A nasty cone with nice properties – new issues in copositive optimization

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Overview

1. Review: IP Methods, Barriers, LP and SDP
2. Linear Conic, and Copositive Optimization (COP)
3. NP-hard problems represented as COPs
4. Copositivity tests and certificates
5. Approximation hierarchies – a survey

Review: IP Revolution in Linear Optimization

Linear Optimization Problem (LP):
n variables in a vector $\mathbf{x} \in \mathbb{R}^n$, linear objective $\mathbf{c}^\top \mathbf{x}$;
m linear constraints $A\mathbf{x} = \mathbf{b}$ ($m < n$ linear equations);
nonnegativity constraints $\mathbf{x} \geq \mathbf{o}$: means $\min_i x_i \geq 0$.

Simplex Algorithm **[Dantzig '47]**: many variables $(n - m)$ zero;
exchange vertices of feasible set (polyhedron) until optimality.
In almost all practical cases, $\leq 3m$ exchange steps necessary.
Nasty examples **[Klee/Minty '72]**: can need up to 2^m steps.

Interior Point (IP) Algorithms: all n variables positive;
[Yudin/Nemirovski/Shor '76+, Khachian '79+]: ellipsoid m.
Only $K(m+n)^2$ steps necessary in worst case but impractical !

Barrier functions: IP methods made practical

Projective methods **[Dikin '67], [Karmarkar '84]**:
polynomial & practical.

Also can approximate in worst case optimal solution to arbitrary accuracy in polynomial time.

Modern variants:

Barrier function $\beta(\mathbf{x}) = -\sum_i \log(x_i) \nearrow \infty$ if $x_i \searrow 0$ ensures $x_i > 0$ if incorporated into objective:

$$\min\left\{\mathbf{c}^\top \mathbf{x} + \gamma\beta(\mathbf{x}) : A\mathbf{x} = \mathbf{b}\right\}$$ nonlinear, with parameter $\gamma > 0$.

Given γ, solve this only approximately; decrease γ and iterate!

Many computing issues, success with increased computation power.

Semidefinite Optimization (SDP) versus LP

Instead of vector $\mathbf{x}$ now symmetric matrix $X = X^\top$ of variables;
instead of $\mathbf{x} \geq \mathbf{o}$ now psd. constraint $X \succeq O$: means $\lambda_{\text{min}}(X) \geq 0$.

Again logarithmic barrier

$$\beta(X) = -\log \det X = -\textstyle\sum_i \log \lambda_i(X) \ \nearrow \infty \quad \text{if} \quad \lambda_{\text{min}}(X) \searrow 0\,.$$

Again linear objective and m linear constraints:

$$\min \{\langle C, X\rangle : \langle A_i, X\rangle = b_i \,(i = 1..m)\,,\ X \succeq O\}\ ,$$

where $\langle C, X\rangle = \text{trace}\ (CX) = \sum_{i,j} C_{ij}X_{ij}$.

Recall that LP can be written as

$$\min \{\langle C, X\rangle : \langle A_i, X\rangle = b_i \,(i = 1..m)\,,\ X \geq O\}\ .$$

General form of conic linear optimization

Let $\mathcal{K}$ be a convex cone of X matrices. Conic linear program:

$$\min \{\langle C, X\rangle : \langle A_i, X\rangle = b_i \,(i = 1..m)\,,\ X \in \mathcal{K}\}\ ,\ \text{barrier ??}$$

Familiar cases:

$\mathcal{K} = \mathcal{N} = \left\{X = X^\top : X \geq O\right\} = \mathcal{N}^* \ldots$ LP, barrier: $-\sum_{i,j} \log X_{ij}$,

and

$\mathcal{K} = \mathcal{P} = \left\{X = X^\top : X \succeq O\right\} = \mathcal{P}^* \ldots$ SDP, barrier: $-\sum_i \log \lambda_i(X)$.

In above cases, the dual cone of $\mathcal{K}$,

$$\mathcal{K}^* = \left\{S = S^\top : \langle S, X\rangle \geq 0 \text{ for all } X \in \mathcal{K}\right\}$$

coincides with $\mathcal{K}$ (self-duality), but in general $\mathcal{K}^*$ differs from $\mathcal{K}$.

Copositive optimization (COP), duality

A very special matrix cone:

$$\mathcal{K} = \text{ conv } \left\{ \mathbf{x}\mathbf{x}^\top : \mathbf{x} \in \mathbb{R}^n, \mathbf{x} \geq \mathbf{o} \right\},$$

the cone of completely positive matrices, with its dual cone

$$\mathcal{K}^* = \left\{ S = S^\top \text{ is copositive; means: } \mathbf{x}^\top S \mathbf{x} \geq 0 \text{ if } \mathbf{x} \geq \mathbf{o} \right\} \neq \mathcal{K}.$$

Well known relations:

$$\mathcal{K} \subset \mathcal{P} \cap \mathcal{N} \subset \mathcal{P} + \mathcal{N} \subset \mathcal{K}^* \ldots \text{strict for } n \geq 5.$$

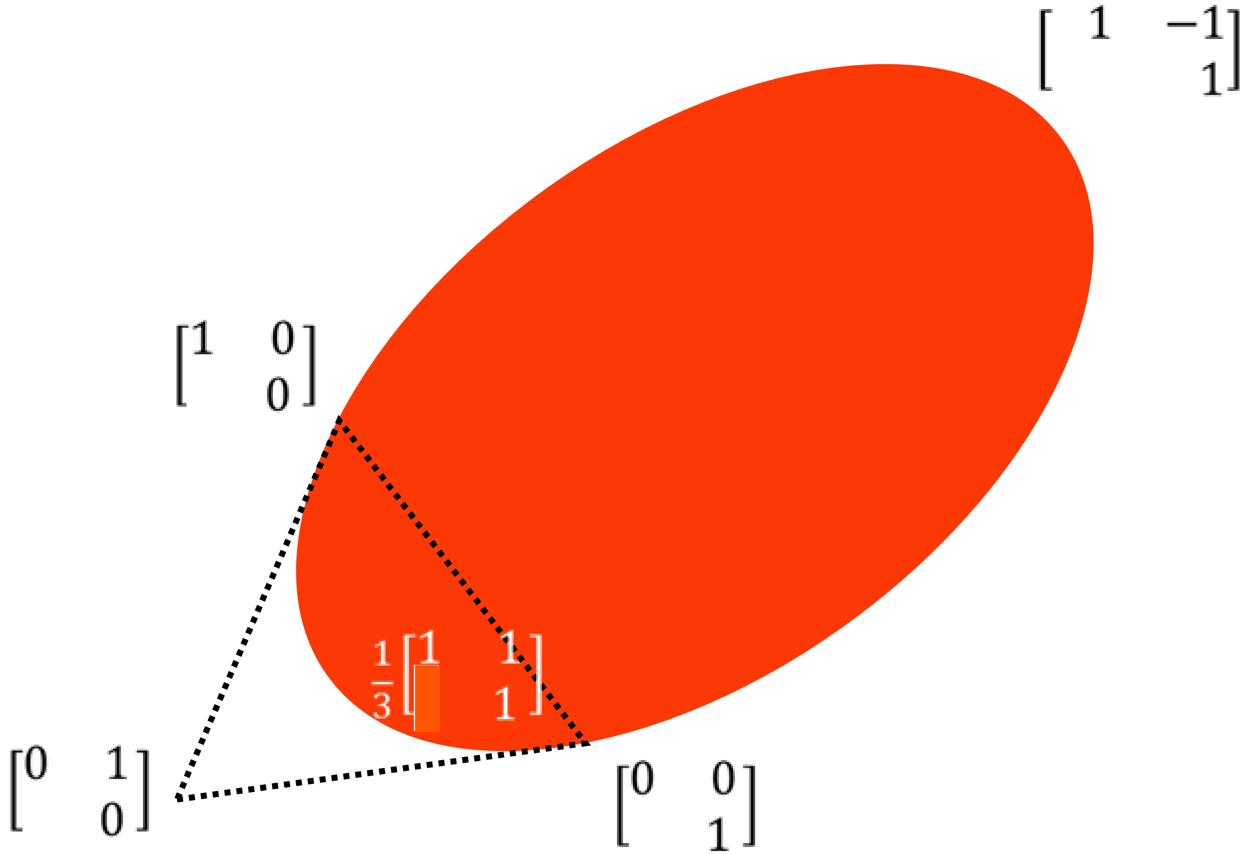
Primal-dual pair in (COP):

$$p^* = \inf \{ \langle C, X \rangle : \langle A_i, X \rangle = b_i \,, \, X \in \mathcal{K} \}$$

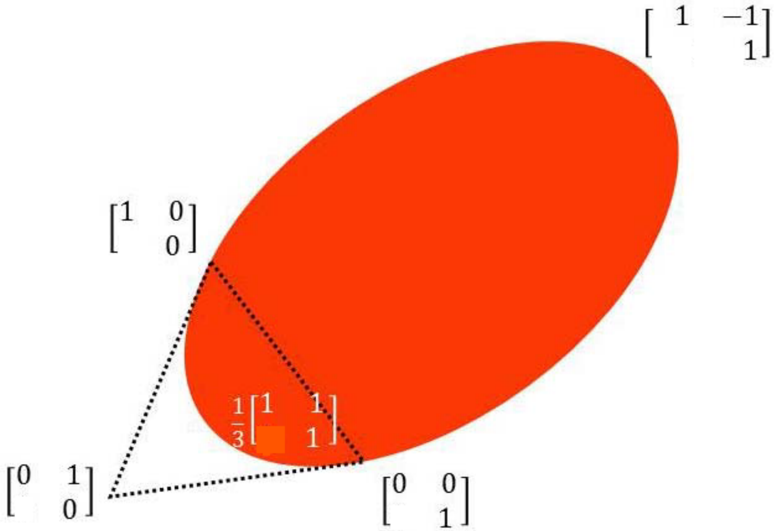
and

$$d^* = \sup \left\{ \mathbf{b}^\top \mathbf{y} : C - \textstyle\sum_i y_i A_i \in \mathcal{K}^* \right\} .$$

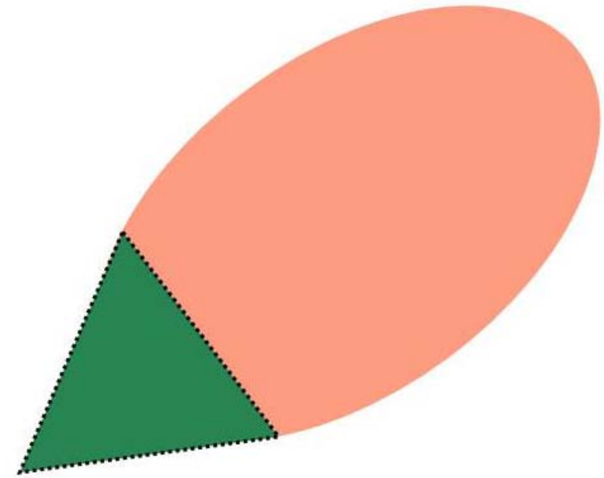
Usual weak ($d^* \leq p^*$) and strong ($d^* = p^*$) duality results hold.



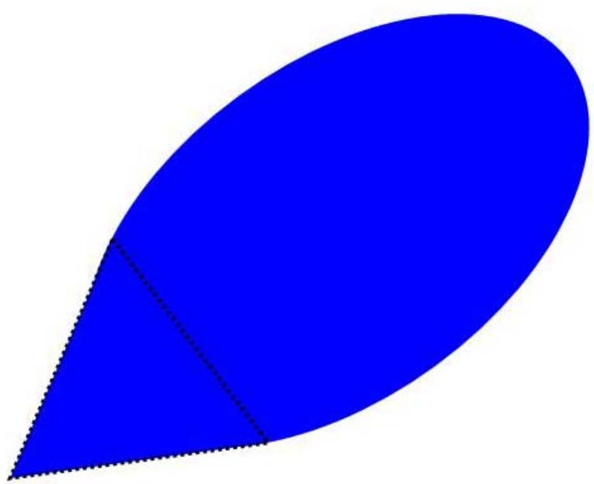
Semidefinite cone $\mathcal{P}$



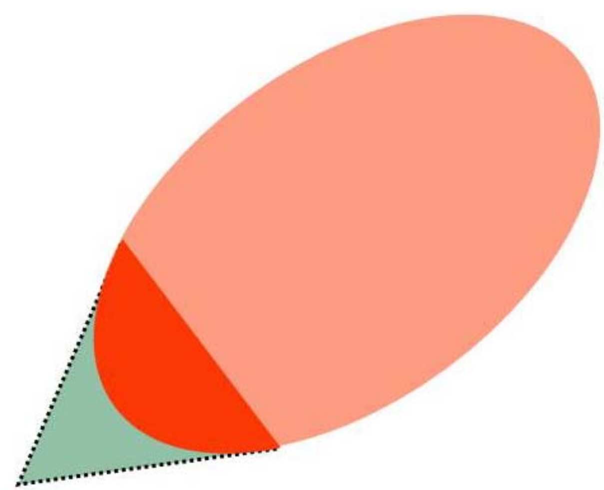
Semidefinite cone $\mathcal{P}$



Nonnegative cone $\mathcal{N}$



Copositive cone $\mathcal{K}^*$



Completely positive cone $\mathcal{K}$

So – why nasty ? (and why nice ?)

Nasty aspects: geometry – while boundaries $\partial\mathcal{P}$ and $\partial\mathcal{N}$ are nice, $\partial\mathcal{K}^*$ is not (contains matrices of full rank, or no zero entries).

Extremal rays of $\mathcal{K}^*$: [Baumert '66, '67, Hildebrand '12];

interior points of $\mathcal{K}^*$: strict copositivity, $\mathbf{x}^\top S\mathbf{x} > 0$ if $\mathbf{x} \in \mathbb{R}^n_+ \setminus \{\mathbf{o}\}$.

Extremal rays of $\mathcal{K}$: $X = \mathbf{x}\mathbf{x}^\top$ with $\mathbf{x} \in \mathbb{R}^n_+$, so have rank one;

interior points of $\mathcal{K}$: [Dür/Still '08], [Dickinson '10].

Nasty aspects: complexity – decision problems
"$S \in \mathcal{K}^*$?" or "$X \in \mathcal{K}$?" are NP-hard [Dickinson/Gijben '13];

caution: not every convex optimization problem is easy !

Why nice ? For instance, because ...

Constrained fractional QPs are COPs

Consider

$$\psi = \min \left\{ f(\mathbf{x}) = \frac{\mathbf{x}^\top C \mathbf{x} + 2\mathbf{c}^\top \mathbf{x} + \gamma}{\mathbf{x}^\top B \mathbf{x} + 2\mathbf{b}^\top \mathbf{x} + \beta} : A\mathbf{x} = \mathbf{a}\,,\ \mathbf{x} \in \mathbb{R}^n_+ \right\}.$$

Applications: engineering (friction and resonance problems – complementary eigenvalues), repair of inconsistent linear systems.

Problem is NP-hard, many inefficient local solutions may coexist.

Theorem [Preisig '96; Amaral/B./Júdice '12]: *We have*

$$\psi = \min \left\{ \langle \overline{C}, X \rangle : \langle \overline{B}, X \rangle = 1\,,\ \langle \overline{A}, X \rangle = 0\,,\ X \in \mathcal{K} \right\},$$

under mild conditions, where

$$\overline{A} = \begin{bmatrix} \mathbf{a}^\top \mathbf{a} & -\mathbf{a}^\top A \\ -A^\top \mathbf{a} & A^\top A \end{bmatrix}, \quad \overline{B} = \begin{bmatrix} \beta & \mathbf{b}^\top \\ \mathbf{b} & B \end{bmatrix}, \quad \overline{C} = \begin{bmatrix} \gamma & \mathbf{c}^\top \\ \mathbf{c} & C \end{bmatrix}.$$

COP formulation of the Maximum Clique Problem (MCP)

Consider an undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with $\#\mathcal{V} = n$ vertices.

Clique $\mathcal{S} \subseteq \mathcal{V}$ is *maximal* if $\mathcal{S}$ is not contained in a larger clique.
Clique $\mathcal{S}^*$ is a *maximum* clique if

$$\#\mathcal{S}^* = \max \{\#\mathcal{T} : \mathcal{T} \text{ clique in } \mathcal{G}\} \, .$$

Finding the *clique number* $\omega(\mathcal{G}) = \#\mathcal{S}^*$ is an NP-complete combinatorial optimization problem, which can be formulated as continuous optimization problem, namely a COP ($E = \mathbf{e}\mathbf{e}^\top$):

Theorem [Motzkin/Straus '65, B.et al.'00]: *For* $Q_\mathcal{G} = E - A_\mathcal{G}$

$$\begin{aligned} \frac{1}{\omega(\mathcal{G})} &= \min \{\langle Q_\mathcal{G}, X\rangle : \langle E, X\rangle = 1\, ,\, X \in \mathcal{K}\} \\ &= \max \{y \in \mathbb{R} : Q_\mathcal{G} - yE \in \mathcal{K}^*\} \, . \end{aligned}$$

Thus: a good barrier for $\mathcal{K}^*$ would reduce MCP to line search !

General Mixed-Binary QPs and copositive programming

Theorem [Burer '09]: *Any Mixed-Binary Quadratic Program*

$$\min\left\{\tfrac{1}{2}\mathbf{x}^\top Q\mathbf{x} + \mathbf{c}^\top\mathbf{x} : A\mathbf{x} = \mathbf{b}\,,\ \mathbf{x} \in \mathbb{R}^n_+\,,\ x_j \in \{0,1\}, \textit{all } j \in B\right\}$$

can (under mild conditions) be expressed as COP:

$$\min\left\{\tfrac{1}{2}\langle \hat{Q}, \hat{X}\rangle : \mathcal{A}(\hat{X}) = \hat{\mathbf{b}}\,,\ X \in \mathcal{K}\right\}$$

where $\hat{X}$ *and* $\hat{Q}$ *are* $(n+1)\times(n+1)$ *matrices, and the size of* $(\mathcal{A}, \hat{\mathbf{b}})$ *is polynomial in the size of* $(A, \mathbf{b})$.

Special cases: continuous QP ($B = \emptyset$) or binary QP – e.g., the Maximum-Cut Problem is a COP:

$$\max\left\{\tfrac{1}{4}\mathbf{y}^\top L\mathbf{y} : \mathbf{y} \in \{-1,1\}^n\right\}.$$

Also QAP and graph partitioning are COPs **[Povh/Rendl '07]**.

Linear mixed-binary problems with uncertain objective

[Natarajan/Teo/Zheng '11] consider mixed-binary LP with stochastic objective function, only the first two moments known:

$$z^* = \sup \left\{ \mathbb{E} \max \left\{ \tilde{\mathbf{c}}^\top \mathbf{x} : A\mathbf{x} = \mathbf{b}\,,\ \mathbf{x} \in \mathbb{R}^n_+ \cap \{0,1\}^B_n \right\} : \tilde{\mathbf{c}} \sim (\boldsymbol{\mu}, \boldsymbol{\Sigma})_+ \right\} ,$$

with $\{0,1\}^B_n = \left\{ \mathbf{x} \in \mathbb{R}^n : x_j \in \{0,1\} \text{ for all } j \in B \right\}$ and where $\tilde{\mathbf{c}} \sim (\boldsymbol{\mu}, \boldsymbol{\Sigma})_+$ means: prob.distr. with support $\mathbb{R}^n_+$ and

$$\mathbb{E}(\tilde{\mathbf{c}}) = \boldsymbol{\mu}\,, \quad \mathbb{E}\left[\tilde{\mathbf{c}}\tilde{\mathbf{c}}^\top\right] = \boldsymbol{\Sigma}\,.$$

Such distributions exist if $\begin{bmatrix} 1 & \boldsymbol{\mu}^\top \\ \boldsymbol{\mu} & \boldsymbol{\Sigma} \end{bmatrix}$ is in the interior of $\mathcal{K}$.

COP formulation of optimization under uncertainty

Under the same conditions as in [Burer '09],

$$z^* = \max\{\mathrm{trace}(Z) \colon A\mathbf{x} = \mathbf{b},\ (AXA^\top)_{ii} = b_i^2 \text{ for all } i \in [1\!:\!n] \text{ and } X_{jj} = x_j \text{ for all } j \in B,\ T_{(\boldsymbol{\mu},\Sigma)}(\mathbf{x}, X, Z) \in \mathcal{K}\},$$

where

$$T_{(\boldsymbol{\mu},\Sigma)}(\mathbf{x}, X, Z) = \begin{bmatrix} 1 & \boldsymbol{\mu}^\top & \mathbf{x}^\top \\ \boldsymbol{\mu} & \boldsymbol{\Sigma} & Z^\top \\ \mathbf{x} & Z & X \end{bmatrix}.$$

For any optimal solution $(\mathbf{x}^*, X^*, Z^*)$, construct sequence $\tilde{\mathbf{c}}_k \in \mathbb{R}^n_+$ such that $\mathbb{E}\tilde{\mathbf{c}}_k \to \boldsymbol{\mu}$ and $\mathbb{E}\left[\tilde{\mathbf{c}}_k \tilde{\mathbf{c}}_k^\top\right] \to \boldsymbol{\Sigma}$ as $k \to \infty$ as well as

$$\mathbb{E}\left[\max\left\{\tilde{\mathbf{c}}_k^\top \mathbf{x} : A\mathbf{x} = \mathbf{b},\ \mathbf{x} \in \mathbb{R}^n_+ \cap \{0,1\}^B_n\right\}\right] \to z^* = \mathrm{trace}(Z^*)\,.$$

Works also if $(\boldsymbol{\mu}, \Sigma)$ are not known exactly but only some bounds.

Convex quadratic underestimators over polytopes

Given indefinite $Q \notin \mathcal{P}$, search for best convex quadratic underestimator of $f(\mathbf{x}) = \mathbf{x}^\top Q\mathbf{x}$ over polytope $P = \text{conv}\,(\mathbf{v}_1, \ldots, \mathbf{v}_n)$.

Copositive approach [Locatelli/Schoen '10]: for $V = [\mathbf{v}_1, \ldots, \mathbf{v}_n]$ let $\mathbf{x} = V\mathbf{v}$ with $\mathbf{v} \in \Delta^n \subseteq \mathbb{R}^n_+$ be barycentric coordinates of $\mathbf{x}$ w.r.t. V, and $Q_P = V^\top QV$. Then search for g_P (or r_P) with

$$f(\mathbf{x}) = q_P(\mathbf{v}) = \mathbf{v}^\top Q_P\mathbf{v} \geq r_P(\mathbf{v}) = \mathbf{v}^\top U_P\mathbf{v} = g_P(\mathbf{x}) \text{ for all } \mathbf{x} \in P$$

where $g_P(\mathbf{x}) = \mathbf{x}^\top S\mathbf{x} + 2\mathbf{c}^\top\mathbf{x} + \gamma$ with $S \in \mathcal{P}$ and

$$U_P = U_P(S, \mathbf{c}, \gamma) = V^\top SV + (V^\top\mathbf{c})\mathbf{e}^\top + \mathbf{e}(V^\top\mathbf{c}) + \gamma\mathbf{e}\mathbf{e}^\top .$$

So $f(\mathbf{x}) \geq g_P(\mathbf{x})$ for all $\mathbf{x} \in P$ means $Q_P - U_P \in \mathcal{K}^*$.

Tight convex QP-underestimators by SDP-COP

Now $g_P(\mathbf{x}) = r_P(\mathbf{v})$ is best such underestimator of $f(\mathbf{x}) = q_P(\mathbf{v})$ if and only if volume difference (integrated convexity gap)

$$\int_\Delta \mathbf{v}^\top (Q_P - U_P)\mathbf{v}\,\mathrm{d}\mathbf{v} = \int_\Delta [q_P(\mathbf{v}) - r_P(\mathbf{v})]\,\mathrm{d}\mathbf{v} \text{ is minimal.}$$

But $\int_\Delta \mathbf{v}^\top A\mathbf{v}\,\mathrm{d}\mathbf{v} = \frac{2}{(n+1)!}\langle E, A\rangle$ holds for any A, so end up in

$$\begin{array}{rcll} \langle E, Q_P - U_P\rangle & \to & \text{min !} & \text{... convexity gap} \\ U_P & = & V^\top S V + (V^\top \mathbf{c})\mathbf{e}^\top + \mathbf{e}(V^\top \mathbf{c}) + \gamma \mathbf{e}\mathbf{e}^\top & \\ (S, \mathbf{c}, \gamma) & \in & \mathcal{P} \times \mathbb{R}^n \times \mathbb{R} & \text{... convexity} \\ Q_P - U_P & \in & \mathcal{K}^* & \text{... underestimation} \end{array}$$

... lends itself naturally to relaxation of $\mathcal{K}^*$ like $\mathcal{P} + \mathcal{N}$. Here it suffices even to require $Q_P - U_P \in \mathcal{N}$ [Locatelli/Schoen '10].

Positive and negative certificates in COP

Positive certificate ($S = C - \sum_i y_i A_i \in \mathcal{K}^*$, i.e., is copositive) gives valid lower bound in COPs by weak duality:

$$\mathbf{b}^\top \mathbf{y} \leq d^* \leq p^* \leq \langle C, X \rangle \quad \text{for all feasible } X \in \mathcal{K}\,.$$

Negative certificates/basic principle from duality: if $\langle X, S \rangle < 0$,

$$X \in \mathcal{K} \;\Rightarrow\; S \notin \mathcal{K}^* \quad \text{while} \quad S \in \mathcal{K}^* \;\Rightarrow\; X \notin \mathcal{K}\,.$$

Simpler variant of the first: *violating vector* $\mathbf{v} \in \mathbb{R}^n_+$ with $\mathbf{v}^\top S \mathbf{v} < 0$ shows $S \notin \mathcal{K}^*$, and moreover yields improving feasible direction in global nonconvex QPs:

Theorem [B.'92]: *Consider local, nonglobal solution $\bar{\mathbf{x}}$ to a QP. If $\mathbf{v}$ is viol.vector for suitable S, $t > 0$ (polyn.-time construction), then $f(\bar{\mathbf{x}} + t\mathbf{v}) < f(\bar{\mathbf{x}})$ ... escape from inefficient solution $\bar{\mathbf{x}}$.*

Copositivity certificates: preprocessing

Theorem [B.'87]: *For any row i, we have*

(a) *If $S_{ii} < 0$, then $\mathbf{v} = \mathbf{e}_i$ is a violating vector;*

(b) *if $S_{ii} = 0 > S_{ij}$, then $\mathbf{v} = (S_{jj} + 1)\mathbf{e}_i - S_{ij}\mathbf{e}_j$ is violating;*

(c) *if $S_{ij} \geq 0$ for all j, then $S \in \mathcal{K}^*$ iff $R = [S_{jk}]_{j,k\neq i}$ copositive;*
$\mathbf{u} = [u_j]_{j\neq i}$ *violating for $R \Rightarrow \mathbf{v} = [0, \mathbf{u}] \in \mathbb{R}^n_+$ violating for S.*

(d) *if $S_{ij} \leq 0 < S_{ii}$ for all $j \neq i$, then $S \in \mathcal{K}^*$ iff*

$$T = [S_{ii}S_{jk} - S_{ij}S_{ik}]_{j,k\neq i} \text{ is copositive;}$$

$$\begin{aligned} \mathbf{w} &= [w_j]_{j\neq i} \text{ violating for } T \Rightarrow \\ \mathbf{v} &= [-\textstyle\sum_{j\neq i} S_{ij}w_j, S_{ii}\mathbf{w}] \in \mathbb{R}^n_+ \text{ violating for } S\,; \end{aligned}$$

(e) *if $S_{ij} < -\sqrt{S_{ii}S_{jj}} < 0$, then $\mathbf{v} = \sqrt{S_{jj}}\,\mathbf{e}_i + \sqrt{S_{ii}}\,\mathbf{e}_j$ is violating.*

After preprocessing ...

... and preceding simple sign tests, drop appropriate rows/columns; it remains to test (possibly smaller) S for copositivity where

(a,b,c) all diagonal entries $S_{ii} > 0$;

(c,d) sign of entries (off the diagonal) change in every row; and

(e) every negative entry $S_{ij} \geq -\sqrt{S_{ii}S_{jj}}$.

Final simplification (D any positive-definite diagonal matrix):

S is copositive if and only if

$$S' = \left[\frac{S_{ij}}{\sqrt{S_{ii}S_{jj}}}\right]_{i,j} \quad (= D^{-1}SD^{-1})$$

is copositive. We have $S'_{ii} = 1$ and $S'_{ij} \geq -1$ for all i, j.

A normal form for copositive matrices

For any symmetric matrix S define the negative sign-graph $\mathcal{G}_-(S)$ via the adjacency matrix: $A_{ij} = 1$ if and only if $S_{ij} < 0$, $i \neq j$.

Theorem: *If S is copositive with $S_{ii} > 0$ for all i, then there are: a matrix $N = N^\top$ with no negative elements; a positive-definite diagonal matrix D; and a loopless undirected graph $\mathcal{G}$ such that*

$$S = D[I_n - A_{\mathcal{G}}]D + N\,.$$

We can choose diag $N = \mathbf{o}$ and diag $D^2 =$ diag S.

Proof. Take $\mathcal{G} = \mathcal{G}_-(S)$ (no other choice) and use $S'_{ij} \geq -1$.

Easy copositivity detection

Theorem: *After ordering S_{ii} such that they increase with i, get*

$$S = \begin{bmatrix} O & O \\ O & D[I_r - A_{\mathcal{G}}]D \end{bmatrix} + N\,,$$

where $r \le n$ with equality iff the O blocks are not there.

[Pardalos/Vavasis'91]: QP with one neg.eigenvalue is NP-hard.

How about: copositivity detection with one negative entry ?

This is easy, even with $\le n$ negatives, if fairly distributed !

Theorem: *Suppose S contains at most one negative element per row. Then $S \in \mathcal{K}^*$ iff $S_{ii} \ge 0$ and $S_{ij} \ge -\sqrt{S_{ii}S_{jj}}$ for all i, j. In fact, then $S \in \mathcal{P} + \mathcal{N}$.*

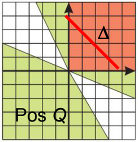
Extends linear-time detection for tridiagonal matrices **[B.'00]**.

Difference-of-convex (d.c.) approach to copositivity

Given: simplex $\Delta = \text{conv}\,(\mathbf{w}_1, \ldots, \mathbf{w}_n)$, matrix Q;
test Δ-copositivity of Q: is $\mathbf{x}^\top Q\mathbf{x} \geq 0$ for all $\mathbf{x} \in \Delta$?
D.c. decomposition: $Q = Q_+ - Q_-$ with $\left\{Q_+, Q_-\right\} \subset \mathcal{P}$.
Non-convex positivity cone Pos $Q = \left\{\mathbf{x} \in \mathbb{R}^n : \mathbf{x}^\top Q_- \mathbf{x} \leq \mathbf{x}^\top Q_+ \mathbf{x}\right\}$:

$$Q \text{ is } \Delta\text{-copositive} \quad \Longleftrightarrow \quad \Delta \subset \text{Pos } Q\,,$$

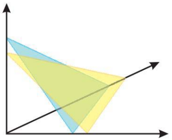
any $\mathbf{v} \in \mathbb{R}_+\Delta \setminus$ Pos Q is a violating vector.



Convex QP-copositivity tests approximate Pos Q:

Suppose for simplicity that both Q_+ and Q_- are nonsingular.
Rescale $\mathbf{v}_i^- = \frac{1}{\sqrt{\mathbf{w}_i^\top Q_- \mathbf{w}_i}}\mathbf{w}_i$; if $\min_i (\mathbf{v}_i^-)^\top Q_+ (\mathbf{v}_i^-) < 1$, a violating vector in Δ is found; else proceed to solve following convex QP.

D.c.-based convex QP tests for copositivity



Solve convex QP over rescaled simplex

$$\mu_\Delta^- = \min\left\{\mathbf{v}^\top Q_+ \mathbf{v} : \mathbf{v} \in \text{conv}\,(\mathbf{v}_1^-, \ldots, \mathbf{v}_n^-)\right\}.$$

If $\mu_\Delta^- \geq 1$, then Q is Δ-copositive;

else use solution to above QP for ω-subdivision of Δ, branch.

Another convex QP works in parallel: renormalize differently, $\mathbf{v}_i^+ = \frac{1}{\sqrt{\mathbf{w}_i^\top Q_+ \mathbf{w}_i}}\mathbf{w}_i$; if $s^2 = \max_i (\mathbf{v}_i^+)^\top Q_- (\mathbf{v}_i^+) > 1$, a violating vector in Δ is found; else proceed to solve following convex QP:

$$\mu_\Delta^+ = \min\left\{\mathbf{v}^\top Q_- \mathbf{v} : \mathbf{v} \in \text{conv}\,(\mathbf{v}_1^+, \ldots, \mathbf{v}_n^+)\right\}.$$

If $\mu_\Delta^+ \leq s^2$, then Q is Δ-copositive; else branch as above.

LP-based shortcut at the root

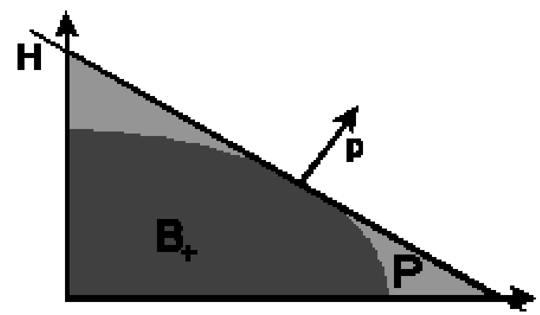
Consider *convex maximization* QP

$$\mu^+ = \sup\left\{\mathbf{x}^\top Q_- \mathbf{x} : \mathbf{x}^\top Q_+ \mathbf{x} \le 1\,,\ \mathbf{x} \in \mathbb{R}^n_+\right\}\,.$$

If $\mu^+ \le 1$, then Q is copositive; now include convex set

$$B_+ = \left\{\mathbf{x} \in \mathbb{R}^n_+ : \mathbf{x}^\top Q_+ \mathbf{x} \le 1\right\}$$

into polytope $P = \text{conv}\,(\mathbf{z}_0, \ldots, \mathbf{z}_n) \supset B_+$.



Then

$$\mu^+ \le \max\left\{\mathbf{x}^\top Q_- \mathbf{x} : \mathbf{x} \in P\right\} = \max_i \mathbf{z}_i^\top Q_- \mathbf{z}_i\,.$$

P is easily found if $\mathbf{p} = Q_+ \mathbf{x} \in \text{int}\ \mathbb{R}^n_+$ for some $\mathbf{x} \in \partial B_+$. Search for this $\mathbf{p}$ by LP with arbitrary $\mathbf{f}$, e.g., $\mathbf{f} = \mathbf{e} = [1, \ldots, 1]^\top$:

$$\max\left\{\mathbf{f}^\top \mathbf{x} : Q_+ \mathbf{x} \ge \mathbf{e}\,,\ \mathbf{x} \ge \mathbf{o}\right\}\,.$$

Sufficient copositivity condition

Theorem [B./Eichfelder '12]: *Given a d.c.d.* $Q = Q_+ - Q_-$, *choose an* $\mathbf{x} \in \mathbb{R}^n_+$ *such that* $\mathbf{p} = Q_+\mathbf{x}$ *has only positive entries. If*

$$(Q_-)_{ii}\, \mathbf{x}^\top Q_+ \mathbf{x} \le (Q_+\mathbf{x})_i^2 \quad \textit{for all } i\,,$$

then Q *is copositive.*

Simulation: 5000 random matrices in $\mathcal{P} + \mathcal{N}$, sizes up to 200; with the choice $\mathbf{f} = Q_+\mathbf{e}$, only one (!) failed the test.

Even without using the LP, the simple choice of $\mathbf{x} = \mathbf{e}$ worked in some cases:
almost 2000 matrices satisfied $\min_i (Q_+\mathbf{e})_i > 0$,
over 1250 of these passed above test.

Lyapunov functions for switched systems

Consider a linear ODE

$$\dot{\mathbf{x}}(t) = A\mathbf{x}(t) \quad \text{with } \mathbf{x}(0) = \mathbf{x}_0\,.$$

System is asymptotically stable if there is a quadratic Lyapunov function $\mathbf{x}^\top P\mathbf{x}$ where P is positive-definite.
This is the case if and only if $AP + PA$ is negative-definite.

Additional constraints $C\mathbf{x}(t) \geq \mathbf{o}$ on trajectories:
above definiteness criterion on P is too strict.

Switched systems

$$\dot{\mathbf{x}}(t) = A_i\mathbf{x}(t) \quad \text{such that } C_i\mathbf{x}(t) \geq \mathbf{o}\,, \qquad \text{with } \mathbf{x}(0) = \mathbf{x}_0\,, i = 1, 2\,.$$

Find P such that

$$\left.\begin{array}{rcl} \mathbf{x}^\top P\mathbf{x} & > & 0 \\ \mathbf{x}^\top(A_iP + PA_i)\mathbf{x} & < & 0 \end{array}\right\} \text{ for all } \mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{o}\} \text{ with } C_i\mathbf{x} \geq \mathbf{o}\,.$$

Simplicial decomposition – copositive formulation

Consider compact basis

$$B_i = \{\mathbf{x} \in \mathbb{R}^n : C_i\mathbf{x} \geq \mathbf{o}\,, \|\mathbf{x}\|_1 = 1\}\ ,$$

simplicial decompositions $\mathcal{D}_i = \left\{\Delta_{i,j}\right\}$ of B_i,

$V_i = \bigcup_j \operatorname{ext}\,(\Delta_{\mathrm{i,j}})$ the set of all vertices of simplices in $\mathcal{D}_i$,

E_i the set of all (undirected) edges of simplices in $\mathcal{D}_i$.

Then P satisfies the above stability condition if and only if P solves the following system of strict linear inequalities for some suitable $\mathcal{D}_i$ [Bundfuss/Dür '09a]:

$$\left.\begin{array}{rcll} \mathbf{v}^\top P\mathbf{v} & > & 0 & \text{for all } \mathbf{v} \in V_1 \cup V_2 \\ \mathbf{u}^\top P\mathbf{v} & > & 0 & \text{for all } \{\mathbf{u},\mathbf{v}\} \in E_1 \cup E_2 \\ \mathbf{v}^\top(A_iP + PA_i)\mathbf{v} & < & 0 & \text{for all } \mathbf{v} \in V_i\,,\ i = 1,2\,, \\ \mathbf{u}^\top(A_iP + PA_i)\mathbf{v} & < & 0 & \text{for all } \{\mathbf{u},\mathbf{v}\} \in E_i\,,\ i = 1,2\,. \end{array}\right\}$$

Existence resolved – reduction to finite linear system

Any solution P to the above system provides a constructive approach to establishing asymptotic stability.

This reduction to a finite system resolves existence question of copositive quadratic Lyapunov functions, posed as an open problem [Camlıbel/Schumacher '04].

Can be also used for:

- copositivity detection [Bundfuss/Dür '08]
  – challenged by [B./Eichfelder '12];

- copositive optimization: given objective function C, adaptive construction of the partition $\mathcal{D}_i$ [Bundfuss/Dür 09b].

Approximation hierarchies; positivity cones

... use (direct or adaptive) discretization methods, sum-of-squares conditions, and moment approaches.

For an arbitrary (possibly finite) subset $T \subseteq \mathbb{R}^n_+$, define

$$\mathcal{P}os(T) := \left\{ S = S^\top : \mathbf{y}^\top S \mathbf{y} \geq 0 \text{ for all } \mathbf{y} \in T \right\} .$$

Obvious: $\mathcal{K}^* \subseteq \mathcal{P}os(T)$ ... polyhedral if T finite.

Already used: $\mathcal{K}^* = \mathcal{P}os(B)$ for any base B of $\mathbb{R}^n_+$ (e.g. $B = \Delta^n$).

Interesting: $\mathcal{K}^* = \mathcal{P}os(\mathbb{N}^n)$ [Buchheim et al.'12].

Instead $\mathbb{N}^n$ finite grid, or equivalent on the standard simplex Δ^n:

$$\mathbb{N}^n_r = \left\{ \mathbf{m} \in \mathbb{N}^n : \sum_{i=1}^n m_i = r \right\} \quad \text{or} \quad \Delta^n_d = \tfrac{1}{d+2} \mathbb{N}^n_{d+2} \subset \Delta^n .$$

Direct discretizations

First (outer) discretization [B./deKlerk'02]:

$$\mathcal{E}_d := \mathcal{P}os(\Delta_d^n) \searrow \mathcal{K}^* \quad \text{as } d \to \infty\,.$$

Refinement [Yıldırım '11]:

$$\mathcal{Y}_d := \mathcal{P}os(\bigcup_{k=0}^{d} \Delta_k^n) \subset \mathcal{E}_d\,,$$

so also $\mathcal{Y}_d \searrow \mathcal{K}^*$ as $d \to \infty$.

Both grids finite – polyhedral approximations, tractable via LP:

$$|\Delta_k^n| = \mathfrak{O}(n^k) \quad \text{polynomial in } n\,.$$

Adaptive outer discretizations

Hierarchy $\mathcal{H}_d$ of nested simplicial partitions of Δ^n, as before let $S_\Delta = V_\Delta^\top S V_\Delta$ and define [Bundfuss/Dür '08,'09b]

$$\mathcal{B}_d := \left\{ S = S^\top : \text{diag } S_\Delta \geq \mathbf{o} \text{ for all } \Delta \in \mathcal{H}_d \right\} ,$$

since diag $S_\Delta = [\mathbf{v}_i^\top S \mathbf{v}_i]$. Again can show under mild conditions: polyhedral $\mathcal{B}_d \searrow \mathcal{K}^*$ as $d \to \infty$.

[B./Teo/Dür '12]: take (lower-level) outer approx. $\mathcal{M} \supseteq \mathcal{K}^*$, replace condition diag $S_\Delta \geq \mathbf{o}$ with $S_\Delta \in \mathcal{M}$ (above: $\mathcal{M} = \left\{ T = T^\top : \text{diag } T \geq \mathbf{o} \right\}$), and define

$$\mathcal{B}_d(\mathcal{M}) := \left\{ S = S^\top : S_\Delta \in \mathcal{M} \text{ for all } \Delta \in \mathcal{H}_d \right\}$$

... more general outer discretization, but no longer polyhedral if $\mathcal{M}$ is not a polyhedral cone.

Partition hierarchy $\mathcal{H}_d$ can be chosen to adapt to objective.

Adaptive inner discretizations

Inner discretization: again based on $\mathcal{H}_d$, now use as above result

$$\mathcal{P}os(\Delta) = \left\{ S = S^\top : S_\Delta \in \mathcal{K}^* \right\}$$

and

$$\begin{aligned} \mathcal{K}^* &= \mathcal{P}os(\Delta^n) = \bigcap_{\Delta \in \mathcal{H}_d} \mathcal{P}os(\Delta) \\ &= \left\{ S = S^\top : S_\Delta \in \mathcal{K}^* \text{ for all } \Delta \in \mathcal{H}_d \right\} . \end{aligned}$$

Now, employing a (lower-level) inner approx. $\mathcal{M} \subset \mathcal{K}^*$, define

$$\mathcal{D}_d(\mathcal{M}) := \left\{ S = S^\top : S_\Delta \in \mathcal{M} \text{ for all } \Delta \in \mathcal{H}_d \right\} .$$

[Bundfuss/Dür '08] took $\mathcal{M} = \mathcal{N}$ while [Sponsel et al.'12] take general $\mathcal{M}$, e.g. $\mathcal{M} = \mathcal{P} + \mathcal{N}$ ($\mathcal{M} = \mathcal{P}$ does not help).

Exhaustivity: $\mathcal{D}_d(\mathcal{M}) \nearrow \mathcal{K}^*$ as $d \to \infty$, if $\mathcal{H}_d$ behaves well.

Sum-of-squares approximation hierarchy

Recall $S \in \mathcal{K}^*$ if f $\mathbf{y}^\top S\mathbf{y} \geq 0$ for all $\mathbf{y}$ s.t. $y_i = x_i^2$, some $\mathbf{x} \in \mathbb{R}^n$.
This is guaranteed if n-variable polynomial of degree $2(d+2)$

$$p_S^{(d)}(\mathbf{x}) = (\sum x_i^2)^d \mathbf{y}^\top S \mathbf{y} = (\sum x_i^2)^d \sum_{j,k} S_{jk} x_j^2 x_k^2$$

is nonnegative for all $\mathbf{x} \in \mathbb{R}^n$. Guaranteed if

(a) $p_S^{(d)}$ has no negative coefficients; or if

(b) $p_S^{(d)}$ is a sum-of-squares (s.o.s.): $p_S^{(d)}(\mathbf{x}) = \sum_i [f_i(\mathbf{x})]^2$.

Approximation cones [Parrilo '00, '03]:

$$\mathcal{I}_d := \{S = S^\top : p_S^{(d)} \text{ satisfies (a)}\},$$

$$\mathcal{S}_d := \{S = S^\top : p_S^{(d)} \text{ satisfies (b)}\}.$$

LMI representation of s.o.s. approximation cones

Again exhaustivity: $\mathcal{S}_d$, $\mathcal{I}_d \nearrow \mathcal{K}^*$ as $d \to \infty$. Further, $\mathcal{I}_d$ is a polyhedral cone while $\mathcal{S}_d$ can be described via LMI's: w.lo.g. $p_S^{(d)}(\mathbf{x}) = \sum_i [h_i(\mathbf{x})]^2$ with homogeneous polynomials h_i:

$$h_i(\mathbf{x}) = \widehat{\mathbf{a}}_i^\top \widehat{\mathbf{x}} \quad \text{with} \quad \widehat{\mathbf{x}} = [\mathbf{x}^\mathbf{m}]_{\mathbf{m}\in\mathbb{N}^n_{d+2}}$$

the vector of monomials $\mathbf{x}^\mathbf{m} = \prod_{i=1}^n x_i^{m_i}$ of degree $d+2$ in $\mathbf{x}$. Thus

$$p_S^{(d)}(\mathbf{x}) = \sum_i \left[\widehat{\mathbf{a}}_\mathbf{i}^\top \widehat{\mathbf{x}}\right]^2 = \widehat{\mathbf{x}}^\top M_S^{(d)}\, \widehat{\mathbf{x}}\,,$$

where $M_S^{(d)}$ is a symmetric matrix of large order $r = \binom{n+d+1}{d+2}$, which obviously must be psd. Conversely any such psd. matrix (not unique!) gives a s.o.s. Thus $\mathcal{S}_d = \left\{S = S^\top : M_S^{(d)} \in \mathcal{P}\right\}$.

Refinements of s.o.s. hierarchy

Proceeding to a more compact LMI description, [Peña et al.'07] introduced

$$\mathcal{Q}_d := \{S = S^\top : (\mathbf{e}^\top \mathbf{x})^d \mathbf{x}^\top S \mathbf{x} = \sum_{\mathbf{m} \in \mathbb{N}_d^n} \mathbf{x}^{\mathbf{m}} (\mathbf{x}^\top Q_{\mathbf{m}} \mathbf{x}) \quad \text{with} \quad Q_{\mathbf{m}} \in \mathcal{P} + \mathcal{N}, \text{ all } \mathbf{m} \in \mathbb{N}_d^n\},$$

to arrive at $\mathcal{I}_d \subset \mathcal{Q}_d \subset \mathcal{S}_d$. Admits a recursive description, too.

Tensor description of the higher-order duals $[\mathcal{Q}_d]^*$, and $[\mathcal{I}_d]^*$ provided in [Dong '10], yield outer approximation hierarchy for $\mathcal{K}$.

These LMI descriptions allow for tractable (well, for small d) SDP implementations in $\mathfrak{O}(n^{2(d+2)})$ variables – expensive but sometimes efficient (cf. Lovász' θ for stability number). Additional methods like warmstarting required [Engau et al.'12].

Lasserre's moment approach

... starts with elementary observation: select T with $\mathbb{R}_+ T = \mathbb{R}^n_+$; if μ is an arbitrary Borel measure on T, and $S = S^\top$, then

$$\mathbf{x}^\top S \mathbf{x} \geq 0 \text{ for all } \mathbf{x} \in \mathbb{R}^n_+ \quad \text{implies} \quad \int_T (\mathbf{x}^\top S \mathbf{x}) \, \mu(\mathrm{d}\mathbf{x}) \geq 0 \, .$$

Reverse implication not true for single μ;
idea: require $\int_T (\mathbf{x}^\top S \mathbf{x}) \, \mu(\mathrm{d}\mathbf{x}) \geq 0$ for large enough class of μ's.

Trivial: all point measures on T. Does not help.

[Lasserre '00, '11]: One choice is $T = \mathbb{R}^n_+$,

$$\left\{ \mu : \frac{\mathrm{d}\mu}{\mathrm{d}\mathbf{x}}(\mathbf{x}) = [g(\mathbf{x})]^2 \exp(-\mathbf{e}^\top \mathbf{x}) \, , \; g \text{ a polynomial in } \mathbf{x} \right\} .$$

LMI representation of moment condition

Let $I(d,n) = \bigcup_{k=0}^{d} \mathbb{N}_d^n$ with $s = \mathfrak{O}(n^d)$ elements. Then degree d polynomial $g(\mathbf{x}) = \widehat{\mathbf{c}}^\top \widehat{\mathbf{x}}$ with $\widehat{\mathbf{x}} = [\mathbf{x}^{\mathbf{k}}]_{\mathbf{k}\in I(d,n)}$, and with above $\mu_{\widehat{\mathbf{c}}}(\mathrm{d}\mathbf{x}) = [g(\mathbf{x})]^2 \exp(-\mathbf{e}^\top \mathbf{x})\mathrm{d}\mathbf{x}$ get $\int\limits_T (\mathbf{x}^\top S \mathbf{x})\, \mu(\mathrm{d}\mathbf{x}) = \widehat{\mathbf{c}}^\top M_d(S)\, \widehat{\mathbf{c}}$ with large $s \times s$ matrix linear in S:

$$M_d(S) = \left[\sum_{i,j} S_{ij}\, y_{\mathbf{k}+\mathbf{m}+\mathbf{e}_i+\mathbf{e}_j} \right]_{(\mathbf{k},\mathbf{m})\in I(d,n)^2}$$

where $y_{\mathbf{m}} = \int_T \mathbf{x}^{\mathbf{m}} \exp(-\mathbf{e}^\top \mathbf{x})\mathrm{d}\mathbf{x} = \prod_i (m_i)!$ for all $\mathbf{m} \in \mathbb{N}^n$.

With this choice of T and $\mu_{\widehat{\mathbf{c}}}$'s it holds that

$$S \in \mathcal{K}^* \quad \iff \quad M_d(S) \in \mathcal{P} \text{ for all } d\,.$$

Gives rise to Lasserre's LMI approximation cone

$$\mathcal{L}_d(\mu_\cdot, T) := \left\{ S = S^\top : M_d(S) \in \mathcal{P} \right\} \searrow \mathcal{K}^* \text{ as } d \to \infty\,.$$

Recent refinement of moment method

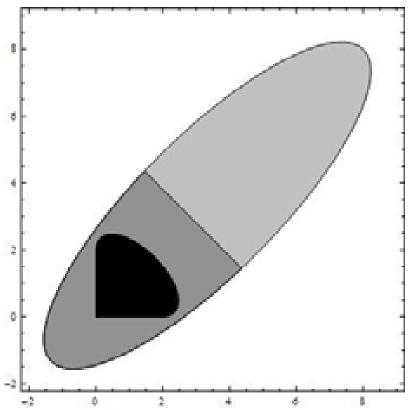
Observation [Dickinson/Povh '12]: $S \in \mathcal{K}^*$ implies even

$$M_d(S) = \int_T (\mathbf{x}^\top S \mathbf{x}) \exp(-\mathbf{e}^\top \mathbf{x})\, \hat{\mathbf{x}}\, \hat{\mathbf{x}}^\top \, \mathrm{d}\mathbf{x} \ \in \mathcal{K}\,,$$

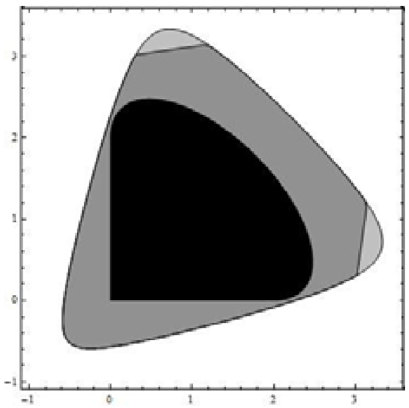
since it is limit of convex combinations of $\hat{\mathbf{z}}\,\hat{\mathbf{z}}^\top$ with $\hat{\mathbf{z}} \in \mathbb{R}^s_+$.

So can also take a tractable cone $\mathcal{A}$ with $\mathcal{K} \subset \mathcal{A} \subset \mathcal{P}$, a (lower-level) outer approximation of $\mathcal{K}$, e.g. $\mathcal{A} = \mathcal{P} \cap \mathcal{N}$, to obtain tighter outer approximation of $\mathcal{K}^*$:

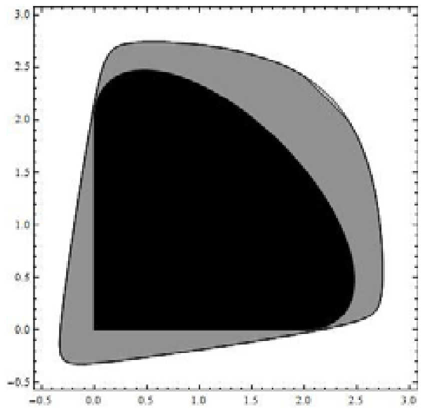
$$\mathcal{K}^* \subset \mathcal{L}_d(\mu_\cdot, T; \mathcal{A}) := \left\{ S = S^\top : M_d(S) \in \mathcal{A} \right\} \subset \mathcal{L}_d(\mu_\cdot, T)\,.$$



(a) d=1



(b) d=2



(c) d=3

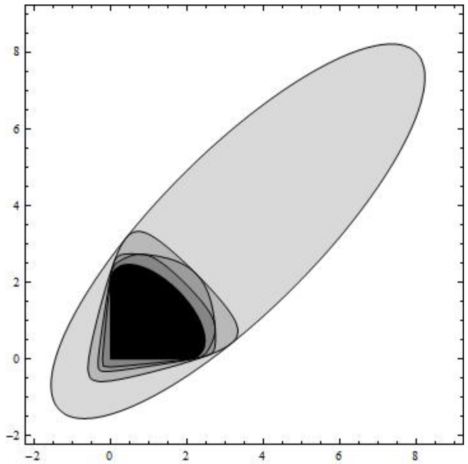
Survey of approximation constructions

Name	symbol	mode	method	remarks
B./de Klerk	$\mathcal{E}$	outer	LP	rational grid for Δ^n
Yıldırım	$\mathcal{Y}$	outer	LP	$\mathcal{Y} \subset \mathcal{E}$, grid
Bundfuss/Dür	$\mathcal{B}$	outer	LP	simplicial partition
B./Dür/Teo	$\mathcal{B}(\mathcal{M})$	outer	LP	$\mathcal{M} \supset \mathcal{K}^*$
Bundfuss/Dür	$\mathcal{D}$	inner	LP	simplicial partition
Sponsel et al.	$\mathcal{D}(\mathcal{M})$	inner	LP	$\mathcal{M} \subset \mathcal{K}^*$
Parrilo et al.	$\mathcal{I}$	inner	LP	coeff $p_S^{(d)} \geq \mathbf{o}$
Parrilo et al.	$\mathcal{S}$	inner	SDP	$p_S^{(d)}$ is a s.o.s.
Peña et al.	$\mathcal{Q}$	inner	SDP	$\mathcal{I} \subset \mathcal{Q} \subset \mathcal{S}$
Lasserre	$\mathcal{L}(\mu, T)$	outer	SDP	μ-moments over T
Dickinson/Povh	$\mathcal{L}(\mu, T; \mathcal{A})$	outer	SDP	$\mathcal{L}(\mu, T; \mathcal{A}) \subset \mathcal{L}(\mu, T)$

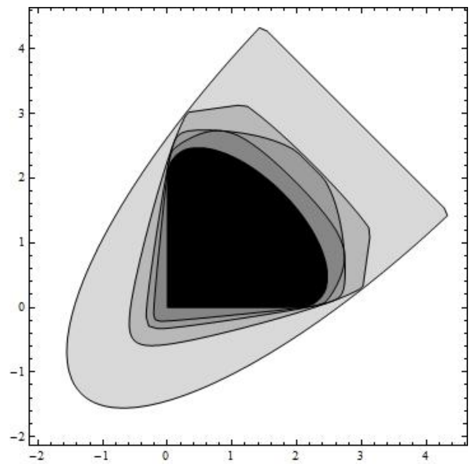
Compact overview of approximation constructions

mode/method	LP	SDP
outer	$\mathcal{E}$, $\mathcal{Y}$, $\mathcal{B}(\mathcal{M})$	$\mathcal{L}(\mu, T; \mathcal{A})$
inner	$\mathcal{I}$, $\mathcal{D}(\mathcal{M})$	$\mathcal{S}$, $\mathcal{Q}$

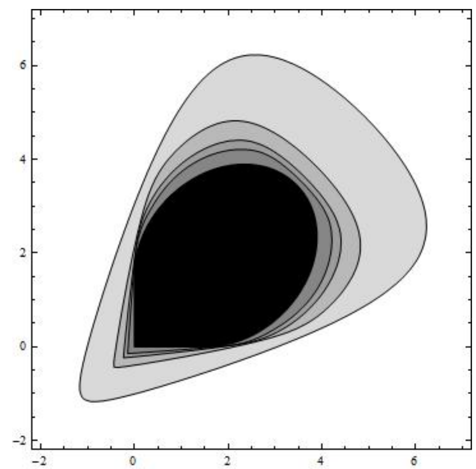
Yet to explore: vary also $\mathcal{M}$, $\mathcal{A}$ and (T, μ) with d, cf. [Dickinson/Povh '12], [B./Dür/Teo '12].



$\mathcal{A} = \mathcal{P}$



$\mathcal{A} = \mathcal{P} \cap \mathcal{N}$



$(T, \mu) = ([0,1]^n, \lambda^n)$

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