日本オペレーションズ・リサーチ学会
2021年 春季研究発表会

Completely Positive Factorization via Orthogonality Constrained Problem

申請中　筑波大学大学院システム情報工学研究科　*頼志堅　RAI Shiken
01703540　筑波大学システム情報系　吉瀬章子　YOSHISE Akiko

1. Introduction

An $n \times n$ real symmetric matrix A is completely positive if for some $r \in \mathbb{N}$ there exists an entrywise nonnegative matrix $B \in \mathbb{R}^{n \times r}$ such that $A = BB^T$. In this case, such B is called a CP-factorization of A. This manuscript is devoted to obtaining a CP-factorization for a given completely positive matrix.

We propose a new numerical method, which stems from the fact that CP-factorization problem can be reformulated as a feasibility problem. Our method is remarkably faster than most of the other CP-factorization algorithms. It also is reliable for the most given completely positive matrices.

2. Applications of $\mathcal{CP}_n$

We refer to $\mathcal{CP}_n$ as the set of all $n \times n$ completely positive matrices. The dual of $\mathcal{CP}_n$ gives rise to the set of copositive matrices, defined if the quadratic form $x^T Ax$ is nonnegative for all nonnegative vectors x. We denote the set of all $n \times n$ copositive matrices by $\mathcal{COP}_n$. It is well known that $\mathcal{CP}_n$ and $\mathcal{COP}_n$ are convex cone, and dual mutually with inner product $\langle A, B\rangle := \operatorname{trace}(A^T B)$. Moreover, they are proper, i.e., (i) closed; (ii) if both $X, -X$ are contained, then $X = O$; (iii) nonempty interior.

In general, conic optimization is a subfield of convex optimization that studies minimization of a linear function over the proper cones, including the familiar positive orthant, positive semidefinite cone and the second-order cone. By the previous results, we can consider so-called copositive program as an example of conic optimization.

In particular, copositive program is closely related to many nonconvex NP-hard quadratic and combinatorial optimizations. As a simplest interpretation, consider the standard quadratic optimization: $\min \left\{ x^T Mx \mid e^T x = 1, x \in \mathbb{R}^n_+ \right\}$, here $M \in \mathcal{S}_n$ is possibly indefinite, and e denotes the all ones vector. Bomze et al. [1] were the first to establish the following equivalent reformulation,

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

3. CP-factorization Problem

Note that neither $\mathcal{COP}_n$ nor $\mathcal{CP}_n$ is self-dual. The primal-dual interior point methodology for conic optimization does not work as it is. Besides this fact, there are many fundamental open problems in copositive and completely positive cones. A typical one is the checking membership in $\mathcal{CP}_n$, which was shown to be NP-hard. In this paper, we focus on a fundamental problem of $\mathcal{CP}_n$—finding a CP-factorization for any given $A \in \mathcal{CP}_n$. This offers a natural criterion for whether a matrix is completely positive.

4. Preliminaries

Define cp-rank of $A \in \mathcal{CP}_n$ as the minimum of the number of columns for all CP-factorization of A, and write as $\operatorname{cp}(A)$. Many authors have studied the upper bound of cp-rank for all $A \in \mathcal{CP}_n$ in order n. For example, $\operatorname{cp}(A) \le n(n+1) - 4$ for $n \ge 2$. It is easy to see that $r \in \mathbb{N}$, $r \ge \operatorname{cp}(A)$ if and only if A has a CP-factorization B with r columns.

Assume that $A \in \mathcal{CP}_n, r \ge \operatorname{cp}(A), A = BB^T$ where initial decomposition $B \in \mathbb{R}^{n \times r}$ is possibly not nonnegative. The following lemma from [4] is very essential.

Lemma 4.1 *Let B, C are $n \times r$ matrices. Then $BB^T = CC^T$ if and only if there is an $r \times r$ orthogonal matrix X such that $BX = C$.*

Thus, finding a CP-factorization of A can then be formulated as the following feasibility problem:

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

where $\mathcal{O}_r$ denotes the set of $r \times r$ orthogonal matrices. Note that this idea was proposed by Groetzner and Dür [3].

5. The New Method

For solving (1), we first consider the following problem:

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

Apparently, (1) is feasible if and only if $\exists X \in \mathcal{O}_r$ such that $\min\,(BX)_{ij} \geq 0$. Our strategy for (2) is roughly as follows:

1. Introduce a differentiable approximation to replace the nonsmooth minimum function.
2. Utilize a state-of-the-art curvilinear search method, that aims to solve the general orthogonality constrained optimization.

5.1. Smooth Approximation—LSE

First, let us concentrate on some facts about the approximate function, namely LogSumExp, given by $LSE_\rho(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$,

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

which can approximate the minimum function as parameter $\rho \to -\infty$ by the following proposition.

Proposition 5.1 *Suppose $\rho < 0$, and $\min x_i$ is the minimum entry of $\mathbf{x}$. For all $\mathbf{x} \in \mathbb{R}^n$, we have*

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

2. $\lim\limits_{\rho \to -\infty} LSE_\rho(\mathbf{x}) = \min x_i$.

3. $\rho_2 < \rho_1 < 0$ *implies* $LSE_{\rho_1}(\mathbf{x}) < LSE_{\rho_2}(\mathbf{x})$.

In the end, we approximate (2) by (3):

$$\begin{array}{ll} \max & LSE_\rho\,(BX) \\ \text{s.t.} & X \in \mathcal{O}_r. \end{array} \tag{3}$$

And if t and t_ρ are global maximum of (2) and (3), respectively, we have $0 < t - t_\rho \leq -\frac{1}{\rho}\log(nr)$.

5.2. A Curvilinear Search Method

We attempt to optimize problem (3) for finding a feasible solution X such that $\min(BX)_{ij} \geq 0$. We apply the famous curvilinear search method proposed by Wen and Yin [2], which is designed for

$$\min_{X \in \mathbb{R}^{n \times p}} \mathcal{F}(X), \text{ s.t. } X^T X = I, \tag{4}$$

where $\mathcal{F}(X) : \mathbb{R}^{n \times p} \to \mathbb{R}$ is differentiable. The constraint set $X^T X = I$ is also called Stiefel manifold. (3) is completely the above structure.

We briefly review this method. On the Stiefel manifold, the curve starting from the current point can maintain the orthogonality with any step size. Simultaneously, as long as the current point is not a local minimizer, the objective value can always be reduced in a certain step size. The step size is prepared using the Armijo-Wolfe rule as in standard line search.

6. Conclusion

In this article, we proposed a new CP-factorization method. As we will explain in our presentation, a lot of numerical experiments shows that the new method is much faster than most of the other CP-factorization algorithms.

参考文献

[1] Bomze, Immanuel M., Mirjam Dür, Etienne De Klerk, Cornelis Roos, Arie J. Quist, and Tamás Terlaky. On copositive programming and standard quadratic optimization problems. *Journal of Global Optimization*, 18, no. 4 (2000): 301-320.

[2] Wen, Zaiwen, and Wotao Yin. A feasible method for optimization with orthogonality constraints. *Mathematical Programming*, 142, no. 1-2 (2013): 397-434.

[3] Groetzner, Patrick, and Mirjam Dür. A factorization method for completely positive matrices. *Linear Algebra and its Applications*, 591 (2020): 1-24.

[4] Xu, Changqing. Completely positive matrices. *Linear Algebra and its Applications*, 379 (2004): 319-327.