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Cone-Constrained Singular Value Problems

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Dedicated to Roger J-B Wets on the occasion of his 85th birthday.

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The singular values of a matrix A of size $m \times n$ can be seen as the critical values of the bilinear form $\langle u, Av\rangle$ with u and v ranging over the unit spheres of $\mathbb{R}^m$ and $\mathbb{R}^n$, respectively. If u and v are further restricted by closed convex cones P and Q, respectively, then the criticality conditions are: $P \ni u \perp (Av - \sigma u) \in P^*$, $Q \ni v \perp (A^\top u - \sigma v) \in Q^*$. This is a coupled system of complementarity problems involving a pair of cones and their dual cones. The parameter σ is called a singular value of A relative to (P, Q). The purpose of our work is to study this new concept of singular value. The analysis of such a coupled system is motivated by a number of applications. By way of illustration, we consider a nonnegative Principal Component Analysis problem.

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1. Introduction

Singular values and singular vectors play a central role in the analysis of a large variety of linear algebra problems involving rectangular matrices. Singular vectors, either left-singular or right-singular, are always assumed to be of unit length. Such a normalization condition is useful in many ways. The essential difference between our work and the linear algebra literature is that, in addition to normalization, we impose on each singular vector a constraint of conic type. The need of imposing constraints of conic type arises for instance in the area of Principal Component Analysis (PCA), cf. Example 1.5. Before entering into the theory of cone-constrained singular vectors, we say a few words on the unconstrained case. Let $\mathbb{S}_d$ be the unit sphere of $\mathbb{R}^d$ and $\mathbb{M}_{m,n}$ be the space of real matrices of size $m \times n$. The set $\Sigma(A)$ of singular values of a matrix $A \in \mathbb{M}_{m,n}$ is defined as follows: a real number σ is a *singular value* of A if there exists a pair $(u, v) \in \mathbb{S}_m \times \mathbb{S}_n$ such that

$$Av = \sigma u\,,\ A^\top u = \sigma v, \tag{1}$$

where the superscript $\top$ stands for transposition.

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In such a case, (u,v,σ) is called a *singular triplet* of A and u (respectively, v) is called a left-singular (respectively, right-singular) vector of A. We do not ask σ to be nonnegative, as done by linear algebraists. The reason is that we work in a cone-constrained setting in which the existence of nonnegative singular values is not automatically guaranteed. For grasping the meaning of a singular value of A, consider the problem of finding the critical points of the bilinear form $\langle u, Av\rangle$ on the bi-sphere $\mathbb{S}_m \times \mathbb{S}_n$. By a standard variational argument, (u,v) is a critical point of f on $\mathbb{S}_m \times \mathbb{S}_n$ if and only if $(u,v) \in \mathbb{S}_m \times \mathbb{S}_n$ and

$$Av = \gamma_1 u\,,\;\; A^\top u = \gamma_2 v \tag{2}$$

for some pair $(\gamma_1,\gamma_2) \in \mathbb{R}^2$. The scalars γ_1 and γ_2 are Lagrange multipliers associated to the equality constraints $\|u\|^2 - 1 = 0$ and $\|v\|^2 - 1 = 0$, respectively. The system (2) is obtained by equating to zero the gradient

$$\nabla L(u,v) \;=\; (\nabla_u L(u,v), \nabla_v L(u,v)) \;=\; \big(Av - \gamma_1 u, A^\top u - \gamma_2 v\big) \tag{3}$$

of the Lagrangian function

$$L(u,v) \;=\; \langle u, Av\rangle - \tfrac{\gamma_1}{2}\left(\|u\|^2 - 1\right) - \tfrac{\gamma_2}{2}\left(\|v\|^2 - 1\right). \tag{4}$$

Clearly, $\gamma_1 = \langle u, Av\rangle$ is equal to $\gamma_2 = \langle v, A^\top u\rangle$. If the common Lagrange multiplier is denoted by σ, then we recover (1) and see that $\sigma = \langle u, Av\rangle$ is a critical value of f on $\mathbb{S}_m \times \mathbb{S}_n$.

1.1. The cone-constrained version

Let $\mathcal{C}_d$ be the set of nonzero closed convex cones in $\mathbb{R}^d$. Let $P \in \mathcal{C}_m$ and $Q \in \mathcal{C}_n$ be a pair of cones intended to constraint u and v, respectively. The criticality (or stationarity) conditions for the minimization problem

$$\alpha \;=\; \min_{\substack{u\in P\cap\mathbb{S}_m\\ v\in Q\cap\mathbb{S}_n}} \langle u, Av\rangle \tag{5}$$

take the form of a coupled system of variational inequalities, namely,

$$\begin{cases} u \in P\,, \;\; \langle A\,v - \sigma u\,,\, u' - u\rangle \geq 0 \;\text{ for all }\; u' \in P\,,\\ v \in Q\,, \;\; \langle A^\top u - \sigma v, v' - v\rangle \geq 0 \;\text{ for all }\; v' \in Q\,. \end{cases}$$

Since P and Q are cones, such a system of variational inequalities can be reformulated as a system of complementarity problems

$$\begin{cases} P \ni u \perp (A\,v - \sigma u) \;\in P^*,\\ Q \ni v \perp (A^\top u - \sigma v) \in Q^* \end{cases} \tag{6}$$

involving the dual cones P^* and Q^*. The maximization problem

$$\beta \;=\; \max_{\substack{u\in P\cap\mathbb{S}_m\\ v\in Q\cap\mathbb{S}_n}} \langle u, Av\rangle \tag{7}$$

leads to a criticality model of the same kind, but involving polar cones:

$$\begin{cases} P \ni u \perp (A\,v - \sigma u) \ \ \in P^\circ, \\ Q \ni v \perp (A^\top u - \sigma v) \in Q^\circ. \end{cases} \tag{8}$$

If P and Q are linear subspaces, then both (6) and (8) reduce to

$$u \in P\,,\ v \in Q\,,\ Av - \sigma u \in P^\perp,\ A^\top u - \sigma v \in Q^\perp, \tag{9}$$

where $L^\perp$ is the orthogonal complement of L. If (P,Q) is not a pair of linear subspaces, then (6) and (8) are not quite the same model. However, since $P^\circ = -P^*$ and $Q^\circ = -Q^*$, one can pass easily from one model to the other. For avoiding repetitions, we focus on dual cones.

Definition 1.1. A real number σ is a *singular value* of A relative to (P,Q) if the system (6) holds for some $(u,v) \in \mathbb{S}_m \times \mathbb{S}_n$. In such a case, u (respectively, v) is called a *left-singular* (respectively, *right-singular*) *vector* of A relative to (P,Q).

The notation $\Sigma(A,P,Q)$ stands for the set of singular values of A relative to (P,Q). A similar set $\Sigma_\circ(A,P,Q)$ of "polar" singular values can be defined by using (8).

Since
$$\Sigma_\circ(A,P,Q) = -\Sigma(-A,P,Q)\,,$$

there is no loss of generality in working with singular values as introduced in Definition 1.1. As can be seen in the proof of Proposition 1.2, if $(u,v,\sigma) \in \mathbb{S}_m \times \mathbb{S}_n \times \mathbb{R}$ satisfies (6), then the term $\sigma = \langle u, Av\rangle$ is a critical value of (5). We could eliminate the variable σ and reformulate (6) as a conic system

$$u \in P\,,\ \ v \in Q\,,\ \ Av - \langle u, Av\rangle\, u \in P^*\,,\ \ A^\top u - \langle u, Av\rangle\, v \in Q^*$$

in the unknown pair (u,v). Such a reduction strategy obscures somehow the presentation of our results and, therefore, we prefer to keep σ in a visible place.

Proposition 1.2. $\Sigma(A,P,Q)$ *is a nonempty compact subset of the real line.*

Proof. The solution set to (5) is nonempty and compact. A necessary condition for $(u,v) \in \mathbb{S}_m \times \mathbb{S}_n$ to be a solution to (5) is that $(u,v) \in P \times Q$ and

$$\langle \nabla L(u,v), (u',v') - (u,v)\rangle \geq 0 \quad \text{for all } \ (u',v') \in P \times Q\,,$$

where L is the Lagrangian function (4). By substituting (3) into the above variational inequality and simplifying, we get

$$\begin{cases} P \ni u \perp (A\,v - \gamma_1 u) \ \ \in P^*, \\ Q \ni v \perp (A^\top u - \gamma_2 v) \in Q^*, \end{cases} \tag{10}$$

with $\gamma_1 = \langle u, Av\rangle$ equal to $\gamma_2 = \langle v, A^\top u\rangle$. The set $\Sigma(A,P,Q)$ is nonempty because it contains this common Lagrange multiplier. That $\Sigma(A,P,Q)$ is compact is clear. $\square$

Remark 1.3. Amri and Seeger [4] consider a more general minimization problem

$$\min_{\substack{u\in P\cap\mathbb{S}_m\\ v\in Q\cap\mathbb{S}_n}} \left\langle \begin{bmatrix} u \\ v \end{bmatrix}, \begin{bmatrix} W_{1,1} & W_{1,2} \\ W_{2,1} & W_{2,2} \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} \right\rangle$$

involving a block structured symmetric matrix W. The corresponding criticality conditions

$$P \ni u \perp (W_{1,1}u + W_{1,2}v - \gamma_1 u) \in P^*,$$
$$Q \ni v \perp (W_{2,1}u + W_{2,2}v - \gamma_2 v) \in Q^*$$

look similar to (10), but now the Lagrange multipliers γ_1 and γ_2 may not be equal. Incidentally, the pair (γ_1, γ_2) is called a bi-eigenvalue of W relative to (P, Q). □

There is a wide variety of interesting optimization problems that can be cast in the minimization format (5) or in the maximization format (7). We briefly mention a few important examples.

Example 1.4. Iusem and Seeger [10, 11, 12, 13] develop the theory of critical angles of a convex cone. Such a theory is based on the criticality conditions for the optimization problem

$$\cos\theta_K = \min_{u,v\in K\cap\mathbb{S}_n} \langle u, v\rangle$$

defining the maximal angle θ_K of a cone $K \in \mathcal{C}_n$. In terms of the multivalued map Σ, the set of critical angles of K is given by $\Omega(K) = \{\arccos\sigma : \sigma \in \Sigma(I_n, K, K)\}$, where I_n is the identity matrix of order n. Seeger and Sossa [24, 25] discuss the case of two cones:

$$\cos[\Theta_{\max}(P,Q)] = \min_{\substack{u\in P\cap\mathbb{S}_n\\ v\in Q\cap\mathbb{S}_n}} \langle u, v\rangle\,, \tag{11}$$

see also the recent contributions of Orlitzky [17] and Bauschke et al. [5]. Problem (11) can be treated in tandem with the analogous problem

$$\cos[\Theta_{\min}(P,Q)] = \max_{\substack{u\in P\cap\mathbb{S}_n\\ v\in Q\cap\mathbb{S}_n}} \langle u, v\rangle \tag{12}$$

defining the minimal angle $\Theta_{\min}(P,Q)$ between P and Q. Both cones are of course in the same space, namely, $\mathbb{R}^n$. Note that (11) and (12) are obtained by setting $A = I_n$ in (5) and (7), respectively. □

Example 1.5. Consider a sample $\{x_t\}_{t=1}^m$ generated by an n-dimensional zero-mean random vector. We may suppose that each data point x_t is a nonzero vector. The Principal Component Analysis (PCA) of such a sample consists in finding a direction of maximum variability:

$$\max_{\|v\|=1} \sum_{t=1}^m \langle x_t, v\rangle^2.$$

Zass and Shashua [30] and Montanari and Richard [16] examine the constrained version

$$\max_{\substack{\|v\|=1\\ v\geq 0}} \sum_{t=1}^m \langle x_t, v\rangle^2, \tag{13}$$

where $v \geq 0$ means that each component of v is nonnegative.

Note that $\sum_{t=1}^{m}\langle x_t, v\rangle^2 = \|X^\top v\|^2$, where $X = [x_1,\ldots,x_m]$ contains x_t in the t-th column. By passing to the square root in (13), we get the equivalent problem

$$\omega = \max_{\substack{\|u\|=1,\, \|v\|=1\\ v\geq 0}} \langle u, X^\top v\rangle\,, \tag{14}$$

which is a particular case of (7). Here v is cone-constrained, but u moves freely on the unit sphere. $\square$

Example 1.6. Let $\mathbb{M}_{m,n}$ be equipped with the Frobenius norm $\|X\| = \left[\mathrm{tr}(X^\top X)\right]^{1/2}$. The rank-one approximation problem

$$\min_{\substack{\|u\|=1,\, \|v\|=1\\ \sigma\in\mathbb{R}}} \|A-\sigma uv^\top\|^2$$

consists in approximating a nonzero matrix A by a rank-one matrix (in fact, by a matrix of rank at most one). Interesting variants of this problem are obtained by imposing further constraints on the vectors u and v (sparsity, nonnegativity, etc). Consider for instance the cone-constrained version

$$\min_{\substack{u\in\mathbb{S}_m\cap P,\, v\in\mathbb{S}_n\cap Q\\ \sigma\in\mathbb{R}}} \|A-\sigma uv^\top\|^2, \tag{15}$$

which we rewrite as $$\min_{\sigma\in\mathbb{R}} \underbrace{\min_{\substack{u\in\mathbb{S}_m\cap P\\ v\in\mathbb{S}_n\cap Q}} \|A-\sigma uv^\top\|^2}_{h(\sigma)}.$$

Dax [6] observes that $\|A-\sigma uv^\top\|^2 = \|A\|^2 - 2\sigma\langle u, Av\rangle + \sigma^2$ for all $(u,v)\in\mathbb{S}_m\times\mathbb{S}_n$. If we fix σ and pass to the minimum on each side of this equality, then we get

$$h(\sigma) = \begin{cases} \|A\|^2 - 2\beta\sigma + \sigma^2 & \text{if } \sigma\geq 0\,,\\ \|A\|^2 - 2\alpha\sigma + \sigma^2 & \text{if } \sigma\leq 0\,, \end{cases} \tag{16}$$

where α and β are given by (5) and (7), respectively. Clearly, $\alpha\leq\beta$. Minimizing the univariate function h is easy:

$$\mathrm{argmin}_{\sigma\in\mathbb{R}}\, h(\sigma) = \begin{cases} \{\alpha\} & \text{if } \alpha+\beta<0\,,\\ \{\beta\} & \text{if } \alpha+\beta>0\,,\\ \{\alpha,\beta\} & \text{if } \alpha+\beta=0\,. \end{cases}$$

As a solution to (15), we get a triplet (u_0, v_0, σ_0), where σ_0 is a minimizer of h and (u_0, v_0) is a solution to (7) (respectively, (5)) if $\sigma_0\geq 0$ (respectively, $\sigma_0\leq 0$). The sign and actual value of σ_0 depend on α and β, see Section 4.1 for some concrete examples. $\square$

In addition to the three examples just mentioned, we have found several references dealing with a problem that can be cast in the abstract format

$$\max_{\substack{u\in P\cap\mathbb{S}_m\\ v\in Q\cap\mathbb{S}_n}} f(\langle u, Av\rangle)$$

with $f(t) = |t|$ or $f(t) = t^2$. See Deshpande et al. [7, Theorem 3] for an example involving the absolute value function and Tenenhaus [28] for the case of the square function. For both choices of f, we end up with a combination of (5) and (7). For instance,

$$\max_{\substack{u\in P\cap\mathbb{S}_m\\ v\in Q\cap\mathbb{S}_n}} |\langle u, Av\rangle| \;=\; \max\left\{ \max_{\substack{u\in P\cap\mathbb{S}_m\\ v\in Q\cap\mathbb{S}_n}} \langle u, Av\rangle\,,\; -\min_{\substack{u\in P\cap\mathbb{S}_m\\ v\in Q\cap\mathbb{S}_n}} \langle u, Av\rangle \right\} \;=\; \max\{\beta, -\alpha\}\,.$$

So, there is a strong motivation for studying problem (5) or the maximization counter-part (7).

2. General theory of cone-constrained singular vectors

The dimensions m and n may be different. Without loss of generality, we may assume that $m \leq n$ or, if we prefer, that $m \geq n$. Indeed, in view of the equality

$$\Sigma(A, P, Q) = \Sigma(A^\top, Q, P)\,, \tag{17}$$

we can shift the attention from A to $A^\top$ if necessary. We refer to (17) as the transposition transfer formula. Another interesting rule for the multivalued map Σ concerns the replacement of P and Q by the cones $R_1(P) = \{R_1 u : u \in P\}$ and $R_2(Q) = \{R_2 v : v \in Q\}$, where R_1 and R_2 are orthogonal matrices of order m and n, respectively. It is easy to check that

$$\Sigma(A, R_1(P), R_2(Q)) \;=\; \Sigma(R_1^\top A R_2, P, Q)\,.$$

So, we can rotate P and Q if it is convenient to do so. For instance, if we are given a self-dual revolution cone P and a self-dual simplicial cone Q, then there is no loss of generality in assuming that P is the standard Lorentz cone in upward position and Q is the usual nonnegative orthant. The next proposition implies that if P and Q are linear subspaces, then we are back to a classical setting in which singular vectors are unconstrained.

Proposition 2.1. *Let P and Q be linear subspaces. Then*

$$\Sigma(A, P, Q) = \Sigma\left(M^\top A N\right), \tag{18}$$

where M is a matrix whose columns form an orthonormal basis of P and N is a matrix whose columns form an orthonormal basis of Q. In particular,

$$\mathrm{card}\,[\Sigma(A, P, Q)] \leq 2\min\{\dim P, \dim Q\}.$$

Proof. Let $p = \dim P$ and $q = \dim Q$. Consider the change of variables $u = M\xi$ and $v = N\eta$. Since $M^\top M = I_p$ and $N^\top N = I_q$, we have $\|u\| = \|\xi\|$ and $\|v\| = \|\eta\|$. Hence, $(u, v) \in \mathbb{S}_m \times \mathbb{S}_n$ satisfies (9) if and only if $(\xi, \eta) \in \mathbb{S}_p \times \mathbb{S}_q$ satisfies

$$AN\eta - \sigma M\xi \in \mathrm{Ker}(M^\top), \quad \text{and} \quad A^\top M\xi - \sigma N\eta \in \mathrm{Ker}(N^\top)$$

or, equivalently, $M^\top A N\,\eta = \sigma\xi$ and $(M^\top A N)^\top \xi = \sigma\eta$. This proves (18). The matrix $M^\top A N$ being of size $p \times q$, it has at most $2\min\{p, q\}$ singular values. The factor 2 is because we are also counting negative singular values. □

We are in a truly cone-constrained setting if at least one of the cones is not a linear subspace. A closed convex cone that is not a linear subspace could have finitely many or infinitely many faces. The last case occurs if the cone is non-polyhedral. In what follows, $\mathcal{F}(P)$ is the set of nonzero faces of P and span$F$ is the linear span of a face F. A set is countable if it is finite or has the same cardinality as the set of positive integers.

Theorem 2.2. *We always have*

$$\Sigma(A,P,Q) \;\subseteq\; \bigcup_{\substack{F\in\mathcal{F}(P)\\ G\in\mathcal{F}(Q)}} \Sigma(A,\mathrm{span}F,\mathrm{span}\,G\,)\,. \tag{19}$$

In particular, if P and Q are polyhedral (*respectively, have countably many faces*), *then $\Sigma(A,P,Q)$ is finite* (*respectively, countable*).

Proof. Inclusion (19) is obtained by applying [4, Proposition 3.1] to the particular case

$$\begin{bmatrix} W_{1,1} & W_{1,2} \\ W_{2,1} & W_{2,2} \end{bmatrix} = \begin{bmatrix} 0 & A \\ A^\top & 0 \end{bmatrix}.$$

The last part of the theorem follows from (19) and Proposition 2.1. If P and Q are polyhedral, then

$$\mathrm{card}[\Sigma(A,P,Q)] \;\leq\; 2\sum_{k=1}^{d_P}\sum_{\ell=1}^{d_Q} f_P(k) f_Q(\ell)\min\{k,\ell\}\,, \tag{20}$$

where d_P is the dimension of the span of P and $f_P(k)$ is the number of k-dimensional faces of P. The upper bound (20) may not be sharp, but shows that $\Sigma(A,P,Q)$ is a finite set. If P and Q have countably many faces, then $\Sigma(A,P,Q)$ is contained in a countable union of finite sets and, therefore, it is countable. $\square$

In a non-polyhedral setting, $\Sigma(A,P,Q)$ could be countable infinite or even uncountable. For instance, Iusem and Seeger [11, Theorem 2] construct a non-polyhedral cone $K \in \mathcal{C}_3$ whose set of critical angles is uncountable. The practical evaluation of $\Sigma(A,P,Q)$ could be nightmarish if the cones P and Q are not nicely structured.

2.1. Stability issues

It is natural to ask what happens with the set $\Sigma(A,P,Q)$ if the matrix A and the cones P and Q are subject to small perturbations. For the sake of convenience, we introduce the notation

$$\mathcal{D}_{m,n} = \mathbb{M}_{m,n} \times \mathcal{C}_m \times \mathcal{C}_n.$$

We could view $\Sigma : \mathcal{D}_{m,n} \to 2^{\mathbb{R}}$ as an ordinary function with values in the power set $2^{\mathbb{R}}$, but we prefer to consider $\Sigma : \mathcal{D}_{m,n} \rightrightarrows \mathbb{R}$ as a multivalued map. Hence, upper and lower semicontinuity are to be understood in the traditional multivalued sense, cf. Rockafellar and Wets [20, p. 193]. The vector space $\mathbb{M}_{m,n}$ is finite dimensional, so we can equip it with any norm. For measuring the distance between two closed convex cones in $\mathbb{R}^n$, we consider the uniform metric

$$\delta_n(Q_1,Q_2) = \max_{w\in\mathbb{S}_n} |\mathrm{dist}(w,Q_1) - \mathrm{dist}(w,Q_2)|\,.$$

Convergence with respect to the uniform metric is equivalent to convergence in the Painlevé-Kuratowski sense, cf. [14] or [20, Section 4].

The proposition below uses the metric

$$\Delta((A_1,P_1,Q_1),(A_2,P_2,Q_2)) = \max\{\|A_1-A_2\|,\delta_m(P_1,P_2),\delta_n(Q_1,Q_2)\}$$

to measure the distance between two elements of $\mathcal{D}_{m,n}$.

Proposition 2.3. *Let* $\max\{m,n\}\geq 1$. *Then the map* $\Sigma:\mathcal{D}_{m,n}\rightrightarrows\mathbb{R}$ *is upper semicontinuous, but not lower semicontinuous.*

Proof. The graph of the multivalued map Σ is defined as the set

$$\mathrm{gr}(\Sigma)=\{(A,P,Q,\sigma):\sigma\in\Sigma(A,P,Q)\}.$$

We claim that such a set is closed in the Cartesian product $\mathcal{D}_{m,n}\times\mathbb{R}$.
Let $\{(A_k,P_k,Q_k,\sigma_k)\}_k$ be a sequence in $\mathrm{gr}(\Sigma)$ such that

$$\|A_k-A\|\to 0\,,\ \delta_m(P_k,P)\to 0\,,\ \delta_n(Q_k,Q)\to 0\,,\ |\sigma_k-\sigma|\to 0 \tag{21}$$

with $(A,P,Q,\sigma)\in\mathcal{D}_{m,n}\times\mathbb{R}$. For each k, there exists $(u_k,v_k)\in\mathbb{S}_m\times\mathbb{S}_n$ such that

$$\begin{cases} P_k \ni u_k \perp (A_k v_k-\sigma_k u_k)\in P_k^*\,,\\ Q_k\ni v_k\perp (A_k^\top u_k-\sigma_k v_k)\in Q_k^*\,. \end{cases} \tag{22}$$

The bi-sphere $\mathbb{S}_m\times\mathbb{S}_n$ being compact, we may suppose that $\{u_k\}_k$ and $\{v_k\}_k$ converge to unit vectors u and v, respectively. On the other hand, by using (21) and the Walkup-Wets Isometry Theorem [29], we deduce that $\delta_m(P_k^*,P^*)\to 0$ and $\delta_n(Q_k^*,Q^*)\to 0$. A passage to the limit in (22) leads to (6). Hence, $\sigma\in\Sigma(A,P,Q)$ and $\mathrm{gr}(\Sigma)$ is closed. On the other hand, we observe that if Ω is a nonempty bounded set in the space $\mathbb{M}_{m,n}$, then there exists a constant c (depending just on Ω) such that

$$\max\{|\sigma|:\sigma\in\Sigma(A,P,Q)\}\ \leq\ \max_{\|v\|=1}\|Av\|\ \leq\ c$$

for all $(A,P,Q)\in\Omega\times\mathcal{C}_m\times\mathcal{C}_n$. Hence, Σ maps bounded sets into bounded sets. But mapping bounded sets into bounded sets and having a closed graph is sufficient for a multivalued map to be upper semicontinuous, cf. [20, Theorem 5.19]. Building a counterexample for the lower semicontinuity of Σ offers no difficulty. □

2.2. Link to the theory of cone-spectra of square matrices

The theory of cone-constrained singular values for rectangular matrices has some analogies with the theory of cone-constrained eigenvalues for square matrices as developed by the first author, but the differences are important enough to justify a separate treatment. We would like to mention that it is not always a good strategy to convert a singular value problem into an eigenvalue problem. This observation is specially relevant in a cone-constrained context. The next definition is taken from Seeger [21]. Let $\mathbb{M}_d$ be the space of square matrices of order d.

Definition 2.4. Let $K\in\mathcal{C}_d$ and $E\in\mathbb{M}_d$. A real number λ is a K-*eigenvalue* of E if

$$K\ni x\perp(Ex-\lambda x)\in K^* \tag{23}$$

has a nonzero solution $x\in\mathbb{R}^d$, called a K-*eigenvector* of E. The set of K-eigenvalues of E is denoted by $\mathrm{Sp}(E,K)$ and it is called the K-*spectrum* of E. □

A nonzero solution x to (23) can always be normalized so that $\|x\| = 1$. The matrix E in Definition 2.4 does not need to be symmetric, but it must be square. Note that $\mathrm{Sp}(E, \mathbb{R}^d)$ corresponds to the set of real eigenvalues of E. There is an abundant literature devoted to the analysis and numerical computation of cone-spectra. See for instance [3, 21, 22, 23, 26, 27] for theoretical issues and [1, 2, 8, 15, 18, 19] for algorithmic aspects. In some of these references, the preference is given to the polarized K-spectrum

$$\mathrm{Sp}_\circ(E, K) = -\mathrm{Sp}(-E, K)\,.$$

It is natural to ask whether $\Sigma(A, P, Q)$ can be obtained by solving a cone-constrained eigenvalue problem like (23). The first idea that comes to mind is to reformulate (6) as

$$P \times Q \ni \begin{bmatrix} u \\ v \end{bmatrix} \perp \left(\begin{bmatrix} 0 & A \\ A^\top & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} - \sigma \begin{bmatrix} u \\ v \end{bmatrix} \right) \in (P \times Q)^*, \tag{24}$$

where $P \times Q$ is the Cartesian product of P and Q. The next proposition shows that, except for a detail, $\Sigma(A, P, Q)$ can be recovered by computing the spectrum relative to $P \times Q$ of the Jordan-Wielandt matrix

$$E_A = \begin{bmatrix} 0 & A \\ A^\top & 0 \end{bmatrix},$$

which is a symmetric matrix of order $m + n$.

Proposition 2.5. *We have*

$$\mathrm{Sp}(E_A, P \times Q) \backslash \{0\} \subseteq \Sigma(A, P, Q) \subseteq \mathrm{Sp}(E_A, P \times Q)\,. \tag{25}$$

Proof. The product space $\mathbb{R}^m \times \mathbb{R}^n$ is identified with $\mathbb{R}^{m+n}$. Hence, $P \times Q$ is viewed as a nonzero closed convex cone in $\mathbb{R}^{m+n}$. Its dual cone is equal to $P^* \times Q^*$ and (24) is indeed an equivalent reformulation of (6). We prove the first inclusion in (25), the second one being obvious. Let $\sigma \neq 0$ be such that (24) holds for a nonzero vector $(u, v) \in \mathbb{R}^{m+n}$. We claim that $u \neq 0$ and $v \neq 0$. Suppose for instance that $u = 0$. In such a case, (24) says that $Av \in P^*$ and $Q \ni v \perp (-\sigma v) \in Q^*$. In particular, $-\sigma\|v\|^2 = 0$. Hence, $v = 0$ and we contradict that (u, v) is a nonzero vector. In conclusion, both u and v are nonzero as claimed. Next, by using the orthogonality conditions

$$\langle u, Av - \sigma u\rangle = 0\,,\ \langle v, A^\top u - \sigma v\rangle = 0\,,$$

we get $\sigma\|u\|^2 = \langle u, Av\rangle = \langle v, A^\top u\rangle = \sigma\|v\|^2$. Hence, u and v have the same length and, consequently, we may assume that $\|u\| = \|v\| = 1$. We deduce that σ is an element of $\Sigma(A, P, Q)$. $\square$

The sets $\Sigma(A, P, Q)$ and $\mathrm{Sp}(E_A, P \times Q)$ could be different, but, if there is a difference at all, then such a difference is only minor: the value 0 may be in the second set and not in the first. The transformation of a cone-constrained singular value problem to a (nearly) equivalent symmetric cone-constrained eigenvalue problem is not always a convenient strategy. A priori, there is no reason to believe that computing $\mathrm{Sp}(E_A, P \times Q)$ is easier than computing $\Sigma(A, P, Q)$. In fact, the Cartesian product $P \times Q$ may not preserve some good properties of the component cones P

and Q. For instance, the Cartesian product of two ellipsoidal cones is no longer an ellipsoidal cone. The computation of $\mathrm{Sp}(E_A, P\times Q)$ could be problematic also from a dimensionality point of view. Indeed, the Jordan-Wielandt matrix E_A has as much as $(m+n)^2$ entries. The existing algorithms for computing cone-spectra should be adapted to the block structured matrix E_A. This being said, Proposition 2.5 could be of interest from a theoretical point of view. For instance, it is known that $\mathrm{Sp}(E, K)$ is a finite set for all E if the cone K is polyhedral, cf. [21]. By using the second inclusion in (25), we deduce that $\Sigma(A, P, Q)$ is a finite set for all A if the cones P and Q are polyhedral, cf. Theorem 2.2. Even if the Jordan-Wielandt matrix E_A is problematic from a dimensionality point of view, it has nonetheless a number of interesting applications, see for instance the proof of the next proposition.

Recall that a nonzero closed convex cone K is non-obtuse if any two unit vectors in K form an angle of 90 degrees at most.

Proposition 2.6. *Let P and Q be non-obtuse. Then there is at most one $\sigma \in \mathbb{R}$ for which the system*

$$Av = \sigma u\,,\ A^\top u = \sigma v\,,\ u \in \mathrm{int}(P)\,,\ v \in \mathrm{int}(Q). \tag{26}$$

is solvable in the unknown (u, v).

Proof. This result is about uniqueness and not about existence. If (u, v, σ) satisfies (26), then

$$\begin{bmatrix} 0 & A \\ A^\top & 0 \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix} = \sigma \begin{bmatrix} u \\ v \end{bmatrix}, \quad \begin{bmatrix} u \\ v \end{bmatrix} \in \mathrm{int}(P\times Q).$$

The Cartesian product of two non-obtuse cones being non-obtuse, it follows that $P\times Q$ is non-obtuse and, therefore, it cannot accommodate two orthogonal vectors in its interior. Hence, the symmetric matrix E_A has at most one eigenvalue with associated eigenvector in $\mathrm{int}(P\times Q)$. $\square$

2.3. Constraints on right-singular vectors only

If P is the whole space $\mathbb{R}^m$, then (6) becomes a hybrid complementarity problem

$$Av \;=\; \sigma u \tag{27}$$

$$Q \ni v \;\perp\; (A^\top u - \sigma v) \in Q^*. \tag{28}$$

Here v is a cone-constrained unit vector, but u lies anywhere on the unit sphere. We encountered already such a situation in Example 1.5. The nonnegative PCA concerns a maximization problem and, consistently, (28) is to be written with the polar cone of Q. We continue however with the strategy of giving the priority to minimization problems and dual cones. The next theorem characterizes the set

$$\Sigma^{\mathrm{right}}(A, Q) \;=\; \Sigma(A, \mathbb{R}^m, Q)\,,$$

where the superscript underlines that only right-singular vectors are cone-constrained.

Theorem 2.7. *Depending on the sign of σ, there are three possibilities:*

(a) $0 \in \Sigma^{\rm right}(A,Q)$ *if and only if there exists* $(u,v) \in \mathbb{S}_m \times \mathbb{S}_n$ *such that* $A^\top u \in Q^*$, $v \in Q$, $Av = 0$.

(b) *Let σ be positive. Then* $\sigma \in \Sigma^{\rm right}(A,Q)$ *if and only if* $\sigma^2 \in {\rm Sp}(A^\top A, Q)$.

(c) *Let σ be negative. Then* $\sigma \in \Sigma^{\rm right}(A,Q)$ *if and only if* $\sigma^2 \in {\rm Sp}_\circ(A^\top A, Q)$.

Proof. (a) By setting $\sigma = 0$ in (27)–(28), we get

$$Av = 0\,,\ \ Q \ni v \perp (A^\top u) \in Q^*. \tag{29}$$

Since $\langle v, A^\top u\rangle = 0$ holds automatically if $Av = 0$, system (29) says that $A^\top u \in Q^*$ and $v \in Q \cap {\rm Ker}A$.

(b) Let σ be positive. By substituting $u = (1/\sigma)Av$ into (28), we get

$$Q \ni v \perp (1/\sigma)(A^\top Av - \sigma^2 v) \in Q^*. \tag{30}$$

Since Q^* is a cone, we can drop the positive term $(1/\sigma)$ and write instead

$$Q \ni v \perp (A^\top Av - \sigma^2 v) \in Q^*. \tag{31}$$

We now draw some conclusions. If (u,v,σ) is a singular triplet of A relative to $(\mathbb{R}^m, Q)$, then $v \in \mathbb{S}_n$ satisfies (31) and, therefore, $\sigma^2 \in {\rm Sp}(A^\top A, Q)$. Conversely, let $\sigma^2 \in {\rm Sp}(A^\top A, Q)$. Hence, (31) holds for some nonzero v, which can be normalized so that $\|v\| = 1$. If $Av = 0$, the orthogonality condition in (31) yields $-\sigma^2\|v\|^2 = 0$, contradicting that v is a unit vector. We deduce now that $Av \neq 0$, in which case $u = (1/\sigma)Av$ is nonzero and (u,v,σ) satisfies (27)–(28). We now observe that

$$\sigma^2\|u\|^2 = \|\sigma u\|^2 = \|Av\|^2 = \langle v, A^\top Av\rangle = \sigma^2\|v\|^2,$$

the last equality being due to the orthogonality condition in (31). Hence, u is also a unit vector and (u,v,σ) is a singular triplet of A relative to $(\mathbb{R}^m, Q)$. *Part* (c). Let σ be negative. We write (30) in the form

$$Q \ni v \perp -(1/\sigma)((-A^\top A)v - (-\sigma^2)v) \in Q^*$$

and drop the positive term $-(1/\sigma)$. The remaining part of the proof is as in part (b). $\square$

${\rm Sp}(A^\top A, Q)$ and ${\rm Sp}_\circ(A^\top A, Q)$ are different in general. Computing the first set (respectively, the second set) is a matter of finding the Q-eigenvalues of a positive semidefinite (respectively, negative semidefinite) symmetric matrix of order n. This is done with *ad hoc* algorithms of the theory of cone-spectra. A similar theorem characterizes $\Sigma^{\rm left}(A,P) = \Sigma(A,P,\mathbb{R}^n)$. The transposition transfer formula (17) yields $\Sigma^{\rm left}(A,P) = \Sigma^{\rm right}(A^\top, P)$, so we are back to a right cone-constrained setting.

2.4. The smallest element of $\Sigma(A,P,Q)$

A question that arises in a number of situations is that of finding a constant $\gamma \in \mathbb{R}$ such that

$$\langle u, Av\rangle \geq \gamma\,\|u\|\,\|v\| \qquad \text{for all } u \in P,\ v \in Q. \tag{32}$$

Such a constant always exists and corresponds to a lower bound for the rectangular quotient

$$r(u,v) \;=\; \frac{\langle u, Av\rangle}{\|u\|\,\|v\|} \tag{33}$$

when u and v are nonzero vectors ranging over P and Q, respectively. The term (33) plays somehow the same role as the Rayleigh quotient associated to a quadratic function. The next result is easy and, therefore, its proof is omitted.

Proposition 2.8. *The term α in* (5) *is equal to the largest possible γ in* (32)*. Furthermore,*

$$\alpha \;=\; \min_{\sigma\in\Sigma(A,P,Q)} \sigma\,.$$

We mention Proposition 2.8 just to show the link between the general inequality (32) and the theory of cone-constrained singular values. The case $\gamma = 0$ in inequality (32) is of special interest. If $\langle u, Av\rangle \geq 0$ for all $u \in P$ and $v \in Q$, then A is called nonnegative relative to (P,Q). Such a nonnegativity concept for rectangular matrices is classical. It is well known that the set of nonnegative matrices relative to (P,Q) is a closed convex cone, namely,

$$\pi(Q,P^*) = \{A \in \mathbb{M}_{m,n} : A(Q) \subseteq P^*\}\,.$$

The next corollary is a straightforward consequence of Proposition 2.8.

Corollary 2.9. *$A(Q) \subseteq P^*$ if and only if each element of $\Sigma(A,P,Q)$ is nonnegative.*

Example 2.10. The Lorentz cone $\mathbb{L}_d = \{x \in \mathbb{R}^d : \left[x_1^2 + \ldots + x_{d-1}^2\right]^{1/2} \leq x_d\}$ is a non-polyhedral self-dual cone. Each element of $\mathrm{LSV}(A) = \Sigma(A,\mathbb{L}_m,\mathbb{L}_n)$ is called a Lorentz singular value of A. Explaining how to compute the entire set $\mathrm{LSV}(A)$ is space consuming, so we leave this specific task to a separate note. A question addressed in Hildebrand [9] is that of characterizing

$$\pi(\mathbb{L}_n,\mathbb{L}_m) = \{A \in \mathbb{M}_{m,n} : A(\mathbb{L}_n) \subseteq \mathbb{L}_m\}\,.$$

Corollary 2.9 asserts that $A(\mathbb{L}_n) \subseteq \mathbb{L}_m$ if and only if each Lorentz singular value of A is nonnegative. This observation is not as explicit as Hildebrand's result [9, Lemma 3.6], but it sheds a different light on the problem. In essence, the issue at hand is that of determining the sign of the smallest Lorentz singular value of A.

2.5. Assumptions ensuring the finiteness of $\Sigma(A,P,Q)$

As mentioned already, if (P,Q) is a pair of polyhedral cones, then $\Sigma(A,P,Q)$ is finite for all $A \in \mathbb{M}_{m,n}$. The same conclusion may not be true if at least one of the cones is non-polyhedral.

Proposition 2.11. *For all $m \geq 3$ and $n \geq 3$, there exists $(A,P,Q) \in \mathbb{M}_{m,n}\times\mathcal{C}_m\times\mathcal{C}_n$ such that $\Sigma(A,P,Q)$ is infinite.*

Proof. By using formula (17) if necessary, we may suppose that $m \leq n$. We take $P = \mathbb{R}^m$ and prove the existence of $(A,Q) \in \mathbb{M}_{m,n} \times \mathcal{C}_n$ such that $\Sigma^{\mathrm{right}}(A,Q)$ is infinite. Seeger [23, Theorem 6] asserts that if $E \in \mathbb{M}_n$ is a symmetric matrix admitting an eigenvalue that is multiple and different from the largest one, then there exists a non-polyhedral cone $Q \in \mathcal{C}_n$ such that $\mathrm{Sp}(E, Q)$ is infinite. By way of example, consider the rank-one matrix $E_n = \mathrm{Diag}[1, 0, \ldots, 0]$ of order n. Such a symmetric matrix has 1 as simple eigenvalue and 0 as eigenvalue of multiplicity $n-1$. See the proof of [23, Theorem 6] for the construction of Q. Let $A = [E_m \,|\, O\,]$ be formed with the rank-one matrix E_m of order m and a zero block of size $m \times (n-m)$. Of course, the zero block does not show up if $m = n$. Since $A^\top A = E_n$, the set $\mathrm{Sp}(A^\top A, Q)$ contains infinitely many elements. Such elements are nonnegative, because $A^\top A$ is positive semidefinite. Thanks to Theorem 2.7 (b), we can write

$$\{\sqrt{\lambda} : \lambda \in \mathrm{Sp}(A^\top A, Q) \backslash \{0\}\} \subseteq \Sigma^{\mathrm{right}}(A, Q).$$

This proves that $\Sigma^{\mathrm{right}}(A, Q)$ is infinite. □

A non-polyhedral example of finiteness is given in the next proposition.

Proposition 2.12. *Let P be a linear subspace and Q be a revolution cone (or viceversa). Then $\Sigma(A, P, Q)$ is finite for all $A \in \mathbb{M}_{m,n}$.*

Proof. Suppose, for instance, that P is a p-dimensional linear subspace of $\mathbb{R}^m$ and Q is a revolution cone in $\mathbb{R}^n$. If we define the matrix M as in Proposition 2.1 and introduce the change of variables $u = M\xi$, then $\|u\| = \|\xi\|$ and (6) becomes

$$M^\top A v = \sigma \xi\,, \quad Q \ni v \perp (A^\top M \xi - \sigma v) \in Q^*.$$

Hence, $\Sigma(A, P, Q) = \Sigma^{\mathrm{right}}(M^\top A, Q)$ and Theorem 2.7 shows that $\Sigma(A, P, Q) \backslash \{0\}$ is the union of the sets

$$\begin{aligned} W_+ &= \{\sqrt{\lambda} : \lambda \in \mathrm{Sp}(E, Q) \backslash \{0\}\}\,, \\ W_- &= \{-\sqrt{\lambda} : \lambda \in \mathrm{Sp}_\circ(E, Q) \backslash \{0\}\}\,, \end{aligned}$$

where $E = A^\top M M^\top A$ is a positive semidefinite symmetric matrix. But, Seeger [22, Proposition 5] shows that a symmetric matrix cannot have infinitely many eigenvalues relative to a revolution cone. Hence, $W_\pm$ are finite sets and so is $\Sigma(A, P, Q)$. □

3. Pareto singular values

The Pareto cone (or nonnegative orthant) of the space $\mathbb{R}^d$ is denoted by Π_d. Of special importance is the singular value analysis of a rectangular matrix relative to a pair (Π_m, Π_n) of Pareto cones. The complementarity model (6) takes in this case the form

$$\begin{cases} 0 \leq u \perp (Av - \sigma u) \ \geq 0\,, \\ 0 \leq v \perp (A^\top u - \sigma v) \geq 0\,. \end{cases} \tag{34}$$

The above system corresponds to the criticality conditions for the minimization problem

$$\varrho_{\min}(A) = \min_{\substack{\|u\|=1,\, \|v\|=1 \\ u \geq 0,\, v \geq 0}} \langle u, Av \rangle\,. \tag{35}$$

The criticality conditions for the maximization problem

$$\varrho_{\max}(A) = \max_{\substack{\|u\|=1,\, \|v\|=1 \\ u \geq 0,\, v \geq 0}} \langle u, Av \rangle \tag{36}$$

are similar to (34), except that the right-hand side inequalities are reversed.

Any element of $\mathrm{PSV}(A) = \Sigma(A, \Pi_m, \Pi_n)$ is called a *Pareto singular value* of A. Proposition 2.8 implies that

$$\varrho_{\min}(A) = \min_{\sigma \in \mathrm{PSV}(A)} \sigma . \tag{37}$$

Note that $\varrho_{\max}(A)$ may not be in $\mathrm{PSV}(A)$. In fact, $\varrho_{\max}(A)$ is the largest element of the polarized version $\mathrm{PSV}_\circ(A) = -\mathrm{PSV}(-A)$. In general, $\Sigma(A)$ and $\mathrm{PSV}(A)$ are non-comparable with respect to set inclusion, i.e., neither set is contained in the other. For subsequent use, we record below a lemma that relates classical, Perronian, and Pareto singular values. Some comments on notation and terminology are in order. The spectral norm of a rectangular matrix A is defined by

$$\sigma_{\max}(A) = \left[\lambda_{\max}(A^\top A)\right]^{1/2} = \max_{\|v\|=1} \|Av\| .$$

This notation is consistent with the fact that $\sigma_{\max}(A)$ is the largest singular value of A. A real number σ is called a Perronian singular value of A if there exists $(u, v) \in \mathbb{S}_m \times \mathbb{S}_n$ such that

$$Av = \sigma u\,, \ A^\top u = \sigma v\,, \tag{38}$$

$$u > 0\,, \ v > 0\,, \tag{39}$$

where $u > 0$ means that each component of u is positive. Condition (39) says that u and v are in the interior of Π_m and Π_n, respectively. For this reason, a Perronian singular value is also called an interior-type singular value. Consistently, we use the notation

$$\mathrm{ISV}(A) = \{\sigma \in \mathbb{R} : \sigma \text{ is a Perronian singular value}\}\,,$$

where the first letter is a reminder of "Interior-type".

Lemma 3.1. $\Sigma(A)$ *and* $\mathrm{PSV}(A)$ *are nonempty sets with* $\mathrm{ISV}(A) \subseteq \Sigma(A) \cap \mathrm{PSV}(A)$. *Furthermore,*

(a) $\mathrm{ISV}(A)$ *is either empty or a singleton.*

(b) *If A is positive, then* $\mathrm{ISV}(A) = \{\sigma_{\max}(A)\}$.

Proof. $\Sigma(A)$ and $\mathrm{PSV}(A)$ are nonempty by Proposition 1.2 and the announced inclusion is obvious. Pareto cones are non-obtuse and, therefore, Proposition 2.6 implies that $\mathrm{ISV}(A)$ contains one element at most. Finally, suppose that A is positive. In such a case, $A^\top A$ is positive and the Perron theorem ensures that $A^\top A v_0 = \lambda_{\max}(A^\top A)\, v_0$ for some unit vector $v_0 > 0$. Note that $Av_0 > 0$. If $\sigma_0 = \sigma_{\max}(A)$ and $u_0 = (1/\sigma_0)Av_0$, then (u_0, v_0, σ_0) satisfies (38)–(39) and $\|u_0\| = (1/\sigma_0)\|Av_0\| = 1$. Hence, $\mathrm{ISV}(A)$ contains $\sigma_{\max}(A)$ as unique element. □

The next theorem fully characterizes $\mathrm{PSV}(A)$. For the sake of convenience, we introduce the sets $\langle d \rangle = \{1, 2, \ldots, d\}$ and

$$\mathcal{J}(m, n) = \{(I, J) : \emptyset \neq I \subseteq \langle m \rangle,\ \emptyset \neq J \subseteq \langle n \rangle\}.$$

For (I, J) as above, let $A^{I,J}$ be the submatrix of A obtained by keeping the entries $a_{i,j}$ with $i \in I$ and $j \in J$. In particular, $A^{\langle m \rangle, \langle n \rangle} = A$.

Theorem 3.2. *A real number σ belongs to* $\mathrm{PSV}(A)$ *if and only if there exist* $(I,J) \in \mathcal{J}(m,n)$ *and vectors* $\xi \in \mathbb{R}^{|I|}$ *and* $\eta \in \mathbb{R}^{|J|}$ *such that*

$$A^{I,J}\eta = \sigma\xi\,, \tag{40}$$

$$(A^{I,J})^\top \xi = \sigma\eta\,, \tag{41}$$

$$\xi > 0,\ \eta > 0\,, \tag{42}$$

$$\textstyle\sum_{j\in J} a_{i,j}\,\eta_j \geq 0 \quad \forall i \in \langle m\rangle\backslash I\,, \tag{43}$$

$$\textstyle\sum_{i\in I} a_{i,j}\,\xi_i \geq 0 \quad \forall j \in \langle n\rangle\backslash J\,. \tag{44}$$

Furthermore, the above system can be written with the extra conditions $\|\xi\| = 1$ *and* $\|\eta\| = 1$.

Proof. Let $\sigma \in \mathrm{PSV}(A)$. Then, there exists $(u,v) \in \mathbb{S}_m \times \mathbb{S}_n$ satisfying (34) or, equivalently,

$$u_i \geq 0,\ v_j \geq 0\,, \tag{45}$$

$$(Av - \sigma u)_i \geq 0\,, \tag{46}$$

$$(A^\top u - \sigma v)_j \geq 0\,, \tag{47}$$

$$u_i(Av - \sigma u)_i = 0\,, \tag{48}$$

$$v_j(A^\top u - \sigma v)_j = 0\,, \tag{49}$$

for all $i \in \langle m\rangle$ and $j \in \langle n\rangle$. Let $I = \{i \in \langle m\rangle : u_i > 0\}$ and $J = \{j \in \langle n\rangle : v_j > 0\}$. Furthermore, let $\xi \in \mathbb{R}^{|I|}$ and $\eta \in \mathbb{R}^{|J|}$ be defined by $\xi_i = u_i$ for all $i \in I$ and $\eta_j = v_j$ for all $j \in J$. Hence, (42) is true, (48)–(49) yields (40)–(41), and (46)–(47) yields (43)–(44). This takes care of the "only if" part of the theorem. Note that ξ and η are unit vectors because u and v are unit vectors. Conversely, let $\sigma \in \mathbb{R}$ be such that (40)–(44) is true for nonempty index sets $I \subseteq \langle m\rangle$ and $J \subseteq \langle n\rangle$ and vectors $\xi \in \mathbb{R}^{|I|}$ and $\eta \in \mathbb{R}^{|J|}$. We claim that there is no loss of generality in assuming that ξ and η are unit vectors. The claim is obvious if $\sigma = 0$. If $\sigma \neq 0$, then we can write

$$\|\xi\|^2 = \langle \xi,\xi\rangle = (1/\sigma)\langle \xi, A^{I,J}\eta\rangle = (1/\sigma)\langle (A^{I,J})^\top\xi, \eta\rangle = (1/\sigma)\langle \sigma\eta,\eta\rangle = \|\eta\|^2.$$

Since ξ and η have the same length, we can take $\|\xi\| = \|\eta\| = 1$. Routine work shows that σ is a Pareto singular value of A with associated Pareto singular vectors $u \in \mathbb{S}_m$ and $v \in \mathbb{S}_n$ given by

$$u_i = \begin{cases} \xi_i & \text{if } i \in I \\ 0 & \text{if } i \in \langle m\rangle\backslash I \end{cases}, \quad v_j = \begin{cases} \eta_j & \text{if } j \in J \\ 0 & \text{if } j \in \langle n\rangle\backslash I \end{cases},$$

respectively. □

The system (40)–(44) says that σ is a singular value of $A^{I,J}$ with associated singular vectors ξ and η that are positive and satisfy the slackness inequalities (SIs) mentioned in (43)–(44). The next proposition is obtained by neglecting the SIs. Note that (43) holds vacuously if $I = \langle m\rangle$ and (44) holds vacuously if $J = \langle n\rangle$.

Proposition 3.3. *If σ is a Pareto singular value of A, then σ is a Perronian singular value of some submatrix of A. In other words,*

$$\mathrm{PSV}(A) \subseteq \bigcup_{(I,J)\in\mathcal{J}(m,n)} \mathrm{ISV}\left(A^{I,J}\right). \tag{50}$$

Furthermore,

(a) *If A is nonnegative, then* (50) *holds as an equality.*

(b) *If A is positive, then*

$$\mathrm{PSV}(A) = \left\{\sigma_{\max}\left(A^{I,J}\right) : (I,J) \in \mathcal{J}(m,n)\right\}, \tag{51}$$

$$\sigma_{\max}(A) = \max_{\sigma\in\mathrm{PSV}(A)} \sigma. \tag{52}$$

Proof. Inclusion (50) is a consequence of Theorem 3.2. Such an inclusion is usually strict. However, if A is nonnegative, then (43)–(44) holds automatically and (50) becomes an equality. If A is positive, then each submatrix $A^{I,J}$ is positive and Lemma 3.1 (b) yields $\mathrm{ISV}\left(A^{I,J}\right) = \{\sigma_{\max}(A^{I,J})\}$. The equality version of (50) yields then (51). Formula (52) is a consequence of (51) and the fact that we have $\sigma_{\max}\left(A^{I,J}\right) \leq \sigma_{\max}(A)$ for all $(I,J) \in \mathcal{J}(m,n)$. □

In spite of their resemblance, formulas (37) and (52) are somehow different in spirit. For instance, (37) is true for all matrix A, whereas (52) may be false if A is not positive. The next example explains how to compute $\mathrm{PSV}(A)$ when A is arbitrary.

Example 3.4. Consider the small size matrix

$$A = \begin{bmatrix} -1 & 1 & 1 \\ 1 & 2 & 1 \end{bmatrix}. \tag{53}$$

By examining the system (40)–(44) for each choice of (I,J), we get 9 Pareto singular values:

$$\sigma_1 = 2.645751\,,\ \sigma_2 = 2.618034\,,\ \sigma_3 = 2.449490\,,\ \sigma_4 = 2.302776\,,\ \sigma_5 = 2.236068\,,$$
$$\sigma_6 = 2.000000\,,\ \ \sigma_7 = 1.414214\,,\ \ \sigma_8 = 1.000000\,,\ \ \sigma_9 = -1.000000\,.$$

By way of example, if we take $I = \{2\}$ and $J = \{2,3\}$, then

$$\begin{aligned}
(40) &\ \Rightarrow\ 2\eta_2 + \eta_3 = \sigma\xi_2\,,\\
(41) &\ \Rightarrow\ 2\xi_2 = \sigma\,\eta_2\,,\ \xi_2 = \sigma\,\eta_3\,,\\
(42) &\ \Rightarrow\ \xi_2 > 0\,,\ \eta_2 > 0\,,\ \eta_3 > 0\,,\\
(43) &\ \Rightarrow\ \eta_2 + \eta_3 \geq 0\,,\\
(44) &\ \Rightarrow\ \xi_2 \geq 0\,.
\end{aligned}$$

We obtain $\xi_2 = 1$, $(\eta_2, \eta_3) = (1/\sqrt{5})\,(2,1)$, and $\sigma = \sqrt{5} = 2.236068$. □

A natural question is that of estimating the expression

$$\mathfrak{s}(m,n) = \max_{A\in\mathbb{M}_{m,n}} \mathrm{card}[\mathrm{PSV}(A)]\,,$$

i.e., the largest possible number of Pareto singular values of a matrix of size $m \times n$.

The transposition transfer formula (17) implies that $\mathfrak{s}(m,n)$ is symmetric in the variables m and n. The next theorem gives an explicit formula for $\mathfrak{s}(m,n)$.

Theorem 3.5. *For all $m,n \geq 1$, we have $\mathfrak{s}(m,n) = (2^m - 1)(2^n - 1)$.*

Proof. The term $\Gamma(m,n) = (2^m - 1)(2^n - 1)$ is equal to the cardinality of $\mathcal{J}(m,n)$. Hence,

$$\mathrm{card}[\mathrm{PSV}(A)] \;\leq \sum_{(I,J)\in\mathcal{J}(m,n)} \mathrm{card}[\,\mathrm{ISV}(A^{I,J})] \;\leq\; \Gamma(m,n) \tag{54}$$

for all $A \in \mathbb{M}_{m,n}$. The first inequality in (54) is due to Proposition 3.3, whereas the second one is because each submatrix $A^{I,J}$ has at most one Perronian singular value, cf. Lemma 3.1 (a). Next, we prove the existence of a matrix $A \in \mathbb{M}_{m,n}$ such that

$$\mathrm{card}[\mathrm{PSV}(A)] \;=\; \Gamma(m,n). \tag{55}$$

Proposition 3.3 (b) shows that a positive matrix A of size $m \times n$ satisfies (55) if and only if all the submatrices $A^{I,J}$ have a different spectral norm, i.e.,

$$\sigma_{\max}\left(A^{I_0,J_0}\right) \neq \sigma_{\max}\left(A^{I_1,J_1}\right) \quad \text{if } \;(I_0,J_0) \neq (I_1,J_1). \tag{56}$$

An example of positive matrix as in (56) is $A = ab^\top$, where $a \in \mathbb{R}^m$ and $b \in \mathbb{R}^n$ are positive vectors such that $\|a_{I_0}\|\,\|b_{J_0}\| \neq \|a_{I_1}\|\,\|b_{J_1}\|$ if $(I_0,J_0) \neq (I_1,J_1)$. The notation a_I refers to the vector formed with the entries of a indexed by I. The definition of b_J is analogous. Note that $\sigma_{\max}\left((ab^\top)^{I,J}\right) = \sigma_{\max}\left(a_I\, b_J^\top\right) = \|a_I\|\,\|b_J\|$ for all $(I,J) \in \mathcal{J}(m,n)$. □

4. Applications

4.1. Nonnegative rank-one approximation

Consider again the cone-constrained rank-one approximation problem presented in Example 1.6. If P and Q are Pareto cones, then (15) becomes the nonnegative rank-one approximation problem

$$\min_{\substack{\|u\|=1,\,\|v\|=1\\ u\geq 0,\,v\geq 0,\,\sigma\in\mathbb{R}}} \|A - \sigma uv^\top\|^2. \tag{57}$$

Solving (57) is a matter of handling simultaneously the optimization problems (35) and (36). Two small size examples will help to understand our way of handling (57).

Example 4.1. Except for one of its entries, the matrix

$$A = \begin{bmatrix} -1 & -8 \\ -4 & 2 \end{bmatrix}$$

looks negative. It is reasonable to conjecture that σ is negative for any optimal solution (u,v,σ) to (57). A direct application of Theorem 3.2 shows that $\mathrm{PSV}(A) = \{-\sqrt{65}, -\sqrt{17}\,\}$. Furthermore,

$$\alpha \;=\; \varrho_{\min}(A) \;=\; \min_{\substack{\|u\|=1,\,\|v\|=1\\ u\geq 0,\,v\geq 0}} \langle u, Av\rangle \;=\; \min_{\sigma\in\mathrm{PSV}(A)} \sigma \;=\; -\sqrt{65}\,,$$

where the first minimum is attained with $u = (1,0)$ and $v = (1/\sqrt{65}\,)(1,8)$. By applying Theorem 3.2 again, we get $\mathrm{PSV}_\circ(A) = -\mathrm{PSV}(-A) = -\{-2,\, 1,\, \sqrt{17}\,\}$ and

$$\beta \;=\; \varrho_{\max}(A) \;=\; \max_{\substack{\|u\|=1,\, \|v\|=1\\ u\geq 0,\, v\geq 0}} \langle u, Av\rangle \;=\; \max_{\sigma\in \mathrm{PSV}_\circ(A)} \sigma \;=\; 2\,,$$

where the first maximum is attained with $u = (0,1)$ and $v = (0,1)$. We now consider the function h given by (16). Since $\alpha + \beta < 0$, the minimum of h is attained at $\sigma_0 = \alpha$ and, consequently,

$$\sigma_0 u_0 v_0^\top \;=\; -\sqrt{65}\begin{bmatrix} 1\\ 0\end{bmatrix}\begin{bmatrix} 1/\sqrt{65}\\ 8/\sqrt{65}\end{bmatrix}^\top \;=\; \begin{bmatrix} -1 & -8\\ 0 & 0\end{bmatrix}$$

is the optimal matrix sought in (57). □

Example 4.2. Let A be given by (53). The Pareto singular values of this matrix were computed in Example 3.4. By proceeding as in Example 4.1, we get

$$\begin{aligned} \alpha &= \varrho_{\min}(A) \;=-1\,, \quad u = (1,0)\,,\; v = (1,0,0)\\ \beta &= \varrho_{\max}(A) = \sqrt{7}\,, \quad u = (1/\sqrt{245}\,)(7,\,14)\,,\; v = (1/\sqrt{35}\,)(1,5,3)\,. \end{aligned}$$

This time $\alpha + \beta > 0$. Hence, the minimum of h is attained at $\sigma_0 = \beta$ and we have, consequently,

$$\sigma_0 u_0 v_0^\top \;=\; \sqrt{7}\begin{bmatrix} 7/\sqrt{245}\\ 14/\sqrt{245}\end{bmatrix}\begin{bmatrix} 1/\sqrt{35}\\ 5/\sqrt{35}\\ 3/\sqrt{35}\end{bmatrix}^\top \;=\; \begin{bmatrix} 0.2 & 1 & 0.6\\ 0.4 & 2 & 1.2\end{bmatrix} \tag{58}$$

is the optimal matrix sought in (57). In this example, $\varrho_{\max}(A)$ is equal to the largest singular value of A and, therefore, (58) is the best rank-one approximation of A. In other words, the nonnegativity constraints in (57) are redundant. This is not surprising altogether, because we are dealing with a matrix A that is positive, except for a single entry (whose absolute value is not too large). □

4.2. Nonnegative PCA

We now examine more closely the nonnegative PCA problem (14) considered in Example 1.5, except that such a maximization problem is brought to the minimization format

$$\vartheta \;=\; \min_{\substack{\|u\|=1,\, \|v\|=1\\ v\geq 0}} \langle u, Av\rangle\,. \tag{59}$$

In the above line, $A = -X^\top$, where $X = [x_1, \ldots, x_m]$ is the data matrix of the PCA problem. The minus sign in front of $X^\top$ appears while passing from maximization to minimization. Note also that the optimal value of (14) is $\omega = -\vartheta$. The criticality conditions for (59) are

$$Av = \sigma u\,,\;\; 0 \leq v \perp (A^\top u - \sigma v) \geq 0\,,$$

where (u, v) is sought on the bi-sphere $\mathbb{S}_m \times \mathbb{S}_n$.

We are interested in finding not just the minimal value ϑ, but the entire collection

$$\Sigma^{\text{right}}(A, \Pi_n) = \Sigma(A, \mathbb{R}^m, \Pi_n) \tag{60}$$

of critical values of (59). In the next proposition, $A^{|J} = A^{\langle m\rangle, J}$ denotes the submatrix of A obtained by keeping the columns indexed by J (rows are not deleted). In particular, $A^{|J} = A$ if $J = \langle n\rangle$.

Proposition 4.3. *A real number σ is a critical value of (59) if and only if there exist a vector $u \in \mathbb{S}_m$, a nonempty index set $J \subseteq \langle n\rangle$, and a vector $\eta \in \mathbb{R}^{|J|}$, such that*

$$A^{|J}\eta = \sigma u \tag{61}$$

$$(A^{|J})^\top u = \sigma\eta \tag{62}$$

$$\eta > 0 \tag{63}$$

$$\textstyle\sum_{i=1}^m a_{i,j}\, u_i \geq 0 \quad \forall j \in \langle n\rangle \backslash J. \tag{64}$$

Furthermore, the above system can be written with the extra condition $\|\eta\| = 1$.

Proof. Clearly, $\sigma \in \mathrm{PSV}^{\text{right}}(A)$ if and only if there exists $(u, v) \in \mathbb{S}_m \times \mathbb{S}_n$ satisfying $Av = \sigma u$ and

$$v_j \geq 0\,, \quad (A^\top u - \sigma v)_j \geq 0\,, \quad v_j(A^\top u - \sigma v)_j = 0$$

for all $j \in \langle n\rangle$. Geometrically speaking, u is anywhere on the sphere $\mathbb{S}_m$, but v must be in the relative interior of one of the faces

$$F_J = \{v \in \Pi_n : v_j = 0 \text{ for all } j \in \langle n\rangle \backslash J\}$$

of the Pareto cone Π_n. So, we set $J = \{j \in \langle n\rangle : v_j > 0\}$ and proceed as in the proof of Theorem 3.2. The details are omitted for avoiding repetitions. □

It is possible to compute (60) with a case-by-case analysis based on Proposition 4.3. In order to explain our method, we consider a nonnegative PCA problem involving hundred nonzero data points in a three dimensional space. In other words, $(m, n) = (100, 3)$. Since $n = 3$, there are $7 = 2^3 - 1$ ways of choosing the index set J, namely,

$$\underbrace{\{1\}, \{2\}, \{3\}}_{|J|=1}, \quad \underbrace{\{1, 2\}, \{1, 3\}, \{2, 3\}}_{|J|=2}, \quad \underbrace{\{1, 2, 3\}}_{|J|=3}.$$

We must solve the system (61)–(64) for each choice of J. The case $|J| = 1$ is trivial. Consider for instance $J = \{1\}$. So, $A^{|J} = a_1$ is the first column of A (which we suppose nonzero, otherwise $\sigma = 0$ and we are done). The vector η in (61)–(63) is in fact a scalar, so we take $\eta = 1$ and get $(u, \sigma) = \pm\,(\|a_1\|^{-1}a_1,\ \|a_1\|)$. For each of these potential solutions, we check the SIs

$$\sum_{i=1}^{100} a_{i,j}\, u_i \geq 0 \quad \text{for } \ j \in \{2, 3\}\,.$$

The case $|J| = 2$ is more subtle. Consider for instance $J = \{1, 2\}$. So, $A^{|J}$ is formed with the first two columns of A. The system (61)–(62) is a classical singular value problem for a matrix of size 100×2. We must check that the right-singular vector $\eta \in \mathbb{R}^2$ is positive and that the left-singular vector $u \in \mathbb{R}^{100}$ satisfies the SI

$$\sum_{i=1}^{100} a_{i,3}\, u_i \geq 0\,.$$

If $|J| = 3$, then we get a classical singular value problem (1) for a matrix of size 100×3, but we must check that the right-singular vector $v \in \mathbb{R}^3$ is positive. The cost of evaluating $\Sigma(A, \mathbb{R}^{100}, \Pi_3)$ is roughly as follows:

$$\begin{cases} 3 \times (\text{checking 2 SIs}) \\ 3 \times (\text{solving a SVP of size } 100 \times 2 \text{ and checking 1 SI}) \\ 1 \times (\text{ solving a SVP of size } 100 \times 3), \end{cases}$$

where SVP is the acronym of (classical) Singular Value Problem. Numerical testing with Gaussian data points suggests that the cost of evaluating $\Sigma(A, \mathbb{R}^m, \Pi_n)$ grows exponentially in n. The figures shown in Table 1 correspond to CPU times measured in milliseconds. All our numerical experiments were carried in macOS Catalina with a processor 3.4 GHz Intel Core i5, Memory(RAM) 8 Gb. The codes were implemented with Matlab R2017a.

	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$
$m = 100$	0.6	1.3	2.8	5.7	12	22
$m = 200$	0.9	2.1	4.7	10	22	48
$m = 300$	1.3	3.0	6.8	15	33	75
$m = 400$	1.8	4.3	9.7	21	47	103

Table 1: CPU time for finding all the critical values of problem (59).
Method based on Proposition 4.3.

We may dispense with Proposition 4.3 and compute the set (60) by relying instead on Theorem 2.7. If we use this alternative method, then we must form the $n \times n$ matrix $E = XX^\top$ and determine $\mathrm{Sp}(E, \Pi_n)$ and $\mathrm{Sp}_\circ(E, \Pi_n)$. The numerical task of computing a set of the form $\mathrm{Sp}(E, \Pi_n)$, called the Pareto spectrum of E, is done with a case-by-case technique developed in [21, Theorem 4.1]. What we have to do is to work out the system

$$E^{J,J} w = \lambda w\,, \quad w > 0\,, \quad \sum_{j \in J} e_{i,j}\, w_j \geq 0 \ \ \forall i \in \langle n \rangle \backslash J$$

for different choices of J. Here w is an unknown vector in $\mathbb{R}^{|J|}$. Each nonzero real λ found in this way yields a positive element $\sigma = \sqrt{\lambda}$ of the set (60). The polarized version $\mathrm{Sp}_\circ(E, \Pi_n)$ is treated by writing the SIs in the reverse order:

$$E^{J,J} w = \lambda w\,, \quad w > 0\,, \quad \sum_{j \in J} e_{i,j}\, w_j \leq 0 \ \ \forall i \in \langle n \rangle \backslash J.$$

A nonzero real λ as above yields a negative element $\sigma = -\sqrt{\lambda}$ of the set (60). Computing $\mathrm{Sp}(E, \Pi_n)$ or $\mathrm{Sp}_\circ(E, \Pi_n)$ offers no difficulty if n is of moderate size, say $n \leq 20$. The number m of data points can be as large as one wishes, provided we are able to carry out the matrix product $XX^\top$. Besides computing $\mathrm{Sp}(E,\Pi_n)$ and $\mathrm{Sp}_\circ(E,\Pi_n)$, we must check whether 0 is a critical value of (59), i.e., whether there are nonzero vectors u and v such that $A^\top u \geq 0$ and $Av = 0, v \geq 0$, respectively. Note, however, that the value ω given by (14) is positive. Equivalently, the value ϑ given by (59) is negative. Hence,

$$\vartheta = \min_{\lambda \in \mathrm{Sp}_\circ(E,\Pi_n)} -\sqrt{\lambda} = -\left[\max_{\lambda \in \mathrm{Sp}_\circ(E,\Pi_n)} \lambda\right]^{1/2}$$

and, therefore, we can focus on the computation of $\mathrm{Sp}_\circ(E,\Pi_n)$. Table 2 displays the CPU time (in milliseconds) needed for computing $\mathrm{Sp}_\circ(E,\Pi_n)$. The data points are generated by a Gaussian random vector.

n	3	4	5	6	7	8
CPU time	0.5	0.9	1.5	3.2	5.6	10.6

Table 2: CPU time for finding all the negative critical values of (59). Method based on Theorem 2.7.

The choice of m is irrelevant in Table 2. The computation of $XX^\top$ is almost instantaneous, but we must be aware that, when m is too large, such a matrix product could be subject to rounding errors. If $XX^\top$ is available with enough precision, then we recommend the method based on Theorem 2, which is significantly faster than the method based on Proposition 4.3.

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