Using orthogonally structured positive bases for constructing positive k-spanning sets with cosine measure guarantees

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Abstract

Positive spanning sets span a given vector space by nonnegative linear combinations of their elements. These have attracted significant attention in recent years, owing to their extensive use in derivative-free optimization. In this setting, the quality of a positive spanning set is assessed through its cosine measure, a geometric quantity that expresses how well such a set covers the space of interest. In this paper, we investigate the construction of positive k-spanning sets with geometrical guarantees. Our results build on recently identified positive spanning sets, called orthogonally structured positive bases. We first describe how to identify such sets and compute their cosine measures efficiently. We then focus our study on positive k-spanning sets, for which we provide a complete description, as well as a new notion of cosine measure that accounts for the resilient nature of such sets. 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.

Keywords Positive spanning sets; Positive k-spanning sets; Positive bases; Positive k-bases; Cosine measure; k-cosine measure; Derivative-free optimization.

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1 Introduction

Positive spanning sets, or PSSs, are sets of vectors that span a space of interest through non-negative linear combinations. These sets were first investigated by Davis [4], with a particular emphasis on inclusion-wise minimal PSSs, also called positive bases [4, 15]. Such a restriction guarantees bounds on the minimal and maximal size of a positive basis [1, 4]. PSSs of this form are now well understood in the literature [18]. Any positive basis is amenable to a decomposition into minimal positive bases over subspaces [21], a result that recently lead to the characterization of nicely structured positive bases [7], hereafter called orthogonally structured positive bases, or OSPBs.

Positive spanning sets and positive bases are now a standard tool to develop derivative-free optimization algorithms [5, 3]. The idea is to use directions from a PSS in replacement for derivative information. In that setting, it becomes critical to quantify how well directions from a PSS cover the space of interest, which is typically assessed through the cosine measure of this PSS [11, 10]. In general, no closed form expression is available for this cosine measure, yet various computing techniques have been proposed [6, 19]. In particular, a deterministic algorithm to compute the cosine measure of any PSS was recently proposed by Hare and Jarry-Bolduc [6]. The cosine measure of certain positive bases is known, along with upper bounds for positive bases of minimal and maximal sizes [16, 18]. The intermediate size case is less understood, even though recent progress was made in the case of orthogonally structured positive bases [7].

Meanwhile, another category of positive spanning sets introduced in the 1970s has received little attention in the literature. Those sets, called positive k-spanning sets (PkSSs), can be viewed as resilient PSSs, since at least k of their elements must be removed in order to make them lose their positively spanning property [12]. Unlike standard PSSs, only partial results are known regarding inclusion-wise minimal PkSS. These results depart from those for PSSs as they rely on polytope theory [13, 22]. Moreover, the construction of PkSSs based on PSSs has not been fully explored. To the best of our knowledge, the cosine measure of PkSSs has not been investigated, which partly prevents those sets from being used in derivative-free algorithms.

In this paper, we investigate positive k-spanning sets through the lens of orthogonally structured positive bases and cosine measure. To this end, we refine previous results on OSPBs so as to obtain an efficient cosine measure calculation technique. We then explain how the notion of cosine measure can be generalized to account for the positive k-spanning property, thereby introducing a quantity called the k-cosine measure. To the best of our knowledge, this definition is new in both the derivative-free optimization and the positive spanning set literature. By combining those elements, we are able to build positive k-spanning sets from OSPBs as well as to provide a bound on their k-cosine measures. Our results pave the way for using positive k-spanning sets in derivative-free algorithms.

The rest of this paper is organized as follows. Section 2 summarizes important properties of positive spanning sets, including their characterization through the cosine measure, with a particular focus on the subclass of orthogonally structured positive bases (OSPBs). Section 3 describes an efficient way to compute the cosine measure of an OSPB based on leveraging its decomposition. Section 4 formalizes the main properties associated with positive k-spanning sets, introduces the k-cosine measure to help studying these sets and uses OSPBs to design PkSSs with guaranteed k-cosine measure. Section 5 summarizes our findings and provides several perspectives of our work.

Notations Throughout this paper, we will work in the Euclidean space $\mathbb{R}^n$ with $n \geq 2$, or a linear subspace thereof, denoted by $\mathbb{L} \subset \mathbb{R}^n$. More generally, blackboard bold letters will be used to designate infinite-valued sets, such as linear (sub)spaces and half-spaces. The Minkowski sum $\{\mathbf{a} + \mathbf{b}, (\mathbf{a}, \mathbf{b}) \in \mathbb{A} \times \mathbb{B}\}$ of two spaces $\mathbb{A}$ and $\mathbb{B}$ will be denoted by $\mathbb{A} + \mathbb{B}$ or by $\mathbb{A} \perp \mathbb{B}$ if the two spaces are orthogonal to one another. The orthogonal to a given subspace $\mathbb{A}$ will be denoted accordingly by $\mathbb{A}^\perp$. In order to allow for repetition among their elements, positive spanning sets will be seen as families of vectors. We will use calligraphic letters such as $\mathcal{D}$ to denote finite families of vectors. Given a family $\mathcal{D} \subset \mathbb{R}^n$, the linear span of this family (*i.e.* the set of linear combinations of its elements) will be denoted by $\operatorname{span}(\mathcal{D})$. Bold lowercase (resp. uppercase) letters will be used to designate vectors (resp. matrices). 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 $\mathcal{I}_n := \{\mathbf{e}_1, \dots, \mathbf{e}_n\}$ will denote the family formed by coordinate basis vectors in $\mathbb{R}^n$. Given a family $\mathcal{D}_a$ of vectors in $\mathbb{R}^n$, we will use $\mathbf{D}_a$ to denote a matrix with n rows and whose columns correspond to the elements in $\mathcal{D}_a$, in no particular order unless otherwise stated. We will use $\mathcal{D}_a \setminus \{\mathbf{d}\}$ to denote a family obtained from $\mathcal{D}$ by removing exactly **one** instance of the vector $\mathbf{d}$. For instance, $\{\mathbf{d}, \mathbf{d}, \mathbf{d}'\} \setminus \{\mathbf{d}\} = \{\mathbf{d}, \mathbf{d}'\}$. Finally, the notation $[\![1, m]\!]$ will refer to the set $\{1, \dots, m\}$.

2 Background on positive spanning sets

In this section, we introduce the main concepts and results on positive spanning sets that will be used throughout the paper. Section 2.1 defines positive spanning sets and positive bases. Section 2.2 introduces the concept of orthogonally structured positive bases, that were first studied under a different name [7]. Section 2.3 provides the definition of the cosine measure of a positive spanning set, along with its value for several commonly used positive bases.

2.1 Positive spanning sets and positive bases

In this section, we recall the definitions of positive spanning sets and positive bases, based on the seminal paper of Davis [4].

Definition 2.1 (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 family of vectors $\mathcal{D} = \{\mathbf{d}_1, \mathbf{d}_2, \cdots, \mathbf{d}_m\}$ in $\mathbb{L}$, denoted* $\operatorname{pspan}(\mathcal{D})$, *is the set*

$$\operatorname{pspan}(\mathcal{D}) := \{\mathbf{u} \in \mathbb{L} : \mathbf{u} = \alpha_1 \mathbf{d}_1 + \cdots + \alpha_m \mathbf{d}_m \mid \forall i \in [\![1, m]\!], \alpha_i \geq 0\}.$$

A positive spanning set *(PSS) of $\mathbb{L}$ is a family of vectors $\mathcal{D}$ such that* $\operatorname{pspan}(\mathcal{D}) = \mathbb{L}$.

When $\mathbb{L}$ is not specified, a positive spanning set is understood as positively spanning $\mathbb{R}^n$. Throughout the paper, we only consider positive spanning sets formed of nonzero vectors. Note, however, that we do not force all elements of a positive spanning set to be distinct. The next two lemmas are well known and describe basic properties of positive spanning sets.

Lemma 2.1 [18, Theorem 2.5] *Let $\mathcal{D}$ be a finite set of vectors in a subspace $\mathbb{L}$ of $\mathbb{R}^n$. The following statements are equivalent:*

(i) $\mathcal{D}$ is a PSS of $\mathbb{L}$.

(ii) For every nonzero vector $\mathbf{u} \in \mathbb{L}$, there exists an element $\mathbf{d} \in \mathcal{D}$ such that $\mathbf{u}^\top \mathbf{d} > 0$.

*(iii) span$(\mathcal{D}) = \mathbb{L}$ and $\mathbf{0}_n$ can be written as a **positive** linear combination of the elements of $\mathcal{D}$.*

Lemma 2.2 [4, Theorem 3.7] *If $\mathcal{D}$ is a PSS of $\mathbb{L}$, then for any $\mathbf{d} \in \mathcal{D}$ the set $\mathcal{D} \backslash \{\mathbf{d}\}$ linearly spans $\mathbb{L}$.*

Note that Lemma 2.2 implies that a PSS must contain at least $\dim(\mathbb{L}) + 1$ vectors. There is no upper bound on the number of elements that a PSS may contain, but such a restriction holds for a subclass of positive spanning sets called positive bases.

Definition 2.2 (Positive basis) *Let $\mathbb{L}$ be a linear subspace of $\mathbb{R}^n$ of dimension $\ell \geq 1$. A* positive basis *of $\mathbb{L}$ of size $\ell + s$, denoted $\mathcal{D}_{\mathbb{L},s}$, is a PSS of $\mathbb{L}$ with $\ell + s$ elements satisfying:*

$$\forall \mathbf{d} \in \mathcal{D}_{\mathbb{L},s}, \quad \text{pspan}\left(\mathcal{D}_{\mathbb{L},s} \backslash \{\mathbf{d}\}\right) \neq \mathbb{L}.$$

When $\mathbb{L} = \mathbb{R}^n$, such a set will be denoted by $\mathcal{D}_{n,s}$.

In other words, positive bases of $\mathbb{L}$ are inclusion-wise minimal positive spanning sets of $\mathbb{L}$ [3]. Positive bases can also be defined thanks to the notion of positive independence.

Definition 2.3 (Positive independence) *Let $\mathbb{L}$ be a linear subspace of $\mathbb{R}^n$ of dimension $\ell \geq 1$. A family of vectors $\mathcal{D}$ in $\mathbb{L}$ is* positively independent *if, for any $\mathbf{d} \in \mathcal{D}$, there exists a vector $\mathbf{u} \in \mathbb{L}$ such that $\mathbf{u}^\top \mathbf{d} > 0$ and $\mathbf{u}^\top \mathbf{v} \leq 0$ for any $\mathbf{v} \in \mathcal{D} \setminus \{\mathbf{d}\}$.*

A positive basis of $\mathbb{L}$ is thus a positively independent PSS of $\mathbb{L}$.In the case $\mathbb{L} = \mathbb{R}^n$, we simply say that $\mathcal{D}_{n,s}$ is a positive basis (of size $n + s$).

One can show that the size of a positive basis of a subspace $\mathbb{L}$ is at least $\dim(\mathbb{L}) + 1$ and at most $2\dim(\mathbb{L})$ [2, 4].

Definition 2.4 *Let $\mathbb{L}$ be a linear subspace of $\mathbb{R}^n$ of dimension $\ell \geq 1$ and $1 \leq s \leq \ell$. A positive basis $\mathcal{D}_{\mathbb{L},s}$ of $\mathbb{L}$ is called* minimal *if $s = 1$, in which case we denote it by $\mathcal{D}_{\mathbb{L}} = \mathcal{D}_{\mathbb{L},1}$. The positive basis is called* maximal *if $s = \ell$. If $1 < s < \ell$, we say that the positive basis has* intermediate size.

Maximal and minimal positive bases have a well-understood structure [2, 17]. The structure of an arbitrary positive basis can however be quite complicated to analyze. In the next section, we describe a decomposition formula for positive bases that identifies a favorable structure.

2.2 Orthogonally structured positive bases

A complete characterization of positive bases can be provided through a subspace decomposition [21]. Such a decomposition is based upon the concept of critical vectors defined below.

Definition 2.5 (Critical vectors) *Let $\mathbb{L}$ be a subspace of $\mathbb{R}^n$ and $\mathcal{D}_{\mathbb{L},s}$ be a positive basis of $\mathbb{L}$. A vector $\mathbf{c} \in \mathbb{L}$ is called a* critical vector *of $\mathcal{D}_{\mathbb{L},s}$ if it cannot replace an element of $\mathcal{D}_{\mathbb{L},s}$ to form a positive spanning set, i.e.*

$$\forall \mathbf{d} \in \mathcal{D}_{\mathbb{L},s}, \quad \text{pspan}\left((\mathcal{D}_{\mathbb{L},s} \setminus \{\mathbf{d}\}) \cup \{\mathbf{c}\}\right) \neq \mathbb{L}.$$

Note that the zero vector is a critical vector for every positive basis of $\mathbb{L}$, and that it is the only critical vector for a maximal positive basis [21]. Moreover, if $\mathcal{D}_{\mathbb{L}}$ is a minimal positive basis and $\dim(\mathbb{L}) \geq 2$, the set of critical vectors (known as the complete critical set) is given by

$$-\bigcup_{i \neq j} \operatorname{pspan}\left(\mathcal{D}_{\mathbb{L}} \setminus \{\mathbf{d}_i, \mathbf{d}_j\}\right).$$

Using critical vectors, one may decompose any positive basis as a union of minimal positive bases. Theorem 2.1 gives the result for a positive basis in $\mathbb{R}^n$, by adapting the original decomposition result due to Romanowicz [21, Theorem 1] (see also [7, Lemma 25]).

Theorem 2.1 (Structure of a positive basis) *Suppose that $n \geq 2$, $s \geq 1$, and consider a positive basis $\mathcal{D}_{n,s}$ of $\mathbb{R}^n$. Then, either $s = 1$ or there exist subspaces $\mathbb{L}_1, \dots, \mathbb{L}_s$ of $\mathbb{R}^n$ such that $\mathbb{R}^n = \mathbb{L}_1 + \mathbb{L}_2 + \cdots + \mathbb{L}_s$ and $\mathbb{L}_i \cap \mathbb{L}_j = \{\mathbf{0}\}$ for any $i \neq j$, and there exist s associated minimal positive bases $\mathcal{D}_{\mathbb{L}_1}, \dots, \mathcal{D}_{\mathbb{L}_s}$ such that*

$$\mathcal{D}_{n,s} \;=\; \mathcal{D}_{\mathbb{L}_1} \cup (\mathcal{D}_{\mathbb{L}_2} + \mathbf{c}_1) \cup \cdots \cup (\mathcal{D}_{\mathbb{L}_s} + \mathbf{c}_{s-1}), \tag{1}$$

where for any $j = 1, \dots, s-1$, we let $\mathcal{D}_{\mathbb{L}_{j+1}} + \mathbf{c}_j := \left\{\mathbf{d} + \mathbf{c}_j \;\middle|\; \mathbf{d} \in \mathcal{D}_{\mathbb{L}_{j+1}}\right\}$, and the vector $\mathbf{c}_j \in \mathbb{L}_1 + \cdots + \mathbb{L}_j$ is a critical vector for $\mathcal{D}_{\mathbb{L}_1} \cup \bigcup_{i=2}^{j} (\mathcal{D}_{\mathbb{L}_i} + \mathbf{c}_{i-1})$.

The result of Theorem 2.1 is actually an equivalence, in that any set that admits the decomposition (1) is a non-minimal positive basis of $\mathbb{R}^n$ [21, Theorem 1]. The example below provides an illustration for both Definition 2.5 and Theorem 2.1. One can easily check that the stated vector is indeed critical, and that the proposed decomposition matches (1).

Example 2.1 *Consider the following positive basis of $\mathbb{R}^4$:*

$$\mathcal{D}_{4,2} = \left\{ \begin{bmatrix}1\\0\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\\0\end{bmatrix}, \begin{bmatrix}-1\\-1\\2\\2\end{bmatrix}, \begin{bmatrix}1\\1\\-4\\-4\end{bmatrix} \begin{bmatrix}0\\0\\1\\0\end{bmatrix}, \begin{bmatrix}0\\0\\0\\1\end{bmatrix} \right\}.$$

The first four vectors of this set form a minimal positive basis for $\{[x\ y\ z\ z]^\top, (x,y,z) \in \mathbb{R}^3\}$ that admits $[0\ 0\ 0.5\ 0.5]^\top$ as a critical vector. Therefore, a decomposition of the form (1) for $\mathcal{D}_{4,2}$ is:

$$\mathcal{D}_{4,2} = \left\{ \begin{bmatrix}1\\0\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\\0\end{bmatrix}, \begin{bmatrix}-1\\-1\\2\\2\end{bmatrix}, \begin{bmatrix}1\\1\\-4\\-4\end{bmatrix} \right\} \bigcup \left(\left\{ \begin{bmatrix}0\\0\\0.5\\-0.5\end{bmatrix}, \begin{bmatrix}0\\0\\-0.5\\0.5\end{bmatrix} \right\} + \left\{ \begin{bmatrix}0\\0\\0.5\\0.5\end{bmatrix} \right\} \right).$$

In general, however, the decomposition (1) is hard to compute, 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 [7], leading to Definition 2.6 below.

Definition 2.6 (Orthogonally structured positive bases) *Suppose that $n \geq 2$, and consider a positive basis $\mathcal{D}_{n,s}$ of $\mathbb{R}^n$. If there exist subspaces $\mathbb{L}_1, \dots, \mathbb{L}_s$ of $\mathbb{R}^n$ such that $\mathbb{R}^n = \mathbb{L}_1 \perp \mathbb{L}_2 \perp \cdots \perp \mathbb{L}_s$ and associated minimal positive bases $\mathcal{D}_{\mathbb{L}_1}, \dots, \mathcal{D}_{\mathbb{L}_s}$ such that*

$$\mathcal{D}_{n,s} \;=\; \mathcal{D}_{\mathbb{L}_1} \cup \mathcal{D}_{\mathbb{L}_2} \cup \cdots \cup \mathcal{D}_{\mathbb{L}_s}, \tag{2}$$

then $\mathcal{D}_{n,s}$ is called an orthogonally structured positive basis*, or OSPB.*

By construction, note that for any $1 \leq i < j \leq s$, any pair of elements $(\mathbf{d}, \mathbf{d}') \in \mathcal{D}_{\mathbb{L}_i} \times \mathcal{D}_{\mathbb{L}_j}$ 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 [7]. As will be shown in Section 3, it is also possible to compute their cosine measure in an efficient manner.

2.3 The cosine measure

To end this background section, we define the cosine measure, a metric associated with a given family of vectors.

Definition 2.7 (Cosine measure and cosine vector set) *Let $\mathcal{D}$ be a family of nonzero vectors in $\mathbb{R}^n$. The* cosine measure *of $\mathcal{D}$ is given by*

$$\operatorname{cm}(\mathcal{D}) = \min_{\substack{\|\mathbf{u}\|=1 \\ \mathbf{u} \in \mathbb{R}^n}} \max_{\mathbf{d} \in \mathcal{D}} \frac{\mathbf{u}^\top \mathbf{d}}{\|\mathbf{d}\|}.$$

The cosine vector set *associated with $\mathcal{D}$ is given by*

$$c\mathcal{V}(\mathcal{D}) = \operatorname*{arg\,min}_{\substack{\|\mathbf{u}\|=1 \\ \mathbf{u} \in \mathbb{R}^n}} \max_{\mathbf{d} \in \mathcal{D}} \frac{\mathbf{u}^\top \mathbf{d}}{\|\mathbf{d}\|}.$$

The cosine measure and cosine vector set provide insights on the geometry of the elements of $\mathcal{D}$ in the space. Such concepts are of particular interest in the case of positive spanning sets, as shown by the result of Proposition 2.1. Its proof can be found in key references in derivative-free optimization [2, 3], but note that our analysis in Section 4 provides a more general proof in the context of positive k-spanning sets.

Proposition 2.1 *Let $\mathcal{D}$ be a finite family of vectors in $\mathbb{R}^n$. Then $\mathcal{D}$ is a positive spanning set in $\mathbb{R}^n$ if and only if $\operatorname{cm}(\mathcal{D}) > 0$.*

Proposition 2.1 shows that the positive spanning property can be checked by computing the cosine measure. The value of the cosine measure further characterizes how well that set covers the space, which is a relevant information in derivative-free algorithms [10]. Both observations motivate the search for efficient techniques to compute the cosine measure.

We end this section by providing several examples of cosine measures for orthogonally structured positive bases, that form the core interest of this paper. We focus on building those positive bases from the coordinate vectors. A classical choice for a maximal positive basis consists in selecting the coordinate vectors and their negatives. In that case, it is known [16] that

$$\mathrm{cm}\left(\mathcal{I}_n \cup -\mathcal{I}_n\right) = \mathrm{cm}\left(\{\mathbf{e}_1,\dots,\mathbf{e}_n,-\mathbf{e}_1,\dots,-\mathbf{e}_n\}\right) = \frac{1}{\sqrt{n}}.$$

One can also consider a minimal positive basis formed by the coordinate vectors and the sum of their negatives. Then, we have

$$\mathrm{cm}\left(\mathcal{I}_n \cup \left\{-\sum_{i=1}^n \mathbf{e}_i\right\}\right) = \mathrm{cm}\left(\left\{\mathbf{e}_1,\dots,\mathbf{e}_n,-\sum_{i=1}^n \mathbf{e}_i\right\}\right) = \frac{1}{\sqrt{n^2+2(n-1)\sqrt{n}}}.$$

To the best of our knowledge, the latter formula has only been recently established in [9, 20], and no formal proof is available in the literature. In the next section, we will develop an efficient cosine measure calculation technique for orthogonally structured positive bases that will provide a proof of this result as a byproduct.

3 Computing OSPBs and their cosine measure

In this section, we describe how orthogonally structured positive bases can be identified using the decomposition introduced in the previous section. We also leverage this decomposition to design algorithms for detecting the OSPB structure and computing the cosine measure of a given OSPB.

3.1 Structure and detection of OSPBs

The favorable structure of an OSPB can be revealed through the properties of its matrix representations, and in particular the Gram matrices associated with an OSPB, in the sense of Definition 3.1 below.

Definition 3.1 (Gram matrix) *Let $\mathcal{S}$ be a finite family of m vectors in $\mathbb{R}^n$ and $\mathbf{S} \in \mathbb{R}^{n\times m}$ a matrix representation of this family. The Gram matrix of $\mathcal{S}$ associated with $\mathbf{S}$ is the matrix $\mathbf{G}(\mathbf{S}) = \mathbf{S}^\top \mathbf{S}$.*

Given a Gram matrix $\mathbf{G}(\mathbf{S})$ of $\mathcal{S}$, any Gram matrix of $\mathcal{S}$ has the form $\mathbf{P}^\top\mathbf{G}(\mathbf{S})\mathbf{P}$ where $\mathbf{P}$ is a permutation matrix. We will show that when $\mathcal{S}$ is an OSPB, there exists a Gram matrix with a block-diagonal structure that reveals the decomposition of the basis, and thus its OSPB nature.

Theorem 3.1 *Let $n \geq 2$, $s \geq 2$ and $\mathcal{D}_{n,s} \subset \mathbb{R}^n$ be a positive basis. Then, $\mathcal{D}_{n,s}$ is orthogonally structured if and only if one of its Gram matrices $\mathbf{G}(\mathcal{D}_{n,s})$ can be written as a block diagonal matrix with s diagonal blocks.*

Proof. Suppose first that $\mathcal{D}_{n,s}$ is an OSPB associated to the decomposition

$$\mathcal{D}_{n,s} = \mathcal{D}_{\mathbb{L}_1} \cup \mathcal{D}_{\mathbb{L}_2} \cup \cdots \cup \mathcal{D}_{\mathbb{L}_s}.$$

Let $\mathbf{D}_{n,s}$ be a matrix representation of $\mathcal{D}_{n,s}$ such that $\mathbf{D}_{n,s} = \begin{bmatrix}\mathbf{D}_{\mathbb{L}_1} & \dots & \mathbf{D}_{\mathbb{L}_s}\end{bmatrix}$, where $\mathbf{D}_{\mathbb{L}_i}$ is a matrix representation of $\mathcal{D}_{\mathbb{L}_i}$ for every $i = 1,\dots,s$. By orthogonality of those matrices, 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 matrix representation $\mathbf{D}_{n,s}$ of $\mathcal{D}_{n,s}$ such that $\mathbf{G}(\mathbf{D}_{n,s})$ is block diagonal with s blocks. Then, by considering a partitioning with respect to those diagonal blocks, one can decompose $\mathbf{D}_{n,s}$ into $\begin{bmatrix}\mathbf{S}_1 & \dots & \mathbf{S}_s\end{bmatrix}$ so that $\mathbf{G}(\mathbf{D}_{n,s}) = \operatorname{diag}(\mathbf{G}(\mathbf{S}_1), \dots, \mathbf{G}(\mathbf{S}_s))$. By definition of the Gram matrix, this structure implies that the columns of $\mathbf{S}_i$ and $\mathbf{S}_j$ are orthogonal for any $i \neq j$, thus we only need to show that each $\mathbf{S}_i$ is a minimal positive basis for its linear span. To this end, we use the fact that $\mathcal{D}_{n,s}$ is positively spanning. By Lemma 2.1(ii), there exists a vector $\mathbf{u} \in \mathbb{R}^{n+s}$ with positive coefficients such that $\mathbf{D}_{n,s}\mathbf{u} = \mathbf{0}_n$. By decomposing the vector $\mathbf{u}$ into s vectors $\mathbf{u}_1, \dots, \mathbf{u}_s$ according to the decomposition $\begin{bmatrix}\mathbf{S}_1 & \dots & \mathbf{S}_s\end{bmatrix}$, we obtain that

$$\mathbf{D}_{n,s}\mathbf{u} = \sum_{i=1}^{n} \mathbf{S}_i \mathbf{u}_i = \mathbf{0}_n. \tag{3}$$

By orthogonality of the $\mathbf{S}_i$ matrices, the property (3) is equivalent to

$$\mathbf{S}_i \mathbf{u}_i = \mathbf{0}_n \ \forall i = 1, \dots, s.$$

Using again Lemma 2.1(ii), this latter property is equivalent to $\mathcal{S}_i$ being a PSS for its linear span. Let n_i be the dimension of this span, and m_i the number of elements in $\mathcal{S}_i$. Since the $\mathbf{S}_i$ are orthogonal and the columns of $\mathbf{D}_{n,s}$ span $\mathbb{R}^n$, 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 $i \in [\![1, s]\!]$, we conclude that $m_i = n_i + 1$, and thus every $\mathcal{S}_i$ is a minimal positive basis. $\square$

Note that the characterization stated by Theorem 3.1 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 3.1 *Let $n \geq 2$, $s \geq 1$ and $\mathcal{D}_{n,s}$ be a positive basis in $\mathbb{R}^n$. Let $\mathbf{D}_{n,s}$ be a matrix representation of $\mathcal{D}_{n,s}$. If there exists a permutation matrix $\mathbf{P} \in \mathbb{R}^{(n+s)\times(n+s)}$ such that the Gram matrix $\mathbf{G}(\mathbf{D}_{n,s}\mathbf{P})$ is block diagonal with s blocks, then $\mathcal{D}_{n,s}$ is an OSPB, and its decomposition* (2) *is given by the columns of $\mathbf{D}_{n,s}\mathbf{P}$ in that order.*

Corollary 3.1 provides a principled way of detecting the OSPB structure, by checking all possible permutations of the elements in the 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 non-zero 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 [14] and can be solved in polynomial time [8].

3.2 Cosine measure of an orthogonally structured positive basis

As seen in the previous section, orthogonally structured positive bases admit a decomposition into minimal positive bases that are orthogonal to one another. In this section, we investigate how this particular structure allows for efficient computation of the cosine measure.

Our approach builds on the algorithm introduced by Hare and Jarry-Bolduc [6], 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 consists of a loop over all possible linear bases contained in the positive spanning set. More formally, given a positive spanning set $\mathcal{D}$ in $\mathbb{R}^n$ and a linear basis $\mathcal{B} \subset \mathcal{D}$, we let $\mathbf{D}$ be a matrix representation of $\mathcal{D}$, and $\mathbf{B}$ the associated representation of $\mathcal{B}$. One then defines

$$\gamma_{\mathcal{B}} := \frac{1}{\sqrt{\mathbf{1}_n^\top \mathbf{G}(\mathbf{B})^{-1}\mathbf{1}_n}} \quad \text{and} \quad \mathbf{u}_{\mathcal{B}} := \gamma_{\mathcal{B}} \mathbf{B}^{-\top}\mathbf{1}_n. \tag{4}$$

The vector $\mathbf{u}_{\mathcal{B}}$ is the only unitary vector such that $\mathbf{u}_{\mathcal{B}}^\top \frac{\mathbf{d}}{\|\mathbf{d}\|} = \gamma_{\mathcal{B}}$ for all $\mathbf{d} \in \mathcal{B}$ [6, Lemmas 12 and 13]. Computing the quantities (4) for all linear bases contained in $\mathcal{D}$ then gives both the cosine measure and the cosine vector set for $\mathcal{D}$ [6, Theorem 19]. Indeed, we have

$$\mathrm{cm}\,(\mathcal{D}) = \min_{\substack{\mathcal{B} \subset \mathcal{D} \\ \mathcal{B} \textit{ basis of } \mathbb{R}^n}} \max_{\mathbf{d} \in \mathcal{D}} \mathbf{u}_{\mathcal{B}}^\top \frac{\mathbf{d}}{\|\mathbf{d}\|}, \tag{5}$$

while the cosine vector set is given by

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

The next proposition shows how, when dealing with OSPBs, formula (5) can be simplified to give a more direct link between the quantities $\gamma_{\mathcal{B}}$ and the cosine measure.

Proposition 3.1 *Let $\mathcal{D}_{n,s}$ be an OSPB of $\mathbb{R}^n$ and $\mathcal{D}_{\mathbb{L}_1}, \dots, \mathcal{D}_{\mathbb{L}_s}$ be a decomposition of $\mathcal{D}_{n,s}$ into minimal positive bases. Then,*

$$\mathrm{cm}\,(\mathcal{D}_{n,s}) = \min_{\substack{\mathcal{B}_n \subset \mathcal{D}_{n,s} \\ \mathcal{B}_n \textit{ basis of } \mathbb{R}^n}} \gamma_{\mathcal{B}_n} \quad \textit{and} \quad c\mathcal{V}(\mathcal{D}_{n,s}) = \{\mathbf{u}_{\mathcal{B}_n} : \gamma_{\mathcal{B}_n} = \mathrm{cm}\,(\mathcal{D}_{n,s})\},$$

where $\gamma_{\mathcal{B}_n}$ and $\mathbf{u}_{\mathcal{B}_n}$ are computed according to (4).

Proof. Using the decomposition of $\mathcal{D}_{n,s}$, any linear basis $\mathcal{B}_n$ of $\mathbb{R}^n$ contained in $\mathcal{D}_{n,s}$ can be decomposed as $\mathcal{B}_n = \mathcal{B}_{\mathbb{L}_1} \cup \cdots \cup \mathcal{B}_{\mathbb{L}_s}$ where $\mathcal{B}_{\mathbb{L}_i} \subset \mathcal{D}_{\mathbb{L}_i}$ is a linear basis of $\mathbb{L}_i$. By construction, the vector $\mathbf{u}_{\mathcal{B}_n}$ makes a positive dot product with every element of $\mathcal{B}_n$ (and thus with every element of any $\mathcal{B}_{\mathbb{L}_i}$) equal to γ_n. Consequently, the vector $\mathbf{u}_{\mathcal{B}_n}$ lies in the positive span of $\mathcal{B}_n$, and its projection on any subspace $\mathbb{L}_i$ lies in the positive span of $\mathcal{B}_{\mathbb{L}_i}$.

Meanwhile, for any $i \in [\![1, s]\!]$, there exists $\mathbf{d}_i \in \mathcal{D}_{\mathbb{L}_i}$ such that $\mathcal{B}_{\mathbb{L}_i} = \mathcal{D}_{\mathbb{L}_i} \setminus \{\mathbf{d}_i\}$, and this vector satisfies $\mathbf{u}_{\mathcal{B}_n}^\top \mathbf{d}_i < 0$ per Lemma 2.1(*ii*), leading to

$$\max_{\mathbf{d} \in \mathcal{D}_n} \frac{\mathbf{u}_{\mathcal{B}_n}^\top \mathbf{d}}{\|\mathbf{d}\|} = \max_{i \in [\![1,s]\!]} \left\{ \max_{\mathbf{d} \in \mathcal{D}_{\mathbb{L}_i}} \frac{\mathbf{u}_{\mathcal{B}_n}^\top \mathbf{d}}{\|\mathbf{d}\|} \right\} = \max_{i \in [\![1,s]\!]} \left\{ \max_{\mathbf{d} \in \mathcal{B}_{\mathbb{L}_i}} \frac{\mathbf{u}_{\mathcal{B}_n}^\top \mathbf{d}}{\|\mathbf{d}\|} \right\} = \max_{\mathbf{d} \in \mathcal{B}_n} \frac{\mathbf{u}_{\mathcal{B}_n}^\top \mathbf{d}}{\|\mathbf{d}\|} = \gamma_n,$$

where the second equality comes from $\mathbf{u}_{\mathcal{B}_n}^\top \mathbf{d}_i < 0$ and $\max_{\mathbf{d} \in \mathcal{D}_n} \mathbf{u}_{\mathcal{B}_n}^\top \mathbf{d} > 0$, and the last equality holds by definition of γ_n. Recalling that $\mathrm{cm}\,(\mathcal{D}_n)$ is given by (5) concludes the proof. □

One drawback of the approach described so far is that it requires to compute the quantities (4) for all linear bases including 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 3.2 *Let $\mathcal{D}_{n,s}$ be an OSPB of $\mathbb{R}^n$ and $\mathcal{D}_{\mathbb{L}_1}, \ldots, \mathcal{D}_{\mathbb{L}_s}$ be a decomposition of $\mathcal{D}_{n,s}$ into minimal positive bases. Let $\mathcal{B}_n$ be a linear basis contained in $\mathcal{D}_{n,s}$ such that $\mathcal{B}_n = \cup_{i=1}^s \mathcal{B}_{\mathbb{L}_i}$, where every $\mathcal{B}_{\mathbb{L}_i}$ is a linear basis of the subspace corresponding to $\mathcal{D}_{\mathbb{L}_i}$. For each basis $\mathcal{B}_{\mathbb{L}_i}$, define*

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

where $\mathbf{B}_{\mathbb{L}_i}$ is a matrix representation of $\mathcal{B}_{\mathbb{L}_i}$ and $\mathbf{1}_{\mathbb{L}_i}$ denotes the vector of all ones in $\mathbb{R}^{\dim(\mathbb{L}_i)}$. Then,

$$\gamma_{\mathcal{B}_n} = \frac{1}{\sqrt{\sum_{i=1}^s \gamma_{\mathcal{B}_{\mathbb{L}_i}}^{-2}}} = \frac{1}{\sqrt{\sum_{i=1}^s \mathbf{1}_{\mathbb{L}_i}^\top \mathbf{G}(\mathbf{B}_{\mathbb{L}_i})^{-1} \mathbf{1}_{\mathbb{L}_i}}}, \tag{6}$$

with $\gamma_{\mathcal{B}_n}$ being defined as in (4).

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

$$\operatorname{cm}(\mathcal{D}_{n,s}) = \frac{1}{\sqrt{\sum_{i=1}^s \max_{\mathbf{d}_i \in \mathcal{D}_{\mathbb{L}_i}} \gamma_{\mathcal{D}_{\mathbb{L}_i} \setminus \{\mathbf{d}_i\}}^{-2}}} \tag{7}$$

and

$$c\mathcal{V}(\mathcal{D}_{n,s}) = \left\{ \mathbf{u}_{\mathcal{B}_n} : \mathcal{B}_n = \cup_{i=1}^s \mathcal{B}_{\mathbb{L}_i}, \quad \mathbf{u}_{\mathcal{B}_n} = \frac{[\mathbf{B}_{\mathbb{L}_1} \ \cdots \ \mathbf{B}_{\mathbb{L}_s}]^{-\top} \mathbf{1}_n}{\sqrt{\sum_{i=1}^s \gamma_{\mathcal{B}_{\mathbb{L}_i}}^{-2}}} \right\} \tag{8}$$

respectively.

Proof. Let $\mathbf{B}_n$ be a matrix representation of $\mathcal{B}_n$ such that $\mathbf{B}_n = \left[\mathbf{B}_{\mathbb{L}_1} \cdots \mathbf{B}_{\mathbb{L}_s}\right]$. Then, the Gram matrix of $\mathbf{B}_n$ is $\mathbf{G}(\mathbf{B}_n) = \operatorname{diag}(\mathbf{G}(\mathbf{B}_{\mathbb{L}_1}), \cdots, \mathbf{G}(\mathbf{B}_{\mathbb{L}_s}))$, implying that

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

which proves (6).

Recall now that every linear basis $\mathcal{B}_{\mathbb{L}_i}$ can be written as $\mathcal{D}_{\mathbb{L}_i} \setminus \{\mathbf{d}_i\}$ for some $\mathbf{d}_i \in \mathcal{D}_{\mathbb{L}_i}$. Combining this property together with (6) and Proposition 3.1, we obtain

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

proving (7).

Finally, combining (7) with the result of Proposition 3.1 on the cosine vector set gives

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

Using a matrix representation $\mathbf{B}_n = \left[\mathbf{B}_{\mathbb{L}_1} \cdots \mathbf{B}_{\mathbb{L}_s}\right]$ along with the formula (4) for $\mathbf{u}_{\mathcal{B}_n}$ leads to

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

which is precisely (8). □

On a broader level, Theorem 3.2 shows that any calculation for a linear basis contained in an OSPB reduces to calculations on bases contained in 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 $\mathcal{D}_{n,s}$ of $\mathbb{R}^n$ with normalized vectors.

2 **Step 1.** Compute a decomposition $\mathcal{D}_{n,s} = \mathcal{D}_{\mathbb{L}_1} \cup \cdots \cup \mathcal{D}_{\mathbb{L}_s}$ of $\mathcal{D}_{n,s}$ into s minimal positive bases $\mathcal{D}_{\mathbb{L}_i}$ on subspaces of $\mathbb{R}^n$.

3 **Step 2.** For every $i \in [\![1, s]\!]$, compute

$$\beta_{\mathbb{L}_i} = \max_{\mathbf{d}\in\mathcal{D}_{\mathbb{L}_i}} \gamma_{\mathcal{D}_{\mathbb{L}_i}\setminus\{\mathbf{d}\}}^{-2} \quad \text{and} \quad \mathcal{A}_i = \operatorname*{arg\,max}_{\mathbf{d}\in\mathcal{D}_{\mathbb{L}_i}} \gamma_{\mathcal{D}_{\mathbb{L}_i}\setminus\{\mathbf{d}\}}^{-2}.$$

For all $\mathbf{d} \in \mathcal{A}_i$, note $\mathcal{B}_{\mathbb{L}_i}^{(\mathbf{d})} = \mathcal{D}_{\mathbb{L}_i} \setminus \{\mathbf{d}\}$.

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

$$\mathrm{cm}\,(\mathcal{D}_{n,s}) = \frac{1}{\sqrt{\sum_{i=1}^{s}\beta_{\mathbb{L}_i}}} \tag{9}$$

and the cosine vector set

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

where $\mathbf{B}_{\mathbb{L}_i}^{(\mathbf{d})}$ is a matrix representation of $\mathcal{B}_{\mathbb{L}_i}^{(\mathbf{d})}$.

In essence, Algorithm 1 is quite similar to the generic method proposed for positive spanning sets [6]. 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 $\mathcal{D}_{\mathbb{L}_i}$ involved in the decomposition, the algorithm considers $|\mathcal{D}_{\mathbb{L}_i}|$ positive bases, and computes the quantities of interest (4) for each of those (which amounts to inverting or solving a linear system involving the associated Gram matrix). Overall, Algorithm 1 thus checks $\sum_{i=1}^{s} |\mathcal{D}_{\mathbb{L}_i}| = |\mathcal{D}_{n,s}| = n + s$ bases to compute the cosine measure (9). This result represents a significant 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 [6]. We also recall from Section 3.1 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 $\mathcal{I}_n \cup \{-\mathbf{1}_n\}$. In this case, the calculation becomes easy thanks to the orthogonality of the vectors within $\mathcal{I}_n \cup \{-\mathbf{1}\}$. Although the value (10) was recently stated [9, 20] and checked numerically using the method of Hare and Jarry-Bolduc [6], to the best of our knowledge the formal proof below is new.

Lemma 3.1 *The cosine measure of the OSPB $\mathcal{I}_n \cup \{-\mathbf{1}_n\}$ is given by*

$$\operatorname{cm}\left(\mathcal{I}_n \cup \{-\mathbf{1}_n\}\right) = \frac{1}{\sqrt{n^2 + 2(n-1)\sqrt{n}}}. \tag{10}$$

Proof. For sake of simplicity, we normalize the last vector in the set (which does not change the value of the cosine measure) and we let $\mathcal{D}_n = \mathcal{I}_n \cup \{-\frac{1}{\sqrt{n}}\mathbf{1}_n\}$ in the rest of the proof. Since $\mathcal{D}_n$ is a positive basis, it follows that

$$\operatorname{cm}\left(\mathcal{D}_n\right) = \min_{\mathbf{d} \in \mathcal{D}_n} \gamma_{\mathcal{D}_n \setminus \{\mathbf{d}\}},$$

Two cases are to be considered. Suppose first that $\mathbf{d} = -\frac{1}{\sqrt{n}}\mathbf{1}_n$, so that $\mathcal{D}_n \setminus \{\mathbf{d}\} = \mathcal{I}_n$. Then, any matrix representation of that basis $\mathbf{B}$ is such that $\mathbf{G}(\mathbf{B}) = \mathbf{I}_n$. Consequently,

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

Suppose now that $\mathbf{d} = \mathbf{e}_i$ for some $i \in [\![1, \ldots, n]\!]$. In that case, considering the matrix representation $\mathbf{B}_i = \begin{bmatrix} \mathbf{e}_1 & \cdots & \mathbf{e}_{i-1} & \mathbf{e}_{i+1} & \cdots & \mathbf{e}_n & -\frac{1}{\sqrt{n}}\mathbf{1}_n \end{bmatrix}$, 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 $i \in [\![1, n]\!]$, we have

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

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 $\gamma_{\mathcal{D}_n \setminus \{\mathbf{e}_i\}} = \frac{1}{\sqrt{n^2 + 2(n-1)\sqrt{n}}}$. 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 in the case of positive k-spanning sets.

4 Positive k-spanning sets and k-cosine measure

In this section, we are interested in positive spanning sets that retain their positively spanning ability when one or more of their elements are removed. Those sets were originally termed *positive k-spanning sets* [13], and we adopt the same terminology. Section 4.1 recalls the key definitions for positive k-spanning sets and positive k-bases, while Section 4.2 introduces the k-cosine measure, a generalization of the cosine measure from Section 2.3. Finally, Section 4.3 illustrates how to construct sets with guaranteed k-cosine measure based on OSPBs.

4.1 Positive k-spanning property

Our goal for this section is to provide a summary of results on positive k-spanning sets that mimic the standard ones for positive spanning sets. We start by defining the property of interest.

Definition 4.1 (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 finite family of vectors $\mathcal{D}$ in $\mathbb{L}$, denoted* $\operatorname{pspan}_k(\mathcal{D})$*, is the set*

$$\operatorname{pspan}_k(\mathcal{D}) := \bigcap_{\substack{\mathcal{S} \subset \mathcal{D} \\ |\mathcal{S}| \geq |\mathcal{D}|-k+1}} \operatorname{pspan}(\mathcal{S}).$$

A positive k-spanning set *(PkSS) of $\mathbb{L}$ is a family of vectors $\mathcal{D}$ such that* $\operatorname{pspan}_k(\mathcal{D}) = \mathbb{L}$.

As for Definition 2.1, when $\mathbb{L}$ is not specified, a PkSS should be understood as a PkSS of $\mathbb{R}^n$. By construction, any PkSS of $\mathbb{L}$ must contain a PSS of $\mathbb{L}$, and therefore is a PSS of $\mathbb{L}$ itself. Moreover, the notions of positive k-span and PkSS with $k = 1$ coincide with that of positive span and PSS from Definition 2.1. Similar to PSSs, we will omit the subspace of interest when $\mathbb{L} = \mathbb{R}^n$.

The notion of positive spanning set is inherently connected to that of spanning set, a standard concept in linear algebra. We provide below a counterpart notion associated with PkSSs.

Definition 4.2 (k-span and k-spanning set) *Let $\mathcal{D}$ be a finite family of vectors in $\mathbb{R}^n$. the* k-span *of $\mathcal{D}$, denoted* $\operatorname{span}_k(\mathcal{D})$*, is defined by*

$$\operatorname{span}_k(\mathcal{D}) \;=\; \bigcap_{\substack{\mathcal{S} \subset \mathcal{D} \\ |\mathcal{S}| \geq |\mathcal{D}|-k+1}} \operatorname{span}(\mathcal{S}).$$

Given a subspace $\mathbb{L}$ of $\mathbb{R}^n$, a k-spanning set *of $\mathbb{L}$ is a family of vectors $\mathcal{D}$ such that* $\operatorname{span}_k(\mathcal{D}) = \mathbb{L}$.

Using the two definitions above, we can generalize the results of Lemma 2.1 and Lemma 2.2 to positive k-spanning sets. The proof is omitted as it merely amounts to combining the definitions with these two lemmas.

Lemma 4.1 *Let $\mathbb{L}$ be a subspace of $\mathbb{R}^n$ and $\mathcal{D}$ a finite family of vectors in $\mathbb{L}$. Let $k \in \mathbb{N}$ satisfy $1 \leq k \leq |\mathcal{D}|$. The following statements are equivalent:*

(i) $\mathcal{D}$ is a PkSS of $\mathbb{L}$.

(ii) For any nonzero vector $\mathbf{u} \in \mathbb{L}$, there exist k elements $\mathbf{d}_1, \dots, \mathbf{d}_k$ of $\mathcal{D}$ such that $\mathbf{u}^\top \mathbf{d}_i > 0$ for all $i \in [\![1, k]\!]$.

(iii) $\text{span}_k(\mathcal{D}) = \mathbb{L}$ *and for any* $\mathcal{S} \subset \mathcal{D}$ *of cardinality* $|\mathcal{D}| - k + 1$*, the vector* $\mathbf{0}_n$ *can be written as a* ***positive*** *linear combination of the elements of* $\mathcal{S}$*.*

Lemma 4.2 *Let* $\mathbb{L}$ *be a subspace of* $\mathbb{R}^n$ *and let the finite set* $\mathcal{D}$ *be a PkSS for* $\mathbb{L}$*. Then, for any* $\mathbf{d} \in \mathcal{D}$*, the* k*-span of the family* $\mathcal{D} \setminus \{\mathbf{d}\}$ *is* $\mathbb{L}$*.*

The equivalence between statements (i) and (ii) from Lemma 4.1 motivates the term "positive k-spanning sets". Indeed, given a PkSS and a vector in the subspace it positively k-spans, there exist k elements of the PkSS that make an acute angle with that vector. Note however that the equivalence between statements (i) and (iii), as well as Definition 4.1, both provide an alternate characterization, namely that a PkSS is a PSS that retains this property when removing $k-1$ of its elements. This latter characterization implies that a PkSS must contain at least $n+k$ vectors, although this bound is only tight when $k=1$. Indeed, in [13, Corollary 5] it is shown that the minimal size of a positive k-spanning set in a subspace of dimension ℓ is $2k + \ell - 1$.

Throughout Section 2, 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.

Definition 4.3 (Positive k-basis) *Let* $\mathbb{L}$ *be a linear subspace of* $\mathbb{R}^n$*. A* positive k-basis *of* $\mathbb{L}$ *is a PkSS* $\mathcal{D}$ *of* $\mathbb{L}$ *satisfying*

$$\forall \mathbf{d} \in \mathcal{D}, \quad \text{pspan}_k \left(\mathcal{D} \setminus \{\mathbf{d}\}\right) \neq \mathbb{L}.$$

Positive k-bases can be thought as inclusion-wise minimal positive k-spanning sets (similarly to the characterization of positive bases from Section 2.1). We showed earlier how the notion of positive independence can be used to give an alternative definition for positive bases. Let us generalize this idea and introduce the concept of positive k-independence, used to characterize positive k-bases.

Definition 4.4 (Positive k-independence) *Let* $\mathbb{L}$ *be a linear subspace of* $\mathbb{R}^n$ *of dimension* $\ell \geq 1$ *and let* $k \geq 1$*. A family of vectors* $\mathcal{D}$ *in* $\mathbb{L}$ *is* positively k-independent *if* $|\mathcal{D}| \geq k$ *and, for any* $\mathbf{d} \in \mathcal{D}$*, there exists a vector* $\mathbf{u} \in \mathbb{L}$ *having a positive dot product with* ***exactly*** k *elements of* $\mathcal{D}$*, including* $\mathbf{d}$*.*

Using this new concept, positive k-bases can alternatively be defined as positively k-independent PkSSs. We mention in passing that the upper bound on the size of a positive k-basis has yet to be determined, though it is known to exceed $2k\ell$ for an ℓ-dimensional subspace [22].

4.2 The k-cosine measure

This section aims at generalizing the cosine measure from Section 2.3 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 4.5.

Definition 4.5 (k-cosine measure) *Let* $\mathcal{D}$ *be a finite family of nonzero vectors in* $\mathbb{R}^n$ *and let* $k \in \mathbb{N}$ *satisfy* $1 \leq k \leq |\mathcal{D}|$*. The* k-cosine measure *of* $\mathcal{D}$ *is given by*

$$\text{cm}_k\left(\mathcal{D}\right) = \min_{\substack{\|\mathbf{u}\|=1 \\ \mathbf{u} \in \mathbb{R}^n}} \max_{\substack{\mathcal{S} \subset \mathcal{D} \\ |\mathcal{S}|=k}} \min_{\mathbf{d} \in \mathcal{S}} \frac{\mathbf{u}^\top \mathbf{d}}{\|\mathbf{d}\|}.$$

The k-cosine vector set *associated with* $\mathcal{D}$ *is given by*

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

Note that Definition 2.7 is a special case of Definition 4.5 corresponding to $k = 1$. In its general form, this definition expresses how well the vectors of the family of interest are spread in the space through subsets of k vectors, which is related to property (*ii*) in Lemma 4.1. Our next result shows that this quantity characterizes PkSSs.

Theorem 4.1 *Let* $\mathcal{D}$ *be a finite family of vectors in* $\mathbb{R}^n$ *and let* $k \in \mathbb{N}$ *satisfy* $1 \leq k \leq |\mathcal{D}|$. *Then* $\mathcal{D}$ *is a positive* k*-spanning set in* $\mathbb{R}^n$ *if and only if* $\mathrm{cm}_k(\mathcal{D}) > 0$.

Proof. Without loss of generality we assume that all the elements of $\mathcal{D}$ are unit vectors.

Suppose first that $\mathcal{D}$ is a $PkSS$. Then, by Lemma 4.1, for any unit vector $\mathbf{u} \in \mathbb{R}^n$, there exist k vectors in $\mathcal{D}$ that make a positive dot product with $\mathbf{u}$. Let $\mathcal{S}_\mathbf{u}$ be a subset of $\mathcal{D}$ consisting of these k vectors. By construction, we have $\min_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d} > 0$ and thus

$$\max_{\substack{\mathcal{S}\subset\mathcal{D}\\ |\mathcal{S}|=k}} \min_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d} \geq \min_{\mathbf{d}\in\mathcal{S}_\mathbf{u}} \mathbf{u}^\top \mathbf{d} > 0.$$

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

Conversely, suppose that $\mathrm{cm}_k(\mathcal{D}) > 0$. Our goal is to show that $\mathcal{D}$ satisfies statement (*ii*) from Lemma 4.1. For any unit vector $\mathbf{u}$, we have by assumption that

$$\max_{\substack{\mathcal{S}\subset\mathcal{D}\\ |\mathcal{S}|=k}} \min_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d} > 0. \tag{11}$$

Let $\bar{\mathcal{S}}_1$ be a subset of $\mathcal{D}$ such that $|\bar{\mathcal{S}}_1| = |\mathcal{D}| - k + 1$. Then, (11) implies that

$$\max_{\substack{\mathcal{S}\subset\bar{\mathcal{S}}_1\\ |\mathcal{S}|=1}} \min_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d} = \max_{\mathbf{d}\in\bar{\mathcal{S}}_1} \mathbf{u}^\top \mathbf{d} > 0,$$

hence there exists a vector $\bar{\mathbf{d}}_1 \in \bar{\mathcal{S}}_1$ such that $\mathbf{u}^\top \bar{\mathbf{d}}_1 > 0$. Consider now a set $\bar{\mathcal{S}}_2$ such that $\bar{\mathcal{S}}_2 = |\mathcal{D}| - k + 1$ and $\bar{\mathbf{d}}_1 \notin \bar{\mathcal{S}}_2$. Applying the same reasoning as above shows that there must exist $\bar{\mathbf{d}}_2 \in \bar{\mathcal{S}}_2$ such that $\mathbf{u}^\top \bar{\mathbf{d}}_2 > 0$. Overall, we can repeat the process k times, showing that there must exist at least k elements of $\mathcal{D}$ that make a positive dot product with $\mathbf{u}$. Since the result applies to any unit vector, we have shown Lemma 4.1(*ii*), and thus that $\mathcal{D}$ is a PkSS. $\square$

As announced in Section 2.3, the proof of Theorem 4.1 covers that of Proposition 2.1 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 4.2 *Let* $\mathcal{D}$ *be a finite family of nonzero vectors in* $\mathbb{R}^n$ *and let* $k \in \mathbb{N}$ *satisfy* $1 \leq k \leq |\mathcal{D}|$. *Then,*

$$\mathrm{cm}_k(\mathcal{D}) = \min_{\substack{\mathcal{S}\subset\mathcal{D}\\ |\mathcal{S}|=|\mathcal{D}|-k+1}} \mathrm{cm}(\mathcal{S}). \tag{12}$$

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

$$\min_{\|\mathbf{u}\|=1} \max_{\substack{\mathcal{S}\subset\mathcal{D}\\|\mathcal{S}|=k}} \min_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d} = \min_{\substack{\mathcal{S}\subset\mathcal{D}\\|\mathcal{S}|=m-k+1}} \operatorname{cm}(\mathcal{S}),$$

we prove the equivalent statement

$$\min_{\|\mathbf{u}\|=1} \max_{\substack{\mathcal{S}\subset\mathcal{D}\\|\mathcal{S}|=k}} \min_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d} = \min_{\|\mathbf{u}\|=1} \min_{\substack{\mathcal{S}\subset\mathcal{D}\\|\mathcal{S}|=m-k+1}} \max_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d}. \tag{13}$$

To this end, let $\mathbf{u}$ be a unit vector in $\mathbb{R}^n$. We reorder the elements of $\mathcal{D}$ so that $\mathbf{u}^\top \mathbf{d}_1 \geq \dots \mathbf{u}^\top \mathbf{d}_m$ and we define $\mathcal{S}_k^- = \{\mathbf{d}_1, \dots, \mathbf{d}_k\}$ and $\mathcal{S}_k^+ = \{\mathbf{d}_k, \dots, \mathbf{d}_m\}$. By construction, one has

$$\mathbf{u}^\top \mathbf{d}_k = \min_{\mathbf{d}\in\mathcal{S}_k^-} \mathbf{u}^\top \mathbf{d} = \max_{\mathbf{d}\in\mathcal{S}_k^+} \mathbf{u}^\top \mathbf{d}. \tag{14}$$

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

$$\mathcal{S}_k^- \in \operatorname*{arg\,max}_{\substack{\mathcal{S}\subset\mathcal{D}\\|\mathcal{S}|=k}} \min_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d} \quad \text{and} \quad \mathcal{S}_k^+ \in \operatorname*{arg\,min}_{\substack{\mathcal{S}\subset\mathcal{D}\\|\mathcal{S}|=|\mathcal{D}|-k+1}} \max_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d}. \tag{15}$$

Combining (14) and (15) gives

$$\max_{\substack{\mathcal{S}\subset\mathcal{D}\\|\mathcal{S}|=k}} \min_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d} = \min_{\substack{\mathcal{S}\subset\mathcal{D}\\|\mathcal{S}|=|\mathcal{D}|-k+1}} \max_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d}. \tag{16}$$

Since (16) holds for any unit vector $\mathbf{u} \in \mathbb{R}^n$, it follows that

$$\min_{\|\mathbf{u}\|=1} \max_{\substack{\mathcal{S}\subset\mathcal{D}\\|\mathcal{S}|=k}} \min_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d} = \min_{\|\mathbf{u}\|=1} \min_{\substack{\mathcal{S}\subset\mathcal{D}\\|\mathcal{S}|=|\mathcal{D}|-k+1}} \max_{\mathbf{d}\in\mathcal{S}} \mathbf{u}^\top \mathbf{d},$$

which is precisely (13) and, as a result, proves (12). □

The formula (12) is associated with another characterization of PkSSs, namely that provided by Definition 4.1. In essence, the k-cosine measure of a family $\mathcal{D}$ is the minimum among all subsets of $\mathcal{D}$ with cardinality $|\mathcal{D}| - k + 1$. A useful corollary of that result is that for any $k \geq 2$, one has

$$\operatorname{cm}(\mathcal{D}) = \operatorname{cm}_1(\mathcal{D}) \geq \operatorname{cm}_2(\mathcal{D}) \geq \dots \geq \operatorname{cm}_k(\mathcal{D}).$$

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

4.3 Building positive k-spanning sets using 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 elements of the set. The purpose of this section is to introduce a more generic approach based on rotation matrices that allows for all vectors to be distinct.

Proposition 4.1 *Let $\mathcal{D}_{n,s}$ be an OSPB of $\mathbb{R}^n$ with $s \in [\![1,n]\!]$. Let $\mathbf{R}^{(1)}, \dots, \mathbf{R}^{(k)}$ be k rotation matrices in $\mathbb{R}^{n\times n}$, and define $\mathcal{D}_{n,s}^{(j)}$ as the family of vectors obtained by applying $\mathbf{R}^{(j)}$ to each vector in $\mathcal{D}_{n,s}$ for any $j \in [\![1,k]\!]$. Then, the set $\mathcal{D}_{n,s}^{(1:k)} = \bigcup_{j=1}^{k} \mathcal{D}_{n,s}^{(j)}$ is a positive k-spanning set with*

$$\mathrm{cm}_k\left(\mathcal{D}_{n,s}^{(1:k)}\right) \geq \mathrm{cm}\left(\mathcal{D}_{n,s}\right). \tag{17}$$

Proof. First, note that applying a rotation to every vector in a family does not change its cosine measure since rotations preserve angles, hence $\mathrm{cm}\left(\mathcal{D}_{n,s}^{(j)}\right) = \mathrm{cm}\left(\mathcal{D}_{n,s}\right)$ for every $j \in [\![1,k]\!]$.

Consider a family $\mathcal{S} \subset \mathcal{D}_{n,s}^{(1:k)}$ with $|\mathcal{S}| = \left|\mathcal{D}_{n,s}^{(1:k)}\right| - k + 1$. By the pigeonhole principle, this set must contain one of the k positive bases obtained by rotation. Letting $\mathcal{D}_{n,s}^{(j_\mathcal{S})}$ denote that positive basis, we have $\mathrm{cm}\left(\mathcal{S}\right) \geq \mathrm{cm}\left(\mathcal{D}_{n,s}^{(j_\mathcal{S})}\right) = \mathrm{cm}\left(\mathcal{D}_{n,s}\right)$. Using Theorem 4.2, we obtain that

$$\mathrm{cm}_k\left(\mathcal{D}_{n,s}^{(1:k)}\right) = \min_{\substack{\mathcal{S}\subset\mathcal{D}_{n,s}^{(1:k)} \\ |\mathcal{S}| = \left|\mathcal{D}_{n,s}^{(1:k)}\right| - k + 1}} \mathrm{cm}\left(\mathcal{S}\right) \geq \mathrm{cm}\left(\mathcal{D}_{n,s}\right).$$

In particular, this proves $\mathrm{cm}_k\left(\mathcal{D}_{n,s}^{(1:k)}\right) > 0$, hence this set being positively k-spanning now follows from Theorem 4.1. $\square$

Several remarks are in order regarding Proposition 4.1. First, note that the result extends to any positive spanning set, but we focus on OSPBs since in that case (17) 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 $\mathcal{D}_{n,s}$ are used, the resulting family is a positive k-basis and relation (17) holds with equality. As a result, its k-cosine measure can be computed in polynomial time using Algorithm 1. In general, however, the family generated through Proposition 4.1 is not necessarily a positive k-basis. For instance, if $n = 2$, setting $\mathcal{D}_2 = \{\mathcal{I}_2, -\mathbf{1}\}$, $k = 2$, $\mathbf{R}_1 = \mathbf{I}_2$ and $\mathbf{R}_2 = \begin{bmatrix} 1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{bmatrix}$ yields a family that is a positive 2-spanning set but not a positive 2-basis.

We now present a strategy based on 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, 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 *Let $\mathcal{D}_\mathbb{L} = \{\mathbf{d}_1, \dots, \mathbf{d}_{\ell+1}\}$ 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*

$$\forall i \in [\![1, \ell+1]\!], \quad \mathbf{d}_i^\top \mathbf{v}_i > 0 \quad \textit{and} \quad \forall 1 \leq j < i \leq \ell+1, \quad \mathbf{d}_i^\top \mathbf{v}_j < 0. \tag{18}$$

Proof. By Lemma 2.1(ii), the zero vector $\mathbf{0}_n$ can be obtained by a positive linear combination of all elements in $\mathcal{D}_\mathbb{L}$. Without loss of generality, we rescale the elements of $\mathcal{D}_\mathbb{L}$ to ensure that $\sum_{i=1}^{\ell+1} \mathbf{d}_i = \mathbf{0}_n$. Now, since $\mathcal{D}_\mathbb{L}$ is a minimal positive basis, the set $\mathcal{D}_\mathbb{L} \backslash \{\mathbf{d}_{\ell+1}\}$ is a linear basis of

$\mathbb{L}$. Suppose that we augment this set with $n-\ell$ vectors to form a basis $\mathcal{B}_n$ of $\mathbb{R}^n$, and let $\mathbf{B}_n$ be a matrix representation of that basis such that the first ℓ columns correspond to $\mathbf{d}_1,\dots,\mathbf{d}_\ell$. Then, we have $\mathbf{d}_i = \mathbf{B}_n\mathbf{e}_i$ for any $i \in [\![1,\ell]\!]$, while $\mathbf{d}_{n+1} = -\mathbf{B}_n\left(\sum_{j=1}^{\ell}\mathbf{e}_j\right)$, 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

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

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 $i \in [\![1,\ell]\!]$ 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 (18) holds.

In addition, for any $1 \le j < i \le \ell+1$, 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 (18) also holds. □

Note that Lemma 4.3 is not equivalent to Definition 2.3 as the inequalities in (18) are strict.

Our second technical result uses the result of Lemma 4.3 to define a quantity characteristic of the angles between vectors in a minimal positive basis.

Lemma 4.4 *Suppose that $n \ge \ell \ge 2$ and let $\mathcal{D}_{\mathbb{L}} = \{\mathbf{d}_1,\dots,\mathbf{d}_{\ell+1}\}$ 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 (18). For any pair $(i,i') \in [\![1,\ell+1]\!]^2$, let $\mathbf{d}_{i,i'}$ be the orthogonal projection of $\mathbf{d}_i$ on $\mathbb{L}\cap\{\mathbf{v}_{i'}\}^\perp$. Then, the quantity $\rho_{\mathcal{D}_{\mathbb{L}}} := \max_{i,i' \le \ell+1} \frac{\mathbf{d}_i^\top\mathbf{d}_{i,i'}}{\|\mathbf{d}_i\|\|\mathbf{d}_{i,i'}\|}$ 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 $\mathbf{d}_i^\top\mathbf{d}_{i,i'} \ge 0$, hence $\rho_{\mathcal{D}_{\mathbb{L}}} \ge 0$. Moreover, for any pair $1 \le i \le i' \le \ell+1$, we have $\mathbf{d}_i^\top\mathbf{v}_{i'} \ne 0$ by (18), hence $\mathbf{d}_i \notin \mathbb{L}\cap\{\mathbf{v}_j\}^\perp$ and $\frac{\mathbf{d}_i^\top\mathbf{d}_{i,i'}}{\|\mathbf{d}_i\|\|\mathbf{d}_{i,i'}\|} < 1$. As a result, $\rho_{\mathcal{D}_{\mathbb{L}}} < 1$, completing the proof. □

The quantity defined in Lemma 4.4 is instrumental in defining suitable rotations matrices to produce a positive k-basis. The construction is described in Theorem 4.3.

Theorem 4.3 *Suppose that $n \ge \ell \ge 2$ and let $\mathcal{D}_{\mathbb{L}} = \{\mathbf{d}_1,\dots,\mathbf{d}_{\ell+1}\}$ be a minimal positive basis of an ℓ-dimensional subspace $\mathbb{L}$ in $\mathbb{R}^n$. Let $\rho_{\mathcal{D}_{\mathbb{L}}}$ be the quantity defined in Lemma 4.4 for some vectors $\mathbf{v}_1,\dots,\mathbf{v}_{\ell+1}$ satisfying (18). 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) $\mathbf{R}_{\mathbb{L}}^{(j)}\mathbf{u} = \mathbf{u}$, *for any $j \in [\![1,k]\!]$ and any vector $\mathbf{u} \in \mathbb{L}^\perp$,*

(ii) for any pair $(j,j') \in [\![1,k]\!]^2$ and any pair $(i,i') \in [\![1,\ell+1]\!]^2$,

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

(iii) $\dfrac{\left[\mathbf{R}_{\mathbb{L}}^{(j)}\mathbf{d}_i\right]^\top \mathbf{d}_i}{\|\mathbf{R}_{\mathbb{L}}^{(j)}\mathbf{d}_i\|\|\mathbf{d}_i\|} > \rho_{\mathcal{D}_{\mathbb{L}}}$ *for any pair* $(i,j) \in [\![1,\ell+1]\!] \times [\![1,k]\!]$.

Denote by $\mathcal{D}_{\mathbb{L}}^{(j)}$ *the family obtained by applying* $\mathbf{R}_{\mathbb{L}}^{(j)}$ *to each vector in* $\mathcal{D}_{\mathbb{L}}$*. Then, the family* $\mathcal{D}_{\mathbb{L}}^{(1:k)} = \bigcup_{j=1}^{k} \mathcal{D}_{\mathbb{L}}^{(j)}$ *is a positive k-basis of* $\mathbb{L}$ *with no identical elements.*

Proof. Owing to assumptions (i) and (ii), we know that $\mathcal{D}_{\mathbb{L}}^{(1:k)}$ is a subset of $\mathbb{L}$ with pairwise distinct elements. Moreover, Proposition 4.1 guarantees that $\mathcal{D}_{\mathbb{L}}^{(1:k)}$ is a PkSS for $\mathbb{L}$. Therefore we only need to show the positive k-independence of this set.

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

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

where $\mathbf{d}_{i,j}$ is defined as in Lemma 4.4. 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 $j \in [\![1,k]\!]$.

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 vectors in $\mathcal{D}_{\mathbb{L}}^{(1:k)}$. Since any vector $\mathbf{d} \in \mathcal{D}_{\mathbb{L}}^{(1:k)}$ is obtained by applying a rotation to some element $\mathbf{d}_i \in \mathcal{D}_{\mathbb{L}}^{(1:k)}$, we conclude that $\mathcal{D}_{\mathbb{L}}^{(1:k)}$ is positively k-independent, proving the desired result. □

Note that Theorem 4.3 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 4.1 *The first two conditions enforced on the rotation matrices in Theorem 4.3 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 vectors in* $\mathcal{D}_{\mathbb{L}}$*.*

Theorem 4.3 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 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 4.1 *Let $\mathcal{D}_{n,s}$ be an OSPB and let $\mathcal{D}_{\mathbb{L}_1}, \dots, \mathcal{D}_{\mathbb{L}_s}$ be a decomposition* (2) *of $\mathcal{D}_{n,s}$. Assume that for every $i \in [\![1, s]\!]$, $dim(\mathbb{L}_i) > 1$. Let $k \geq 1$ and for every $i \in [\![1, s]\!]$, 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 relative to $\mathcal{D}_{\mathbb{L}_i}$. Then, the set*

$$\mathcal{D}_{n,s}^{(1:k)} = \bigcup_{j=1}^{k} \mathcal{D}_{n,s}^{(j)}, \qquad \textit{with} \quad \mathcal{D}_{n,s}^{(j)} = \bigcup_{i=1}^{s} \mathcal{D}_{\mathbb{L}_i}^{(j)} \quad \forall j \in [\![1, k]\!],$$

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

Corollary 4.1 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 $\mathrm{cm}\left(\mathcal{D}_{n,s}\right)$ 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 above.

Similarly to the result of Theorem 4.3, the result of Corollary 4.1 does not apply to all OSPBs. In particular, the maximal OSPB $\{\mathcal{I}_n, -\mathcal{I}_n\}$ decomposes into n minimal positive bases over one-dimensional subspaces, which precludes the application of Theorem 4.3. Note however that Proposition 4.1 still provides a way to compute PkSSs with cosine measure guarantees for such a maximal OSPB.

5 Conclusion

In this paper, we have studied two classes of positive spanning sets. On the one hand, we have investigated 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, a relatively understudied class of PSSs with resilient properties. We have provided several characterizations of these sets, 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.

Our results open the way for several promising areas of research. We believe that the cosine measure calculation technique can be further improved for positive bases by leveraging their decomposition, although the presence of critical vectors poses a number of challenges to overcome for dealing with positive bases that are not orthogonally structured. Such results would also improve the practical calculation of k-cosine measures. Finally, designing derivative-free optimization techniques based on positive k-spanning sets with guarantees on their k-cosine measure is a natural application of our study, and is the subject of ongoing work.

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