On the positive semidefinite polytope rank

David Trieb

Bachelor Thesis

Betreuer: Tim Netzer

Institut für Mathematik
Universität Innsbruck

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1 Introduction

Note that this bachelor thesis largely follows [2].

If you want to do linear optimization over a polytope, the complexity of many algorithms depends on the size of the representation of the polytope. So, if you have a (complicated) polytope, the idea is to find a simpler convex set of higher dimension which has the polytope as a linear image of it and then optimize over that instead. This motivates following definition:

Definition 1.1.
Let $P \subset \mathbb{R}^n$ be a polytope. For a closed convex cone $C \subset \mathbb{R}^m$ and an affine space $L \subset \mathbb{R}^m$, $C \cap L$ is called a *C-lift* of P, if there exists a linear map $\pi : \mathbb{R}^m \to \mathbb{R}^n$ such that $P = \pi(C \cap L)$.

In this bachelor thesis, we will be interested in the cases $C = \mathbb{R}^k_+ = \{x \in \mathbb{R}^k \mid x_1 \geq 0, \ldots, x_n \geq 0\}$ and especially $C = \mathcal{S}^k_+ = \{M \in \mathbb{R}^{k \times k} \mid M$ symmetric, positive semidefinite$\}$. Note that $\mathbb{R}^k_+$ embeds into $\mathcal{S}^k_+$ via diagonal matrices.
Now one is interested in finding the smallest cone in the families $\{\mathbb{R}^k_+\}$ and $\{\mathcal{S}^k_+\}$, respectively, which allows a lift of a polytope P:

Definition 1.2.
Let $P \subset \mathbb{R}^n$ be a polytope.

(1) The *nonnegative rank* of a polytope is given by $\text{rank}_+(P) := \min(\{k \in \mathbb{N} \mid P$ has $\mathbb{R}^k_+$-lift$\})$.

(2) The *positive semidefinite (psd) rank* of a polytope is given by $\text{rank}_{\text{psd}}(P) := \min(\{k \in \mathbb{N} \mid P$ has $\mathcal{S}^k_+$-lift$\})$.

In order to investigate the properties of the psd rank of a polytope, the following definitions are also needed:

Definition 1.3.
Let $P \subset \mathbb{R}^n$ be a n-dimensional polytope with vertex set $\{p_1, \ldots, p_v\}$ and irredundant inequality representation $P = \{x \in \mathbb{R}^n \mid b_1 - \langle a_1, x\rangle \geq 0, \ldots, b_f - \langle a_f, x\rangle \geq 0\}$, where $b_j \in \mathbb{R}$ and $a_j \in \mathbb{R}^n$ for $j = 1, \ldots, f$.
Then the *slack matrix* $S_P \in \mathbb{R}^{v \times f}$ is given by $(S_P)_{ij} = b_j - \langle a_j, p_i\rangle$.

Short reminder: the polar dual of a cone C is given by

$$C^\circ := \{y \in \mathbb{R}^m \mid \langle x, y\rangle \geq 0 \ \ \forall x \in C\}.$$

Note that both $\mathcal{S}^k_+$ and $\mathbb{R}^k_+$ are self dual cones, i.e. $C = C^\circ$. For symmetric matrices A, B we will use the trace inner product $\langle A, B\rangle = \text{Tr}(AB)$.

Definition 1.4.
Let $M \in \mathbb{R}^{p \times q}_+$ be a nonnegative matrix and C a closed convex cone with its polar dual C°.

(1) A pair of ordered sets $a^1, \dots, a^p \in C$ and $b^1, \dots, b^q \in C^\circ$ is called *C-factorisation* of M, if $M_{ij} = \langle a^i, b^j \rangle$ for all $i = 1, \dots, p$ and $j = 1, \dots, q$.

(2) For $C = \mathcal{S}_+^k$ (respectively, $\mathbb{R}_+^k$), a C-factorisation of M is called a *psd* (respectively, *nonnegative*) *factorisation* of M.

(3) $\operatorname{rank}_{\text{psd}} M := \min(\{k \in \mathbb{N} \mid M \text{ has } \mathcal{S}_+^k\text{-factorisation}\})$ denotes the *psd rank* of M. $\operatorname{rank}_+ M := \min(\{k \in \mathbb{N} \mid M \text{ has } \mathbb{R}_+^k\text{-factorisation}\})$ denotes the *nonnegative rank* of M.

Note that in Definition 1.3 any positive scaling of a facet inequality of P can be used and therefore, if you positively scale the columns of a slack matrix S_P of P, you get a slack matrix of P again. In the following, any such slack matrix is denoted by S_P.

Remark 1.5.
These are some results we will use:

- $\operatorname{rank}_{\text{psd}} P = \operatorname{rank}_{\text{psd}} S_P$ and $\operatorname{rank}_+ P = \operatorname{rank}_+ S_P$. [1], [4]
- $\operatorname{rank}_+ P$ and $\operatorname{rank}_{\text{psd}} P$ are invariant under affine transformations.
- If P° is the polar polytope of P and S_P a slack matrix of P, then $S_P^\intercal$ is (up to row scaling) a slack matrix of P° and therefore, $\operatorname{rank}_{\text{psd}} P = \operatorname{rank}_{\text{psd}} P^\circ$.
- Since $\mathbb{R}_+^k$ embeds into $\mathcal{S}_+^k$ via diagonal matrices it follows $\operatorname{rank}_{\text{psd}} M \leq \operatorname{rank}_+ M$ for $M \in \mathbb{R}_+^{p\times q}$. Together with the first statement of this remark this yields $\operatorname{rank}_{\text{psd}} P \leq \operatorname{rank}_+ P$ for any polytope $P \subset \mathbb{R}^n$.

Proof. • We prove that $\operatorname{rank}_+ P = \operatorname{rank}_+ S_P$. $\operatorname{rank}_{\text{psd}} P = \operatorname{rank}_{\text{psd}} S_P$ can be proven similarly.

(1) $\operatorname{rank}_+ P \geq \operatorname{rank}_+ S_P$:
Let $P = \{x \in \mathbb{R}^n \mid 1 - \langle c_1, x\rangle \geq 0, \dots, 1 - \langle c_f, x\rangle \geq 0\} \subset \mathbb{R}^n$ be a fulldimensional polytope with vertices $p_1, \dots, p_v$ and $\operatorname{rank}_+ P = k$. Then there exists a linear map $\pi : \mathbb{R}^k \to \mathbb{R}^n$ such that $P = \pi(\mathbb{R}_+^k \cap L)$, where L is an affine subspace. Suppose that $L = z + L_0$, where L_0 is a linear subspace. Then P is given by $P = \{x \in \mathbb{R}^n \mid x = \pi(w), w \in \mathbb{R}_+^k \cap (z + L_0)\}$.
Let $\pi^* : \mathbb{R}^n \to \mathbb{R}^k$ be the adjoint of π and assume that $\mathbb{R}_+^k \cap L_0 = \{0\}$ (we may do so, because P is bounded). Then, by strong conic duality:

$$P^\circ = \{x \in \mathbb{R}^n \mid y - \pi^*(x) \in \mathbb{R}_+^k, y \in L_0^\perp, \langle y, z\rangle = 1\}$$

Since $y \in L_0^\perp$, we have $\langle w_i, y\rangle = 1$ for any $w_i \in L_0 + z = L$. Now define $a^i := w_i$ and $b^j := y - \pi^*(c_j)$, where $w_i \in \pi^{-1}(p_i) \cap \mathbb{R}_+^k$ and $y \in L_0^\perp \cap (\mathbb{R}_+^k + \pi^*(c_j))$ with $\langle y, z\rangle = 1$. Such w_i and y do exist and we get

$$\begin{aligned}(S_P)_{ij} &= 1 - \langle c_j, p_i\rangle = 1 - \langle c_j, \pi(w_i)\rangle = 1 - \langle \pi^*(c_j), w_i\rangle = 1 - \langle w_i, y - b^j\rangle = \\ &= 1 - 1 + \langle w_i, b^j\rangle = \langle a^i, b^j\rangle.\end{aligned}$$

As $a^i \in \mathbb{R}_+^k$ and $b^j \in \mathbb{R}_+^k$, we have $\operatorname{rank}_+ S_P \leq k = \operatorname{rank}_+ P$.

(2) $\operatorname{rank}_+ P \leq \operatorname{rank}_+ S_P$:
Let P be a polytope as above. Assume that $\operatorname{rank}_+ S_P = k$. Then there exist $a^1, \ldots, a^v, b^1, \ldots, b^f \in \mathbb{R}^k_+$ such that $(S_P)_{ij} = \langle a^i, b^j \rangle$. Define

$$L := \{(x, y) \in \mathbb{R}^n \times \mathbb{R}^k \mid 1 - \langle x, c_i \rangle = \langle y, b^j \rangle, j = 1, \ldots, f\}.$$

Let $L_k \subset \mathbb{R}^k$ denote the projection onto the second coordinate of L. Note that $a^i \in \mathbb{R}^k_+ \cap L_k$ and $0 \notin L_k$ ($0 \in L_k \Rightarrow \exists x : 1 - \langle x, c_i \rangle = 0$ for all $i = 1, \ldots, f \Rightarrow P^\circ$ is contained in the hyperplane $\{y \mid \langle x, y \rangle = 1\}$, which is a contradiction, because $0 \in P^\circ$).

For all $x \in \mathbb{R}^n$ for which there exist $y \in \mathbb{R}^k_+$ such that $(x, y) \in L$ we have $1 - \langle x, c_i \rangle \geq 0$, $i = 1, \ldots, f \Rightarrow 1 - \langle x, y \rangle \geq 0\ \forall y \in P^\circ \Rightarrow x \in (P^\circ)^\circ = P$.

Claim: $\forall\, y \in \mathbb{R}^k_+ \cap L_k : \exists!\, x_y \in \mathbb{R}^n : (x_y, y) \in L$.
Proof of claim: The existence follows from the definition of L_k. Now let x_y and x'_y be two such points. Since $(x_y, y), (x'_y, y) \in L$, we get $1 - \langle x_y, c_i \rangle = 1 - \langle x'_y, c_i \rangle = \langle y, b^j \rangle$, and thus we obtain for $t \in \mathbb{R}$:

$$1 - \langle t x_y + (1 - t) x'_y, c_i \rangle = 1 - t\langle x_y, c_i \rangle - \langle x'_y, c_i \rangle + t\langle x'_y, c_i \rangle = \langle y, b^j \rangle,$$

i.e., $(t x_y + (1 - t) x'_y, y) \in L$, which means that the line through x_y and x'_y is contained in P, which is a contradiction, unless $x_y = x'_y$.

Therefore, the map $\mathbb{R}^k_+ \cap L_k \to \mathbb{R}^n : y \mapsto x_y$ is well-defined. As this map is affine and $0 \notin L_k$, we may extend it to a linear map $\pi : \mathbb{R}^k \to \mathbb{R}^n$. We have already proven $\pi(\mathbb{R}^k_+ \cap L_k) \subset P$ above. Since for all $i = 1, \ldots, v$, $a^i \in \mathbb{R}^k_+ \cap L_k$, it follows $p_i = \pi(a^i) \in \pi(\mathbb{R}^k_+ \cap L_k)$ and because P is the convex hull of its vertices and $\pi(\mathbb{R}^k_+ \cap L_k)$ is convex, we obtain $C \subset \pi(\mathbb{R}^k_+ \cap L_k)$. Thus $C = \pi(\mathbb{R}^k_+ \cap L_k)$ and we found a $\mathbb{R}^k_+$-lift of P. Hence, $\operatorname{rank}_+ P \leq \operatorname{rank}_+ S_P$.

- Let $P \subset \mathbb{R}^n$ be a n-dimensional polytope with $\operatorname{rank}_{\mathrm{psd}} P = k$. Then there exists a linear map $\pi : \mathcal{S}^k_+ \to \mathbb{R}^n$ such that $P = \pi(\mathcal{S}^k_+ \cap L)$, where $L \subset \mathcal{S}^k_+$ is an affine subspace. Let $\pi_1 : \mathbb{R}^n \to \mathbb{R}^n$ be an affine transformation. Then $\pi_1(P) = z + \pi_2(\pi(\mathcal{S}^k_+ \cap L))$ for some $z \in \mathbb{R}^n$ and a linear function π_2. As the composition $\pi_2 \circ \pi$ is also linear, this means that the polytope $\pi_1(P) - z$ has a $\mathcal{S}^k_+$-lift. Since $\pi_1(P) - z$ can be mapped to P via another affine transformation, it follows $\operatorname{rank}_{\mathrm{psd}} \pi_1(P) - z = k$.

  From the first statement of the remark, we know that $\operatorname{rank}_{\mathrm{psd}} \pi_1(P) - z =$ $= \operatorname{rank}_{\mathrm{psd}} S_{\pi_1(P)-z}$. Now $\pi_1(P) - z$ has the same slack matrix as $\pi_1(P)$ (see Lemma 1.6 below) and we get $k = \operatorname{rank}_{\mathrm{psd}} \pi_1(P) - z = \operatorname{rank}_{\mathrm{psd}} S_{\pi_1(P)-z} = \operatorname{rank}_{\mathrm{psd}} S_{\pi_1(P)} = \operatorname{rank}_{\mathrm{psd}} \pi_1(P)$.

  The proof for $\operatorname{rank}_+ P$ works analogously.

□

Lemma 1.6.
Let $P \subset \mathbb{R}^n$ be a polytope with vertices $p_1, \ldots, p_v$ and inequality representation $P = \{x \in \mathbb{R}^n \mid b_1 - \langle a_1, x \rangle \geq 0, \ldots, b_f - \langle a_f, x \rangle \geq 0\}$, and let $z \in \mathbb{R}^n$. Then $S_P = S_{P+z}$.

Proof. The polytope $P+z$ has vertices $p_1+z,\dots,p_v+z$ and it holds $P+z=\{x\in\mathbb{R}^n \mid b_1-\langle a_1,x\rangle+\langle a_1,z\rangle\geq 0,\dots,b_f-\langle a_f,x\rangle+\langle a_f,z\rangle\geq 0\}$. Therefore, we obtain $(S_{P+z})_{ij}=b_j-\langle a_j,p_i+z\rangle+\langle a_j,z\rangle=b_j-\langle a_j,p_i\rangle-\langle a_j,z\rangle+\langle a_j,z\rangle=(S_P)_{ij}$. □

The following proposition compares psd rank with usual rank:

Proposition 1.7.
[3] Let $M\in\mathbb{R}_+^{p\times q}$. Then

$$\frac{1}{2}\sqrt{1+8\operatorname{rank}M}-\frac{1}{2}\leq\operatorname{rank}_{\text{psd}}M\leq\min(\{p,q\}).$$

Proof. (1) Let $\operatorname{rank}_{\text{psd}}M=k$ and assume that $A^1,\dots,A^p,B^1,\dots,B^q$ give an $\mathcal{S}_+^k$-factorisation of M. For $N\in\mathcal{S}_+^k$ define

$$\operatorname{vec}(N):=\Big(N_{11},N_{22},\dots,N_{kk},\sqrt{2}N_{12},\sqrt{2}N_{13},\dots,\sqrt{2}N_{1k},\\ \sqrt{2}N_{23},\dots,\sqrt{2}N_{2k},\dots,\sqrt{2}N_{34},\dots,\sqrt{2}N_{(k-1)k}\Big).$$

Then $\operatorname{vec}(N)\in\mathbb{R}^{\binom{k+1}{2}}$ and

$$\langle\operatorname{vec}(A^i),\operatorname{vec}(B^j)\rangle=\sum_{l=1}^{k}A^i_{ll}B^j_{ll}+2\sum_{m=1}^{k-1}\sum_{n=m+1}^{k}A^i_{mn}B^j_{mn}=\\ =\sum_{m=1}^{k}\sum_{n=1}^{k}A^i_{mn}B^j_{mn}=\operatorname{Tr}(A^iB^j)=\langle A^i,B^j\rangle=M_{ij}.$$

Thus $\operatorname{rank}M\leq\binom{k+1}{2}$ and it follows

$$\operatorname{rank}M\leq\frac{(k+1)k}{2}\implies 0\leq k^2+k-2\operatorname{rank}M\implies k\geq\frac{-1+\sqrt{1+8\operatorname{rank}M}}{2}.$$

(2) Let e_j denote the jth standard unit vector. Since $\langle\operatorname{diag}(M_{i-}),\operatorname{diag}(e_j)\rangle=$ $=\operatorname{Tr}(\operatorname{diag}(M_{i-})\cdot\operatorname{diag}(e_j))=\langle M_{i-},e_j\rangle=M_{ij}$, there exists an $\mathcal{S}_+^q$-factorisation of M. Similarly, one gets a $\mathcal{S}_+^p$-factorisation of M.

□

2 Hadamard square roots

In this section we will use Hadamard square roots to study the psd rank of nonnegative matrices.

Definition 2.1.
Any matrix whose (i,j)-entry is a square root of the (i,j)-entry of M is called a *Hadamard square root* of M and is denoted by $\sqrt{M}$. In particular, let $\sqrt[+]{M}$ be the all-nonnegative Hadamard square root of M.

The *square root rank* of M is defined as $\operatorname{rank}_{\sqrt{}}M:=\min(\{\operatorname{rank}\sqrt{M}\})$.

Proposition 2.2.
Let $M \in \mathbb{R}_+^{p\times q}$ be a nonnegative matrix. Then $\operatorname{rank}_{\text{psd}} M \leq \operatorname{rank}_{\surd} M$.

Proof. If $\sqrt{M}$ is a Hadamard square root of M of rank r, then there exist vectors $a_1, \dots, a_p$ and $b_1, \dots, b_q \in \mathbb{R}^r$ such that $\left(\sqrt{M}\right)_{ij} = \langle a_i, b_j \rangle$. We obtain

$$M_{ij} = \langle a_i, b_j \rangle^2 = (a_i^\intercal b_j)^2 = \left(\sum_{k=1}^{r} a_{ik} b_{jk}\right)^2 = \sum_{k=1}^{r}\sum_{l=1}^{r} a_{ik}a_{il}b_{jk}b_{jl} =$$
$$= \operatorname{Tr}\left(\begin{pmatrix} a_{i1}^2 & a_{i1}a_{i2} & \cdots & a_{i1}a_{ir} \\ a_{i1}a_{i2} & a_{i2}^2 & \cdots & a_{i2}a_{ir} \\ \vdots & \vdots & \ddots & \vdots \\ a_{i1}a_{ir} & a_{i2}a_{ir} & \cdots & a_{ir}^2 \end{pmatrix} \begin{pmatrix} b_{j1}^2 & b_{j1}b_{j2} & \cdots & b_{j1}b_{jr} \\ b_{j1}b_{j2} & b_{j2}^2 & \cdots & b_{j2}b_{jr} \\ \vdots & \vdots & \ddots & \vdots \\ b_{j1}b_{jr} & b_{j2}b_{jr} & \cdots & b_{jr}^2 \end{pmatrix}\right) =$$
$$= \operatorname{Tr}\left(a_i a_i^\intercal \cdot b_j b_j^\intercal\right) = \left\langle a_i a_i^\intercal, b_j b_j^\intercal \right\rangle$$

and thus get a $\mathcal{S}_+^r$-factorisation of M. Hence, $\operatorname{rank}_{\text{psd}} M \leq r$. □

Example 2.3.
This simple example shows that the upper bound in 2.2 can be strict:
Consider $M := \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$. It holds $\operatorname{rank} M = \operatorname{rank}_{\surd} M = 3$, but $\operatorname{rank}_{\text{psd}} M = 2$, as the follwing $\mathcal{S}_+^2$-factorisation of M shows:

$$A^1 := \begin{pmatrix} 0.5 & -0.5 \\ -0.5 & 1 \end{pmatrix}, A^2 := \begin{pmatrix} 0.5 & 0 \\ 0 & 0 \end{pmatrix}, A^3 := \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$
$$B^1 := \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}, B^2 := \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, B^3 := \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}.$$

One can easily check that $M_{ij} = \langle A^i, B^j \rangle$.

Lemma 2.4.
$k = \operatorname{rank}_{\surd} M$ is the smallest k that admits a $\mathcal{S}_+^k$- factorisation for $M \in \mathbb{R}_+^{p\times q}$ where all factors have rank one.

Proof. (1) If $k = \operatorname{rank}_{\surd} M$, then there exists a Hadamard square root $\sqrt{M}$ of M such that $\operatorname{rank} \sqrt{M} = k$ and the proof of proposition 2.2 gives a $\mathcal{S}_+^k$-factorisation of M where all factors have rank one.

(2) $k \geq \operatorname{rank}_{\surd} M$:
Let $a_1 a_1^\intercal, \dots, a_p a_p^\intercal \in \mathcal{S}_+^k$ and $b_1 b_1^\intercal, \dots, b_q b_q^\intercal \in \mathcal{S}_+^k$ be a $\mathcal{S}_+^k$-factorisation of M with rank one factors. Then $M_{ij} = \langle a_i a_i^\intercal, b_j b_j^\intercal \rangle = \langle a_i, b_j \rangle^2$ and the matrix $\sqrt{M}$ with $\left(\sqrt{M}\right)_{ij} = \langle a_i, b_j \rangle$ is a Hadamard square root of M with $\operatorname{rank} \sqrt{M} \leq k$.

□

Next, we show a method to increase the psd rank of a matrix by one.

Proposition 2.5.
Let $M \in \mathbb{R}_+^{p\times q}$ *with* $\operatorname{rank_{psd}} M = k, w \in \mathbb{R}_+^q$, $\alpha > 0$ *and* $M' := \begin{pmatrix} M & \mathbf{0} \\ w & \alpha \end{pmatrix}$.
Then $\operatorname{rank_{psd}} M' = k+1$. *Furthermore, in any* $\mathcal{S}_+^{k+1}$*-factorisation of* M', *the factor associated to the last column of* M' *is of rank one.*

Proof. (1) First, we show that $\operatorname{rank_{psd}} M'$ cannot be smaller than $k+1$:
Assume that there is a $\mathcal{S}_+^k$-factorisation of M' with factors $A_1, \ldots, A_p, A \in \mathcal{S}_+^k$ associated to its rows and $B_1, \ldots, B_q, B \in \mathcal{S}_+^k$ associated to its columns. From $\langle A, B\rangle = \alpha \neq 0$ we get $A \neq 0 \neq B$. Let $r = \operatorname{rank} B > 0$. Then there exists an orthogonal matrix U such that $U^{-1}BU = \operatorname{diag}(\lambda_1, \ldots, \lambda_r, 0, \ldots, 0) =: D$, where $\lambda_1, \ldots, \lambda_r$ are the positive eigenvalues of B. Let $A_i' := U^{-1}A_iU \in \mathcal{S}_+^k \ \forall i = 1, \ldots, p$. Then $\forall i = 1, \ldots, p$:

$$\langle D, A_i'\rangle = \langle U^{-1}BU, U^{-1}A_iU\rangle = \operatorname{Tr}(U^{-1}BA_iU) = \operatorname{Tr}(BA_i) = \langle B, A_i\rangle = 0.$$

Because the diagonal entries of A_i' are nonnegative and those of D positive, the first r diagonal entries of A_i' must be zero, since $\operatorname{Tr}(DA_i') = 0$. Since A_i' is psd, it follows that the first r rows and columns of A_i' are all zero (if this were not the case, there would be at least one negative eigenvalue of A_i'). For $B_j' := U^{-1}B_jU, j = 1, \ldots, q$ we have

$$\langle A_i', B_j'\rangle = \operatorname{Tr}(U^{-1}A_iUU^{-1}B_jU) = \operatorname{Tr}(U^{-1}A_iB_jU) = \operatorname{Tr}(A_iB_j) = \langle A_i, B_j\rangle = M_{ij}$$

$\forall i = 1, \ldots, p$ and $j = 1, \ldots, q$. Since A_i' only has nonzero entries in its bottom right $(k-r)\times(k-r)$-block, it follows that $M_{ij} = \langle \overline{A_i}, \overline{B_j}\rangle$, where $\overline{A_i}$ and $\overline{B_j}$ are the bottom right $(k-r)\times(k-r)$-submatrices of A_i' and B_j' respectively. Now we have found a $\mathcal{S}_+^{k-r}$-factorisation of M which is a contradiction to $\operatorname{rank_{psd}} M = k$. Therefore, $\operatorname{rank_{psd}} M' \geq k+1$.

(2) If $A_1, \ldots, A_p, B_1, \ldots, B_q \in \mathcal{S}_+^k$ is an $\mathcal{S}_+^k$-factorisation of M, then $A_1', \ldots, A_p', A'$, $B_1', \ldots, B_q', B' \in \mathcal{S}_+^{k+1}$ is an $\mathcal{S}_+^{k+1}$-factorisation of M', where

$$A_i' := \begin{pmatrix} A_i & \mathbf{0} \\ \mathbf{0} & 0 \end{pmatrix}, B_j' := \begin{pmatrix} B_j & \mathbf{0} \\ \mathbf{0} & w_j \end{pmatrix}, A' := \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 1 \end{pmatrix}, B' := \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \alpha \end{pmatrix}.$$

This proofs that $\operatorname{rank_{psd}} M' = k+1$.

(3) Now let B be the matrix associated to the last column of M' in a $\mathcal{S}_+^{k+1}$-factorisation of M'. Since $\alpha > 0$, $B \neq 0$. So, let $r = \operatorname{rank} B > 0$. By applying the same arguments as above, we get a $\mathcal{S}_+^{k+1-r}$-factorisation of M. Because of $\operatorname{rank_{psd}} M = k$ and $r > 0$, $r = \operatorname{rank} B$ must be one.

□

Example 2.6.
If $M \in \mathbb{R}_+^{n\times n}$ is a diagonal matrix with positive entries, then $\operatorname{rank}_{\mathrm{psd}} M = n$. Furthermore, each factor of any $\mathcal{S}_+^n$-factorisation of M is of rank one.

Proof. The proof is by induction on n. For $n = 1$, the first statement is trivially true. If $\operatorname{rank}_{\mathrm{psd}} M = n$ for a diagonal matrix $M \in \mathbb{R}_+^{n\times n}$ with positive entries, then $\operatorname{rank}_{\mathrm{psd}} M' = n+1$, where $M' = \begin{pmatrix} M & \mathbf{0} \\ \mathbf{0} & \alpha \end{pmatrix}$ and $\alpha > 0$ by Proposition 2.5. That each factor of a $\mathcal{S}_+^n$-factorisation of M must have rank one follows from the second part of Proposition 2.5 applied to M and $M^\intercal$. □

3 Psd ranks of polytopes

For this section, let $P \subset \mathbb{R}^n$ be a n-dimensional polytope.

Lemma 3.1.
$\operatorname{rank} S_P = n + 1$.

Proof. If the vertices of P are $p_1, \ldots, p_v$ and $P = \{x \in \mathbb{R}^n \mid b_1 - \langle a_1, x\rangle \geq 0, \ldots, b_f - \langle a_f, x\rangle \geq 0\}$ is an irredundant inequality representation, then $(S_P)_{ij} = b_j - \langle a_j, p_i\rangle$ and

$$S_P = \begin{pmatrix} 1 & p_1^\intercal \\ \vdots & \vdots \\ 1 & p_v^\intercal \end{pmatrix} \begin{pmatrix} b_1 & \cdots & b_f \\ -a_1 & \cdots & -a_f \end{pmatrix}.$$

Call the first factor F and the second one G.

Since P is a n-dimensional polytope, there exist $n+1$ vertices of P such that no vertex lies in the linear span of the other n vertices, implying that $\operatorname{rank} F \geq n + 1$ and thus, because $F \in \mathbb{R}^{v\times(n+1)}$, $\operatorname{rank} F = n + 1$.

Now assume that $\operatorname{rank} G \leq n$. Then there exists a nonzero $c \in \mathbb{R}^{n+1}$ such that $c^\intercal G = (0, \ldots, 0)$. If $c_1 \neq 0$, then normalise c such that $c_1 = 1$ and set $c' := (c_2, \ldots, c_{n+1})^\intercal$. Then, for all j: $b_j - \langle a_j, c'\rangle = 0$, implying that c' lies on every facet of P, which is a contradiction. If $c_1 = 0$, it follows $\langle a_j, c'\rangle = 0$ (c' as above) for all $j = 1, \ldots, f$. This means that c' (as a vector) is parallel to every facet of P, which is a contradiction, since P is fulldimensional. Thus, $\operatorname{rank} G = n + 1$.

As both factors have rank $n + 1$, it also holds $\operatorname{rank} S_P = n + 1$. □

Proposition 3.2.
$\operatorname{rank}_{\mathrm{psd}} P \geq n + 1$. *If equality holds, every $\mathcal{S}_+^{n+1}$-factorisation of S_P has only rank one factors.*

Proof. The proof is by induction on the dimension n. For $n = 1$, P is a line segment with vertices p_1, p_2 and facets f_1, f_2, where $p_1 = f_2$ and $p_2 = f_1$. Because of $(S_P)_{12} = b_1 - a_1 p_2 = b_1 - a_1 f_1 = 0$, and, analogously, $(S_P)_{21} = 0$, the slack matrix S_P of P is a 2×2 diagonal matrix with positive entries. From Example 2.6 we get that $\operatorname{rank}_{\mathrm{psd}} P = \operatorname{rank}_{\mathrm{psd}} S_P = 2$ and any $\mathcal{S}_+^2$-factorisation only uses rank one factors.

Now suppose the first statement holds up to dimension $n-1$. Let $P \subset \mathbb{R}^n$ be a full-dimensional polytope. Let F be a facet of P with vertices $p_1, \dots, p_s$ and facets $f_1, \dots, f_t$ and slack matrix S_F. Assume that f_j corresponds to the facet F_j of P for $j = 1, \dots, t$. Then, by induction hypothesis, $\operatorname{rank}_{\text{psd}} F \geq n$. Suppose that, if $p \notin F$ is a vertex of P, the top left $(s+1) \times (t+1)$ submatrix of S_P is indexed by $p_1, \dots, p_s, p$ in the rows and $F_1, \dots, F_t, F$ in the columns. We will call that submatrix S'_F. S'_F has the form

$$S'_F = \begin{pmatrix} S_F & \mathbf{0} \\ * & \alpha \end{pmatrix},$$

where $\alpha > 0$. From Proposition 2.5 we get that $\operatorname{rank}_{\text{psd}} S_P \geq \operatorname{rank}_{\text{psd}} S'_F \geq n+1$.

If $\operatorname{rank}_{\text{psd}} P = n+1$, then there exists a $\mathcal{S}_+^{n+1}$-factorisation of S_P, and therefore of S'_F. By Proposition 2.5, the factor corresponding to the facet F must be of rank one. Applying this argumentation to all facets F of P, it follows that all factors indexed by the facets of P have rank one. Recall that $S_P^\intercal$ is, up to row scaling, a slack matrix of the polar dual polytope P° and therefore, all factors corresponding to the vertices of P also have rank one. □

Corollary 3.3.
If a facet of a polytope P has psd rank k, then $\operatorname{rank}_{\text{psd}} P \geq k+1$. Especially, if $P \subset \mathbb{R}^n$ is a n-dimensional polytope with psd rank $n+1$, then, for every i-dimensional face F of P, $\operatorname{rank}_{\text{psd}} F = i+1$. □

Theorem 3.4.
$\operatorname{rank}_{\text{psd}} P = n+1$ *if and only if* $\operatorname{rank}_{\sqrt{}} S_P = n+1$.

Proof. By remark 1.5, $\operatorname{rank}_{\text{psd}} P = \operatorname{rank}_{\text{psd}} S_P$. If $\operatorname{rank}_{\sqrt{}} S_P = n+1$, then, by Proposition 2.2, $\operatorname{rank}_{\text{psd}} P = \operatorname{rank}_{\text{psd}} S_P \leq \operatorname{rank}_{\sqrt{}} S_P = n+1$ and $\operatorname{rank}_{\text{psd}} P \geq n+1$ (Proposition 3.2) implies $\operatorname{rank}_{\text{psd}} = n+1$.

On the other hand, if $\operatorname{rank}_{\text{psd}} P = n+1$, then there exists a $\mathcal{S}_+^{n+1}$-factorisation of S_P, whose factors are by Proposition 3.2 all of rank one. By Lemma 2.4, $\operatorname{rank}_{\sqrt{}} S_P \geq n+1$. Since $\operatorname{rank}_{\text{psd}} S_P \leq \operatorname{rank}_{\sqrt{}} S_P$, $\operatorname{rank}_{\sqrt{}} S_P = n+1$. □

Example 3.5.
Consider the pentagon P with vertices

$$p_1 = (0,0), p_2 = (1,0), p_3 = (2,1), p_4 = (1,2), p_5 = (0,1)$$

and inequality representation

$$P = \left\{ \begin{pmatrix} x \\ y \end{pmatrix} \in \mathbb{R}^2 \;\middle|\; -\left\langle \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \begin{pmatrix} x \\ y \end{pmatrix} \right\rangle \geq 0, 1 - \left\langle \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \begin{pmatrix} x \\ y \end{pmatrix} \right\rangle \geq 0, \right.$$
$$\left. 3 - \left\langle \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} x \\ y \end{pmatrix} \right\rangle \geq 0, 1 - \left\langle \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \begin{pmatrix} x \\ y \end{pmatrix} \right\rangle \geq 0, -\left\langle \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \begin{pmatrix} x \\ y \end{pmatrix} \right\rangle \geq 0 \right\}.$$

Then we obtain the slack matrix

$$S_P = \begin{pmatrix} 0 & 4 & 12 & 4 & 0 \\ 0 & 0 & 8 & 8 & 2 \\ 2 & 0 & 0 & 8 & 4 \\ 4 & 8 & 0 & 0 & 2 \\ 2 & 8 & 8 & 0 & 0 \end{pmatrix}$$

(the inequalities have been multiplied by 2, 4, 4, 4, and 2, respectively). Theorem 4.5 will show that the psd rank of P is at least four. Due to the following $\mathcal{S}_+^4$-factorisation of P we have $\operatorname{rank}_{\mathrm{psd}} P = 4$:
It holds $(S_P)_{ij} = \langle A^i, B^j \rangle$ with A^i, B^j as follows:

$$A^1 := \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 1 & -1 \\ 0 & 1 & 1 & -1 \\ 0 & -1 & -1 & 1 \end{pmatrix}, A^2 := \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}, A^3 := \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix},$$

$$A^4 := \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}, A^5 := \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix},$$

$$B^1 := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}, B^2 := \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}, B^3 := \begin{pmatrix} 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix},$$

$$B^4 := \begin{pmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{pmatrix}, B^5 := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Now let us look at $\operatorname{rank}_{\sqrt{}} S_P$. Let

$$S := \begin{pmatrix} 0 & a & b & c & 0 \\ 0 & 0 & d & e & f \\ g & 0 & 0 & h & i \\ j & k & 0 & 0 & l \\ m & n & o & 0 & 0 \end{pmatrix}.$$

Then there exists a Hadamard square root of S_P with rank ≤ 4 if and only if there exists a solution to this system of equations:

$$\det(S) = 0, a^2 = 4, b^2 = 12, c^2 = 4, \ldots, o^2 = 8.$$

Using a computer one can easily check that this system of equations has no solution and it follows $\operatorname{rank}_{\sqrt{}} S_P = 5$.

Thus, the psd rank of a polytope may be smaller than the square root rank of its slack matrix.

Example 3.6.
Consider a pentagonal pyramid $PP \subset \mathbb{R}^3$ with the pentagon P from Example 3.5 as the base. The vertices of PP are

$$p_1 = \begin{pmatrix}0\\0\\0\end{pmatrix}, p_2 = \begin{pmatrix}1\\0\\0\end{pmatrix}, p_3 = \begin{pmatrix}2\\1\\0\end{pmatrix}, p_4 = \begin{pmatrix}1\\2\\0\end{pmatrix}, p_5 = \begin{pmatrix}0\\1\\0\end{pmatrix}, p_6 = \begin{pmatrix}1\\1\\1\end{pmatrix}$$

and it holds

$$PP = \{(x, y, z) \in \mathbb{R}^3 \mid y - z \geq 0, 1 - x + y - z \geq 0, 3 - x - y - z \geq 0, \\ 1 + x - y - z \geq 0, x - z \geq 0, z \geq 0\}.$$

Since P is a facet of PP and $\operatorname{rank}_{\text{psd}} P = 4$ (see above), we get from Corollary 3.3 that $\operatorname{rank}_{\text{psd}} PP \geq 5$. A slack matrix of PP is given by

$$S_{PP} = \begin{pmatrix}0 & 4 & 12 & 4 & 0 & 0\\ 0 & 0 & 8 & 8 & 2 & 0\\ 2 & 0 & 0 & 8 & 4 & 0\\ 4 & 8 & 0 & 0 & 2 & 0\\ 2 & 8 & 8 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 2\end{pmatrix}.$$

The top left 5×5 submatrix of S_{PP} is equal to S_P and thus, by Proposition 2.5, $\operatorname{rank}_{\text{psd}} PP = \operatorname{rank}_{\text{psd}} S_{PP} = 5$.

Example 3.7.
Let $H \subset \mathbb{R}^2$ be a regular hexagon with vertices

$$p_1 = \begin{pmatrix}1\\0\end{pmatrix}, p_2 = \begin{pmatrix}\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix}, p_3 = \begin{pmatrix}\frac{-1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix}, p_4 = \begin{pmatrix}-1\\0\end{pmatrix}, p_5 = \begin{pmatrix}\frac{-1}{2}\\ \frac{-\sqrt{3}}{2}\end{pmatrix}, p_6 = \begin{pmatrix}\frac{1}{2}\\ \frac{-\sqrt{3}}{2}\end{pmatrix}$$

and inequality representation

$$H = \Bigg\{ \begin{pmatrix}x\\y\end{pmatrix} \in \mathbb{R}^2 \;\Bigg|\; 2 - \left\langle \begin{pmatrix}2\\2/\sqrt{3}\end{pmatrix}, \begin{pmatrix}x\\y\end{pmatrix} \right\rangle \geq 0, 2 - \left\langle \begin{pmatrix}0\\4/\sqrt{3}\end{pmatrix}, \begin{pmatrix}x\\y\end{pmatrix} \right\rangle \geq 0, \\ 2 - \left\langle \begin{pmatrix}-2\\2/\sqrt{3}\end{pmatrix}, \begin{pmatrix}x\\y\end{pmatrix} \right\rangle \geq 0, 2 - \left\langle \begin{pmatrix}-2\\-2/\sqrt{3}\end{pmatrix}, \begin{pmatrix}x\\y\end{pmatrix} \right\rangle \geq 0, \\ 2 - \left\langle \begin{pmatrix}0\\-4/\sqrt{3}\end{pmatrix}, \begin{pmatrix}x\\y\end{pmatrix} \right\rangle \geq 0, 2 - \left\langle \begin{pmatrix}2\\-2/\sqrt{3}\end{pmatrix}, \begin{pmatrix}x\\y\end{pmatrix} \right\rangle \geq 0 \Bigg\}.$$

The slack matrix S_H of H is then given by

$$S_H = \begin{pmatrix}0 & 2 & 4 & 4 & 2 & 0\\ 0 & 0 & 2 & 4 & 4 & 2\\ 2 & 0 & 0 & 2 & 4 & 4\\ 4 & 2 & 0 & 0 & 2 & 4\\ 4 & 4 & 2 & 0 & 0 & 2\\ 2 & 4 & 4 & 2 & 0 & 0\end{pmatrix}.$$

It holds $\operatorname{rank} \sqrt[+]{S_H} = 5$, while the following Hadamard square root of H has rank four:

$$\begin{pmatrix} 0 & \sqrt{2} & 2 & 2 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} & 2 & 2 & \sqrt{2} \\ \sqrt{2} & 0 & 0 & \sqrt{2} & 2 & 2 \\ -2 & -\sqrt{2} & 0 & 0 & \sqrt{2} & 2 \\ 2 & -2 & -\sqrt{2} & 0 & 0 & \sqrt{2} \\ \sqrt{2} & 2 & -2 & -\sqrt{2} & 0 & 0 \end{pmatrix}.$$

This example shows that it is not enough to compute $\operatorname{rank} \sqrt[+]{S_P}$ in order to get $\operatorname{rank}_{\sqrt{}} S_P$.

Example 3.8.
Let H be as in Example 3.7. In Proposition 3.2 and Theorem 3.4 we have shown that if P is an n-dimensional polytope with $\operatorname{rank}_{\text{psd}} P = n+1$, then $\operatorname{rank}_{\text{psd}} P = \operatorname{rank}_{\sqrt{}} P$ and all $\mathcal{S}_+^{n+1}$-factorisations of S_P have only rank one factors.

From Theorem 4.5 we have that $\operatorname{rank}_{\text{psd}} H \geq 4$, hence we get from Theorem 3.4 that the square root rank of S_H is at least four and since we have seen a Hadamard square root of S_H of rank four in the example above, it holds $\operatorname{rank}_{\sqrt{}} S_H = 4$. We also get from Theorem 4.5 that $\operatorname{rank}_{\text{psd}} H \geq 4$ and the following $\mathcal{S}_+^4$-factorisation proofs that $\operatorname{rank}_{\text{psd}} H = 4$:

$$A^1 := \begin{pmatrix} 1 & -1 & 0 & 1 \\ -1 & 1 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 1 & -1 & 0 & 1 \end{pmatrix}, A^2 := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & -1 \\ 0 & 1 & 1 & -1 \\ 0 & -1 & -1 & 1 \end{pmatrix}, A^3 := \begin{pmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$A^4 := \begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{pmatrix}, A^5 := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 1 \\ 0 & -1 & 1 & -1 \\ 0 & 1 & -1 & 1 \end{pmatrix}, A^6 := \begin{pmatrix} 1 & -1 & 1 & 0 \\ -1 & 1 & -1 & 0 \\ 1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$B^1 := \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, B^2 := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}, B^3 := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$B^4 := \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, B^5 := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}, B^6 := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Note that $\operatorname{rank} A^i = 2$ for all $i = 1, \ldots, 6$.

Thus, there can be $\mathcal{S}_+^{\operatorname{rank}_{\text{psd}} P}$-factorisations of a slack matrix S_P of a polytope P, where there are factors with rank greater than one even if $\operatorname{rank}_{\text{psd}} P = \operatorname{rank}_{\sqrt{}} P$.

4 Polytopes of minimum psd rank

For a n-dimensional polytope $P \subset \mathbb{R}^n$, $\operatorname{rank}_+ P \geq n+1$ and the only n-dimensional polytopes that achieve the lower bound of $n+1$ are simplices. In this section, we will see that there are several classes of polytopes that achieve the minimum psd rank of $n+1$.

Definition 4.1.
A full fulldimensional polytope $P \subset \mathbb{R}^n$ is called *2-level* if its slack matrixes entries are all 0 or 1.

Remark 4.2.
A polytope P is 2-level if and only if for every facet F of P, all vertices of P lie on the union of the facet F and one hyperplane parallel to the hyperplane containing F. For example, any n-dimensional cube is 2-level.

Corollary 4.3.
If P is a n-dimensional 2-level polytope, then $\operatorname{rank}_{\text{psd}} P = n+1$ and every $\mathcal{S}_+^{n+1}$-factorisation of P only has factors of rank one.

Proof. Let S_P be a slack matrix of a n-dimensional 2-level polytope P. We have $\operatorname{rank}_{\sqrt{}} S_P \leq \operatorname{rank} \sqrt[+]{S_P} = \operatorname{rank} S_P = n+1$ and therefore, by Proposition 2.2, $\operatorname{rank}_{\text{psd}} S_P \leq \operatorname{rank}_{\sqrt{}} S_P \leq n+1$ and thus $\operatorname{rank}_{\text{psd}} P = \operatorname{rank}_{\text{psd}} S_P = n+1$. The second statement follows from Proposition 3.2. □

Theorem 4.4.
For any fulldimensional polytope $P \subset \mathbb{R}^n$ with $n+2$ vertices we have $\operatorname{rank}_{\text{psd}} P = n+1$.

Proof. Let P be a polytope with $n+2$ vertices and f facets. Then $S_P \in \mathbb{R}_+^{(n+2)\times f}$ and $\operatorname{rank} S_P = n+1$. Since $\operatorname{rank} S_P = n+1$, there exist $a_i \in \mathbb{R}$ (not all of them equal to zero) such that $\sum_{i=1}^{n+2} a_i (S_P)_{i-} = (0,\dots,0)$. Because every vertex lies on at least n different facets, each column of S_P has at least n zeros. Thus, considering above equation componentwise, we have that for all $j = 1,\dots,f$ there exist $i_1, i_2 \in \{1,\dots,n+2\}$ such that $a_{i_1}(S_P)_{i_1 j} + a_{i_2}(S_P)_{i_2 j} = 0$. Now let $b_i := \operatorname{sgn}(a_i)\sqrt{|a_i|}$. Then $b_{i_1}\sqrt{(S_P)_{i_1 j}} + b_{i_2}\sqrt{(S_P)_{i_2 j}} = 0$. Since this is true for all components, we get that $\sum_{i=1}^{n+2} b_i \sqrt{(S_P)_{i-}} = (0,\dots,0)$ and thus $\operatorname{rank} \sqrt[+]{S_P} = n+1 = \operatorname{rank}_{\sqrt{}} S_P$. This together with Theorem 3.4 proves the statement. □

Theorem 4.5.
Let $P \subset \mathbb{R}^2$ be a 2-dimensional polytope. Then $\operatorname{rank}_{\text{psd}} P = 3 \iff P$ has at most four vertices.

Proof. "$\Leftarrow$": Follows from 4.4.

"$\Rightarrow$": Let $P \subset \mathbb{R}^2$ be a polytope with at least 5 vertices. Since the psd rank is invariant under affine transformations we can assume that two facets of P are given by $f_1 = \{(x,y) \in \mathbb{R}^2 \mid x \geq 0\}$ and $f_2 = \{(x,y) \in \mathbb{R}^2 \mid y \geq 0\}$ with vertices $v_1 = (0,0)$, $v_2 = (0,1)$ and $v_3 = (1,0)$. Furthermore, let $v_4 = (a,b)$ and $v_5 = (c,d)$ be the vertices sharing an edge with $(0,1)$ and $(1,0)$, respectively. These two edges are given by $f_3 = \{(x,y) \in \mathbb{R}^2 \mid y \leq \frac{b-1}{a}x + 1\} = \{(x,y) \in \mathbb{R}^2 \mid a + (b-1)x - ay \geq 0\}$ and $f_4 = \{(x,y) \in \mathbb{R}^2 \mid y \geq \frac{d}{c-1}(x-1)\} = \{(x,y) \in \mathbb{R}^2 \mid (c-1)y - d(x-1) \geq 0\}$. Then, the 5×4 submatrix S'_P of S_P indexed by these vertices and facets is given by

$$S'_P = \begin{pmatrix} 0 & 0 & a & d \\ 0 & 1 & 0 & c-1+d \\ 1 & 0 & a+b-1 & 0 \\ a & b & 0 & cb-b-da+d \\ c & d & bc-c-ad+a & 0 \end{pmatrix}.$$

We now show that $\operatorname{rank}_{\sqrt{}} S_P \geq 4$. Theorem 3.4 then yields $\operatorname{rank}_{\text{psd}} P > 3$, which proves the statement.

It is enough to show that any Hadamard square root H of the top left 4×4 submatrix of S'_P has rank four. Assume that

$$H = \begin{pmatrix} 0 & 0 & \pm\sqrt{a} & \pm\sqrt{d} \\ 0 & \pm 1 & 0 & \pm\sqrt{c-1+d} \\ \pm 1 & 0 & \pm\sqrt{a+b-1} & 0 \\ \pm\sqrt{a} & \pm\sqrt{b} & 0 & \pm\sqrt{cb-b-da+d} \end{pmatrix}$$

has rank three. It is obvious that the first three rows are independent, hence we can write the fourth row as a linear combination of the first three and it must hold

$$\begin{aligned} H_{4-} &= \pm\sqrt{a}H_{3-} \pm \sqrt{b}H_{2-} \mp \sqrt{a+b-1}H_{1-} = \\ &= \left(\pm\sqrt{a}, \pm\sqrt{b}, 0, \mp\sqrt{d(a+b-1)} \pm \sqrt{b(d+c-1)}\right). \end{aligned}$$

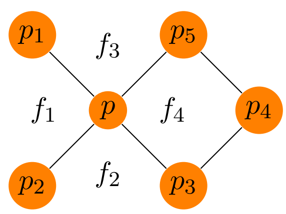
Let $\alpha := b(d+c-1)$ and $\beta := d(a+b-1)$. Thus

$$H_{44} = \pm\sqrt{cb-b-da+d} = \pm\sqrt{\alpha-\beta} \stackrel{!}{=} \pm\sqrt{\alpha} \mp \sqrt{\beta},$$

and this implies $\alpha = \beta \to bc - b = da - d \to \frac{b}{a-1} = \frac{d}{c-1}$. Hence, the slopes of the lines between (a,b) and $(1,0)$, and (c,d) and $(1,0)$ are the same, meaning that $(a,b),(c,d)$ and $(1,0)$ are collinear and cannot be all vertices, except when $(a,b) = (c,d)$. □

Lemma 4.6.
Let $P \subset \mathbb{R}^3$ be a fulldimensional polytope with psd rank four and p be a vertex of P of degree four. Then the four faces incident to p are all triangles.

Proof. Assume that one of the four faces is not a triangle. By Corollary 3.3, this face has psd rank 3 and hence, by Theorem 4.5, it is a quadrilateral. Thus, P contains the configuration



where $p_1, \dots, p_5$ are vertices of P. According to Lemma 3.1, $\operatorname{rank} S_P = 4$. Since $\operatorname{rank}_{\text{psd}} P = 4$, by Theorem 3.4, there exists a Hadamard square root $\sqrt{S_P}$ of S_P of rank four. Let f_1, f_2, f_3 and f_4 be the faces of P containing the vertices p, p_1, p_2; p, p_2, p_3; p, p_1, p_5 and p, p_3, p_4, p_5, respectively and M be the 5×4 - submatrix of $\sqrt{S_P}$ indexed by p, p_1, p_2, p_3, p_4 in the rows and f_1, f_2, f_3, f_4 in the columns. Then, by scaling the columns of S_P accordingly, it holds

$$M = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & a \\ 1 & 0 & b & 0 \\ c & d & e & 0 \end{pmatrix},$$

where $a, b, c, d, e > 0$. Since the four rows of $\sqrt{S_P}$ (and S_P) corresponding to the first four rows of M are clearly independent, we can write the row of $\sqrt{S_P}$ (and S_P) corresponding to the fifth row of M as a linear combination of the other four. This yields the conditions $d + ae = abc$ (for $\sqrt{S_P}$) and $d^2 + a^2e^2 = a^2b^2c^2$ (for S_P), implying $d^2 + a^2e^2 = d^2 + a^2e^2 + 2ade$ and thus $ade = 0$, which is a contradiction to $a, b, c, d, e > 0$. $\square$

Definition 4.7.
Let $\mathfrak{F}(P)$ denote the set of all faces of a polytope P. Two polytopes Q and Q' are called *combinatorially equivalent*, if there exists an isomorphism $f : \mathfrak{F}(Q) \to \mathfrak{F}(Q')$ which preserves the partial order given by inclusion.

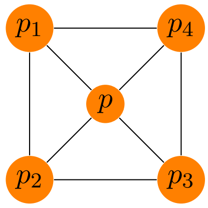
Remark 4.8.
Roughly speaking, two polytopes that are combinatorially equivalent have the same number of faces of each dimension arranged in the same way. For example, every three-dimensional polytope with six two-dimensional quadrilateral faces is combinatorially equivalent to a cube.

Theorem 4.9.
A fulldimensional polytope $P \subset \mathbb{R}^3$ with $\operatorname{rank}_{\text{psd}} P = 4$ is combinatorially equivalent to an octahedron, bisimplex, simplex, quadrilateral pyramid, triangular prism, or cube.

Proof. Let v, e, f be the number of vertices, edges, and faces of P, respectively. Further, $v_t := \#\{v \mid v \text{ vertex of } P, \deg v = 3\}$, $v_q := \#\{v \mid v \text{ vertex of } P, \deg v = 4\}$, $f_t := \#\{f \mid f \text{ triangular face of } P\}$ and $f_q := \#\{f \mid f \text{ quadrangular face of } P\}$. By counting the edges on each face, $2e = 3f_t + 4f_q$, and thus (by considering P°), we also have $2e = 3v_t + 4v_q$. Since $v - e + f = 2$ (Euler's formula) and $v = v_t + v_q$, $f = f_t + f_q$, we get $2e = 2v_t + 2v_q + 2f_t + 2f_q - 4$ and thus: $3v_t + 4v_q = 2v_t + 2v_q + 2f_t + 2f_q - 4 \Rightarrow v_t = 2f_t + 2f_q - 4 - 2v_q$, and analogously, $f_t = 2v_t + 2v_q - 4 - 2f_q$, from which we get that v_t and f_t are even and $v_t + f_t = 2v_t + 2f_t - 8 \Rightarrow v_t + f_t = 8$. Therefore, the only polytopes we have to consider are polytopes, where (v_t, f_t) equals $(0, 8)$, $(2, 6)$, $(4, 4)$, $(6, 2)$ and $(8, 0)$.

(1) $(v_t, f_t) = (0, 8)$: In this case, every vertex of P has degree four. From Lemma 4.6 we get that all faces of P must be triangular. An octahedron is the only polytope in $\mathbb{R}^3$ that satisfies these conditions.

(2) $(v_t, f_t) = (2, 6)$: Here, there must be at least one vertex p of P of degree four, and thus, by Lemma 4.6, P contains the following structure:



(a)

Since $v_t = 2$, at least two of the vertices p_1, p_2, p_3, p_4 have degree four. Now assume, that two of those degree four vertices (let's say, p_1 and p_2) are adjacent. Then, again by Lemma 4.6, p_1 and p_2 are contained in four faces which are triangles, implying that p_1 and p_2 each lie on two triangular faces not shown in the figure. Since p_1 already shares a face with p_2, they can only share at most one of the four extra triangular faces, meaning that there must be at least 7 triangular faces, which is a contradiction to $f_t = 6$.
Thus, only two out of p_1, p_2, p_3, p_4 have degree four and those two are nonadjacent. Again, both lie on two extra triangular faces not shown in the figure, and because of $f_t = 6$, they must share both of them. Consequently, P is a bisimplex

(3) $(v_t, f_t) = (4, 4)$: If $v_q = 0$, then there are only four vertices in total and the polytope must be a simplex. If $v_q > 0$, then, by Lemma 4.6, P contains structure (a). Since $f_t = 4$, p_i must have degree three, $i = 1, 2, 3, 4$ (if one of the p_i's had the degree four, then there would be too many triangular faces). Therefore, the polytope is a quadrilateral pyramid.

(4) $(v_t, f_t) = (6, 2)$: Then, for the polar dual of P we have $(v_t, f_t) = (2, 6)$, hence, the polar dual of P is a bisimplex and thus, P is a combinatorial triangular prism.

(5) $(v_t, f_t) = (8, 0)$: Again, for the polar dual of P: $(v_t, f_t) = (0, 8)$. Thus P is the polar dual of an octahedron, i.e. a cube.

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