A SIMPLEX ALGORITHM FOR RATIONAL CP-FACTORIZATION

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ABSTRACT. In this paper we provide an algorithm, similar to the simplex algorithm, which determines a rational cp-factorization of a given matrix, whenever the matrix allows such a factorization. This algorithm can be used to show that every integral completely positive $2 \times 2$ matrix has an integral cp-factorization.

1. Introduction

Copositive programming gives a common framework to formulate many difficult optimization problems as convex conic ones. In fact, many NP-hard problems are known to have such reformulations (see for example the surveys [3, 10]). All the difficulty of these problems appears to be “converted” into the difficulty of understanding the cone of copositive matrices $\text{COP}_n$ which consists of all symmetric $n \times n$ matrices $B \in \mathcal{S}^n$ with $x^T B x \geq 0$ for all $x \in \mathbb{R}^n_{\geq 0}$. Its dual cone is the cone

$$\text{CP}_n = \text{cone}\{xx^T : x \in \mathbb{R}^n_{\geq 0}\}$$

of completely positive $n \times n$ matrices. Therefore, it seems no surprise that many basic questions about this cone are still open and appear to be very difficult.

One important problem is to find an algorithmic test deciding whether or not a given symmetric matrix $A$ is completely positive. If possible one would like to obtain a certificate for either $A \in \text{CP}_n$ or $A \not\in \text{CP}_n$. Dickinson and Gijben [7] showed that this (strong) membership problem is NP-hard.

In terms of the definitions the most natural certificate for $A \in \text{CP}_n$ is giving a cp-factorization

$$A = \sum_{i=1}^m x_i x_i^T \quad \text{with} \quad x_1, \ldots, x_m \in \mathbb{R}^n_{\geq 0}.$$ 

For $A \not\in \text{CP}_n$ it is natural to give a separating hyperplane defined by a matrix $B \in \text{COP}_n$ so that the inner product of $A$ and $B$ satisfies $\langle B, A \rangle < 0$.

From the algorithmic side, different ideas have been proposed, in particular by Jarre and Schmallowsky [19], Nie [24], Sponsel and Dür [28], Elser [12], Groetzner and Dür [15], and Anstreicher, Burer, and Dickinson [6, Section 3.3]. Latter approach is based on the ellipsoid method, while all others are non-exact numerical heuristics.

In this paper, in Section 3 we describe a new procedure that is based on pivoting like the simplex algorithm. For the defining the pivoting we apply the notion of the
copositive minimum which we introduce in Section 2. Our algorithm works for all matrices in the cone
\[ \mathcal{C}P_n = \text{cone}\{xx^T : x \in \mathbb{Q}^n_{\geq 0}\}. \]
Moreover, we conjecture that it always computes certificates, if the input matrix
is not completely positive. In contrast to the non-exact approaches mentioned above, (the exception being the approach by Anstreicher, Burer and Dickinson whose factorization method is based on the ellipsoid method), our algorithm uses
rational numbers only if the input matrix is rational and so does not face numerical
instabilities. As a consequence, to the best of our knowledge, our algorithm is
currently the only one that can find a rational cp-factorization whenever it exists.
In [6] a similar result was obtained, but restricted to matrices in the interior of
\( \mathcal{C}P_n \).
If the input matrix \( A \) integral, one can also ask if it admits an integral cp-factorization, i.e. a cp-factorization of the form \( A = \sum_{i=1}^{m} x_i x_i^T \) with \( x_i \in \mathbb{Z}^n_{\geq 0} \) and \( i = 1, \ldots, m \). For \( n \geq 3 \) it is known that there are integral matrices \( A \in \mathcal{C}P_n \) which do not have an integral cp-factorization, see [1, Theorem 6.4]. For \( n = 2 \) it was conjectured by Berman and Shaked-Monderer [1, Conjecture 6.13] that every integral matrix \( A \in \mathcal{C}P_2 \) possesses an integral cp-factorization. This conjecture was recently proved by Laffey and Simgoc [21]. In Section 4 we show that our simplex algorithm can be used to give a short, alternative proof of this result.
In Section 5 we describe how an implementation of our algorithm performs on
some examples.

2. THE COPOSITIVE MINIMUM AND COPOSITIVE PERFECT MATRICES

By \( S^n \) we denote the Euclidean vector space of symmetric \( n \times n \) matrices with
inner product \( \langle A, B \rangle = \text{Trace}(AB) = \sum_{i,j=1}^{n} A_{ij} B_{ij} \). With respect to this inner
product we have the following duality relations between the cone of copositive
matrices and the cone of completely positive matrices
\[ \mathcal{C}OP_n = (\mathcal{C}P_n)^* = \{ B \in S^n : \langle A, B \rangle \geq 0 \text{ for all } A \in \mathcal{C}P_n \}, \]
and
\[ \mathcal{C}P_n = (\mathcal{C}OP_n)^*. \]
So, in order to show that a given symmetric matrix \( A \) is not completely positive, it
suffices to find a copositive matrix \( B \in \mathcal{C}OP_n \) with \( \langle B, A \rangle < 0 \). We call \( B \) a separating witness for \( A \notin \mathcal{C}P_n \) in this case, because the linear hyperplane orthogonal
to \( B \) separates \( A \) and \( \mathcal{C}P_n \).
Using the notation \( B[x] \) for \( x^T Bx = \langle B, xx^T \rangle \), we obtain
\[ \mathcal{C}OP_n = \{ B \in S^n : B[x] \geq 0 \text{ for all } x \in \mathbb{R}^n_{\geq 0} \}. \]

Definition 2.1. For a symmetric matrix \( B \in S^n \) we define the copositive minimum as
\[ \min_{\mathcal{C}OP}(B) = \inf \{ B[v] : v \in \mathbb{Z}^n_{\geq 0} \setminus \{0\} \}, \]
and we denote the set of vectors attaining it by
\[ \text{Min}_{\mathcal{C}OP}(B) = \{ v \in \mathbb{Z}^n_{\geq 0} : B[v] = \min_{\mathcal{C}OP}(B) \}. \]

The following proposition shows that matrices in the interior of the cone of
copositive matrices attain their copositive minimum.
Lemma 2.2. Let $B$ be a matrix in the interior of the cone of copositive matrices. Then, the copositive minimum of $B$ is strictly positive and it is attained by only finitely many vectors.

Proof. Since $B$ is copositive, we have the inequality $\min_{\mathbb{COP}} (B) \geq 0$. Suppose that $\min_{\mathbb{COP}} (B) = 0$. Then there is a sequence $v_i \in \mathbb{Z}_{\geq 0} \setminus \{0\}$ of pairwise distinct lattice vectors such that $B[v_i]$ tends to zero when $i$ tends to infinity. From the sequence $v_i$ we construct a new sequence $u_i$ of vectors on the unit sphere $S^{n-1}$ by setting $v_i = \|v_i\| u_i$. The sequence $u_i$ belongs to the compact set $\mathbb{R}_{\geq 0} \cap S^{n-1}$. Thus, by taking a subsequence if necessary, we may assume that $u_i$ converges to a point $u \in \mathbb{R}_{\geq 0} \cap S^{n-1}$. The sequence of norms $\|v_i\|$ tends to infinity since the set of lattice vectors of bounded norm is finite. Thus we get

$$0 = \lim_{i \to \infty} B[v_i] = \lim_{i \to \infty} \|v_i\|^2 B[u_i],$$

which implies that $B[u] = 0$, contradicting our assumption $B \in \text{int}(\mathbb{COP}_n)$. Hence, $\min_{\mathbb{COP}} (B) > 0$.

By the same argument one can show that $\text{Min}_{\mathbb{COP}} (B)$ only contains finitely many vectors. $\square$

In our previous paper [9] and in this paper the set

$\mathcal{R} = \{ B \in S^n : \langle B, vv^T \rangle \geq 1 \text{ for all } v \in \mathbb{Z}_{\geq 0} \setminus \{0\} \}$

plays a central role. In [9, Lemma 2.3] we showed that $\mathcal{R}$ is contained in the interior of the cone of copositive matrices. Thus, we can rewrite $\mathcal{R}$ as

$$\mathcal{R} = \{ B \in S^n : \min_{\mathbb{COP}} (B) \geq 1 \}.$$  (1)

Furthermore, in [9, Lemma 2.4] we showed that for $A \in \text{int}(\mathbb{CP}_n)$ and all sufficiently large $\lambda > 0$ the set

$$\mathcal{P}(A, \lambda) = \{ B \in \mathcal{R} : \langle A, B \rangle \leq \lambda \}$$

is a full-dimensional polytope.

In principle (cf. [9, Proof of Theorem 1.1]), this gives a way to compute a cp-factorization for a given matrix $A \in \text{int}(\mathbb{CP}_n)$ by solving the linear program

$$\min \{ \langle A, B \rangle : B \in \mathcal{P}(A, \lambda) \} :$$

This is because the minimum is attained at a vertex $B^*$ of $\mathcal{P}(A, \lambda)$ if and only if $A$ is contained in the (inner) normal cone

$$\mathcal{V}(B^*) = \text{cone} \{ vv^T : v \in \text{Min}_{\mathbb{COP}} B^* \}$$

of $\mathcal{R}$ at $B^*$. For a rational matrix $A \in \text{int}(\mathbb{CP}_n)$ we obtain a rational cp-factorization in this way, that is, a decomposition of the form

$$A = \sum_{i=1}^{m} \alpha_i v_i v_i^T \quad \text{with } \alpha_i \in \mathbb{Q}_{\geq 0} \text{ and } v_i \in \mathbb{Z}_{\geq 0}^n, \quad \text{for } i = 1, \ldots, m.$$  (3)

However, for solving the linear program (2) one needs an explicit finite algorithmic description of the set $\mathcal{P}(A, \lambda)$, for example by a finite list of linear inequalities. The proof of the polyhedrality of $\mathcal{P}(A, \lambda)$ in [9, Lemma 2.4] relies on an indirect compactness argument (similar to the one in the proof of Lemma 2.2) which does not yield such an explicit algorithmic description. In the remainder of this paper we are therefore concerned with finding a finite list of linear inequalities.
The following definitions and the algorithm in the following section are inspired by Voronoi’s classical algorithm for the classification of perfect positive definite quadratic forms. These can for instance be used to classify all locally densest lattice sphere packings (see for example [22] or [27]). In (3) we use the letter $V$ to denote the normal cone of a vertex, as it is a generalization of the Voronoi cone used in the classical setting. In fact, our generalization of Voronoi’s work can be viewed as an example of a broader framework described by Opgenorth [25]. In analogy with Voronoi’s theory for positive definite quadratic forms we define the notion of perfectness for copositive matrices:

**Definition 2.3.** A copositive matrix $B \in \text{int}(\text{COP}_n)$ is called $\text{COP}$-perfect if it is uniquely determined by its copositive minimum $\min_{\text{COP}} B$ and the set $\text{Min}_{\text{COP}} B$ attaining it.

In other words, $B \in \text{int}(\text{COP}_n)$ is $\text{COP}$-perfect if and only if it is the unique solution of the system of linear equations

$$\langle B, vv^T \rangle = \min_{\text{COP}} B, \text{ for all } v \in \text{Min}_{\text{COP}} B.$$  

In fact, $\text{COP}$-perfect matrix are, up to scaling, the vertices of $\mathbb{R}$.

**Lemma 2.4.** $\text{COP}$-perfect matrices exist in all dimensions (dimension $n = 1$ being trivial): For dimension $n \geq 2$ the following matrix

$$Q_{\text{A}_n} = \begin{pmatrix} 2 & -1 & 0 & \ldots & 0 \\ -1 & 2 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 2 & -1 \\ 0 & \ldots & 0 & -1 & 2 \end{pmatrix}$$  

is $\text{COP}$-perfect; $\frac{1}{2}Q_{\text{A}_n}$ is a vertex of $\mathbb{R}$.

**Proof.** The matrix $Q_{\text{A}_n}$ is positive definite since

$$Q_{\text{A}_n}[x] = x_1^2 + \sum_{i=1}^{n-1} (x_i - x_{i+1})^2 + x_n^2$$

is a sum of squares. Thus $Q_{\text{A}_n}$ lies in the interior of the copositive cone. Furthermore,

$$\min_{\text{COP}} Q_{\text{A}_n} = 2 \text{ with } \text{Min}_{\text{COP}} Q_{\text{A}_n} = \left\{ \sum_{i=j}^{k} e_i : 1 \leq j \leq k \leq n \right\},$$

where $e_i$ is the $i$-th standard unit basis vector of $\mathbb{R}^n$. Thus, the $\binom{n+1}{2}$ vectors attaining the copositive minimum have a continued sequence of 1s in their coordinates and otherwise 0s. Now it is easy to see that the rank-1-matrices

$$\left( \sum_{i=j}^{k} e_i \right) \left( \sum_{i=j}^{k} e_i \right)^T,$$  

where $1 \leq j \leq k \leq n$,

are linearly independent and span the space of symmetric matrices which shows that $Q_{\text{A}_n}$ is $\text{COP}$-perfect. \qed
The matrix $Q_{A_n}$ is also known as a Gram matrix of the root lattice $A_n$, a very important lattice, for instance in the theory of sphere packings (see for example [3]).

3. The algorithm

In this section we show how one can solve the linear program [2]. Our algorithm is similar to the simplex algorithm for linear programming. It walks along a path of subsequently constructed COP-perfect matrices, which are vertices of the polyhedral set $\mathcal{R}$ that are connected by edges of $\mathcal{R}$.

**Input:** $A \in \tilde{CP}_n \ [ A \in S^n_{>0} ]$

**Output:** If $A \in \tilde{CP}_n$, then a cp-factorization of $A$ is returned
(a set $v_1, \ldots, v_m \in \mathbb{Z}^n_\geq$ and $\alpha_i \in \mathbb{R}_\geq$ with $A = \sum_{i=1}^m \alpha_i v_i v_i^T$)

[ If $A \notin CP_n$, then a separating witness is returned (a matrix $W \in COP_n$ with $\langle W, A \rangle < 0$) ]

1. Choose an initial COP-perfect matrix $B_P \in \mathcal{R}$.

2. if $\langle B_P, A \rangle < 0$ then output $A \notin CP_n$ (with witness $W = B_P$ )

3. if $A \in V(B_P)$ then output $A \in \tilde{CP}_n$ (with cp-factorization)

4. Determine a generator $R$ of an extreme ray of $(V(B_P))^*$ with $\langle A, R \rangle < 0$.

5. if $R \in COP_n$ then output $A \notin CP_n$ (with witness $W = R$ )

6. Use Algorithm 2 to determine the contiguous COP-perfect matrix $B_N := B_P + \lambda R$ with $\lambda > 0$ and $\min_{CP}(B_N) = 1$.

7. Set $B_P := B_N$ and goto 2.

**Algorithm 1.** Algorithm to find a cp-factorization [ or a separating witness ]

3.1. Description of the algorithm. In Algorithm 1 we distinguish between two different kinds of inputs, as indicated by the brackets [ . . . ]. If $A \in \tilde{CP}_n$, then the algorithm always terminates when choosing the right pivots $R$ in Step 4 (cf. Theorem 3.2). If $A$ is in the cone $S^n_{>0}$ of positive definite matrices, then we can use Step 2 and Step 5 to certify $A \notin CP_n$ with a witness matrix $W$. However, we do not know yet if Algorithm 1 always terminates in this case (cf. Conjecture 3.3).

In the following we describe the steps of Algorithm 1 in more detail:

In **Step 1**, we can choose for instance the initial vertex $B_P = \frac{1}{2}Q_{A_n}$ of $\mathcal{R}$ with $Q_{A_n}$ as in (4). Then the algorithm subsequently constructs vertices of $\mathcal{R}$.

In **Step 2** we check whether or not the current COP-perfect matrix is already a separating witness. By this, the algorithm subsequently constructs an outer approximation of the $CP_n$ cone:

$$CP_n \subseteq \{ Q \in S^n : \langle Q, B \rangle \geq 0 \text{ for all constructed vertices } B \text{ of } \mathcal{R} \}$$

We shall show in Theorem 3.1 that this procedure gives a tighter and tighter outer approximation of the completely positive cone which eventually converges.

In **Step 3** we determine whether $A$ lies in the polyhedral cone $V(B_P)$. This can be done by solving an auxiliary linear program

$$\min \{ \langle A, Q \rangle : Q \in V(B_P) \} .$$
The minimum equals 0 if and only if $A$ lies in $\mathcal{V}(B_P)$. If $A \in \mathcal{V}(B_P)$, then we can find non-negative coefficients $\lambda_v$, with $v \in \text{Min}_{\text{COP}}(B_P)$, to get a cp-factorization

$$A = \sum_{v \in \text{Min}_{\text{COP}}(B_P)} \lambda_v v v^T.$$ 

Using an algorithmic version of Carathéodory’s theorem we can choose a subset $\{v_1, \ldots, v_m\} \subset \text{Min}_{\text{COP}}(B_P)$ so that we get a rational cp-factorization $A = \sum_{i=1}^m \alpha_i v_i v_i^T$ with positive rational numbers $\alpha_i$.

If the minimum of the auxiliary linear program (5) is negative we can find in Step 4 a generator $R$ of an extreme ray of $(\mathcal{V}(B_P))^*$ with $\langle A, R \rangle < 0$. Here, several choices of $R$ with $\langle A, R/\|R\| \rangle$ minimal, where $\|R\|^2 = \langle R, R \rangle$. Also a random choice of $R$ among the extreme rays of $(\mathcal{V}(B_P))^*$ with $\langle A, R \rangle < 0$ seems to perform quite well.

In Step 5 it is checked whether or not $R$ is a separating witness for $A$, that is, if not only $\langle A, R \rangle < 0$ but also $R \in \text{COP}_n$ holds. We will explain the copositivity test of $R$ in Section 3.3.

In Step 6 Algorithm 2 is used to determine in direction of $R \notin \text{COP}_n$ a new contiguous $\text{COP}$-perfect matrix $B_N$ of $B_P$, that is, a neighboring vertex of $B_P$ on $\mathcal{R}$, connected via an edge in direction $R$. Note that such a vertex exists (and $\mathcal{R}$ is not unbounded in the direction of $R$) under the assumption $R \notin \text{COP}_n$, because $\mathcal{R} \subseteq \text{int}(\text{COP}_n)$, see [9, Lemma 2.3].

Finally, we observe that since $\langle A, R \rangle < 0$, we have $\langle A, B_N \rangle < \langle A, B_P \rangle$ in each iteration (Steps 2 through 6) of the algorithm.

### 3.2. Computing contiguous $\text{COP}$-perfect matrices

Our algorithm for computing contiguous $\text{COP}$-perfect matrices is inspired by a corresponding algorithm for computing contiguous perfect positive definite quadratic forms which is a subroutine in Voronoi’s classical algorithm. In fact, the following algorithm is, after performing obvious changes, essentially identical with the one in [8, Section 6, Erratum to algorithm of Section 2.3].

Computationally the most involved parts of Algorithm 2 are checking if a matrix lies in the interior of the cone of copositive matrices, and if so, computing its copositive minimum $\min_{\text{COP}}$ and all vectors $\text{Min}_{\text{COP}}$ attaining it. We discuss these tasks in Sections 3.3 and 3.4.

In the first while loop of Algorithm 2 lower and upper bounds $l$ and $u$ for the desired value $\lambda$ are computed, such that $B_P + lR$ and $B_P + uR$ are lying in $\text{int}(\text{COP}_n)$ satisfying

$$\min_{\text{COP}}(B_P + lR) = \min_{\text{COP}}(B_P) > \min_{\text{COP}}(B_P + uR).$$

In the second while loop, the exact value of $\lambda$ is determined. Note that replacing the assignment of $u$ by the simpler assignment $u := \gamma$ corresponds to a binary search coming at least arbitrarily close to $\lambda$. However, it may never reach the exact value. The assignment of $u$ ensures that $\langle B_P + uR \rangle[v] \geq 1$ for all $v \in \mathbb{Z}_{\geq 0}^n$. 


**Input:** COP-perfect matrix $B_P \in \mathcal{R}$, generator $R \not\in \text{COP}_n$ of extreme ray of the polyhedral cone $(\mathcal{V}(B_P))^*$

**Output:** Neighboring vertex $B_N$ of $B_P$ on $\mathcal{R}$, connected via an edge in direction $R$, i.e.

$$B_N = B_P + \lambda R \text{ with } \lambda > 0, \min_{\text{COP}}(B_N) = 1, \min_{\text{COP}}(B_N) \not\subseteq \min_{\text{COP}}(B_P).$$

1. $(l, u) := (0, 1)$
2. while $B_P + uR \not\in \text{int}(\text{COP}_n)$ or $\min_{\text{COP}}(B_P + uR) = 1$ do
   - if $B_P + uR \not\in \text{int}(\text{COP}_n)$ then $u := (l + u)/2$
   - else $(l, u) := (u, 2u)$
3. while $\min_{\text{COP}}(B_P + lR) \subseteq \min_{\text{COP}} B_P$ do
   - $\gamma := (l + u)/2$
   - if $\min_{\text{COP}}(B_P + \gamma R) = 1$ then $l := \gamma$
   - else $u := \min \{1 - B_P[v]/R[v] : v \in \min_{\text{COP}}(B_P + \gamma R), R[v] < 0\} \cup \{\gamma\}$
   - if $\min_{\text{COP}}(B_P + uR) = 1$ then $l := u$
4. output $\lambda := l, B_N := B_P + \lambda R$.

**Algorithm 2.** Determination of a contiguous COP-perfect matrix.

### 3.3 Checking copositivity.

From a complexity point of view, checking whether or not a given symmetric matrix is copositive is known to be co-NP-complete by a result of Murty and Kabadi [23].

Nevertheless, in our algorithms we need to check whether or not a given symmetric matrix lies in the cone of copositive matrices (Step 5 in Algorithm 1) or in its interior (Step 2 of Algorithm 2). From a practical point of view, this can be checked by the following recursive characterization of Gaddum [14, Theorem 3.1 and 3.2]: By

$$\Delta = \left\{ x \in \mathbb{R}^n : x \geq 0, \sum_{i=1}^{n} x_i = 1 \right\}$$

we denote the $(n-1)$-dimensional standard simplex in dimension $n$. A matrix $B \in \mathcal{S}_n$ lies in COP$_n$ (in int(COP$_n$)) if and only if every of its principal minors of size $(n-1) \times (n-1)$ lies in COP$_n$ (in int(COP$_{n-1}$)) and the value

$$v = \max_{x \in \Delta} \min_{y \in \Delta} x^T By = \min_{y \in \Delta} \max_{x \in \Delta} x^T By,$$

of the two-player game with payoff matrix $B$ is non-negative (strictly positive).

One can compute the value of $v$ in (6) by a linear program:

$$v = \max\{\lambda : \lambda \in \mathbb{R}, y \in \Delta, By \geq \lambda e\},$$

where $e = (1, \ldots, 1)^T$ is the all-ones vector.

### 3.4 Computing the copositive minimum.

Once we know that a given symmetric matrix $B$ lies in the interior of the copositive cone (i.e. after Step 2 of Algorithm 2) we apply the idea of simplex partitioning initially developed by Bundfuss and Dür [2] to compute its copositive minimum $\min_{\text{COP}}(B)$ and all vectors $\min_{\text{COP}}(B)$ attaining it.
First we recall some facts and results from [2]. A family \( \mathcal{P} = \{\Delta^1, \ldots, \Delta^m\} \) of simplices is called a simplicial partitioning of the standard simplex \( \Delta \) if
\[
\Delta = \bigcup_{i=1}^{m} \Delta^i \quad \text{with} \quad \text{int}(\Delta^i) \cap \text{int}(\Delta^j) = \emptyset \quad \text{whenever} \quad i \neq j.
\]

Let \( v_1^k, \ldots, v_n^k \) be the vertices of simplex \( \Delta^k \). It is easy to verify that if a symmetric matrix \( B \in S^n \) satisfies the strict inequalities
\[
(v_i^k)^T B v_j^k > 0 \quad \text{for all} \quad i, j = 1, \ldots, n, \quad \text{and} \quad k = 1, \ldots, m,
\]
then it lies in \( \text{int}(\text{COP}_n) \). Bundfuss and Dür [2, Theorem 2] proved the following converse: Suppose \( B \in \text{int}(\text{COP}_n) \), then there exists an \( \epsilon > 0 \) so that for all finite simplex partitions \( \mathcal{P} = \{\Delta^1, \ldots, \Delta^m\} \) of \( \Delta \), where the diameter of every simplex \( \Delta^k \) is at most \( \epsilon \), strict inequalities (7) hold. Here, the diameter of \( \Delta^k \) is defined as
\[
\max\{||v_i^k - v_j^k|| : i, j = 1, \ldots, n\}.
\]

We assume now that \( B \in \text{int}(\text{COP}_n) \) and that we have a finite simplex partition \( \mathcal{P} \) so that (7) holds. We furthermore assume that all the vertices \( v_i^k \) have rational coordinates. Such a simplex partition exists as shown by Bundfuss and Dür [2, Algorithm 2].

Each simplex \( \Delta^k = \text{conv}\{v_1^k, \ldots, v_n^k\} \) defines a simplicial cone by \( \text{cone}\{v_1^k, \ldots, v_n^k\} \). From now on we only work with the simplicial cones and not with the simplices any more, so we may scale the rational \( v_i^k \)'s to have integral coordinates.

The goal is now to find all integer vectors \( v \) in \( \Delta^k \) which minimize \( B[v] \). To do this we adapt the algorithm of Fincke and Pohst [13], which solves the shortest lattice vector problem. It is the corresponding problem for positive semidefinite matrices. The adapted algorithm will solve the following problem: Given a matrix \( B \in \text{int}(\text{COP}_n) \) and a simplicial cone, which is generated by integer vectors \( v_1, \ldots, v_n \) so that \( v_i^T B v_j \geq 0 \) holds, and given a positive constant \( M \), find all integer vectors \( v \) in the cone so that \( B[v] \leq M \) holds. Then by reducing \( M \) successively to \( B[v] \), whenever such a non-trivial integer vector \( v \) is found, we can find the copositive minimum of \( B \) in the simplicial cone, as well as all integer vectors attaining it.

The first step of the algorithm is to compute the Hermite normal form of the matrix \( V \) which contains the the vectors \( v_1, \ldots, v_n \) as it columns. (see for example Kannan and Bachem [20] or Schrijver [26], where it is shown that computing the Hermite normal form can be done in polynomial time). We find a unimodular matrix \( U \in GL_n(\mathbb{Z}) \) such that \( UV = W \) holds, where \( W \) is an upper triangular matrix with columns \( w_1, \ldots, w_n \) and coefficients \( W_{i,j} \). Then,
\[
0 < S_{i,i}, 0 \leq S_{i,j} \quad \text{with} \quad S_{i,j} = v_i^T B v_j = w_i^T (U^{-1})^T B U^{-1} w_j.
\]

By \( B' \) we denote the matrix \( (U^{-1})^T B U^{-1} \).

We want to find all vectors \( v \in \text{cone}\{v_1, \ldots, v_n\} \cap \mathbb{Z}^n \) so that \( B[v] \leq M \). In other words, the goal is to find all rational coefficients \( \alpha_1, \ldots, \alpha_n \) satisfying the following three properties:

(i) \( \alpha_1, \ldots, \alpha_n \geq 0 \),
(ii) \( \sum_{i=1}^{n} \alpha_i v_i \in \mathbb{Z}^n \),
(iii) \( B[\sum_{i=1}^{n} \alpha_i v_i] \leq M \).
Since matrix $U$ lies in $\text{GL}_n(\mathbb{Z})$, a vector $\sum_{i=1}^{n} \alpha_i v_i$ is integral if and only if $\sum_{i=1}^{n} \alpha_i w_i$ is integral. Looking at the last vector componentwise we have

$$\sum_{i=1}^{n} \alpha_i w_i = \left( \sum_{j=1}^{n} \alpha_j W_{1,j}, \sum_{j=2}^{n} \alpha_j W_{2,j}, \ldots, \alpha_{n-1} W_{n-1,n-1} + \alpha_n W_{n-1,n}, \alpha_n W_{n,n} \right).$$

We first consider the possible values of the last coefficient $\alpha_n$, and then continue to other coefficients $\alpha_{n-1}, \ldots, \alpha_1$, one by one via a backtracking search. Conditions (i) and (ii) imply that

$$\alpha_n \in \{ k/W_{n,n} : k = 0, 1, 2, \ldots \}.$$ 

Condition (iii) gives an upper bound for $\alpha_n$: Write $\alpha = (\alpha_1, \ldots, \alpha_n)^T$, then

$$M \geq (V\alpha)^T B' V\alpha = \alpha^T W'B' W\alpha = B' \left[ \sum_{i=1}^{n} \alpha_i w_i \right] \geq B' [\alpha_n w_n] = \alpha_n^2 B'[w_n],$$

where the last inequality follows from (3). Hence, $\alpha_n \leq \sqrt{M/B'[w_n]}$ and so

$$\alpha_n \in \{ k/W_{n,n} : k = 0, 1, \ldots, \left[ \sqrt{M/B'[w_n]} \right] W_{n,n} \}.$$ 

Now suppose $\alpha_n$ is fixed. We want to compute all possible values of the coefficient $\alpha_{n-1}$. Then the second but last coefficient $\alpha_{n-1} W_{n-1,n-1} + \alpha_n W_{n-1,n}$ should be integral and $\alpha_{n-1}$ should be non-negative. Thus,

$$\alpha_{n-1} \in \{ (k - \alpha_n W_{n-1,n})/W_{n-1,n-1} : k = [\alpha_n W_{n-1,n}], [\alpha_n W_{n-1,n}] + 1, \ldots \}.$$ 

Again we use condition (iii) to get an upper bound for $\alpha_{n-1}$:

$$M \geq B' \left[ \sum_{i=1}^{n-1} \alpha_i w_i \right] \geq B' [\alpha_{n-1} w_{n-1} + \alpha_n w_n]$$

$$= \alpha_{n-1}^2 B'[w_{n-1}] + 2\alpha_{n-1} \alpha_n w_{n-1} B'[w_n] + \alpha_n^2 B'[w_n],$$

and solving the corresponding quadratic equation gives the desired upper bound.

Now suppose $\alpha_n$ and $\alpha_{n-1}$ are fixed. We want to compute all possible values of the coefficient $\alpha_{n-2}$ and we can proceed inductively.

3.5. Analysis of the algorithm. In the following we prove some features of the algorithm.

We start with a general result which gives a tight outer approximation of the cone of completely positive matrices in terms of the boundary structure (its 1-skeleton to be precise) of the convex set $\mathcal{R}$.

Theorem 3.1. We have

$$\mathcal{CP}_n = \{ Q \in S^n : \langle Q, B \rangle \geq 0 \text{ for all vertices and for all generators of extreme rays } B \text{ of } \mathcal{R} \}.$$ (9)

Proof. Clearly, by [9] Lemma 2.3, the left hand side is contained in the right hand side because all vertices and all generators of extreme rays of $\mathcal{R}$ are elements of the (interior of the) copositive cone.

In order to show the reverse inclusion we use the fact

$$\mathcal{CP}_n = (\text{CO}_n)^* = (\text{int}(\text{CO}_n))^*,$$

where the identity $K^* = (\text{int}(K))^*$ is generally true for full dimensional convex cones.
Suppose for contradiction, we may assume that there is a \( Q \) in the right hand side of (9), for which there is a matrix \( B \in \text{int}(\text{COP}_n) \) so that \( \langle Q, B \rangle < 0 \) holds. By Lemma 2.2 and appropriate positive scaling we may assume without loss of generality that \( B \) lies in \( R \). Therefore, we find vertices \( B_1, \ldots, B_k \) of \( R \) (\( \text{COP} \)-perfect matrices) and generators \( R_1, \ldots, R_l \) of extreme rays of \( R \) such that

\[
B = \lambda_1 B_1 + \cdots + \lambda_k B_k + \mu_1 R_1 + \cdots + \mu_l R_l,
\]

with suitable positive coefficients \( \lambda_i \) and \( \mu_i \), satisfying  \( \lambda_1 + \cdots + \lambda_k = 1 \).

Because \( Q \) lies in the right hand side of (9), \( \langle Q, B_i \rangle \geq 0 \) and \( \langle Q, R_i \rangle \geq 0 \) for all \( i \), and hence \( \langle Q, B \rangle \geq 0 \) contradicting our initial assumption.

\section*{Theorem 3.2.}
For a rational \( A \in \tilde{\text{CP}}_n \), Algorithm [1] with suitable choices in Step 4 ends after finitely many iterations giving a rational cp-factorization of \( A \).

\begin{proof}
For \( A \in \text{int}(\text{COP}_n) \subseteq \tilde{\text{CP}}_n \) the assertion follows from Lemma 2.4 in [9].

So let us assume \( A \in \text{bd} \text{COP}_n \cap \tilde{\text{CP}}_n \). Then \( A \) is in the relative interior of a proper face \( F \) of \( \text{COP}_n \), spanned by finitely many rank-1 matrices \( xx^\top \) with \( x \in \mathbb{Z}^n_{\geq 0} \). This face \( F \) is contained in at least one cone \( \mathcal{V}(B_P) \) of a perfect matrix \( B_P \) (being w.l.o.g. a vertex of \( R \)). In fact, in any neighborhood of \( A \) there are interior points of \( \text{COP}_n \), which are contained in one of the cones \( \mathcal{V}(B_P) \), having \( F \) as one of its faces.

Let \( \{R_1, R_2, \ldots \} \) be a possible sequence of generators of rays constructed in Step 4 of Algorithm [1]. For all of these generators, the inequality \( \langle A, R_i \rangle < 0 \) holds. For \( k \) such generators, the conditions \( \langle Q, R_i \rangle < 0 \) for \( i = 1, \ldots, k \) are not only satisfied for \( Q = A \), but also for all \( Q \) in an \( \varepsilon \)-neighborhood of \( A \) (with a suitable \( \varepsilon \) depending on \( k \)). For any \( k \), this neighborhood also contains points of \( \text{int}(\mathcal{V}(B_P)) \subseteq \text{int}(\text{COP}_n) \). For these interior points \( Q \), however, Algorithm [1] finishes after at most finitely many steps (when checking for \( Q \in \mathcal{V}(B_P) \) in Step 3). Thus, for some finite number of suitable choices in Step 4, the algorithm also ends for \( A \) (when checking for \( A \in \mathcal{V}(B_P) \), and then returning \( X = \text{Min}_{\text{COP}}(B_P) \)).

In principle we could use breadth-first-search in Step 4 of Algorithm [1] to ensure finite termination, but this of course would be far less efficient.

For the case of \( A \notin \text{COP}_n \), we do not yet know if it is possible that Algorithm [1] does not provide a separating witness \( W \) after finitely many iterations. With a suitable chosen rule in Step 4, however, we conjecture that the computation finishes with a certificate:

\section*{Conjecture 3.3.}
For \( A \notin \text{COP}_n \), Algorithm [2] with a suitable “pivot rule” in Step 4 ends after finitely many iterations with a separating witness \( W \).

We close this subsection with a few observations that can be made in the remaining “non-rational boundary cases”, that is, for \( A \in \text{bd} \text{COP}_n \setminus \text{COP}_n \). In this case, Algorithm [1] may not terminate after finitely many steps, as shown in a 2-dimensional example in the following section. Assuming there is an infinite sequence of vertices \( B_P^{(i)} \) of \( R \) constructed in Algorithm [1], we know however at least the following:

(i) The perfect matrix \( B_P^{(i)} \) is in \( \{B \in \text{COP}_n : \langle B_P^{(i-1)}, A \rangle > \langle B, A \rangle \geq 0 \} \).

(ii) The norms \( \|B_P^{(i)}\| \) are unbounded. Otherwise – following the arguments in the proof of Lemma 2.4 in [9] – we could construct a convergent subsequence with limit \( B \in R \), for which we could then find a \( u \in \mathbb{R}^n_{\geq 0} \) of norm \( |u| = 1 \) with \( B[u] = 0 \) (contradicting \( B \in \text{int}(\text{COP}_n) \)).
A simplex algorithm for rational cp-factorization

Figure 1. Subdivision of $\mathcal{CP}_2$ by Voronoi cones $\mathcal{V}(B_P)$. Matrices $A = (a_{ij})$ are drawn with 2-dimensional coordinates

$$(x, y) = \frac{1}{a_{11} + a_{22}} (a_{11} - a_{22}, a_{12}).$$

Integers $\alpha, \beta$ indicate that the shown point is on a ray spanned by the rank-1 matrix $A = vv^T$ with $v = (\alpha, \beta)^T$.

(iii) $B_{P(i)} / \|B_{P(i)}\|$ contains a convergent subsequence with limit $B \in \{ X \in S^n : \langle X, A \rangle = 0 \}$. It can be shown that this $B$ is in $\text{bd} \mathcal{CP}_n$. Infinite sequences of vertices $B_{P(i)}$ of $\mathcal{R}$ with such a limit $B$ exist. For $n = 2$ we give an example in Section 4 in which $A$ is from the “irrational boundary part” $(\text{bd} \mathcal{CP}_n) \setminus \mathcal{CP}_n$.

4. A 2-DIMENSIONAL EXAMPLE

In this section we demonstrate how Algorithm 1 works for $n = 2$. Thereby, we discover a relation of our algorithm to beautiful classical results in elementary number theory. In particular, we consider the case when the input matrix $A$ lies on the boundary of $\mathcal{CP}_2$. For $n = 2$ the boundary cases can be understood (up to scaling) to lie on a half circle, see Figure 1.

The boundary of $\mathcal{CP}_2$ splits into a part of diagonal matrices

$$A = \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} \quad \text{with} \quad \alpha, \beta \geq 0$$

and into rank-1 matrices $A = xx^T$. In the first case, Algorithm 1 finishes already in its first iteration, if we use $Q_{A_2}$ as a starting perfect matrix, where

\begin{equation}
Q_{A_2} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad \text{Min}_{\mathcal{CP}}(Q_{A_2}) = \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right\}.
\end{equation}

Let us consider the other boundary cases for $n = 2$, where $A = xx^T$ is a rank-1 matrix. Without loss of generality we can assume that $x = (\alpha, 1)^T$. As we explain in the following, Algorithm 1 will terminate after finitely many iterations

\[1\] Strictly speaking we should use $\frac{1}{2} Q_{A_2}$ here. If we use $Q_{A_2}$ instead, then the algorithm produces integral matrices and vertices of $2\mathcal{R}$. 
with a COP-perfect matrix $B_P$ satisfying $x \in \text{Min}_{\text{COP}} B_P$ when $\alpha$ is rational. For irrational $\alpha$ the algorithm will not terminate.

The first observation is that Algorithm 1 subsequently replaces a COP-perfect matrix $B_P$ by a contiguous COP-perfect matrix $B_N$ in a way that one of the three vectors in $\text{Min}_{\text{COP}}(B_P)$ is replaced by the sum of the remaining two. Let $B_P$ be a copositive matrix with

$$\text{Min}_{\text{COP}} B_P = \left\{ \begin{pmatrix} a \\ b \end{pmatrix}, \begin{pmatrix} c \\ d \end{pmatrix}, \begin{pmatrix} e \\ f \end{pmatrix} \right\}.  \tag{11}$$

Then, $\det \begin{pmatrix} a & c \\ b & d \end{pmatrix} = \pm 1$ and we get a contiguous COP-perfect matrix $B_N$ with

$$\text{Min}_{\text{COP}} B_N = \left\{ \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}, \begin{pmatrix} a + c \\ b + d \end{pmatrix} \right\} \neq \text{Min}_{\text{COP}} B_P$$

by

$$B_N = B_P + 4 \begin{pmatrix} bd & \frac{1}{2}(ad + bc) \\ -\frac{1}{2}(ad + bc) & ac \end{pmatrix}.$$

For instance, starting with $B_P = Q_{\lambda_2}$ as in (10),

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{is replaced by} \quad \begin{pmatrix} 1 \\ 2 \end{pmatrix} \quad \text{if} \quad \alpha < 1 \quad \text{yielding} \quad B_N = \begin{pmatrix} 6 & -3 \\ -3 & 2 \end{pmatrix},$$

or

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{is replaced by} \quad \begin{pmatrix} 2 \\ 1 \end{pmatrix} \quad \text{if} \quad \alpha > 1 \quad \text{yielding} \quad B_N = \begin{pmatrix} 2 & -3 \\ -3 & 6 \end{pmatrix}.$$  

Note that for $\alpha = 1$, Algorithm 1 also finishes already in the first iteration. The way these vectors are constructed corresponds to the way the famous Farey sequence is obtained. This relation between the Farey diagram/sequence and quadratic forms was first investigated in a classical paper of Adolf Hurwitz [18] in 1894 inspired by a lecture of Felix Klein; see also the book by Hatcher [16], which contains the proofs.

For concreteness, let us choose $\alpha = \sqrt{2}$. Then $\text{Min}_{\text{COP}}(B_P)$ is changed by replacing a suitable vector subsequently with

$$\begin{pmatrix} 2 \\ 1 \end{pmatrix}, \begin{pmatrix} 3 \\ 2 \end{pmatrix}, \begin{pmatrix} 4 \\ 3 \end{pmatrix}, \begin{pmatrix} 7 \\ 5 \end{pmatrix}, \begin{pmatrix} 10 \\ 7 \end{pmatrix}, \begin{pmatrix} 17 \\ 12 \end{pmatrix}, \begin{pmatrix} 24 \\ 17 \end{pmatrix}, \begin{pmatrix} 41 \\ 29 \end{pmatrix}, \begin{pmatrix} 58 \\ 41 \end{pmatrix}, \begin{pmatrix} 99 \\ 70 \end{pmatrix}, \ldots$$

Note that there is always a unique choice in Step 4 in case $A$ is a $2 \times 2$ rank-1 matrix. Note also that the vectors represent fractions that converge to $\sqrt{2}$. Every second vector corresponds to a convergent of the continued fraction of $\sqrt{2}$. For instance,

$$99/70 = 1 + \cfrac{1}{2 + \cfrac{1}{2 + \cfrac{1}{2 + \frac{1}{2}}}}.$$

The COP-perfect matrix after ten iterations of the algorithm is

$$B_{P}^{(10)} = \begin{pmatrix} 4756 & -6726 \\ -6726 & 9512 \end{pmatrix}.$$
It can be shown that the matrices $B_P^{(i)}$ converge to a multiple of

$$B = \begin{pmatrix} 1 & -\sqrt{2} \\ -\sqrt{2} & 2 \end{pmatrix}$$

satisfying $\langle A, B \rangle = 0$ and $\langle X, B \rangle \geq 0$ for all $X \in \mathcal{CP}_2$.

However, every one of the infinitely many perfect matrices $B_P^{(i)}$ satisfies

$$\langle X, B_P^{(i)} \rangle > 0 \text{ for all } X \in \mathcal{CP}_2.$$  

Laffey and Šimogoc [21] showed that every integral matrix $A \in \mathcal{CP}_2$ possesses an integral cp-factorization. This can also be seen as follows: If $B_P$ is a copositive matrix with (11) then the matrices

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix}, \begin{pmatrix} c & d \\ d & c \end{pmatrix}, \begin{pmatrix} e & f \\ f & e \end{pmatrix}$$

form a Hilbert basis of the convex cone which they generate. This means that every integral matrix in this cone is an integral combination of the three matrices above. To show this, one immediately verifies this fact in the special case of $B_P = Q_{\lambda_2}$. Then all the other cones are equivalent by conjugating with a matrix in $\text{GL}_2(\mathbb{Z})$.

5. Computational Experiments

We implemented our algorithm. The source code, written in C++, is available on GitHub [17]. In this section we report on the performance on several examples, most of them previously discussed in the literature. Generally, the running time of the procedure is hard to predict. The number of necessary iterations in Algorithm 1 drastically varies in the considered examples. Most of the computational time is taken by the computation of the copositive minimum as described in Section 3.4.

5.1. Matrices in the interior. For matrices in the interior of the completely positive cone, our algorithm terminates with a certificate in form of a cp-factorization. Note that in [11] and in [5] characterizations of matrices in the interior of the completely positive cone are given. For example, we have that $A \in \text{int}(\mathcal{CP}_n)$ if and only if $A$ has a factorization $A = BB^T$ with $B > 0$ and rank $B = n$.

The matrix

$$\begin{pmatrix} 6 & 7 & 8 & 9 & 10 & 11 \\ 7 & 9 & 10 & 11 & 12 & 13 \\ 8 & 10 & 12 & 13 & 14 & 15 \\ 9 & 11 & 13 & 15 & 16 & 17 \\ 10 & 12 & 14 & 16 & 18 & 19 \\ 11 & 13 & 15 & 17 & 19 & 21 \end{pmatrix}$$

for example lies in the interior of $\mathcal{CP}_6$, as it has a cp-factorization with vectors $(1, 1, 1, 1, 1, 1)$, $(1, 1, 1, 1, 2)$, $(1, 1, 1, 2, 2)$, $(1, 1, 2, 2, 2)$ and $(1, 2, 2, 2, 2)$. It is found after 8 iterations of our algorithm.

5.2. Matrices on the boundary. For matrices in $\mathcal{CP}_n$ there exists a cp-factorization by definition. However, on the boundary of the cone these are often difficult to find.
The following example is from [15] and lies in the boundary of $\tilde{\text{CP}}_5$:

\[
\begin{pmatrix}
8 & 5 & 1 & 1 & 5 \\
5 & 8 & 5 & 1 & 1 \\
1 & 5 & 8 & 5 & 1 \\
1 & 1 & 5 & 8 & 5 \\
5 & 1 & 1 & 5 & 8
\end{pmatrix}
\]

Starting from $Q_{A_5}$, our algorithm needs 5 iterations to find the cp-factorization with the ten vectors $(0, 0, 0, 1, 1), (0, 0, 1, 1, 0), (0, 0, 1, 2, 1), (0, 1, 1, 0, 0), (0, 1, 2, 1, 0), (1, 0, 0, 0, 1), (1, 0, 0, 1, 2), (1, 1, 0, 0, 0), (1, 2, 1, 0, 0)$ and $(2, 1, 0, 0, 1)$.

While the above example can be solved within seconds on a standard computer, the matrix

\[
\begin{pmatrix}
41 & 43 & 80 & 56 & 50 \\
43 & 62 & 89 & 78 & 51 \\
80 & 89 & 162 & 120 & 93 \\
56 & 78 & 120 & 104 & 62 \\
50 & 51 & 93 & 62 & 65
\end{pmatrix}
\]

from Example 7.2 in [15] took roughly 10 days and 70 iterations to find a factorization with only three vectors $(3, 5, 8, 8, 2), (4, 1, 7, 2, 5)$ and $(4, 6, 7, 6, 6)$. Both algorithms suggested in [15] were not able to find any cp-factorization.

We also considered the following family of completely positive $(n + m) \times (n + m)$ matrices, generalizing the family of examples considered in [19]: The matrices

\[
\begin{pmatrix}
 n \text{Id}_m & J_{m,n} \\
 J_{n,m} & m \text{Id}_n
\end{pmatrix},
\]

with $J_\cdot$, denoting an all-ones matrix of suitable size, are known to have cp-rank $nm$, that is, they have a cp-factorization with $nm$ vectors, but not with less. These factorizations are found by our algorithm with starting $\text{COP}$-perfect matrix $Q_{A_{m+n}}$ for all $n, m \leq 3$ in less than 6 iterations.

### 5.3. Matrices that are not completely positive.

For matrices that are not completely positive, our algorithm can find a certificate in form of a witness matrix that is copositive.

The following example is taken from [24, Example 6.2].

\[
A = \begin{pmatrix}
1 & 1 & 0 & 0 & 1 \\
1 & 2 & 1 & 0 & 0 \\
0 & 1 & 2 & 1 & 0 \\
0 & 0 & 1 & 2 & 1 \\
1 & 0 & 0 & 1 & 6
\end{pmatrix}
\]

is positive semidefinite, but not completely positive. Starting from $Q_{A_5}$, our algorithm needs 18 iterations to find the copositive witness matrix

\[
B = \begin{pmatrix}
363/5 & -2126/35 & 2879/70 & 608/21 & -4519/210 \\
-2126/35 & 1787/35 & -347/10 & 1025/12 & 253/14 \\
2879/70 & -347/10 & 829/35 & -1748/105 & 371/30 \\
608/21 & 1025/12 & -1748/105 & 1237/105 & -601/70 \\
-4519/210 & 253/14 & 371/30 & -601/70 & 671/105
\end{pmatrix}
\]

with $\langle A, B \rangle = -2/5$, verifying $A \not\in \text{CP}_5$. 
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