposition 2.1.1, it follows that the matrix \mathbf{M}_ℓ is a PSS. \square

Our characterization of positive bases will consist in identifying critical matrices within a matrix decomposition, called the critical structure, that applies to any IN matrix.

Definition 3.4.3 (Critical structure) *Let $\mathbf{M} \in \mathbb{R}^{n \times (n+s)}$ be an IN matrix as described in (3.6). There exist positive integers n_1, \dots, n_s satisfying $n_1 + \dots + n_s = n$ and matrices $\mathbf{X}_1, \dots, \mathbf{X}_{s-1}$ such that*

$$\mathbf{M} = \begin{bmatrix} \mathbf{M}_1 \\ \dots \\ \mathbf{M}_s \end{bmatrix}, \quad \begin{cases} \mathbf{M}_1 = [\mathbf{I}_{n_1} & \mathbf{O} & -\mathbf{1}_{n_1} & \mathbf{X}_1] \\ \mathbf{M}_i = [\mathbf{O} & \mathbf{I}_{n_i} & \mathbf{O} & -\mathbf{1}_{n_i} & \mathbf{X}_i] \\ \mathbf{M}_s = [\mathbf{O} & \mathbf{I}_{n_s} & -\mathbf{1}_{n_s}] \end{cases} \quad \text{if } i \in \llbracket 2, s-1 \rrbracket \quad (3.7)$$

in which blocks of zeroes of arbitrary sizes are noted \mathbf{O} . The structure described by equation (3.7) is called the critical structure of \mathbf{M} .

When $s = 1$, \mathbf{M} has the trivial structure $\mathbf{M} = \mathbf{M}_1 = [\mathbf{I}_n \quad -\mathbf{1}_n]$, which does not involve any arbitrary block \mathbf{X}_i , and it is then immediate that \mathbf{M} is a positive basis. In the general case, however, assessing whether an IN matrix $\mathbf{M} \in \mathbb{R}^{n \times (n+s)}$ with $\ell = n$ and $k = s \geq 2$ is a positive basis amounts to checking the critical nature of the blocks $\mathbf{X}_1, \dots, \mathbf{X}_{s-1}$.

Theorem 3.4.1 *Let $\mathbf{M} \in \mathbb{R}^{n \times (n+s)}$ be an IN matrix as described in (3.6). Then, \mathbf{M} is a positive basis if and only if and each block \mathbf{X}_i in the critical structure (3.7) is a critical matrix in \mathbb{R}^{n_i} .*

Proof. We first proceed by contraposition and suppose that there exists $i \in \llbracket 1, s-1 \rrbracket$ such that \mathbf{X}_i is *not* critical. Then, there exist $j_0 \in \llbracket 1, n_i + 1 \rrbracket$ and $\mathbf{v} \in \text{pspan}(\mathbf{X}_i)$ such that the matrix obtained by replacing the j_0^{th} column of $[\mathbf{I}_{n_i} \quad -\mathbf{1}_{n_i}]$ with \mathbf{v} is a PSS. Let j be the index of this column in \mathbf{M}_i , let \mathbf{m}_j be the j^{th} column of \mathbf{M} and let \mathbf{M}' be the matrix obtained by removing \mathbf{m}_j from \mathbf{M} . Consider the matrix $\mathbf{M}'' = \begin{bmatrix} \mathbf{X}_i \\ \mathbf{O} \end{bmatrix}$ with $m' = n - m - n_i$ rows, where $m = n_1 + \dots + n_{i-1}$ so that \mathbf{M}'' is a submatrix of \mathbf{M}' . Using that $\mathbf{v} \in \text{pspan}(\mathbf{X}_i)$, it follows that

$$\mathbf{M}' \mathbf{u} = \begin{bmatrix} \mathbf{x} \\ \mathbf{v} \\ \mathbf{0}_{m'} \end{bmatrix} \quad \text{with } \mathbf{u} \geq \mathbf{0}_{n+s-1} \quad \text{and } \mathbf{x} \in \mathbb{R}^m. \quad (3.8)$$

Moreover, there exists a PSS $\hat{\mathbf{M}}$ of \mathbb{R}^m and a zero matrix \mathbf{O} such that $\begin{bmatrix} \hat{\mathbf{M}} \\ \mathbf{O} \end{bmatrix}$ is contained in \mathbf{M}' . Therefore equation (3.8) has a solution for any $\mathbf{x} \in \mathbb{R}^m$ and in particular, one can choose \mathbf{u} such that $\mathbf{M}'\mathbf{u} = \mathbf{m}_j$. In other words, $\mathbf{m}_j \in \text{pspan}(\mathbf{M}')$, thus \mathbf{M}' is a PSS and \mathbf{M} is not a positive basis.

Conversely, suppose that all matrices $\{\mathbf{X}_i\}_{i \in \llbracket 1, s-1 \rrbracket}$ are critical. Let \mathbf{c} be

a column of \mathbf{M} and let $\mathbf{M}' = \begin{bmatrix} \mathbf{M}'_1 \\ \dots \\ \mathbf{M}'_s \end{bmatrix}$ be the matrix obtained from \mathbf{M} by

removing \mathbf{c} . By construction of \mathbf{M}' , there exists $i \in \llbracket 1, s-1 \rrbracket$ such that one of the columns of $\begin{bmatrix} \mathbf{I}_{n_i} & -\mathbf{1}_{n_i} \end{bmatrix}$ is not a column of \mathbf{M}'_i . Let \mathbf{v}_i denote that column. By criticality of \mathbf{X}_i , $\mathbf{v}_i \notin \text{pspan}(\mathbf{M}'_i)$, and thus \mathbf{M}'_i is not a PSS. As a result, \mathbf{M} is no longer a PSS when one of its columns is removed, and thus it is a positive basis. \square

It follows from Theorem 3.4.1 that characterizing positive bases in \mathbb{R}^n reduces to describing critical matrices in \mathbb{R}^m for all $m \leq n$. The next proposition lists such matrices in dimension $n \leq 3$, and will be used to characterize positive bases of near-maximal size.

Proposition 3.4.2

- (i) $\mathbf{X} \in \mathbb{R}^{1 \times m}$ is critical if and only if it is the zero matrix.
- (ii) $\mathbf{X} \in \mathbb{R}^{2 \times m}$ is critical if and only if $\text{col}(\mathbf{X})$ is contained in one of the critical cones defining $\mathcal{K}(\mathbb{R}^2)$.
- (iii) $\mathbf{X} \in \mathbb{R}^{3 \times m}$ is critical if and only if $\text{col}(\mathbf{X})$ is contained in one of the critical cones defining $\mathcal{K}(\mathbb{R}^3)$ or in $\text{span}(\mathbf{e}_i + \mathbf{e}_j)$ for some $(i, j) \in \llbracket 1, 3 \rrbracket^2$, $i < j$.

Proof. In all cases, the reverse implication is immediate, thus we focus on proving the direct implication. To this end, we recall that a critical matrix $\mathbf{X} \in \mathbb{R}^{n \times m}$ satisfies $\text{col}(\mathbf{X}) \subset \text{pspan}(\mathbf{X}) \subset \mathcal{K}(\mathbb{R}^n)$ by definition.

(i) Since $\mathcal{K}(\mathbb{R}^1) = \{0\}$, the result is immediate.

(ii) We start by proving that for any two columns \mathbf{x} and \mathbf{y} of a critical matrix \mathbf{X} , one of the critical cones defining $\mathcal{K}(\mathbb{R}^2)$ contains them both. We proceed by contradiction: suppose the existence of two columns \mathbf{x} and \mathbf{y} which are not contained in a same critical cone and for the sake of simplicity, suppose that $\mathbf{x} \in \mathcal{K}_1(\mathbb{R}^2)$. Then $[\mathbf{x}]_2 < 0$, as $\mathbf{x} \neq \mathbf{0}_2$. Now, if $\mathbf{y} \in \mathcal{K}_2(\mathbb{R}^2)$ then $\mathbf{x} + \mathbf{y}$ is not critical since $\mathbf{x} + \mathbf{y} < \mathbf{0}_2$. Similarly, if $\mathbf{y} \in \mathcal{K}_{1,2}(\mathbb{R}^2)$ then $\frac{-[\mathbf{y}]_1}{[\mathbf{x}]_2}\mathbf{x} + \mathbf{y}$ is not critical as it is a positive multiple of \mathbf{e}_2 . Both cases are absurd and the preliminary result is proved.

Now, suppose that $\text{col}(\mathbf{X})$ is not entirely contained in any of the critical cones defining $\mathcal{K}(\mathbb{R}^2)$. Then there exists three (non-necessarily distinct) columns \mathbf{x} , \mathbf{y} and \mathbf{z} of \mathbf{X} with $\mathbf{x} \notin \mathcal{K}_1(\mathbb{R}^2)$, $\mathbf{y} \notin \mathcal{K}_2(\mathbb{R}^2)$ and $\mathbf{z} \notin \mathcal{K}_{1,2}(\mathbb{R}^2)$.

Then the two vectors \mathbf{x} and \mathbf{y} must be contained in $\mathcal{K}_{1,2}(\mathbb{R}^2)$ and similarly, \mathbf{x} and \mathbf{z} must be two elements of $\mathcal{K}_2(\mathbb{R}^2)$. Since $\mathcal{K}_{1,2}(\mathbb{R}^2) \cap \mathcal{K}_2(\mathbb{R}^2) = \{\mathbf{0}_2\}$ we obtain $\mathbf{x} = \mathbf{0}_2$, a contradiction as $\mathbf{0}_2 \in \mathcal{K}_1(\mathbb{R}^2)$.

(iii) Let $\mathcal{S} = \{\mathcal{K}_i(\mathbb{R}^3), \mathcal{K}_{i,j}(\mathbb{R}^3), \text{span}(\mathbf{e}_i + \mathbf{e}_j) \text{ with } i, j \in \llbracket 1, 3 \rrbracket\}$.

We start by proving that for any two columns \mathbf{x} and \mathbf{y} of a critical matrix \mathbf{X} , some element of \mathcal{S} contains them both. We proceed by contradiction and assume the existence of two columns \mathbf{x} and \mathbf{y} which do not satisfy this property.

- First, suppose that $\mathbf{x} \in \mathcal{K}_1(\mathbb{R}^3)$. Let $\{i, j\} = \{2, 3\}$ and note that if $\mathbf{y} \in \mathcal{K}_i(\mathbb{R}^3)$ then $\mathbf{x} + \mathbf{y} < \mathbf{0}_3$, a contradiction as this vector would not be critical. Therefore \mathbf{y} is not contained in any of the cones $\mathcal{K}_i(\mathbb{R}^3)$. In particular, the maximal coordinate of \mathbf{y} must be positive and non-unique as $\mathbf{y} \in \mathcal{K}(\mathbb{R}^3)$.

If $\mathbf{y} \in \mathcal{K}_{1,2}(\mathbb{R}^3)$, then $\mathbf{x} \in \mathcal{K}_1(\mathbb{R}^3) \setminus \mathcal{K}_{1,2}(\mathbb{R}^3)$ and so $[\mathbf{x}]_2 < 0$. As a consequence, if $[\mathbf{y}]_3 < [\mathbf{y}]_1$, then for $\varepsilon > 0$ sufficiently small, $\mathbf{z}_\varepsilon = \varepsilon \mathbf{x} + \mathbf{y}$ is not critical. If $[\mathbf{y}]_3 = [\mathbf{y}]_1$ then $\mathbf{y} \in \mathcal{K}_{1,2}(\mathbb{R}^3) \cap \mathcal{K}_{1,3}(\mathbb{R}^3)$ therefore $\mathbf{x} \notin \mathcal{K}_{1,3}(\mathbb{R}^3)$, which entails $[\mathbf{x}]_3 < 0$. In that case the vector $\mathbf{x} + \mathbf{y}$ is not critical as its maximal coordinate is positive and unique. Both cases contradict the criticality of \mathbf{X} , therefore $\mathbf{y} \notin \mathcal{K}_{1,2}(\mathbb{R}^3)$ and by a similar reasoning, $\mathbf{y} \notin \mathcal{K}_{1,3}(\mathbb{R}^3)$.

If $\mathbf{y} \in \mathcal{K}_{2,3}(\mathbb{R}^3) \setminus \mathcal{K}_{1,2}(\mathbb{R}^3)$, three cases are to be considered. First, suppose that $[\mathbf{y}]_1 = 0$ and $[\mathbf{x}]_2 = [\mathbf{x}]_3$. Then \mathbf{x} and \mathbf{y} are both in $\text{span}(\mathbf{e}_2 + \mathbf{e}_3)$, a contradiction. Second, if $[\mathbf{y}]_1 = 0$ and $[\mathbf{x}]_2 \neq [\mathbf{x}]_3$, then without loss of generality $[\mathbf{x}]_2 < [\mathbf{x}]_3$ so the vector $\mathbf{x} + \left| \frac{[\mathbf{x}]_2}{[\mathbf{y}]_2} \right| \mathbf{y}$ is non-critical: it is a positive multiple of \mathbf{e}_3 . Third, if $[\mathbf{y}]_1 \neq 0$ then for a sufficiently large $\varepsilon > 0$, $\varepsilon \mathbf{x} + \mathbf{y}$ is non-critical. Each of the three cases leads to a contradiction, therefore we conclude that $\mathbf{y} \notin \mathcal{K}_{2,3}(\mathbb{R}^3)$.

From all that precedes, the critical vector \mathbf{y} is not contained in any of the critical cones which define $\mathcal{K}(\mathbb{R}^3)$, an absurdity: by contradiction, we proved that $\mathbf{x} \notin \mathcal{K}_1(\mathbb{R}^3)$. This last result easily generalizes, and we now know that none of the critical cones $\mathcal{K}_i(\mathbb{R}^3), i \leq 3$ contains any of the two vectors \mathbf{x} and \mathbf{y} .

- Now, suppose that $\mathbf{x} \in \mathcal{K}_{1,2}(\mathbb{R}^3)$. If $\mathbf{y} \in \mathcal{K}_{1,3}(\mathbb{R}^3)$, the vector $\mathbf{x} + \mathbf{y}$ is non-critical: from $\mathbf{x} \notin \mathcal{K}_{1,3}(\mathbb{R}^3)$ we deduce that the first coordinate of $\mathbf{x} + \mathbf{y}$ is positive and strictly larger than the other two. By a similar reasoning, if $\mathbf{y} \in \mathcal{K}_{2,3}(\mathbb{R}^3)$ $\mathbf{x} + \mathbf{y}$ is non-critical. In the end we conclude that \mathbf{y} cannot be contained in any of the critical cones that define $\mathcal{K}(\mathbb{R}^3)$, an absurdity as \mathbf{y} is a critical vector. Therefore $\mathbf{x} \notin \mathcal{K}_{1,2}(\mathbb{R}^3)$ and the result easily generalizes to $\mathcal{K}_{1,3}(\mathbb{R}^3)$ and $\mathcal{K}_{2,3}(\mathbb{R}^3)$.

By definition of \mathbf{X} the vector \mathbf{x} must be critical, yet we proved that it is not contained in any of the critical cones, a clear contradiction. In conclusion, for any pair (\mathbf{x}, \mathbf{y}) of columns of \mathbf{X} , there must exist an element S of \mathcal{S} that contains them both.

We are now ready to prove the main result. We proceed by con-

tradiction and assume that $\text{col}(\mathbf{X})$ is not contained in any set $S \in \mathcal{S}$. In that case, each column \mathbf{x} of \mathbf{X} must be at the intersection of at least two distinct sets S_1 and S_2 of \mathcal{S} . Then \mathbf{x} is contained in some set $T \in \mathcal{T}$, where $\mathcal{T} = \{\text{pspan}(-\mathbf{e}_i), \text{pspan}(\mathbf{1}_3), \text{span}(\mathbf{e}_i + \mathbf{e}_j) \text{ with } i \neq j\}$. Moreover, it is easy to verify that for any two distinct sets $T_1 \in \mathcal{T}, T_2 \in \mathcal{T}$ and any two nonzero vectors $\mathbf{x} \in T_1, \mathbf{y} \in T_2$, there exist some value $\varepsilon > 0$ such that $\mathbf{x} + \varepsilon\mathbf{y}$ is not an element of any $T \in \mathcal{T}$. Therefore $\text{col}(\mathbf{X})$ must be a subset some set $T \in \mathcal{T}$, a contradiction as any such set T satisfies $T \subset S$, for some $S \in \mathcal{S}$. \square

Proposition 3.4.2 and Theorem 3.4.1 can be used to characterize positive bases in \mathbb{R}^n with critical structure (3.7) consisting of blocks \mathbf{M}_i with at most three rows. When all blocks \mathbf{M}_i have one row, we recover the result of Proposition 2.2.2 since all \mathbf{X}_i blocks are necessarily zero matrices. Tackling the other two cases requires the following auxiliary result.

Lemma 3.4.2 *Suppose $n \geq 2$. Any positive basis $\mathbf{D}_{n,s}$ is structurally equivalent to an IN matrix as described in (3.6) whose critical structure (3.7) satisfies $\text{col}(\mathbf{X}_i) \subset \mathcal{K}_1(\mathbb{R}^2)$ whenever $n_i = 2$, and $\text{col}(\mathbf{X}_i) \subset \mathcal{K}_1(\mathbb{R}^3)$ or $\text{col}(\mathbf{X}_i) \subset \text{span}(\mathbf{e}_2 + \mathbf{e}_3)$ whenever $n_i = 3$.*

Proof. Let $\mathbf{M} \equiv \mathbf{D}_{n,s}$ be an IN matrix satisfying (3.6). Suppose that one of the blocks \mathbf{M}_i in its critical structure (3.7) has two rows and let $m_i = n_1 + \dots + n_{i-1} + 1$ be the index of its first row in \mathbf{M} . Since $\mathbf{D}_{n,s}$ is a positive basis, the block \mathbf{X}_i is critical for \mathbb{R}^2 per Theorem 3.4.1. If $\text{col}(\mathbf{X}_i) \subset \mathcal{K}_1(\mathbb{R}^2)$ there is nothing to prove. Otherwise, we must have $\text{col}(\mathbf{X}_i) \subset \mathcal{K}_2(\mathbb{R}^2)$ or $\text{col}(\mathbf{X}_i) \subset \mathcal{K}_{1,2}(\mathbb{R}^2)$ by Proposition 3.4.2. If $\text{col}(\mathbf{X}_i) \subset \mathcal{K}_2(\mathbb{R}^2)$, permuting the rows and columns of indices m_i and $m_i + 1$ in \mathbf{M} (as well as other columns if needed) creates a new matrix \mathbf{M}' whose critical structure (3.7) satisfies $\text{col}(\mathbf{X}'_i) \subset \mathcal{K}_1(\mathbb{R}^2)$ and $\mathbf{X}'_j = \mathbf{X}_j$ whenever $j \neq i$. If $\text{col}(\mathbf{X}_i) \subset \mathcal{K}_{1,2}(\mathbb{R}^2)$, replacing the $(m_i + 1)^{\text{th}}$ row of \mathbf{M} by its opposite and adding this new row to that of index m_i creates again a matrix \mathbf{M}' with the desired critical structure up to further column permutation.

Suppose now that the block \mathbf{M}_i has three rows. Since \mathbf{X}_i must be critical for \mathbb{R}^3 , its columns must lie in one of the sets stated in Proposition 3.4.2. If $\text{col}(\mathbf{X}_i) \subset \text{span}(\mathbf{e}_2 + \mathbf{e}_3)$ or $\text{col}(\mathbf{X}_i) \subset \mathcal{K}_1(\mathbb{R}^3)$, the desired conclusion follows. More generally, if $\text{col}(\mathbf{X}_i) \subset \text{span}(\mathbf{e}_j + \mathbf{e}_k)$ or $\text{col}(\mathbf{X}_i) \subset \mathcal{K}_j(\mathbb{R}^3)$ for any (j, k) in $\llbracket 1, 3 \rrbracket$, permutations of rows and columns can be applied to \mathbf{M} to obtain a matrix \mathbf{M}' whose critical structure (3.7) satisfies $\text{col}(\mathbf{X}'_i) \subset \mathcal{K}_1(\mathbb{R}^3)$ or $\text{col}(\mathbf{X}'_i) \subset \text{span}(\mathbf{e}_2 + \mathbf{e}_3)$ as well as $\mathbf{X}'_j = \mathbf{X}_j$ whenever $j \neq i$. By Proposition 3.4.2 and without loss of generality, the only remaining case to consider is that where $\text{col}(\mathbf{X}_i) \subset \mathcal{K}_{1,2}(\mathbb{R}^3)$. In that case, up to column permutations, the matrix \mathbf{M}' described above can be obtained by replacing the m_i^{th} row of \mathbf{M} by its opposite and then adding it to the rows of index $(m_i + 1)$ and $(m_i + 2)$. \square

We are now equipped with the necessary tools to extend the results of Corollary 2.2.1 and Proposition 2.2.2 and to other sizes of positive bases.

3.4.3 Structure of nearly extreme-size positive bases

Having shown in Section 3.4.2 how the structure of any positive basis connects to the critical structure of its associated IN matrix, we now apply these results to fully characterize positive bases of size $2\ell - 1$, $2\ell - 2$ and $\ell + 2$ of an ℓ -dimensional subspace of \mathbb{R}^n . To our knowledge, those descriptions are novel in both the positive spanning set and the minimal strongly edge-connected digraph literature. For this reason, we state every result using positive bases then provide an equivalent for strongly edge-connected digraphs, starting with the size $2\ell - 1$.

Theorem 3.4.2 *Let $n \geq \ell \geq 2$. A matrix $\mathbf{D}_{\mathbb{L}, \ell-1} \in \mathbb{R}^{n \times (2\ell-1)}$ is a positive basis for some ℓ -dimensional linear space $\mathbb{L} \subset \mathbb{R}^n$ if and only if there exists a non-positive vector $\mathbf{x} \in \mathbb{R}^{\ell-2}$ such that*

$$\mathbf{D}_{\mathbb{L}, \ell-1} \equiv \begin{bmatrix} \mathbf{I}_\ell & \mathbf{N} \\ \mathbf{0}_{n-\ell, \ell} & \mathbf{0}_{n-\ell, \ell-1} \end{bmatrix}, \quad \text{with } \mathbf{N} = \begin{bmatrix} -1 & \mathbf{0}_{\ell-2}^\top \\ -1 & \mathbf{x}^\top \\ \mathbf{0}_{\ell-2} & -\mathbf{I}_{\ell-2} \end{bmatrix}. \quad (3.9)$$

Proof. We only prove the result when $\ell = n$ as the reasoning easily adapts to all other cases. If $\ell = n$ and $\mathbf{D}_{\mathbb{L}, \ell-1}$ satisfies (3.9), the result holds. Conversely, let $\mathbf{D}_{n, n-1}$ be a positive basis and $\mathbf{M} = [\mathbf{I}_n \ \mathbf{N}]$ be the associated IN matrix through (3.6). Since $\mathbf{N} \in \mathbb{R}^{n \times (n-1)}$, the critical structure (3.7) of \mathbf{M} must consist of $n - 1$ blocks $\mathbf{M}_i \in \mathbb{R}^{n_i \times (2n-1)}$. Using $n_1 + \dots + n_{n-1} = n$, it follows that exactly one of the blocks \mathbf{M}_i has two rows while the others have one. By Theorem 3.4.1 and Proposition 3.4.2 each block \mathbf{X}_i must be critical and those with one row are zero matrices. Finally, Lemma 3.4.2 implies that the unique block \mathbf{X}_i on two rows can be transformed into a matrix $\begin{bmatrix} \mathbf{0}_{\ell-2}^\top \\ \mathbf{x}^\top \end{bmatrix}$ where $\mathbf{x} \in \mathbb{R}^{\ell-2}$ is non-positive, hence the conclusion. \square

An implication of Theorem 3.4.2 in terms of strongly edge-connected digraphs is given below, and illustrated through Example 3.4.2.

Corollary 3.4.1 *A digraph $G = (V, A)$ on n vertices and $2n - 3$ arcs is minimally strongly edge-connected if and only if it is the union of a bi-directed forest F with a graph $G \setminus F$ such that*

- (i) $G \setminus F$ consists of circuits of size 3, all sharing a common arc $a \in A$.
- (ii) Each tree in F contains exactly one vertex of $G \setminus F$.

Proof. Suppose that G is minimally strongly edge-connected and let $\mathbf{M} = \mathbf{D}_{n-1, n-2}$ in $\mathbb{R}^{(n-1) \times (2n-3)}$ be an associated network matrix. By Theorem 3.4.2, $\mathbf{M} \equiv \tilde{\mathbf{M}} = [\mathbf{I}_{n-1} \quad \mathbf{N}]$, with $\mathbf{N} = \begin{bmatrix} -1 & \mathbf{0}_{n-3}^\top \\ -1 & \mathbf{x}^\top \\ \mathbf{0}_{n-3} & -\mathbf{I}_{n-3} \end{bmatrix}$ and $\mathbf{x} \leq \mathbf{0}_{n-3}$.

By Lemma 3.4.1, $\tilde{\mathbf{M}}$ can be assumed to be a network matrix, implying $\mathbf{x} \in \{-1, 0\}^{n-3}$. Write $A = \{a_1, \dots, a_n\}$ so that the i^{th} column of $\tilde{\mathbf{M}}$ is associated to a_i , for all i . Recalling that $\{a_{i_1}, \dots, a_{i_k}\} \subset A$ is a circuit in G if and only if it is associated to an inclusion-wise minimal set of columns in $\tilde{\mathbf{M}}$ which add up to $\mathbf{0}_{n-1}$. Based on this remark, we observe that $\{a_1, a_2, a_n\}$ is a circuit of size 3 in G . Moreover, any other circuit of this size in G is given by $\{a_2, a_{i+2}, a_{n+i}\}$ where $i \in \llbracket 1, n-3 \rrbracket$ satisfies $[\mathbf{x}]_i = -1$. We denote by $G' = (V', A')$ the union of these circuits and we let $|A'| = m$. Now, consider the spanning tree $T = (V, \hat{A})$ associated to $\tilde{\mathbf{M}}$. T can be decomposed as the union of $T \cap G'$ with a sequence $(T_j)_{j \leq m}$ of pairwise disjoint trees, each touching a unique vertex in G' . It is easy to see that each arc in any tree T_j is part of a circuit of size 2. Indeed, any such arc a_i must satisfy $i \in \llbracket 3, n-1 \rrbracket$ and $[\mathbf{x}]_{i-2} = 0$, and as such is contained in a circuit $\{a_i, a_{n+i-2}\}$. We have thus established (i) and (ii).

Conversely, if a graph G admits such a decomposition, it must be edge-connected and $\tilde{\mathbf{M}}$ is a network matrix for G . Since $\tilde{\mathbf{M}}$ is a positive basis, it follows that G is minimally strongly edge-connected. \square

Example 3.4.2 Figure 3.11 provides an example of a minimally strongly edge-connected digraph on $n = 9$ vertices, and $2n - 3 = 15$ arcs. The bi-directed forest F is represented in black while the circuits of $G \setminus F$ are in blue.

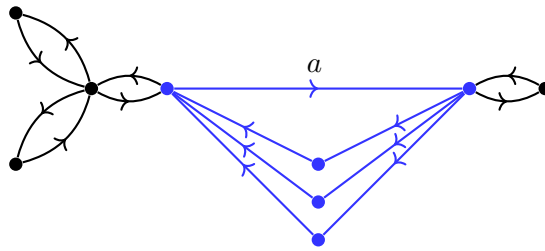


Figure 3.11. Minimally strongly edge-connected with $|A| = 2n - 3$

We now turn to positive bases of size $2\ell - 2$ and the associated strongly edge-connected digraphs. Recall how the critical structure (3.7) associated to a positive basis $\mathbf{D}_{n, n-1}$ consists of blocks \mathbf{M}_i with two rows or less - an essential element to the proof of Theorem 3.4.2. Likewise, it can be observed that the critical structure of an IN matrix associated to a positive basis $\mathbf{D}_{n, n-2}$ through (3.6) consists of blocks on three rows or less: if one of

those blocks has three rows, it is unique and the others all possess exactly one row. Otherwise, exactly two blocks are on two rows while the others are on one. By combining these observations with the results of Theorem 3.4.1, Proposition 3.4.2 and Lemma 3.4.2 we obtain the following characterization - whose proof is omitted as being nearly identical to that of Theorem 3.4.2.

Theorem 3.4.3 *Let $n \geq \ell \geq 3$. Then $\mathbf{D}_{\mathbb{L}, \ell-2} \in \mathbb{R}^{n \times (2\ell-2)}$ is a positive basis for some ℓ -dimensional space $\mathbb{L} \subset \mathbb{R}^n$ if and only if $\mathbf{D}_{\mathbb{L}, \ell-2} \equiv$*

$$\begin{bmatrix} \mathbf{I}_\ell & \mathbf{N} \\ \mathbf{0}_{n-\ell, \ell} & \mathbf{0}_{n-\ell, \ell-2} \end{bmatrix} \text{ with}$$

$$\mathbf{N} = \begin{bmatrix} -1 & \mathbf{0}_{\ell-3}^\top \\ -1 & \mathbf{x}_1^\top \\ -1 & \mathbf{x}_2^\top \\ \mathbf{0}_{\ell-3} & -\mathbf{I}_{\ell-3} \end{bmatrix}, \quad \mathbf{N} = \begin{bmatrix} -1 & \mathbf{0}_{\ell-3}^\top \\ -1 & \mathbf{x}^\top \\ -1 & \mathbf{x}^\top \\ \mathbf{0}_{\ell-3} & -\mathbf{I}_{\ell-3} \end{bmatrix} \quad \text{or} \quad \mathbf{N} = \begin{bmatrix} -1 & 0 & \mathbf{0}_{\ell-4}^\top \\ -1 & 0 & \mathbf{x}_3^\top \\ 0 & -1 & \mathbf{0}_{\ell-4}^\top \\ 0 & -1 & \mathbf{x}_4^\top \\ \mathbf{0}_{\ell-4} & \mathbf{0}_{\ell-4} & -\mathbf{I}_{\ell-4} \end{bmatrix},$$

where $\mathbf{x}_1 \in \mathbb{R}^{\ell-3}$, $\mathbf{x}_2 \in \mathbb{R}^{\ell-3}$, $\mathbf{x}_3 \in \mathbb{R}^{\ell-4}$, $\mathbf{x}_4 \in \mathbb{R}^{\ell-4}$ are non-positive and $\mathbf{x} \in \mathbb{R}^{\ell-3}$ is arbitrary.

Theorem 3.4.3 bears important consequences on the structure of minimally strongly edge-connected digraphs, as described in the following corollary.

Corollary 3.4.2 *A digraph $G = (V, A)$ on n vertices and $2n - 4$ arcs is minimally strongly edge-connected if and only if $G = F \cup H$, where F is a bi-directed forest whose trees all contain exactly one vertex of H , and the digraph H is constructed through one of the two procedures below.*

- | | |
|--|---|
| <p>i) Draw a circuit $\{a_1, a_2, a_3, a_n\}$, where $a_1 = (u_1, u_2)$, $a_2 = (u_2, u_3)$, $a_3 = (u_3, u_4)$ and $a_n = (u_4, u_1)$.</p> <p>ii) Add an arbitrary number of vertices v_i and for all i, draw exactly one of the two paths $\{(u_2, v_i), (v_i, u_4)\}$ and $\{(u_4, v_i), (v_i, u_2)\}$.</p> <p>iii) If no path $\{(u_2, v_i), (v_i, u_4)\}$ was ever drawn: add an arbitrary number of vertices w_j and for all j, draw exactly one of the two paths $\{(u_3, w_j), (w_j, u_2)\}$ and $\{(u_4, w_j), (w_j, u_3)\}$.</p> | <p>i') Draw two edge-disjoint circuits $\{a_1, a_2, a_n\}$ and $\{a_3, a_4, a_{n+1}\}$, where $a_1 = (u_1, u_2)$, $a_2 = (u_2, u_3)$, $a_3 = (v_1, v_2)$ and $v_4 = (v_2, v_3)$. The arcs a_1 and a_3 are allowed to share a common vertex.</p> <p>ii') If a_1 and a_3 are vertex disjoint, draw a bi-directed path from one endpoint of a_1 to one endpoint of a_3.</p> <p>iii') Add an arbitrary number of vertices w_j and for all j, draw exactly one of the two paths $\{(u_2, w_j), (w_j, u_1)\}$ and $\{(v_2, w_j), (w_j, v_1)\}$.</p> |
|--|---|

Proof. Suppose that G is minimally strongly edge-connected and let $\mathbf{M} = \mathbf{D}_{n-1, n-3} \in \mathbb{R}^{(n-1) \times (2n-4)}$ be an associated network matrix. By Theorem 3.4.3, $\mathbf{M} \equiv \tilde{\mathbf{M}} = [\mathbf{I}_{n-1} \quad \mathbf{N}]$ with

$$\mathbf{N} = \begin{bmatrix} -1 & \mathbf{0}_{n-4}^\top \\ -1 & \mathbf{x}_1^\top \\ -1 & \mathbf{x}_2^\top \\ \mathbf{0}_{n-4} & -\mathbf{I}_{n-4} \end{bmatrix}, \quad \mathbf{N} = \begin{bmatrix} -1 & \mathbf{0}_{n-4}^\top \\ -1 & \mathbf{x}^\top \\ -1 & \mathbf{x}^\top \\ \mathbf{0}_{n-4} & -\mathbf{I}_{n-4} \end{bmatrix} \quad \text{or} \quad \mathbf{N} = \begin{bmatrix} -1 & 0 & \mathbf{0}_{n-5}^\top \\ -1 & 0 & \mathbf{x}_3^\top \\ 0 & -1 & \mathbf{0}_{n-5}^\top \\ 0 & -1 & \mathbf{x}_4^\top \\ \mathbf{0}_{n-5} & \mathbf{0}_{n-5} & -\mathbf{I}_{n-5} \end{bmatrix},$$

$\mathbf{x}_1 \in \mathbb{R}^{n-4}$, $\mathbf{x}_2 \in \mathbb{R}^{n-4}$, $\mathbf{x}_3 \in \mathbb{R}^{n-5}$, $\mathbf{x}_4 \in \mathbb{R}^{n-5}$ being non-positive and $\mathbf{x} \in \mathbb{R}^{n-4}$ being arbitrary. By Lemma 3.4.1, $\tilde{\mathbf{M}}$ can be assumed to be a network matrix for G and for some spanning tree $\tilde{T} = (V, \tilde{A})$, $\tilde{A} \subset A$. Thus $\mathbf{x} \in \llbracket -1, 1 \rrbracket^{n-4}$ and $\mathbf{x}_1 \in \{-1, 0\}^{n-4}$, $\mathbf{x}_2 \in \{-1, 0\}^{n-4}$, $\mathbf{x}_3 \in \{-1, 0\}^{n-5}$, $\mathbf{x}_4 \in \{-1, 0\}^{n-5}$. Write $A = \{a_1, \dots, a_n\}$ so that the i^{th} column of $\tilde{\mathbf{M}}$ is associated to a_i , for all i . Clearly, each circuit of size 2 in G can be associated to a pair of columns $\{\mathbf{e}_i, -\mathbf{e}_i\} \subset \text{col}(\tilde{\mathbf{M}})$, where \mathbf{e}_i designates some canonical vector. Since G is minimally strongly edge-connected, the union of these circuits forms a bi-directed forest F in which every tree must be connected to $G \setminus F$ in some way. Based on the structure of \mathbf{N} , we see that the digraph $G \setminus F$ consists of at most two connected components. If the number of components is equal to 1, owing to the fact that G is minimally strongly edge-connected, each tree in F must share exactly one vertex with $G \setminus F$. On the other hand, if that number is equal to 2, then one of the trees in F must share exactly one vertex with each of the two components. Each of the three possible structures for the matrix \mathbf{N} were listed at the beginning of this proof. Each of those is now to be considered.

- First, suppose that \mathbf{N} has the left-most structure. Then $G \setminus F$ contains a circuit of size 4, given by $\{a_1, a_2, a_3, a_n\}$. This corresponds to the first step of the left-most procedure. For $i \in \llbracket 1, 3 \rrbracket$ we write $a_i = (u_i, u_{i+1})$, and so $a_n = (u_4, u_1)$. Let \mathcal{S}_1 (resp. \mathcal{S}_2) be the set of indices i such that $[\mathbf{x}_1]_i = -1$ (resp. $[\mathbf{x}_2]_i = -1$). Now, consider any other arc of $G \setminus F$ and denote by $u \notin \{u_1, \dots, u_4\}$ one of its two extremities. Owing to the structure of \mathbf{N} , the arc must be contained in a circuit of size 3 or 4 in $G \setminus F$. If it is part of a circuit of size 4, then $\mathcal{S}_1 \cap \mathcal{S}_2 \neq \emptyset$ as this circuit is given by $\{a_2, a_3, a_{i+3}, a_{n-1+i}\}$ for some $i \in \mathcal{S}_1 \cap \mathcal{S}_2$. Alternatively, the circuit can be written as $\{(u_2, u_3), (u_3, u_4), (u_4, u), (u, u_2)\}$ and therefore the arc is some path $\{(u_4, u), (u, u_2)\}$, as announced in step *ii*) of the left-most procedure. Alternatively, the arc could be contained in a circuit of size 3. Then $\mathcal{S}_1 \neq \mathcal{S}_2$ and this circuit is given by $\{a_2, a_{i+3}, a_{n-1+i}\}$, $i \in \mathcal{S}_1 \setminus \mathcal{S}_2$, or by $\{a_3, a_{j+3}, a_{n-1+j}\}$, $j \in \mathcal{S}_2 \setminus \mathcal{S}_1$. Alternatively we write the circuit as $\{(u_2, u_3), (u_3, u), (u, u_2)\}$ and $\{(u_3, u_4), (u_4, u), (u, u_3)\}$ and we easily identify that the arc must be contained in one of the paths described in step *iii*) of the left-most procedure. In conclusion, the digraph $G \setminus F$ can be obtained by following steps *i*), *ii*) and *iii*).

• Now, suppose that \mathbf{N} has the center-most structure. Once again, the circuit $\{a_1, a_2, a_3, a_n\}$ is contained in $G \setminus F$, which corresponds to the first step of the left-most procedure. Any other arc in $G \setminus F$ is contained in some circuit of size 4 having one of the two forms $\{a_2, a_3, a_{i+3}, a_{n-1+i}\}$, where $[\mathbf{x}]_i = -1$ or $\{a_1, a_n, a_{j+3}, a_{n-1+j}\}$, where $[\mathbf{x}]_j = 1$. Such circuits contain a path $\{(u_4, v_i), (v_i, u_2)\}$, $v_i \in V$ or a path $\{(u_2, v_j), (v_j, u_4)\}$, $v_j \in V$, as described in step *ii*) of the left-most procedure. Therefore $G \setminus F$ is obtained by following steps *i*), *ii*) and *iii*).

• Finally, suppose that \mathbf{N} has the right-most structure. If some $i \in \llbracket 1, n-5 \rrbracket$ satisfies $[\mathbf{x}_3]_i = [\mathbf{x}_4]_i = -1$, then \mathbf{N} is structurally equivalent to a matrix with the left-most structure, for which the result is already proved. Suppose instead that \mathbf{x}_3 and \mathbf{x}_4 do not share any negative entry. In that case, $G \setminus F$ contains two circuits of size 3, given by $\{a_1, a_2, a_n\}$ and $\{a_3, a_4, a_{n+1}\}$. Note that $G \setminus F$ does not possess any circuit of size 4. Write $a_1 = (u_1, u_2)$, $a_2 = (u_2, u_3)$, $a_3 = (v_1, v_2)$ and $a_4 = (v_2, v_3)$. Then $a_n = (u_3, u_1)$ and $a_{n+1} = (v_3, v_1)$. This corresponds to the first step of the right-most procedure. Since G is strongly edge-connected, the two circuits must either share a common vertex or be connected by some bi-directed path, as indicated in step *ii'*). Now, consider any other arc in $G \setminus F$. This arc is contained in some circuit of size 3, which we either express as $\{a_2, a_{i+4}, a_{n+1+i}\}$ (where $i \in \llbracket 1, n-5 \rrbracket$ satisfies $[\mathbf{x}_3]_i = -1$) or as $\{a_4, a_{i+4}, a_{n+1+i}\}$ (where $[\mathbf{x}_4]_i = -1$). The circuit can be rewritten as $\{(u_2, u_3), (u_3, u), (u, u_2)\}$ or $\{(v_2, v_3), (v_3, u), (u, v_2)\}$, $u \in V$, therefore we recognize that the arc must be contained in one of the paths described in step *iii'*) of the right-most procedure.

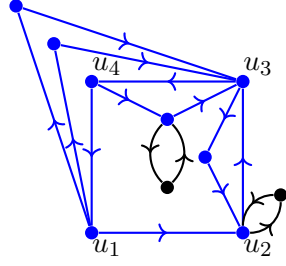
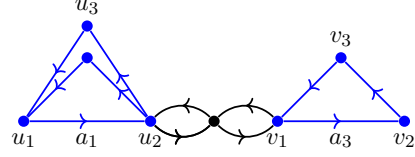
Conversely, consider any digraph G constructed using one of the two procedures. Then G admits the positive basis $\tilde{\mathbf{M}}$ as a network matrix therefore it is minimally strongly edge-connected, by Corollary 3.2.1. \square

The following example illustrates the result of Corollary 3.4.2: each of the two digraphs below was obtained through one of the two procedures described in the corollary.

Example 3.4.3 *Figures 3.12 and 3.13 below show two minimally strongly edge-connected digraphs on n vertices and $2n-4$ arcs, with $n = 8$ and $n = 18$. In both cases, the circuits of size 3 and 4 are drawn in blue. Note that Figure 3.12 is obtained through the left-most procedure in Corollary 3.4.2 while Figure 3.13 is obtained through the right most procedure.*

Let us now investigate the structure of positive bases of smaller size: the next theorem characterizes bases of size $\ell + 2$.

Theorem 3.4.4 *Let $n \geq \ell \geq 2$. A matrix $\mathbf{D}_{\mathbb{L},2} \in \mathbb{R}^{n \times (\ell+2)}$ is a positive basis for some ℓ -dimensional linear space $\mathbb{L} \subset \mathbb{R}^n$ if and only if there exists*

Figure 3.12. $|A| = 2n - 4$ Figure 3.13. $|A| = 2n - 4$

a non-positive vector $\mathbf{x} \in \mathbb{R}^k$, $k \in [1, \ell - 1]$ satisfying $[\mathbf{x}]_1 = 0$ and such that

$$\mathbf{D}_{L,2} \equiv \begin{bmatrix} \mathbf{I}_\ell & \mathbf{N} \\ \mathbf{0}_{n-\ell,\ell} & \mathbf{0}_{n-\ell,2} \end{bmatrix} \quad \text{with} \quad \mathbf{N} = \begin{bmatrix} -\mathbf{1}_k & \mathbf{x} \\ \mathbf{0}_{\ell-k} & -\mathbf{1}_{\ell-k} \end{bmatrix}.$$

Proof. As for Theorem 3.4.2, the converse implication is trivial and will not be proved. Moreover, we assume that $\ell = n$ as the general result is easily deduced from this specific case. Consider a positive basis $\mathbf{D}_{n,2}$ of size $n + 2$ in \mathbb{R}^n and any IN matrix $\mathbf{M} = [\mathbf{I}_n \ \mathbf{N}]$ associated to it through (3.6). Note $\mathbf{N} = \begin{bmatrix} -\mathbf{1}_k & \mathbf{w} \\ \mathbf{0}_{n-k} & -\mathbf{1}_{n-k} \end{bmatrix}$, where $k \in [1, n - 1]$ and $\mathbf{w} \in \mathbb{R}^k$ is arbitrary. By Theorem 3.4.1, \mathbf{w} is critical and so, if this vector is non-positive, one of its coordinates must be zero. In this case, the result is proved after permuting rows and columns in \mathbf{M} .

Otherwise and by definition of a critical vector, the maximal entry of \mathbf{w} must be non-unique and positive. Let $[\mathbf{w}]_i = [\mathbf{w}]_j > 0$ be two maximal entries; denote by \mathbf{u} and \mathbf{v} the two columns of \mathbf{N} . One easily checks that $\mathcal{B} = \{\mathbf{u}, \mathbf{e}_1, \dots, \mathbf{e}_n\} \setminus \{\mathbf{e}_i\}$ is a linear basis for \mathbb{R}^n , moreover

$$\mathbf{e}_i = -\mathbf{u} - \sum_{\ell=1, \ell \neq i}^k \mathbf{e}_\ell \quad \text{and} \quad \mathbf{v} = -[\mathbf{v}]_i \mathbf{u} + \sum_{\ell=1, \ell \neq i}^k ([\mathbf{v}]_\ell - [\mathbf{v}]_i) \mathbf{e}_\ell - \sum_{\ell=k+1}^n \mathbf{e}_\ell.$$

Note that each coefficient in the linear combination associated to \mathbf{e}_i is non-positive. Similarly, the linear combination associated to \mathbf{v} is non-positive as $[\mathbf{v}]_i = [\mathbf{w}]_i$ is a maximal entry of \mathbf{v} , and this combination is not strictly negative as $[\mathbf{v}]_j - [\mathbf{v}]_i = 0$. In consequence, letting $\mathbf{B} \in \mathbb{R}^{n \times n}$ satisfy $\text{col}(\mathbf{B}) = \mathcal{B}$, we see that up to rows and columns permutation, the matrix $\mathbf{B}^{-1}\mathbf{M}$ has the announced structure. Since $\mathbf{D}_{n,2} \equiv \mathbf{B}^{-1}\mathbf{M}$, the result is proved. \square

Through the use of Lemma 3.4.1, the previous theorem is easily translated into a statement on minimally strongly edge-connected digraphs.

Corollary 3.4.3 *A digraph $G = (V, A)$ on n vertices and $n + 1$ arcs is minimally strongly edge-connected if and only if it is the union of two*

circuits whose intersection defines an elementary path - potentially reduced to a single vertex - in G .

Proof. We only prove the direct implication as the converse is trivial. Let $\mathbf{M} = \mathbf{D}_{n-1,2}$ in $\mathbb{R}^{(n-1) \times (n+1)}$ be a network matrix associated to the minimally strongly edge-connected graph G . By Theorem 3.4.4, $\mathbf{M} \equiv \tilde{\mathbf{M}} = [\mathbf{I}_{n-1} \quad \mathbf{N}]$ with

$$\mathbf{N} = \begin{bmatrix} -\mathbf{1}_k & \mathbf{x} \\ \mathbf{0}_{n-1-k} & -\mathbf{1}_{n-1-k} \end{bmatrix} \quad \text{and} \quad \mathbf{x} \leq \mathbf{0}_k, \quad k \geq 1, \quad [\mathbf{x}]_1 \neq 0.$$

Using Lemma 3.4.1 we assume $\tilde{\mathbf{M}}$ to be a network matrix, therefore $\mathbf{x} \in \{-1, 0\}^k$. Write $A = \{a_1, \dots, a_n\}$ and suppose that the i^{th} column of $\tilde{\mathbf{M}}$ is associated to a_i , for all i .

Based on the structure of $\tilde{\mathbf{M}}$, the digraph G contains a circuit of size $k + 1$, namely $\mathcal{C}_1 = \{a_1, \dots, a_k, a_n\}$. Moreover \mathcal{C}_2 is a circuit in G , where $\mathcal{C}_2 = \{a_{i_1}, \dots, a_{i_m}, a_{k+1}, \dots, a_{n-1}, a_{n+1}\}$ and $\{i_1, \dots, i_m\} \subset \llbracket 2, k \rrbracket$ is the - potentially empty - set of indices i such that $[\mathbf{x}]_i = -1$. We show that $\mathcal{C}_1 \cap \mathcal{C}_2$ is an elementary path. For $i \leq 2$, let $V_i \subset V$ be the set of extremities of the arcs in \mathcal{C}_i and let $v \in V_1$. Consider the sequence given by $G_0 = (\{v\}, \emptyset)$, $G_1 = (V_1, \mathcal{C}_1)$, $G_2 = (V_1 \cup V_2, \mathcal{C}_1 \cup \mathcal{C}_2)$. As $\mathcal{C}_1 \cup \mathcal{C}_2 = A$, the sequence defines an ear-decomposition for G . In particular $(\mathcal{C}_1 \cup \mathcal{C}_2) \setminus \mathcal{C}_1 = \mathcal{C}_2 \setminus \mathcal{C}_1$ is an ear of G that defines a $u - v$ path between two vertices in V . Then, since \mathcal{C}_2 is a circuit, we find that $(\mathcal{C}_1 \cup \mathcal{C}_2) \cap \mathcal{C}_1 = \mathcal{C}_1 \cap \mathcal{C}_2$ must be an elementary $v - u$ path. \square

Proposition 2.2.2, Corollary 2.2.1 as well as Theorems 3.4.2 and 3.4.4 together imply that any positive basis $\mathbf{D}_{n,s}$, $n \leq 4$ is associated through (3.6) to an IN matrix $[\mathbf{I}_n \quad \mathbf{N}]$ where \mathbf{N} has non-positive entries. Although positive bases can always be generated from such IN matrix structures [64, Theorem 5.4], we emphasize that the equivalence no longer holds in dimension 5 or higher, as could be anticipated from Theorem 3.4.3. Indeed, the matrix $\mathbf{D}_{5,8} = [\mathbf{I}_5 \quad -\mathbf{e}_1 - \mathbf{e}_2 - \mathbf{e}_3 \quad -\mathbf{e}_2 - \mathbf{e}_3 - \mathbf{e}_4 \quad \mathbf{e}_2 + \mathbf{e}_3 - \mathbf{e}_5]$ is both a positive basis and a network matrix, yet it cannot be associated through (3.6) to any IN matrix with a non-positive \mathbf{N} block.

3.5 PkSSs and k-strong edge connectivity

The previous sections of this chapter have highlighted the relationship between positive spanning sets and directed graphs. We now expand on this relationship in hope of finding new properties for PkSSs.

3.5.1 k -strongly edge-connected digraphs

Akin to the relationship between PKSSs and positive spanning sets, the notion of k -strong edge connection in digraphs can be seen as generalizing that of strong edge-connection.

Definition 3.5.1 (k -strongly edge-connected digraph) A digraph $G = (V, A)$ with $|A| \geq k - 1$ is k -strongly edge-connected whenever it is strongly edge-connected and remains so upon arbitrarily removing $k - 1$ arcs or less.

As should be clear from the definition, being strongly edge-connected is equivalent to being 1-strongly edge-connected. By creating k copies of the arcs of a strongly edge-connected digraph, one easily creates a k -strongly edge-connected digraph. Other examples are provided below.

Example 3.5.1 The two digraphs on 5 vertices below are 2-strongly edge-connected.

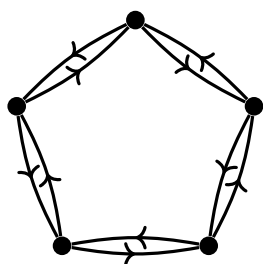


Figure 3.14. 2-strongly edge-connected

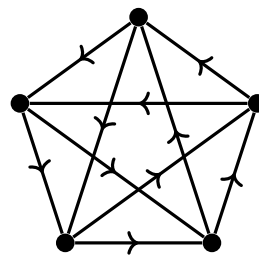


Figure 3.15. 2-strongly edge-connected

Alternatively, k -strongly edge-connected digraphs are sometimes defined based on the following theorem - which can be seen as a corollary to Menger's theorem [29].

Theorem 3.5.1 [70, Theorem 15.4] A digraph $G = (V, A)$ is k -strongly edge-connected if and only if there exist k arc-disjoint paths between any two vertices u and v .

Theorem 3.5.1 is easily illustrated by the two digraphs given in Figures 3.14 and 3.15. Moreover note that removing an arbitrary arc from any of these graphs makes them lose their 2-strong connectivity. In that sense, we say that they are minimal for this property.

Definition 3.5.2 (Minimally k -strongly edge-connected digraph) A digraph G is minimally k -strongly edge-connected whenever it is k -strongly edge-connected and loses this property upon arbitrarily removing one arc.

It is well known that the number of arcs in a minimally k -strongly edge-connected digraph on n vertices is not fixed. The lower bound can easily be

proved to be kn [10, Section 5.6]. The exact value of the upper bound was determined by Dalmazzo [18] and generalizes that given in Proposition 3.1.1.

Proposition 3.5.1 [18, Corollary to Theorem 2] *Let $G = (V, A)$ be minimally k -strongly edge-connected on $n \geq 2$ vertices. Then*

$$kn \leq |A| \leq 2k(n - 1). \tag{3.10}$$

As stated in Proposition 3.1.1, bi-directed trees are the only strongly edge-connected digraphs on $n \geq 2$ vertices with $|A| = 2(n - 1)$. The result generalizes to minimally k -strongly edge-connected digraphs.

Proposition 3.5.2 [18, Theorem 4] *Let $G = (V, A)$ be minimally k -strongly edge-connected on $n \geq 2$ vertices. If $|A| = 2k(n - 1)$, then G is obtained by replacing each edge of a tree with $2k$ arcs, k in each direction.*

Figures 3.16 and 3.17 below provide two examples of minimally 2-strongly edge-connected digraphs with a maximal number of arcs: each contains 4 vertices and 16 arcs. As per Proposition 3.5.2, they are the only two minimally 2-strongly edge-connected digraphs of such size.

Example 3.5.2 *In the two figures below, a doubled arrow tip indicates that an arc is doubled.*

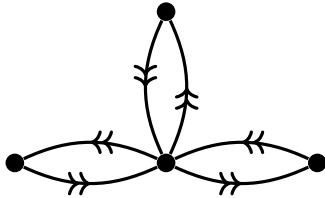


Figure 3.16. $|A| = 2k(n - 1)$



Figure 3.17. $|A| = 2k(n - 1)$

When considering minimally strongly edge-connected digraphs with no duplicated arcs, note that the upper bound given in Proposition 3.5.1 can be reduced [11]. A variety of scientific articles revolve around finding algorithms to recognize k -strongly edge-connected digraphs [78, 82]. The general properties of k -strongly edge-connected digraphs are discussed at length in [10, Section 5.6].

We conclude this section with a result bridging undirected graphs with k -strongly edge-connected, directed ones, adapted from a theorem by Nash-Williams [58]. We start by defining a concept of interest.

Definition 3.5.3 (k -edge-connected graph) *Let $G = (V, E)$ be undirected. We say that G is k -edge-connected if it is connected and remains so upon arbitrarily removing $(k - 1)$ edges or less.*

Cycles are basic examples of 2-edge-connected graphs. Note that these can easily be oriented into 1-strongly edge-connected digraphs, by turning them into circuits. Nash-Williams [58] proved that the result generalizes to $2k$ -edge-connected graphs.

Theorem 3.5.2 [58, Theorem 1] *Let $k \geq 1$, let $G = (V, E)$ be a $2k$ -edge-connected undirected graph on n vertices. Then G can be oriented into a k -strongly edge-connected digraph.*

Example 3.5.3 *The 2-edge-connected, undirected graph below can easily be transformed into a strongly edge-connected digraph, as shown in Figure 3.10.*

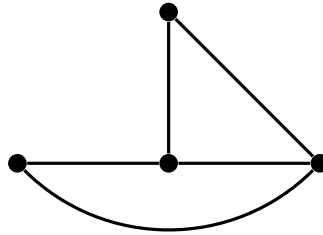


Figure 3.18. 2-edge-connected, undirected graph

3.5.2 Links with positive k -spanning sets and positive k -bases

The relationship between PSSs and strongly edge-connected digraphs generalizes to positive k -spanning sets: the next proposition is deduced from Theorem 3.2.1 and Proposition 3.2.1.

Proposition 3.5.3 *Let $T = (V, \hat{A})$ be an oriented spanning tree contained in a digraph $G = (V, A)$. The associated network matrix $\mathbf{M} \in \mathbb{R}^{n \times m}$ is a $PkSS$ for \mathbb{R}^n if and only if G is k -strongly edge-connected.*

Proof. Suppose that G is k -strongly edge-connected and let $\tilde{\mathbf{M}}$ be obtained from \mathbf{M} by removing $k - 1$ columns or less. In order to show that \mathbf{M} is positively k -spanning, it suffices to show that $\tilde{\mathbf{M}}$ is a PSS. Name a_{i_1} to $a_{i_{k-1}}$ the arcs of G associated to the columns of \mathbf{M} that were removed.

First, suppose that $\{a_{i_1}, \dots, a_{i_{k-1}}\} \cap \hat{A} = \emptyset$. Then $\tilde{\mathbf{M}}$ is the network matrix associated to $\tilde{G} = (V, A \setminus \{a_{i_1}, \dots, a_{i_{k-1}}\})$ and to T . Since G is k -strongly edge-connected, then \tilde{G} must be strongly edge-connected; by Theorem 3.2.1, $\tilde{\mathbf{M}}$ is a PSS.

Suppose now that $\{a_{i_1}, \dots, a_{i_{k-1}}\} \cap \hat{A} \neq \emptyset$ and let $T' = (V, \hat{A}')$ denote a spanning tree of G whose set of arcs does not intersect $\{a_{i_1}, \dots, a_{i_{k-1}}\}$. By Proposition 3.2.1, the network matrix \mathbf{M}' associated to G and T' satisfies $\mathbf{M}' \equiv \mathbf{M}$. Thus $\tilde{\mathbf{M}}$ is structurally equivalent to a submatrix $\tilde{\mathbf{M}}'$ of \mathbf{M}' . Moreover $\tilde{\mathbf{M}}'$ is the network matrix associated to \tilde{G} and to T' . In turn, it is a PSS and so $\tilde{\mathbf{M}}$ is also a PSS.

Conversely, suppose that $\tilde{\mathbf{M}}$ is a PkSS. The previous reasoning can be reversed to deduce that G must be k -strongly edge-connected. \square

We easily derive from Proposition 3.5.3 that the network matrix of a minimally k -strongly edge-connected digraph is a positive k -basis. Exploiting this result and that of Proposition 3.5.2, one can describe the structure of a specific type of positive k -basis. Indeed, we see that all positive k -bases $\mathbf{D} \in \mathbb{R}^{n \times 2kn}$ that are structurally equivalent to the network matrix of some minimally k -strongly edge-connected digraph are obtained by stacking together copies of a maximal positive basis.

Example 3.5.4 *The matrix $\mathbf{D} = [\mathbf{I}_3 \quad -\mathbf{I}_3 \quad \mathbf{I}_3 \quad -\mathbf{I}_3] = [\mathbf{D}_{3,3} \quad \mathbf{D}_{3,3}]$ is both a positive 2-basis and a network matrix associated to the minimally 2-strongly edge-connected digraph G given in Figure 3.16.*

In spite of these promising results, the relationship between digraphs and positive k -bases quickly reaches its first limitation. Indeed, for $k \geq 2$, there is no clear correspondence between the size of minimally k -strongly edge-connected digraphs and that of positive k -bases in \mathbb{R}^n - see Propositions 2.3.2 and 2.3.6. Using a broader approach, let us now investigate the general properties of k -strongly edge-connected digraphs with the hope of finding an analog for PkSSs.

Partitioning matrices

We first take interest in Theorem 3.5.1, stating that any two vertices of a k -strongly edge-connected digraphs are connected to each other through k disjoint paths. An equivalent property for matrices is defined thereafter.

Definition 3.5.4 (Partitionable matrix) *Let $k \geq 1$ and $\mathbf{x} \in \mathbb{R}^n$. A matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$ is (\mathbf{x}, k) -partitionable if $\mathbf{D} \equiv [\mathbf{D}_{\mathbf{x},1} \quad \dots \quad \mathbf{D}_{\mathbf{x},k}]$, where \mathbf{x} is contained in the positive span of each block $\mathbf{D}_{\mathbf{x},i}$. We say that \mathbf{D} is k -partitionable if it is (\mathbf{x}, k) -partitionable for all $\mathbf{x} \in \mathbb{R}^n$.*

It immediately follows from Definition 3.5.4 that all k -partitionable matrices are positively k -spanning. Letting $\mathbf{D}_{n,s} \in \mathbb{R}^{n \times (n+s)}$ be a positive basis in \mathbb{R}^n , a trivial example of a k -partitionable matrix in \mathbb{R}^n is given by $[\mathbf{D}_{n,s} \quad \dots \quad \mathbf{D}_{n,s}]$. In particular, we note that the network matrix of a minimally k -strongly edge-connected digraph of maximal size is k -partitionable. In dimension 2 and more however, the columns of k -partitionable PkSSs can usually not be decomposed in such a fashion: a counter example is given by the pentagon represented in Figure 2.9. While the associated positive 2-basis $\mathbf{D} \in \mathbb{R}^{2 \times 5}$ is 2-partitionable, it is clear that the matrix cannot be decomposed into a union of two PSSs as \mathbf{D} only possesses five columns.

In the case of digraphs, we note that an analog negative result applies: arbitrary k -strongly edge-connected digraphs $G = (V, A)$ cannot always be

decomposed into a union of strongly edge-connected digraphs $G_i = (V, A_i)$, $i \leq k$.

Example 3.5.5 *The directed graph $G = (V, A)$ represented in Figure 3.19 below cannot be partitioned into a union of two strongly edge-connected digraphs on five vertices.*

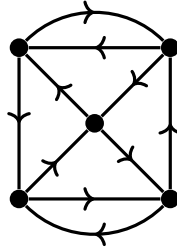


Figure 3.19. Minimally 2-strongly edge-connected

We indicated earlier that all k -partitionable matrices were positively k -spanning. The converse implication, which generalizes the result of Theorem 3.5.1, can be proved to be true in low dimensions.

Proposition 3.5.4 *Let $n \leq 2$. All $PkSS$ s in \mathbb{R}^n are k -partitionable.*

Proof. The result trivially holds when $n = 1$ as any $PkSS$ in \mathbb{R} is structurally equivalent to a matrix which contains k copies of the positive basis $[1 \ -1]$ in its columns.

Now, let $\mathbf{x} \in \mathbb{R}^2$ and let $\mathbf{D} = [\mathbf{d}_1 \ \dots \ \mathbf{d}_m] \in \mathbb{R}^{2 \times m}$ be a positive k -spanning set, whose columns are assumed to be nonzero. We make the additional assumption that $\mathbf{x} \neq \mathbf{0}_2$, as \mathbf{D} is clearly $(\mathbf{0}_2, k)$ -partitionable.

Let $\Theta(\mathbf{u}, \mathbf{v}) \in [0, 2\pi[$ denote the angle between two nonzero vectors \mathbf{u} and \mathbf{v} . Without loss of generality, we assume to have $\Theta(\mathbf{x}, \mathbf{d}_i) \leq \Theta(\mathbf{x}, \mathbf{d}_{i+1})$ for all i and we let $\mathbf{M}_i = [\mathbf{d}_i \ \mathbf{d}_{m-k+i}]$. Then $\mathbf{x} \in \text{pspan}(\mathbf{M}_i)$ for all $i \leq k$, and so the matrix \mathbf{D} is (\mathbf{x}, k) -partitionable. □

Example 3.5.6 *The regular heptagon $[\mathbf{d}_1 \ \dots \ \mathbf{d}_7]$ represented below is a 3-partitionable $P3SS$ in \mathbb{R}^2 . For instance, the vector \mathbf{x} is contained in each of the three cones $\text{pspan}([\mathbf{d}_1 \ \mathbf{d}_5])$, $\text{pspan}([\mathbf{d}_2 \ \mathbf{d}_6])$ and $\text{pspan}([\mathbf{d}_3 \ \mathbf{d}_7])$.*

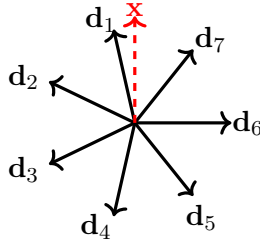


Figure 3.20. 3-partitionable P3SS

Note that the result of Proposition 3.5.4 does not hold anymore in higher dimensions, as illustrated by the next counter-example.

Example 3.5.7 The P2SS $\mathbf{D} = \begin{bmatrix} 1 & 0 & -1 & -1 & 1 & 0 & 0 \\ 0 & 1 & -1 & -3 & 2 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 \end{bmatrix}$ in \mathbb{R}^3 , whose columns consist of a lifted pentagon and of two copies of the vector $-\mathbf{e}_3$, is not $(\mathbf{e}_3, 2)$ -partitionable. In turn, \mathbf{D} is not 2-partitionable.

Reorienting matrices

We now turn our attention towards Theorem 3.5.2, stating that all $2k$ -edge-connected undirected graphs can be oriented into k -strongly edge-connected digraphs. Our aim is to translate this result into an equivalent one which applies to a particular class of matrix, defined thereafter.

Definition 3.5.5 (k -spanning set) A matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$ with $m \geq k$ is a k -spanning set in \mathbb{R}^n (alternatively, we say that \mathbf{D} is k -spanning) if it is linearly spanning and remains so upon arbitrarily removing $k - 1$ columns or less. If no proper submatrix of \mathbf{M} is k -spanning in \mathbb{R}^n , we say that \mathbf{M} is minimally k -spanning.

k -spanning and minimally k -spanning matrices can be thought of as the counterpart to positive k -spanning sets and positive k -bases. Our main interest resides in k -spanning network matrices. Using Theorem 3.2.1 and since all PkSSs are k -spanning, a first example is given by the network matrix of any k -strongly edge-connected digraph. In order to generalize Theorem 3.5.2, we now apply the concept of reorientation to matrices.

Definition 3.5.6 (Reoriented matrix) A matrix $\tilde{\mathbf{M}} \in \mathbb{R}^{n \times m}$ is a reorientation of $\mathbf{M} \in \mathbb{R}^{n \times m}$ if it can be obtained by arbitrarily replacing columns in \mathbf{M} with their opposite.

The relationship between reorientations of digraphs and matrices is discussed in the next proposition.

Proposition 3.5.5 Let $T = (V, \hat{A})$ be a spanning tree contained in a digraph $G = (V, A)$ on $n + 1$ vertices and let $\mathbf{M}_1 = [\mathbf{I}_n \ \mathbf{X}_1]$ be the associated network matrix. Any network matrix \mathbf{M}_2 associated to some orientation of G and T is structurally equivalent to a reorientation of \mathbf{M}_1 .

Proof. Let $\tilde{G} = (V, A)$ be the orientation of G to which \mathbf{M}_1 is associated. Let $\tilde{T} = (V, \hat{A})$ be the associated orientation of T . Any other orientation of G and T can be obtained by iteratively changing the direction of arcs in \tilde{G} . Let $a_i \in A$ and let $\mathbf{c}_i \in \text{col}(\mathbf{M})$ be the column associated to a_i .

Upon reorienting a_i , we change the sign of \mathbf{c}_i to create a new matrix \mathbf{M} which represents the relationships between the arcs of the modified digraph. If $a_i \notin \hat{A}$, then $\mathbf{c}_i \in \text{col}(\mathbf{X}_1)$ and $\mathbf{M} = \mathbf{M}_2$ is thus a network matrix. On the other hand if $a_i \in \hat{A}$, then \mathbf{M} does not possess an identity block anymore as $\mathbf{c}_i = \mathbf{e}_i \in \text{col}(\mathbf{I}_n)$. We then change the sign of the i^{th} row of \mathbf{M} to obtain the network matrix $\mathbf{M}_2 = [\mathbf{I}_n \ \mathbf{X}_2] \equiv \mathbf{M}$. \square

Example 3.5.8 The network matrix \mathbf{M}_2 below is structurally equivalent to a reorientation of the matrix \mathbf{M} given in Figure 3.10. Indeed, \mathbf{M}_2 is obtained from \mathbf{M} by successively changing the sign of the first row and the first column.

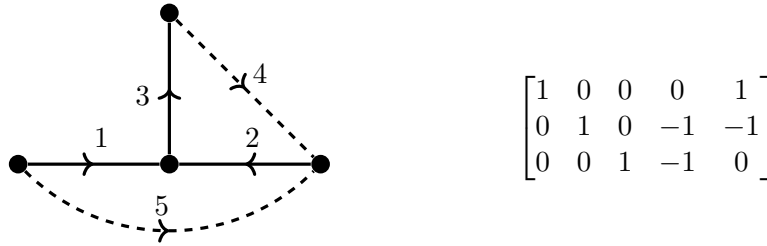


Figure 3.21. Digraph, spanning tree and network matrix

Note that two network matrices $[\mathbf{I}_n \ \mathbf{X}_1]$ and $[\mathbf{I}_n \ \mathbf{X}_2]$ are associated to two orientations of the same digraph and spanning tree if and only if \mathbf{X}_2 is obtained from \mathbf{X}_1 by switching the signs of some rows and columns. Let us now restate Theorem 3.5.2 in terms of network matrices.

Proposition 3.5.6 Let $\mathbf{M} = [\mathbf{I}_n \ \mathbf{X}]$ be a $2k$ -spanning network matrix. Then \mathbf{M} admits a reorientation into a $PkSS$.

Proof. Let $G = (V, A)$ be the digraph associated to \mathbf{M} . Based on Theorem 3.5.2 and Proposition 3.5.5, the result is proved upon showing that the underlying undirected graph $\tilde{G} = (V, E)$ is $2k$ -edge-connected. The proof of this last statement is essentially identical to that of Proposition 3.5.3. \square

In the remainder of this section, we investigate the properties of $2k$ -spanning matrices in \mathbb{R}^n , with the hope of generalizing the result of Propo-

sition 3.5.6 to non-network matrices. We start by proving that when $k = 1$, the result holds for all $2k$ -spanning sets.

Proposition 3.5.7 *Let $\mathbf{M} \in \mathbb{R}^{n \times m}$ be 2 -spanning. Then \mathbf{M} admits a reorientation into a PSS.*

Proof. Consider a matrix $\mathbf{N} = [\mathbf{I}_n \ \mathbf{X}] \in \mathbb{R}^{n \times m}$ satisfying $\mathbf{N} \equiv \mathbf{M}$. Then \mathbf{M} admits a reorientation into a PSS if and only if \mathbf{N} shares this same property. As \mathbf{M} is 2 -spanning, so must be \mathbf{N} . Thus for all $i \in [1, n]$, the block \mathbf{X} admits a column whose i^{th} entry is nonzero. Therefore there exists a vector $\mathbf{v} \in \text{pspan}(\mathbf{X})$ which satisfies $[\mathbf{v}]_i \neq 0$, for all $i \leq n$. Now, consider the diagonal matrix $\mathbf{B} \in \mathbb{R}^{n \times n}$ defined by $[\mathbf{B}]_{i,i} = \text{sgn}(-[\mathbf{v}]_i)$, for all $i \leq n$. By construction, the matrix $[\mathbf{B} \ \mathbf{v}] \equiv [\mathbf{I}_n \ -\mathbf{1}_n]$ is a minimal positive basis in \mathbb{R}^n . Thus $\tilde{\mathbf{N}} = [\mathbf{B} \ \mathbf{X}]$ is reorientation of \mathbf{N} into a PSS, as each column of $[\mathbf{B} \ \mathbf{v}]$ is contained in $\text{pspan}(\tilde{\mathbf{N}})$. \square

Example 3.5.9 *The matrix $\mathbf{M} = \begin{bmatrix} 1 & 2 & 3 & 3 & 5 \\ 4 & 5 & 6 & 9 & 11 \\ 7 & 9 & 9 & 16 & 18 \end{bmatrix}$, which is 2 -spanning*

in \mathbb{R}^3 , is structurally equivalent to $\mathbf{N} = [\mathbf{I}_3 \ \mathbf{e}_1 + \mathbf{e}_2 \ \mathbf{e}_2 + \mathbf{e}_3]$. We reorient \mathbf{N} into a PSS by considering the matrix $\tilde{\mathbf{N}} = [\mathbf{I}_3 \ -(\mathbf{e}_1 + \mathbf{e}_2) \ -(\mathbf{e}_2 + \mathbf{e}_3)]$.

Since $\tilde{\mathbf{N}} \equiv \begin{bmatrix} 1 & 2 & 3 & -3 & -5 \\ 4 & 5 & 6 & -9 & -11 \\ 7 & 8 & 9 & -15 & -17 \end{bmatrix}$, we found a reorientation $\tilde{\mathbf{M}}$ of \mathbf{M} into a

PSS. While $\tilde{\mathbf{M}} \equiv \tilde{\mathbf{N}}$ is a positive basis, we note that the 2 -spanning matrix \mathbf{M} was surprisingly not minimal.

One can easily verify that $k+n-1$ is the lowest attainable size for the number of columns of a minimal k -spanning set $\mathbf{M} \in \mathbb{R}^{n \times m}$. On the other hand, it is known that the maximal possible size is given by $m = kn$ and that minimal k -spanning sets of such size consist of k scalar multiples of a linear basis [49, page 3]. Based on these observations, the result of Proposition 3.5.7 can be generalized to all values of k , in dimension 2.

Proposition 3.5.8 *Let $n \leq 2$. For all $k \geq 1$, all $2k$ -spanning sets \mathbf{M} in \mathbb{R}^n admit a reorientation into a PkSS.*

Proof. First, suppose that $n = 1$. Then \mathbf{M} possesses $2k$ nonzero entries or more, as it is $2k$ -spanning. Reorient \mathbf{M} to ensure that k of these coefficients are positive and k other are negative. The matrix $\tilde{\mathbf{M}}$ thus obtained is a PkSS in \mathbb{R} .

Now let $n = 2$ and let $\mathbf{M} = [\mathbf{c}_1 \ \dots \ \mathbf{c}_m] \in \mathbb{R}^{2 \times m}$ be $2k$ -spanning. Clearly, $m \geq 2k + 1$. For the sake of simplicity, we assume \mathbf{M} to be *minimally* $2k$ -spanning; in particular, each column \mathbf{c}_i is nonzero. For any two

nonzero vectors \mathbf{u} and \mathbf{v} in \mathbb{R}^2 , we denote by $\Theta(\mathbf{u}, \mathbf{v}) \in [0, 2\pi[$ the angle from \mathbf{u} to \mathbf{v} . We reorder the columns of \mathbf{M} and if necessary, reorient them to ensure $0 \leq \Theta(\mathbf{e}_1, \mathbf{c}_1) \leq \Theta(\mathbf{e}_1, \mathbf{c}_2) \leq \dots \leq \Theta(\mathbf{e}_1, \mathbf{c}_m) < \pi$.

Initially, we assume each column \mathbf{c}_i to be unique. Then $m = 2k + 1$ and we claim that the matrix $\tilde{\mathbf{M}} = [\mathbf{c}_1 \quad -\mathbf{c}_2 \quad \mathbf{c}_3 \quad \dots \quad -\mathbf{c}_{2k} \quad \mathbf{c}_{2k+1}]$ is a PkSS. Indeed and by construction, any submatrix of $\tilde{\mathbf{M}}$ constituted of three columns of indices $i_1 < i_2 < i_3$ with i_1 and i_3 both odd and i_2 even (resp. i_1 and i_3 both even and i_2 odd) is positively spanning. Upon removing $k - 1$ columns of $\tilde{\mathbf{M}}$, at least one such triplet is preserved in the resulting matrix \mathbf{N} , thus \mathbf{N} is a PSS and so $\tilde{\mathbf{M}}$ is positively k -spanning.

Now, we assume some column \mathbf{c}_i of \mathbf{M} to be non-unique. As \mathbf{M} is *minimally* $2k$ -spanning, some other column $\mathbf{c}_j \neq \mathbf{c}_i$ must also be non-unique. Two cases are to be considered. First, assume that *each* column \mathbf{c}_ℓ is non-unique. Then \mathbf{M} is a $2k$ -spanning set of maximal size $4kn$ and consists of two copies of a k -spanning set. By orienting these two copies in opposite directions, we obtain a PkSS $\tilde{\mathbf{M}}$. Last, we assume the existence of some index ℓ such that \mathbf{c}_ℓ is unique. Then, the submatrix $\mathbf{N} = [\mathbf{c}_i \quad \mathbf{c}_j \quad \mathbf{c}_\ell]$ of \mathbf{M} is 2-spanning; up to permuting columns we write $\mathbf{M} = [\mathbf{N} \quad \tilde{\mathbf{M}}]$. Using Proposition 3.5.7, we reorient \mathbf{N} into a PSS. We now wish to orient the matrix $\tilde{\mathbf{M}}$ into a $P(k - 1)$ SS. This reorientation can be achieved through a recursive reasoning, upon observing that $\tilde{\mathbf{M}}$ is $2(k - 1)$ -spanning. \square

Example 3.5.10 Figure 3.22 below shows a 4-spanning set \mathbf{M} of size 5 in \mathbb{R}^2 . The vectors are reoriented in Figure 3.23 to ensure $\Theta(\mathbf{e}_1, \tilde{\mathbf{c}}_i) < \pi$, for all i . Finally, each vector $\tilde{\mathbf{c}}_i$ of even index is reoriented. We obtain the P2SS given in Figure 3.24.

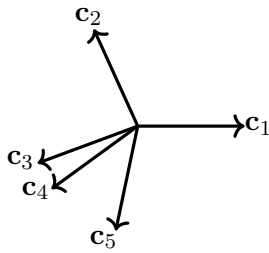


Figure 3.22

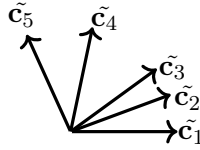


Figure 3.23

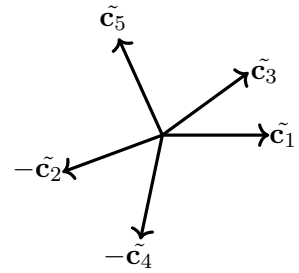


Figure 3.24

Now, consider the minimal 4-spanning set of size 7 given in Figure 3.25. Combined with \mathbf{c}_4 , the two redundant vectors \mathbf{c}_1 and \mathbf{c}_5 form a 2-spanning set which we orient into a PSS. The four remaining vectors $\mathbf{c}_2 = \mathbf{c}_3$ and $\mathbf{c}_6 = \mathbf{c}_7$ are non-unique and reoriented into a positive basis $\mathbf{D}_{2,2}$ to obtain the P2SS given in Figure 3.26.

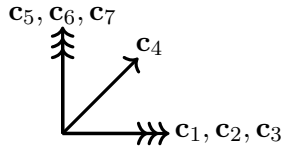


Figure 3.25

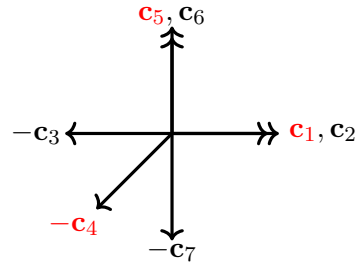


Figure 3.26

We conclude this section with a counter-example illustrating that in the general case, for larger values of k and n , $2k$ -spanning sets in \mathbb{R}^n cannot be reoriented into Pk SSs.

Example 3.5.11 The matrix $\mathbf{M} = \begin{bmatrix} 1 & 0 & 0 & 2 & 1 & 1 \\ 0 & 1 & 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 1 & 1 & 2 \end{bmatrix}$ is 4-spanning, yet cannot be reoriented into a $P2SS$. Indeed, by Lemma 2.3.1 and by symmetry any such reorientation would be equivalent to $\tilde{\mathbf{M}} = \begin{bmatrix} 1 & 0 & 0 & -2 & -1 & 1 \\ 0 & 1 & 0 & -1 & -2 & 1 \\ 0 & 0 & 1 & -1 & -1 & 2 \end{bmatrix}$.

Name $\tilde{\mathbf{M}}_{\mathbf{e}_2}$ the matrix obtained from $\tilde{\mathbf{M}}$ by removing the column \mathbf{e}_2 . Then each element \mathbf{v} of $\text{pspan}(\tilde{\mathbf{M}}_{\mathbf{e}_2})$ satisfies $[\mathbf{v}]_2 \leq [\mathbf{v}]_3$, thus $\tilde{\mathbf{M}}_{\mathbf{e}_2}$ is not a PSS and $\tilde{\mathbf{M}}$ is not a $P2SS$.

3.6 Summary of Chapter 3

Throughout this chapter, we studied the links between graphs and positive spanning sets. We showed that the properties of *strongly edge-connected digraphs*, a concept which extends that of connectivity in undirected graphs, could be used to characterize PSS s and positive bases. We analyzed the main properties of such graphs in Section 3.1, where we took a particular interest in the characterization of strong connectivity through ear-decompositions - see Section 3.1.2.

The bridging between graphs and PSS s was accomplished in Section 3.2 using *network matrices*: we showed in Section 3.2.2 that a network matrix was positively spanning on the condition that the associated digraph was strongly edge-connected. This was the object of Theorem 3.2.1, which corresponds to the first contribution of this chapter. Building on this theorem, we showed in Section 3.3 the existence of an analog result to the ear-decomposition of strongly edge-connected digraphs, applied to PSS s. This result, stated in Theorem 3.3.1, characterizes positive spanning sets and was successfully derived upon studying the properties of *circuits* in matrices - see Section 3.3.1.

Aiming to refine Theorem 3.3.1 into a characterization of positive bases, we studied in Section 3.4.2 the notion of *criticality*, which we had already encountered in Chapter 2. Upon successfully characterizing the critical families for linear spaces of low dimension in Proposition 3.4.2, we were able to properly describe the structure of positive bases of sizes $2n - 1$, $2n - 2$ and $n + 2$ in \mathbb{R}^n in Section 3.4.3; in turn, we used these newfound results to characterize strongly edge-connected digraphs of near extreme sizes.

In the last section of this chapter, we discussed the link between positive k -spanning sets and k -strongly edge-connected digraphs, a resilient class of strongly edge-connected digraphs whose properties are listed in Section 3.5.1. While the result of Theorem 3.2.1 was easily generalized, we quickly realized that no decomposition result for PkSSs could be derived from the study of positively k -spanning network matrices. Instead, we investigated generalizations of some usual properties of k -strongly edge-connected digraphs - see Theorems 3.5.1 and 3.5.2. Menger's theorem states that two vertices in a k -strongly edge-connected digraph are connected through k pairwise disjoint oriented paths. We showed in Section 3.5.2 that the analog matrix property, defined in Definition 3.5.4, was satisfied by all PkSSs in dimension 2 or less but did not hold anymore in higher dimensions. Similarly, we saw that although all $2k$ -connected graphs could be reoriented into strongly k -connected digraphs, the analog property for $2k$ -spanning sets - see Definitions 3.5.5 and 3.5.6 - could only hold for low values of k and n . Most of the content from Sections 3.1 to Section 3.4 have been accepted for publication in **Discrete applied mathematics** [17]. New contributions of this thesis are found in Theorem 3.4.3 and Corollary 3.4.2.

Chapter 4

Cosine measures and positive spanning sets

This chapter focuses on the *cosine measure*, a tool which quantifies how well the directions induced by the set of columns of a matrix cover the Euclidean space and whose main properties are discussed in Section 4.1.2. Various computational techniques have been proposed for determining the cosine measure of a matrix [31, 65], a problem which was recently shown to be APX-hard [38]. We take a particular interest in an algorithm by Hare and Jarry-Bolduc, which we describe in Section 4.1.2. We then focus on a recently identified class of positive spanning sets, called orthogonally structured positive bases (OSPBs). First, we describe in Section 4.2 how to identify such matrices and compute their cosine measures efficiently by improving on Hare and Jarry-Bolduc’s algorithm. Then, in Section 4.3, we turn towards studying positive k -spanning sets, for which we provide a new notion of cosine measure that accounts for the resilient nature of such matrices. By combining our results, we are able to use orthogonally structured positive bases to create positive k -spanning sets with guarantees on the value of their cosine measures.

4.1 The cosine measure

4.1.1 Definition and examples

Positive spanning sets and positive bases are now a standard tool used by derivative-free optimization algorithms [15, 6]. The idea is to use directions induced by the set of columns of a PSS in replacement for derivative information. In that setting, it becomes critical to quantify how well these directions cover the space of interest, which is typically assessed through the

cosine measure of this PSS [43, 40].

Definition 4.1.1 (Cosine measure and cosine vector set) Let \mathbf{D} be a matrix with nonzero columns $\mathbb{R}^{n \times m}$. The cosine measure and the associated cosine vector set of \mathbf{D} , noted $\text{cm}(\mathbf{D})$ and $c\mathcal{V}(\mathbf{D})$, are given by

$$\text{cm}(\mathbf{D}) = \min_{\substack{\|\mathbf{u}\|=1 \\ \mathbf{u} \in \mathbb{R}^n}} \max_{\mathbf{d} \in \text{col}(\mathbf{D})} \frac{\mathbf{u}^\top \mathbf{d}}{\|\mathbf{d}\|} \quad \text{and} \quad c\mathcal{V}(\mathbf{D}) = \arg \min_{\substack{\|\mathbf{u}\|=1 \\ \mathbf{u} \in \mathbb{R}^n}} \max_{\mathbf{d} \in \text{col}(\mathbf{D})} \frac{\mathbf{u}^\top \mathbf{d}}{\|\mathbf{d}\|}.$$

The cosine vector set of a matrix \mathbf{D} consists of all unitary vectors \mathbf{v} whose angular distance to their closest neighbor in $\text{col}(\mathbf{D})$ is maximized. The value $\text{cm}(\mathbf{D})$ is given by the cosine of the angle between any such vector \mathbf{v} and its closest neighbor in $\text{col}(\mathbf{D})$.

Example 4.1.1 Consider the basis $\mathbf{D} = [\mathbf{d}_1 \ \mathbf{d}_2 \ \mathbf{d}_3] = \begin{bmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2} \end{bmatrix}$ whose columns are represented in the figure below. Then the vector $\mathbf{v} = -\mathbf{d}_3$ is contained in $c\mathcal{V}(\mathbf{D})$ as the angular distance between \mathbf{v} and its closest neighbor in $\text{col}(\mathbf{D})$ is maximal. We find that $\text{cm}(\mathbf{D}) = \cos(\frac{\pi}{3}) = \frac{1}{2}$.

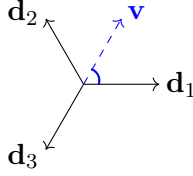


Figure 4.1. A PSS in \mathbb{R}^2 .

The cosine measure and cosine vector set are of particular interest in the case of positive spanning sets, as shown by the result of Proposition 4.1.1. Its proof can be found in key references in derivative-free optimization [6, 15]. Note that our analysis in Section 4.3 provides a more general proof in the context of positive k -spanning sets.

Proposition 4.1.1 A matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$ is a positive spanning set in \mathbb{R}^n if and only if $\text{cm}(\mathbf{D}) > 0$.

An illustration that positive spanning sets have a positive cosine measure is provided in Example 4.1.1. Conversely, the cosine measure of the non positively spanning matrix $\tilde{\mathbf{D}} = [\mathbf{d}'_1 \ \mathbf{d}'_2 \ \mathbf{d}'_3]$ represented in Figure 2.2 is negative as the angle between $\mathbf{v}' = -\mathbf{d}'_1$ and each column of $\tilde{\mathbf{D}}$ is obtuse. Proposition 4.1.1 shows that the positive spanning property can be checked by computing the cosine measure. This value further characterizes how well the set $\text{col}(\mathbf{D})$ covers the space, which is a relevant information in derivative-free algorithms [40]. Both observations motivate the search for efficient

techniques to compute the cosine measure. We note that the definition of the cosine measure can be adapted to help recognize positive spanning sets for proper subspaces of \mathbb{R}^n [7]. Our approach in Section 4.3 will introduce a new tool that allows for the recognition of positive k -spanning sets.

We conclude this section with results on the cosine measure of positive bases of extremal sizes in \mathbb{R}^n .

Proposition 4.1.2 [57, Theorem 2] *Let $\mathbf{D}_{n,n}$ be a maximal positive basis in \mathbb{R}^n . Then $\text{cm}(\mathbf{D}_{n,n}) \leq \frac{1}{\sqrt{n}}$.*

The bound given in Proposition 4.1.2 is tight, as it is attained by the positive basis $[\mathbf{I}_n \quad -\mathbf{I}_n]$. In the case of bases of minimal, a similar result can be derived.

Proposition 4.1.3 [57, Theorem 1] *Let \mathbf{D}_n be a minimal positive basis in \mathbb{R}^n . Then $\text{cm}(\mathbf{D}_n) \leq \frac{1}{n}$.*

Again, the bound given in Proposition 4.1.3 is tight: it is attained by all positive bases with uniform angles, such as the one given in Example 4.1.1. In the case of the minimal positive basis formed by the coordinate vectors and the sum of their negatives, we find

$$\text{cm}([\mathbf{I}_n \quad -\mathbf{1}_n]) = \frac{1}{\sqrt{n^2 + 2(n-1)\sqrt{n}}}.$$

To the best of our knowledge, this formula has only been recently established [37, 67] and no formal proof is available in the literature. In the next section, we will develop an efficient cosine measure calculation technique for specific positive bases, that will provide a proof of this result as a byproduct.

4.1.2 Computing the cosine measure

Finding the cosine measure of a matrix \mathbf{D} by relying on the formula given in Definition 4.1.1 would require an infinite amount of computations: those of each dot product between unitary vectors in \mathbb{R}^n with columns of \mathbf{D} . To address this challenge, several algorithms have been proposed [31, 65]. We now summarize the one introduced by Hare and Jarry-Bolduc.

For a positive spanning set $\mathbf{D} \in \mathbb{R}^{n \times m}$, the algorithm revolves around the observation that each element \mathbf{u} of $c\mathcal{V}(\mathbf{D})$ admits a non-unique closest neighbor in $\text{col}(\mathbf{D})$.

Lemma 4.1.1 [31, Corollary 19] *Let $\mathbf{D} \in \mathbb{R}^{n \times m}$ be positively spanning and let $\mathbf{u} \in c\mathcal{V}(\mathbf{D})$. The set $\arg \max_{\mathbf{d} \in \text{col}(\mathbf{D})} \frac{\mathbf{u}^\top \mathbf{d}}{\|\mathbf{d}\|}$ contains a linear basis of \mathbb{R}^n .*

Note that the result of Lemma 4.1.1 generalizes to all linearly spanning sets.

Example 4.1.2 Let $\mathbf{D} = [\mathbf{d}_1 \ \mathbf{d}_2 \ \mathbf{d}_3]$ be the PSS associated to Figure 2.1. Then the cosine vector $\mathbf{v} \in c\mathcal{V}(\mathbf{D})$ is equidistant from \mathbf{d}_1 and \mathbf{d}_2 , which form a linear basis of \mathbb{R}^2 .

Although the matrix \mathbf{D}' from Figure 2.2 is not a PSS, it is linearly spanning and \mathbf{v}' is as distant as possible its two closest neighbors \mathbf{d}'_2 and \mathbf{d}'_3 in $\text{col}(\mathbf{D}')$. Together, these vectors form a linear basis.

Each linear basis \mathbf{B} of \mathbb{R}^n can be associated to a unique unit vector $\mathbf{u}_{\mathbf{B}}$ that is equidistant to each column of \mathbf{B} and whose dot product with these vectors is positive. The exact value of this dot product can be expressed in terms of the Gram matrix of \mathbf{B} , as shown in Lemma 4.1.2.

Definition 4.1.2 (Gram matrix) Let $\mathbf{M} \in \mathbb{R}^{n \times m}$. The Gram matrix of \mathbf{M} is the matrix $\mathbf{G}(\mathbf{M}) = \mathbf{M}^\top \mathbf{M} \in \mathbb{R}^{m \times m}$.

Lemma 4.1.2 [31, Lemma 12 and 13] Let $\mathbf{B} = [\mathbf{b}_1 \ \dots \ \mathbf{b}_n] \in \mathbb{R}^{n \times n}$ be a linear basis. There exists a unique unit vector $\mathbf{u}_{\mathbf{B}} \in \mathbb{R}^n$ whose dot product with each \mathbf{b}_i is positive and satisfies $\frac{\mathbf{u}_{\mathbf{B}}^\top \mathbf{b}_i}{\|\mathbf{b}_i\|} = \frac{\mathbf{u}_{\mathbf{B}}^\top \mathbf{b}_j}{\|\mathbf{b}_j\|}$, for all i and j . Moreover, letting $\gamma_{\mathbf{B}} = \frac{\mathbf{u}_{\mathbf{B}}^\top \mathbf{b}_1}{\|\mathbf{b}_1\|}$, we have

$$\gamma_{\mathbf{B}} = \frac{1}{\sqrt{\mathbf{1}_n^\top \mathbf{G}(\mathbf{B})^{-1} \mathbf{1}_n}} \quad \text{and} \quad \mathbf{u}_{\mathbf{B}} = \gamma_{\mathbf{B}} \mathbf{B}^{-\top} \mathbf{1}_n. \quad (4.1)$$

Computing the quantities (4.1) for all linear bases formed by columns of \mathbf{D} then gives both the cosine measure and the cosine vector set for \mathbf{D} [31, Theorem 20]. Indeed, we have

$$\text{cm}(\mathbf{D}) = \min_{\substack{\text{col}(\mathbf{B}) \subset \text{col}(\mathbf{D}) \\ \mathbf{B} \text{ linear basis of } \mathbb{R}^n}} \max_{\mathbf{d} \in \text{col}(\mathbf{D})} \mathbf{u}_{\mathbf{B}}^\top \frac{\mathbf{d}}{\|\mathbf{d}\|}, \quad (4.2)$$

while the cosine vector set is given by

$$c\mathcal{V}(\mathbf{D}) = \left\{ \mathbf{u}_{\mathbf{B}} : \max_{\mathbf{d} \in \text{col}(\mathbf{D})} \mathbf{u}_{\mathbf{B}}^\top \frac{\mathbf{d}}{\|\mathbf{d}\|} = \text{cm}(\mathbf{D}) \right\}.$$

In the next section of this chapter, we investigate a class of positive spanning sets for which these values can be quickly computed.

4.2 Orthogonally structured positive bases and cosine measure

Theorem 2.2.1 showed that each positive basis in \mathbb{R}^n could be decomposed into a union of altered minimal bases of smaller linear spaces. Let us now exploit this result to improve the efficiency of Hare and Jarry-Bolduc's Algorithm to specific cases.

4.2.1 Structure and detection of OSPBs

For arbitrary positive bases, computing the Romanowicz decomposition given in (2.4) is hard as it requires to determine the critical vectors and the subspaces \mathbb{L}_i , that need not be orthogonal to one another. These considerations have lead researchers to consider a subclass of positive bases with a nicer decomposition [33], leading to Definition 4.2.1 below.

Definition 4.2.1 (Orthogonally structured positive basis, OSPB)

Suppose that $n \geq 2$ and consider a positive basis $\mathbf{D}_{n,s}$ of \mathbb{R}^n . If there exist subspaces $\mathbb{L}_1, \dots, \mathbb{L}_s$ of \mathbb{R}^n such that $\mathbb{R}^n = \mathbb{L}_1 \perp \mathbb{L}_2 \perp \dots \perp \mathbb{L}_s$ and associated minimal positive bases $\mathbf{D}_{\mathbb{L}_1}, \dots, \mathbf{D}_{\mathbb{L}_s}$ such that

$$\mathbf{D}_{n,s} \equiv [\mathbf{D}_{\mathbb{L}_1} \quad \mathbf{D}_{\mathbb{L}_2} \quad \dots \quad \mathbf{D}_{\mathbb{L}_s}], \quad (4.3)$$

where the structural equivalence only involves permutations of columns, then $\mathbf{D}_{n,s}$ is called an orthogonally structured positive basis or OSPB.

By construction, note that for any $1 \leq i < j \leq s$, any pair of columns $(\mathbf{d}, \mathbf{d}') \in \text{col}(\mathbf{D}_{\mathbb{L}_i}) \times \text{col}(\mathbf{D}_{\mathbb{L}_j})$ satisfies $\mathbf{d}^\top \mathbf{d}' = 0$.

The class of orthogonally structured positive bases includes common positive bases, such as minimal ones and certain maximal positive bases such as those formed by the coordinate vectors and their negatives in \mathbb{R}^n . More OSPBs can be obtained via numerical procedures, even for intermediate sizes [33].

Example 4.2.1 The positive basis $\mathbf{D}_{3,2} = \begin{bmatrix} 1 & -1 & 2 & -1 & -1 \\ 1 & -1 & -1 & 1 & 0 \\ 1 & -1 & -1 & 0 & 1 \end{bmatrix}$ is an

OSPB. Indeed, for $\mathbb{L}_1 = \text{span}([\mathbf{1}_3])$ and $\mathbb{L}_2 = \text{span}([\mathbf{e}_1 - \mathbf{e}_2 \quad \mathbf{e}_1 - \mathbf{e}_3])$, we see that the two linear spaces \mathbb{L}_1 and \mathbb{L}_2 are orthogonal to one another, that the first two columns of $\mathbf{D}_{3,2}$ form a minimal positive basis for \mathbb{L}_1 and that the last three columns form a minimal positive basis for \mathbb{L}_2 .

While computing the cosine measure of an arbitrary matrix is APX-hard [38], we will show in Section 4.2.2 that it can be computed in polynomial time for OSPBs.

The favorable structure of an OSPB can be revealed through the properties of the associated Gram matrix. We will show that when \mathbf{D} is an OSPB, its columns can be permuted to obtain a matrix $\tilde{\mathbf{D}} = \mathbf{D}\mathbf{P}$ whose Gram matrix $\mathbf{G}(\tilde{\mathbf{D}}) = \mathbf{P}^\top \mathbf{G}(\mathbf{D})\mathbf{P}$ possesses a block-diagonal structure which reveals the decomposition of the basis, and thus its OSPB nature.

Theorem 4.2.1 Let $n \geq 2$, $s \geq 2$. The positive basis $\mathbf{D}_{n,s}$ is orthogonally structured if and only if there exists a permutation matrix $\mathbf{P} \in \mathbb{R}^{(n+s) \times (n+s)}$ such that $\mathbf{G}(\mathbf{D}_{n,s}\mathbf{P})$ can be written as a block diagonal matrix with s diagonal blocks.

Proof. Suppose first that $\mathbf{D}_{n,s}$ is an OSPB, with

$$\mathbf{D}_{n,s} \equiv [\mathbf{D}_{\mathbb{L}_1} \quad \mathbf{D}_{\mathbb{L}_2} \quad \cdots \quad \mathbf{D}_{\mathbb{L}_s}].$$

For each permutation matrix $\mathbf{P} \in \mathbb{R}^{(n+s) \times (n+s)}$, the matrix $\mathbf{D}_{n,s}\mathbf{P}$ is an OSPB associated to the same decomposition. Therefore without loss of generality we assume the structural equivalence above to be an equality. By orthogonality of the matrices $\mathbf{D}_{\mathbb{L}_i}$, the Gram matrix $\mathbf{G}(\mathbf{D}_{n,s}) = \mathbf{D}_{n,s}^\top \mathbf{D}_{n,s}$ is then block diagonal with s blocks corresponding to $\mathbf{G}(\mathbf{D}_{\mathbb{L}_1}), \dots, \mathbf{G}(\mathbf{D}_{\mathbb{L}_s})$, and thus the desired result holds.

Conversely, suppose that there exists a permutation matrix \mathbf{P} matrix such that the matrix $\mathbf{G}(\mathbf{D}_{n,s}\mathbf{P}) = \mathbf{P}^\top \mathbf{G}(\mathbf{D}_{n,s})\mathbf{P}$ is block diagonal with s blocks. Then, by considering a partitioning with respect to those diagonal blocks, one can write $\mathbf{D}_{n,s}\mathbf{P} = [\mathbf{M}_1 \quad \cdots \quad \mathbf{M}_s]$ so that $\mathbf{G}(\mathbf{D}_{n,s}\mathbf{P}) = \text{diag}(\mathbf{G}(\mathbf{M}_1), \dots, \mathbf{G}(\mathbf{M}_s))$. By definition of the Gram matrix, this structure implies that the columns of \mathbf{M}_i and \mathbf{M}_j are orthogonal for any $i \neq j$, thus we only need to show that each \mathbf{M}_i is a minimal positive basis for its linear span. To this end, we use the fact that $\mathbf{D}_{n,s}\mathbf{P}$ is positively spanning. By Proposition 2.1.1(iii), there exists a vector $\mathbf{x} \in \mathbb{R}^{n+s}$ with positive coefficients such that $\mathbf{D}_{n,s}\mathbf{P}\mathbf{x} = \mathbf{0}_n$. By decomposing the vector \mathbf{x} into s vectors $\mathbf{x}_1, \dots, \mathbf{x}_s$ according to the decomposition $[\mathbf{M}_1 \quad \cdots \quad \mathbf{M}_s]$, we obtain that

$$\mathbf{D}_{n,s}\mathbf{P}\mathbf{x} = \sum_{i=1}^s \mathbf{M}_i \mathbf{x}_i = \mathbf{0}_n. \quad (4.4)$$

By orthogonality of the columns of the matrices \mathbf{M}_i , the property (4.4) is equivalent to

$$\mathbf{M}_i \mathbf{x}_i = \mathbf{0}_n \quad \forall i \in \llbracket 1, s \rrbracket.$$

Using again Proposition 2.1.1(iii), this latter property is equivalent to \mathbf{M}_i being a PSS for its linear span. Let n_i be the dimension of this span, and m_i the number of columns in \mathbf{M}_i . Since the \mathbf{M}_i are orthogonal and since $\text{span}(\mathbf{D}_{n,s}\mathbf{P}) = \mathbb{R}^n$, we must have $\sum_{i=1}^s n_i = n$. In addition, we also have $\sum_{i=1}^s m_i = n + s = \sum_{i=1}^s n_i + s$. Since $m_i > n_i$ for all $i \in \llbracket 1, s \rrbracket$, we conclude that $m_i = n_i + 1$, and thus every \mathbf{M}_i is a minimal positive basis. \square

Note that the characterization stated by Theorem 4.2.1 trivially holds for minimal positive bases. This theorem thus provides a characterization of the OSPB property through Gram matrices. One can then use this result to determine whether a positive basis has an orthogonal structure and, in that event, to highlight the associated decomposition.

Corollary 4.2.1 *Let $n \geq 2$, $s \geq 1$ and $\mathbf{D}_{n,s}$ be a positive basis in \mathbb{R}^n . If there exists a permutation matrix $\mathbf{P} \in \mathbb{R}^{(n+s) \times (n+s)}$ such that $\mathbf{G}(\mathbf{D}_{n,s}\mathbf{P})$ is block diagonal with s blocks, then $\mathbf{D}_{n,s}$ is an OSPB, and its decomposition (4.3) is given by $\mathbf{D}_{n,s}\mathbf{P}$.*

Corollary 4.2.1 provides a principled way of detecting the OSPB structure, by checking all possible permutations of the columns of the positive basis. Although this is not the focus of this work, we remark that it can be done in an efficient manner by considering a graph whose Laplacian matrix \mathbf{L} has nonzero coordinates in the exact same rows and columns as $\mathbf{G}(\mathbf{D}_{n,s})$. Indeed, the problem of finding the permutation for matrix \mathbf{L} reduces to that of finding the number of connected components in the graph [51] and can be solved in polynomial time [35].

4.2.2 Cosine measure of an OSPB

Orthogonally structured positive bases were defined as matrices which admit a decomposition into minimal positive bases that are orthogonal to one another. We now investigate how this particular structure allows for efficient computation of the cosine measure.

Our approach builds on the algorithm by Hare and Jarry-Bolduc [31], that computes the cosine measure of any positive spanning set in finite time (though the computation time may be exponential in the problem dimension). This procedure, which consists of a loop over all possible linear bases \mathbf{B} formed by columns of the positive spanning set, was detailed in Section 4.1. The next proposition shows how, when dealing with OSPBs, formula (4.2) can be simplified to give a more direct link between the quantities $\gamma_{\mathbf{B}}$ and the cosine measure.

Proposition 4.2.1 *Let $\mathbf{D}_{n,s}$ be an OSPB associated to the decomposition $[\mathbf{D}_{\mathbb{L}_1} \ \dots \ \mathbf{D}_{\mathbb{L}_s}]$ of minimal positive bases. Then*

$$\text{cm}(\mathbf{D}_{n,s}) = \min_{\substack{\text{col}(\mathbf{B}) \subset \text{col}(\mathbf{D}_{n,s}) \\ \mathbf{B} \text{ linear basis of } \mathbb{R}^n}} \gamma_{\mathbf{B}} \quad \text{and} \quad \text{cV}(\mathbf{D}_{n,s}) = \{\mathbf{u}_{\mathbf{B}} : \gamma_{\mathbf{B}} = \text{cm}(\mathbf{D}_{n,s})\},$$

$$\text{where } \gamma_{\mathbf{B}} = \frac{1}{\sqrt{\mathbf{1}_n \mathbf{G}(\mathbf{B})^{-1} \mathbf{1}_n^{\top}}} \quad \text{and} \quad \mathbf{u}_{\mathbf{B}} = \gamma_{\mathbf{B}} \mathbf{B}^{-\top} \mathbf{1}_n.$$

Proof. Using the decomposition of $\mathbf{D}_{n,s}$, any linear basis \mathbf{B} of \mathbb{R}^n formed by columns of $\mathbf{D}_{n,s}$ can be permuted into $[\mathbf{B}_{\mathbb{L}_1} \ \dots \ \mathbf{B}_{\mathbb{L}_s}]$, where for all i , $\text{col}(\mathbf{B}_{\mathbb{L}_i}) \subset \text{col}(\mathbf{D}_{\mathbb{L}_i})$ and $\mathbf{B}_{\mathbb{L}_i}$ is a linear basis of \mathbb{L}_i . By construction, the vector $\mathbf{u}_{\mathbf{B}}$ makes a positive dot product with every column \mathbf{b}_i of \mathbf{B} (and thus with every column of each $\mathbf{B}_{\mathbb{L}_i}$) equal to $\gamma_{\mathbf{B}} \|\mathbf{b}_i\|$. Consequently, the vector $\mathbf{u}_{\mathbf{B}}$ lies in the positive span of \mathbf{B} , and its projection on any subspace \mathbb{L}_i lies in the positive span of $\mathbf{B}_{\mathbb{L}_i}$.

Meanwhile, for any $i \in \llbracket 1, s \rrbracket$, there exists $\mathbf{d}_i \in \text{col}(\mathbf{D}_{\mathbb{L}_i})$ such that $\text{col}(\mathbf{B}_{\mathbb{L}_i}) = \text{col}(\mathbf{D}_{\mathbb{L}_i}) \setminus \{\mathbf{d}_i\}$, and this vector satisfies $\mathbf{u}_{\mathbf{B}}^{\top} \mathbf{d}_i < 0$ per Proposition 2.1.1(iii), leading to

$$\max_{\mathbf{d} \in \text{col}(\mathbf{D}_{n,s})} \frac{\mathbf{u}_{\mathbf{B}}^{\top} \mathbf{d}}{\|\mathbf{d}\|} = \max_{i \in \llbracket 1, s \rrbracket} \left\{ \max_{\mathbf{d} \in \text{col}(\mathbf{D}_{\mathbb{L}_i})} \frac{\mathbf{u}_{\mathbf{B}}^{\top} \mathbf{d}}{\|\mathbf{d}\|} \right\} = \max_{i \in \llbracket 1, s \rrbracket} \left\{ \max_{\mathbf{d} \in \text{col}(\mathbf{B}_{\mathbb{L}_i})} \frac{\mathbf{u}_{\mathbf{B}}^{\top} \mathbf{d}}{\|\mathbf{d}\|} \right\}$$

$$= \max_{\mathbf{d} \in \text{col}(\mathbf{B})} \frac{\mathbf{u}_{\mathbf{B}}^{\top} \mathbf{d}}{\|\mathbf{d}\|} = \gamma_{\mathbf{B}},$$

where the second equality comes from $\mathbf{u}_{\mathbf{B}}^{\top} \mathbf{d}_i < 0$ and $\max_{\mathbf{d} \in \mathbf{D}_{n,s}} \mathbf{u}_{\mathbf{B}}^{\top} \mathbf{d} > 0$, and the last equality holds by definition of $\gamma_{\mathbf{B}}$. Recalling that $\text{cm}(\mathbf{D}_{n,s})$ is given by (4.2) concludes the proof. \square

One drawback of the approach described so far is that it requires computing the quantities (4.1) for all linear bases contained in the positive spanning set of interest. In the case of OSPBs, we show below that the number of linear bases to be considered can be greatly reduced by leveraging to their decomposition into minimal positive bases.

Theorem 4.2.2 *Let $\mathbf{D}_{n,s}$ be an OSPB of \mathbb{R}^n associated to the decomposition $[\mathbf{D}_{\mathbb{L}_1} \ \dots \ \mathbf{D}_{\mathbb{L}_s}]$. Let \mathbf{B} be a linear basis of \mathbb{R}^n formed by columns of $\mathbf{D}_{n,s}$ and such that $\text{col}(\mathbf{B}) = \cup_{i=1}^s \text{col}(\mathbf{B}_{\mathbb{L}_i})$, where every $\mathbf{B}_{\mathbb{L}_i}$ is a linear basis of the subspace corresponding to $\mathbf{D}_{\mathbb{L}_i}$. For each basis $\mathbf{B}_{\mathbb{L}_i}$, define*

$$\gamma_{\mathbf{B}_{\mathbb{L}_i}} = \frac{1}{\sqrt{\mathbf{1}_{\mathbb{L}_i}^{\top} \mathbf{G}(\mathbf{B}_{\mathbb{L}_i})^{-1} \mathbf{1}_{\mathbb{L}_i}}},$$

where $\mathbf{1}_{\mathbb{L}_i}$ denotes the vector of all ones in $\mathbb{R}^{\dim(\mathbb{L}_i)}$. Then,

$$\gamma_{\mathbf{B}} = \frac{1}{\sqrt{\sum_{i=1}^s \gamma_{\mathbf{B}_{\mathbb{L}_i}}^{-2}}} = \frac{1}{\sqrt{\sum_{i=1}^s \mathbf{1}_{\mathbb{L}_i}^{\top} \mathbf{G}(\mathbf{B}_{\mathbb{L}_i})^{-1} \mathbf{1}_{\mathbb{L}_i}}}, \quad (4.5)$$

with $\gamma_{\mathbf{B}}$ being defined as in (4.1).

As a result, the cosine measure and cosine vector set of $\mathbf{D}_{n,s}$ are given by

$$\text{cm}(\mathbf{D}_{n,s}) = \frac{1}{\sqrt{\sum_{i=1}^s \max_{\mathbf{d}_i \in \text{col}(\mathbf{D}_{\mathbb{L}_i})} \gamma_{\mathbf{D}_{\mathbb{L}_i, \mathbf{d}_i}}^{-2}}}, \quad (4.6)$$

where $\mathbf{D}_{\mathbb{L}_i, \mathbf{d}_i}$ denotes the linear basis obtained from $\mathbf{D}_{\mathbb{L}_i}$ by removing the column \mathbf{d}_i , and

$$c\mathcal{V}(\mathbf{D}_{n,s}) = \left\{ \mathbf{u}_{\mathbf{B}} = \frac{[\mathbf{B}_{\mathbb{L}_1} \ \dots \ \mathbf{B}_{\mathbb{L}_s}]^{-\top} \mathbf{1}_n}{\sqrt{\sum_{i=1}^s \gamma_{\mathbf{B}_{\mathbb{L}_i}}^{-2}}} : \text{col}(\mathbf{B}) = \bigcup_{i=1}^s \text{col}(\mathbf{B}_{\mathbb{L}_i}) \right\}. \quad (4.7)$$

Proof. The cosine measure and cosine vector set of $\mathbf{D}_{n,s}$ are preserved upon permuting columns. Therefore and without loss of generality, we assume the structural equivalence $\mathbf{D}_{n,s} \equiv [\mathbf{D}_{\mathbb{L}_1} \ \dots \ \mathbf{D}_{\mathbb{L}_s}]$ to be an equality. Consider any linear basis \mathbf{B} of \mathbb{R}^n formed by columns of

$\mathbf{D}_{n,s}$ and write $\mathbf{B} = [\mathbf{B}_{\mathbb{L}_1} \cdots \mathbf{B}_{\mathbb{L}_s}]$. Then, the Gram matrix of \mathbf{B} satisfies $\mathbf{G}(\mathbf{B}) = \text{diag}(\mathbf{G}(\mathbf{B}_{\mathbb{L}_1}), \dots, \mathbf{G}(\mathbf{B}_{\mathbb{L}_s}))$, implying that

$$\begin{aligned} \gamma_{\mathbf{B}} &= \frac{1}{\sqrt{\mathbf{1}_n^\top \mathbf{G}(\mathbf{B})^{-1} \mathbf{1}_n}} = \frac{1}{\sqrt{\mathbf{1}_n^\top \text{diag}(\mathbf{G}(\mathbf{B}_{\mathbb{L}_1}), \dots, \mathbf{G}(\mathbf{B}_{\mathbb{L}_s}))^{-1} \mathbf{1}_n}} \\ &= \frac{1}{\sqrt{\mathbf{1}_n^\top \text{diag}(\mathbf{G}(\mathbf{B}_{\mathbb{L}_1})^{-1}, \dots, \mathbf{G}(\mathbf{B}_{\mathbb{L}_s})^{-1}) \mathbf{1}_n}} \\ &= \frac{1}{\sqrt{\sum_{i=1}^s \mathbf{1}_{\mathbb{L}_i}^\top \mathbf{G}(\mathbf{B}_{\mathbb{L}_i})^{-1} \mathbf{1}_{\mathbb{L}_i}}}, \end{aligned}$$

which proves (4.5).

In the rest of this proof and for each positive basis $\mathbf{D}_{\mathbb{L}_i}$, we use the notation $\mathbf{D}_{\mathbb{L}_i, \mathbf{d}}$ to designate the matrix obtained from $\mathbf{D}_{\mathbb{L}_i}$ by removing the column \mathbf{d} . Recall that every linear basis $\mathbf{B}_{\mathbb{L}_i}$ can be expressed in such a way. We combine this property together with (4.5) and Proposition 4.2.1 to obtain

$$\begin{aligned} \text{cm}(\mathbf{D}_{n,s}) &= \min_{\substack{\text{col}(\mathbf{B}) \subset \text{col}(\mathbf{D}_{n,s}) \\ \mathbf{B} \text{ linear basis of } \mathbb{R}^n}} \gamma_{\mathbf{B}} = \min_{\substack{\mathbf{B}_{\mathbb{L}_1}, \dots, \mathbf{B}_{\mathbb{L}_s} \\ \text{col}(\mathbf{B}_{\mathbb{L}_i}) = \text{col}(\mathbf{D}_{\mathbb{L}_i}) \setminus \{\mathbf{d}_i\}}} \frac{1}{\sqrt{\sum_{i=1}^s \gamma_{\mathbf{B}_{\mathbb{L}_i}}^{-2}}} \\ &= \min_{\substack{\mathbf{d}_1, \dots, \mathbf{d}_s \\ \mathbf{d}_i \in \text{col}(\mathbf{D}_{\mathbb{L}_i})}} \frac{1}{\sqrt{\sum_{i=1}^s \gamma_{\mathbf{D}_{\mathbb{L}_i, \mathbf{d}_i}}^{-2}}} \\ &= \frac{1}{\sqrt{\sum_{i=1}^s \max_{\mathbf{d}_i \in \text{col}(\mathbf{D}_{\mathbb{L}_i})} \gamma_{\mathbf{D}_{\mathbb{L}_i, \mathbf{d}_i}}^{-2}}}, \end{aligned}$$

proving (4.6).

Finally, combining (4.6) with the result of Proposition 4.2.1 on the cosine vector set gives

$$\begin{aligned} c\mathcal{V}(\mathbf{D}_{n,s}) &= \{\mathbf{u}_{\mathbf{B}} : \gamma_{\mathbf{B}} = \text{cm}(\mathbf{D}_{n,s})\} \\ &= \left\{ \mathbf{u}_{\mathbf{B}} : \text{col}(\mathbf{B}) = \bigcup_{i=1}^s \text{col}(\mathbf{B}_{\mathbb{L}_i}), \quad \frac{1}{\sqrt{\sum_{i=1}^s \gamma_{\mathbf{B}_{\mathbb{L}_i}}^{-2}}} = \text{cm}(\mathbf{D}_{n,s}) \right\} \end{aligned}$$

Using the formula (4.1) for $\mathbf{u}_{\mathbf{B}}$ leads to

$$\begin{aligned} c\mathcal{V}(\mathbf{D}_{n,s}) &= \left\{ \mathbf{u}_{\mathbf{B}} : \text{col}(\mathbf{B}) = \bigcup_{i=1}^s \text{col}(\mathbf{B}_{\mathbb{L}_i}), \quad \mathbf{u}_{\mathbf{B}} = \gamma_{\mathbf{B}} [\mathbf{B}_{\mathbb{L}_1} \cdots \mathbf{B}_{\mathbb{L}_s}]^{-\top} \mathbf{1}_n \right\} \\ &= \left\{ \mathbf{u}_{\mathbf{B}} : \text{col}(\mathbf{B}) = \bigcup_{i=1}^s \text{col}(\mathbf{B}_{\mathbb{L}_i}), \quad \mathbf{u}_{\mathbf{B}} = \frac{[\mathbf{B}_{\mathbb{L}_1} \cdots \mathbf{B}_{\mathbb{L}_s}]^{-\top} \mathbf{1}_n}{\sqrt{\sum_{i=1}^s \gamma_{\mathbf{B}_{\mathbb{L}_i}}^{-2}}} \right\}, \end{aligned}$$

which is precisely (4.7). \square

On a broader level, Theorem 4.2.2 shows that any calculation for a linear basis being a submatrix of an OSPB reduces to calculations on bases which are submatrices of each of the minimal positive bases in its decomposition. This observation leads to a principled way of computing the cosine measure from the OSPB decomposition, as described in Algorithm 1.

Algorithm 1: Cosine measure of an orthogonally structured positive basis

- 1 *Input:* An orthogonally structured positive basis $\mathbf{D}_{n,s}$ with normalized columns.
- 2 **Step 1.** Compute a decomposition $\mathbf{D}_{n,s} \equiv [\mathbf{D}_{\mathbb{L}_1} \ \cdots \ \mathbf{D}_{\mathbb{L}_s}]$ of the matrix into s minimal positive bases $\mathbf{D}_{\mathbb{L}_i}$ on subspaces of \mathbb{R}^n .
- 3 **Step 2.** For every $i \in \llbracket 1, s \rrbracket$, compute

$$\beta_{\mathbb{L}_i} = \max_{\mathbf{d} \in \text{col}(\mathbf{D}_{\mathbb{L}_i})} \gamma_{\mathbf{D}_{\mathbb{L}_i, \mathbf{d}}}^{-2} \quad \text{and} \quad \mathcal{A}_i = \arg \max_{\mathbf{d} \in \text{col}(\mathbf{D}_{\mathbb{L}_i})} \gamma_{\mathbf{D}_{\mathbb{L}_i, \mathbf{d}}}^{-2},$$

where $\mathbf{D}_{\mathbb{L}_i, \mathbf{d}}$ is obtained from $\mathbf{D}_{\mathbb{L}_i}$ by removing the column \mathbf{d} . For all $\mathbf{d} \in \mathcal{A}_i$, write $\mathbf{B}_{\mathbb{L}_i}^{(\mathbf{d})} = \mathbf{D}_{\mathbb{L}_i, \mathbf{d}}$.

- 4 **Step 3.** Return the cosine measure

$$\text{cm}(\mathbf{D}_{n,s}) = \frac{1}{\sqrt{\sum_{i=1}^s \beta_{\mathbb{L}_i}}} \quad (4.8)$$

and the cosine vector set

$$c\mathcal{V}(\mathbf{D}_{n,s}) = \bigcup_{(\mathbf{d}_1, \dots, \mathbf{d}_s) \in \mathcal{A}_1 \times \cdots \times \mathcal{A}_s} \left\{ \mathbf{u} \in \mathbb{R}^n, \mathbf{u} = \frac{[\mathbf{B}_{\mathbb{L}_1}^{(\mathbf{d}_1)} \ \cdots \ \mathbf{B}_{\mathbb{L}_s}^{(\mathbf{d}_s)}]^{-\top} \mathbf{1}_n}{\sqrt{\sum_{i=1}^s \beta_{\mathbb{L}_i}}} \right\}.$$

In essence, Algorithm 1 is quite similar to the generic method proposed for positive spanning sets [31]. However, Algorithm 1 reduces the computation of the cosine measure to that over minimal positive bases, which leads to significantly cheaper calculations. Indeed, for any minimal positive basis $\mathbf{D}_{\mathbb{L}_i}$ involved in the decomposition, the algorithm considers $\dim(\mathbb{L}_i)+1$ linear bases, and computes the quantities of interest (4.1) for each of those (which amounts to inverting or solving a linear system involving the associated Gram matrix). Overall, Algorithm 1 thus checks $\sum_{i=1}^s (\dim(\mathbb{L}_i) + 1) = n + s$ bases to compute the cosine measure (4.8). This result represents a sig-

nificant improvement over the $\binom{n+s}{n}$ possible bases that are potentially required when the OSPB decomposition is not exploited, as in the algorithm for generic PSSs [31]. We also recall from Section 4.2.1 that Step 1 in Algorithm 1 can be performed in polynomial time.

To end this section, we illustrate how Algorithm 1 results in a straightforward calculation in the case of some minimal positive bases, by computing explicitly the cosine measure of the minimal positive basis $[\mathbf{I}_n \quad -\mathbf{1}_n]$. In this case, the calculation becomes easy thanks to the orthogonality of the columns within the matrix. Although the value (4.9) was recently stated [37, 67] and checked numerically using the method of Hare and Jarry-Bolduc [31], to the best of our knowledge the formal proof below is new.

Lemma 4.2.1 *The cosine measure of the OSPB $[\mathbf{I}_n \quad -\mathbf{1}_n]$ is given by*

$$\text{cm}([\mathbf{I}_n \quad -\mathbf{1}_n]) = \frac{1}{\sqrt{n^2 + 2(n-1)\sqrt{n}}}. \quad (4.9)$$

Proof. For the sake of simplicity, we normalize the last column of the matrix (which does not change the value of the cosine measure) and consider $\mathbf{D}_n = [\mathbf{I}_n \quad -\frac{1}{\sqrt{n}}\mathbf{1}_n]$. Since \mathbf{D}_n is a positive basis, it follows that

$$\text{cm}(\mathbf{D}_n) = \min_{i \leq n+1} \gamma_{\mathbf{B}_i},$$

where \mathbf{B}_i designates the matrix obtained from \mathbf{D}_n by removing the column of index i . Two cases are to be considered. Suppose first that $i = n+1$, so that $\mathbf{B}_i = \mathbf{I}_n$. Then the Gram matrix of \mathbf{B}_i satisfies $\mathbf{G}(\mathbf{B}_i) = \mathbf{G}(\mathbf{I}_n) = \mathbf{I}_n$. Consequently,

$$\gamma_{\mathbf{B}_i} = \frac{1}{\sqrt{\mathbf{1}_n^\top \mathbf{G}(\mathbf{B}_i)^{-1} \mathbf{1}_n}} = \frac{1}{\sqrt{\mathbf{1}_n^\top \mathbf{1}_n}} = \frac{1}{\sqrt{n}}.$$

Suppose now that $i \in \llbracket 1, n \rrbracket$. Then $\mathbf{B}_i = [\mathbf{e}_1 \quad \cdots \quad \mathbf{e}_{i-1} \quad \mathbf{e}_{i+1} \quad \cdots \quad \mathbf{e}_n \quad -\frac{1}{\sqrt{n}}\mathbf{1}_n]$ and we obtain that

$$\mathbf{G}(\mathbf{B}_i) = \begin{bmatrix} \mathbf{I}_{n-1} & -\frac{1}{\sqrt{n}}\mathbf{1}_{n-1} \\ -\frac{1}{\sqrt{n}}\mathbf{1}_{n-1}^\top & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{G}(\mathbf{B}_i)^{-1} = \begin{bmatrix} \mathbf{I}_{n-1} + \mathbf{1}_{n-1}\mathbf{1}_{n-1}^\top & \sqrt{n}\mathbf{1}_{n-1} \\ \sqrt{n}\mathbf{1}_{n-1}^\top & n \end{bmatrix}$$

Since these formulas do not depend on i , we obtain that for all $i \in \llbracket 1, n \rrbracket$, we have

$$\gamma_{\mathbf{B}_i} = \frac{1}{\sqrt{\mathbf{1}_n^\top \mathbf{G}(\mathbf{B}_i)^{-1} \mathbf{1}_n}} = \frac{1}{\sqrt{\sum_{j=1}^n \sum_{\ell=1}^n [\mathbf{G}(\mathbf{B}_i)^{-1}]_{j,\ell}}}.$$

Summing all coefficients of $\mathbf{G}(\mathbf{B}_i)^{-1}$ gives $n-1 + (n-1)^2 + 2(n-1)\sqrt{n} + n = n^2 + 2(n-1)\sqrt{n}$, hence $\gamma_{\mathbf{B}_i} = \frac{1}{\sqrt{n^2 + 2(n-1)\sqrt{n}}}$. Comparing this value with

$\frac{1}{\sqrt{n}}$ yields the desired conclusion. \square

Algorithm 1 allows for efficient calculation of cosine measures for specific positive spanning sets that originate from OSPBs, as we will establish in Section 4.3 in the case of positive k -spanning sets.

4.3 The k -cosine measure for positive k -spanning sets

4.3.1 A cosine measure for PkSSs

This section aims at generalizing the cosine measure from Section 4.1 to positive k -spanning sets so that it characterizes the positive k -spanning property. Our proposal, called the k -cosine measure, is described in Definition 4.3.1.

Definition 4.3.1 (k -cosine measure) Let $\mathbf{D} \in \mathbb{R}^{n \times m}$ be a matrix whose columns are nonzero and let $k \in \mathbb{N}$ satisfy $1 \leq k \leq m$. The k -cosine measure of \mathbf{D} is given by

$$\text{cm}_k(\mathbf{D}) = \min_{\substack{\|\mathbf{u}\|=1 \\ \mathbf{u} \in \mathbb{R}^n}} \max_{\substack{\mathbf{S} \in \mathbb{R}^{n \times k} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \min_{\mathbf{d} \in \text{col}(\mathbf{S})} \frac{\mathbf{u}^\top \mathbf{d}}{\|\mathbf{d}\|},$$

The k -cosine vector set associated with \mathbf{D} is given by

$$c\mathcal{V}_k(\mathbf{D}) = \arg \min_{\substack{\|\mathbf{u}\|=1 \\ \mathbf{u} \in \mathbb{R}^n}} \max_{\substack{\mathbf{S} \in \mathbb{R}^{n \times k} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \min_{\mathbf{d} \in \text{col}(\mathbf{S})} \frac{\mathbf{u}^\top \mathbf{d}}{\|\mathbf{d}\|}.$$

Note that Definition 4.1.1 is a special case of Definition 4.3.1 corresponding to $k = 1$. In its general form, this definition expresses how well the columns of the matrix of interest are spread in the space through submatrices of k columns, which is related to Proposition 2.3.1. Our next result shows that this quantity characterizes PkSSs.

Theorem 4.3.1 Let $\mathbf{D} \in \mathbb{R}^{n \times m}$ be a matrix with nonzero columns and let $k \in \mathbb{N}$ satisfy $1 \leq k \leq m$. Then \mathbf{D} is a positive k -spanning set in \mathbb{R}^n if and only if $\text{cm}_k(\mathbf{D}) > 0$.

Proof. Without loss of generality we assume each column of \mathbf{D} to be a unit vector.

Suppose first that \mathbf{D} is a PkSS. Then, by Proposition 2.3.1, for any unit vector $\mathbf{u} \in \mathbb{R}^n$, there exist k columns of \mathbf{D} that make a positive dot product

with \mathbf{u} . Let $\mathcal{S}_{\mathbf{u}}$ be a set consisting of such columns. By construction, we have $\min_{\mathbf{d} \in \mathcal{S}_{\mathbf{u}}} \mathbf{u}^\top \mathbf{d} > 0$ and thus

$$\max_{\substack{\mathbf{S} \in \mathbb{R}^{n \times k} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \min_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d} \geq \min_{\mathbf{d} \in \mathcal{S}_{\mathbf{u}}} \mathbf{u}^\top \mathbf{d} > 0.$$

Since the result holds for any unit vector \mathbf{u} , we conclude that $\text{cm}_k(\mathbf{D}) > 0$.

Conversely, suppose that $\text{cm}_k(\mathbf{D}) > 0$. For any unit vector \mathbf{u} , we have by assumption that

$$\max_{\substack{\mathbf{S} \in \mathbb{R}^{n \times k} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \min_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d} > 0. \quad (4.10)$$

In other words, at least k columns of \mathbf{D} have a positive dot product with \mathbf{u} . Thus by Proposition 2.3.1, \mathbf{D} is a positive k -spanning set. \square

As announced in Section 4.1, the proof of Theorem 4.3.1 covers that of Proposition 4.1.1 as the special case $k = 1$.

To end this section, we provide an alternate definition of the k -cosine measure that connects this notion to the cosine measure.

Theorem 4.3.2 *Let $\mathbf{D} \in \mathbb{R}^{n \times m}$ be a matrix with nonzero columns and let $k \in \mathbb{N}$ satisfy $1 \leq k \leq m$. Then*

$$\text{cm}_k(\mathbf{D}) = \min_{\substack{\mathbf{S} \in \mathbb{R}^{n \times (m-k+1)} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \text{cm}(\mathbf{S}). \quad (4.11)$$

Proof. Without loss of generality, we assume that $\mathbf{D} = [\mathbf{d}_1 \ \dots \ \mathbf{d}_m]$ where each \mathbf{d}_i is a unit vector. In order to show that

$$\min_{\|\mathbf{u}\|=1} \max_{\substack{\mathbf{S} \in \mathbb{R}^{n \times k} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \min_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d} = \min_{\substack{\mathbf{S} \in \mathbb{R}^{n \times (m-k+1)} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \text{cm}(\mathbf{S}),$$

we prove the equivalent statement

$$\min_{\|\mathbf{u}\|=1} \max_{\substack{\mathbf{S} \in \mathbb{R}^{n \times k} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \min_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d} = \min_{\|\mathbf{u}\|=1} \min_{\substack{\mathbf{S} \in \mathbb{R}^{n \times (m-k+1)} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \max_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d}. \quad (4.12)$$

To this end, let \mathbf{u} be a unit vector in \mathbb{R}^n . We reorder the columns of \mathbf{D} so that for all $i \leq m-1$, $\mathbf{u}^\top \mathbf{d}_i \geq \mathbf{u}^\top \mathbf{d}_{i+1}$ and we define $\mathbf{S}_k^- = [\mathbf{d}_1 \ \dots \ \mathbf{d}_k]$ and $\mathbf{S}_k^+ = [\mathbf{d}_k \ \dots \ \mathbf{d}_m]$. By construction, one has

$$\mathbf{u}^\top \mathbf{d}_k = \min_{\mathbf{d} \in \text{col}(\mathbf{S}_k^-)} \mathbf{u}^\top \mathbf{d} = \max_{\mathbf{d} \in \text{col}(\mathbf{S}_k^+)} \mathbf{u}^\top \mathbf{d}. \quad (4.13)$$

Moreover, the definitions of \mathbf{S}_k^- and \mathbf{S}_k^+ also imply that

$$\mathbf{S}_k^- \in \underset{\substack{\mathbf{S} \in \mathbb{R}^{n \times k} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}}{\arg \max} \min_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d} \quad \text{and} \quad \mathbf{S}_k^+ \in \underset{\substack{\mathbf{S} \in \mathbb{R}^{n \times (m-k+1)} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}}{\arg \min} \max_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d}. \quad (4.14)$$

Combining (4.13) and (4.14) gives

$$\max_{\substack{\mathbf{S} \in \mathbb{R}^{n \times k} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \min_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d} = \min_{\substack{\mathbf{S} \in \mathbb{R}^{n \times (m-k+1)} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \max_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d}. \quad (4.15)$$

Since (4.15) holds for any unit vector $\mathbf{u} \in \mathbb{R}^n$, it follows that

$$\min_{\|\mathbf{u}\|=1} \max_{\substack{\mathbf{S} \in \mathbb{R}^{n \times k} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \min_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d} = \min_{\|\mathbf{u}\|=1} \min_{\substack{\mathbf{S} \in \mathbb{R}^{n \times (m-k+1)} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}}} \max_{\mathbf{d} \in \text{col}(\mathbf{S})} \mathbf{u}^\top \mathbf{d},$$

which is precisely (4.12) and, as a result, proves (4.11). \square

The formula (4.11) is associated with another characterization of Pk SSs, namely that provided by Definition 2.3.1. In essence, the k -cosine measure of a matrix $\mathbf{D} \in \mathbb{R}^{n \times m}$ is the minimum value of the cosine measure among all submatrices of \mathbf{D} with $m - k + 1$ columns. A useful corollary of that result is that

$$\text{cm}(\mathbf{D}) = \text{cm}_1(\mathbf{D}) \geq \text{cm}_2(\mathbf{D}) \geq \cdots \geq \text{cm}_m(\mathbf{D}) = -1.$$

In the next section, we will show how Pk SSs built using OSPBs satisfy stronger properties associated with the k -cosine measure.

4.3.2 Building Pk SSs from OSPBS

In this section, we describe how OSPBs can be used to generate positive k -spanning sets or positive k -bases with guarantees on their k -cosine measure.

A first approach towards constructing positive k -spanning sets consists in duplicating the same PSS k times, so that every direction remains even after taking out $k - 1$ elements. However, such a strategy creates redundancy among the columns of the matrix. The purpose of this section is to introduce a more generic approach based on rotation matrices that allows for all columns to be distinct.

Proposition 4.3.1 *Let $\mathbf{D}_{n,s}$ be an OSPB of \mathbb{R}^n with $s \in \llbracket 1, n \rrbracket$. Let $\mathbf{R}^{(1)}, \dots, \mathbf{R}^{(k)}$ be k rotation matrices in $\mathbb{R}^{n \times n}$, and define $\mathbf{D}_{n,s}^{(j)} := \mathbf{R}^{(j)} \mathbf{D}_{n,s}$ for any $j \in \llbracket 1, k \rrbracket$. Then, the matrix $\mathbf{D}_{n,s}^{(1:k)} = \begin{bmatrix} \mathbf{D}_{n,s}^{(1)} & \dots & \mathbf{D}_{n,s}^{(k)} \end{bmatrix}$ is a positive k -spanning set with*

$$\text{cm}_k \left(\mathbf{D}_{n,s}^{(1:k)} \right) \geq \text{cm}(\mathbf{D}_{n,s}). \quad (4.16)$$

Proof. First, note that applying a rotation to a matrix does not change its cosine measure since rotations preserve angles, hence $\text{cm}(\mathbf{D}_{n,s}^{(j)}) = \text{cm}(\mathbf{D}_{n,s})$ for every $j \in \llbracket 1, k \rrbracket$.

Consider a submatrix \mathbf{S} of $\mathbf{D}_{n,s}^{(1:k)}$ with $|\text{col}(\mathbf{S})| = |\text{col}(\mathbf{D}_{n,s}^{(1:k)})| - k + 1$. By the pigeonhole principle, one of the k positive bases obtained by rotation must be a submatrix of \mathbf{S} . Letting $\mathbf{D}_{n,s}^{(js)}$ denote that positive basis, we have $\text{cm}(\mathbf{S}) \geq \text{cm}(\mathbf{D}_{n,s}^{(js)}) = \text{cm}(\mathbf{D}_{n,s})$. Using Theorem 4.3.2, we obtain that

$$\text{cm}_k(\mathbf{D}_{n,s}^{(1:k)}) = \min_{\substack{\mathbf{S} \in \mathbb{R}^{n \times (k(n+s)-k+1)} \\ \mathbf{S} \text{ submatrix of } \mathbf{D}_{n,s}^{(1:k)}}} \text{cm}(\mathbf{S}) \geq \text{cm}(\mathbf{D}_{n,s}).$$

In particular, this proves $\text{cm}_k(\mathbf{D}_{n,s}^{(1:k)}) > 0$, hence this matrix being positively k -spanning now follows from Theorem 4.3.1. \square

Several remarks are in order regarding Proposition 4.3.1. First, note that the result extends to any positive spanning set, but we focus on OSPBs since in that case (4.16) gives a lower bound on the k -cosine measure that can be computed in polynomial time. Moreover, when $\mathbf{R}_1 = \dots = \mathbf{R}_k = \mathbf{I}_n$, i.e. when k identical copies of $\mathbf{D}_{n,s}$ are used, the resulting matrix is a positive k -basis and relation (4.16) holds with equality. As a result, its k -cosine measure can be computed in polynomial time using Algorithm 1. In general, however, the matrix generated through Proposition 4.3.1 is not necessarily a positive k -basis. For instance, if $n = 2$, setting $\mathbf{D}_2 = [\mathbf{I}_2 \quad -\mathbf{1}_n]$, $k = 2$, $\mathbf{R}_1 = \mathbf{I}_2$ and $\mathbf{R}_2 = \begin{bmatrix} 1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{bmatrix}$ yields a matrix that is a positive 2-spanning set but not a positive 2-basis.

In order to obtain a method which uses rotations to systematically create positive k -bases, we first introduce a geometric characterization of these matrices.

Definition 4.3.2 (Positive k -independence) *A matrix $\mathbf{D} = [\mathbf{d}_1 \ \dots \ \mathbf{d}_m]$ in $\mathbb{R}^{n \times m}$ is positively k -independent if for any $\mathbf{d} \in \text{col}(\mathbf{D})$, there exists a vector $\mathbf{u} \in \mathbb{R}^n$ having a positive dot product with \mathbf{d} and at most $k - 1$ other columns of \mathbf{D} .*

Using Farkas's Lemma, it should be clear that the notion of positive k -independence in \mathbb{R}^n generalizes that of positive independence given in Definition 2.1.2. In particular, the concept of positive 1-independence is equivalent to that of positive independence. Positive k -bases are characterized as positively k -independent $PkSSs$.

As announced, we now present a strategy to create positive k -bases with rotations, tailored to OSPBs. Recall that OSPBs can be decomposed into

minimal positive bases over orthogonal subspaces. Our proposal consists in applying separate rotations to each of those minimal positive bases. Our key result is described in Theorem 4.3.3, and shows that one can define a strategy for rotating a minimal positive basis to obtain a positive k -basis. The proof relies on two technical results, the first one being an intrinsic property of minimal positive bases.

Lemma 4.3.1 *Let $\mathbf{D}_{\mathbb{L}} = [\mathbf{d}_1 \ \dots \ \mathbf{d}_{\ell+1}]$ be a minimal positive basis of an ℓ -dimensional subspace \mathbb{L} in \mathbb{R}^n . Then, there exists $\mathbf{v}_1, \dots, \mathbf{v}_{\ell+1} \in \mathbb{L}$ satisfying*

$$\forall i \in \llbracket 1, \ell + 1 \rrbracket, \quad \mathbf{d}_i^\top \mathbf{v}_i > 0 \quad \text{and} \quad \forall 1 \leq j < i \leq \ell + 1, \quad \mathbf{d}_i^\top \mathbf{v}_j < 0. \quad (4.17)$$

Proof. By Proposition 2.1.1, the zero vector $\mathbf{0}_n$ can be obtained by a positive linear combination of all columns of $\mathbf{D}_{\mathbb{L}}$. Without loss of generality, we rescale the columns of $\mathbf{D}_{\mathbb{L}}$ to ensure that $\sum_{i=1}^{\ell+1} \mathbf{d}_i = \mathbf{0}_n$. Now, since $\mathbf{D}_{\mathbb{L}}$ is a minimal positive basis, the matrix $\mathbf{D}_{\mathbb{L}, \mathbf{d}_{\ell+1}}$ obtained from $\mathbf{D}_{\mathbb{L}}$ by removing the column $\mathbf{d}_{\ell+1}$ is a linear basis of \mathbb{L} . Suppose that we augment this matrix with $n - \ell$ additional columns to form a basis \mathbf{B} of \mathbb{R}^n . Then, we have $\mathbf{d}_i = \mathbf{B}\mathbf{e}_i$ for any $i \in \llbracket 1, \ell \rrbracket$, while $\mathbf{d}_{\ell+1} = -\mathbf{B} \left(\sum_{j=1}^{\ell} \mathbf{e}_j \right)$, where we recall that $\mathbf{e}_1, \dots, \mathbf{e}_\ell$ are the first ℓ vectors of the canonical basis.

We now define the vectors

$$\begin{cases} \mathbf{v}_i &= \mathbf{B}^{-\top} \left(-\sum_{j=1}^{\ell} \mathbf{e}_j + (\ell + 1)\mathbf{e}_i \right) & i \in \llbracket 1, \ell \rrbracket \\ \mathbf{v}_{\ell+1} &= -\mathbf{B}^{-\top} \sum_{j=1}^{\ell} \mathbf{e}_j. \end{cases}$$

Using orthogonality of the coordinate vectors in \mathbb{R}^n , we have that $\mathbf{d}_i^\top \mathbf{v}_i = \ell \|\mathbf{e}_i\|^2 = \ell > 0$ for every $i \in \llbracket 1, \ell \rrbracket$ and $\mathbf{v}_{\ell+1}^\top \mathbf{d}_{\ell+1} = \left\| \sum_{j=1}^{\ell} \mathbf{e}_j \right\|^2 > 0$. As a result, the first part of (4.17) holds.

In addition, for any $1 \leq j < i \leq \ell + 1$, we obtain that $\mathbf{d}_i^\top \mathbf{v}_j = -\|\mathbf{e}_i\|^2 = -1 < 0$ if $i < \ell + 1$ and

$$\mathbf{d}_{\ell+1}^\top \mathbf{v}_j = \left\| \sum_{i=1}^{\ell} \mathbf{e}_i \right\|^2 - (\ell + 1)\|\mathbf{e}_j\|^2 = \sum_{i=1}^{\ell} \|\mathbf{e}_i\|^2 - (\ell + 1)\|\mathbf{e}_j\|^2 = \ell - (\ell + 1) = -1 < 0,$$

thus the second part of (4.17) also holds. \square

Our second technical result uses the result of Lemma 4.3.1 to define a quantity characteristic of the angles between columns of a minimal positive basis.

Lemma 4.3.2 *Suppose that $n \geq \ell \geq 2$ and let $\mathbf{D}_{\mathbb{L}} = [\mathbf{d}_1 \ \dots \ \mathbf{d}_{\ell+1}]$ be a minimal positive basis of a ℓ -dimensional subspace \mathbb{L} in \mathbb{R}^n . Let $\mathbf{v}_1, \dots, \mathbf{v}_{\ell+1}$*

be vectors in \mathbb{L} that satisfy (4.17). For any pair $(i, i') \in \llbracket 1, \ell + 1 \rrbracket^2$, let $\mathbf{d}_{i,i'}$ be the orthogonal projection of \mathbf{d}_i on $\mathbb{L} \cap \{\mathbf{v}_{i'}\}^\perp$. Then, the quantity $\rho_{\mathbf{D}_{\mathbb{L}}} := \max_{i,i' \leq \ell+1} \frac{\mathbf{d}_i^\top \mathbf{d}_{i,i'}}{\|\mathbf{d}_i\| \|\mathbf{d}_{i,i'}\|}$ lies in the interval $[0, 1)$.

Proof. Since $\mathbf{d}_{i,i'}$ is a projection of \mathbf{d}_i for any pair (i, i') , we have that $\mathbf{d}_i^\top \mathbf{d}_{i,i'} \geq 0$, hence $\rho_{\mathbf{D}_{\mathbb{L}}} \geq 0$. Moreover, for any pair $1 \leq i \leq i' \leq \ell + 1$, we have $\mathbf{d}_i^\top \mathbf{v}_{i'} \neq 0$ by (4.17), hence $\mathbf{d}_i \notin \mathbb{L} \cap \{\mathbf{v}_{i'}\}^\perp$ and $\frac{\mathbf{d}_i^\top \mathbf{d}_{i,i'}}{\|\mathbf{d}_i\| \|\mathbf{d}_{i,i'}\|} < 1$. As a result, $\rho_{\mathbf{D}_{\mathbb{L}}} < 1$, completing the proof. \square

The quantity defined in Lemma 4.3.2 is instrumental in defining suitable rotations matrices to produce a positive k -basis. The construction is described in Theorem 4.3.3.

Theorem 4.3.3 *Suppose that $n \geq \ell \geq 2$ and let $\mathbf{D}_{\mathbb{L}} = [\mathbf{d}_1 \ \dots \ \mathbf{d}_{\ell+1}]$ be a minimal positive basis of an ℓ -dimensional subspace \mathbb{L} in \mathbb{R}^n . Let $\rho_{\mathbf{D}_{\mathbb{L}}}$ be the quantity defined in Lemma 4.3.2 for some vectors $\mathbf{v}_1, \dots, \mathbf{v}_{\ell+1}$ satisfying (4.17). Finally, let $\mathbf{R}_{\mathbb{L}}^{(1)}, \dots, \mathbf{R}_{\mathbb{L}}^{(k)}$ be k rotation matrices in $\mathbb{R}^{n \times n}$ such that*

$$(i) \ \mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{u} = \mathbf{u}, \quad \text{for any } j \in \llbracket 1, k \rrbracket \text{ and any vector } \mathbf{u} \in \mathbb{L}^\perp,$$

$$(ii) \ \text{for any pair } (j, j') \in \llbracket 1, k \rrbracket^2 \text{ and any pair } (i, i') \in \llbracket 1, \ell + 1 \rrbracket^2,$$

$$\frac{[\mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_i]^\top \mathbf{R}_{\mathbb{L}}^{(j')} \mathbf{d}_{i'}}{\|\mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_i\| \|\mathbf{R}_{\mathbb{L}}^{(j')} \mathbf{d}_{i'}\|} = 1 \quad \Leftrightarrow \quad j = j' \text{ and } i = i',$$

$$(iii) \ \frac{[\mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_i]^\top \mathbf{d}_i}{\|\mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_i\| \|\mathbf{d}_i\|} > \rho_{\mathbf{D}_{\mathbb{L}}} \quad \text{for any pair } (i, j) \in \llbracket 1, \ell + 1 \rrbracket \times \llbracket 1, k \rrbracket.$$

Let $\mathbf{D}_{\mathbb{L}}^{(j)} := \mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{D}_{\mathbb{L}}$, for all j . Then, the matrix $\mathbf{D}_{\mathbb{L}}^{(1:k)} = [\mathbf{D}_{\mathbb{L}}^{(1)} \ \dots \ \mathbf{D}_{\mathbb{L}}^{(k)}]$ is a positive k -basis of \mathbb{L} with no identical columns.

Proof. Owing to assumptions (i) and (ii), we know that the columns of $\mathbf{D}_{\mathbb{L}}^{(1:k)}$ are contained in \mathbb{L} and pairwise distinct. Moreover, Proposition 4.3.1 guarantees that $\mathbf{D}_{\mathbb{L}}^{(1:k)}$ is a $PkSS$ for \mathbb{L} . Therefore we only need to show the positive k -independence of this matrix.

To this end, we consider an index $i \in \llbracket 1, \ell + 1 \rrbracket$ and show that the vector \mathbf{v}_i makes a positive dot product with exactly k columns of $\mathbf{D}_{\mathbb{L}}^{(1:k)}$, these columns being $\mathbf{R}_{\mathbb{L}}^{(1)} \mathbf{d}_i, \dots, \mathbf{R}_{\mathbb{L}}^{(k)} \mathbf{d}_i$. For any $j \in \llbracket 1, k \rrbracket$, we deduce from condition (iii) in the theorem's statement that

$$\frac{[\mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_i]^\top \mathbf{d}_i}{\|\mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_i\| \|\mathbf{d}_i\|} > \rho_{\mathbf{D}_{\mathbb{L}}} \geq \frac{\mathbf{d}_i^\top \mathbf{d}_{i,j}}{\|\mathbf{d}_i\| \|\mathbf{d}_{i,j}\|},$$

where $\mathbf{d}_{i,j}$ is defined as in Lemma 4.3.2. Letting $\Theta(\mathbf{u}, \mathbf{u}')$ denote the angle (with values in $[0, \pi]$) between two elements \mathbf{u} and \mathbf{u}' in \mathbb{R}^n , the above property translates to $\Theta(\mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_i, \mathbf{d}_i) < \Theta(\mathbf{d}_i, \mathbf{d}_{i,j})$. Using now that $\Theta(\mathbf{u}, \mathbf{u}') \leq \Theta(\mathbf{u}, \mathbf{u}'') + \Theta(\mathbf{u}'', \mathbf{u}')$ for any vector triplet $(\mathbf{u}, \mathbf{u}', \mathbf{u}'') \in (\mathbb{R}^n)^3$, we obtain

$$\Theta(\mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_i, \mathbf{v}_i) \leq \Theta(\mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_i, \mathbf{d}_i) + \Theta(\mathbf{d}_i, \mathbf{v}_i) < \Theta(\mathbf{d}_{i,i}, \mathbf{d}_i) + \Theta(\mathbf{d}_i, \mathbf{v}_i) = \frac{\pi}{2},$$

where the last equality comes from the fact that $\mathbf{d}_{i,i}$ and \mathbf{v}_i are orthogonal vectors. We have thus established that $\mathbf{v}_i^\top \mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_i > 0$ for all $j \in \llbracket 1, k \rrbracket$.

It now remains to show that $\mathbf{v}_i^\top \mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_{i'} \leq 0$ for any $i' \neq i$. First, using the same argument as above yields $\Theta(\mathbf{v}_i, \mathbf{d}_{i'}) = \frac{\pi}{2} + \Theta(\mathbf{d}_{i',i}, \mathbf{d}_{i'})$ as well as $\Theta(\mathbf{v}_i, \mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_{i'}) \geq \Theta(\mathbf{v}_i, \mathbf{d}_{i'}) - \Theta(\mathbf{d}_{i'}, \mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_{i'})$. Applying condition (iii), we find that $\Theta(\mathbf{d}_{i'}, \mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_{i'}) < \Theta(\mathbf{d}_{i'}, \mathbf{d}_{i',i})$, which finally leads to

$$\Theta(\mathbf{v}_i, \mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_{i'}) \geq \Theta(\mathbf{v}_i, \mathbf{d}_{i'}) - \Theta(\mathbf{d}_{i'}, \mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_{i'}) > \frac{\pi}{2},$$

hence $\mathbf{v}_i^\top \mathbf{R}_{\mathbb{L}}^{(j)} \mathbf{d}_{i'} \leq 0$. Overall, we have established that the vector \mathbf{v}_i makes a positive scalar product with exactly k columns in $\mathbf{D}_{\mathbb{L}}^{(1:k)}$. Since any vector $\mathbf{d} \in \text{col}(\mathbf{D}_{\mathbb{L}}^{(1:k)})$ is obtained by applying a rotation to some element $\mathbf{d}_i \in \text{col}(\mathbf{D}_{\mathbb{L}}^{(1:k)})$, we conclude that $\mathbf{D}_{\mathbb{L}}^{(1:k)}$ is positively k -independent, proving the desired result. \square

Note that Theorem 4.3.3 only applies when $\ell \geq 2$ (thus requiring $n \geq 2$ as well). Indeed, when the subspace \mathbb{L} has dimension 1, none of the three conditions (i), (ii) and (iii) can be fulfilled.

Remark 4.3.1 *The first two conditions enforced on the rotation matrices in Theorem 4.3.3 are designed to produce distinct vectors in \mathbb{L} without affecting the orthogonal complement of \mathbb{L} in \mathbb{R}^n . Indeed, condition (i) guarantees that the rotation leaves any vector orthogonal to \mathbb{L} invariant. Condition (ii) enforces that all vectors produced by applying the rotations are distinct since the angle between two different vectors has cosine less than 1. Finally, condition (iii) ensures that the vectors are positively k -independent. These conditions can be ensured through careful control of the eigenvalues of those rotation matrices, according to the angles between the columns of $\mathbf{D}_{\mathbb{L}}$.*

Theorem 4.3.3 provides a principled way of building positive k -bases from minimal positive bases. This approach naturally extends to OSPBs through their decomposition into orthogonal minimal positive bases. Using the technique described in Theorem 4.3.3 one can define rotation matrices that act on a single subspace from the decomposition of the OSPB without affecting the remaining subspaces thanks to orthogonality. The next corollary states the result.

Corollary 4.3.1 *Let $\mathbf{D}_{n,s} \equiv [\mathbf{D}_{\mathbb{L}_1} \ \dots \ \mathbf{D}_{\mathbb{L}_s}]$ be an OSPB, decomposed as in (4.3). Assume that for every $i \in \llbracket 1, s \rrbracket$, $\dim(\mathbb{L}_i) > 1$. Let $k \geq 1$ and for every $i \in \llbracket 1, s \rrbracket$, let $\mathbf{R}_{\mathbb{L}_i}^{(1)}, \dots, \mathbf{R}_{\mathbb{L}_i}^{(k)}$ be k rotation matrices satisfying the properties (i), (ii) and (iii) from Theorem 4.3.3 relative to $\mathbf{D}_{\mathbb{L}_i}$. Then,*

$$\mathbf{D}_{n,s}^{(1:k)} = \left[\mathbf{D}_{n,s}^{(1)} \ \dots \ \mathbf{D}_{n,s}^{(k)} \right], \quad \text{with } \mathbf{D}_{n,s}^{(j)} = \left[\mathbf{D}_{\mathbb{L}_i}^{(1)} \ \dots \ \mathbf{D}_{\mathbb{L}_i}^{(s)} \right] \quad \forall j \in \llbracket 1, k \rrbracket,$$

is a positive k -basis with $\text{cm}_k \left(\mathbf{D}_{n,s}^{(1:k)} \right) \geq \text{cm} \left(\mathbf{D}_{n,s} \right)$.

Corollary 4.3.1 thus provides a useful strategy to design positive k -bases with guaranteed k -cosine measure, since a lower bound on that quantity is given by $\text{cm}(\mathbf{D}_{n,s})$ and that measure can be efficiently computed through Algorithm 1. In particular, applying this strategy to a minimal positive basis yields a simple way of generating a positive k -basis with $k(n+1)$ vectors, as shown by Theorem 4.3.3 above.

Similarly to the result of Theorem 4.3.3, the result of Corollary 4.3.1 does not apply to all OSPBs. In particular, the maximal OSPB $[\mathbf{I}_n \ -\mathbf{I}_n]$ decomposes into n minimal positive bases over one-dimensional subspaces, which precludes the application of Theorem 4.3.3. Note however that Proposition 4.3.1 still provides a way to compute PkSSs with cosine measure guarantees for such a maximal OSPB.

4.4 Summary of Chapter 4

In this chapter, we have studied two classes of positive spanning sets through the lens of the cosine measure, a tool that allows for a geometric characterization of PSSs, as highlighted in Section 4.1.2. On the one hand, we have investigated in Section 4.2 orthogonally structured positive bases, that possess a favorable structure in that they decompose into minimal positive bases over orthogonal subspaces. By exploiting this property, we described an algorithm that computes this structure as well as the value of the cosine measure in polynomial time, thereby improving an existing procedure for generic positive spanning sets. On the other hand, we have conducted a detailed study of positive k -spanning sets in Section 4.3 and provided several characterizations of these matrices, including the generalization of the cosine measure through the k -cosine measure. We have also leveraged OSPBs to build positive k -spanning sets with guarantees on their k -cosine measure based on rotations. The results contained in this chapter have been published in **Linear Algebra and its Applications** [32].

Chapter 5

Using positive k -spanning sets in derivative-free optimization

Positive spanning sets are an important tool for derivative-free optimization, a subset of continuous optimization that aims at minimizing a function using only its values. In this chapter, we discuss the benefit of using positive k -spanning sets over generic PSSs within a derivative-free algorithm.

Throughout the chapter, we focus on a particular class of methods in derivative-free optimization, namely direct-search methods. We provide background material for both direct-search methods and derivative-free optimization in Section 5.1.

5.1 Derivative-free optimization and direct-search

5.1.1 Derivative-free optimization techniques

Continuous optimization is a fundamental tool in the field of mathematical programming and operations research. It involves finding the optimal solution to problems with continuous variables, which are ubiquitous in various scientific and engineering applications. Given a real valued function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, we consider the minimization problem

$$\underset{\mathbf{x} \in \mathbb{R}^n}{\text{minimize}} f(\mathbf{x}). \quad (5.1)$$

Without any convexity assumption on the function f , optimization algorithms on differentiable functions such as gradient descent seek a first-order critical point, i.e. a vector $\mathbf{x} \in \mathbb{R}^n$ such that $\nabla f(\mathbf{x}) = \mathbf{0}_n$ [81]. In certain cases, however, gradient information cannot be exploited, thereby precluding the use of gradient-type methods. The difficulty may reside in the properties of the function itself, in that derivative values could either not exist

or be hard to compute numerically, sometimes taking weeks for a single evaluation. Additionally, the presence of noise can render gradient descent methods inefficient, as it prevents the computation of derivative values to be done accurately.

Derivative-free optimization methods have been developed to circumvent these issues [15, 6]. Such methods have recently gained in popularity owing to the increasing complexity in mathematical modeling [1, 66]. They can be broadly divided into model-based methods and direct-search methods, although hybrid approaches are becoming increasingly popular [41]. Model-based algorithms build a model of the objective function from past evaluations in order to assess the next point to evaluate. Typical choices for such models include polynomial interpolation or regression models. A good model provides accurate approximations to the objective function and its derivatives (gradients and beyond when applicable). For continuously differentiable functions, examples of such models are obtained through simplex gradients [6, Definition 9.5] or polynomial models obtained by interpolation or regression using a set of function values f [15]. For a recent overview of model-based methods, we refer the reader to the survey by Larson, Menickelly and Wild [42, Section 2.2].

The second class of methods and the focus of this chapter is that of direct-search methods. Those algorithms proceed through successive function evaluations. Early approaches centered on evaluating f at the vertices of a simplex, which is systematically modified at each iteration. This is the basis of *simplicial methods* and of their well-known adaptation by Nelder and Mead, which has remained widely used since its introduction sixty years ago [6, Chapter 5] [59]. Alternatively, direct-search methods are sometimes based on functions evaluations in a close neighborhood of the current candidate solution. The properties of such methods, labeled as *directional*, are described in Section 5.1.2.

5.1.2 Directional direct-search methods

Given a candidate vector \mathbf{x}_j for solving (5.1) and a positive spanning set \mathbf{D} , directional direct-search methods look for an improved candidate solution \mathbf{x}_{j+1} among the neighbors of \mathbf{x}_j in the directions induced by \mathbf{D} . The associated algorithms are typically built around two main steps, repeated iteratively [15, 6].

First, the *search step* consists in looking for \mathbf{x}_{j+1} through function evaluations at a finite number of trial points in the space. This optional step can drastically improve the performance of the method and allows heuristic subroutines to be embedded within the algorithm. In cases where the search step is unsuccessful, a *poll step* is subsequently applied, where the function

value at \mathbf{x}_j is compared to that of its close neighbors. Algorithm 2 combines those two steps in an iterative framework.

Algorithm 2: Directional direct-search algorithm

- 1 *Input:* $f : \mathbb{R}^n \rightarrow \mathbb{R}$ function to be minimized, $\mathbf{x}_0 \in \mathbb{R}^n$, $\alpha_0 > 0$,
 $\rho : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ nonnegative function.
 - 2 For $j = 0, 1, 2, \dots$, choose a positive spanning set $\mathbf{D}^{(j)}$ and:
 - 3 **Search step:** Evaluate f at a each point of a finite set $\mathcal{S}_j \subset \mathbb{R}^n$. If a point $\mathbf{z} \in \mathcal{S}_j$ satisfies $f(\mathbf{z}) < f(\mathbf{x}_j) - \rho(\alpha_j)$, set $\mathbf{x}_{j+1} = \mathbf{z}$, declare the iteration successful and skip the poll step. Otherwise, proceed with the poll step.
 - 4 **Poll step:** define a poll set $\mathcal{P}_j = \{\mathbf{x}_j + \alpha_j \mathbf{d}, \mathbf{d} \in \text{col}(\mathbf{D}^{(j)})\}$ and evaluate f at the poll points. If one of these points satisfies $f(\mathbf{x}_j + \alpha_j \mathbf{d}) < f(\mathbf{x}_j) - \rho(\alpha_j)$, set $\mathbf{x}_{j+1} = \mathbf{x}_j + \alpha_j \mathbf{d}$ and declare the iteration successful. Otherwise, declare the iteration unsuccessful and set $\mathbf{x}_{j+1} = \mathbf{x}_j$.
 - 5 **Parameter update:** If the iteration was successful, set $\alpha_{j+1} \geq \alpha_j$. Otherwise, set $\alpha_{j+1} \leq \alpha_j$.
-

An iteration of Algorithm 2 is deemed *successful* if the search step (resp. poll step) identifies a point \mathbf{z} for which the function value $f(\mathbf{z})$ is sufficiently less than $f(\mathbf{x}_j)$; otherwise, the iteration is deemed *unsuccessful*. The nonnegative function ρ serves as a tool to ensure this sufficient decrease condition [15, Section 7.7]. In the remainder of this chapter, we shall always choose ρ as a forcing function.

Definition 5.1.1 (Forcing function) *A function $\rho : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is called forcing if it is continuous, non-decreasing and satisfies $\lim_{\alpha \rightarrow 0_+} \frac{\rho(\alpha)}{\alpha} = 0$*

Typical examples of forcing functions are given by those of the form $\rho(\alpha) = c\alpha^q$, where $q > 1$ and c is positive. In the next sections, we shall take a particular interest in the choice $\rho(\alpha) = \frac{\alpha^2}{2}$.

In order to implement the search step (resp. poll step) of Algorithm 2, one can compute the values $f(\mathbf{z})$, $\mathbf{z} \in \mathcal{S}_j$ (resp. $\mathbf{z} \in \mathcal{P}_j$) successively or through parallel evaluations. In the former case, the *opportunistic* strategy consists in terminating the step as soon as any point \mathbf{z} is found such that $f(\mathbf{z}) < f(\mathbf{x}_j) - \rho(\alpha_j)$, allowing for a reduction on the number of function evaluations required at each iteration. In the case of parallel evaluations, a *complete* strategy can sometimes be favored, where each poll point is evaluated.

We now briefly review classical directional direct-search algorithms. Our first example is given by the *coordinate search*, an implementation of Algo-

rithm 2 where the positive basis $[\mathbf{I}_n \quad -\mathbf{I}_n]$ is chosen at each step and the forcing function is $\rho(\alpha) = 0$. When the objective function f is assumed to have bounded level sets, a convergence result is derived.

Definition 5.1.2 (Bounded level sets) *Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$. We say that f has bounded level sets if for each $y \in \mathbb{R}$, the set $\{\mathbf{x} \in \mathbb{R}^n, f(\mathbf{x}) \leq y\}$ is bounded.*

Proposition 5.1.1 *[6, Theorem 3.4] Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be continuously differentiable with bounded level sets. Consider the sequence of unsuccessful iterates $(\mathbf{x}_j)_{j>0}$ obtained through an implementation of Algorithm 2 in which each successful iteration sets $\alpha_{j+1} = \alpha_j$, each unsuccessful iteration sets $\alpha_{j+1} = \frac{1}{2}\alpha_j$ and the positive basis $[\mathbf{I}_n \quad -\mathbf{I}_n]$ is chosen at each poll step. Then $\{\mathbf{x}_j\}$ possesses an accumulation point $\hat{\mathbf{x}}$ such that $\nabla f(\hat{\mathbf{x}}) = 0$.*

In the general framework of direct-search, note that the PSS $\mathbf{D}^{(j)}$ used in the poll step is allowed to be modified at each iteration.

We stated earlier that the search step of Algorithm 2 was optional. In the absence of such a step, we highlight that the choice of the candidate solution \mathbf{x}_0 given as an input to the algorithms yields an impact on the convergence speed. Indeed, each new candidate \mathbf{x}_{j+1} for minimizing f generated by the poll step is chosen in a close neighborhood of the incumbent solution \mathbf{x}_j . In cases where the input \mathbf{x}_0 is distant from each critical point \mathbf{x}^* of f , the number of steps required for Algorithm 2 to converge can be considerably high. By implementing a search step, one can ensure the exploration of points further away from the current candidate solution. More generally, this additional step can improve the performance of the algorithm without compromising its convergence guarantees. For instance, applying the correct heuristic at each iteration of the search step can sometimes help Algorithm 2 converge towards a global minimizer of the objective function f , as opposed to a local one [6, Section 7.2]. Implementations of the search step can be done through the use of a mesh.

Definition 5.1.3 (Mesh) *Let $\mathbf{D} \in \mathbb{R}^{n \times m}$ be a positive spanning set. The mesh generated by \mathbf{D} , centered at the incumbent solution $\mathbf{x}_j \in \mathbb{R}^n$ of coarseness $\alpha_j > 0$ is defined by $\mathcal{M}_j = \{\mathbf{x}_j + \alpha_j \mathbf{D}\mathbf{y} : \mathbf{y} \in \mathbb{N}^m\} \subset \mathbb{R}^n$.*

Mesh-based methods are then built from Algorithm 2 by ensuring that each iteration of the algorithm starts with a search step in which the finite set \mathcal{S}_j is contained in the mesh \mathcal{M}_j . This is the object of the generalized pattern search algorithm [75]. Under the right assumptions, the generalized pattern search algorithm can again be proved to converge [4]. The following proposition is derived from a result by Audet and Hare [6, Theorem 7.7].

Proposition 5.1.2 *Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be continuously differentiable with bounded level sets. Consider the sequence of iterates $(\mathbf{x}_j)_{j>0}$ obtained through*

an implementation of Algorithm 2 in which each set \mathcal{S}_j generated at the search step is contained in the mesh \mathcal{M}_j , each successful iteration sets $\alpha_{j+1} = 2\alpha_j$ and each unsuccessful iteration sets $\alpha_{j+1} = \frac{1}{2}\alpha_j$. Then $(\mathbf{x}_j)_{j>0}$ possesses an accumulation point $\hat{\mathbf{x}}$ such that $\nabla f(\hat{\mathbf{x}}) = 0$.

Note that generalized pattern search algorithms were extended into a family of algorithms labeled *mesh adaptive direct-search* (MADS) [5]. Such algorithms involve the presence of a frame, used to determine which positive spanning set should be chosen at each poll step of the algorithm [6, Chapter 8].

5.1.3 Complexity results for direct-search

In this section, we review the standard complexity results for direct-search based on sufficient decrease and positive spanning sets, based on the original paper of Vicente [77]. We consider the following implementation of Algorithm 2, which uses opportunistic polling and in which, for the sake of simplicity, the search step was removed. Note moreover that the values of the forcing function ρ and the parameter α_0 have been fixed for simplicity.

Algorithm 3: Direct-search algorithm with sufficient decrease

- 1 *Input:* $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $\mathbf{x}_0 \in \mathbb{R}^n$, $\alpha_0 = 1$.
 - 2 For $j = 0, 1, 2, \dots$, choose a positive spanning set $\mathbf{D}^{(j)}$ and:
 - 3 **Poll step:** define a poll set $\mathcal{P}_j = \{\mathbf{x}_j + \alpha_j \mathbf{d}, \mathbf{d} \in \text{col}(\mathbf{D}^{(j)})\}$ and start evaluating f at the poll points. If one of these points satisfies $f(\mathbf{x}_j + \alpha_j \mathbf{d}) < f(\mathbf{x}_j) - \frac{\alpha_j^2}{2}$, then stop polling, set $\mathbf{x}_{j+1} = \mathbf{x}_j + \alpha_j \mathbf{d}$ and declare the iteration successful. Otherwise, declare the iteration unsuccessful and set $\mathbf{x}_{j+1} = \mathbf{x}_j$.
 - 4 **Parameter update:** If the iteration was successful, set $\alpha_{j+1} = \alpha_j$. Otherwise, set $\alpha_{j+1} = \frac{1}{2}\alpha_j$.
-

In order to study the complexity of Algorithm 3, we will now consider additional assumptions on the inputs. We emphasize that each complexity result presented in this section would remain true in the presence of a search step.

Assumption 5.1.1 *The objective function f has bounded level sets. It is continuously differentiable and ∇f is a Lipschitz continuous function associated to the constant $L > 0$.*

In addition to the objective function f , each positive spanning set considered in Algorithm 3 should satisfy specific properties.

Assumption 5.1.2 *There exists two constants $\kappa > 0$ and $m \in \mathbb{N}$ such that each positive spanning set $\mathbf{D}^{(j)}$ in the algorithm satisfies $\text{cm}(\mathbf{D}^{(j)}) \geq \kappa$ and possesses at most m columns. Each of these columns is a unit vector.*

As stated in Proposition 5.1.1, the coordinate search algorithm applied to a continuously differentiable objective function f that has bounded level sets generates an infinite sequence of unsuccessful iterates, which admits an accumulation point that is critical for f . The following theorem generalizes the result to Algorithm 3 and gives an upper bound on the norm of the gradient of each candidate solution \mathbf{x}_j associated to an unsuccessful iteration.

Theorem 5.1.1 *[77, Lemma 1 & Theorem 1] Under Assumptions 5.1.1 and 5.1.2, Algorithm 3 contains infinitely many unsuccessful iterations. Letting j_0 denote the index of any unsuccessful iteration of Algorithm 3, we have*

$$\|\nabla f(\mathbf{x}_{j_0})\| \leq \frac{\alpha_{j_0}(L+1)}{2\kappa}.$$

The value of the parameter α_j is halved at each unsuccessful iteration and remains unchanged when the iteration is successful. In consequence, note that the value $\frac{\alpha_{j_0}(L+1)}{2\kappa}$ given in Theorem 5.1.1 must converge to 0 and thus, Algorithm 3 can be used to find a critical point for the objective function f . In order to determine the worst case complexity of Algorithm 3, Vicente computed upper bounds on the number of successful and unsuccessful iterations needed for convergence and combined these values [77, Corollary 1]. The following theorem summarizes this initial complexity result by showing the dependence in the cosine measure.

Theorem 5.1.2 *[24, Theorem 3.2.1] Consider any application of Algorithm 3 under Assumptions 5.1.1 and 5.1.2 and let $\varepsilon > 0$. The algorithm finds a solution \mathbf{x}_j satisfying $\|\nabla f(\mathbf{x}_j)\| \leq \varepsilon$ after at most $\mathcal{O}(\kappa^{-2}\varepsilon^{-2})$ iterations and thus, at most $\mathcal{O}(m\kappa^{-2}\varepsilon^{-2})$ function evaluations. The value of the constant in each $\mathcal{O}(\cdot)$ can be fully expressed in terms of f_{low} and L*

The bounds given in Theorem 5.1.2 exhibit a factor $m\kappa^{-2}$, that involves both the cardinality and the cosine measure of the positive spanning set(s) at hand. Both m and κ depend on the problem dimension n , and one aims at selecting PSSs that yield the lowest value of $m\kappa^{-2}$ possible. The next theorem can be used to identify the optimal PSS to be considered.

Theorem 5.1.3 *[25, Theorem 4.1] There exists a constant $c > 0$ such that $m \text{cm}(\mathbf{D})^{-2} \geq cn^2$, for each PSS $\mathbf{D} \in \mathbb{R}^{n \times m}$.*

Consider any implementation of Algorithm 3 under Assumptions 5.1.1 and 5.1.2. We saw in Theorem 5.1.2, that the number of functions evaluation was bounded above by $\mathcal{O}(m\kappa^{-2}\varepsilon^{-2})$. As an immediate consequence to Theorem 5.1.3, we see that this bound can at best be reduced to $\mathcal{O}(n^{-2}\varepsilon^{-2})$, when choosing PSSs that minimize the value $m \text{cm}(\mathbf{D}^{(j)})^{-2}$ at each iteration.

Example 5.1.1 Consider Algorithm 3 under Assumptions 5.1.1 and 5.1.2 in which the positive basis \mathbf{D}_n is chosen at each poll step. The cosine measure of the positive basis $\mathbf{D}_n = [\mathbf{I}_n \quad -\mathbf{1}_n]$ was computed in Chapter 4, where we showed that $\text{cm}(\mathbf{D}_n) = \frac{1}{\sqrt{n^2+2(n-1)\sqrt{n}}}$. The size of this positive basis is given by $m = n + 1$; we find $m \text{cm}(\mathbf{D}_n)^{-2} = \mathcal{O}(n^3)$.

By Theorem 5.1.2, for any $\varepsilon > 0$, after at most $\mathcal{O}(n^3\varepsilon^{-2})$ function evaluations, the algorithm has found a solution \mathbf{x}_j satisfying $\|\nabla f(\mathbf{x}_j)\| \leq \varepsilon$.

The cosine measure of the maximal positive basis $\mathbf{D}_{n,n} = [\mathbf{I}_n \quad -\mathbf{I}_n]$ was shown in Chapter 4 to be equal to $\frac{1}{\sqrt{n}}$. Thus, letting $m = 2n$ we find $m \text{cm}(\mathbf{D}_n) = 2n^2$. Using Theorem 5.1.3, we deduce that the coordinate search algorithm, in which each iteration of the poll step consists in using the positive basis $[\mathbf{I}_n \quad -\mathbf{I}_n]$ has an optimal worst-case complexity order.

Corollary 5.1.1 [77, Corollary 2] Consider any application of Algorithm 3 under Assumptions 5.1.1 and 5.1.2 and let $\varepsilon > 0$. Assume that the positive basis $[\mathbf{I}_n \quad -\mathbf{I}_n]$ is chosen at each poll step. After at most $\mathcal{O}(n^2\varepsilon^{-2})$ function evaluations, the algorithm has found a solution \mathbf{x}_j satisfying $\|\nabla f(\mathbf{x}_j)\| \leq \varepsilon$.

5.2 Algorithm based on positive k -spanning sets

5.2.1 Parallel evaluations and stragglers

Our motivation for using positive k -spanning sets in direct-search stems from *parallel computing*, a paradigm in which the computations performed at each iteration of an algorithm are carried out simultaneously across multiple processors.

Direct-search schemes have been adapted to parallel environments in several ways. First, recall that a basic framework such as that of Algorithm 2 either relies on opportunistic or complete polling, as discussed in Section 5.1.2. Because complete polling is more expensive in terms of function values, opportunistic is often preferred in sequential environments. In the context of parallel computing, however, these extra computations can sometimes allow for a reduction of the total running time. Perhaps surprisingly, these can also help reduce the total number of function evaluations needed for convergence [23]. More recently, asynchronous variants of these parallel evaluations procedures, that allow for opportunistic polling, have shown practical benefit [36, 39, 8].

Recall that derivative-free optimization methods are employed when the gradient ∇f of the objective function is difficult to compute or does not exist. We now consider cases where the function evaluations themselves are costly or unreliable. For instance, in optimal aeroacoustic shape design, a single evaluation may take an entire day [52]. In other cases, such as minimizing helicopter rotor blade vibrations [13], the function may fail to return a

value in more than two thirds of the trials due to hidden constraints [14]. To address these issues, we consider parallelized implementations of Algorithm 3, where each function evaluation is assigned on a separate processor. We impose a fixed time limit $T > 0$. At each step, any processor that either fails or takes longer than T seconds to complete its function evaluation is designated as a *straggler*, an expression that we borrow from the machine learning literature [73]. In the presence of stragglers, the convergence of Algorithm 3 is no longer guaranteed. Indeed, a number of values may be missing at every poll step, and thus the poll step may no longer consists of evaluations in directions forming a PSS. In the next section, we shall see how positive k -spanning sets can be exploited to maintain convergence results in such settings.

5.2.2 Algorithmic framework

We now present a derivative-free algorithm which exploits the resilient nature of positive k -spanning sets, and handles the presence of stragglers. The full description is provided in Algorithm 4.

Algorithm 4: Direct-search algorithm with PkSSs

- 1 *Input:* $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $\mathbf{x}_0 \in \mathbb{R}^n$, $\alpha_0 = 1$, $k \geq 2$.
 - 2 For $j = 0, 1, 2, \dots$, choose a positive k -spanning set $\mathbf{D}^{(j)}$ and:
 - 3 **Poll step:** define a poll set $\mathcal{P}_j = \{\mathbf{x}_j + \alpha_j \mathbf{d}, \mathbf{d} \in \text{col}(\mathbf{D}^{(j)})\}$ and start evaluating f at the poll points. If one of these points satisfies $f(\mathbf{x}_j + \alpha_j \mathbf{d}) < f(\mathbf{x}_j) - \frac{\alpha_j^2}{2}$, then stop polling, set $\mathbf{x}_{j+1} = \mathbf{x}_j + \alpha_j \mathbf{d}$ and declare the iteration successful. Otherwise, declare the iteration unsuccessful and set $\mathbf{x}_{j+1} = \mathbf{x}_j$.
 - 4 **Parameter update:** If the iteration was successful, set $\alpha_{j+1} = \alpha_j$. Otherwise, set $\alpha_{j+1} = \frac{\alpha_j}{2}$.
-

In a nutshell, Algorithm 4 is obtained from Algorithm 3 by replacing each PSS $\mathbf{D}^{(j)}$ with a PkSS. As before, we study the complexity of Algorithm 4 under Assumption 5.1.1. The assumption on the PSSs involved in Algorithm 3 is replaced with a similar one on positive k -spanning sets.

Assumption 5.2.1 *There exists two constants $\kappa > 0$ and $m \in \mathbb{N}$ such that each positive k -spanning set $\mathbf{D}^{(j)}$ in Algorithm 4 satisfies $\text{cm}_k(\mathbf{D}^{(j)}) \geq \kappa$ and possesses at most m columns. Each of these columns is a unit vector.*

Last, we allow for the presence of failed evaluations in the poll step of each iteration. The number of stragglers is bounded above.

Assumption 5.2.2 *For $j = 0, 1, 2, \dots$, the poll set contains at most $k - 1$ stragglers.*

The complexity of Algorithm 4 under Assumptions 5.1.1, 5.2.1 and 5.2.2 is investigated in the next section of this chapter.

5.2.3 Complexity analysis

In order to study the complexity of Algorithm 4, we exploit the similarities that it shares with Algorithm 3.

Theorem 5.2.1 *Consider any application of Algorithm 4 under Assumptions 5.1.1, 5.2.1 and 5.2.2 and let $\varepsilon > 0$. The algorithm finds a solution \mathbf{x}_j satisfying $\|\nabla f(\mathbf{x}_j)\| \leq \varepsilon$ after at most $\mathcal{O}(\kappa^{-2}\varepsilon^{-2})$ iterations and thus, at most $\mathcal{O}(m\kappa^{-2}\varepsilon^{-2})$ function evaluations. The value of the constant in each $\mathcal{O}(\cdot)$ can be fully expressed in terms of f_{low} and L .*

Proof. Each matrix $\mathbf{D}^{(j)}$ considered in Algorithm 4 is a PkSS and in particular, these matrices are also positively spanning. Denote by $\tilde{\mathbf{D}}^{(j)}$ the matrix obtained by removing from $\mathbf{D}^{(j)}$ each column \mathbf{d} associated to a failed evaluation of the quantity $f(\mathbf{x}_j + \alpha_j \mathbf{d})$. By Assumption 5.2.2, $\tilde{\mathbf{D}}^{(j)}$ is obtained from $\mathbf{D}^{(j)}$ by removing at most $k - 1$ columns, therefore $\tilde{\mathbf{D}}^{(j)}$ is a PSS. Finally, as per Assumption 5.2.1 we have $\text{cm}_k(\mathbf{D}^{(j)}) \geq \kappa$ therefore by Theorem 4.3.2 we find $\text{cm}(\tilde{\mathbf{D}}^{(j)}) \geq \kappa$.

In the end, under the three assumptions that were considered, applying Algorithm 4 amounts to applying Algorithm 3 under Assumptions 5.1.1 and 5.1.2. By Theorem 5.1.2, we obtain the expected result. \square

In line with the results found in Section 5.1.3, we observe that the worst case complexity of Algorithm 4, in terms of function evaluations, is dependent on the value of the ratio $\frac{m}{\kappa^2}$, which should be minimized. In the case of Algorithm 3, we saw in Theorem 5.1.3 that for $k = 1$ the ratio was in $\Omega(n^2)$. The proof of this result, by Dodangeh, Vicente and Zhang, uses sphere coverings [25]. We now adapt this line of reasoning to cases where $k > 1$, in order to determine the optimal order of worst case complexity of Algorithm 4. We will show that this ratio is in $\Omega(\frac{n^2 m}{m-k+1})$. We start with preliminary results.

Lemma 5.2.1 [25, Generalized from Lemma 4.1] *Let $k \geq 1$ and consider any PkSS $\mathbf{D} \in \mathbb{R}^{n \times m}$ with unit columns. Let $\tilde{m} \in \llbracket m - k + 1, m \rrbracket$ and let $\tilde{\mathbf{D}} = [\tilde{\mathbf{d}}_1 \ \dots \ \tilde{\mathbf{d}}_{\tilde{m}}] \in \mathbb{R}^{n \times \tilde{m}}$ be a PSS with $\text{col}(\tilde{\mathbf{D}}) \subset \text{col}(\mathbf{D})$. The union of the spherical caps centered at each $\tilde{\mathbf{d}}_i$ with geodesic radius $\arccos(\text{cm}_k(\mathbf{D}))$ covers the sphere $\mathbb{S}^{n-1} \subset \mathbb{R}^n$.*

Proof. When $k = 1$, we observe that $\tilde{m} = m$ and in consequence, the positive spanning set $\tilde{\mathbf{D}}$ is given by $\tilde{\mathbf{D}} = \mathbf{D}$. Moreover, the value $\text{cm}_k(\mathbf{D})$ corresponds to the cosine measure of \mathbf{D} . As so, this case is a restatement of [25, Lemma 4.1], whose proof we omit.

Now, suppose that $k \geq 2$ and let $\mathbf{D} \in \mathbb{R}^{n \times m}$ be a PkSS. Consider any positive spanning set $\tilde{\mathbf{D}}$ of size $\tilde{m} \in \llbracket m - k + 1, m \rrbracket$ with $\text{col}(\tilde{\mathbf{D}}) \subset \text{col}(\mathbf{D})$. By Theorem 4.3.2, we have $\text{cm}(\tilde{\mathbf{D}}) \geq \text{cm}_k(\mathbf{D})$ and thus, $\arccos(\text{cm}(\tilde{\mathbf{D}})) \leq \arccos(\text{cm}_k(\mathbf{D}))$. Moreover, by [25, Lemma 4.1], we know the sphere \mathbb{S}^{n-1} to be covered by the spherical caps centered at each $\tilde{\mathbf{d}}_i$ with geodesic radius $\arccos(\text{cm}(\tilde{\mathbf{D}}))$. Since $\arccos(\text{cm}(\tilde{\mathbf{D}})) \leq \arccos(\text{cm}_k(\mathbf{D}))$, the covering of the sphere \mathbb{S}^{n-1} is maintained upon setting the radii of each spherical cap to $\arccos(\text{cm}_k(\mathbf{D}))$. \square

An upper bound on the k -cosine measure of positive k -spanning sets can be deduced by combining Lemma 5.2.1 with the following result.

Lemma 5.2.2 [25, Lemma 4.2] *Any covering of the sphere \mathbb{S}^{n-1} by $\tilde{m} \geq n+1$ spherical caps of geodesic radius ϕ satisfies $\cos(\phi) \leq c\sqrt{n^{-1}\log(n^{-1}\tilde{m})}$, for some constant $c > 0$.*

Observe that each PSS obtained by removing at most $k - 1$ column from a PkSS $\mathbf{D} \in \mathbb{R}^{n \times m}$ has size $\tilde{m} \geq n + 1$. As announced, an upper bound on the k -cosine measure of \mathbf{D} can then be derived from Lemmas 5.2.1 and 5.2.2.

Lemma 5.2.3 [25, Generalized from Lemma 4.3] *Any PkSS $\mathbf{D} \in \mathbb{R}^{n \times m}$ satisfies $\text{cm}_k(\mathbf{D}) \leq c\sqrt{n^{-1}\log(n^{-1}(m - k + 1))} \leq cn^{-1}\sqrt{m - k + 1}$, for some constant $c > 0$.*

From the inequality $\text{cm}_k(\mathbf{D}) \leq cn^{-1}\sqrt{m - k + 1}$, it is easy to deduce a lower bound on the value of the ratio $\frac{m}{\text{cm}_k(\mathbf{D})^2}$, for any PkSS $\mathbf{D} \in \mathbb{R}^{n \times m}$.

Theorem 5.2.2 *Each PkSS $\mathbf{D} \in \mathbb{R}^{n \times m}$ satisfies $m \text{cm}_k(\mathbf{D})^{-2} = \Omega(\frac{n^2 m}{m - k + 1})$.*

As implied by Theorem 5.2.2, using positive k -spanning sets $\mathbf{D}^{(j)} \in \mathbb{R}^{n \times m}$ which minimize the ratio $m \text{cm}_k(\mathbf{D}^{(j)})^{-2}$ can help reducing the upper bound on the number of function evaluations needed for Algorithm 4 to converge. Theorem 5.2.2 suggests that the bound $\mathcal{O}(\frac{n^2 m}{m - k + 1} \varepsilon^{-2})$ can be attained by considering the appropriate PkSS.

In the case of positive k -spanning sets of minimal size $m = 2k + n - 1$, where $n > 0$ is fixed, we find $\Omega(\frac{n^2 m}{m - k + 1}) = \Omega(n^2(1 + \frac{k-1}{k+n}))$. Note this ratio approaches $\Omega(2n^2)$ for large values of k .

Alternatively, when the parameter $k > 0$ is negligible compared to the size of the PkSS, the lower bound on the ratio $m \text{cm}_k(\mathbf{D})^{-2}$ greatly simplifies as we obtain $m \text{cm}_k(\mathbf{D})^{-2} = \Omega(\frac{n^2 m}{m - k + 1}) = \Omega(n^2)$. This last scenario hints at the existence of a positive k -spanning set that reduces the worst case complexity for Algorithm 4 to $\mathcal{O}(n^2 \varepsilon^{-2})$.

Special choices of PkSSs Let $\mathbf{D}_{n,s} = [\mathbf{D}_{\mathbb{L}_1} \ \dots \ \mathbf{D}_{\mathbb{L}_s}] \in \mathbb{R}^{n \times (n+s)}$ be an OSPB decomposed as in (2.4). Suppose that each linear space \mathbb{L}_i satisfies $\dim(\mathbb{L}_i) > 1$. A systematic method for building positive k -spanning sets of size $k(n+s)$ with a k -cosine measure bounded below by $\kappa = \text{cm}(\mathbf{D}_{n,s})$ was presented in Corollary 4.3.1. Using this procedure on a minimal positive basis with $\text{cm}(\mathbf{D}_n) = \frac{1}{n}$ allows for the construction of a PkSS $\mathbf{D}_n^{(1:k)} \in \mathbb{R}^{n \times k(n+1)}$ for which we find $m \text{cm}_k(\mathbf{D}_n^{(1:k)})^{-2} \leq 2kn^3$. Consequently, using at each iteration of Algorithm 4 yields a complexity in $\mathcal{O}(2kn^3\varepsilon^{-2})$ in terms of function evaluations.

Note that for positive k -spanning sets of size $m = k(n+1)$, the bound in Theorem 5.2.3 is re-expressed as $\Omega(n^2(1 + \frac{k-1}{kn+1}))$ and simplifies into $\Omega(n^2(1 + \frac{1}{n}))$ for large values of k . This observation suggests the existence of PkSSs of size $n(k+1)$ that could yield a complexity bound in $\mathcal{O}(n^2(1 + \frac{1}{n})\varepsilon^{-2})$ function evaluations, an improvement over that associated to $\mathbf{D}_n^{(1:k)}$.

Consider now $\mathbf{D}_{n,n} = [\mathbf{I}_n \ -\mathbf{I}_n]$. For each $i \leq k$, we choose an orthogonal matrix \mathbf{P}_i and let $\mathbf{M}_i = \mathbf{P}_i \mathbf{D}_{n,n}$. Finally, we let $\mathbf{D}_{n,n}^{(1:k)} = [\mathbf{M}_1 \ \dots \ \mathbf{M}_k]$. Then, letting $m = 2kn$, the PkSS $\mathbf{D}_{n,n}^{(1:k)} \in \mathbb{R}^{n \times m}$ satisfies $m \text{cm}_k(\mathbf{D}_{n,n}^{(1:k)})^{-2} \leq 2kn^2$. Using $\mathbf{D}_{n,n}^{(1:k)}$ at every iteration of Algorithm 4 yields a complexity in $\mathcal{O}(2kn^2\varepsilon^{-2})$ in terms of function evaluations. For small values of k , we observe that this value approaches the theoretical lower bound $\mathcal{O}(n^2\varepsilon^{-2})$ that was previously mentioned.

5.3 Summary of Chapter 5

This chapter presented an application of the results from Chapter 4.3 to derivative-free optimization algorithms. We highlighted in Section 5.1.1 how such methods are employed for minimizing functions that are noisy or whose derivative is expensive to evaluate. We showed in Section 5.1.2 how positive spanning sets play a crucial role for directional direct-search algorithms: the directions they define are used to find new candidate solutions for minimizing the objective. The worst case complexity of such algorithms is known to depend on the cosine measure and the size of the PSSs used in the implementation. In that regard, we computed in Example 5.1.1 the worst case complexity associated to the use of the positive basis $[\mathbf{I}_n \ -\mathbf{1}_n]$ at each iteration of a directional direct-search algorithm.

Section 5.2.1 is motivated by parallel computing, which helps reducing the running time of algorithms by performing calculations simultaneously across multiple processors. We considered in implementations of direct-search algorithms which allow for the presence of *stragglers*, that is, functions evaluations which fail or which are particularly time consuming. For naive

approaches such as that described in Algorithm 3, allowing for failed evaluations compromises convergence guarantees. The issue was tackled in Section 5.2, where we introduced a new algorithm that exploits the resilient nature of positive k -spanning sets to account for the presence of stragglers. Last, we saw in Sections 5.2.2 and 5.2.3 that under the proper assumptions on the Pk SSs to be considered, the convergence of Algorithm 4 could be guaranteed for the same classes of objective functions as Algorithm 3. An upper bound on the worst case complexity of this new algorithm was found in Theorem 5.2.1, where we showed that this complexity is dependent on the k -cosine measure of the Pk SSs considered in the implementation.

Chapter 6

Conclusion

6.1 Summary of the thesis

Throughout this manuscript, we investigated the structural properties of positive spanning sets. An important relationship between such sets and strongly connected digraphs was exhibited in Chapter 3, allowing for a novel decomposition result for PSSs and positive bases. We showed that the result could be leveraged and combined with properties on critical matrices - see Definition 3.4.2 - to derive a characterization of positive bases in \mathbb{R}^n . By doing so, we were able to give a complete description of bases of near-extreme sizes, as summarized in the table below.

Size of the positive basis	Associated structure
$n + 1$ (minimal)	See [64, Theorem 6.1]
$n + 2$	Theorem 3.4.4 (Contribution)
$n + 3$ to $2n - 3$	Unknown
$2n - 2$	Theorem 3.4.3 (Contribution)
$2n - 1$	Theorem 3.4.2 (Contribution)
$2n$ (maximal)	See [64, Theorem 6.3]

In turn, we obtained a characterization of minimally strongly connected digraphs on n vertices and m arcs for each m in $\{n + 1, 2n - 3, 2n - 4\}$. Chapter 2 highlighted how positive k -spanning sets were typically built through the use of Gale diagrams. An alternative construction method was introduced in Section 2.3.3 and allowed for a characterization of positive 2-bases of minimal size in \mathbb{R}^n .

The last two chapters of this manuscript took concern in the uses of positive (k -)spanning sets in optimization algorithms. Chapter 4 introduced a method for computing the cosine measure of specific PSSs in polynomial time. More importantly, it presented a simple method for constructing positive k -bases with a structure particularly well-suited for use in direct-search algorithms. These results were exploited in Chapter 5, where we presented an optimization algorithm which uses the properties of Pk SSs to guarantee convergence even in the presence of failed evaluations. Theoretical bounds on the complexity of this algorithm were provided, though numerical experiments remain to be conducted.

6.2 Perspectives

The third chapter of this thesis leveraged classical results in graph theory to derive new characterizations of positive spanning sets. Similarly, the structure of positive bases of near-extreme sizes was successfully described by exploiting the properties of critical matrices, which remain understudied. A deeper understanding on the properties of these matrices should facilitate the characterization of broader categories of positive bases. On that note, this manuscript took concern in the study of critical matrices having at most three rows. This work could naturally be expanded to matrices with larger amount of rows. Alternatively, a study on the properties of critical matrices with a small amount of columns could help achieve a better understanding of their structure. As a last note on critical matrices, we emphasize that the IN matrix associated to an arbitrary positive basis \mathbf{D} through (3.6) is non-unique. In consequence, the critical structure (3.7) associated to \mathbf{D} is itself non-unique and in particular, the sizes of each critical block can change from one decomposition of the positive basis to another. Developing methods for finding an optimal critical structure (3.7) of \mathbf{D} - that is, one in which each critical block is of relatively small size - could be an interesting direction for future works.

Although a relationship between positive k -spanning sets and strongly k -edge connected digraphs was discussed in Section 3.5, the results derived from this relationship do not appear to be as strong as those obtained for positive spanning sets. Alternative approaches should be favored in order to study Pk SSs. On that note, previous authors aimed at finding the maximal possible size of positive k -bases through polytope theory. This promising approach has already led to the finding of a finite upper bound on the size of positive k -bases. A deeper analysis on the properties of $(k-1)$ -unneighborly polytopes - see Definition 2.3.7 - could help reduce this bound, as positive k -bases are characterized as being Gale diagrams for such polytopes. Alternatively, we note that the problem of finding the size of a maximal positive basis in \mathbb{R}^n is easily tackled through the use of a linear programming ar-

gument. Determining whether this argument can be generalized for larger values of k should prove as an interesting challenge.

Results with regard to the $(k-)$ cosine measure of positive $(k-)$ spanning sets were detailed in Chapters 4 and 5. While general methods for computing the cosine measure of a given set are exponential, we showed that this complexity could be drastically reduced for OSPBs - see Definition 4.2.1. The existence of other classes of positive spanning sets with a cosine measure that can quickly be computed remains to be determined. On that matter, a first attempt could consist in exploring results related to the structural equivalence between matrices. Indeed, the cosine measure of a matrix \mathbf{D} is entirely determined by that of a structurally equivalent matrix $\tilde{\mathbf{D}} \equiv \mathbf{D}$ and by the nonsingular matrix \mathbf{B} involved in this structural equivalence. In particular, when \mathbf{B} is orthogonal the two matrices share an equal cosine measure. Alternative hypotheses on the properties of the nonsingular matrix \mathbf{B} could be associated to similar formulas connecting the cosine measures of the two matrices. In turn and for matrices that are structurally equivalent to OSPBs, the computation of the cosine measure could sometimes be greatly simplified.

The k -cosine measure is a novel tool whose properties remain to be studied in depth. The structure of positive k -bases of minimal whose k -cosine measure is maximal - and the value of this k -cosine measure - are easily determined when $k = 1$. Future research could aim at generalizing these results to all values of k . In the more general case however, the task of computing the k -cosine measure of an arbitrary PkSS is particularly tedious. A more reasonable challenge would consist in assessing upper and lower bounds on this value.

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RÉSUMÉ

Les familles positivement génératrices (PSSs) sont définies par leur capacité à engendrer l'entière de l'espace euclidien par des combinaisons linéaires à coefficients positifs ou nuls. De telles familles de vecteurs jouent un rôle important dans le cadre de l'optimisation continue, et plus particulièrement dans celui de l'optimisation sans dérivées. Dans ce contexte, les algorithmes directionnels de recherche directe se basent sur l'utilisation de PSSs pour explorer l'espace en quête d'un extremum de la fonction à optimiser. Les performances de ces algorithmes sont impactées par la taille des PSSs considérés, mais aussi par la dispersion de leurs éléments dans l'espace, évaluée par leur mesure cosinus. Les bornes de complexité se voient ainsi réduites pour des familles alliant une faible cardinalité à une mesure cosinus élevée. À ce jour, il n'existe pourtant ni de caractérisation satisfaisante des bases positives - nom donné aux PSSs minimaux en termes d'inclusion - ni d'algorithme polynomial permettant d'évaluer la mesure cosinus d'une famille de vecteurs.

Dans ce manuscrit, nous nous attachons à examiner chacun de ces deux problèmes, par l'étude théorique des propriétés des familles positivement génératrices. Dans un premier temps, nous explorons les relations liant les matrices de réseaux de graphes fortement connexes aux représentations matricielles des PSSs. Nous exhibons ainsi une nouvelle caractérisation de ces familles, que nous affinons dans le but de caractériser les bases positives. Par la suite, nous démontrons l'existence d'algorithmes polynomiaux permettant de déterminer la mesure cosinus de certaines classes de bases positives. Nous démontrons qu'il est possible, à l'aide de ces familles, de construire des PSSs résilients qui conservent une mesure cosinus satisfaisante lorsqu'on retire un certain nombre de leurs éléments. Enfin, nous introduisons un nouvel algorithme de recherche directe, plus robuste que ses prédécesseurs, basé sur l'utilisation de ces PSSs résilients.

MOTS CLÉS

Famille positivement génératrice, base positive, graphe fortement connexe, mesure cosinus, diagramme de Gale, optimisation continue, optimisation sans dérivées, recherche directe directionnelle

ABSTRACT

Positive spanning sets (PSSs) are defined by their ability to generate the entire Euclidean space through linear combinations with nonnegative coefficients. Such families of vectors play an important role in the framework of continuous optimization, and more specifically in derivative-free optimization. In this context, directional direct-search algorithms rely on the use of PSSs to explore the space in search of an extremum of the objective function. The performance of these algorithms is influenced not only by the size of the PSSs to be considered, but also by the spread of their elements in space, assessed through their cosine measure. Complexity bounds can thus be lowered for families that combine low cardinality with a high cosine measure. To date, however, there exists neither a satisfactory characterization of positive bases - PSSs that are inclusion-wise minimal - nor a polynomial time algorithm for evaluating the cosine measure of a family of vectors.

In this manuscript, we examine each of these two problems through a theoretical study of the properties of positive spanning sets. First, we explore the relationships between network matrices of strongly connected digraphs and the matrix representations of PSSs. In doing so, we establish a new characterization of these families, which we refine to characterize positive bases. Next, we prove the existence of polynomial time algorithms able to determine the cosine measure of certain classes of positive bases. Using these families, we show that it is possible to construct resilient PSSs which preserve a satisfactory cosine measure upon losing some of their elements. Finally, we introduce a new direct-search algorithm, more robust than its predecessors, based on the use of such resilient PSSs.

KEYWORDS

Positive spanning set, positive basis, strongly connected digraph, cosine measure, Gale diagram, continuous optimization, derivative-free optimization, directional direct-search