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COMPLETE POSITIVITY OVER THE RATIONALS

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ABSTRACT. A matrix A is called completely positive if $A = BB^T$, where the entries of B are nonnegative. A is called completely positive over the rationals, if in addition the entries of B are rational numbers. Consider a completely positive matrix A with rational entries. It is an open question whether every such A is completely positive over the rationals. We survey results that may be helpful in solving this question.

1. INTRODUCTION

A matrix A is called *completely positive* (CP) if it can be decomposed as $A = BB^T$, where B is a nonnegative matrix. Equivalently, $A = \sum_{i=1}^k \mathbf{b}_i \mathbf{b}_i^T$, where the \mathbf{b}_i 's are the columns of B, that is, A can be written as the sum of rank 1 completely positive matrices. The smallest number of rank 1 matrices in such a sum is called the *cp*-rank of A, and is denoted by cpr A. The $n \times n$ completely positive matrices form a closed convex cone, denoted by $C\mathcal{P}_n$. The interior of $C\mathcal{P}_n$ is

int
$$\mathcal{CP}_n = \{BB^T : \operatorname{rank} B = n \text{ and } B > 0\},\$$

see [13, Theorem 3.8]. A reference on CP matrices and the cp-rank is [6].

Combinatorial optimization problems which are NP-hard in general, can be written as linear programs in which the variables are CP matrices [10], see the surveys [15, 8]. This makes the study of CP matrices an interesting meeting point of the communities of linear algebraists and optimization researchers. This short paper was inspired by Prof. Ben-Israel's important contributions to both Optimization Theory and Matrix Theory.

The analysis of the complex problem of determining complete positivity suggests the study of the analogues of complete positivity and cp-rank over the rationals. A matrix A is called *completely positive over the rationals* (*CP over the rationals*) if it can be decomposed as $A = BB^T$, where the entries of B are nonnegative rational numbers. This concept was introduced in [5]. In this paper we study the following natural conjecture.

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Conjecture 1. Every rational completely positive matrix is completely positive over the rationals.

By definition, a matrix A is completely positive over the rationals if $A = \sum_{i=1}^{k} \mathbf{b}_i \mathbf{b}_i^T$, where the vectors \mathbf{b}_i are rational and nonnegative. An alternative approach is to say that A is completely positive over the rationals if it can be decomposed in the form

(1.1)
$$A = \sum_{i=1}^{m} d_i \mathbf{x}_i \mathbf{x}_i^T,$$

where each d_i is a nonnegative rational number and each \mathbf{x}_i is a nonnegative rational vector. That is,

(1.2)
$$A = XDX^T,$$

where $X = (\mathbf{x}_1 | \dots | \mathbf{x}_m)$ is a nonnegative rational matrix, and $D = \text{Diag}(d_1, \dots, d_m)$ is a diagonal nonnegative rational matrix.

These two approaches are equivalent: consider $\frac{p}{q}\mathbf{x}\mathbf{x}^{T}$ where p, q are positive integers and the vector \mathbf{x} is rational and nonnegative. Then according to Lagrange's four-square theorem there exist nonnegative integers s_1, \ldots, s_4 such that $pq = s_1^2 + s_2^2 + s_3^2 + s_4^2$, and we get

$$\frac{p}{q} \mathbf{x} \mathbf{x}^T = \frac{pq}{q^2} \mathbf{x} \mathbf{x}^T = \frac{s_1^2 + s_2^2 + s_3^2 + s_4^2}{q^2} \mathbf{x} \mathbf{x}^T = \sum_{i=1}^4 \left(\frac{s_i}{q} \mathbf{x}\right) \left(\frac{s_i}{q} \mathbf{x}\right)^T.$$

Note that the number of rank-one matrices needed in the decompositions $A = \sum \mathbf{b}_i \mathbf{b}_i^T$ and $A = \sum \mathbf{d}_i \mathbf{x}_i \mathbf{x}_i^T$ may differ by a factor of up to 4, as can be seen in the above construction. An explicit example is

$$A = \begin{pmatrix} 7 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot 7 \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}^{T} = \begin{pmatrix} 2 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}^{T},$$

where no smaller decomposition exists, since for any positive integer q, the number $7q^2$ cannot be represented as a sum of less than four squares. For the definition of the rational cp-rank, we prefer to work with rational decompositions of the form (1.1). That is, for a matrix A that is completely positive over the rationals, the rational cp-rank of A, rcpr A, is the minimal number of summands in (1.1) (i.e., the minimal number of columns of X in (1.2)). We refer to a decomposition in the form (1.1) as a rational cp-decomposition. Note that rank $A \leq \operatorname{cpr} A \leq \operatorname{rcpr} A$ for every matrix A which is CP over the rationals.

The following discussion may suggest that the truth of Conjecture 1 is not obvious. A matrix A is called *completely positive over the integers* if it can be decomposed as $A = BB^{T}$, where the entries of B are nonnegative integers. It has been recently shown in [20] that every 2×2 integral completely positive matrix is completely positive over the integers, but this is no longer true for matrices of order greater than 2. The matrices

$$\left(\begin{array}{rrrr} 1 & 1 & 1 \\ 1 & a & 0 \\ 1 & 0 & b \end{array}\right), \quad \text{with } a, b \text{ integers, } a \ge 2, b \ge 2$$

and

$$\begin{pmatrix} 2 & 3 & 1 \\ 3 & 5 & 3 \\ 1 & 3 & c \end{pmatrix}, \text{ with } c \text{ integer, } c \ge 5,$$

are integral and completely positive, but not completely positive over the integers, and hence the analogue of Conjecture 1 is not true for complete positivity over the integers. These examples are special cases of the following theorem.

Theorem 1.1 ([11]). For every graph G that is not a disjoint union of paths on two vertices and isolated vertices there exists an integral completely positive matrix that is not completely positive over the integers, whose graph is G. (For the definition of the graph of a matrix, see Section 3.)

Conjecture 1, however, is strongly supported by the following result of Dutour Sikirić, Schürmann and Vallentin [16].

Theorem 1.2 ([16]). Every rational matrix that lies in the interior of CP_n is completely positive over the rationals.

By this theorem, it remains to consider rational matrices on the boundary of \mathcal{CP}_n . In this paper we collect some results that may be helpful in this consideration. The rest of the paper is divided into three parts. In Section 2 we make some basic observations which are useful in the study of Conjecture 1. In Section 3 we survey results on necessary conditions and sufficient conditions for a symmetric nonnegative matrix to be completely positive, and we show that under these conditions, rational completely positive matrices are completely positive over the rationals. In Section 4 we give upper bounds for rcpr A and show that for $n \geq 3$ there exist $n \times n$ matrices A for which rcpr A > cpr A.

2. Rational complete positivity — basic tools

It is well known that if A is a rational positive semidefinite matrix, then the Cholesky algorithm can be used to obtain a decomposition $A = XDX^T$, where D is a nonnegative diagonal matrix, and both X and D are rational matrices. This obviously implies:

Observation 2.1. Let A be a rational completely positive matrix, and let $A = XDX^T$ be its Cholesky factorization. If X is nonnegative, then A is completely positive over the rationals and rcpr $A = \operatorname{rank} A$.

A related result is the following:

Observation 2.2. If a matrix of the form

$$A = \left(\begin{array}{cc} B & C^T \\ C & E \end{array}\right),$$

is positive semidefinite and rational and E is nonsingular, then both the Schur complement $A/E = B - C^T E^{-1}C$ and the matrix

$$\left(\begin{array}{cc} C^T E^{-1} C & C^T \\ C & E \end{array}\right)$$

are rational positive semidefinite matrices. If both are CP over the rationals, then A is also CP over the rationals.

More generally, this holds for the generalized Schur complement, when E is not necessarily nonsingular and the Moore-Penrose generalized inverse E^{\dagger} is used instead of E^{-1} . As A is positive semidefinite, C = EY. The matrix Y, whose columns are solutions to linear systems with rational coefficients, may be taken to be rational. Thus $C^{T}E^{\dagger}C = Y^{T}EE^{\dagger}EY = Y^{T}EY$ is rational. For details about the Moore-Penrose generalized inverse see [7].

Most of the basic tools used in the study of complete positivity (see [6, Section 2.1]) also hold in the rational case. In particular,

- If A_1, A_2 are CP over the rationals and d_1, d_2 are nonnegative rational numbers, then $A := d_1A_1 + d_2A_2$ is CP over the rationals.
- Let $A = A_1 \oplus A_2$. Then A has a rational cp-decomposition if and only if both A_1 and A_2 have such decompositions.
- Let P be a permutation matrix. Then A has a rational cp-decomposition if and only if the matrix $P^T A P$ has.

Also, the property of being completely positive over the rationals is invariant under diagonal scaling by a nonnegative rational diagonal matrix:

• Let *D* be a *rational* diagonal matrix with positive diagonal entries. Then *A* has a rational cp-decomposition if and only if the matrix *DAD* has.

In the study of (real) complete positivity, diagonal scaling is often used to conveniently replace a matrix A by a matrix DAD whose diagonal entries all equal 1. However, for a rational positive semidefinite matrix A, the matrix D used in this scaling is not necessarily rational, nor is it necessarily of the form \sqrt{dD} with a rational diagonal matrix D and a positive rational number d. Therefore, known results on complete positivity need to be carefully checked for validity in the rational case. The next three lemmas assert that some basic techniques carry over from (real) complete positivity to the rational case.

First, since the inverse of a nonsingular rational matrix is rational, it is easy to see that the following rational version of [6, Proposition 3.3] holds:

Lemma 2.3. Let A be a symmetric rational matrix and let S be a nonsingular rational matrix with S^{-1} nonnegative. If SAS^{T} is completely positive over the rationals, then A is completely positive over the rationals.

This, in turn, can be used to prove (exactly as in the real case) the following rational version of [6, Lemma 3.5] which is originally due to Loewy and Tam [21].

Lemma 2.4. Let A be a positive semidefinite and nonnegative rational matrix. Suppose that for some $1 \le p \ne q \le n$ the support of row p of A is not empty, and contained in the support of row q. Let

$$\mu = \min_{a_{pj} > 0} \frac{a_{qj}}{a_{pj}}.$$

Let S be an $n \times n$ rational matrix with all diagonal entries equal to 1, and all other entries zero except for $S_{ap} = -\mu$. Then we have:

- (a) SAS^T is rational, positive semidefinite and nonnegative, and rank $(SAS^T) = rank(A)$.
- (b) If $a_{ij} = 0$ for some $1 \le i, j \le n$, then $(SAS^T)_{ij} = 0$.
- (c) There is at least one additional zero entry in row q of SAS^T , compared to row q of A.

The following useful lemma is by Barioli [2], and the proof of its rational version follows the original proof exactly, using Observation 2.1 (see also [6, Lemma 2.1]):

Lemma 2.5. Let A be completely positive over the rationals, and let B be a rational positive semidefinite matrix which is zero except for a 2×2 principal submatrix. If A + B is nonnegative, then A + B is completely positive over the rationals.

3. Sufficient conditions for rational complete positivity

We start with a few definitions. Let A be an $n \times n$ symmetric nonnegative matrix. The *comparison matrix of* A is defined by

$$[M(A)]_{ij} = \begin{cases} a_{ij} & \text{if } i = j; \\ -a_{ij} & \text{if } i \neq j; \end{cases}$$

The graph of A, denoted by G(A), has n vertices and an edge between i and j if and only if $a_{ij} > 0$. The graph that consists of n-2 triangles sharing a common base is denoted by T_n . A graph G is *completely positive* if it does not have an odd cycle of length greater than 4. This means that each block of the graph is either bipartite, or a T_k , or has at most 4 vertices (recall that a block of a graph is a subgraph that has no cut vertex, which is maximal with respect to this property). In the following theorem we group together necessary conditions and sufficient conditions for a real matrix to be completely positive.

Theorem 3.1. Let A be a symmetric nonnegative matrix.

- (a) A sufficient condition for A to be completely positive is that M(A) is positive semidefinite. If G(A) is triangle free, then this sufficient condition is also necessary.
- (b) A necessary condition for A to be completely positive is that A is positive semidefinite. If G(A) is completely positive, then this necessary condition is also sufficient.

Part (a) was proved by Drew, Johnson and Loewy [14]. Part (b) was proved by Ando [1] and by Kogan and Berman [19]. The proof of Kogan and Berman is based on the proof for the case $n \leq 4$ in [23], on the proof for bipartite graphs [3], and on [4].

The proofs of the following results are similar to those for real completely positive matrices (see [6, Section 2.3]). We include these proofs to demonstrate how to bypass diagonal scaling by diagonal matrices which may not be rational.

Theorem 3.2. Let A be an $n \times n$ rational completely positive matrix. Then A is completely positive over the rationals in any of the following cases:

(a) rank
$$A \leq 2$$

(b)
$$n \le 3$$
,

- (c) n = 4,
- (d) A is diagonally dominant,
- (e) M(A) is positive semidefinite,
- (f) G(A) is triangle free,
- (g) $G(A) = T_n$,
- (h) G(A) is completely positive.
- Proof. (a) If rank(A) = 1, then A is completely positive over the rationals by Observation 2.1. If rank(A) = 2, then $A = BB^T$, where $B \ge 0$ has two columns [6, Theorem 3.1]. It is shown in [17] that here exists an orthogonal 2×2 matrix Q such that $BQ \ge 0$ and BQ has a row with only one positive entry, say row i. By permuting rows and columns of A if necessary, we may assume that i = 1. Then in the Cholesky decomposition $A = \sum_{i=1}^{2} \mathbf{y}_i \mathbf{y}_i^T$, we get that \mathbf{y}_1 is a multiple of the first column of BQ, and thus $(\mathbf{y}_1 \ \mathbf{y}_2) =$ $BQ \ge 0$. Since $\mathbf{y}_1 \mathbf{y}_1^T$ coincides with A in its first row and column, the Cholesky decomposition is a rational cp-decomposition.
 - (b) The case $n \leq 2$ follows from (a), so assume n = 3. It follows from Maxfield and Minc [23] (see also [6, Corollary 2.13]) that there exists a permutation P such that applying the Cholesky decomposition to the rational matrix PAP^T yields a cp-decomposition. This provides a rational decomposition of A due to Observation 2.1.
 - (c) If A has a zero diagonal entry, then the result follows from the case n = 3 in part (b). So suppose that all diagonal entries of A are positive.

If A has a zero off-diagonal entry, we may assume $a_{34} = 0$. Then A has the form

$$A = \left(\begin{array}{cc} B & C^T \\ C & D \end{array}\right),$$

where all blocks are 2×2 and D is a positive diagonal matrix. Let

$$A_1 = \begin{pmatrix} C^T D^{-1} C & C^T \\ C & D \end{pmatrix} \text{ and } A_2 = \begin{pmatrix} A/D & 0 \\ 0 & 0 \end{pmatrix}.$$

Then $A = A_1 + A_2$. Clearly, A_1 is nonnegative, rational and positive semidefinite, and A_2 is rational and positive semidefinite. Since rank $(A_1) = 2$, it follows from (a) that A_1 is completely positive over the rationals, and since A_2 is zero except for a 2×2 principal submatrix, the result follows from Lemma 2.5.

If A is positive, we define

$$\mu = \min_{1 \le j \le n} \frac{a_{1j}}{a_{2j}}.$$

Let S be a 4×4 rational matrix whose diagonal entries are all equal to 1, and whose off-diagonal entries all equal zero except for $s_{12} = -\mu$. Then by Lemma 2.4, SAS^T is a 4×4 matrix which is rational, nonnegative, positive semidefinite and has an off-diagonal zero entry, so by the previous case, SAS^T is completely positive over the rationals. Applying Lemma 2.3 concludes the proof.

(d) If A is diagonaly dominant, the known simple cp-decomposition dating back to Kaykobad [18] is a rational cp-decomposition: Let E_{ij} denote the symmetric matrix whose only nonzero entries are 1's in positions *ii*, *jj*, *ij* and *ji*. Then the decomposition is

$$A = \sum_{1 \le i < j \le n} a_{ij} E_{ij} + \operatorname{Diag}(\delta_1, \dots, \delta_n), \text{ where } \delta_i = a_{ii} - \sum_{\substack{j=1\\ j \ne i}}^n a_{ij} \ge 0.$$

(e) As in the real case, the proof of (e) is by showing that for some rational positive diagonal matrix D, the matrix DAD is diagonally dominant, which is equivalent to showing that DM(A)D is diagonally dominant. Let 1 denotes the vector of all ones.

If M(A) is nonsingular, then there exists a positive diagonal matrix D such that $M(A)D\mathbf{1} > \mathbf{0}$ (e.g., take $D = \text{Diag}(\mathbf{d})$, where \mathbf{d} is the positive eigenvector corresponding to the minimal eigenvalue of M(A)). By slightly perturbing the entries of D if necessary, we may choose D to be rational. This makes DM(A)D a rational strictly diagonally dominant matrix.

On the other hand, if M(A) is singular, then there exists a positive diagonal matrix D such that $DM(A)D\mathbf{1} = \mathbf{0}$. Since $D\mathbf{1}$ is a solution to the rational linear system $M(A)\mathbf{x} = \mathbf{0}$, D may be chosen to be rational. This makes DM(A)D a rational diagonally dominant singular matrix.

- (f) In a cp-factorization $A = BB^T$, $B \ge 0$, each column of B is supported by a clique in the triangle free graph G(A), and therefore has at most two positive entries. Construct a matrix X from B by reversing the sign of the second positive entry in each column whose support is of size 2. Then $XX^T = M(A)$, so M(A) is positive semidefinite. The result therefore follows from (e).
- (g) By applying a suitable permutation if necessary, we may assume that

$$A = \left(\begin{array}{cc} B & C^T \\ C & D \end{array}\right),$$

where D is an $(n-2) \times (n-2)$ rational positive diagonal matrix. Define

$$A_1 = \begin{pmatrix} C^T D^{-1} C & C^T \\ C & D \end{pmatrix} \text{ and } A_2 = \begin{pmatrix} B - C^T D^{-1} C & 0 \\ 0 & 0 \end{pmatrix}.$$

Then $A = A_1 + A_2$. Both A_1 and A_2 are rational positive semidefinite by Observation 2.2. The matrix A_1 is completely positive over the rationals by the following decomposition (which is its Cholesky decomposition):

$$A_1 = \begin{pmatrix} C^T D^{-1} \\ I \end{pmatrix} D \begin{pmatrix} C^T D^{-1} \\ I \end{pmatrix}^T.$$

The result then follows from Lemma 2.5.

(h) If $G(A) = G_1 \cup G_2$, where G_1 and G_2 share exactly one vertex, we may assume that

$$A = \left(\begin{array}{ccc} B & \mathbf{u} & 0\\ \mathbf{u}^T & c & \mathbf{w}^T\\ 0 & \mathbf{w} & E \end{array}\right).$$

n

By Observation 2.2 the matrices

$$A_1 = A/E = \begin{pmatrix} B & \mathbf{u} \\ \mathbf{u}^T & c - \mathbf{w}^T E \mathbf{w} \end{pmatrix} \text{ and } \begin{pmatrix} 0 & 0 & \mathbf{0}^T \\ 0 & \mathbf{w}^T E \mathbf{w} & \mathbf{w}^T \\ \mathbf{0} & \mathbf{w} & E \end{pmatrix}$$

are rational positive semidefinite, and they are nonnegative. The graph of A/E is G_1 , and the graph of $\begin{pmatrix} \mathbf{w}^T E \mathbf{w} & \mathbf{w}^T \\ \mathbf{w} & E \end{pmatrix}$ is G_2 . As G(A) is a completely positive graph, by Theorem 3.1(b) these matrices are completely positive. Thus A is a sum of rational completely positive matrices such that the graphs of their nonzero principal submatrices are the blocks of G(A). Since every block of a completely positive graph is either bipartite, or a T_k , or has at most 4 vertices, the result follows from (f), (g), and (c).

4. RATIONAL CP-RANK

In this section we discuss the rational cp-rank. Since the space of $n \times n$ rational symmetric matrices is an $\frac{1}{2}n(n+1)$ -dimensional linear space over the rationals, we get by Carathéodory's theorem that for every matrix A which is completely positive over the rationals, rcpr $A \leq \frac{1}{2}n(n+1)$. In fact, if we replace in [24] every phrase "... is completely positive" by "... is completely positive over the rationals" we get the following results:

Theorem 4.1. Let A be a rank r matrix which is completely positive over the rationals. If there exists an $r \times r$ nonsingular principal submatrix of A with N zeros above the diagonal, then

$$\operatorname{rcpr} A \le \frac{r(r+1)}{2} - N.$$

In the case that $N \leq 1$, this bound can be reduced by 1:

Theorem 4.2. Let A be a rank r matrix which is completely positive over the rationals, and let $N \in \{0, 1\}$. If there exists an $r \times r$ nonsingular principal submatrix of A with N zeros above the diagonal, then

$$\operatorname{rcpr} A \le \frac{r(r+1)}{2} - N - 1.$$

The proof of Theorem 4.2 uses the fact that the Cholesky decomposition of an inverse *M*-matrix *A* has nonnegative factors [22], and by Observation 2.1, rcpr $A = \operatorname{rank} A$.

The bound $\frac{1}{2}r(r+1) - N$ in Theorem 4.1 is sharp. For example, in the case that A has a diagonal $r \times r$ nonsingular principal submatrix, i.e., $N = \frac{1}{2}r(r-1)$, we have rcpr $A = r = \frac{1}{2}r(r+1) - N$.

From Theorem 4.2, we get the following corollary:

Corollary 4.3. Let A be an $n \times n$ matrix that is completely positive over the rationals. Then $\operatorname{rcpr} A \leq \frac{1}{2}n(n+1) - 1$. **Remark 4.4.** For matrices in $C\mathcal{P}_n$ with $n \geq 7$, the best known upper bound on the (real) cp-rank was shown in [25] (see also [9]) to be $\frac{1}{2}n(n+1) - 5$. However, the proof uses the duality of the closed convex cones $C\mathcal{P}_n$ and its dual (the cone of $n \times n$ copositive matrices), and we do not know an alternative proof that would carry over to the rational case.

We conclude by remarking that the inequality $\operatorname{cpr} A \leq \operatorname{rcpr} A$ may be strict, as in the following example.

Example 4.5. The matrix

$$A = \begin{pmatrix} 3 & 1 & 0 & 1 \\ 1 & 3 & 1 & 0 \\ 0 & 1 & 3 & 1 \\ 1 & 0 & 1 & 3 \end{pmatrix}$$

is completely positive over the rationals since $A = BB^T$ with

$$B = \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \end{pmatrix}$$

It is easy to see that $\operatorname{cpr} A = 4$: we have $\operatorname{cpr} A \leq 4$ by [23], and $\operatorname{cpr} A \geq \operatorname{rank} A = 4$. It follows from [12] that in a minimal cp-decomposition $A = BB^T$, the matrix B must be of the form

$$B = \begin{pmatrix} x & 0 & 0 & 1/w \\ 1/x & y & 0 & 0 \\ 0 & 1/y & z & 0 \\ 0 & 0 & 1/z & w \end{pmatrix},$$

with $x = \sqrt{\frac{3\pm\sqrt{5}}{2}} \notin \mathbb{Q}$. Consequently, rcpr A > 4. In fact, rcpr A = 5 because of the rational cp-decomposition $A = XDX^T$ with

$$X = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 1 & 0 \\ 0 & 0 & 0.5 & 0.4 & 1 \\ 1 & 0 & 1 & 0 & 0 \end{pmatrix} \quad \text{and} \quad D = \text{Diag}(1, 2, 2, 2.5, 2.1).$$

Note that n = 4 is the smallest order for which strict inequality cpr $A < \operatorname{rcpr} A$ may hold, since for A of order $n \leq 3$ there exists a permutation matrix P such that the Cholesky decomposition of $P^T A P$ is a rational cp-decomposition.

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