Computing cone-constrained singular values of matrices

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Hidden structures in dynamical systems optimization and machine learning

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Class of Computational Complexity

$$\min_{\substack{u \in P, \|u\| = 1, \\ v \in Q, \|v\| = 1,}} u^{\top} A v$$

P,Q closed convex cones finitely generated

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Pareto Singular Values min $u^{\top}Av$

 $\min_{\substack{u \ge 0, \|u\| = 1, \\ v \ge 0, \|v\| = 1,}} u^{\top} A v$



Pareto Singular Values

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Conic Angles

$$\min_{\substack{u \in P, \ \|u\| = 1, \\ v \in Q, \ \|v\| = 1, }} u^{\top} v$$







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

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

The minimum conical singular value problem reduces polynomially

to the maximum angle between cones problem

Theorem (G., Glineur 2013)

Let $B \in \{0, 1\}^{m \times n}$ be the bi-adjacency matrix of a bipartite graph with $d \ge \max\{m, n\}$. $\min_{x, y \ge 0} \|B - d(1 - B) - xy^{\top}\|_{F}^{2}$ (Nonnegative Rank 1)

is solved by binary vectors x, y that identify the Maximum Edge Biclique

$$\sigma_0 = (u^*)^\top A v^* = \min_{u,v \ge 0} u^\top A v \quad : \quad \|u\| = \|v\| = 1 \quad \text{(Pareto SV)}$$

has at least one negative entry then $(x^*, y^*) = \sqrt{-\sigma_0}(u^*, v^*)$ is optimal for
$$\min_{x,y \ge 0} \|-A - xy^\top\|_F^2 \quad \text{(Nonnegative Rank 1)}$$

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Theorem (Seeger, S. 2023)

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Maximum Number of Edges in a Bipartite Connected Subgraph

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Nonnegative Rank 1

 $\min_{x,y\geq 0}\|M-xy^\top\|$

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Conic Angles

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





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"Simple" Case:

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





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"Simple" Case:

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

$$\min_{v \in Q, \|v\|=1} u^{\top} v = -\max_{v \in -Q, \|v\|=1} u^{\top} v \implies v = -\frac{\operatorname{Proj}(u, -Q)}{\|\operatorname{Proj}(u, -Q)\|}$$
$$\operatorname{Proj}(u, -Q) \equiv \min_{y \ge 0} \|u - (-H)y\| \quad \langle H \rangle = Q, \text{ NNLS, convex}$$



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if $(u^*)^{\top}v^* < 0$, when is it that one among u, v is a vertex?

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 faces 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 $n \leq 3$ with $u \neq -v$, then at least one among u, v is a vertex





Algorithms

$$\lambda^* = \min_{\substack{u \in P, \|u\| = 1, \\ v \in Q, \|v\| = 1, \\ v \in Q, \|v\| = 1, \\ w \in Q, \|v\| = 1, \\ w = 0, \|Av| = 1, \\ w =$$

Idea: If we know the sets \mathcal{I} , \mathcal{J} of indices for which $x_i^*, y_j^* > 0$, called Active Sets, then a direct gradient computation solves the problem

KKT Conditions:

$$\begin{cases} 0 \le x^* \perp G^\top A H y^* - \lambda^* G^\top G x^* \ge 0\\ 0 \le y^* \perp H^\top A^\top G x^* - \lambda^* H^\top H y^* \ge 0 \\ \|Gx^*\| = \|Hy^*\| = 1 \end{cases} \implies \begin{cases} 0 < \overline{x}, \quad \overline{G}^\top A \overline{H} \overline{y} - \lambda^* \overline{G}^\top \overline{G} \overline{x} = 0\\ 0 < \overline{y}, \quad \overline{H}^\top A^\top \overline{G} \overline{x} - \lambda^* \overline{H}^\top \overline{H} \overline{y} = 0\\ \overline{x} := x_{\mathcal{I}}^*, \overline{y} := y_{\mathcal{J}}^*, \overline{G} := G_{:,\mathcal{I}}, \overline{H} := H_{:,\mathcal{J}} \end{cases}$$

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

For the optimal solution $(u^*, v^*) = (Gx^*, Hy^*) = (\overline{Gx}, \overline{Hy})$ and $\lambda^* = (u^*)^\top A v^*$

$$M^* := \begin{pmatrix} 0 & \overline{H}^{\dagger} A^{\top} \overline{G} \\ \overline{G}^{\dagger} A \overline{H} & 0 \end{pmatrix} \implies M^* \begin{pmatrix} \overline{y} \\ \overline{x} \end{pmatrix} = \lambda^* \begin{pmatrix} \overline{y} \\ \overline{x} \end{pmatrix}$$

where λ^* is the least eigenvalue of M^* (from 2° order KKT)

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Idea: If we know the sets \mathcal{I} , \mathcal{J} of indices for which $x_i^*, y_j^* > 0$, called Active Sets, then a direct gradient computation solves the problem

The Active Set algorithm cycles over all subsets of indices \mathcal{I}, \mathcal{J} and tests if the least eigenvalue of M has a nonnegative eigenvector, giving us upper bounds on λ^* , and the exact solution when \mathcal{I}, \mathcal{J} coincide with the active sets of (x^*, y^*)

Optimizations: $2 < |\mathcal{I}| + |\mathcal{J}| \le m + n - \text{Null}(A^{\top}A - ||A||^2I)$ and \overline{G} , \overline{H} must be full rank

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Input:
$$A \in \mathbb{R}^{m \times n}$$
, $G \in \mathbb{R}^{m \times p}$, $H \in \mathbb{R}^{n \times q}$, $P = \langle G \rangle$, $Q = \langle H \rangle$
Output: $\lambda = \min u^{\top} A v$ such that $||u|| = ||v|| = 1$, $u \in P$, $v \in Q$

1:
$$\lambda = g_i^\top Ah_j = \min_{k,\ell} (G^\top AH)_{k,\ell}, u = g_i, v = h_j, r = \operatorname{Null}(A^\top A - ||A||^2 I_n)$$

2: $\mathscr{I} := \{(\mathcal{I}, \mathcal{J}) : 2 < |\mathcal{I}| + |\mathcal{J}| \le m + n - r, \overline{G} := G_{:,\mathcal{I}} \text{ and } \overline{H} := H_{:,\mathcal{J}} \text{ full column rank}\}$
3: for $(\mathcal{I}, \mathcal{J}) \in \mathscr{I}$, do
4: $A_x = \overline{G}^{\dagger} A^\top \overline{H}, A_y = \overline{H}^{\dagger} A \overline{G}$
5: $A_\lambda = A_y A_x, \ \widetilde{A}_\lambda = A_x \text{ (or } A_\lambda = A_x A_y, \ \widetilde{A}_\lambda = A_y \text{ if } |\mathcal{I}| > |\mathcal{J}|)$
6: if $\rho(A_\lambda) \le \lambda^2$ then Skip to the next $(\mathcal{I}, \mathcal{J}) \in \mathscr{I}$
7: U right eigenspace of $\rho(A_\lambda)$ in $A_\lambda, \mu = -\sqrt{\rho(A_\lambda)}, W = \begin{pmatrix} \widetilde{A}_\lambda U/\mu \\ U \end{pmatrix}$

8: Compute the reduced QR of
$$W = VR$$

9: if
$$(VV^{\top} - I)z = 0$$
, $z \ge 0$, $e^{\top}z = 1$ admits a solution then

10:
$$\lambda = \underline{\mu}, z = [y^\top x^\top]^\top \text{(or } z = [x^\top y^\top]^\top \text{if } |\mathcal{I}| > |\mathcal{J}|)$$

11:
$$u = \overline{G}x/\|\overline{G}x\|, v = \overline{H}y/\|\overline{H}y\|$$

12: end if

13: end for

$$\lambda^* = \min_{\substack{u \in P, \|u\| = 1, \\ v \in Q, \|v\| = 1,}} u^\top A v$$

Idea: We have seen that if we know u^* or v^* , then finding the other is equivalent to solve an easy convex problem

Alternate Projection: starting from an initial feasible point (u_0, v_0) and k = 0

•
$$u_{k+1} = \arg \min_{x \in P} x^\top A v_k$$
 such that $||x||_2 = 1$

- $v_{k+1} = \arg \min_{y \in Q} u_{k+1}^\top A y$ such that $\|y\|_2 = 1$
- k = k + 1

To accelerate the convergence, we add an Extrapolation step after each update

•
$$u_{k+1} = u_{k+1} + \beta(u_{k+1} - u_k)$$

- $v_{k+1} = v_{k+1} + \beta(v_{k+1} v_k)$
- If the objective increases then we decrease β and go back to (u_k, v_k), otherwise we increase β

$$\lambda^* = \min_{\substack{u \in P, \|u\| = 1, \\ v \in Q, \|v\| = 1,}} u^\top A v$$

Idea: We have seen that if we know u^* or v^* , then finding the other is equivalent to solve an easy convex problem

Alternate Projection: starting from an initial feasible point (u_0, v_0) and k = 0

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 such that $\|y\|_2 = 1$

• *k* = *k* + 1

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Input: $A \in \mathbb{R}^{m \times n}$, cones $P \subseteq \mathbb{R}^m$ and $Q \subseteq \mathbb{R}^n$ **Output:** An approximate solution to $\min_{u \in P, v \in Q} u^{\top} A v$ such that $||u||_2 = ||v||_2 = 1$. 1: u = 0, v = 0, $v_e = v_0$, k = 1. 2: while $k \leq K$ and $(||u - u_p||_2 \geq \delta \text{ or } ||v - v_p||_2 \geq \delta)$ do $u_p = u$. % Keep previous iterate in memory 3: $u = \arg \min_{x \in P} x^{\top} A v_e$ such that $||x||_2 = 1$. 4. $u_e = u + \beta(u - u_p)$. % Extrapolated point 5. $v_{\rm p} = v$. % Keep previous iterate in memory 6: $v = \arg \min_{y \in Q} u_e^\top A y$ such that $||y||_2 = 1$. 7. $v_e = v + \beta(v - v_p)$. % Extrapolated point 8. 9: $e_{k} \leftarrow \mu^{\top} A v$. 10: if k > 2 and $e_k > e_{k-1}$ then $u = u_p, v = v_p, \beta = \frac{\beta}{n}.$ 11: else 12: $\beta \leftarrow \min(1, \gamma \beta).$ 13: end if 14: $k \leftarrow k + 1$. 15 16: end while

$$\lambda^{*} = \min_{\substack{u \in P, \|u\| = 1, \\ v \in Q, \|v\| = 1, \\ v \in Q, \|v\| = 1, \\ v \in Q, v \neq 0, \\ v \in Q, v \neq 0, \\ u = \frac{u^{\top}Av}{\|u\| \|v\|} = \min_{\substack{e^{\top}x = 1, x \ge 0, \\ e^{\top}y = 1, y \ge 0, \\ e^{\top}y = 1, y \ge 0, \\ u = \frac{u^{\top}AHy}{\|Gx\| \|Hy\|}}$$

Idea: If the minimum of $f_{\delta}(x, y) := x^{\top} G^{\top} A H y - \delta \|Gx\| \|Hy\|$ over $(x, y) \in \Delta_{p} \times \Delta_{q}$ is $\mu < 0$ then we get a decrease in the objective function

$$\frac{x^{\top}G^{\top}AHy}{\|Gx\|\|Hy\|} = \delta + \frac{\mu}{\|Gx\|\|Hy\|} < \delta$$

Partial Linearization: starting from an initial feasible point (x_0, y_0) and k = 0,

•
$$\delta = \frac{\mathbf{x}_k^\top \mathbf{G}^\top \mathbf{A} \mathbf{H} \mathbf{y}_k}{\|\mathbf{G} \mathbf{x}_k\| \| \mathbf{H} \mathbf{y}_k\|}$$

- Linearize wrt x the function f_δ(x, y_k), penalize it with ||x x_k||² and minimize it to obtain x_{k+1}
- Linearize wrt y the function $f_{\delta}(x_{k+1}, y)$, penalize it with $||y y_k||^2$ and minimize it to obtain y_{k+1}
- k = k + 1

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- Linearize wrt x the function $f_{\delta}(x, y_k)$, penalize it with $||x x_k||^2$ and minimize it to obtain x_{k+1}
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Input: $A \in \mathbb{R}^{m \times n}$, cones $P \subseteq \mathbb{R}^m$ and $Q \subseteq \mathbb{R}^n$ **Output:** An approximate solution to $\min_{u \in P, v \in Q} \langle u, Av \rangle$ such that ||u|| = ||v|| = 11: Set

$$\delta_k := \frac{\langle Gx^k, AHy^k \rangle}{\|Gx^k\| \|Hy^k\|}$$

2: Let $L_1^k(x) := \langle Gx, AHy^k - \delta_k \| Gx^k \|^{-1} \| Hy^k \| Gx^k \rangle$ Compute a solution \tilde{x}^k to the convex program

 $\min L_1^k(x) + \frac{\mu_1}{2} \|x - x^k\|^2$ such that $x \in \Delta_p$

 Let L^k₂(y) := ⟨Hy, A[⊤]Gx^k - δ_k||Gx^k|||Hy^k||⁻¹Hy^k⟩ Compute a solution ỹ^k to the convex program

$$\min L_2^k(y) + rac{\mu_2}{2} \|y - y^k\|^2$$
 such that $y \in \Delta_q$

4: Let $d_1^k := \tilde{x}^k - x^k$ and $d_2^k := \tilde{y}^k - y^k$

5: If $(|L_1^k(d_1^k)| < \delta$ and $|L_2^k(d_2^k)| < \delta)$ or $k \ge K$ terminate Otherwise, let $t_k := \beta \rho^{\ell_k}$, where ℓ_k is the smallest nonnegative integer ℓ such that

$$\Phi(x^{k} + t^{k}d_{1}^{k}, y^{k} + t^{k}d_{2}^{k}) \leq \Phi(x^{k}, y^{k}) + \alpha t_{k}\frac{L_{1}^{k}(d_{1}^{k}) + L_{2}^{k}(d_{2}^{k})}{\|Gx^{k}\|\|Hy^{k}\|}$$

Set $(x^{k+1}, y^{k+1}) := (x^k, y^k) + t_k(d_1^k, d_2^k)$ and k = k + 1. Go to step 1

Experiments

An Example: Schur Cone

We test and compare the following algorithms on several problems:

- Brute Force Active Set
- Alternating projection with extrapolation
- Sequential Regularized Partial Linearization
- Gurobi (exact nonconvex quadratic solver based on McCormick relaxation)

The Schur Cone is generated by the matrix

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

One can prove that the maximum angle between the Schur cone Q and \mathbb{R}^n_+ is achieved by

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

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Schur Cone and Positive Orthant

Table 1: Numerical comparison for Gur and BFAS for different dimensions for the problem of finding the maximum angle between the Schur cone and \mathbb{R}_{+}^{n} . The table reports the optimal objective functions values found in the timelimit (60 seconds) and the actual elapsed time. We also report the exact value for each problem.

п	5	10	20	50
exact	0.852416π	0.897584π	0.928217π	0.954833π
Gur	0.852416π	0.897584π	0.928218π	0.954833π
	0.1134 s	0.2016 s	20.1493 s	60* s
BFAS	0.852416π	0.897584π	0.750000π	0.750000π
	0.3310 s	48.3153 s	60* s	60* s

n	100	200	500
exact	0.968116π	0.977473π	0.985760π
Gur	0.968116π	0.977473 π	0.985756 π
	60* s	60* s	60* s
BFAS	0.750000π	0.750000π	0.750000π
	60* s	60* s	60* s

Schur Cone and Positive Orthant

Table 1: Numerical comparison for Gurobi and BFAS for different dimensions for the problem of finding the maximum angle between the Schur cone and itself. The table reports the optimal objective functions values found in the timelimit (60 seconds) and the actual elapsed time. We also report the exact value for each problem.

п	5	10	20	50
exact	0.800000π	0.900000π	0.950000π	0.980000π
Gur	0.800001π	0.90000 π	0.950000π	0.980000 π
	0.2508 s	60* s	60* s	60* s
BFAS	0.80000π	0.90000π	0.859157π	0.804087π
	0.3856 s	60* s	60* s	60* s

n	100	200	500
exact	0.990000π	0.995000π	0.998000π
Gur	0.936315π	0.994996 π	0.998011π
	60* s	60* s	60* s
BFAS	0.750000π	0.750000π	0.750000π
	60* s	60* s	60* s

Schur Cone and Positive Orthant



Recall that solving the Pareto singular value problem is equivalent to solve the maximum edge biclique problem.

Here we thus test all four algorithms on four bipartite graphs taken from a benchmark dataset¹. All graphs have been randomly generated with a fixed edge density, and then a biclique has been added to them. In particular,

- the first graph is a 100 \times 100 graph with density 0.2 and planted biclique of size 50 \times 50 = 2500,
- the second graph is a 300 \times 300 graph with density 0.3 and planted biclique of size 2 \times 55 = 110,
- the third graph is a 100 \times 100 graph with density 0.71 and planted biclique of size 80 \times 80 = 6400,
- the fourth graph is a 10000 \times 300 graph with density 0.03 and planted biclique of size $22 \times 2 = 44$.

¹Shaham, E.: maximum biclique benchmark. https://github.com/shahamer/ maximum-biclique-benchmark (2019)

Table 1: Numerical comparison for Gurobi, BFAS, E-AO and SRPL for the problem of finding the maximum edge biclique in four different bipartite graphs. The table reports the maximum edgee biclique found in the timelimit (10 seconds) for Gurobi and BFAS. The reported number for E-AO and SRPL are instead the average value found at 10 seconds for 100 runs, and in parentheses the best value found throughout all 100 runs when it differs from the average one. Gurobi cannot be executed on the last graph due to its excessive size.

п	100 imes 100	300 imes 300	100 imes 100	10000×300
Gur	2500	0	310	NA
BFAS	3	2	2	2
E-AO	66	114	87	12
SRPL	2500	114	6400	46(358)

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$$n = 2, 3, 4 \implies \gamma_n = \frac{3}{4}\pi \qquad \lim_{n \to \infty} \gamma_n \uparrow \pi$$

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5	$0.7575 \ \pi$	$0.7575 \ \pi$	18	$0.7699 \ \pi$	0.7670π	Left: Best known lower
6	$0.7575 \ \pi$	$0.7575 \ \pi$	19	$0.7703 \ \pi$	0.7681π	Left. Dest known lower
7	$0.7575~\pi$	$0.7575~\pi$	20	$0.7719~\pi$	0.7719 π	bounds on γ_n
8	$0.7608 \ \pi$	$0.7608 \ \pi$	21	$0.7719\ \pi$	$0.7719\ \pi$	
9	0.7608 π	$0.7608\ \pi$	22	$0.7719\ \pi$	$0.7719\ \pi$	Right: Gurobi solutions
10	$0.7609\ \pi$	$0.7608~\pi$	23	$0.7722~\pi$	$0.7719~\pi$	- In black the exact angle
11	$0.7627 \ \pi$	$0.7627 \ \pi$	24	0.7735 π	$0.7730~\pi$	$\mathcal{SC}^n \cap \mathcal{P}^n \neq \mathcal{SC}^n \cap \mathcal{N}^n$
12	$0.7649 \ \pi$	$0.7649 \ \pi$	25	$0.7735 \ \pi$	$0.7730 \ \pi$	
13	$0.7649\ \pi$	$0.7649\ \pi$	26	0.7735 π	$0.7730~\pi$	- In blue if a previous angle
14	$0.7659\ \pi$	$0.7649\ \pi$	27	$0.7739\ \pi$	$0.7730~\pi$	was bigger then the exact so-
15	0.7678 π	$0.7649\ \pi$	28	$0.7750\ \pi$	$0.7730~\pi$	lution
16	$0.7699 \ \pi$	$0.7670 \ \pi$	29	$0.7750 \ \pi$	$0.7741 \ \pi$	
17	$0.7699\ \pi$	$0.7670\ \pi$	30	0.7757 π	0.7741 π	- In red if it is a lower bound

 Table 2: Numerical comparison of Gur and BFAS for different dimensions for the problem of finding the maximum angle between the PSD cone and the nonnegative symmetric cone, both restricted to the subalgebra of circulant matrices. Timelimit: 60 seconds

n	13	15	17	19	21	23
exact	0.762950π	0.757765π	0.764971π	0.768062π	0.768769π	0.766370π
Gur	0.762950 π	0.757765 π	0.764971 π	0.767876π	0.765409π	0.766370 π
	0.854 s	25.061 s	$60^* s$	60* s	60* s	60* s
BFAS	0.762950π	0.757765π	0.764971π	0.768062π	0.768768π	0.766370π
	0.333 s	0.356 s	1.114 s	4.418 s	19.953 s	60* s

Table 3: Numerical comparison of Gur, BFAS, E-AO and SRPL for the same problem. Timelimit: 10seconds. When the exact value is not available, the best known lower bound is reported with anasterisk

п	17	19	21	23	25	27
exact	0.764971π	0.768062π	0.768769π	0.766370π	$0.767385\pi^*$	$0.768258\pi^*$
Gur	0.764971π	0.759309π	0.765409π	0.766370π	0.767385π	0.760879π
BFAS	0.764971π	0.768062π	0.768768π	0.766370π	0.762620π	0.756841π
E-AO	0.764971π	0.768062π	0.768768π	0.766370π	0.767385π	0.768258π
SRPL	0.764970π	0.768062π	0.768768π	0.766369π	0.767384π	0.768257π

PSD and **SNN** matrices

Since E-AO and SRPL main steps are projections, they can be adapted to the case of NON-polyhedral cones, as long as we know how to compute the projection on such cones We can thus test them on the task to find the maximum angle between the cone of Positive Semi-Definite matrices and the cone of Symmetric Nonnegative matrices

Table 4: Numerical comparison for E-AO and SRPL for different dimensions for the problem of finding the maximum angle between the PSD cone and the nonnegative symmetric cone. The table reports the best and average value found over 10000 random initializations, together with the average elapsed time. We also report the best known value for each dimension.

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п	30	40	50	60
best known	0.7757π	0.7789π	0.7812π	0.7837π
EAO _b	0.7757π	0.7789 π	0.7812π	0.7837 π
EAO _a	0.7741π	0.7768π	0.7790π	0.7805π
	0.111 ± 0.054 s	$0.701\pm0.235~\text{s}$	$1.263\pm0.273~\text{s}$	$2.852\pm0.321~\text{s}$
SRPL _b	0.7757π	0.7789π	0.7812π	0.7837 π
SRPL _a	0.7739π	0.7766π	0.7787π	0.7802π
	0.062 ± 0.025 s	0.155 ± 0.060 s	$\textbf{0.319} \pm 0.130~\text{s}$	$\textbf{0.565} \pm 0.229~\text{s}$

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Thank You!