Copositive Programming and Combinatorial Optimization

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Overview

- The power of copositivity
- Relaxations based on CP
- Heuristics based on CP

The Power of Copositivity

- Copositive matrices
- Copositive programs
- Stable sets, Coloring
- Burer's theorem

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 called completely positive.

$$COP = \{X : X \text{ completely positive}\}$$

COP is closed, convex cone. From the definition we get

$$COP = \text{conv}\{aa^T : a \geq 0\}.$$

For basics, see the book: A. Berman, N. Shaked-Monderer: Completely Positive Matrices, World Scientific 2003

Copositive Matrices

Dual cone COP^* of COP in S_n (sym. matrices):

$$Y \in COP^* \iff \text{tr}XY \geq 0 \;\; \forall X \in COP$$

$$\iff a^T Y a \geq 0 \;\; \forall \text{ vectors } a \geq 0.$$

By definition, this means Y is copositive.

$$CP = \{Y : a^T Y a \geq 0 \; \forall a \geq 0\}$$

CP is dual cone to COP!

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CP is dual cone to COP!
Bad News: $X \notin CP$ is NP-complete decision problem.

Semidefinite matrices PSD: $Y \in PSD \iff a^T Y a \geq 0 \ \forall a$.
Well known facts: • $PSD^* = PSD$ (PSD cone is selfdual.)
• $COP \subset PSD \subset CP$

Semidefinite and Copositive Programs

Problems of the form

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

are called Semidefinite Programs.

Problems of the form

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

or

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

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

Why Copositive Programs ?

Copositive Programs can be used to solve combinatorial optimization problems.

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

$$\alpha(G) = \max\{\langle J, X\rangle : \langle A + I, X\rangle = 1, \quad X \in COP\}$$

$$= \min\{y : y(A + I) - J \in CP\}.$$

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

Proof (1)

$$\frac{1}{\alpha(G)} = \min\{x^T(A+I)x : x \in \Delta\}$$ (Motzkin-Strauss Theorem)

$\Delta = \{x : \ \sum_i x_i = 1, \ x \geq 0\}$ is standard simplex. We get

$$0 = \min\{x^T(A + I - \frac{ee^T}{\alpha})x : \ x \in \Delta\}$$

$$= \min\{x^T(\alpha(A + I) - J)x : \ x \geq 0\}.$$

This shows that $\alpha(A + I) - J$ is copositive. Therefore

$$\inf\{y : \ y(A + I) - J \in CP\} \leq \alpha.$$

Proof (2)

Weak duality of copositive program gives:

$$\sup\{\langle J, X\rangle : \ \langle A+I, X\rangle = 1, \ X \in COP\} \leq$$

$$\leq \inf\{y : \ y(A+I) - J \in CP\} \leq \alpha.$$

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Now let ξ be incidence vector of a stable set of size α. The matrix $\frac{1}{\alpha}\xi\xi^T$ is feasible for the first problem. Therefore

$$\alpha \leq \sup\{\ldots\} \leq \inf\{\ldots\} \leq \alpha.$$

This shows that equality holds throughout and sup and inf are attained.
The recent proof of this result by DeKlerk and Pasechnik does not make explicit use of the Motzkin Strauss Theorem.

Connections to theta function

Theta function (Lovasz (1979)):

$$\vartheta(G) = \max\{\langle J, X \rangle : x_{ij} = 0 \ ij \in E, \text{tr}(X) = 1, X \succeq 0\} \geq \alpha(G).$$

Motivation: If ξ characteristic vector of stable set, then $\frac{1}{\xi^T \xi} \xi \xi^T$ is feasible for above SDP.

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Schrijver (1979) improvement: include $X \geq 0$
In this case we can add up the constraints $x_{ij} = 0$ and get

$$\vartheta'(G) = \max\{\langle J, X\rangle : \langle A, X\rangle = 0, \mathrm{tr}(X) = 1, X \geq 0, X \succeq 0\}.$$

($A \ldots$ adjacency matrix). We have $\vartheta(G) \geq \vartheta'(G) \geq \alpha(G)$.

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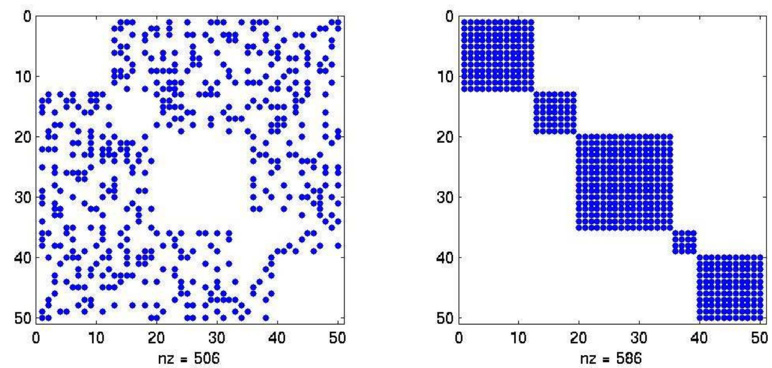
($A \ldots$ adjacency matrix). We have $\vartheta(G) \geq \vartheta'(G) \geq \alpha(G)$.
Replacing the cone $X \geq 0, X \succeq 0$ by $X \in COP$ gives $\alpha(G)$, see before.

Graph Coloring



Adjacency matrix A of a graph (left), associated partitioning (right). The graph can be colored with 5 colors.

- M is k-partition matrix if $\exists P \in \Pi$ such that $P^T M P$ is direct sum of k all-ones blocks.
- Number of colors = number of all-ones blocks = rank of M.

Chromatic number

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- Number of colors = number of all-ones blocks = rank of M.

Therefore chromatic number $\chi(G)$ of graph G can be defined as follows:

$$\chi(G) = \min\{rank(M) : M \text{ is partition matrix}, m_{ij} = 0 \; ij \in E(G)\}.$$

We need a 'better' description of k-partition matrices.

Lemma: M is partition matrix if and only if

$$M = M^T, \; m_{ij} \in \{0, 1\}, (tM - J \succeq 0 \;\Leftrightarrow\; t \geq rank(M)).$$

Proof of Lemma

Proof:

$\Rightarrow$: Nonzero principal minor of $tM - J$ has form

$$tI_s - J_s$$

and $s \leq rank(M)$. Hence $tM - J \succeq 0$ iff $t \geq rank(M)$.

$\Leftarrow$: $t \neq 0$, therefore $m_{ii} = 1$ (so each vertex in one color class). We also have $M \succeq 0$.

$m_{ij} = m_{jk} = 1$ implies $m_{ik} = 1$ because $\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} \not\succeq 0.$

Therefore M is direct sum of all-ones blocks.

Chromatic number

Hence

$\chi(G) = \min\{rank(M) : M$ is partition matrix $, m_{ij} = 0\, ij \in E\} =$

$$\min\{t : M = M^T, m_{ij} \in \{0,1\}, m_{ij} = 0 \forall ij \in E, tM - J \succeq 0\},$$

using the previous lemma.

Leaving out $m_{ij} \in \{0,1\}$ gives SDP lower bound:

$\chi(G) \geq \min\{t : Y - J \succeq 0,\ y_{ii} = t\, \forall i,\ y_{ij} = 0\, ij \in E(G)\} = \vartheta(G).$

This gives the second inequality in the Lovasz sandwich theorem, Lovasz (1979):

$$\omega(G) \leq \vartheta(G) \leq \chi(G).$$

Copositive strengthening

$\chi(G) \geq \min\{t : Y - J \succeq 0,\ y_{ii} = t\ \forall i,\ y_{ij} = 0\ ij \in E\} = \vartheta(G)$.
Note that Y can be interpreted as tM, where M is partition matrix. By construction, we also have $M \in COP$.
Hence we get the following strengthening

$$t'(G) = \min\{t : Y - J \succeq 0, Y \in COP, y_{ii} = t\ \forall i,\ y_{ij} = 0\ ij \in E\}$$

Dukanovic and R. (2006) show that t' is equal to the fractional chromatic number $\chi_f(G)$ of G.

$$\chi(G) \geq \chi_f(G) = t'(G) \geq \vartheta(G)$$

Gvozdenovic and Laurent (2007) show that (unless P=NP), there is no polynomially computable number between $\chi(G)$ and $\chi_f(G)$.

A general copositive modeling theorem

Burer (2007) shows the following general result for the power of copositive programming:
The optimal values of P and C are equal: opt(P) = opt(C)

$$(P) \qquad \min x^T Q x + c^T x$$

$$a_i^T x = b_i,\ x \geq 0,\ x_i \in \{0,1\}\ \forall i \leq m.$$

Here $x \in \mathbb{R}^n$ and $m \leq n$.

$$(C) \qquad \min \mathrm{tr}(QX) + c^T x,\ \text{s.t. } a_i^T x = b_i,$$

$$a_i^T X a_i = b_i^2,\ X_{ii} = x_i\ \forall i \leq m,\ \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in COP$$

Overview

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- Relaxations based on CP
- Heuristics based on CP

Approximating COP

We have now seen the power of copositive programming.

Since optimizing over CP is NP-Hard, it makes sense to get approximations of CP or COP.

• To get relaxations, we need supersets of COP, or inner approximations of CP (and work on the dual cone). The Parrilo hierarchy uses Sum of Squares and provides such an outer approximation of COP (dual viewpiont!).

• We can also consider inner approximations of COP. This can be viewed as a method to generate feasible solutions of combinatorial optimization problems (primal heuristic!).

Relaxations

Inner approximation of CP.

$$CP := \{M : x^T M x \geq 0 \ \forall x \geq 0\}$$

Parrilo (2000) and DeKlerk, Pasechnik (2002) use the following idea to approximate CP from inside:

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

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.

Parrilo hierarchy (2)

Parrilo characterizes SOS for $r = 0, 1$:

$P_0(x)$ is SOS iff $M = P + N$, where $P \succeq 0$ and $N \geq 0$.

$P_1(x)$ is SOS iff $\exists M_1, \dots, M_n$ such that

$$M - M_i \succeq 0$$

$$(M_i)_{ii} = 0 \; \forall i \quad (M_i)_{jj} + 2(M_j)_{ij} = 0 \; \forall i \neq j$$

$$(M_i)_{jk} + (M_j)_{ik} + (M_k)_{ij} \geq 0 \; \forall i < j < k$$

The resulting relaxations are SDP. But the $r = 1$ relaxation involves n matrices and n SDP constraints to certify SOS. This is computationally challenging.

Computational comparison

We consider Hamming graphs and compare the P_0 and the P_1 relaxation of the chromatic number.

graph	n	$r = 0$	$r = 1$	χ
H(7,6)	128	53.33	63.9	64
H(8,6)	256	85.33	127.9	128
H(9,4)	512	51.19	53.9	
H(10,8)	1024	383.99	511.9	512
H(12,4)	4096	211.86	255.5	

Using the automorphism structure of Hamming graphs, the general certificate for $r = 1$ reduces to one additional matrix and one additional SDP constraint. (Computation time: a few minutes!) (see Dukanovic, R.: Math Prog (2008))

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Inner approximations of COP

We consider

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

Remember: COP= $\{X : X = VV^T,\ V \geq 0\}$.

Some previous work by:
• Bomze, DeKlerk, Nesterov, Pasechnik, others:
Get stable sets by approximating COP formulation of the stable set problem using optimization of quadratic over standard simplex, or other local methods.

Incremental version

A general feasible descent approach:
Let $X = VV^T$ with $V \geq 0$ be feasible. Consider the regularized, and convex descent step problem:

$$\min \epsilon \langle C, \Delta X \rangle + (1-\epsilon)\|\Delta X\|^2,$$

$$\text{such that } A(\Delta X) = 0, \quad X + \Delta X \in COP.$$

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For small $\epsilon > 0$ we approach the true optimal solution, because we follow the continuous steepest descent path, projected onto COP.

Unfortunately, this problem is still not tractable. We approximate it by working in the V-space instead of the X-space.

Incremental version: V-space

$$X^+ = (V + \Delta V)(V + \Delta V)^T \text{ hence },$$

$$X = VV^T$$

$$\Delta X = \Delta X(\Delta V) = V\Delta V^T + \Delta V V^T + (\Delta V)(\Delta V^T).$$

Now linearize and make sure ΔV is small.

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$$\Delta X = \Delta X(\Delta V) = V\Delta V^T + \Delta V V^T + (\Delta V)(\Delta V^T).$$

Now linearize and make sure ΔV is small. We get

$$\min \epsilon \langle 2CV, \Delta V\rangle + (1-\epsilon)\|\Delta V\|^2 \text{ such that}$$

$$\langle 2A_i, \Delta V\rangle = b_i - \langle A_i V, V\rangle \ \ \forall i,$$

$$V + \Delta V \geq 0$$

This is convex approximation of nonconvex version in $\Delta X(\Delta V)$.

Correcting the linearization

The linearization obtained by replacing $\Delta X(\Delta V)$ with $V\Delta V^T + \Delta V V^T$ introduces an error both in the cost function and in the constraints $A(X) = b$.

We therefore include corrector iterations of the form

$$\Delta V = \Delta V_{old} + \Delta V_{corr}$$

before actually updating $V \leftarrow V + \Delta V$.

Convex quadratic subproblem

The convex subproblem is of the following form, after appropriate redefinition of data and variables $x = vec(V + \Delta V), \ldots$.

$$\min c^T x + \rho x^T x \text{ such that } Rx = r, \; x \geq 0.$$

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If V is $n \times k$ (k columns generating V), x if of dimension nk and there are m equations.

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If V is $n \times k$ (k columns generating V), x if of dimension nk and there are m equations.
Since Hessian of cost function is identity matrix, this problem can be solved efficiently using interior-point methods. (convex quadratic with sign constraints and linear equations)

Main effort is solving a linear system of order m, essentially independent of n and k.

Test data sets

COP problems coming from formulations of NP-hard problems are too difficult (Stable Set, Coloring, Quadratic Assignment) to test new algorithms.

Would like to have:

Data (A, b, C) and (X, y, Z) such that
- (X, y, Z) is optimal for primal and dual (no duality gap).
- COP is nontrivial (optimum not given by optimizing over semidefiniteness plus nonnegativity)
- generate instances of varying size both in n and m.

Hard part: Z provably copositive !!

A COP generator

Basic idea: Let G be a graph, with $Q_G = A + I$, and (X_G, y_G, Z_G) be optimal solution of

$$\omega(G) = \max\langle J, X\rangle \text{ such that } \langle Q_G, X\rangle = 1,\ X \in COP$$

$$= \min y \text{ such that } yQ_G - J \in CP.$$

We further assume:
• $G = H * K$ (strong graph product of H and K).
• K is perfect and $H = C_5$ (or some other graph with known clique number and $\omega(G) < \vartheta'(G)$).

This implies:
• $\omega(G) = \omega(H)\omega(K)$ (same for ϑ')
• Max cliques in G through Kronecker products from H, K.

COP generator (2)

Then we have:

- $y_G := \omega(H)\omega(K)$ implies $Z_G = y_G Q_G - J \in CP$.
- Let X_H and X_K convex combinations of outer products of characteristic vectors of max cliques in H and K. This implies that $X_G = X_H \otimes X_K \in COP$ is primal optimal.
- Select m and Matrix A of size $m \times n^2$ and set $b = A(X_G)$.
- Set $C := Z_G - A^T(y_G)$.

This implies that (X_G, y_G, Z_G) is optimal for the data set A, b, C and that there is no duality gap, and the problem is nontrivial, because of $\omega(G) < \vartheta'(G)$. Therefore

$$\min\{\ldots, X \in COP\} > \min\{\ldots, X \in PSD \cap N\}$$

Computational results

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

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

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 10^{-5}
60	120	-266.99	-266.48	4 10^{-5}
70	140	-158.74	-157.55	3 10^{-5}
80	160	-703.75	-701.68	5 10^{-5}
100	100	-659.65	-655.20	8 10^{-5}

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

Some experiments with Stable Set

$$\max \langle J, X \rangle \text{ such that } \mathrm{tr}(X) = 1, \; \mathrm{tr}(A_G X) = 0, \; X \in COP$$

Only two equations but many local optima. We consider a selection of graphs from the DIMACS collection. Computation times in the order of a few minutes.

name	n	ω	clique found
keller4	171	11	9
brock200-4	200	17	14
c-fat200-1	200	12	12
c-fat200-5	200	58	58
brock400-1	400	27	24
p-hat500-1	500	9	8

Last Slide

We have seen the power of copositivity.

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.

The number of columns of V does not need to be larger than $\binom{n+1}{2}$, but for practical purposes, this is too large.

Further technical details in a forthcoming paper by I. Bomze, F. Jarre and F. R.: Quadratic factorization heuristics for copositive programming, technical report, (2008).