On the computation of maximal angles between cones

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Class of Computational Complexity

Conical Singular Values

$$\min_{\substack{u \in P,\ \|u\| = 1, \\ v \in Q,\ \|v\| = 1,}} \quad u^\top A v \qquad P, Q \quad \text{closed convex cones, finitely generated}$$

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Polynomial Time
$O(mn^2)$ to compute
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$$\min_{\substack{u \geq 0,\ \|u\| = 1,\\ v \geq 0,\ \|v\| = 1,}} u^\top A v \qquad A \in \mathbb{R}^{m \times n} \qquad \Xi(A) := \{\text{stationary points of the o.p.}\}$$

"Simple" Case: $A \geq 0$

Theorem (Seeger, S. 2023)

$$A \geq 0 \iff \Xi(A) = \{\|B\| : B \trianglelefteq A\}$$

Theorem (Seeger, S. 2023)

The set of matrices $A \in \mathbb{R}_+^{m \times n}$ for which all the submatrices have different norms, is dense, open and its complementary has measure zero on the space of nonnegative matrices

$\implies$ A generic nonnegative matrix has **exponentially** many Pareto Singular Values

Still it does say nothing on the complexity of recovering the minimum, since

$$A \geq 0 \implies \min \Xi(A) = \min_{i,j} A_{i,j}$$

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$$\min_{\substack{u \in P,\ \|u\| = 1, \\ v \in Q,\ \|v\| = 1,}} u^\top v \qquad P, Q \subseteq \mathbb{R}^n \text{ non trivial polyhedral cones}$$

"Simple" Case:

$$\min_{\substack{u \in P,\ \|u\| = 1, \\ v \in Q,\ \|v\| = 1,}} u^\top v \geq 0 \implies u, v \text{ are vertices of } P, Q$$

If one of u, v in the antipodal pair is a vertex then the problem is **Polynomial** in n and the number of generators of P, Q

Theorem (B., G., S. 2024)

Let (u, v) be a stationary point and let $u \in int(F_u)$, $v \in int(F_v)$ where F_u, F_v are facets of P, Q. If $\dim(F_u) + \dim(F_v) > n$ and $v \neq \pm u$, then (u, v) is a saddle point

Corollary (B., G., S. 2024)

If (u, v) is a local minimum in dimension $n \leq 3$, then at least one among u, v is a vertex

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- $\dim(F_u) + \dim(F_v) > n$ then (u, v) is a saddle point
- (u, v) local minimum, $n \leq 3$, then u or v is a vertex

Idea of proof:

- If $\dim(F_u) + \dim(F_v) > n$ then $0 \neq z \in Span(F_u) \cap Span(F_v)$
- The local minima of the restriction to $Span(u, v, z)$ are on the border of F_u or F_v

Counterexample for n $\geq$ 4:

$$P = \langle \begin{pmatrix} 1 & 1 \\ -1 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \rangle \quad Q = \langle \begin{pmatrix} -1 & -1 \\ 0 & 0 \\ 1 & 1 \\ -1 & 1 \end{pmatrix} \rangle \quad u = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad v = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\dim(F_u) = \dim(F_v) = 2 \qquad u^\top v = -\frac{1}{\sqrt{2}} < 0$$

(u, v) is an antipodal pair in the interior part of P and Q

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Hardest Problem

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Lemma (B., G., S. 2024)

Any matrix $A \in \mathbb{R}^{m\times n}$ of spectral norm 1 and $m \geq n$ can be decomposed as $A = U^T V$ where $U, V \in \mathbb{R}^{(m+n)\times n}$ are matrices with orthonormal columns

Proof: Let

$$A = U^T V \qquad U = \begin{pmatrix} I \\ 0 \end{pmatrix} \in \mathbb{R}^{(m+n)\times m} \qquad V := \begin{pmatrix} A \\ C \end{pmatrix} \in \mathbb{R}^{(m+n)\times m}$$

Given the SVD $A = W\Sigma Z^\top$ let $C = (I - \Sigma^\top\Sigma)^{1/2} Z^\top$ so that

$$V^\top V = A^\top A + Z(I - \Sigma^\top \Sigma)Z^\top = ZZ^\top = I$$

i.e. all columns of V are orthogonal to each other and with unitary norm

Notice:

The columns of U are a subset of the canonical basis

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Reduction

$$\min_{u,v} u^\top A v : \quad \|u\| = \|v\| = 1 \qquad u \in P = \langle G \rangle \subseteq \mathbb{R}^n \quad v \in Q = \langle R \rangle \subseteq \mathbb{R}^n$$

$$\min_{x,y} (Gx)^\top A (Ry) : \quad \|Gx\| = \|Ry\| = 1 \qquad x, y \geq 0$$

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From Conical SV to Conic Angles

The minimum conical singular value of dimension n with number of generators a, b for G, R reduces polynomially to the maximum angle between cones of dimension $n + m$ with number of generators a, b for UG, VR

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Reduction from Maximum Edge Biclique to Minimal Pareto Singular Value

Theorem (Seeger, S. 2023)

Let (σ_0, u, v) be the optimal solution of

$$\sigma_0 = \min_{u,v \geq 0} u^\top A v \quad : \quad \|u\| = \|v\| = 1$$

If A has at least one negative entry then $(x, y) = \sqrt{-\sigma_0}(u, v)$ is optimal for

$$\min_{x,y \geq 0} \| - A - xy^\top \|_F^2$$

This shows that the Minimal Pareto Singular Value is **at least as hard** as the Nonnegative Rank 1 Approximation problem

Theorem (G., Glineur 2013)

Let $B \in \{0,1\}^{m \times n}$ be the bi-adjacency matrix of a bipartite graph (N_1, N_2, E) where $B_{i,j} = 1$ iff node i in N_1 and node j in N_2 are connected and $d \geq \max\{m, n\}$.

$$\min_{x,y \geq 0} \|B - d(1 - B) - xy^\top\|_F^2$$

is solved by binary vectors x, y that identify the fully connected subsets $S_1 \subseteq N_1$ and $S_2 \subseteq N_2$ corrisponding to the Maximum Edge Biclique, i.e they maximise $|S_1| \cdot |S_2|$

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$$\sigma_0 = \min_{u,v\geq 0} u^\top A v \quad : \quad \|u\| = \|v\| = 1$$

If A has at least one negative entry then $(x, y) = \sqrt{-\sigma_0}(u, v)$ is optimal for

$$\min_{x,y\geq 0} \| - A - xy^\top \|_F^2$$

This shows that the Minimal Pareto Singular Value is **at least as hard** as the Nonnegative Rank 1 Approximation problem

Theorem (G., Glineur 2013)

Let $B \in \{0, 1\}^{m\times n}$ be the bi-adjacency matrix of a bipartite graph (N_1, N_2, E) where $B_{i,j} = 1$ iff node i in N_1 and node j in N_2 are connected and $d \geq \max\{m, n\}$.

$$\min_{x,y\geq 0} \|B - d(1 - B) - xy^\top \|_F^2$$

is solved by binary vectors x, y that identify the fully connected subsets $S_1 \subseteq N_1$ and $S_2 \subseteq N_2$ corrisponding to the Maximum Edge Biclique, i.e they maximise $|S_1| \cdot |S_2|$

- $\min_{x,y\geq 0} \|B - d(1-B) - xy^\top\|_F^2$ identifies the Maximum Edge Biclique

Idea of Proof:

All the Maximal Bicliques (S_1, S_2) are local minima of $\|B - d(1-B) - xy^\top\|_F^2$ where $x = \chi(S_1)$, $y = \chi(S_2)$ because any extension of $S_1 \times S_2$ gets a $-d$ and

$$(-d - \epsilon)^2 = d^2 + 2d\epsilon + \epsilon^2$$

with the error going up by $d\epsilon$ that is way more then what we gain by removing ϵ from all the ones in a row/column

As a consequence $xy^\top$ has zeros in correspondence of the $-d$ of M and the rest nonzero entries equal to 1, meaning that local minima x, y are indicator for the maximal bicliques

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Everything is Hard

Theorem (Peeters 2003)

The Maximal Edge Biclique problem is NP-hard

Maximal Edge Biclique

Maximum Number of Edges in a Bipartite Connected Subgraph

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Recall:

$$\min_{\substack{u \geq 0,\ \|u\| = 1,\\ v \geq 0,\ \|v\| = 1}} \langle u, Av \rangle = \|A\| \quad \min_{\substack{u \geq 0,\ \|Uu\| = 1,\\ v \geq 0,\ \|Vv\| = 1}} \langle Uu, Vv \rangle = \|A\| \quad \min_{\substack{x \in P,\ \|x\| = 1,\\ y \in Q,\ \|y\| = 1}} \langle x, y \rangle,$$

with $U^\top = \begin{pmatrix} I & 0 \end{pmatrix}$

Theorem (B., G., S. 2024)

The maximum angle between convex closed cones problem

$$\min_{\substack{x \in P,\ \|x\| = 1,\\ y \in Q,\ \|y\| = 1}} \langle x, y \rangle$$

with P being generated by a subset of the canonical basis is NP-hard

Conjecture (B., G., S. 2024)

The maximum angle between the positive orthant and another convex closed cone

$$\min_{\substack{x \geq 0,\ \|x\| = 1,\\ y \in Q,\ \|y\| = 1}} \langle x, y \rangle = -\max_{y \in Q,\ \|y\|=1} \|y^-\|$$

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Quadratic Programming with Gurobi

(Not) a Gurobi AD

GUROBI
OPTIMIZATION

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GUROBI OPTIMIZATION

minimize	$x^T Q x + c^T x + \text{alpha}$	
subject to	$Ax = b$	(linear constraints)
	$\ell \le x \le u$	(bound constraints)
	some x_j integral	(integrality constraints)
	$x^T Qc\, x + q^T x \le \text{beta}$	(quadratic constraints)
	some x_i in SOS	(special ordered set constraints)
	min, max, abs, or, ...	(general constraints)

- ✓ Interfaces with C, C++, Python, Java, Matlab, .NET, R
- × Proprietary, not Open Source
- ✓ Free for Academic use
- × Slower than approximating iterative solvers
- ✓ Solve the problem exactly even in the indefinite case

Uses **McCormick Relaxation**:

$$\min_{(u,v)\in K} \langle u, Av\rangle = \min_{(u,v)\in K} \sum_{i,j} A_{i,j} u_i v_j = \min_{(u,v)\in K, u_i v_j = w_{i,j}} \sum_{i,j} A_{i,j} w_{i,j} \ge \min_{(u_i, v_j, w_{i,j})\in K_{i,j}} \sum_{i,j} A_{i,j} w_{i,j}$$

where $K_{i,j} = \text{Conv}((u_i, v_j, w_{i,j}) : w_{i,j} = u_i v_j,\ \underline{u_i} \le u_i \le \overline{u_i},\ \underline{v_j} \le v_j \le \overline{v_j})$ is a convex polyhedron with at most 4 faces in $\mathbb{R}^3$ and if $(u_i^*, v_j^*, w_{i,j}^*)$ is the relaxed solution,

$$\sum_{i,j} A_{i,j} u_i^* v_j^* \ge \min_{(u,v)\in K} \langle u, Av\rangle \ge \sum_{i,j} A_{i,j} w_{i,j}^* \qquad \text{Err} \le \sum_{i,j} |A_{i,j}|(\overline{u_i} - \underline{u_i})(\overline{v_j} - \underline{v_j})$$

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An Example: Schur Cone

Gurobi easily solves some angles problems, e.g., $P = \mathbb{R}^m_+$ and $Q = \langle H \rangle$, or $P = Q = \langle H \rangle$ where H generates the Schur cone

$$H = \begin{pmatrix} 1 & 0 & \dots & 0 \\ -1 & 1 & \dots & 0 \\ 0 & -1 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 1 \\ 0 & 0 & \dots & -1 \end{pmatrix} \in \mathbb{R}^{n \times n-1} \qquad \langle H \rangle \subseteq e^{\perp}$$

In the first case, Gurobi returns

$$y = e_n \in P \quad x = (a\,a\,\dots\,a\,b) \in Q \quad a = \sqrt{\frac{1}{n(n-1)}} \quad b = -\sqrt{1 - \frac{1}{n}} = x^\top y$$

that can be proved being the maximum angle as

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Maximum Angle between PSD and Nonnegative Symmetric Matrices

Given the inner product $\langle A, B\rangle = Tr(A^\top B)$ on the space of $n \times n$ real symmetric matrices $\mathcal{S}^n$ an open question is the maximum angle between the cone of PSD matrices $\mathcal{P}^n$ and the cone of nonnegative symmetric matrices $\mathcal{N}^n$ for $n \geq 5$

$$\gamma_n := \min_{\substack{A \in \mathcal{P}^n,\, B \in \mathcal{N}^n \\ \|A\|_F = \|B\|_F = 1}} \langle A, B\rangle = -\max_{A\in\mathcal{P}^n, \|A\|_F=1} \|A^-\|_F = -\frac{1}{2} \max_{B\in\mathcal{N}^n, \|B\|_F=1} \|B - \sqrt{B^2}\|_F$$

It is known that

$$n = 2, 3, 4 \implies \gamma_n = -\frac{1}{\sqrt{2}} = \cos\left(\frac{3}{4}\pi\right) \qquad \lim_{n\to\infty} \gamma_n \downarrow -1 = \cos(\pi)$$

This is a lower bound on the maximum angle in the cone of copositive matrices

$$\mathcal{C}^n := \{A \in \mathcal{S}^n \,:\, x^\top Ax \geq 0 \;\forall x \geq 0\}$$

All the algorithms to compute γ_n are iteratively converging to a critical angle, i.e. a stationary point of the optimization problem

For $n \geq 5$ **we only have lower bounds** on the minimum angle

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A Conjecture

Known Antipodal Couples:

$n = 1$: $A_1 = B_1 = 1$

$n = 2$: $A_2 = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \quad B_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$n = 3, 4$: $A_n = \begin{pmatrix} A_2 & 0 \\ 0 & 0 \end{pmatrix} \quad B_n = \begin{pmatrix} B_2 & 0 \\ 0 & 0 \end{pmatrix}$

$n = 5$: (Best Known Stationary Point) F_5 is the Fourier matrix

$$A_n = F_5 \begin{pmatrix} 0 & & & & \\ & 0 & & & \\ & & \frac{1}{\sqrt{2}} & & \\ & & & \frac{1}{\sqrt{2}} & \\ & & & & 0 \end{pmatrix} F_5^H \qquad B_n = \frac{1}{\sqrt{10}}\begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

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Every antipodal pair is block circulant

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Known Antipodal Couples:

$n = 1$: $A_1 = B_1 = 1$

$n = 2$: $A_2 = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \quad B_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$n = 3, 4$: $A_n = \begin{pmatrix} A_2 & 0 \\ 0 & 0 \end{pmatrix} \quad B_n = \begin{pmatrix} B_2 & 0 \\ 0 & 0 \end{pmatrix}$

$n = 5$: (Best Known Stationary Point) F_5 is the Fourier matrix

$$A_n = F_5 \begin{pmatrix} 0 & & & & \\ & 0 & & & \\ & & \frac{1}{\sqrt{2}} & & \\ & & & \frac{1}{\sqrt{2}} & \\ & & & & 0 \end{pmatrix} F_5^H \qquad B_n = \frac{1}{\sqrt{10}}\begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

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Circulant Symmetric Matrices

The algebra of circulant real symmetric matrices $\mathcal{SC}^n$ is the set of

$$\begin{pmatrix} a_0 & a_1 & a_2 & \dots & a_1 \\ a_1 & a_0 & a_1 & \ddots & \vdots \\ a_2 & a_1 & \ddots & \ddots & a_2 \\ \vdots & \ddots & \ddots & a_0 & a_1 \\ a_1 & \dots & a_2 & a_1 & a_0 \end{pmatrix} = a_0 I_n + F_n \operatorname{diag}\left(\sum_{j>0} 2a_j \cos(2\pi ij/n) \right)_{i=0:n-1} F_n^H$$

Properties:

- Both $\mathcal{SC}^n \cap \mathcal{P}^n$ and $\mathcal{SC}^n \cap \mathcal{N}^n$ are finitely generated cones with $\lceil \frac{n+1}{2} \rceil$ generators
- Given $C \in \mathcal{SC}^n \cap \mathcal{P}^n$ its projection C' onto $-\mathcal{N}^n$ is still in $\mathcal{SC}^n$, and the angle between $C, -C'$ is the maximum angle between C and $\mathcal{N}^n$
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Check with Gurobi

If n is odd and $n = 1 + 2m$

$$\min_{\substack{A \in \mathcal{SC}^n \cap \mathcal{P}^n,\ \|A\|_F = 1 \\ B \in \mathcal{SC}^n \cap \mathcal{N}^n,\ \|B\|_F = 1}} \langle A, B \rangle = \min_{\substack{x \geq 0,\ \|x\|_F = 1 \\ y \geq 0,\ \|y\|_F = 1}} \langle x, My \rangle \qquad M = \frac{2}{\sqrt{n}} \left[\cos\left(\frac{2\pi}{n} ij \right) \right]_{i,j=1:m}$$

A similar reduction holds for n even

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A similar reduction holds for n even

5	$0.7575\ \pi$	$0.7575\ \pi$	18	$0.7699\ \pi$	$0.7670\ \pi$
6	$0.7575\ \pi$	$0.7575\ \pi$	19	$0.7703\ \pi$	$0.7681\ \pi$
7	$0.7575\ \pi$	$0.7575\ \pi$	20	$0.7719\ \pi$	$0.7719\ \pi$
8	$0.7608\ \pi$	$0.7608\ \pi$	21	$0.7719\ \pi$	$0.7719\ \pi$
9	$0.7608\ \pi$	$0.7608\ \pi$	22	$0.7719\ \pi$	$0.7719\ \pi$
10	$0.7609\ \pi$	$0.7608\ \pi$	23	$0.7722\ \pi$	$0.7719\ \pi$
11	$0.7627\ \pi$	$0.7627\ \pi$	24	$0.7735\ \pi$	$0.7730\ \pi$
12	$0.7649\ \pi$	$0.7649\ \pi$	25	$0.7735\ \pi$	$0.7730\ \pi$
13	$0.7649\ \pi$	$0.7649\ \pi$	26	$0.7735\ \pi$	$0.7730\ \pi$
14	$0.7659\ \pi$	$0.7649\ \pi$	27	$0.7739\ \pi$	$0.7730\ \pi$
15	$0.7678\ \pi$	$0.7649\ \pi$	28	$0.7750\ \pi$	$0.7730\ \pi$
16	$0.7699\ \pi$	$0.7670\ \pi$	29	$0.7750\ \pi$	$0.7741\ \pi$
17	$0.7699\ \pi$	$0.7670\ \pi$	30	$0.7757\ \pi$	$0.7741\ \pi$

Left: Lower bounds on γ_n

Right:

- In **black** the exact angle $\mathcal{SC}^n \cap \mathcal{P}^n \angle \mathcal{SC}^n \cap \mathcal{N}^n$
- In blue if a previous angle was bigger then the exact solution
- In red if it is a lower bound

Thank You!

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