CP-factorization via Orthogonality Constrained Problem

Zhijian Lai, Akiko Yoshise

University of Tsukuba

August 24, 2020

Zhijian Lai, Akiko Yoshise (University of Tsukuba)

2 Existing Results on \mathcal{CP}_n

Our Approach: CP-factorization via Orthogonality Constrained Problem

- CP-factorization as a nonconvex feasibility problem Groetzner and Dür
- LogSumExp: Smooth Approximation to Min Function
- A curvilinear search method Wen and Yin

4 Numerical Results

2 Existing Results on \mathcal{CP}_n

3 Our Approach: CP-factorization via Orthogonality Constrained Problem

- CP-factorization as a nonconvex feasibility problem Groetzner and Dür
- LogSumExp: Smooth Approximation to Min Function
- A curvilinear search method Wen and Yin

4 Numerical Results

Background: Basic Concepts

Definition 1.1 c.f. [Abraham and Naomi, 2003]

• A matrix $A \in \mathbb{S}_n$ is called *completely positive* if there exists an entrywise nonnegative matrix $B \in \mathbb{R}^{n \times r}$ such that $A = BB^T$. Such B is called a *CP-factorization*.

2 $CP_n := \{BB^\top \in \mathbb{S}_n \mid B \text{ is a nonnegative matrix}\}$ denotes the *completely positive cone*.

Consider the matrix $A_1 \in \mathcal{CP}_3$ where $A_1 = BB^T$.

$$A_1 = \begin{pmatrix} 18 & 9 & 9 \\ 9 & 18 & 9 \\ 9 & 9 & 18 \end{pmatrix}, B = \begin{pmatrix} 4 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 4 \end{pmatrix}.$$

A counterexample

$$A_{2} = \begin{pmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 3 \end{pmatrix} \in \mathcal{S}_{5}^{+} \cap \mathcal{N}_{5} \backslash \mathcal{C}P_{5}.$$

Background: Application of \mathcal{CP}_n

Many nonconvex NP-hard quadratic and combinatorial optimizations have a linear program over CP_n . For example, *standard quadratic optimization*:

$$\min\left\{x^T M x \mid e^T x = 1, x \in \mathbb{R}^n_+\right\},\$$

can equivalently be written as

Standard quadratic optimization by CP_n [Bomze et al., 2000]

$$\min\left\{\langle M, X \rangle \mid \left\langle ee^T, X \right\rangle = 1, X \in \mathcal{CP}_n\right\},\$$

where $M \in S_n$ possibly indefinite, and e is the all ones vector.

An application of above is

Independence number α of a graph G by \mathcal{CP}_n [De Klerk and Pasechnik, 2002]

$$\alpha(G) = \max\left\{ \langle E, X \rangle \mid \langle A + I, X \rangle = 1, X \in \mathcal{CP}_n \right\},\$$

where A is the adjacency matrix of G and E is the all-ones matrix.

Checking membership in CP_n is NP-hard [Dickinson and Gijben, 2014].

RECALL: A matrix $A \in \mathbb{S}_n$ is called *completely positive* if there exists an entrywise nonnegative matrix $B \in \mathbb{R}^{n \times r}$ such that $A = BB^T$. Such B is called a *CP-factorization*.

Our Goal

Given $A \in \mathcal{CP}_n$, find a CP-factorization of A.

Many different methods to CP-factorization problem have studied before.

- Some work well for the matrices with specific property.
 —special sparse matrices [Dickinson and Dür, 2012], rational CP-factorization [Sikirić et al., 2020].
- Some work for all matrices but are numerically expensive. —[Nie, 2014], [Jarre and Schmallowsky, 2009], [Sponsel and Dür, 2014].

2 Existing Results on \mathcal{CP}_n

3 Our Approach: CP-factorization via Orthogonality Constrained Problem

- CP-factorization as a nonconvex feasibility problem Groetzner and Dür
- LogSumExp: Smooth Approximation to Min Function
- A curvilinear search method Wen and Yin

4 Numerical Results

Example 1.2 [Groetzner and Dür, 2020, Example 2.1.]

Consider the matrix $A \in \mathcal{CP}_3$ where $A = B_1 B_1^T = B_2 B_2^T = B_3 B_3^T$.

$$A = \left(\begin{array}{rrrr} 18 & 9 & 9\\ 9 & 18 & 9\\ 9 & 9 & 18 \end{array}\right)$$

Generally, one can have many CP-factorizations, even those numbers of columns differ.

$$B_1 := \begin{pmatrix} 4 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 4 \end{pmatrix}, \quad B_2 := \begin{pmatrix} 3 & 3 & 0 & 0 \\ 3 & 0 & 3 & 0 \\ 3 & 0 & 0 & 3 \end{pmatrix}, \quad B_3 := \begin{pmatrix} 3 & 3 & 0 \\ 3 & 0 & 3 \\ 0 & 3 & 3 \end{pmatrix}.$$

Definition 2.1 c.f. [Abraham and Naomi, 2003]

We define cp-rank of $A \in S_n$ as minimum of the number of columns for CP-factorization B, that is

$$cp(A) := \min_{B} \left\{ r \in \mathbb{N} | \exists B \in \mathbb{R}^{n \times r}, B \ge 0, A = BB^{T} \right\}.$$

Notice that $cp(A) = \infty$ if $A \notin CP_n$. Also define *cp-plus-rank* of $A \in S_n$, that is

$$\operatorname{cp}^+(A) := \min_{B} \left\{ r \in \mathbb{N} | \exists B \in \mathbb{R}^{n \times r}, B > 0, A = BB^T \right\}.$$

Sometimes, we need to distinguish the completely positive matrices in either interior or boundary of \mathcal{CP}^n .

Theorem 2.2 [Dickinson, 2010, Theorem 3.8] For $A \in S_n$, we have $A \in int (\mathcal{CP}^n) \iff cp^+(A) < \infty$ and rank(A) = n.

EL SQA

Existing Results on CP_n : Essential Lemma

Observation: If we have had a CP-factorization B of A with r columns, then we can easily get another CP-factorization \hat{B} of A with r' columns for every positive integer $r' \ge r$. For instance, let k := r' - r, then

$$\widehat{B} := [B, 0_{n \times k}] \ge 0$$
, and $\widehat{B}\widehat{B}^{\top} = BB^{\top} = A$.

Lemma 2.3

Suppose that $A \in \mathbb{S}_n$, $r \in \mathbb{N}$. Then

 $r \ge \operatorname{cp}(A) \iff A$ has a CP-factorization B with r columns.

Essential Lemma 2.4 [Xu, 2004, Lemma 1.]

Let \mathcal{O}_r denote the set of $r \times r$ orthogonal matrices. Suppose that $B, C \in \mathbb{R}^{n \times r}$. Then

$$BB^T = CC^T \iff \exists X \in \mathcal{O}_r \text{ such that } BX = C.$$

2 Existing Results on \mathcal{CP}_n

Our Approach: CP-factorization via Orthogonality Constrained Problem

- CP-factorization as a nonconvex feasibility problem Groetzner and Dür
- LogSumExp: Smooth Approximation to Min Function
- A curvilinear search method Wen and Yin

4 Numerical Results

ELE NOR

2 Existing Results on \mathcal{CP}_n

3 Our Approach: CP-factorization via Orthogonality Constrained Problem

- CP-factorization as a nonconvex feasibility problem Groetzner and Dür
- LogSumExp: Smooth Approximation to Min Function
- A curvilinear search method Wen and Yin

4 Numerical Results

ELE NOR

CP-factorization as a nonconvex feasibility problem

RECALL:

Lemma 2.3 $r \ge cp(A) \iff A$ has a CP-factorization with r columns.

Lemma 2.4 $BB^T = CC^T \iff \exists X \in \mathcal{O}_r \text{ such that } BX = C.$

• a "bad" factorization $B \not\geq 0$

 $A = BB^T$, but B not nonnegative. (spectral decomposition and zero appending to r) \downarrow a suitable orthogonal matrix $X \in \mathcal{O}_r$

2 a "good" factorization $BX \ge 0$

 $A = (BX)(BX)^T$, meanwhile BX nonnegative.

CP-factorization as a nonconvex feasibility problem [Groetzner and Dür, 2020]

find	X
s.t.	$BX \ge 0$
	$X \in \mathcal{O}_r$

where $r \ge cp(A)$, $B \in \mathbb{R}^{n \times r}$ is an arbitrary initial factorization $A = BB^T$ not nonnegative. From Lemma 2.3 and 2.4 we have $A \in \mathcal{CP}_n \iff (1)$ is feasible.

(1)

Our Approach

[Groetzner and Dür, 2020] applied the so-called alternating projection method to (1).

Our Approach to nonconvex feasibility problem (1) [L, 2020]

• We first establish the connection between (1) and (2):

- Introducing a differentiable objective approximation function for the sake of adapting the method below:

$$\min (BX)_{ij} \stackrel{\text{approximate}}{\longrightarrow} LSE_{\rho}(BX)$$

Adopting a state-of-the-art curvilinear search method, which aims to solve the general optimization with orthogonality constrains:

$$\min_{X \in \mathbb{R}^{n \times p}} \mathcal{F}(X), \text{ s.t. } X^T X = I,$$

where $\mathcal{F}(X) : \mathbb{R}^{n \times p} \to \mathbb{R}$ is a differentiable function.

2 Existing Results on \mathcal{CP}_n

Our Approach: CP-factorization via Orthogonality Constrained Problem
 CP-factorization as a nonconvex feasibility problem — Groetzner and Dür

- LogSumExp: Smooth Approximation to Min Function
- A curvilinear search method Wen and Yin

4 Numerical Results

ELE NOR

LogSumExp: Smooth Approximation to Min Function

The LogSumExp (LSE) function is given by $LSE_{\rho}(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$,

$$LSE_{\rho}(\mathbf{x}) = \frac{1}{\rho} \log \left(\sum_{i=1}^{n} \exp \left(\rho x_i \right) \right).$$

Lemma 3.1 — Basic properties of LSE

Suppose that $\rho < 0$, $\mathbf{x} \in \mathbb{R}^n$. The following results indicate that $LSE_{\rho}(\mathbf{x})$ nicely approximates the minimum function from below.

• For all
$$\mathbf{x} \in \mathbb{R}^n$$
, we have $\lim_{\rho \to -\infty} LSE_{\rho}(\mathbf{x}) = \min x_i$.

2 For all $\mathbf{x} \in \mathbb{R}^n$, we have

$$\min x_i + \frac{1}{\rho} \log(n) \le LSE_{\rho}(\mathbf{x}) < \min x_i,$$

i.e., the error item $\epsilon_{\mathbf{x}} := \min x_i - LSE_{\rho}(\mathbf{x})$ is in the interval $(0, -\frac{1}{\rho}\log(n)]$.

ELE SQC

LogSumExp: Smooth Approximation to Min Function

The LogSumExp (LSE) function is given by $LSE_{\rho}(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$,

$$LSE_{\rho}(\mathbf{x}) = \frac{1}{\rho} \log \left(\sum_{i=1}^{n} \exp \left(\rho x_i \right) \right).$$

Example 3.2: Values of $LSE_{\rho}(\mathbf{x})$

n=4	$\rho = -1$	$\rho = -2$	$\rho = -3$	$\rho = -10$
$\mathbf{x}_1 = [5, 2, 6, 3]^t$	1.6381	1.9353	1.9838	1.9999
$\mathbf{x}_2 = [2, 2, 2, 2]^t$	0.6137	1.3068	1.5379	1.8613
$\epsilon_{\rho} := -1/\rho log(n)$	1.3863	0.6931	0.4621	0.1387

We find that the less ρ is, the better approximation effects.

Lemma 3.3 — Basic properties of matrix LSE [L, 2020]

Suppose that $\rho < 0, B \in \mathbb{R}^{n \times r}$, matrix varible $X \in \mathbb{R}^{r \times r}$. The following results indicate that $LSE_{\rho}(BX) : \mathbb{R}^{r \times r} \to \mathbb{R}$ nicely approximates the min $(BX)_{ij}$ from below.

• For all
$$X \in \mathbb{R}^{r \times r}$$
, we have $\lim_{\rho \to -\infty} LSE_{\rho}(BX) = \min(BX)_{ij}$.

2 For all $X \in \mathbb{R}^{r \times r}$, we have

$$\min(BX)_{ij} + \frac{1}{\rho}\log(nr) \le LSE_{\rho}(BX) < \min(BX)_{ij},$$

i.e., the error item $\epsilon_X := \min(BX)_{ij} - LSE_{\rho}(BX)$ is in the interval $(0, -\frac{1}{\rho}\log(nr)]$.

LogSumExp: Smooth Approximation to Min Function

Approximate the problem (2) by problem (3):

$$\begin{array}{ll} \max & \min {(BX)_{ij}} \\ \text{s.t.} & X \in \mathcal{O}_r \end{array} \tag{2} \\ \begin{array}{ll} \max & LSE_{\rho}\left(BX\right) \\ \text{s.t.} & X \in \mathcal{O}_r \end{array} \tag{3}$$

Proposition 3.4 [L, 2020]

Let t resp. t_{ρ} denote global maximum of problem (2) resp. (3), and $\epsilon_{\rho} := -\frac{1}{\rho} \log(nr) > 0$ is maximum error of $LSE_{\rho}(BX)$. Then,

$$0 < t - t_{\rho} \le \epsilon_{\rho}.$$

Proposition 3.5 [L, 2020]

If problem (3) has a feasible solution X such that $LSE_{\rho}(BX) \ge 0$, then

- for the same X, $min (BX)_{ij} > 0$ for problem (2).
- **2** hence, we find a CP factorization $(BX)(BX)^T = A$ with BX > 0.

< ロ > < 同 > < 三 > < 三 > < 三 > < 三 > < 回 > < ○ < ○ </p>

2 Existing Results on \mathcal{CP}_n

3 Our Approach: CP-factorization via Orthogonality Constrained Problem

- CP-factorization as a nonconvex feasibility problem Groetzner and Dür
 LogSumExp: Smooth Approximation to Min Function
- A curvilinear search method Wen and Yin

4 Numerical Results

ELE NOR

A curvilinear search method

Attempting to optimize (3), we apply the famous curvilinear search method, proposed by Wen and Yin [Wen and Yin, 2013], for general optimization with orthogonality constrains:

$$\min_{X \in \mathbb{R}^{n \times p}} \mathcal{F}(X), \text{ s.t. } X^T X = I.$$

Let gradient $G := \mathcal{DF}(X) = \left(\frac{\partial \mathcal{F}(X)}{\partial X_{i,j}}\right)$. The Lagrangian function is $\mathcal{L}(X, \Lambda) = \mathcal{F}(X) - \frac{1}{2} \operatorname{tr} \left(\Lambda \left(X^T X - I\right)\right)$ where $\Lambda \in \mathcal{S}^n$ is lagrangian multiplier.

Lemma 3.5 — First-order optimality conditions [Wen and Yin, 2013, Lemma 1.]

• Suppose that X is a local minimizer of problem above. Then X satisfies the first-order optimality conditions $\mathcal{D}_X \mathcal{L}(X, \Lambda) = G - X G^T X = 0$ and $X^T X = I$ with the associated lagrangian multiplier $\Lambda = G^T X$.

Define

$$\nabla \mathcal{F}(X) := G - X G^T X \text{ and } A := G X^T - X G^T.$$

Then $\nabla \mathcal{F}(X) = AX$. Moreover, $\nabla \mathcal{F}(X) = 0$ if and only if A = 0.

Lemma 3.6 — Update scheme [Wen and Yin, 2013, Lemma 3.]

• X is a feasible point. Given any skew-symmetric matrix $W \in \mathbb{R}^{n \times n}$ (i.e. $W^T = -W$), the matrix $Y(\tau)$ defined below satisfies $Y(\tau)^T Y(\tau) = X^T X$ and Y(0) = X,

$$Y(\tau) = \left(I + \frac{\tau}{2}W\right)^{-1} \left(I - \frac{\tau}{2}W\right) X.$$

 $Y(\tau): \mathbb{R} \to \mathbb{R}^{n \times p}$ is a smooth curve.

2 If set $W = A := GX^T - XG^T$. Then $Y(\tau)$ is a descent curve at $\tau = 0$, that is

$$\mathcal{F}'_{\tau}(Y(0)) := \left. \frac{\partial \mathcal{F}(Y(\tau))}{\partial \tau} \right|_{\tau=0} = -\frac{1}{2} \|A\|_F^2.$$

Since $\nabla \mathcal{F}(X) = 0$ if and only if A = 0, as long as X is yet to be local minimizer, then $\mathcal{F}'_{\tau}(Y(0)) < 0$.

EL SQA

Algorithm 1: CP-factorization via Orthogonality Constrained Problem

Data: Given $A \in \mathcal{CP}_n$, r > cp(A). **Result:** An $n \times r$ CP-factorization of A. Initialization: Choose an initial decomposition $B \in \mathbb{R}^{n \times r}$ and starting point $X_0 \in \mathcal{O}_r$. Set $0 < \theta_1 < \theta_2 < 1, \rho < 0, \epsilon > 0, k \leftarrow 0$: while $\|\nabla \mathcal{F}(X_k)\| > \epsilon$ do Generate $G_k \leftarrow -B^T \frac{\partial LSE_{\rho}(BX_k)}{\partial (BX_k)}, A_k \leftarrow G_k X_k^T - X_k G_k^T, W_k \leftarrow A_k$; Find a step size $\tau_k > 0$ that satisfies the Armijo-Wolfe conditions: $\mathcal{F}\left(Y_{k}\left(\tau_{k}\right)\right) \leq \mathcal{F}\left(Y_{k}(0)\right) + \theta_{1}\tau_{k}\mathcal{F}_{\tau}'\left(Y_{k}(0)\right)$ $\mathcal{F}'_{\tau}\left(Y_k\left(\tau_k\right)\right) > \theta_2 \mathcal{F}'_{\tau}\left(Y_k(0)\right);$ Set $X_{k+1} \leftarrow Y_k(\tau_k), k \leftarrow k+1$;

end

The global convergence of local minimizer is guaranteed in [Wen and Yin, 2013, Theorem 2], that is $\lim_{k\to\infty} \|\nabla \mathcal{F}(X_k)\|_F = 0$.

Image: A matrix

2 Existing Results on \mathcal{CP}_n

3 Our Approach: CP-factorization via Orthogonality Constrained Problem

- CP-factorization as a nonconvex feasibility problem Groetzner and Dür
- LogSumExp: Smooth Approximation to Min Function
- A curvilinear search method Wen and Yin

4 Numerical Results

ELE NOR

Numerical Results

We investigate random instances were generated like [Groetzner and Dür, 2020, Section 7.7]¹.

Table: For every value of n and r, our approach has 100% success rate and is significantly faster than [Groetzner and Dür, 2020] even if our computer is very poor.

		Our Approach ² Intel Core i7-4770 3.40 GHz and 16GB Ram Very poor environment!		[Groetzner and Dür, 2020] 88 Intel Xenon ES-2699 cores (2.2 GHz each) and a total of 0.792 TB Ram	
n	r	av. success rate (%)	av. time (sec.)	av. success rate (%)	av. time (sec.)
50	51	100	0.06	1.1	504
50	151	100	0.27	100	0.9
100	151	100	0.42	100	9.8
100	301	100	1.41	100	4
150	201	100	0.89	83.3	42
200	301	100	2.31	90.9	47

¹Compute *C* by setting $C_{ij} := |B_{ij}|$ for all *i*, *j*, where *B* is a random $n \times k$ matrix based on Matlab command randn and finally we take $A = CC^T$ to be factorized. For randomly generated matrices *A* with several *n* and k = 2n. For $n \le 50$, we used 100 starting points, for n > 50, we used 10 starting points. In each case, we used a maximum of 5000 iterations per starting point. The numbers in columns 3 - 6 represent the average of 100 randomly generated instances. ²Some improvements in practice: Instead of Armijo-Wolfe conditions, we use well-known Barzilai-Borwein step. And a heuristic extension — decreasing of parameter ρ . Also we decide min $(BX_{k+1})_{ij} > 0$ as stopping condition.

Zhijian Lai, Akiko Yoshise (University of Tsukuba)

RIMSmeeting2020

Reference I

[Abraham and Naomi, 2003] Abraham, B. and Naomi, S.-m. (2003). *Completely positive matrices.* World Scientific.

[Bomze et al., 2015] Bomze, I. M., Dickinson, P. J., and Still, G. (2015). The structure of completely positive matrices according to their cp-rank and cp-plus-rank. *Linear algebra and its applications*, 482:191–206.

[Bomze et al., 2000] Bomze, I. M., Dür, M., De Klerk, E., Roos, C., Quist, A. J., and Terlaky, T. (2000). On copositive programming and standard quadratic optimization problems. *Journal of Global Optimization*, 18(4):301–320.

[De Klerk and Pasechnik, 2002] De Klerk, E. and Pasechnik, D. V. (2002). Approximation of the stability number of a graph via copositive programming. *SIAM Journal on Optimization*, 12(4):875–892.

[Dickinson, 2010] Dickinson, P. J. (2010).

An improved characterisation of the interior of the completely positive cone. *Electronic Journal of Linear Algebra*, 20(1):51.

[Dickinson and Dür, 2012] Dickinson, P. J. and Dür, M. (2012). Linear-time complete positivity detection and decomposition of sparse matrices. SIAM Journal on Matrix Analysis and Applications, 33(3):701–720.

Reference II

[Dickinson and Gijben, 2014] Dickinson, P. J. and Gijben, L. (2014).

On the computational complexity of membership problems for the completely positive cone and its dual. *Computational optimization and applications*, 57(2):403–415.

[Groetzner and Dür, 2020] Groetzner, P. and Dür, M. (2020). A factorization method for completely positive matrices. *Linear Algebra and its Applications*, 591:1–24.

[Jarre and Schmallowsky, 2009] Jarre, F. and Schmallowsky, K. (2009). On the computation of c* certificates. Journal of Global Optimization, 45(2):281.

[Nie, 2014] Nie, J. (2014).
 The a-truncated k-moment problem.
 Foundations of Computational Mathematics, 14(6):1243–1276.

[Sikirić et al., 2020] Sikirić, M. D., Schürmann, A., and Vallentin, F. (2020). A simplex algorithm for rational cp-factorization.

Mathematical Programming, pages 1–21.

[Sponsel and Dür, 2014] Sponsel, J. and Dür, M. (2014). Factorization and cutting planes for completely positive matrices by copositive projection. *Mathematical Programming*, 143(1-2):211–229.

- 4 母 ト 4 ヨ ト ヨ ヨ ち の Q ()

 [Wen and Yin, 2013] Wen, Z. and Yin, W. (2013).
 A feasible method for optimization with orthogonality constraints. Mathematical Programming, 142(1-2):397–434.

[Xu, 2004] Xu, C. (2004). Completely positive matrices. Linear algebra and its applications, 379:319–327.

-

A B A B A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 A
 A
 A
 A

ELE DOO

Improvement: BB step and Heuristic extension

In practice, parameter ρ is not as small as possible. Although a smaller ρ gives a much tighter approximation, the speed of convergence, however, often slows.

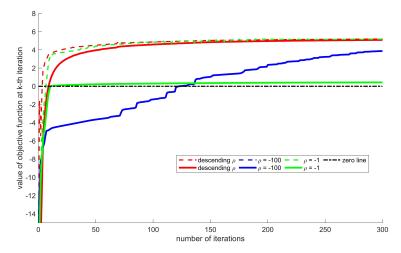


Figure: Value of objective function

RIMSmeeting2020

Lemma [Bomze et al., 2015, Theorem 4.1]

$$\text{For all } A \in \mathcal{CP}_n \text{, we have } \operatorname{cp}(A) \leq \operatorname{cp}_n := \left\{ \begin{array}{ll} n & \text{for } n \in \{2,3,4\} \\ \frac{1}{2}n(n+1) - 4 & \text{for } n \geq 5 \end{array} \right.$$

CP-factorization as a nonconvex feasibility problem [Groetzner and Dür, 2020]

$$\begin{array}{ll} \mbox{find} & X \\ 1 \ \mbox{s.t.} & BX \geq 0 \\ & X \in \mathcal{O}_r \end{array}$$

where $r \ge cp(A)$, $B \in \mathbb{R}^{n \times r}$ is an arbitrary initial factorization $A = BB^T$ not nonnegative. From Lemma 2.3 and 2.4 we have $A \in \mathcal{CP}_n \iff (1)$ is feasible.

ELE NOR

(4)

Proof of Lemma 3.1.

We first show an auxiliary result that is also applied for avoiding numerical overflow on computing value $LSE_{\rho}(\mathbf{x})$ in Algorithm 1. Given $\mathbf{x} \in \mathbb{R}^n$, we have

$$LSE_{\rho}(\mathbf{x}) = \frac{1}{\rho} \log\left(\sum_{i=1}^{n} \exp\left(\rho(x_i - c)\right)\right) + c$$

for all $c \in \mathbb{R}$. It follows from

$$\begin{aligned} \frac{1}{\rho} \log\left(\sum_{i=1}^{n} \exp\left(\rho(x_i - c)\right)\right) + c &= \frac{1}{\rho} \log\left(\exp(-\rho c)\sum_{i=1}^{n} \exp\left(\rho x_i\right)\right) + c \\ &= \frac{1}{\rho} \log\left(\exp(-\rho c)\right) + \frac{1}{\rho} \log\left(\sum_{i=1}^{n} \exp\left(\rho x_i\right)\right) + c \\ &= \frac{1}{\rho} \log\left(\sum_{i=1}^{n} \exp\left(\rho x_i\right)\right). \end{aligned}$$

31/36

In particular, if we let $c := \min x_i$, say x_j , then

$$LSE_{\rho}(\mathbf{x}) = \frac{1}{\rho} \log\left(\sum_{i=1}^{n} \exp\left(\rho(x_i - x_j)\right)\right) + x_j$$
$$= \frac{1}{\rho} \log\left(1 + \sum_{i \neq j}^{n} \exp\left(\rho(x_i - x_j)\right)\right) + x_j.$$
(5)

Since for any $i \neq j$, $\rho(x_i - x_j) \leq 0$ implies $1 < 1 + \sum_{i \neq j}^n \exp(\rho(x_i - x_j)) \leq n$, then the term $\log\left(1 + \sum_{i \neq j}^n \exp(\rho(x_i - x_j))\right)$ is bounded, thus $\lim_{\rho \to -\infty} LSE_{\rho}(\mathbf{x}) = x_j$.

2 Note that x_j denotes $\min x_i$. Due to the equation (5) and

$$\frac{1}{\rho}\log(n) \le \frac{1}{\rho}\log\left(1 + \sum_{i\neq j}^{n}\exp\left(\rho(x_i - x_j)\right)\right) < 0,$$

we have $\frac{1}{\rho}\log(n) \leq LSE_{\rho}(\mathbf{x}) - x_j < 0.$

It is easily seen that the gradient of $LSE_{\rho}(\mathbf{x})$ is the so-called famous "softmax function", and the individual components of it is

$$\left(\frac{\partial LSE_{\rho}(\mathbf{x})}{\partial x_{i}}\right) = \frac{\exp(\rho x_{i})}{\sum_{j=1}^{n} \exp(\rho x_{j})} = \exp\{\rho(x_{i} - LSE_{\rho}(\mathbf{x}))\}.$$
(6)

Notice that we do not use the form $\exp(-\rho LSE_{\rho}(\mathbf{x}))\exp(\rho x_i)$ due to numerical underflow and overflow in Algorithm 1. We only prove the next property to complete the last proof. We declare that for any fixed $\mathbf{x} \in \mathbb{R}^n$, if we regard $LSE_{\rho}(\mathbf{x})$ as a map of variable $\rho \in (-\infty, 0)$, denoted by $LSE_{\mathbf{x}}(\rho)$, then

$$\frac{\partial LSE_{\mathbf{x}}(\rho)}{\partial \rho} < 0$$

for all $\rho \in (-\infty, 0)$. For convenience, we replace $LSE_{\mathbf{x}}(\rho)$ or $LSE_{\rho}(\mathbf{x})$ sometimes with LSE at next procedure. We have

$$\begin{aligned} \frac{\partial LSE_{\mathbf{x}}(\rho)}{\partial \rho} &= -\frac{1}{\rho^2} \log\left(\sum_{i=1}^n \exp\left(\rho x_i\right)\right) + \frac{1}{\rho} \frac{1}{\sum_{i=1}^n \exp\left(\rho x_i\right)} \left(\sum_{i=1}^n x_i \exp\left(\rho x_i\right)\right) \\ &= \frac{1}{\rho} \{-LSE + \exp(-\rho LSE) \left(\sum_{i=1}^n x_i \exp\left(\rho x_i\right)\right)\} \\ &= \frac{1}{\rho} \{\sum_{i=1}^n x_i \exp\{\rho(x_i - LSE)\} - LSE\} \\ &= \frac{1}{\rho} \{\mathbf{x}^T \frac{\partial LSE}{\partial \mathbf{x}} - LSE\} < 0. \end{aligned}$$

For the last inequality, we observe from (6) that $\sum_{i=1}^{n} \frac{\partial LSE}{\partial x_i} = 1$ and every entry $\frac{\partial LSE}{\partial x_i} > 0$, hence the term $\mathbf{x}^T \frac{\partial LSE}{\partial \mathbf{x}}$ is a convex combination of all entries of \mathbf{x} , which implies that $\mathbf{x}^T \frac{\partial LSE}{\partial \mathbf{x}} \ge \min x_i > LSE$.

Proof of Proposition 3.4.

By definition of global maximum and Lemma 3.3 we have

$$LSE_{\rho}(BX^{*}) \le LSE_{\rho}(BX^{*}_{\rho}) = t_{\rho} < \min(BX^{*}_{\rho})_{ij} \le \min(BX^{*})_{ij} = t,$$

thus $0 < t - t_{\rho}$. And $t - t_{\rho} = \min(BX^*)_{ij} - LSE_{\rho}(BX^*_{\rho}) \leq \min(BX^*)_{ij} - LSE_{\rho}(BX^*) \leq \epsilon_{\rho}$.

312

Consider the so-called copositive program (primal problem)

$$\min\left\{\langle C, X \rangle \mid \langle A_i, X \rangle = b_i \ (i = 1, \dots, m), X \in \mathcal{COP}_n\right\},\tag{7}$$

where $COP_n \triangleq \{A \in S_n | x^T A x \ge 0 \text{ for all } x \in \mathbb{R}^n_+\}$ is the cone of so-called copositive matrices. Here S_n is the set of real symmetric $n \times n$ matrices, and the inner product of two matrices $\langle A, B \rangle := \operatorname{trace}(A^T B)$ as usual. The dual problem of (7) is

$$\max\left\{\sum_{i=1}^{m} b_i y_i \mid C - \sum_{i=1}^{m} y_i A_i \in \mathcal{CP}_n, \ y_i \in \mathbb{R}\right\},\tag{8}$$

where CP_n denotes the set of $n \times n$ completely positive matrices, which is a proper cone (i.e., closed, convex, pointed, and full dimensional) and also is the dual cone of COP_n , cf. [Abraham and Naomi, 2003].