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# On the semidefinite representation of real functions applied to symmetric matrices

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## Abstract

We present a new semidefinite representation for the trace of a real function  $f$  applied to symmetric matrices, when a semidefinite representation of the convex (or concave) function  $f$  is known. Our construction is intuitive, and yields a representation that is more compact than the previously known one. We also show with the help of matrix geometric means and a Riemannian metric over the set of positive definite matrices that for a rational exponent  $p$  in the interval  $(0, 1]$ , the matrix  $X$  raised to  $p$  is the largest element of a set represented by linear matrix inequalities. This result further generalizes to the case of the matrix  $A \sharp_p B$ , which is the point of coordinate  $p$  on the geodesic from  $A$  to  $B$ . We give numerical results for a problem inspired from the theory of experimental designs, which show that the new semidefinite programming formulation can yield an important speed-up factor.

**Keywords:** semidefinite representability, optimal experimental designs, SDP, matrix geometric mean

**AMS Classification:** 90C22, 62K05

## 1 Introduction

In this article we discuss semidefinite representations of scalar functions applied to symmetric matrices. We recall that it is possible to extend the definition of a function  $f : I \mapsto \mathbb{R}, x \rightarrow f(x)$ , where  $I$  is a real interval, to the set  $\mathbb{S}_m^I$  of  $m \times m$ -symmetric matrices whose spectrum lies in  $I$  as follows: if  $X = U \text{Diag}(\lambda_1, \dots, \lambda_m) U^T$  is an eigenvalue decomposition of  $X$ , then we define  $f(X) := U \text{Diag}(f(\lambda_1), \dots, f(\lambda_m)) U^T$ . Throughout this article we denote by  $\mathbb{S}_m$  (resp.  $\mathbb{S}_m^+, \mathbb{S}_m^{++}$ ) the set of  $m \times m$  symmetric (resp. positive semidefinite, positive definite) matrices.

If the scalar function  $f$  is semidefinite representable, then a result of Ben-Tal and Nemirovski can be used to construct a semidefinite representation of  $X \rightarrow \text{trace } f(X)$ . Indeed,  $\text{trace } f(X)$  can be rewritten as  $\sum_i f(\lambda_i)$ , which is a symmetric and semidefinite representable function of the eigenvalues of  $X$ , so that Proposition 4.2.1. in [5] applies.

In this article, we show that the semidefinite representation of  $x \rightarrow f(x)$  can be lifted to the matrix case  $X \rightarrow \text{trace } f(X)$  by an intuitive transformation

which involves Kronecker products (Theorem 3.1). For a convex (resp. concave) function, the resulting semidefinite representation of the epigraph (resp. hypograph)

$$\begin{aligned} E &= \{(t, X) \in \mathbb{R} \times \mathbb{S}_m : \text{trace } f(X) \leq t\} \\ \left( \text{resp. } H &= \{(t, X) \in \mathbb{R} \times \mathbb{S}_m : \text{trace } f(X) \geq t\} \right) \end{aligned}$$

is more compact than the one obtained from the general construction of Ben-Tal and Nemirovski, in which the Ky-Fan  $k$ -norms of  $M$  must be bounded for  $k = 1, \dots, m$ . Our numerical results of Section 5 moreover show that the semidefinite programs (SDP) based on the present representation are solved in a shorter time than the former SDP formulations, and they are numerically more stable.

For the case where  $f(x) = x^p : \mathbb{R}^+ \mapsto \mathbb{R}^+$ , where  $p$  is a rational number in  $(0, 1]$ , we shall see that our construction yields a stronger result. Namely, we show in Theorem 4.4 that  $X^p$  has an extremal representation of the form

$$X^p = \max_{\preceq} \{T \in \mathbb{S}_m : T \in \mathcal{S}\},$$

where the set  $\mathcal{S}$  is semidefinite representable and  $\max_{\preceq}$  denotes the largest element with respect to the Löwner ordering, which is defined over  $\mathbb{S}_m$  as follows:

$$A \preceq B \iff (B - A) \in \mathbb{S}_m^+.$$

More generally, our result shows that the matrix  $B \sharp_p A := B^{\frac{1}{2}} (B^{-\frac{1}{2}} A B^{-\frac{1}{2}})^p B^{\frac{1}{2}}$  has an extremal representation. The proof of this result uses the notion of *matrix geometric mean*, and the Banach fixed point theorem in the space  $\mathbb{S}_m^{++}$  equipped with a Riemannian metric.

Our study is motivated by the *theory of optimal experimental designs*, where the general problem to solve takes the form

$$\begin{aligned} \max_{\mathbf{w} \in \mathbb{R}^s} \quad & \Phi_p \left( \sum_{i=1}^s w_i M_i \right), \\ \text{s. t.} \quad & \sum_{i=1}^s w_i = 1, \quad \mathbf{w} \geq \mathbf{0}, \end{aligned} \tag{1}$$

where  $M_1, \dots, M_s$  are given positive semidefinite matrices, and for  $p \in [-\infty, 1]$  the  $\Phi_p$ -criterion is defined over the set of positive definite matrices  $M \in \mathbb{S}_m^{++}$  as

$$\Phi_p(M) = \begin{cases} \lambda_{\min}(M) & \text{for } p = -\infty ; \\ \left( \frac{1}{m} \text{trace } M^p \right)^{\frac{1}{p}} & \text{for } p \in (-\infty, 1], p \neq 0 ; \\ (\det(M))^{\frac{1}{m}} & \text{for } p = 0. \end{cases} \tag{2}$$

The definition of  $\Phi_p$  is extended by continuity to singular matrices  $M \in \mathbb{S}_m^+$ , so that  $\Phi_p(M) = 0$  if  $M$  is singular and  $p \leq 0$ . This design problem arises when an experimenter must select a subset of trials to perform among a set of available experiments, and has many applications in various domains, such as dose-finding in clinical studies [11] or measurements in telecommunication networks [21]. We refer the reader to Pukelsheim [17] for more background on optimal experimental designs.

Note that any semidefinite representation of the function  $M \rightarrow \text{trace } MP$  yields a semidefinite programming (SDP) formulation of Problem (1). The cases  $p = -\infty$ ,  $p = -1$ , and  $p = 0$ , known as  $E$ -,  $A$ - and  $D$ -optimal design problems have been extensively studied in the literature, and SDP formulations are known for these problems [10]. We also point out that lighter Second Order Cone Programming (SOCP) formulations exist for  $p = -1$  and  $p = 0$  [19, 18]. The general case ( $p \in [-\infty, 1]$ ) deserved less attention. However, it was recently noticed by Papp [16] that the SDP formulation can be obtained by using Proposition 4.2.1. in [5]. Our numerical results (cf. Section 5) show that the new SDP formulation from this paper can improve the computation time by several orders of magnitude.

## 2 Preliminaries

In this section, we briefly recall some basic notion about semidefinite representability and matrix geometric means. A *Semidefinite Program* (SDP) is an optimization problem where a linear function  $\mathbf{c}^T \mathbf{x}$  must be maximized, among the vectors  $\mathbf{x}$  belonging to a set  $S$  defined by *linear matrix inequalities* (LMI):

$$S = \{\mathbf{x} \in \mathbb{R}^n : F_0 + \sum_i x_i F_i \succeq 0\}.$$

We now recall the definition of a semidefinite representable set, which was introduced by Ben-Tal and Nemirovski [5]:

**Definition 2.1** (Semidefinite representability). A convex set  $S \subset \mathbb{R}^n$  is said to be *semidefinite representable*, abbreviated *SDr*, if  $S$  is the projection of a set in a higher dimensional space which can be described by LMIs. In other words,  $S$  is *SDr* if and only if there exists symmetric matrices  $F_0, \dots, F_n, F'_1, \dots, F'_{n'}$  such that

$$\mathbf{x} \in S \iff \exists \mathbf{y} \in \mathbb{R}^{n'} : F_0 + \sum_{i=1}^n x_i F_i + \sum_{i=1}^{n'} y_i F'_i \succeq 0.$$

Such an LMI is called a *semidefinite representation* (SDR) of the set  $S$ .

**Definition 2.2** (SDR of a function). A convex (resp. concave) function  $f : S \subset \mathbb{R}^n \mapsto \mathbb{R}$  is said *SDr* if and only if the epigraph of  $f$ ,  $\{(t, \mathbf{x}) : f(\mathbf{x}) \leq t\}$  (resp. the hypograph  $\{(t, \mathbf{x}) : t \leq f(\mathbf{x})\}$ ), is *SDr*.

It follows immediately from these two definitions that the problem of maximizing a concave *SDr* function (or minimizing a convex one) over a *SDr* set can be cast as an SDP.

We now give a short insight on the theory of matrix geometric means and the Riemannian metric of the set of positive definite matrices  $\mathbb{S}_m^{++}$ . We refer the reader to the book of Bhatia [6] and the references therein for more details on this subject. The Geometric mean of two positive definite matrices  $A, B \in \mathbb{S}_m^{++}$  was introduced by Ando [3]:

$$A \sharp B := A^{1/2} (A^{-1/2} B A^{-1/2})^{1/2} A^{1/2}.$$

In the latter paper, Ando shows that  $A \sharp B$  satisfies the following extremal property:

$$A \sharp B = \max_{\succeq} \left\{ X \in \mathbb{S}_m : \begin{pmatrix} A & X \\ X & B \end{pmatrix} \succeq 0 \right\}. \quad (3)$$

The space of positive definite matrices is equipped with the Riemannian metric

$$\delta_2(A, B) = \|\log A^{-1/2} B A^{-1/2}\|_F,$$

where  $\|M\|_F = \sqrt{\text{trace}(M^T M)}$  denotes the Frobenius norm of  $M$ . In this space, there exists a unique geodesic  $[A, B]$  between two matrices  $A$  and  $B$ , which can be parametrized as follows (using the common  $\sharp_t$ -notation):

$$\gamma_{A \rightarrow B}(t) = A \sharp_t B := A^{1/2} (A^{-1/2} B A^{-1/2})^t A^{1/2}, \quad 0 \leq t \leq 1.$$

Note that  $A \sharp B = A \sharp_{\frac{1}{2}} B$  is the midpoint of this geodesic. The geometric mean of two matrices has the following properties:

- *it is commutative:*

$$A \sharp B = B \sharp A; \quad (4)$$

- if  $A$ , and  $B$  commute, then

$$A \sharp B = A^{1/2} B^{1/2}; \quad (5)$$

- the map  $X \rightarrow A \sharp X$  is *operator monotone*, i.e.

$$Y \succeq X \implies A \sharp Y \succeq A \sharp X; \quad (6)$$

- the  $\sharp$ -operator is *invariant under congruent transformation*: for all invertible matrix  $U$  of size  $m$ ,

$$U^T (A \sharp B) U = (U^T A U) \sharp (U^T B U). \quad (7)$$

We also point out that the metric  $\delta_2$  enjoys an important convexity property, which will be useful in the proof of Theorem 4.4:

$$\forall A, B, C, D \in \mathbb{S}_m^{++}, \quad \delta_2(A \sharp B, C \sharp D) \leq \frac{1}{2} \delta_2(A, C) + \frac{1}{2} \delta_2(B, D). \quad (8)$$

### 3 Lifting the SDR of a scalar function

In this section, we show that the *SDR* of a function  $f : I \mapsto \mathbb{R}$  can be transformed in a simple way to a *SDR* of trace  $f : \mathbb{S}_m^I \rightarrow \mathbb{R}$ :

**Theorem 3.1.** *Let  $f : I \mapsto \mathbb{R}$  be a scalar function, where  $I$  is a real interval. Assume that  $f$  admits the following SDR: for all  $x \in I$ ,*

$$f(x) \leq t \iff \exists \mathbf{y} \in \mathbb{R}^n : F_0 + xF_X + tF_T + \sum_{i=1}^n y_i F_i \succeq 0,$$

where the symmetric matrices  $F_0, \dots, F_n, F_X, F_T$  are given. Then, a SDR of the function  $g : \mathbb{S}_m^I \mapsto \mathbb{R}, X \rightarrow \text{trace } f(X)$  is given by: for all  $X \in \mathbb{S}_m^I$ ,

$$\text{trace } f(X) \leq t \iff \exists T, Y_1, \dots, Y_n \in \mathbb{S}_m :$$

$$(i) \quad F_0 \otimes I_m + F_X \otimes X + F_T \otimes T + \sum_{i=1}^n F_i \otimes Y_i \succeq 0;$$

$$(ii) \quad \text{trace } T \leq t,$$

where  $I_m$  denotes the  $m \times m$  identity matrix and  $\otimes$  is the Kronecker product. In other words, the SDR is lifted from scalar to matrices by replacing each scalar by a corresponding matrix block of size  $m \times m$ .

*Proof.* Let  $X$  be an arbitrary matrix in  $\mathbb{S}_m^I$ , and  $X = U \text{Diag}(\boldsymbol{\lambda}) U^T$  be an eigenvalue decomposition of  $X$ .

We first assume that  $\text{trace } f(X) \leq t$ . For  $k = 1, \dots, m$ , define  $t_k = f(\lambda_k)$ . By assumption there exists a vector  $\mathbf{y}^{(k)}$  such that

$$B_k := F_0 + \lambda_k F_X + t_k F_T + \sum_{i=1}^n y_i^{(k)} F_i \succeq 0.$$

Denote by  $\mathcal{B}$  the block diagonal matrix with blocks  $B_1, \dots, B_m$  on the diagonal, and by  $\mathbf{y}_i$  the vector of  $\mathbb{R}^m$  with components  $y_i^{(1)}, \dots, y_i^{(m)}$ . We may write

$$\mathcal{B} = I_m \otimes F_0 + \text{Diag}(\boldsymbol{\lambda}) \otimes F_X + \text{Diag}(\mathbf{t}) \otimes F_T + \sum_{i=1}^n \text{Diag}(\mathbf{y}_i) \otimes F_i \succeq 0.$$

In the previous expression, we may commute the Kronecker products, which is equivalent to pre- and post-multiplying by a permutation matrix:

$$F_0 \otimes I_m + F_X \otimes \text{Diag}(\boldsymbol{\lambda}) + F_T \otimes \text{Diag}(\mathbf{t}) + \sum_{i=1}^n F_i \otimes \text{Diag}(\mathbf{y}_i) \succeq 0.$$

Now, we multiply this expression to the left by the block diagonal matrix  $\text{Diag}(U, \dots, U) = I \otimes U$ , and to the right by its transpose. This gives:

$$F_0 \otimes I_m + F_X \otimes X + F_T \otimes T + \sum_{i=1}^n F_i \otimes Y_i \succeq 0,$$

where we have set  $T = U \text{Diag}(\mathbf{t}) U^T$  and  $Y_i = U \text{Diag}(\mathbf{y}_i) U^T$ . By construction, we have  $T = f(X)$ , so (ii) holds and we have proved the “ $\Rightarrow$ ” part of the theorem.

For the converse part, consider some matrices  $T', Y'_1, \dots, Y'_n \in \mathbb{S}_m$  such that the LMI (i) of the theorem is satisfied. Define  $H_T = T' - T$  and  $H_i = Y'_i - Y_i$ , where  $T = f(X)$  and  $Y_i = U \text{Diag}(\mathbf{y}_i) U^T$  are defined as in the first part of this proof. We will show that  $\text{trace } H_T \geq 0$ , which implies  $\text{trace } T' \geq \text{trace } f(X)$ , and the proof will be complete.

So from (i) we have:

$$F_0 \otimes I_m + F_X \otimes X + F_T \otimes (T + H_T) + \sum_{i=1}^n F_i \otimes (Y_i + H_i) \succeq 0.$$

Again, we multiply this expression to the left by  $I \otimes U^T$  and to the right by  $I \otimes U$ , and then we commute the Kronecker products. This gives:

$$\text{Diag}(B_1, \dots, B_m) + U^T H_T U \otimes F_T + \sum_{i=1}^n U^T H_i U \otimes F_i \succeq 0.$$

For all  $k = 1, \dots, m$ , this implies that the  $k$ th diagonal block is positive semidefinite:

$$B_k + (U^T H_T U)_{k,k} F_T + \sum_{i=1}^n (U^T H_i U)_{k,k} F_i \succeq 0.$$

According to the *SDR* of the scalar function  $f$ , it means that

$$f(\lambda_k) \leq t_k + (U^T H_T U)_{k,k},$$

and since  $f(\lambda_k) = t_k$  we obtain  $(U^T H_T U)_{k,k} \geq 0$ . From there, it is easy to conclude:

$$\text{trace } H_T = \text{trace } H_T U U^T = \text{trace } U^T H_T U = \sum_{k=1}^m (U^T H_T U)_{k,k} \geq 0.$$

□

**Example 3.2.** A *SDR* of the function  $x \rightarrow x^p$ , where  $p \in \mathbb{Q}$  is briefly sketched in [5] (§3.3.1., examples 12 to 15) and given with more details in [1] (§2.3.h). (Note that this function is concave for  $p \in [0, 1]$  and convex for other values of  $p$ .) For example, the epigraph of the convex function  $x \rightarrow x^{-4/3}$  mapping  $(0, \infty)$  onto itself, may be represented as follows: for all  $t \geq 0, x > 0$ :

$$\begin{aligned} x^{-4/3} \leq t &\iff 1 \leq x^4 t^3 \\ &\iff \exists u \geq 0, v \geq 0 : 1 \leq xu, u^2 \leq tv, v^2 \leq t \\ &\iff \exists u \in \mathbb{R}, v \in \mathbb{R} : \begin{pmatrix} x & 1 \\ 1 & u \end{pmatrix} \succeq 0, \begin{pmatrix} t & u \\ u & v \end{pmatrix} \succeq 0, \begin{pmatrix} t & v \\ v & 1 \end{pmatrix} \succeq 0 \end{aligned}$$

For the second equivalence, the “ $\Leftarrow$ ” part is clear and the “ $\Rightarrow$ ” part is obtained by setting  $u = t^{3/4}$  and  $v = t^{1/2}$ . The third equivalence is a standard use of the Schur complement lemma. By using Theorem 3.1, we obtain a *SDR* of the function  $X \rightarrow \text{trace } X^{-4/3}$ :

$$\text{trace } X^{-4/3} \leq t \iff \exists U, V, T \in \mathbb{S}_m : \left\{ \begin{array}{l} \begin{pmatrix} X & I_m \\ I_m & U \end{pmatrix} \succeq 0 \\ \begin{pmatrix} T & U \\ U & V \end{pmatrix} \succeq 0, \\ \begin{pmatrix} T & V \\ V & I_m \end{pmatrix} \succeq 0, \\ \text{trace } T \leq t \end{array} \right.$$

□

Note however that LMI (i) of Theorem 3.1 does not imply the stronger property  $f(X) \preceq T$ . As a counter-example, consider the function  $f(x) = x^4$ , which admits the *SDR*

$$x^4 \leq t \iff \exists u \in \mathbb{R} : \begin{pmatrix} u & x \\ x & 1 \end{pmatrix} \succeq 0, \begin{pmatrix} t & u \\ u & 1 \end{pmatrix} \succeq 0.$$



If we set  $T = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$ ,  $U = \begin{pmatrix} 8 & 8 \\ 8 & 3 \end{pmatrix}$  and  $X = \begin{pmatrix} 73 & 39 \\ 39 & 34 \end{pmatrix}$ , the reader can check that the LMI (i) of Theorem 3.1 holds:

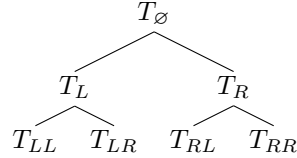
$$\begin{pmatrix} U & X \\ X & I_2 \end{pmatrix} \succeq 0, \quad \begin{pmatrix} T & U \\ U & I_2 \end{pmatrix} \succeq 0,$$

but  $X^4 \not\preceq T$ . In the next section, we show that this stronger property holds for  $f : x \rightarrow x^p$  when  $p \in \mathbb{Q} \cap (0, 1]$ .

## 4 Semidefinite representation of $A \#_p B$

Throughout this section,  $p$  denotes a rational number in  $(0, 1]$ , and we choose two integers  $\alpha$  and  $\beta$  such that  $p = \frac{\alpha}{\beta}$  and  $0 < \alpha \leq \beta$ . We are going to show that the lifted *SDR* of the function  $f_p$  mapping  $\mathbb{R}_+$  onto itself and defined by  $f(x) = x^p$ , also provides an extremal representation of  $X^p$ . In other words, there is a *SDr* set  $\mathcal{S} \subset \mathbb{S}_m^+$  for which  $X^p$  is the largest element with respect to Löwner ordering. In fact, we will prove a stronger statement: for any  $A \in \mathbb{S}_m^+$  and  $B \in \mathbb{S}_m^{++}$ , the matrix  $B \#_p A = B^{\frac{1}{2}} (B^{-\frac{1}{2}} A B^{-\frac{1}{2}})^p B^{\frac{1}{2}}$ , which is the point of coordinate  $p$  on the geodesic from  $B$  to  $A$ , is the largest element of a *SDr* set. The matrix power  $A^p$  arises as the particular case  $B = I_m$ .

To do this, we first present the construction of the *SDR* of  $\tilde{f}_p : (a, b) \rightarrow a^p b^{1-p}$ . As explained in [1], this *SDR* is based on binary trees whose nodes contain variables. Note that in a perfect binary tree, every node of depth  $k$  can be indexed by an element of  $\Gamma_k := \{L, R\}^k$ , which indicates the sequence of *left* or *right* turns needed to reach this node from the root of the tree. For example, a perfect binary tree  $T$  of depth 2 is indexed as follows:



We denote by  $\mathcal{T}_n = \Gamma_0 \cup \dots \cup \Gamma_n$  the set of node indices in a perfect binary trees of depth  $n$ , so that  $(\mathbb{S}_m)^{\mathcal{T}_n}$  represents the set of binary trees of depth  $n$ , whose nodes are matrices of  $\mathbb{S}_m$ . The concatenation of tree indices is denoted by  $\sqcup$ , so that for example,  $LR \sqcup L = LRL \in \Gamma_3$ . We define  $n$  as the integer such that  $2^{n-1} < \beta \leq 2^n$ , and  $\chi_{\alpha, \beta}$  as the following formal sequence of length  $2^n$ , which is formed with characters in the alphabet  $\{A, B, X\}$ :

$$\chi_{\alpha, \beta} := \underbrace{(A, \dots, A)}_{\alpha \text{ times}} \underbrace{(B, \dots, B)}_{(\beta - \alpha) \text{ times}} \underbrace{(X, \dots, X)}_{(2^n - \beta) \text{ times}}.$$

Now, let  $\sigma$  be any one of the permutations of  $\chi_{\alpha, \beta}$ , and let  $A, B$  be two arbitrary matrices (respectively in  $\mathbb{S}_m^+$  and  $\mathbb{S}_m^{++}$ ). The elements of  $\sigma$  are indexed by  $\gamma \in \Gamma_n$ , in the order corresponding to the leaves of a tree of depth  $n$  from left to right. For example, if  $\sigma = (A, B, X, B)$ , we have  $\sigma_{LL} = A$ ,  $\sigma_{RL} = X$ , and  $\sigma_{LR} = \sigma_{RR} = B$ . Let us now define for all  $\gamma \in \Gamma_n$  the function  $\hat{\sigma}_\gamma$ , mapping  $\mathbb{S}_m^+$  to either  $A, B$ , or

$X$  as follows:

$$\forall X \in \mathbb{S}_m^+, \hat{\sigma}_\gamma(X) = \begin{cases} A & \text{if } \sigma_\gamma = \mathbf{A} \\ B & \text{if } \sigma_\gamma = \mathbf{B} \\ X & \text{if } \sigma_\gamma = \mathbf{X} \end{cases} \quad (9)$$

With a slight abuse of notation, we will write  $\sigma_\gamma(X)$  instead of  $\hat{\sigma}_\gamma(X)$  in the remaining of this paper. (So  $\sigma_\gamma$  denotes a character in  $\{\mathbf{A}, \mathbf{B}, \mathbf{X}\}$ , while  $\sigma_\gamma(X)$  denotes the corresponding matrix in  $\mathbb{S}_m^+$ .) Similarly, we will simply write  $\sigma(X)$  to denote the sequence  $(\hat{\sigma}_\gamma(X))_{\gamma \in \Gamma_n}$ .

We can now construct the *SDR* of  $\tilde{f}_p$  (already lifted to  $\mathbb{S}_m^+$  by considering matrix blocks instead of scalar variables). It involves a tree whose root is  $X$ , leaves are defined by  $\sigma$ , and a LMI related to the matrix geometric mean must be satisfied at each node:

$$\begin{aligned} \mathcal{S}(\sigma) = \{X \in \mathbb{S}_m^+ : \exists T \in (\mathbb{S}_m)^{\mathcal{T}_n} : \\ (i) \ T_\emptyset = X; \\ (ii) \ \forall \gamma \in \Gamma_n, \ T_\gamma = \sigma_\gamma(X); \\ (iii) \ \forall k = 0, \dots, n-1, \ \forall \gamma \in \Gamma_k, \ \begin{pmatrix} T_{\gamma \sqcup L} & T_\gamma \\ T_\gamma & T_{\gamma \sqcup R} \end{pmatrix} \succeq 0\} \end{aligned}$$

**Example 4.1.** If  $p = 1/3$ , we have  $\alpha = 1$ ,  $\beta = 3$ ,  $n = 2$ , and  $\sigma$  must contain respectively  $\alpha = 1$ ,  $(\beta - \alpha) = 2$ , and  $(2^n - \beta) = 1$  copies of  $\mathbf{A}, \mathbf{B}$ , and  $\mathbf{X}$ . If  $\sigma = (\mathbf{A}, \mathbf{X}, \mathbf{B}, \mathbf{B})$ , the set  $\mathcal{S}(\sigma)$  is defined through a tree of the form

$$\begin{array}{c} X \\ \swarrow \quad \searrow \\ T_L \quad T_R \\ \swarrow \quad \searrow \quad \swarrow \quad \searrow \\ A \quad X \quad B \quad B \end{array} \quad (10)$$

The property (iii) in the definition of  $\mathcal{S}(\sigma)$  implies that  $T_R$  satisfies

$$\begin{pmatrix} B & T_R \\ T_R & B \end{pmatrix} \succeq 0.$$

So by Equation (3) we have  $T_R \preceq B$ , and the definition of  $\mathcal{S}(\sigma)$  simplifies to:

$$X \in \mathcal{S}(\sigma) \iff \exists T_L \in \mathbb{S}_m : \begin{pmatrix} T_L & X \\ X & B \end{pmatrix} \succeq 0, \begin{pmatrix} A & T_L \\ T_L & X \end{pmatrix} \succeq 0.$$

□

Generally speaking, we point out that the order of the elements in the permutation  $\sigma$  can be chosen such that the definition of  $\mathcal{S}(\sigma)$  involves no more than  $2(n-1) = O(\log \beta)$  LMIs of size  $2m \times 2m$ :

**Proposition 4.2.** *The permutation  $\sigma$  of  $\chi_{\alpha, \beta}$  can always be chosen such that  $\mathcal{S}(\sigma)$  admits an *SDR* involving no more than  $2(n-1) = O(\log \beta)$  LMIs of size  $2m \times 2m$ , and no more than  $2n-3 = O(\log \beta)$  additional variables  $T_\gamma \in \mathbb{S}_m$ .*

A constructive proof of this result is presented in appendix.

Now, as a consequence of Equation (3), observe that property (iii) in the definition of  $\mathcal{S}(\sigma)$  implies  $T_\gamma \preceq T_{\gamma \sqcup L} \# T_{\gamma \sqcup R}$  (if the geometric mean is well defined, i.e.  $T_{\gamma \sqcup L}, T_{\gamma \sqcup R} \in \mathbb{S}_m^{++}$ ). By operator monotonicity of the matrix geometric mean (see (6)), we see that if the matrices  $A, B, X, T_L$  and  $T_R$  of Tree (10) are positive definite, then:

$$X \preceq T_L \# T_R \preceq (A \# X) \# (B \# B).$$

In the general case, we can bound  $X$  from above (with respect to Löwner ordering) by an expression with nested “ $\#$ -operations” in the binary tree whose leaves are defined through  $\sigma$ . Formally, for any two collections  $\varsigma, \varsigma' \in (\mathbb{S}_m^+)^{\Gamma_n}$  of  $2^n$  positive definite matrices indexed by tree indices, i.e.

$$\forall \gamma \in \Gamma_n, \quad \varsigma_\gamma \in \mathbb{S}_m^+, \varsigma'_\gamma \in \mathbb{S}_m^+,$$

we define the juxtaposition  $\varsigma \sqcap \varsigma' \in (\mathbb{S}_m^+)^{\Gamma_{n+1}}$  as follows:

$$\forall \gamma \in \Gamma_n, \quad (\varsigma \sqcap \varsigma')_{L \sqcup \gamma} = \varsigma_\gamma, \quad (\varsigma \sqcap \varsigma')_{R \sqcup \gamma} = \varsigma'_\gamma.$$

Note that if  $n \geq 1$ , any sequence  $\varsigma \in (\mathbb{S}_m^+)^{\Gamma_n}$  can be uniquely decomposed as  $\varsigma = \varsigma^{[L]} \sqcap \varsigma^{[R]}$ , where the subsequences  $\varsigma^{[L]}$  and  $\varsigma^{[R]}$  are elements of  $(\mathbb{S}_m^+)^{\Gamma_{n-1}}$ . This allows us to define inductively the *nested sharp operator*  $\#$ , which acts from  $(\mathbb{S}_m^{++})^{\Gamma_n}$  onto  $\mathbb{S}_m^{++}$  as follows:

$$\begin{cases} \forall \varsigma \in (\mathbb{S}_m^{++})^{\Gamma_0}, & \#(\varsigma) := \varsigma_\emptyset; \\ \forall \varsigma = \varsigma^{[L]} \sqcap \varsigma^{[R]} \in (\mathbb{S}_m^{++})^{\Gamma_n}, \quad n \geq 1, & \#(\varsigma) := (\#(\varsigma^{[L]})) \# (\#(\varsigma^{[R]})). \end{cases}$$

With a straightforward induction, we can now obtain the following lemma:

**Lemma 4.3.** *If  $A$  and  $B$  are positive definite, then*

$$X \in \mathcal{S}(\sigma) \implies X \preceq \#(\sigma(X)).$$

We can finally give the main result of this section:

**Theorem 4.4** (Extremal representation of  $B \#_p A$ ). *Let  $p = \frac{\alpha}{\beta}$ ,  $0 < \alpha \leq \beta$ ,  $\alpha \in \mathbb{N}, \beta \in \mathbb{N}$ ,  $A \in \mathbb{S}_m^+$ ,  $B \in \mathbb{S}_m^{++}$ , and let  $\sigma$  be an arbitrary permutation of  $\chi_{\alpha, \beta}$ . Then,  $B \#_p A$  satisfies the following extremal property*

$$B \#_p A = \max_{\preceq} \{X \in \mathbb{S}_m^+ : X \in \mathcal{S}(\sigma)\}.$$

*Proof.* Let  $A \in \mathbb{S}_m^{++}$  be an arbitrary positive definite matrix. We are first going to show that  $B \#_p A = \max_{\preceq} \{X \in \mathbb{S}_m^{++} : X \in \mathcal{S}(\sigma)\}$ . The general statement where  $A \in \mathbb{S}_m^+$  may be singular will be obtained at the end of this proof by continuity. Our proof relies on the following lemma:

**Lemma 4.5.** *If  $A$  and  $B$  are positive definite, then  $X = B \#_p A$  is a solution of the equation*

$$X = \#(\sigma(X)).$$

*Proof of the lemma.*

Define a sequence  $\sigma'(X)$ , such that for all  $\gamma \in \Gamma_n$ ,

$$\sigma'_\gamma(X) = B^{-\frac{1}{2}} \sigma_\gamma(X) B^{-\frac{1}{2}}.$$

Set  $Y = B^{-\frac{1}{2}}AB^{-\frac{1}{2}}$ , so that the elements of  $\sigma'(B \#_p A)$  are all in  $\{Y, I_m, Y^p\}$ , and hence they commute. A simple induction shows that  $\#(\sigma'(B \#_p A)) = Y^p$  (the geometric means are easy to compute when the matrices commute, see (5)). By congruence invariance (see (7)),

$$\begin{aligned} \#(\sigma(B \#_p A)) &= B^{\frac{1}{2}} \#(\sigma'(B \#_p A)) B^{\frac{1}{2}} \\ &= B^{\frac{1}{2}} Y^p B^{\frac{1}{2}} \\ &= B \#_p A. \end{aligned}$$

□

*Proof of Theorem 4.4 (continued).* Let  $X \in \mathbb{S}_m^{++}$  such that  $X \in \mathcal{S}(\sigma)$ , and let  $T \in (\mathbb{S}_m)^{\mathcal{T}_n}$  be a tree satisfying properties (i) – (iii) of the definition of  $\mathcal{S}(\sigma)$ . Define a new tree  $T'$  as follows:

$$\forall \gamma \in \Gamma_{n-1}, T'_\gamma := T_{\gamma \sqcup L} \# T_{\gamma \sqcup R} \succeq T_\gamma,$$

and

$$\forall \gamma \in \Gamma_k, T'_\gamma := T'_{\gamma \sqcup L} \# T'_{\gamma \sqcup R} \succeq T_\gamma$$

for  $k = (n-2), \dots, 0$ . By construction, the root of  $T'$  is  $X' := T'_\emptyset = \#(\sigma(X)) \succeq X$ . It remains to define the leaves of  $T'$ , which we do according to  $\sigma(X')$ :

$$\forall \gamma \in \Gamma_n, T'_\gamma := \sigma_\gamma(X') \succeq T_\gamma.$$

By construction, it is clear that  $T'$  satisfies the property (iii) of the definition of  $\mathcal{S}(\sigma)$  for the depth levels  $k = 0, \dots, n-2$ . For a  $\gamma \in \Gamma_{n-1}$ , (iii) also holds, because

$$\begin{pmatrix} T'_{\gamma \sqcup L} & T'_\gamma \\ T'_\gamma & T'_{\gamma \sqcup R} \end{pmatrix} \succeq \begin{pmatrix} T_{\gamma \sqcup L} & T'_\gamma \\ T'_\gamma & T_{\gamma \sqcup R} \end{pmatrix} \succeq 0,$$

where the first inequality follows from  $T'_{\gamma \sqcup L} \succeq T_{\gamma \sqcup L}$ ,  $T'_{\gamma \sqcup R} \succeq T_{\gamma \sqcup R}$ , and the second inequality is a consequence of  $T'_\gamma = T_{\gamma \sqcup L} \# T_{\gamma \sqcup R}$ . This shows that  $X'$  belongs to  $\mathcal{S}(\sigma)$ , too.

Define  $h : \mathbb{S}_m^{++} \mapsto \mathbb{S}_m^{++}$ ,  $X \mapsto \#(\sigma(X))$ . So far, we have shown that  $X \in \mathcal{S}(\sigma) \implies [h(X) \succeq X \text{ and } h(X) \in \mathcal{S}(\sigma)]$ . By using the convexity property of the Riemannian metric (Equation (8)), a simple induction shows that  $h$  is a contraction mapping with a contraction factor equal to the fraction of the number of elements of  $\sigma$  that take the value  $X$ :

$$\forall X, X' \in \mathbb{S}_m^{++}, \delta_2(h(X), h(X')) \leq \frac{2^n - \beta}{2^n} \delta_2(X, X') < \delta_2(X, X').$$

Hence, the mapping  $X \mapsto h(X)$  is contractive in the space  $\mathbb{S}_m^{++}$  equipped with the Riemannian metric  $\delta_2$ . It is known that this space is complete (see e.g. [15]), and hence we can apply the Banach fixed point theorem: the fixed point equation  $X = h(X)$  has a unique solution  $X^* \in \mathbb{S}_m^{++}$ . Moreover for all  $X \in \mathbb{S}_m^{++}$  the sequence defined by  $X_0 = X$ ,  $X_{i+1} = h(X_i)$  converges to  $X^*$ . In particular, if  $X \in \mathcal{S}(\sigma)$ , our previous discussion shows that  $X \preceq X^*$ . Moreover, we can construct a tree with leaves defined by  $\sigma(X^*)$ , and such that all non-leaf node is the geometric mean of its two children, so that the root will be  $h(X^*) = X^*$ .

So,  $X^* \in \mathcal{S}(\sigma)$  is the largest element of  $\mathcal{S}(\sigma)$ . Finally, we know from Lemma 4.5 that  $X^* = B \sharp_p A$ .

It remains to show that the statement of the theorem remains valid when the matrix  $A \in \mathbb{S}_m^+$  is singular. We will first show that  $B \sharp_p A \in \mathcal{S}(\sigma)$ . Consider a tree  $T$  with leaves  $\sigma(B \sharp_p A)$ . Since the matrix  $B \sharp_p A = B^{\frac{1}{2}} (B^{-\frac{1}{2}} A B^{-\frac{1}{2}})^p B^{\frac{1}{2}}$  is singular, we may not define the non-leaf nodes of this tree using geometric means. However, observe that every leaf is of the form  $B \sharp_k A$ , with  $k \in \{0, p, 1\}$ . Hence, we define the non-leaf nodes of  $T$  by the following relation: if  $T_{\gamma \sqcup L} = B \sharp_{k_1} A$  and  $T_{\gamma \sqcup R} = B \sharp_{k_2} A$ , then  $T_\gamma := B \sharp_{\frac{k_1+k_2}{2}} A$ . It is easy to check that the property (iii) of the definition of  $\mathcal{S}(\sigma)$  is satisfied for the resulting tree  $T$ . A simple induction shows that the root of this tree is

$$T_\emptyset = B \sharp_{\frac{n_A(\sigma) + p n_X(\sigma)}{2^n}} A,$$

where  $n_A(\sigma)$  and  $n_X(\sigma)$  represent the number of times that  $A$  and  $X$  appear in the sequence  $\sigma$ . Replacing  $n_A(\sigma)$  by  $\alpha$  and  $n_X(\sigma)$  by  $2^n - \beta$ , we find  $T_\emptyset = B \sharp_p A$ . This shows that  $B \sharp_p A \in \mathcal{S}(\sigma)$ .

Until now the matrices  $A$  and  $B$  were fixed, but now we need to let  $A$  vary so we introduce the notation  $\bar{\sigma}_{A'}(X)$  to represent the sequence of length  $2^n$  which is identical to  $\sigma(X)$ , except for the elements  $A$  that are replaced by  $A'$ :

$$(\bar{\sigma}_{A'}(X))_\gamma := \begin{cases} A' & \text{if } \sigma_\gamma = A; \\ B & \text{if } \sigma_\gamma = B; \\ X & \text{if } \sigma_\gamma = X. \end{cases}$$

In particular,  $\bar{\sigma}_A(X) = \sigma(X)$  for all  $X \in \mathbb{S}_m^+$ . We also define the set

$$\bar{\mathcal{S}}(\sigma) := \{(A', X) \in \mathbb{S}_m^+ \times \mathbb{S}_m^+ : X \in \mathcal{S}(\bar{\sigma}_{A'})\}.$$

Note that  $\bar{\mathcal{S}}(\sigma)$  is *SDr* by construction, and hence convex.

Now, choose a sequence  $A_i \in \mathbb{S}_m^+$  such that  $A_i \rightarrow A$  as  $i \rightarrow \infty$ , as well as a sequence  $\epsilon_i > 0$  such that  $\epsilon_i \rightarrow 0$ . We know that  $(A_i, B \sharp_p A_i) \in \bar{\mathcal{S}}(\sigma)$  for all  $i$ . Let  $X \in \mathcal{S}(\sigma)$ , so that  $(A, X) \in \bar{\mathcal{S}}(\sigma)$  and define  $A'_i := (1 - \epsilon_i)A + \epsilon_i A_i$ ,  $X'_i := (1 - \epsilon_i)X + \epsilon_i B \sharp_p A_i$ . By convexity of  $\bar{\mathcal{S}}(\sigma)$ , we have  $(A'_i, X'_i) \in \bar{\mathcal{S}}(\sigma)$ . Moreover, since the matrices  $A'_i$  and  $X'_i$  are positive definite, we know that  $X'_i \preceq B \sharp_p A'_i$ . By taking the limit, we obtain  $X \preceq B \sharp_p A$ . This completes the proof.  $\square$

**Corollary 4.6.** *Let  $p = \frac{\alpha}{\beta}$ ,  $0 < \alpha \leq \beta$ , and for all  $U, X \in \mathbb{S}_m^+$  let  $\sigma_X(U)$  be a permutation of  $\chi_{\alpha, \beta}(X, I_m, U)$  (the order of the elements in  $\sigma_X(U)$  does not depend on  $X$  and  $U$ ). If  $K$  is a  $m \times r$ -matrix, then the concave function  $X \rightarrow \text{trace } K^T X^p K$ , which maps  $\mathbb{S}_m^+$  to  $\mathbb{R}^+$ , has the following semidefinite representation: for all  $X \in \mathbb{S}_m^+$ ,*

$$t \leq \text{trace } K^T X^p K \iff \exists U \in \mathcal{S}(\sigma_X), t \leq \text{trace } K^T U K.$$

*Proof.* If  $t \leq \text{trace } K^T X^p K$ , we set  $U = X^p$ , so that  $t \leq \text{trace } K^T U K$  and by Theorem 4.4  $U \in \mathcal{S}(\sigma_X)$ . Conversely, assume that  $U \in \mathcal{S}(\sigma_X)$ . We know from previous theorem that  $U \preceq X^p$ . Hence, we have  $\langle M, U \rangle \leq \langle M, X^p \rangle$  for all positive semidefinite matrix  $M$ . In particular,

$$\text{trace } K^T U K = \langle K K^T, U \rangle \leq \langle K K^T, X^p \rangle = \text{trace } K^T X^p K,$$

from which the conclusion follows.  $\square$

**Remark 4.7.** In the recent years, many authors have proposed to generalize the definition of matrix geometric means for three or more matrices [4, 7, 9, 8]. In a seminal work, Ando, Li and Mathias [4] have given a list of 10 properties that a “good” geometric mean should satisfy. A natural question arising from this paper is the following: *is there a matrix geometric mean satisfying the ten properties of [4], that coincides with the largest element of a SDR set?* Interestingly, our result can be generalized in a straightforward way to give an extremal representation of the unique fixed point  $F(A_1, \dots, A_N)$  of the map

$$X \rightarrow \# \left( (A_1, A_2, \dots, A_N, \underbrace{X, \dots, X}_{2^n - N}) \right),$$

where the operand of  $\#$  is a sequence of  $(\mathbb{S}_m^{++})^{\Gamma^n}$ , with  $n \in \mathbb{N}$  such that  $2^{n-1} < N \leq 2^n$ . We claim that this fixed point satisfies most of the Ando-Li-Mathias properties, but the permutation invariance is not fulfilled: for a permutation  $\sigma$ ,  $F(A_1, \dots, A_N) \neq F(A_{\sigma(1)}, \dots, A_{\sigma(N)})$  in general.

## 5 Numerical Results

In this section, we compare the CPU time required to solve problems of the form

$$\min_{\substack{\mathbf{w} \geq \mathbf{0} \\ \sum_i w_i = 1}} \text{trace } f\left(\sum_{k=1}^s w_k M_k\right), \quad (P_f)$$

by using the semidefinite representation of Theorem 3.1, and the one of Ben-Tal and Nemirovski [5]. This problem is inspired from the application to optimal experimental design that is presented in the introduction. For the sake of variety, we do not limit ourselves to power functions  $x \rightarrow x^p$  with  $p < 1$ . More precisely, assume that  $f : I \rightarrow \mathbb{R}$  is a convex real valued function defined on the interval  $I$ , an *SDR* of  $f$  is known:

$$\forall x \in I, f(x) \leq t \iff \exists \mathbf{y} \in \mathbb{R}^n : F_0 + xF_X + tF_T + \sum_{i=1}^n y_i F_i \succeq 0,$$

and the matrices  $M_1, \dots, M_s \in \mathbb{S}_m^I$  are given. We compare the efficiency of the following two SDP formulations of Problem  $(P_f)$ : the one with block matrices resulting from Theorem 3.1,

$$\begin{aligned} & \min_{X, T, \{Y_i\}, \mathbf{w}} \text{trace } T && (SDP_f - 1) \\ & \text{s. t.} && F_0 \otimes I_m + F_X \otimes X + F_T \otimes T + \sum_{i=1}^n F_i \otimes Y_i \succeq 0; \\ & && X = \sum_{k=1}^s w_k M_k, \quad \mathbf{w} \geq \mathbf{0}, \quad \sum_{k=1}^s w_k = 1, \end{aligned}$$

$f(x)$	$I$	$m$	CPU time (s) [SeDuMi]		CPU time (s) [MOSEK]	
			$(SDP_f - 1)$	$(SDP_f - 2)$	$(SDP_f - 1)$	$(SDP_f - 2)$
$-x^{\frac{1}{3}}$	$[0, \infty)$	10	0.40	0.80	0.05	0.18
		25	5.16	40.85	0.72	6.92
		40	59.19	<i>706.43</i> <sup>†</sup>	3.47	<i>71.25</i> <sup>b</sup>
$-x^{\frac{2}{5}}$	$[0, \infty)$	10	0.58	1.28	0.08	0.22
		25	20.38	39.57	1.68	5.88
		40	298.90	<i>799.77</i> <sup>†</sup>	<i>19.33</i> <sup>b</sup>	<i>66.69</i> <sup>b</sup>
$x^{\frac{-8}{7}}$	$(0, \infty)$	10	0.49	0.90	0.10	0.19
		25	22.38	<i>40.07</i> <sup>†</sup>	1.65	4.96
		40	357.22	<i>691.75</i> <sup>†</sup>	14.65	61.87
$x^{\frac{7}{4}}$	$[0, \infty)$	10	0.41	1.23	0.07	0.17
		25	8.71	39.95	<i>1.19</i> <sup>b</sup>	<i>5.90</i> <sup>b</sup>
		40	120.16	<i>741.15</i> <sup>†</sup>	<i>6.38</i> <sup>b</sup>	<i>68.63</i> <sup>b</sup>
$\frac{1}{x(1-x)}$	$(0, 1)$	10	0.30	0.76	0.05	0.15
		25	4.31	37.21	0.37	4.97
		40	51.79	<i>607.57</i> <sup>†</sup>	2.27	<i>61.44</i> <sup>b</sup>
$g_{\text{conv}}(x)$	$\mathbb{R}$	10	0.75	1.50	0.12	0.24
		25	63.62	<i>43.08</i> <sup>†</sup>	2.94	4.37
		40	1019.70	<i>903.55</i> <sup>†</sup>	31.06	<i>58.46</i> <sup>b</sup>

Table 1: CPU time of two SDP formulations for Problem  $(P_f)$  with SeDuMi and MOSEK. The second column indicates the interval  $I$  where the function  $f$  is defined, and the third column specifies the size of the matrices  $M_i \in \mathbb{S}_m^I$ . The function  $g_{\text{conv}}$  in the last row is defined in (11). <sup>†</sup>The numbers displayed in italics for SeDuMi indicate that the solver stopped before reaching the optimality tolerance, because of numerical problems. <sup>b</sup>The numbers displayed in italics for MOSEK indicate that the solver returned the near-optimal status.

and the SDP from [5] that bounds each Ky-Fan Norm of  $X$ :

$$\begin{aligned}
& \min_{X, t, x, y, \sigma, \{Z_j\}} \sum_{j=1}^m t_j && (SDP_f - 2) \\
& \text{s. t.} && F_0 + x_j F_X + t_j F_T + \sum_{i=1}^n y_i^{(j)} F_i \succeq 0, \quad (j = 1, \dots, m); \\
& && x_1 \geq x_2 \geq \dots \geq x_m; \\
& && \sum_{k=1}^j x_k - j\sigma_j - \text{trace}(Z_j) \geq 0, \quad (j = 1, \dots, m-1); \\
& && Z_j \succeq 0, \quad (j = 1, \dots, m-1); \\
& && Z_j - X + \sigma_j I_m \succeq 0, \quad (j = 1, \dots, m-1); \\
& && \text{trace } X = \sum_{j=1}^m x_j; \\
& && X = \sum_{k=1}^s w_k M_k, \quad \mathbf{w} \geq \mathbf{0}, \quad \sum_{k=1}^s w_k = 1.
\end{aligned}$$

Our computational results are summarized in Table 1. Besides rational power functions, we have also consider the function  $f : (0, 1) \mapsto \mathbb{R}$ ,  $x \mapsto \frac{1}{x(x-1)}$ ,

which has the *SDR*

$$\begin{aligned} \forall x \in (0, 1), \quad f(x) \leq t &\iff \exists u \in \mathbb{R} : 1 \leq u(1-x), \quad 1 \leq (t-u)x \\ &\iff \exists u \in \mathbb{R} : \begin{pmatrix} u & 1 \\ 1 & 1-x \end{pmatrix} \succeq 0, \quad \begin{pmatrix} t-u & 1 \\ 1 & x \end{pmatrix} \succeq 0, \end{aligned}$$

as well as the convex envelope of a polynomial of degree 6. The fact that convex envelopes of univariate rational functions are *SDr* was proved by Laraki and Lasserre [13]. For the function

$$g_{\text{conv}} : \mathbb{R} \mapsto \mathbb{R}, x \rightarrow \text{convex-envelope}\left(\frac{x^6}{6} - 3\frac{x^4}{2} + 4x^2 + x\right), \quad (11)$$

the *SDR* given in [13] is:

$$\begin{aligned} g_{\text{conv}}(x) \leq t &\iff \exists y_2, \dots, y_6 \in \mathbb{R} : \begin{pmatrix} 1 & x & y_2 & y_3 \\ x & y_2 & y_3 & y_4 \\ y_2 & y_3 & y_4 & y_5 \\ y_3 & y_4 & y_5 & y_6 \end{pmatrix} \succeq 0, \\ &t \geq \frac{y_6}{6} - 3\frac{y_4}{2} + 4y_2 + x. \end{aligned}$$

For all our instances, we have generated  $s = 25$  random matrices  $M_i \in \mathbb{S}_m^I$ . We solved the SDPs by using SeDuMi [22] interfaced by YALMIP [14], and MOSEK 7.0 [2] interfaced by PICOS [20], with the default settings on a PC with 8 processors at 2.2GHz. Our experiments show that the block matrix formulation (*SDP<sub>f</sub> - 1*) improves the CPU time by a factor that vary between 2 and 12 for SeDuMi, and between 1.5 and 27 with MOSEK. An exception is the case  $f = g_{\text{conv}}$  with SeDuMi, but in this case the solver encountered numerical problems with (*SDP<sub>f</sub> - 2*) and stopped the computation before reaching the optimality tolerance.

Also note that SeDuMi was always able to compute an optimal solution with (*SDP<sub>f</sub> - 1*) but not with (*SDP<sub>f</sub> - 2*), and that MOSEK returned the *near-optimal* status twice more often with the formulation (*SDP<sub>f</sub> - 2*). This suggests that the formulation from this paper is numerically more stable.

To confirm this fact, we have computed the behavioural measures studied in [12], for the two SDP formulations of several of the above instances. The authors of this article evidence a positive correlation between the number of interior point method iterations and some measures of the SDP instances, such as the Renegar condition number  $C$  and some geometry measures  $D_p^\epsilon, g_p, D_d^\epsilon, g_d$  related to the primal and dual feasible regions and the norm of the solutions. We used a matlab code written by an author of [12] to compute these behavioural measures and compare them. For all the instances we considered, the Renegar condition number  $C$  was infinite, as well as the geometric measures  $D_p^\epsilon$  and  $g_d$ . However,  $g_p$  and  $D_d^\epsilon$  had finite values for most instances, see Table 2. These quantities are always orders of magnitude smaller for the formulation (*SDP<sub>f</sub> - 1*), which suggests that the formulation of this paper has better numerical properties indeed.



$f(x)$	$D_d^\epsilon$		$g_p$	
	$(SDP_f - 1)$	$(SDP_f - 2)$	$(SDP_f - 1)$	$(SDP_f - 2)$
$-x^{1/3}$	319.2	2438.4	639.0	38292
$-x^{2/5}$	463.5	2115.7	1143.0	38420
$x^{-8/7}$	$+\infty$	$+\infty$	$+\infty$	$+\infty$
$x^{7/4}$	674.4	2087.8	297.4	8117.7
$\frac{x}{1-x}$	167.7	215.2	128.9	4867.8
$g_{\text{conv}}(x)$	1506.8	2582.4	5522.8	12472

Table 2: Behavioural measures  $D_d^\epsilon$  and  $g_p$  of [12], computed for the same instances as in Table 1, for  $m = 25$ .

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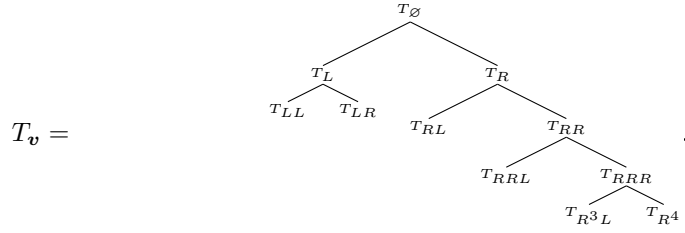
## Appendix

*Proof of Proposition 4.2.* To prove this result, we need to present an alternative construction of  $\mathcal{S}(\sigma)$  which relies on the concept of *proper binary trees* rather than *perfect binary trees*. In contrast to the latter, all the leaves of a proper binary tree do not necessarily have the same depth, but every non-leaf node must still have exactly two children. In other words, in a proper binary tree every node has either 0 or 2 children.

Now, let  $\mathbf{v} \in \mathbb{N}^n$ . It is easy to see that there exists a proper binary tree with  $v_k$  leaves of depth  $k$  only if

$$\sum_{k=1}^n v_k 2^{n-k} = 2^n. \quad (12)$$

Let us denote by  $T_{\mathbf{v}}$  the proper binary tree where the  $v_k$  leaves of depth  $k$  are as far left as possible. We denote by  $\Gamma_{\mathbf{v}}$  the set of indices of all nodes in  $T_{\mathbf{v}}$ . This set can be partitioned as  $\Gamma_{\mathbf{v}} = \Gamma_{\mathbf{v}}^{\Delta} \uplus \Gamma_{\mathbf{v}}^{\circ}$ , where  $\Gamma_{\mathbf{v}}^{\Delta}$  (resp.  $\Gamma_{\mathbf{v}}^{\circ}$ ) denotes the set of indices of the leaves (resp. non-leaf nodes). For example, the leftmost proper binary tree associated to the vector  $\mathbf{v} = [0, 3, 1, 2]$  is



So the set of leaves and non-leaf nodes indices are

$$\Gamma_{\mathbf{v}}^{\Delta} = \{LL, LR, RL, RRL, R^3L, R^4\}$$

$$\Gamma_{\mathbf{v}}^{\circ} = \{\emptyset, L, R, RR, R^3\}$$

Now let  $\sigma \in \{A, B, X\}^{\Gamma_{\mathbf{v}}^{\Delta}}$  be a sequence of characters indexed in  $\Gamma_{\mathbf{v}}^{\Delta}$ . As before we make a slight abuse of notation and we write  $\sigma_{\gamma}(X)$  for the matrix  $\hat{\sigma}_{\gamma}(X)$  corresponding to the character  $\sigma_{\gamma}$  (see (9)). We can now define a new set  $\mathcal{S}_{\mathbf{v}}(\sigma)$  based on proper binary trees:

$$\begin{aligned} \mathcal{S}_{\mathbf{v}}(\sigma) = \{X \in \mathbb{S}_m^+ : \exists T \in (\mathbb{S}_m^+)^{\Gamma_{\mathbf{v}}} \\ (i) \ T_{\emptyset} = X; \\ (ii) \ \forall \gamma \in \Gamma_{\mathbf{v}}^{\Delta}, \ T_{\gamma} = \sigma_{\gamma}(X); \\ (iii) \ \forall \gamma \in \Gamma_{\mathbf{v}}^{\circ}, \ \begin{pmatrix} T_{\gamma \sqcup L} & T_{\gamma} \\ T_{\gamma} & T_{\gamma \sqcup R} \end{pmatrix} \succeq 0\} \end{aligned}$$

The sets  $\mathcal{S}_{\mathbf{v}}$  and  $\mathcal{S}$  are related by the following lemma:

**Lemma 6.1.** *Let  $\mathbf{v}$  be a vector of  $\mathbb{N}^n$  satisfying Equation (12), and  $\sigma \in \{A, B, X\}^{\Gamma_{\mathbf{v}}^{\Delta}}$  be a sequence of characters indexed by the leaves of  $T_{\mathbf{v}}$ . Define a new character sequence  $\varsigma \in \{A, B, X\}^{\Gamma_n}$ , such that for every descendant  $\gamma = \gamma' \sqcup \gamma'' \in \Gamma_n$  of a node  $\gamma' \in \Gamma_{\mathbf{v}}^{\Delta}$ ,  $\varsigma_{\gamma} := \sigma_{\gamma'}$ . Then,*

$$\mathcal{S}_{\mathbf{v}}(\sigma) = \mathcal{S}(\varsigma).$$

*Proof of the lemma.* First note that by definition,  $\mathcal{S}(\varsigma) = \mathcal{S}_{[0, \dots, 0, 2^n]}(\varsigma)$  for all  $\varsigma \in \Gamma_n$ .

Now, let  $\sigma'$  and  $\mathbf{v}'$  be as in the lemma, i.e.  $\mathbf{v}'$  satisfies (12) and  $\sigma' \in \{\mathbf{A}, \mathbf{B}, \mathbf{X}\}^{\Gamma_{\mathbf{v}'}}$ . Assume that  $\sigma'$  assigns the same character to the two leftmost sibling leaves of depth  $k > 1$ . In other words, the leftmost non-leaf node  $\gamma_0$  of  $\Gamma_{\mathbf{v}'}^{\odot} \cap \Gamma_{k-1}$  is such that

$$(\gamma_0 \sqcup L) \in \Gamma_{\mathbf{v}'}^{\Delta}, \quad (\gamma_0 \sqcup R) \in \Gamma_{\mathbf{v}'}^{\Delta}, \quad \sigma'_{\gamma_0 \sqcup L} = \sigma'_{\gamma_0 \sqcup R}.$$

Define  $\mathbf{v}'' := [v'_1, v'_2, \dots, v'_{k-1} + 1, v'_k - 2, \dots, v'_n]$ . Note that by construction,  $\Gamma_{\mathbf{v}''}^{\Delta} = \Gamma_{\mathbf{v}'}^{\Delta} \cup \{\gamma_0\} \setminus \{\gamma_0 \sqcup L, \gamma_0 \sqcup R\}$ , and define  $\sigma'' \in \{\mathbf{A}, \mathbf{B}, \mathbf{X}\}^{\Gamma_{\mathbf{v}''}}$  as follows:

$$\forall \gamma \in \Gamma_{\mathbf{v}''}^{\Delta}, \quad \sigma''_{\gamma} = \begin{cases} \sigma'_{\gamma_0 \sqcup L} & \text{if } \gamma = \gamma_0; \\ \sigma'_{\gamma} & \text{otherwise.} \end{cases}$$

We are next going to show that  $\mathcal{S}_{\mathbf{v}'}(\sigma') = \mathcal{S}_{\mathbf{v}''}(\sigma'')$ . Then, by applying this transformation several times starting from  $\mathcal{S}(\varsigma) = \mathcal{S}_{[0, \dots, 0, 2^n]}(\varsigma)$ , we will be able to remove successively all identical siblings in  $\varsigma$  until we get the set  $\mathcal{S}_{\mathbf{v}}(\sigma)$  from the lemma.

Denote by  $\bar{\gamma}$  the parent node of  $\gamma_0$ , and by  $\gamma_1$  the sibling node of  $\gamma_0$  (i.e.,  $\gamma_0 = \bar{\gamma} \sqcup L$  and  $\gamma_1 = \bar{\gamma} \sqcup R$ ). Let  $X \in \mathcal{S}_{\mathbf{v}'}(\sigma')$ , and let  $T$  be a tree satisfying the conditions (i), (ii), (iii) of the definition of  $\mathcal{S}_{\mathbf{v}'}$ . In particular,  $T$  must satisfy

$$\begin{pmatrix} \sigma'_{\gamma_0 \sqcup L}(X) & T_{\gamma_0} \\ T_{\gamma_0} & \sigma'_{\gamma_0 \sqcup L}(X) \end{pmatrix} \succeq 0 \text{ and } \begin{pmatrix} T_{\gamma_0} & T_{\bar{\gamma}} \\ T_{\bar{\gamma}} & T_{\gamma_1} \end{pmatrix} \succeq 0 \quad (13)$$

(recall that  $\sigma'_{\gamma_0 \sqcup L} = \sigma'_{\gamma_0 \sqcup R}$ ). The first LMI implies  $T_{\gamma_0} \preceq \sigma'_{\gamma_0 \sqcup L}(X)$ , (see (3)), and so the second LMI is still satisfied if we replace the block  $T_{\gamma_0}$  by  $\sigma'_{\gamma_0 \sqcup L}(X)$ . No other LMI involves  $T_{\gamma_0}$  in the definition of  $\mathcal{S}_{\mathbf{v}'}$ . Hence we can replace these two LMIs by

$$\begin{pmatrix} \sigma'_{\gamma_0 \sqcup L}(X) & T_{\bar{\gamma}} \\ T_{\bar{\gamma}} & T_{\gamma_1} \end{pmatrix} \succeq 0,$$

which results in the set of conditions that  $T$  must satisfy to guarantee  $X \in \mathcal{S}_{\mathbf{v}''}(\sigma'')$ , because  $\sigma'_{\gamma_0 \sqcup L} = \sigma''_{\gamma_0}$ . So  $\mathcal{S}_{\mathbf{v}'}(\sigma') \subseteq \mathcal{S}_{\mathbf{v}''}(\sigma'')$ .

Conversely if  $X \in \mathcal{S}_{\mathbf{v}''}(\sigma'')$  and  $T$  satisfies (i), (ii), (iii) of the definition of  $\mathcal{S}_{\mathbf{v}''}$ , then we have  $T_{\gamma_0} = \sigma''_{\gamma_0}(X) = \sigma'_{\gamma_0 \sqcup L}(X)$ . So the two LMIs of Equation (13) are satisfied, and  $X \in \mathcal{S}_{\mathbf{v}'}(\sigma')$ . This shows  $\mathcal{S}_{\mathbf{v}''}(\sigma'') \subseteq \mathcal{S}_{\mathbf{v}'}(\sigma')$  and the proof of the lemma is complete.  $\square$

*Proof of Proposition 4.2 (continued).*

Let  $n_{\mathbf{A}} := \alpha$ ,  $n_{\mathbf{B}} := \beta - \alpha$  and  $n_{\mathbf{X}} := 2^n - \beta$  represent the number of occurrences of  $\mathbf{A}, \mathbf{B}$  and  $\mathbf{X}$  in  $\chi_{\alpha, \beta}$  (Recall that  $n$  is the largest integer such that  $2^{n-1} < \beta \leq 2^n$ ). Let the binary representation of these numbers be

$$n_{\mathbf{A}} = \sum_{k \in K_{\mathbf{A}}} 2^k, \quad n_{\mathbf{B}} = \sum_{k \in K_{\mathbf{B}}} 2^k, \quad \text{and} \quad n_{\mathbf{X}} = \sum_{k \in K_{\mathbf{X}}} 2^k,$$

where  $K_{\mathbf{A}}, K_{\mathbf{B}}$  and  $K_{\mathbf{X}}$  are (finite) subsets of  $\mathbb{N}$ . We define  $\mathbf{v} \in \mathbb{N}^n$  as follows:

$$\forall n \in \{1, \dots, n\}, \quad v_k = \left| \{Z \in \{\mathbf{A}, \mathbf{B}, \mathbf{X}\} : (n - k) \in K_Z\} \right|,$$

where  $|\cdot|$  denotes the cardinality of a set. By construction, the vector  $\mathbf{v}$  satisfies (12). Let  $\sigma \in \{\mathbf{A}, \mathbf{B}, \mathbf{X}\}^{\Gamma_{\mathbf{v}}^{\Delta}}$  be a sequence of characters such that the following sets coincide:

$$\forall k \in \{1, \dots, n\}, \quad \{\mathbf{Z} \in \{\mathbf{A}, \mathbf{B}, \mathbf{X}\} : (n-k) \in K_{\mathbf{Z}}\} = \{\sigma_{\gamma} : \gamma \in \Gamma_{\mathbf{v}}^{\Delta} \cap \Gamma_k\}.$$

In other words, there is a leaf  $\gamma \in \Gamma_{\mathbf{v}}^{\Delta}$  of depth  $k$  such that  $\sigma_{\gamma}$  takes the value  $\mathbf{Z} \in \{\mathbf{A}, \mathbf{B}, \mathbf{X}\}$  if and only if  $(n-k) \in K_{\mathbf{Z}}$ . It is easy to see that every leaf  $\gamma$  of depth  $k$  yields  $2^{n-k}$  leaves with the value  $\sigma_{\gamma}$  in the expanded sequence  $\varsigma$  of Lemma 6.1. So by construction,  $\varsigma$  contains  $\sum_{(n-k) \in K_{\mathbf{Z}}} 2^{n-k} = \sum_{k \in K_{\mathbf{Z}}} 2^k = n_{\mathbf{Z}}$  times the character  $\mathbf{Z}$ , i.e.  $\varsigma$  is a permutation of  $\chi_{\alpha, \beta}$ . By Lemma 6.1  $\mathcal{S}(\varsigma)$  admits the *SDR* provided in the definition of  $\mathcal{S}_{\mathbf{v}}(\sigma)$ , and it remains to show that it involves no more than  $2(n-1)$  LMIs and  $2n-3$  additional variables  $T_{\gamma} \in \mathbb{S}_m$ .

It is only necessary to add a new variable  $T_{\gamma}$  in the *SDR* when  $\gamma \in \Gamma_{\mathbf{v}}^{\circ} \setminus \{\emptyset\}$ , i.e., every non-leaf node at the exception of the root (for the other nodes  $\gamma \in \Gamma_{\mathbf{v}}^{\Delta} \cup \{\emptyset\}$ , by property (i) – (ii) the variable  $T_{\gamma}$  can be replaced by the constant  $A$  or  $B$ , or by the variable  $X$ ). So the number of LMIs required to define  $\mathcal{S}_{\mathbf{v}}(\sigma)$  is  $|\Gamma_{\mathbf{v}}^{\circ}|$  and the number of additional variables  $T_{\gamma} \in \mathbb{S}_m$  involved in the *SDR* is  $|\Gamma_{\mathbf{v}}^{\circ}| - 1$ .

Let us now bound the number of non-leaf nodes in  $\Gamma_{\mathbf{v}}$ . Let  $k \in \{1, \dots, n\}$ . By construction the characters of depth  $k$ , i.e.  $\{\sigma_{\gamma} : \gamma \in \Gamma_{\mathbf{v}}^{\Delta} \cap \Gamma_k\}$ , are all distinct, so they are no more than 3. Since the leaves are as far left as possible, if  $v_k \geq 2$  then two of the leaves must be siblings, and this implies that there are at most 2 non-leaf nodes at depth  $k-1$ . For the depth levels  $k=0$  and  $k=n-1$ , we can even bound the number of non-leaf-nodes by 1 (this is trivial for  $k=0$ ). Assume *ad absurdum* that  $v_n = 3$ . Then  $n_{\mathbf{A}}, n_{\mathbf{B}}$  and  $n_{\mathbf{X}}$  are odd numbers, so their sum is an odd number. But  $n_{\mathbf{A}} + n_{\mathbf{B}} + n_{\mathbf{X}} = 2^n$  must be even, which is a contradiction. So the number of leaves of depth  $n$  is  $v_n \leq 2$ , and the number of non-leave nodes of depth  $n-1$  is at most 1. To sum up, there is at most 1 non-leaf node at levels  $k=0$  and  $k=n-1$ , and at most 2 such nodes at levels  $k=1, \dots, n-2$ , so we obtain  $|\Gamma_{\mathbf{v}}^{\circ}| \leq 2(n-1)$ .

Before concluding the proof, we point out that this bound can be attained. For example, take  $\alpha = 3, \beta = 5$ , so that  $n = 3, n_{\mathbf{A}} = n_{\mathbf{X}} = 3$  and  $n_{\mathbf{B}} = 2$ . This yields  $\mathbf{v} = [0, 3, 2]$ , and  $|\Gamma_{\mathbf{v}}^{\circ}| = 4 = 2(n-1)$ .  $\square$