Positive k-spanning sets and their use in Derivative Free Optimization

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1. Positive Spanning Sets

2. Cosine measure

3. Positive k-Spanning Sets

4. k-cosine measure

Applications

Question

Let $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ *be a smooth function. How can we minimize* $f(x)$ *?*

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If the elements of D are well spread in $\mathbb{R}^n$, the algorithm will converge.

Positive Spanning Sets and Positive Bases

Definition

A **PSS** spans $\mathbb{R}^n$ with positive linear combinations.
A **positive basis** is minimal for this property.

Remark

If the columns of matrix M *form a PSS, we say that* M *is a PSS.*

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Examples in $\mathbb{R}^2$

$\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix}$ *is a positive basis.*

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$\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix}$ *is a positive basis.* $\begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix}$ *too.*

e.g: $\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} 3 \\ 0 \\ 0 \\ 4 \end{bmatrix} = \begin{bmatrix} 3 \\ -4 \end{bmatrix}$ *and* $\begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} 7 \\ 0 \\ 4 \end{bmatrix} = \begin{bmatrix} 3 \\ -4 \end{bmatrix}$.

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$\begin{bmatrix} 1 & 0 & -2 & 1 \\ 0 & 1 & 1 & -2 \end{bmatrix}$ *is...* $\begin{bmatrix} 1 \\ 0 \\ 0 \\ 2 \end{bmatrix}$

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$\begin{bmatrix} 1 & 0 & -2 & 1 \\ 0 & 1 & 1 & -2 \end{bmatrix}$ *is a PSS.* $\begin{bmatrix} 0 & -2 & 1 \\ 1 & 1 & -2 \end{bmatrix}$ *is a positive basis.*

Remark

If the columns of matrix M *form a PSS, we say that* M *is a PSS.*

Cardinal

Proposition

The smallest possible size for a positive basis of $\mathbb{R}^n$ *is* $n+1$*.*
The biggest possible size is $2n$*.*

Proof (idea)

- *Lower bound: a PSS must clearly be larger than a linear basis.*
- *Upper bound: Trickier. Proven using linear programming arguments.*

Farkas Lemma

Lemma

Let $\mathrm{M} \in \mathbb{R}^{n,m}$*, let* $\mathrm{b} \in \mathbb{R}^{n}$*. Exactly one of the two following assertions is true:*

- *Equation* $\mathrm{M}\mathrm{x} = \mathrm{b}$ *has a solution* $\mathrm{x} \geq 0$*.*
- *Inequation* $\mathrm{y}^\top \mathrm{M} \geq 0$ *has a solution* y *such that* $\mathrm{y}^\top \mathrm{b} < 0$*.*

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- *Equation* $\mathrm{M}\mathrm{x} = \mathrm{b}$ *has a solution* $\mathrm{x} \geq 0$*. Always true for PSSs.*
- *Inequation* $\mathrm{y}^\top \mathrm{M} \geq 0$ *has a solution* y *such that* $\mathrm{y}^\top \mathrm{b} < 0$.

Remark

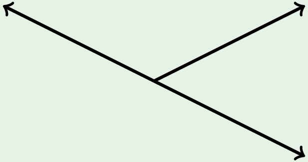
When M *is a PSS, the second assertion is false for all* b *!*

Characterization of PSSs

Characterization

M *is a PSS* $\iff$ *There is no* $\mathrm{y} \neq 0$ *such that* $\mathrm{y}^\top \mathrm{M} \geq 0^\top$.

Examples in $\mathbb{R}^2$



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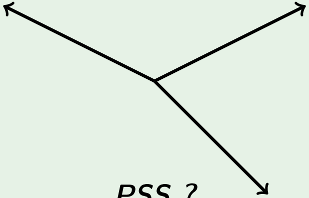

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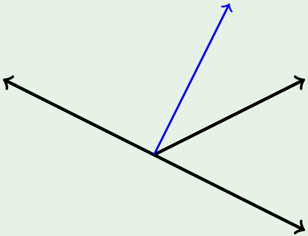

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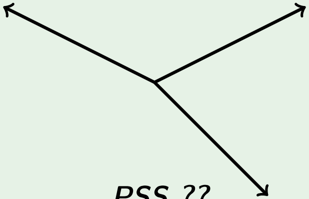

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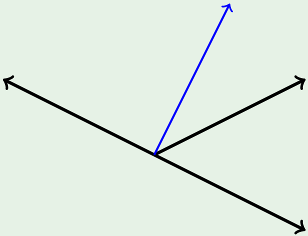

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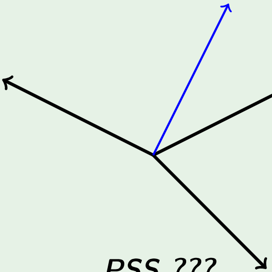

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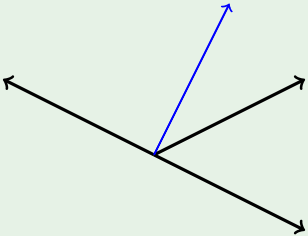

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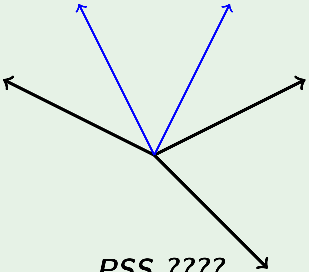


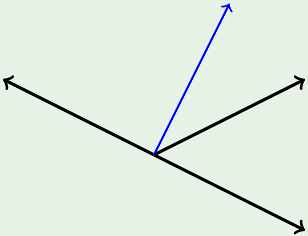
PSS ????

Characterization of PSSs

Characterization

M *is a PSS* $\iff$ *There is no* $y \neq 0$ *having an acute angle with every element of* M*. Only a* ***finite*** *number of checks are required !*

Examples in $\mathbb{R}^2$



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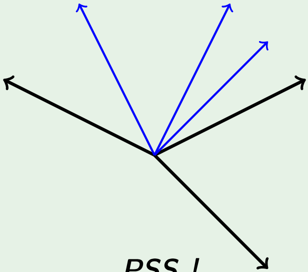

PSS !

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Characterizing PSSs via the cosine measure

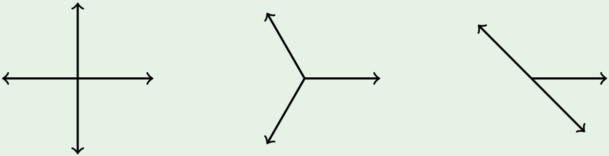
Definition

Let $M = \{\mathrm{d_1}, \ldots, \mathrm{d_m}\} \subset \mathbb{R}^n$. The **cosine measure** of M is defined as:

$$cm(M) := \min_{\mathrm{v} \neq 0} \max_{i \in [1,m]} \frac{\mathrm{d_i}^\top \mathrm{v}}{\|\mathrm{d_i}\|.\|\mathrm{v}\|}.$$

Characterization

M is a PSS $\iff cm(M) > 0$.



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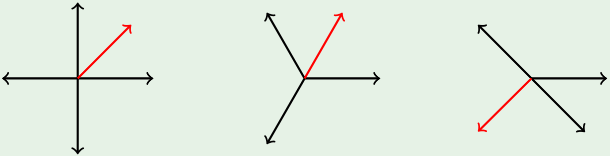

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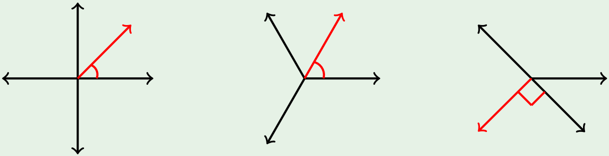

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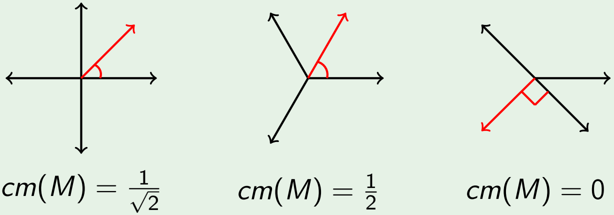

$cm(M) = \frac{1}{\sqrt{2}}$ $\quad$ $cm(M) = \frac{1}{2}$ $\quad$ $cm(M) = 0$

Computing the cosine measure

Theorem

Let $D_{\mathbb{R}^n}$ be a positive basis of $\mathbb{R}^n$.

- *If $|D_{\mathbb{R}^n}| = 2n$, then $cm(D_{\mathbb{R}^n}) \leq \frac{1}{\sqrt{n}}$.*
- *If $|D_{\mathbb{R}^n}| = n + 1$ then $cm(D_{\mathbb{R}^n}) \leq \frac{1}{n}$.*

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- It is better to use PSSs whose cosine measure is close to 1 for optimization purposes...
- ...However, algorithms to find the cosine measure of a PSS are exponential in time.

Orthogonally structured positive bases

Definition

Positive basis $D_{\mathbb{R}^n}$ of $\mathbb{R}^n$ is an OSPB if:

- It can be written as a partition of positive bases for smaller linear spaces:

$$D_{\mathbb{R}^n} = D_{\mathbb{L}_1} \cup \cdots \cup D_{\mathbb{L}_s}.$$

- These bases are pairwise orthogonal and of minimal size.

Examples

$$\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix} \quad \begin{bmatrix} 0 & 1 & 4 & 0 & -5 \\ 2 & 0 & 0 & -2 & 0 \\ 0 & 3 & 5 & 0 & -8 \end{bmatrix} \quad \begin{bmatrix} 1 & -1 & 2 & -1 & -1 \\ 1 & -1 & -1 & 1 & 0 \\ 1 & -1 & -1 & 0 & 1 \end{bmatrix}.$$

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Theorem (new !)

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Algorithm: cosine measure of an OSPB

- *Step 1: Find an orthogonal decomposition for your basis.*
- *Step 2: For any set $D_{\mathbb{L}_i}$ in the decomposition, compute its induced cosine measure c_i.*
- *Step 3: Return $\frac{1}{\sqrt{\sum_i c_i^{-2}}}$.*

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What if we have trouble computing $f(x_0 + \alpha d_i)$?

Positive k-spanning sets, Positive k-bases

Definition

A **PkSS** remains positively spanning when $k-1$ of its elements are removed. A **positive k-basis** is a minimal PkSS.

Examples of positive 2-bases in $\mathbb{R}^2$

$$\begin{bmatrix} 1 & 0 & -1 & 1 & 0 & -1 \\ 0 & 1 & -1 & 0 & 1 & -1 \end{bmatrix} \qquad \begin{bmatrix} 1 & 0 & -1 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 & 1 & -1 \end{bmatrix}$$

Remark

$P1SS \iff PSS$

Positive k-spanning sets, Positive k-bases

Definition

At least k elements must be removed from a **PkSS** before it stops being positively spanning. A **positive k-basis** is a minimal PkSS.

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Alternative definition

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M *is a PkSS* $\iff$ *For all* $y \neq 0$, *vector* $y^\top M$ *has at least* k *positive coordinates.*

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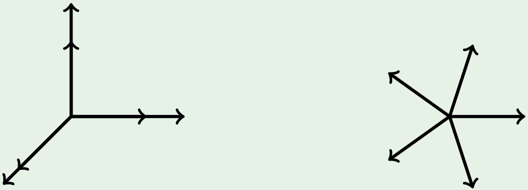

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M *is a PkSS* $\iff$ *For all* $y \neq 0$*, vector* $y^\top M$ *has at least* k *positive coordinates.* $\iff$ y *makes an acute angle with at least* k *elements of M.*

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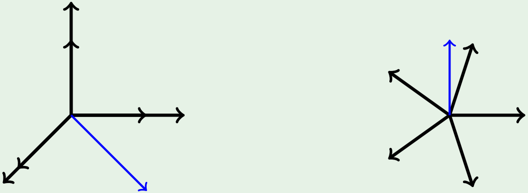

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M *is a PkSS* $\iff$ *For any hyperplane, at least* k *elements of* M *point on each side of the hyperplane.*

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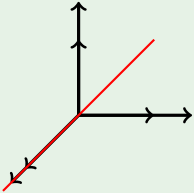

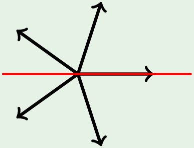

Cardinal of positive k-bases

Proposition

Let $D_{\mathbb{R}^n}$ be a positive basis of $\mathbb{R}^n$. Then $n + 1 \leq |D_{\mathbb{R}^n}| \leq 2n$.

Can this be generalized ?

Let us try...

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- *The hyperplane characterization implies a lower bound of $2k + n - 1$ on the size of a PkSS. Tight (Marcus, 1984).*
- *Digraphs can be used to create positive k-bases. In that case, the maximal size is $2kn$.*

PkSSs and Polytope theory

Definition

Let $\mathrm{M} \in \mathbb{M}_{n,m}(\mathbb{R})$. Any full rank matrix B such that $\mathrm{M}\mathrm{B}^\top = 0$ is called a **Gale diagram** of M.

Theorem

Vertices of a well chosen polytope.

Suppose $M = \begin{bmatrix} & P & \\ 1 & \dots & 1 \end{bmatrix}$. *Then any Gale diagram of* M *is a PkSS.*

Polytopes and cardinality of positive k-bases

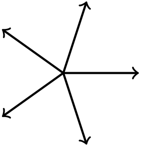
Theorem

Let $D^{(k)}_{\mathbb{R}^n}$ be a positive k-basis of $\mathbb{R}^n$. Then :

$$2k + n - 1 \leq |D^{(k)}_{\mathbb{R}^n}| \leq kn(n+1)^{k-1}$$

Remark

- *The lower bound is tight (eg: pentagon).*
- *The upper bound might not be. (Wotzlaw, 2009)*



A new tool for characterizing PkSSs

Definition (new !)

Let $k \geq 1$ *and* $\mathsf{M} \subset \mathbb{R}^n \backslash \{0\}$*. The* k*-cosine measure of* M *is:*

$$cm_k(\mathsf{M}) := \min_{\mathsf{v} \neq 0} \max_{\substack{\mathsf{S} \subset \mathsf{M} \\ |\mathsf{S}| = k}} \min_{\mathsf{s} \in \mathsf{S}} \frac{\mathsf{s}^\top \mathsf{v}}{\|\mathsf{s}\| . \|\mathsf{v}\|}.$$

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Theorem

M *is a PkSS if and only if* $cm_k(\mathsf{M}) > 0$*.*

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$$cm_k(\mathsf{M}) = \min_{\substack{\mathsf{S} \subset \mathsf{M} \\ |\mathsf{S}| = |\mathsf{M}| - k + 1}} cm(\mathsf{S}).$$

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- $cm_k(\mathsf{M})$ *is computed by finding a vector as far as possible from its* k^{th} *closest neighbor in* M.

Examples

Remark

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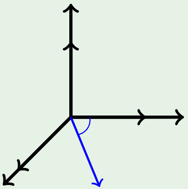
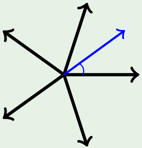
Computing the cosine measure:

Examples



$cos(\frac{3\pi}{8}) \simeq 0.38$



$cos(\frac{2\pi}{10}) \simeq 0.809$

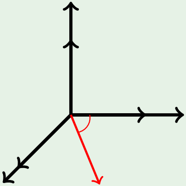
Examples

Remark

$cm_2(\mathrm{M})$ is computed by finding a vector as far as possible from its second closest neighbor in M*.*

Computing the 2-cosine measure:

Examples



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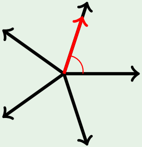


$cos(\frac{2\pi}{5}) \simeq 0.309$

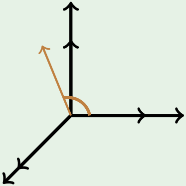
Examples

Remark

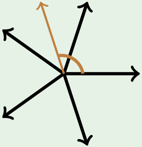
$cm_3(\mathrm{M})$ is computed by finding a vector as far as possible from its third closest neighbor in M.

Computing the 3-cosine measure:

Examples



$cos(\frac{5\pi}{8}) \simeq -0.38$



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Basic remarks of the k-cosine measure

There is no easy way to compute the k-cosine measure of a given family.
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- *Let $k < l$. Then $cm_k(\mathrm{M}) \geq cm_l(\mathrm{M})$.*

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- *Let* $k < l$*. Then* $cm_k(\mathrm{M}) \geq cm_l(\mathrm{M})$*.*
- *Let* $\mathrm{N} \subseteq \mathrm{M}$*. Then* $cm_k(\mathrm{N}) \leq cm_k(\mathrm{M})$*.*

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- *Let* $k < l$*. Then* $cm_k(\mathrm{M}) \geq cm_l(\mathrm{M})$.
- *Let* $\mathrm{N} \subseteq \mathrm{M}$*. Then* $cm_k(\mathrm{N}) \leq cm_k(\mathrm{M})$.
- *If* $cm(\mathrm{M}) = \alpha$*, duplicating M creates a PkSS whose k-cosine measure is* α*.*

Rotating PSSs

Proposition

Let $D_{\mathbb{R}^n} \subset \mathbb{R}^n \backslash \{0\}$ *be an OSPB. Stacking together* k *rotations of* $D_{\mathbb{R}^n}$ *creates a PkSS* $D_{\mathbb{R}^n}^{(k)}$ *satisfying:*

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Unfortunately, this PkSS might not be a positive k-basis.

Rotating minimal bases

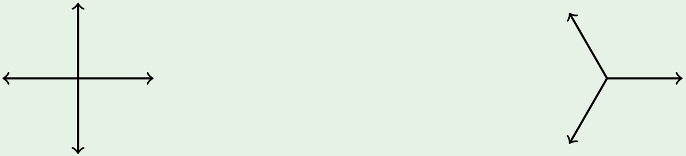
Theorem

Rotating minimal positive bases can create positive k-bases.

Idea: apply small rotations.

Note: this technique only works for minimal positive bases !

Examples in $\mathbb{R}^2$



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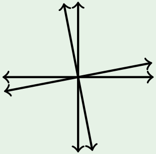
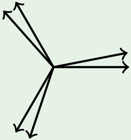


$\Longleftarrow$ *non-minimal P2SS!*



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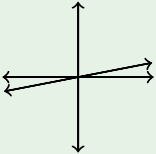

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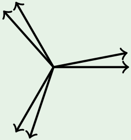

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Perspectives

- Finding new ways to build "nice" PkSSs.
- Using PkSSs in Derivative Free Algorithms.

Thanks for your attention !