Quadratic factorization heuristics for copositive programming

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Outline

- Brief Intro to Semidef. and Copositive Programming
- Complete Positivity and Combinatorial Optimization
- Approximating Completely Positive Matrices
- A Nonconvex Quadratic Reformulation
- A Local Method for the Nonconvex Program
- Conclusion

Notation

Scalar product of two matrices A, B:

$$\langle A, B\rangle := \textbf{trace } A^T B \equiv \sum_{i,j} A_{i,j} B_{i,j}$$

inducing the Frobenius norm $\|A\|_F := (\langle A, A\rangle)^{1/2}$.

$\mathcal{S}^n$ symmetric $n \times n$-matrices.
$\mathcal{S}^n_+ = \{X \in \mathcal{S}^n \mid X \succeq 0\}$ positive semidefinite matrices.

Copositive Matrices

A matrix symmetric Y is called copositive if

$$a^T Y a \geq 0 \; \forall a \geq 0.$$

Cone of copsitive matrices:

$$\mathcal{C} = \{Y \in \mathcal{S}^n \mid a^T Y a \geq 0 \; \forall a \geq 0\}.$$

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Challenge: $X \notin \mathcal{C}$ is NP-complete decision problem.

Dual cone

Dual cone $\mathcal{C}^*$ of $\mathcal{C}$ in $\mathcal{S}^n$:

$$X \in \mathcal{C}^* \iff \langle X, Y \rangle \geq 0 \;\; \forall Y \in \mathcal{C}$$

$$\iff X \in \textbf{conv}\{aa^T \mid a \geq 0\}.$$

Such X is called completely positive.

$\mathcal{C}^*$ is the cone of completely positive matrices, a closed, convex cone.

Completely Positive Matrices

Let $A = (a_1, \ldots, a_k)$ be a nonnegative $n \times k$ matrix, then

$$X = a_1 a_1^T + \ldots + a_k a_k^T = AA^T$$

is completely positive.

By Caratheodory's theorem, for any $X \in \mathcal{C}^*$ there is a nonnegative A as above with $k \leq n(n+1)/2$.

Basic Reference:

A. Berman, N. Shaked-Monderer:
Completely Positive Matrices, World Scientific 2003

Semidefinite and Copositive Programs

Problems of the form

$$\min\langle C, X\rangle \text{ s.t. } A(X) = b,\ X \in \mathcal{S}_+^n$$

are called Semidefinite Programs.

Problems of the form

$$\min\langle C, X\rangle \text{ s.t. } A(X) = b,\ X \in \mathcal{C}$$

or

$$\min\langle C, X\rangle \text{ s.t. } A(X) = b,\ X \in \mathcal{C}^*$$

are called Copositive Programs, because the primal or the dual involves copositive matrices.

Interior-Point Methods

Semidefinite programs can be efficiently solved by interior point algorithms. One particular form of interior point method is based on so-called Dikin ellipsoids:

For a given point Y in the interior of $\mathcal{S}^n_+$ define the “largest” ellipsoid E_Y such that $Y + E_Y$ is contained in $\mathcal{S}^n_+$.

$$E_Y := \{S \mid \mathrm{trace}(SY^{-1}SY^{-1}) \leq 1\}$$

$$= \{S \mid \|Y^{-1/2}SY^{-1/2}\|_F^2 \leq 1\}.$$

$$= \{S \mid \|Y^{-1}S\|_F^2 \leq 1\}.$$

Concept of Dikin interior point algorithm

Minimizing a linear objective function over the intersection of an ellipsoid with an affine subspace is easy. (Solving a system of linear equations).

Given X^k in the interior of $\mathcal{S}^n_+$ with $A(X) = b$ let ΔX be the solution of

$$\min\{\langle C, \Delta X\rangle \quad | \quad A(\Delta X) = 0\,,\ \Delta X \in E_{X^k}\}$$

and set $X^{k+1} = X^k + \frac{1}{2}\Delta X$. (Step length $\frac{1}{2}$.)

Convergence

For linear programs and fixed step length of at most $\frac{2}{3}$ the Dikin algorithm converges to an optimal solution. Counterexamples for longer step lengths.
(Tsuchiya et al)

For semidefinite problems there exist examples where this variant of interior point method converges to non-optimal points (Muramatsu).

(Use other interior point methods based on barrier functions or primal-dual systems.)

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Why Copositive Programs ?

Copositive Programs can be used to solve combinatorial optimization problems.

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Copositive Programs can be used to solve combinatorial optimization problems.

• Stable Set Problem:
Let A be adjacency matrix of graph, E be all ones matrix.
Theorem (DeKlerk and Pasechnik (SIOPT 2002))

$$\alpha(G) = \max\{\langle E, X\rangle : \langle A + I, X\rangle = 1, \quad X \in \mathcal{C}^*\}$$

$$= \min\{y : y(A + I) - E \in \mathcal{C}\}.$$

This is a copositive program with only one equation (in the primal problem).
– a simple consequence of the Motzkin-Straus Theorem.

Semidefinite relaxation –

Consider the (nonconvex) problem

$$\min\left\{x^\top Qx + 2c^\top x \mid a_i{}^\top x = b_i\,,\ i = 1:m\,,\ x \geq 0\right\}.$$

with add. constraints $x_i \in \{0,1\}$ for $i \in B$.

Think of $X = xx^\top$ so that $x^\top Qx = \langle Q, X\rangle$ and solve

$$\min\left\{\langle Q, X\rangle + 2c^\top x \ \middle|\ \begin{array}{ll} & a_i^\top X a_i = b_i^2,\ a_i^\top x = b_i,\quad i = 1:m \\ \begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} \succeq 0, & \qquad x_i = X_{i,i} \text{ for } i \in B \end{array}\right\}.$$

– *versus copositive Reformulation:*

If the domain is bounded the copositive relaxation

$$\min \left\{ \langle Q, X \rangle + 2c^\top x \;\middle|\; \begin{array}{ll} a_i^\top X a_i = b_i^2,\ a_i^\top x = b_i, & i = 1:m \\ \begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} \in \mathcal{C}^*, & x_i = X_{i,i} \text{ for } i \in B \end{array} \right\}$$

is exact (Burer 2007).

Hence copositive programs form an NP-hard problem class.

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Approximating $\mathcal{C}^*$

We have now seen the power of copositive programming.

Since optimizing over $\mathcal{C}$ is NP-Hard, it makes sense to get approximations of $\mathcal{C}$ or $\mathcal{C}^*$.

• To get relaxations, we need supersets of $\mathcal{C}^*$, or inner approximations of $\mathcal{C}$ (and work on the dual cone). The Parrilo hierarchy uses Sum of Squares and provides such an outer approximation of $\mathcal{C}^*$ (dual viewpiont!).

• We can also consider inner approximations of $\mathcal{C}^*$. This can be viewed as a method to generate feasible solutions of combinatorial optimization problems (primal heuristic!).

Relaxations

Inner approximation of $\mathcal{C}$.

$$\mathcal{C} = \{M \mid x^T M x \geq 0 \; \forall x \geq 0\}.$$

Parrilo (2000) and DeKlerk, Pasechnik (2002) use the following idea to approximate $\mathcal{C}$ from inside:

$$M \in \mathcal{C} \text{ iff } P(x) := \sum_{ij} x_i^2 x_j^2 m_{ij} \geq 0 \;\; \forall x.$$

A sufficient condition for this to hold is that $P(x)$ has a sum of squares (SOS) representation.

Theorem Parrilo (2000) : $P(x)$ has SOS iff $M = P + N$, where $P \succeq 0$ and $N \geq 0$.

Parrilo hierarchy

To get tighter approximations, Parrilo proposes to consider SOS representations of

$$P_r(x) := (\sum_i x_i^2)^r P(x)$$

for $r = 0, 1, \ldots$. (For $r = 0$ we get the previous case.) Mathematical motivation by an old result of Polya.

Theorem Polya (1928):
If M strictly copositive then $P_r(x)$ is SOS for some sufficiently large r.

Inner approximations of $\mathcal{C}^*$

Some previous work by:

- Bomze, DeKlerk, Nesterov, Pasechnik, others:
Get stable sets by approximating $\mathcal{C}^*$ formulation of the stable set problem using optimization of quadratic over standard simplex, or other local methods.

- Bundschuh, Dür (2008): linear inner and outer approximations of $\mathcal{C}$

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The (dual of the) copositive program

Recall the (dual form of the) copositive program:

(CP) $\qquad \min\langle C, X\rangle$ **s.t.** $A(X) = b,\ X \in \mathcal{C}^*,$

Here, the linear constraints can be represented by m symmetric matrices A_i:

$$A(X) = \begin{pmatrix} \langle A_1, X\rangle \\ \vdots \\ \langle A_m, X\rangle \end{pmatrix}.$$

Assumption

We assume that the feasible set of the "copositive" program (CP) is bounded and satisfies Slater's condition, i.e. that there exists a matrix X in the interior of $\mathcal{C}^*$ satisfying the linear equations $\langle A_i, X\rangle = b_i\ ,\ i = 1 : m$. These assumptions imply the existence of an optimal solution of (CP) and of its dual.

A feasible descent method

- Given $X^j \in \mathcal{C}^*$ with $\langle A_i, X^j \rangle = b_i$ and $\varepsilon \in (0,1)$ consider the *regularized problem*

$$(RP) \qquad \begin{array}{rl} \min & \varepsilon\langle C, \Delta X\rangle + (1-\varepsilon)\|\Delta X\|_j^2 \\ \text{s.t.} & \langle A_i, \Delta X\rangle = 0\,,\ i = 1:m \\ & X^j + \Delta X \in \mathcal{C}^* \end{array}$$

  which has a strictly convex objective function and a unique optimal solution denoted by ΔX^j.
- The norm $\| \;.\; \|_j$ may change at each iteration.
- For large $\varepsilon < 1$ the point $X^j + \Delta X^j$ approaches a solution of the copositive problem (CP).

Outer iteration

$$X^{j+1} := X^j + \Delta X^j$$

Lemma

If the norms $\| \, . \, \|_j$ satisfy a global bound,

$$\exists M < \infty : \qquad \|H\|_j^2 \leq M\|H\|^2 \quad \forall \; H = H^\top \;\; \forall \; j$$

then the following result holds true:

Let $\bar{X}$ be any limit point of the sequence X^j. Then $\bar{X}$ solves the copositive program (CP).

Inner iteration

Assume $X^j = VV^\top$ with $V \geq 0$.
Write $X^{j+1} = (V + \Delta V)(V + \Delta V)^\top$, i.e.

$$\Delta X = \Delta X(\Delta V) := V \Delta V^\top + \Delta V V^\top + \Delta V \Delta V^\top, .$$

Thus, the regularized problem (RP) is equivalent to the nonconvex program

$$(NC) \qquad \begin{array}{rl} \min & \varepsilon \langle C, \Delta X(\Delta V) \rangle + (1 - \varepsilon) \|\Delta X(\Delta V)\|_j^2 \\ \text{s.t.} & \langle A_i, \Delta X(\Delta V) \rangle = 0 \,, \; i = 1 : m \\ & V + \Delta V \geq O \,. \end{array}$$

Caution

By construction, the regularized problem (RP) and the nonconvex program (NC) are equivalent.
(RP) has a unique local – and global – optimal solution.
However, (NC) may have multiple local (nonglobal) solutions;

the equivalence only refers to the global solution of (NC).

Eliminating ΔX

- Replace the norm $\|\Delta X(\Delta V)\|_j$ with the (semi-) norm

$$\|\Delta V\|_V := \|V\Delta V^\top + \Delta V V^\top\|$$

$$\approx \|V\Delta V^\top + \Delta V V^\top + \Delta V \Delta V^\top\| = \|\Delta X(\Delta V)\|.$$

- If the Frobenius norm $\|\Delta V\|$ is used instead of $\|\Delta V\|_V$ the subproblems are very sparse.

We obtain

$$\begin{array}{ll} \min & \varepsilon\,[2\langle CV\,,\Delta V\rangle + \langle C\Delta V\,,\Delta V\rangle] + (1-\varepsilon)\|\Delta V\|^2 \\ \text{s.t.} & \langle A_i\Delta V\,,\Delta V\rangle + 2\langle A_i V\,,\Delta V\rangle = 0\,,\ i = 1:m \\ & V + \Delta V \in I\!R_+^{n\times k} \end{array}$$

which is equivalent to (RP) and (NC) when $\|\Delta X\|_j$ is replaced with the regularization term $\|\Delta V\|$.

Finally,

Since $\|\Delta V\|$ is small when $\epsilon > 0$ is small, we linearize the quadratic constraints (ignore the term $\Delta V \Delta V^\top$)
$\Rightarrow$ Linearized Problem (LP)
(plus a simple convex quadratic objective)

Fixed point iteration to satisfy the constraints:

$$
\begin{array}{rl}
\min & \varepsilon \langle C(2V + \Delta V^{old}), \Delta V \rangle + (1-\varepsilon) \|\Delta V^{old} + \Delta V\|^2 + \tau_l \|\Delta V\|^2 \\
\text{s.t.} & \langle A_i(2V + \Delta V^{old}), \Delta V \rangle = \tilde{s}_i \,, \; i = 1 : m \\
 & V + \Delta V^{old} + \Delta V \in \mathbb{R}_+^{n \times k} \,,
\end{array}
$$

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Input: $\varepsilon \leq 1/2$ and $V \geq O$ with $\langle A_i, VV^\top \rangle = b_i$ for all i.

1. Set $\Delta V^{old} := O$ and $\tilde{s}_i := 0$ for all i. Set $l = 1$ and $\tau_1 := 1$.
2. Solve the linearized problem (LP) and denote the optimal solution by ΔV^l.
3. Update $\Delta V^{old} := \Delta V^{old} + \Delta V^l$ and $\tilde{s}_i := b_i - \langle A_i(2V + \Delta V^{old}), V + \Delta V^{old} \rangle$.
4. If $\|\Delta V^{old}\| > 1$ set $\varepsilon = \varepsilon/2$.
5. If $\|\Delta V^l\| \approx 0$: Stop, $\Delta V := \Delta V^{old} + \Delta V^l$ approximately solves (NC) locally.
6. Else update $l := l + 1$, $\tau_l := l$, and go to Step 2.

Subproblems (inner loop)

$$\begin{aligned} \min \quad & \langle \tilde{C}, \Delta V \rangle + \rho \|\Delta V\|^2 \\ \text{s.t.} \quad & \langle \tilde{A}_i, \Delta V \rangle = \tilde{s}_i \,, \; i = 1:m \,, \\ & V + \Delta V \in I\!\!R_+^{n \times k} \,, \end{aligned}$$

a strictly convex quadratic problem over a polyhedron. In vector form,

$$\min \left\{ \tilde{c}^\top x + \rho x^\top x : \tilde{a}_i^\top x = \tilde{s}_i \,, \; i = 1:m \,, \; x + v \geq o \right\}.$$

When m is small, $n \leq 500$ and $k \leq 1000$ this can be solved on a standard PC.

A negative example:

(Remember – this is an NP-hard problem.)

If rank $(V) < \frac{n}{2}$ then the mapping $\Delta V \mapsto V \Delta V^\top + \Delta V V^\top$ is not surjective, and hence, there does not exist a Lipschitz continuous function $\Delta V_\delta \mapsto \Delta X_\delta$. (This lack of Lipschitz continuity was exploited when constructing examples such that (NC) has local solutions even for tiny $\epsilon > 0$.)

Lemma:

If V is a rectangular matrix such that $VV^T \succ 0$, then the map $\Delta V \mapsto V \Delta V^\top + \Delta V V^\top$ is surjective.

A Dikin ellipsoid approach

- Let $V > O$. The Dikin ellipsoid E_V for the set $\{V \geq O\}$ is defined by

$$E_V := \{\Delta V \ \mid \ \|\Delta V / V\|_F \leq 1\},$$

where the division $\Delta V / V$ is taken componentwise.

Dikin-type algorithm

Let $V > O$ be given with $VV^\top \succ O$.
Select some small value $\epsilon \in (0,1)$ and $\tilde{\varepsilon} > 0$.
Set $\tilde{s}_i := b_i - \langle A_i V, V\rangle$ and $l := 0$.

1. Solve

$$\begin{aligned} \min \quad & \langle 2CV, \Delta V\rangle \\ \text{s.t.} \quad & \langle 2A_i V, \Delta V\rangle = \tilde{s}_i\,, \; i = 1:m \\ & \Delta V \in \epsilon E_V\,, \end{aligned}$$

   and denote the optimal solution by ΔV^l.

2. Update $V := V + \Delta V^l$ and $\tilde{s}_i := b_i - \langle A_i V, V\rangle$.
3. Update $l := l + 1$. If $\|\Delta V\|_2 < \tilde{\varepsilon}$ stop, else go to Step 1.

Computational results (here $k = 2n$)

A sample instance with $n = 60,\ m = 100$.

$z_{sdp} = -9600, 82, \quad z_{sdp+nonneg} = -172.19, z_{cop} = -69.75$

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it	|b-A(X)|	f(x)
1	0.002251	-68.7274
5	0.000014	-69.5523
10	0.000001	-69.6444
15	0.000001	-69.6887
20	0.000000	-69.6963

The number of inner iterations was set to 5, column 1 shows the outer iteration count.

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But starting point: $V0 = .95$ Vopt $+ .05$ rand

Computational results (2)

Example (continued). recall $n = 60,\ m = 100$.

$z_{sdp} = -9600, 82,\quad z_{sdp+nonneg} = -172.19, z_{cop} = -69.75$

start	iter	|b-A(X)|	f(x)
(a)	20	0.000000	-69.696
(b)	20	0.000002	-69.631
(c)	50	0.000008	-69.402

Different starting points:

(a) V = .95 * V_{opt} + .05 * rand

(b) V = .90 * V_{opt} + .10 * rand

(c) V = rand(n, 2n)

Random Starting Point

Example (continued), $n = 60,\ m = 100$.

$z_{sdp} = -9600,82,\quad z_{sdp+nonneg} = -172.19,$ $z_{cop} = -69.75$

it	|b-A(X)|	f(x)
1	6.121227	1831.5750
5	0.021658	101.1745
10	0.002940	-43.4477
20	0.000147	-67.0989
30	0.000041	-68.7546
40	0.000015	-69.2360
50	0.000008	-69.4025

Starting point: $V0 = rand(n, 2n)$

More results

n	m	opt	found	$\|b - A(X)\|$
50	100	314.48	314.90	$4 \cdot 10^{-5}$
60	120	-266.99	-266.48	$4 \cdot 10^{-5}$
70	140	-158.74	-157.55	$3 \cdot 10^{-5}$
80	160	-703.75	-701.68	$5 \cdot 10^{-5}$
100	100	-659.65	-655.20	$8 \cdot 10^{-5}$

Starting point in all cases: rand(n,2n)
Inner iterations: 5
Outer iterations: 30

The code works on random instances. Now some more serious experiments.

Dikin vs. QP-formulation

Comp. pos. reformulation of max-clique problem:

$\max\langle E, X\rangle$ such that $\text{trace }(X) = 1,\ \text{trace }(A_G X) = 0,\ X \in \mathcal{C}^*$

Only two equations but many local optima.
Computation times in the order of a few minutes.

Problem	Nodes	Max-Clique	QP	Dikin
brock200_4	200	17	16.00	12.97
c-fat200-1	200	12	12.00	11.92
c-fat200-5	200	58	58.00	56.21
hamming6-2	64	32	32.00	32.00
hamming8-2	256	128	128.0	124.4
keller4	171	11	9	6.971

Table 1: Comparison, QP-formulation – Dikin

Sufficient condition for Non-copositivity

To show that $M \notin \mathcal{C}$, consider

$$\min\{x^T M x \mid e^T x = 1,\ x \geq 0\}$$

and try to solve this through

$$\min\{\langle M, X\rangle \mid e^T x = 1, \langle E, X\rangle = 1, \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \mathcal{C}^*\}.$$

Our method is local, but once we have feasible solution with negative value, we have a certificate for $M \notin \mathcal{C}$.

We apply this to get another heuristic for stable sets.

Stable sets - second approach

If we can show that for some integer t

$$Q = t(A + I) - J$$

is not copositive, then $\alpha(G) \geq t + 1.$

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If we can show that for some integer t

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is not copositive, then $\alpha(G) \geq t + 1$. Hence we consider $\min\{x^T Q x : e^T x = 1, x \geq 0\}$ and translate this into

$$\min\{\langle Q, X\rangle : e^T x = 1, \langle J, X\rangle = 1, \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \mathcal{C}^*\}.$$

If we find solution with value < 0, then we have certificate that $\alpha(G) \geq t + 1$.

Stable sets - second approach

If we can show that for some integer t

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$$\min\{\langle Q, X\rangle : e^T x = 1, \langle J, X\rangle = 1, \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \mathcal{C}^*\}.$$

If we find solution with value < 0, then we have certificate that $\alpha(G) \geq t + 1$.

• Note that we prove existence of stable set of size $t + 1$, without actually providing such a set.

Further (preliminary) experiments

Some DIMACS graphs (use $k = 50$ – very quick)

name	n	ω	direct	dual
san200-1	200	30	30	30
san200-2	200	18	14	14
san200-3	200	70	70	70
san200-4	200	60	60	60
san200-5	200	44	35	44
phat500-1	500	9	9	9
phat500-2	500	36	36	36
phat500-3	500	$\geq$ 50	48	49

Some more results (direct approach):

Some DIMACS graphs (use $k = 50$ – very quick)

name	n	ω	direct
brock200-1	200	21	20
brock200-2	200	12	10
brock200-3	200	15	13
brock200-4	200	17	16
brock400-1	400	27	24
brock400-2	400	29	23
brock400-3	400	31	23
brock400-4	400	33	24

Last Slide

We have seen the power of copositivity.
Copositive Programming is an exciting new field with many open research problems.

Relaxations: The Parrilo hierarchy is computationally too expensive. Other way to approximate CP?

Heuristics: Unfortunately, the subproblem may have local solutions, which are not local minima for the original descent step problem.

Further technical details in a forthcoming paper by I. Bomze, F. J. and F. Rendl.: Quadratic factorization heuristics for copositive programming, technical report, (2009).