Separating Doubly Nonnegative and Completely Positive Matrices

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CP and DNN matrices

Let $\mathcal{S}_n$ denote the set of $n \times n$ real symmetric matrices, $\mathcal{S}_n^+$ denote the cone of $n \times n$ real symmetric positive semidefinite matrices and $\mathcal{N}_n$ denote the cone of symmetric nonnegative $n \times n$ matrices.

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- Dual of $\mathcal{C}_n$ is the cone of $n \times n$ copositive matrices, $\mathcal{C}_n^* = \{X \in \mathcal{S}_n \mid y^T X y \geq 0 \;\forall\, y \in \Re_n^+\}$.

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Clear that

$$\mathcal{C}_n \subseteq \mathcal{D}_n, \qquad \mathcal{D}_n^* = \mathcal{S}_n^+ + \mathcal{N}_n \subseteq \mathcal{C}_n^*,$$

and these inclusions are in fact strict for $n > 4$.

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- $\mathcal{D}_n$ is a tractable relaxation of $\mathcal{C}_n$. Expect that solution of relaxed problem will be $X \in \mathcal{D}_n \setminus \mathcal{C}_n$.
- Note that least n where problem occurs is $n = 5$.

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The main result on CP graphs is the following:

Proposition 1. [KB93] *An undirected graph on n vertices is a CP graph if and only if it contains no odd cycle of length 5 or greater.*

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- Extreme rays of $\mathcal{D}_5$ are either rank-one matrices in $\mathcal{C}_5$, or rank-three "extremely bad" matrices where $G(X)$ is a 5-cycle (every vertex in $G(X)$ has degree two).
- Any such extremely bad matrix can be separated from $\mathcal{C}_5$ by a transformation of the Horn matrix

$$H := \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix} \in \mathcal{C}_5^* \setminus \mathcal{D}_5^*.$$

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An even more general separation procedure that applies to *any* $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ is described in [BD10]. In this talk we will describe the procedure from [DA10] for $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$, $X \not> 0$, and its generalization to larger matrices having block structure.

A separation procedure for the 5×5 case

Assume that $X \in \mathcal{D}_5$, $X \not\succeq 0$. After a symmetric permutation and diagonal scaling, X may be assumed to have the form

$$X = \begin{pmatrix} X_{11} & \alpha_1 & \alpha_2 \\ \alpha_1^T & 1 & 0 \\ \alpha_2^T & 0 & 1 \end{pmatrix}, \tag{1}$$

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Theorem 1. [BX04, Theorem 2.1] *Let $X \in \mathcal{D}_5$ have the form (1). Then $X \in \mathcal{C}_5$ if and only if there are matrices A_{11} and A_{22} such that $X_{11} = A_{11} + A_{22}$, and*

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In [BX04], Theorem 1 is utilized only as a proof mechanism, but we now show that it has algorithmic consequences as well.

Theorem 2. *Assume that* $X \in \mathcal{D}_5$ *has the form* (1). *Then* $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ *if and only if there is a matrix*

$$V = \begin{pmatrix} V_{11} & \beta_1 & \beta_2 \\ \beta_1^T & \gamma_1 & 0 \\ \beta_2^T & 0 & \gamma_2 \end{pmatrix} \quad \textit{such that} \quad \begin{pmatrix} V_{11} & \beta_i \\ \beta_i^T & \gamma_i \end{pmatrix} \in \mathcal{D}_4^*, \quad i = 1, 2,$$

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- However cannot conclude that $V \in \mathcal{C}_5^*$ because $V \bullet \tilde{X} \geq 0$ only holds for $\tilde{X}$ of the form (1), in particular, $\tilde{x}_{45} = 0$.
- Fortunately, by [HJR05, Theorem 1], V can easily be "completed" to obtain a copositive matrix that still separates X from $\mathcal{C}_5$.

Theorem 3. *Suppose that* $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ *has the form* (1), *and* V *satisfies the conditions of Theorem 2. Define*

$$V(s) = \begin{pmatrix} V_{11} & \beta_1 & \beta_2 \\ \beta_1^T & \gamma_1 & s \\ \beta_2^T & s & \gamma_2 \end{pmatrix}.$$

Then $V(s) \bullet X < 0$ *for any* s, *and* $V(s) \in \mathcal{C}_5^*$ *for* $s \geq \sqrt{\gamma_1 \gamma_2}$.

Separation for larger matrices with block structure

Procedure for 5 case where $X \not\succeq 0$ can be generalized to larger matrices with block structure. Assume X has the form

$$X = \begin{pmatrix} X_{11} & X_{12} & X_{13} & \dots & X_{1k} \\ X_{12}^T & X_{22} & 0 & \dots & 0 \\ X_{13}^T & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ X_{1k}^T & 0 & \dots & 0 & X_{kk} \end{pmatrix}, \tag{2}$$

where $k \geq 3$, each X_{ii} is an $n_i \times n_i$ matrix, and $\sum_{i=1}^{k} n_i = n$.

Lemma 1. *Suppose that $X \in \mathcal{D}_n$ has the form (2), $k \geq 3$, and let*

$$X^i = \begin{pmatrix} X_{11} & X_{1i} \\ X_{1i}^T & X_{ii} \end{pmatrix}, i = 2, \ldots, k.$$

Then $X \in \mathcal{C}_n$ if and only if there are matrices A_{ii}, $i = 2, \ldots, k$ such that $\sum_{i=2}^k A_{ii} = X_{11}$, and

$$\begin{pmatrix} A_{ii} & X_{1i} \\ X_{1i}^T & X_{ii} \end{pmatrix} \in \mathcal{C}_{n_1+n_i}, \quad i = 2, \ldots, k.$$

Moreover, if $G(X^i)$ is a CP graph for each $i = 2, \ldots, k$, then the above statement remains true with $\mathcal{C}_{n_1+n_i}$ replaced by $\mathcal{D}_{n_1+n_i}$.

Theorem 4. *Suppose that* $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ *has the form* (2), *where* $G(X^i)$ *is a CP graph,* $i = 2, \ldots, k$. *Then there is a matrix* V, *also of the form* (2), *such that*

$$\begin{pmatrix} V_{11} & V_{1i} \\ V_{1i}^T & V_{ii} \end{pmatrix} \in \mathcal{D}^*_{n_1+n_i}, \quad i = 2, \ldots, k,$$

and $V \bullet X < 0$. *Moreover, if* $\gamma_i = \mathrm{diag}(\mathrm{Diag}(V_{ii})^{.5})$, *then the matrix*

$$\tilde{V} = \begin{pmatrix} V_{11} & \ldots & V_{1k} \\ \vdots & \ddots & \vdots \\ V_{1k}^T & \ldots & V_{kk} \end{pmatrix},$$

where $V_{ij} = \gamma_i \gamma_j^T$, $2 \le i \ne j \le k$, *has* $\tilde{V} \in \mathcal{C}_n^*$ *and* $\tilde{V} \bullet X = V \bullet X < 0$.

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- Theorem 4 may provide a cut separating a given $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ even when the sufficient conditions for generating such a cut are not satisfied. In particular, a cut may be found even when the condition that X^i is a CP graph for each i is not satisfied.

A second case where block structure can be used to generate cuts for a matrix $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ is when X has the form

$$X = \begin{pmatrix} I & X_{12} & X_{13} & \dots & X_{1k} \\ X_{12}^T & I & X_{23} & \dots & X_{2k} \\ X_{13}^T & X_{23}^T & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & X_{(k-1)k} \\ X_{1k}^T & X_{2k}^T & \dots & X_{(k-1)k}^T & I \end{pmatrix}, \tag{3}$$

where $k \geq 2$, each X_{ij} is an $n_i \times n_j$ matrix, and $\sum_{i=1}^k n_i = n$. The structure in (3) corresponds to a partitioning of the vertices $\{1, 2, \dots, n\}$ into k stable sets in $G(X)$, of size $n_1, \dots, n_k$ (note that $n_i = 1$ is allowed).

Applications

Example 1: Consider the box-constrained QP problem

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To describe a CP-formulation of QPB, define matrices

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By the result of [Bur09], QPB can then be written in the form

$$\begin{array}{lll}(\text{QPB}_{\text{CP}}) & \max & Q \bullet X + c^T x \\ & \text{s.t.} & x + s = e, \quad \text{Diag}(X + 2Z + S) = e, \\ & & Y^+ \in \mathcal{C}_{2n+1}.\end{array}$$

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- Constraints from Boolean Quadric Polytope (BQP) are valid for off-diagonal components of X [BL09]. For $n = 3$, BQP is completely determined by triangle inequalities and RLT constraints. However, can still be a gap when using SDP+RLT+TRI relaxation.

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- Constraints from Boolean Quadric Polytope (BQP) are valid for off-diagonal components of X [BL09]. For $n = 3$, BQP is completely determined by triangle inequalities and RLT constraints. However, can still be a gap when using SDP+RLT+TRI relaxation.
- Example from [BL09] with $n = 3$ has optimal value for QPB of 1.0, value for SDP+RLT+TRI relaxation of 1.093. Solution matrix Y^+ has 5×5 principal submatrix that is *not* strictly positive, and is *not* CP. Can obtain cut from Theorem 3, re-solve problem, and repeat.

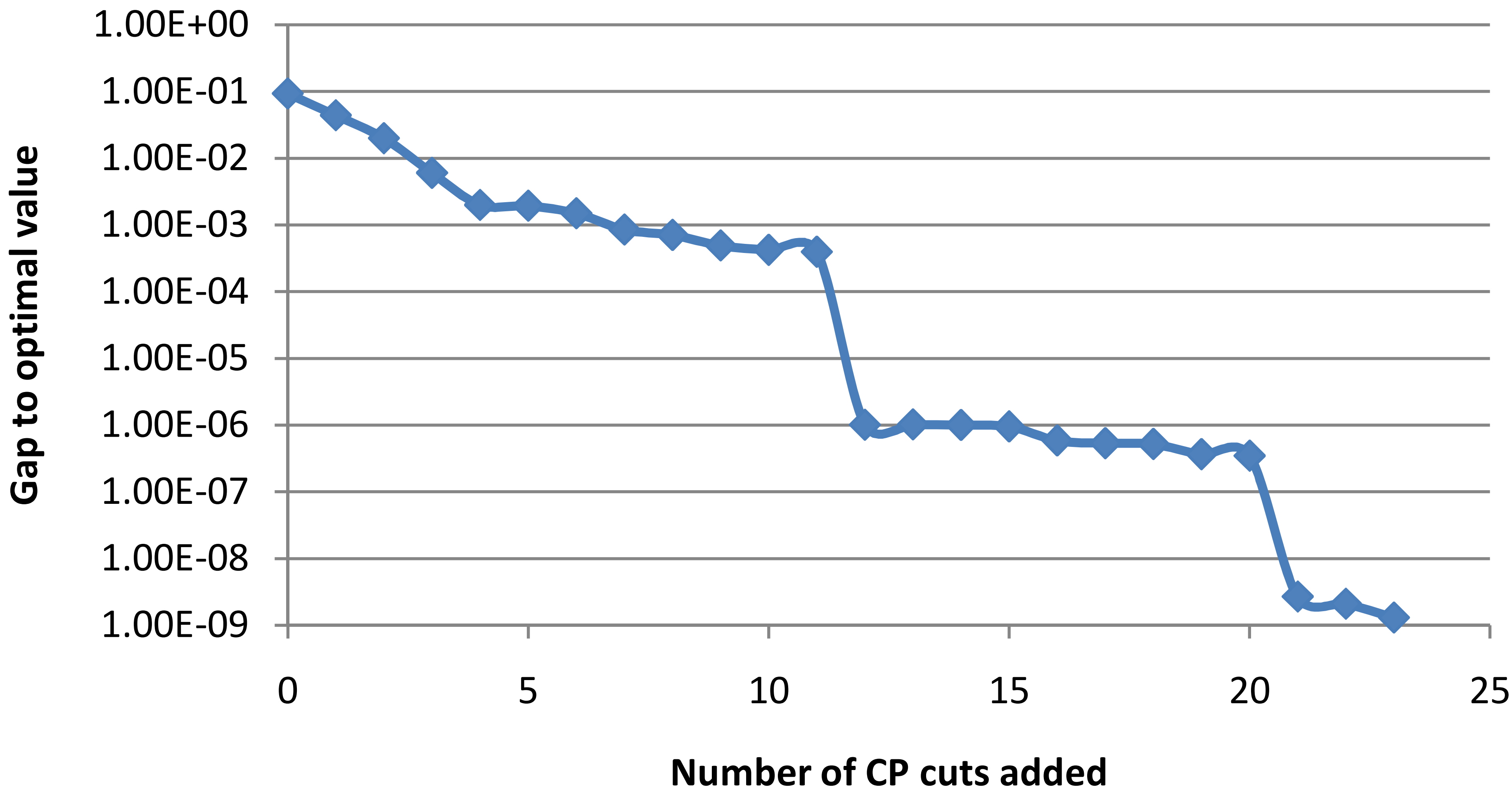

Figure 1: Gap to optimal value for Burer-Letchford QPB problem ($n = 3$)

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Relaxing $\mathcal{C}_n$ to $\mathcal{D}_n$ results in the Lovász-Schrijver bound

$$(\vartheta')^{-1} = \min\left\{(I + A) \bullet X : ee^T \bullet X = 1, X \in \mathcal{D}_n\right\}. \tag{5}$$

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- Using the cone $\mathcal{K}_{12}^{1}$ to approximate the dual of (4) provides no improvement [BdK02].
- For the solution matrix $X \in \mathcal{D}_{12}$ from (5), cannot find cut based on first block structure (2). However *can* find a cut based on (3). Adding this cut and re-solving, gap to $1/\alpha = \frac{1}{3}$ is approximately 2×10^{-8}.

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