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Computable representations for convex hulls of low-dimensional quadratic forms

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Abstract Let $\mathscr{C}$ be the convex hull of points $\{\binom{1}{x}\binom{1}{x}^T \,|\, x \in \mathscr{F} \subset \Re^n\}$. Representing or approximating $\mathscr{C}$ is a fundamental problem for global optimization algorithms based on convex relaxations of products of variables. If $n \le 4$ and $\mathscr{F}$ is a simplex, then $\mathscr{C}$ has a computable representation in terms of matrices X that are doubly nonnegative (positive semidefinite and componentwise nonnegative). If $n = 2$ and $\mathscr{F}$ is a box, then $\mathscr{C}$ has a representation that combines semidefiniteness with constraints on product terms obtained from the reformulation-linearization technique (RLT). The simplex result generalizes known representations for the convex hull of $\{(x_1, x_2, x_1x_2) \,|\, x \in \mathscr{F}\}$ when $\mathscr{F} \subset \Re^2$ is a triangle, while the result for box constraints generalizes the well-known fact that in this case the RLT constraints generate the convex hull of $\{(x_1, x_2, x_1x_2) \,|\, x \in \mathscr{F}\}$. When $n = 3$ and $\mathscr{F}$ is a box, a representation for $\mathscr{C}$ can be obtained by utilizing the simplex result for $n = 4$ in conjunction with a triangulation of the box.

Keywords Quadratic form · convex hull · convex envelope · global optimization · semidefinite programming

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1 Introduction

Let $\mathscr{C}$ be the convex hull of $\{\binom{1}{x}\binom{1}{x}^T \mid x \in \mathscr{F} \subset \Re^n\}$. Representing or approximating $\mathscr{C}$ is a fundamental problem for global optimization methods based on convex relaxations of products of variables, for example the popular BARON algorithm [11]. Typically the set $\mathscr{F}$ has a simple structure, often obtained via a partitioning of the underlying feasible set. In this paper we consider the two most common choices for $\mathscr{F}$, a simplex and a box, and obtain computable representations for $\mathscr{C}$ in low dimensions.

For the case where $\mathscr{F}$ is a regular simplex and $n \le 4$, $\mathscr{C}$ has a representation involving $n \times n$ matrices that are doubly nonnegative (positive semidefinite and componentwise nonnegative). This result is a straightforward consequence of existing theory for completely positive matrices, but to our knowledge does not appear in the literature. A known counterexample shows that the representation for $\mathscr{C}$ does not hold when $n > 4$. As a corollary of the result for a simplex, we obtain a representation for the case where $\mathscr{F}$ is a triangle in $\Re^2$ or tetrahedron in $\Re^3$. The problem of representing the convex hull of $\{(x_1, x_2, x_1x_2) \mid x \in \mathscr{F}\}$, where $\mathscr{F} \subset \Re^2$ is a triangle was considered in [8]. Our result both generalizes and simplifies the analysis in [8], which itself extends the earlier work of [13].

A well-known result in the global optimization literature is that when $\mathscr{F} \subset \Re^2$ is a box, the constraints on the product term x_1x_2 that arise from the *reformulation–linearization technique* (RLT) give the convex hull of $\{(x_1, x_2, x_1x_2) \mid x \in \mathscr{F}\}$ (see for example [12] or [8] and references therein). We extend this result by showing that when $\mathscr{F} \subset \Re^2$ is a box, $\mathscr{C}$ can be represented using a combination of the RLT constraints and semidefiniteness. Our proof utilizes a recent paper [5] that gives a representation for nonconvex quadratic programming problems involving completely positive matrices. We also give an example to show that the given representation for $\mathscr{C}$ does not hold when $n > 2$.

We next show that for $n \le 3$ a representation for $\mathscr{C}$ can be obtained when $\mathscr{F}$ is any triangulated polytope. This result is primarily of interest in cases where $\mathscr{F}$ is simple enough so that a triangulation of low cardinality can be easily computed. For example, in the case where $\mathscr{F} \subset \Re^3$ is a box (i.e., the 3-cube), we obtain a computable, disjunctive representation of $\mathscr{C}$ by utilizing a triangulation of the 3-cube.

Finally, we perform an exploratory analysis of $\mathscr{C}$ when $\mathscr{F}$ is the 3-cube, the smallest case (mentioned above) where our suggested representation for $\mathscr{C}$ based on RLT constraints and semidefiniteness is not exact. We derive several new cutting planes and demonstrate their ability to characterize certain portions of $\mathscr{C}$. However, using the computable, disjunctive representation of $\mathscr{C}$, we establish that the derived cutting planes are still not sufficient to capture $\mathscr{C}$ exactly.

Notation. We use e to denote a column vector of arbitrary dimension with each component equal to one, and let $E = ee^T$. We use PSD to denote the cone of $m \times m$ symmetric positive semidefinite matrices. We sometimes write $X \succeq 0$ in place of $X \in$ PSD. We use DNN to denote the cone of $m \times m$ doubly nonnegative matrices ($X \in$ DNN $\iff X \succeq 0,\ X \ge 0$), and CP to denote the cone of $m \times m$ completely positive matrices ($X \in$ CP $\iff X = \sum_{i=1}^k x_i x_i^T$, $x_i \in \Re^m_+$, $i = 1, \ldots, k$). In all cases the dimension m is implicit. For conforming matrices A and X the matrix inner product is denoted $A \bullet X = \text{tr}(AX^T)$ and for an $m \times m$ matrix A, $\text{diag}(A) \in \Re^m$ is the vector whose ith component is a_{ii}. We use $\text{Conv}\{\cdot\}$ to denote the convex hull.

2 Simplex constraint

In this section we consider a feasible set of the form $\mathscr{F} = \mathscr{S} = \{x \geq 0 \,|\, e^T x = 1\}$. The problem of minimizing a general quadratic $x^T Q x + c^T x$ over $x \in \mathscr{S}$ is often referred to as standard quadratic programming (QPS) [2,4,3]. The problem is known to be NP-hard, since for example computing the maximum stable set in a graph can be written in the form QPS [9]. In [3] an exact formulation for QPS problems is given in terms of completely positive matrices. Note that if $x \geq 0$, $e^T x = 1$ and $X = xx^T$, then $X \in \text{CP}$ and $E \bullet X = 1$. Moreover one can assume without loss of generality that $c = 0$ since for $x \in \mathscr{S}$, $c^T x$ can be written as a quadratic form $\frac{1}{2} x^T (ce^T + ec^T) x$. These observations suggest writing QPS in the form

$$\min\ Q \bullet X, \quad E \bullet X = 1, \quad X \in \text{CP}. \tag{1}$$

The fact that (1) gives an exact formulation of QPS relies on the following result.

Proposition 1 [3, Lemma 4.5] *The extreme points of the set* $\{X \in \text{CP} \,|\, E \bullet X = 1\}$ *are the rank-one matrices* $X = xx^T$, $x \in \mathscr{S}$.

The fact that (1) is an exact formulation of QPS, and that QPS is itself NP-Hard, implies that in general optimization over CP is difficult. However it is known that in low dimensions matrices in CP have a tractable representation. It is clear that for any n,

$$\text{CP} \subset \text{DNN} \subset \text{DNN}^* \subset \text{CP}^*, \tag{2}$$

where CP^* is the cone of copositive matrices, and DNN^* is the cone of matrices that can be written as the sum of a semidefinite matrix and a nonnegative matrix. In general the inclusions in (2) are strict, but for $n \leq 4$ the following result implies that $\text{CP} = \text{DNN}$ and $\text{CP}^* = \text{DNN}^*$. Approximation results for QPS with $n > 4$ based on a hierarchy of cones between DNN^* and CP^* are given in [4].

Proposition 2 [7] *To any symmetric matrix* X *associate an undirected graph* $G(X)$ *with edge set* $\{\{i,j\} \,|\, i \neq j, X_{ij} \neq 0\}$, *and call a loopless graph* G completely positive *if any matrix* $X \in \text{DNN}$ *with* $G(X) = G$ *also has* $X \in \text{CP}$. *Then* G *is completely positive if and only if* G *contains no odd cycle of length greater than 4.*

Using Propositions 1 and 2 together we obtain a tractable representation of $\mathscr{C}$ for $n \leq 4$. Define

$$\mathscr{D}_S = \left\{ \begin{pmatrix} 1 & e^T X \\ Xe & X \end{pmatrix} \,\middle|\, X \in \text{DNN}, E \bullet X = 1 \right\}.$$

Theorem 1 *Let* $\mathscr{C} = \text{Conv}\{\binom{1}{x}\binom{1}{x}^T \,|\, x \in \mathscr{S} \subset \Re^n\}$. *Then* $\mathscr{C} \subset \mathscr{D}_S$, *and* $\mathscr{C} = \mathscr{D}_S$ *for* $n \leq 4$.

Proof It is obvious that if $x \in \mathscr{S}$ then $\binom{1}{x}\binom{1}{x}^T \in \mathscr{D}_S$, and since $\mathscr{D}_S$ is convex we immediately have $\mathscr{C} \subset \mathscr{D}_S$. Next suppose that $n \leq 4$, $X \in$ DNN, $E \bullet X = 1$ and that X is an extreme point with respect to these constraints. Then $X \in$ CP by Proposition 2, and moreover X must be an extreme point of $\{X \in \text{CP} \,|\, E \bullet X = 1\}$. Then $X = xx^T, x \in \mathscr{S}$ by Proposition 1, so

$$\begin{pmatrix} 1 & e^T X \\ Xe & X \end{pmatrix} = \begin{pmatrix} 1 & x^T \\ x & xx^T \end{pmatrix} \in \mathscr{C}.$$

Thus every extreme point of $\mathscr{D}_S$ is in $\mathscr{C}$, and since $\mathscr{D}_S$ is compact it follows that $\mathscr{D}_S \in \mathscr{C}$. □

Another immediate consequence of Propositions 1 and 2 is that for $n \leq 4$, a QPS problem with $c = 0$ is equivalent to the problem

$$\min\, Q \bullet X, \quad E \bullet X = 1, \quad X \in \text{DNN}.$$

In [4, Example 5.1] it is shown that this equivalence may not hold when $n > 4$, implying that the inclusion $\mathscr{C} \subset \mathscr{D}_S$ can be strict when $n > 4$.

Let $\mathscr{T}$ denote the convex hull of $n+1$ affinely independent points in $\Re^n$ (so $\mathscr{T}$ is a triangle in $\Re^2$ or a tetrahedron in $\Re^3$). Since there is an invertible affine mapping from $\mathscr{T} \in \Re^n$ to $\mathscr{S} \in \Re^{n+1}$, a version of Theorem 1 can be written for $x \in \mathscr{T}$. This representation is of some independent interest, and will be used in Section 4, so we give it explicitly in the corollary below. Let the affinely independent points of $\mathscr{T}$ be given by $a_j \in \Re^n$, $j = 1, \ldots, n+1$, and let A be the matrix whose jth column is a_j. Then $\mathscr{T} = \{y \in \Re^n \,|\, y = Ax,\ x \in \mathscr{S} \subset \Re^{n+1}\}$. Define

$$\mathscr{D}_T = \left\{ \begin{pmatrix} 1 & e^T X A^T \\ AXe & AXA^T \end{pmatrix} \,\middle|\, X \in \text{DNN}, E \bullet X = 1 \right\}.$$

Corollary 1 *Let* $\mathscr{C} = \text{Conv}\{\binom{1}{x}\binom{1}{x}^T \,|\, x \in \mathscr{T} \subset \Re^n\}$. *Then* $\mathscr{C} \subset \mathscr{D}_T$, *and* $\mathscr{C} = \mathscr{D}_T$ *for* $n \leq 3$.

3 Box constraints

In this section we consider a feasible set of the form $\mathscr{F} = \mathscr{B} = \{x \,|\, 0 \leq x \leq e\}$. Minimization of a quadratic function over $\mathscr{B}$ is commonly referred to as box-constrained quadratic programming (QPB). QPB has been heavily studied in the global optimization literature; see for example [15] and references therein. For $x \in \mathscr{B}$ consider a matrix Y of the form

$$Y = \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix}. \tag{3}$$

If $X = xx^T$ then certainly $Y \succeq 0$, and multiplying together the upper and lower bound inequalities on x_i and x_j produces the additional constraints

$$X_{ij} \leq x_i, \tag{4a}$$
$$X_{ij} \leq x_j, \tag{4b}$$
$$X_{ij} \geq 0, \tag{4c}$$
$$X_{ij} \geq x_i + x_j - 1. \tag{4d}$$

The constraints (4) arise when applying the reformulation-linearization technique [12] to QPB. Consequently we will refer to (4) as the RLT constraints, and write $Y \in \text{RLT}$ to denote that a matrix of the form (3) satisfies the constraints (4). Note that for $i = j$ the upper bounds (4a) and (4b) are identical, and the lower bounds (4c) and (4d) are dominated by the inequality $X_{ii} \geq x_i^2$ that is implied by $Y \succeq 0$ (the use of this convex, nonlinear inequality was suggested in [14]). It is also easy to see that the RLT constraints imply that $0 \leq x \leq e$; this is a special case of a general result for RLT [12, Proposition 8.1].

For a matrix Y as in (3), consider the matrices

$$T = \begin{pmatrix} 1 & 0 \\ 0 & I \\ e & -I \end{pmatrix}, \qquad Y^+ = TYT^T = \begin{pmatrix} 1 & x^T & s(x)^T \\ x & X & Z(x,X) \\ s(x) & Z(x,X)^T & S(x,X) \end{pmatrix}, \tag{5}$$

where $s(x) := e - x$, $Z(x,X) := xe^T - X$ and $S(x,X) := ee^T - xe^T - ex^T + X$. It is then clear that $Y \succeq 0 \Leftrightarrow Y^+ \succeq 0$. Moreover it is straightforward to show that the RLT upper bounds (4a)–(4b) are equivalent to $Z(x,X) \geq 0$, while the lower bounds (4d) are equivalent to $S(x,X) \geq 0$. Consequently $Y \in \text{PSD} \cap \text{RLT}$ if and only if $Y^+ \in \text{DNN}$, where Y^+ is given by (5).

Matrices of the form

$$\begin{pmatrix} 1 & x^T & s^T \\ x & X & Z \\ s & Z^T & S \end{pmatrix} \tag{6}$$

also arise in the representation of $\mathscr{C}$ given in [5]. The methodology of [5] requires that all constraints be written as equalities, so nonnegative slack variables must be explicitly added to inequality constraints. Consequently let

$$\mathscr{C}^+ = \text{Conv}\left\{ \begin{pmatrix} 1 \\ x \\ s \end{pmatrix} \begin{pmatrix} 1 \\ x \\ s \end{pmatrix}^T \middle| x \geq 0,\ s \geq 0,\ x + s = e \right\}. \tag{7}$$

The main result of [5] gives a representation of $\mathscr{C}^+$ that imposes complete positivity, the original linear equality constraints $x + s = e$ and their squared counterparts. Note that squaring the constraint $x_i + s_i = 1$ results in a constraint $X_{ii} + 2Z_{ii} + S_{ii} = 1$ on the components of (6).

Proposition 3 [5] *Let* $\mathscr{C}^+$ *be given as in* (7). *Then*

$$\mathscr{C}^+ = \left\{ \begin{pmatrix} 1 & x^T & s^T \\ x & X & Z \\ s & Z^T & S \end{pmatrix} \in \text{CP} \,|\, x + s = e, \text{diag}(X + 2Z + S) = e \right\}.$$

Using Propositions 2 and 3, we can obtain a computable representation of $\mathscr{C}$ for $n = 2$. Define

$$\mathscr{D}_B = \left\{ Y = \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \middle| Y \in \text{PSD} \cap \text{RLT} \right\}.$$

Theorem 2 *Let* $\mathscr{C} = \text{Conv}\{\binom{1}{x}\binom{1}{x}^T \,|\, x \in \mathscr{B} \subset \Re^n\}$. *Then* $\mathscr{C} \subset \mathscr{D}_B$, *and* $\mathscr{C} = \mathscr{D}_B$ *for* $n = 2$.

Proof It is obvious that if $x \in \mathscr{B}$ then $\binom{1}{x}\binom{1}{x}^T \in \mathscr{D}_B$, and since $\mathscr{D}_B$ is convex we immediately have $\mathscr{C} \subset \mathscr{D}_B$. Next suppose that $Y \in \mathrm{PSD} \cap \mathrm{RLT}$. Then $Y^+ \in \mathrm{DNN}$, where Y^+ is defined as in (5). We wish to show that Y^+ is in $\mathscr{C}^+$ as described in Proposition 3, which will imply $Y \in \mathscr{C}$.

Let $s = s(x) = e - x$, $Z = Z(x,X) = xe^T - X$ and $S = S(x,X) = ee^T - xe^T - ex^T + X$. For $n = 2$, Proposition 2 then implies that

$$\begin{pmatrix} X & Z \\ Z^T & S \end{pmatrix} \in \mathrm{CP},$$

and therefore there are $x_i \geq 0$, $s_i \geq 0$, $i = 1, \ldots k$ so that

$$\begin{pmatrix} X & Z \\ Z^T & S \end{pmatrix} = \sum_{i=1}^{k} \begin{pmatrix} x_i \\ s_i \end{pmatrix} \begin{pmatrix} x_i \\ s_i \end{pmatrix}^T.$$

Note that since $Z = xe^T - X$ and $S = ee^T - xe^T - ex^T - X$ we have $x = \frac{1}{2}(Xe + Ze)$ and $s = \frac{1}{2}(Se + Z^T e)$. Defining $\lambda_i = \frac{1}{2}e^T(x_i + s_i)$, $i = 1, \ldots, k$ it follows that

$$Y^+ = \begin{pmatrix} \frac{1}{2}e^T & \frac{1}{2}e^T \\ I & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} X & Z \\ Z^T & S \end{pmatrix} \begin{pmatrix} \frac{1}{2}e & I & 0 \\ \frac{1}{2}e & 0 & I \end{pmatrix} = \sum_{i=1}^{k} \begin{pmatrix} \lambda_i \\ x_i \\ s_i \end{pmatrix} \begin{pmatrix} \lambda_i \\ x_i \\ s_i \end{pmatrix}^T \in \mathrm{CP}.$$

Moreover $x + s = e$ by construction and $\mathrm{diag}(X + 2Z + S) = e$ from (5), so $Y^+ \in \mathscr{C}^+$ by Proposition 3. □

In addition to the proof above based on Propositions 2 and 3, it is also possible to prove Theorem 2 using the theory for extreme points of semidefinite programs from [10]. We prefer the proof given since it is both simpler and more closely related to the analysis for the case $\mathscr{F} = \mathscr{S}$ given in the previous section.

In many cases of interest, the constraint $x \in \mathscr{B} = \{x \,|\, 0 \leq x \leq e\}$ is replaced by the constraint that x lie in a hyper-rectangle: $x \in \mathscr{R} = \{x \,|\, l \leq x \leq u\}$. Since there is an invertible affine transformation between $\mathscr{B}$ and $\mathscr{R}$ it is easy to write a version of Theorem 2 for $x \in \mathscr{R}$. In fact it can be shown that for $x \in \mathscr{R}$, Theorem 2 holds exactly as stated if the condition $Y \in \mathrm{RLT}$, where Y has the form (3), is taken to mean that x and X satisfy the general RLT constraints

$$\begin{aligned} X_{ij} - l_i x_j - u_j x_i &\leq -l_i u_j, \\ X_{ij} - l_j x_i - u_i x_j &\leq -l_j u_i, \\ X_{ij} - l_i x_j - l_j x_i &\geq -l_i l_j, \\ X_{ij} - u_i x_j - u_j x_i &\geq -u_i u_j, \end{aligned}$$

in place of (4). (An approximation result for the case $\mathscr{R} = \{x \,|\, -e \leq x \leq e\}$ that uses $Y \succeq 0$ and simple upper bounds on $\mathrm{diag}(X)$ is given in [16].) It is also possible to generalize Theorem 2 to the case where $\mathscr{F}$ is a parallelepiped, but since this case does not commonly occur in practice we omit the details.

In [6] explicit formulas are given for the convex (lower) and concave (upper) envelopes of a bivariate quadratic function over a rectangle $\mathscr{R} \subset \Re^2$. The methodology of [6] requires an analysis of different cases, one of which partitions the rectangle into three different regions, each of which is the domain for a piece of the convex or concave envelope. Compared to Theorem 2, the approach in [6] has the advantage that explicit formulas are obtained, but the disadvantage that the case analysis and possible partitioning of the rectangle depend on the particular quadratic form being analyzed.

It follows from Theorem 2 that for $n = 2$ and a quadratic objective $c^T x + x^T Qx$, the solution value of QPB is equal to

$$\min \tilde{Q} \bullet Y, \quad Y \in \text{PSD} \cap \text{RLT}, \tag{8}$$

where Y has the form (3) and

$$\tilde{Q} = \begin{pmatrix} 0 & \frac{1}{2}c^T \\ \frac{1}{2}c & Q \end{pmatrix}.$$

If Theorem 2 were true for $n > 2$, then (8) would continue to give the solution value for QPB for any c and Q. We have determined that this is false. For example, for $n = 3$ the QPB problem with

$$c = 0, \qquad Q = \frac{1}{3}ee^T - I = \begin{pmatrix} -2/3 & 1/3 & 1/3 \\ 1/3 & -2/3 & 1/3 \\ 1/3 & 1/3 & -2/3 \end{pmatrix} \tag{9}$$

has solution value $-2/3$ (obtained by evaluating the quadratic at the extreme points of $\mathscr{B}$, since $Q \preceq 0$), while the problem (8) has a solution value of $-3/4$. We will investigate the effect of adding constraints based on (9) and certain transformations of (9) in Section 4.

Although (8) may not be equivalent to QPB for $n > 2$, we have found that for randomly generated problems with $n = 3$ the exact solution value of QPB is almost always given by (8). In the next section we show that an exact disjunctive representation for $\mathscr{C}$ when $\mathscr{F} = \mathscr{B} \subset \Re^3$ can be obtained by applying Corollary 1 to a triangulation of $\mathscr{B}$. For larger n we have found that the lower bound from (8) is often quite sharp. For example, in 15 problems of size $n = 30$ from [15], the percentage gap between the exact solution value and the value from (8) has a maximum of 3.06%, is 0.00% on 8 instances and averages 0.41% [1].

4 Triangulated polytopes and the 3-cube

In this section we consider the case where $\mathscr{F} \subset \Re^n$ is a triangulated polytope. In particular we assume that $\mathscr{F} = \mathscr{P} = \cup_{i=1}^k \mathscr{T}_i$, where each $\mathscr{T}_i$ is the convex hull of $n+1$ affinely independent points. Letting the coordinates of these points be the columns of an $n \times (n+1)$ matrix A_i, we have $\mathscr{T}_i = \{y \in \Re^n \,|\, y = A_i x,\ x \in \mathscr{S} \subset \Re^{n+1}\}$ for each i. Since any polytope can be triangulated, the methodology described here is quite general. However we are primarily interested in low-dimensional cases where $\mathscr{F}$ has a simple enough structure so that a triangulation can be explicitly given. Define

$$\mathscr{D}_P = \left\{ \sum_{i=1}^k \begin{pmatrix} \lambda_i & e^T X_i A_i^T \\ A_i X_i e & A_i X_i A_i^T \end{pmatrix} \,\middle|\, \sum_{i=1}^k \lambda_i = 1, X_i \in \text{DNN}, E \bullet X_i = \lambda_i, i = 1, \ldots, k \right\}.$$

Theorem 3 *Let $\mathscr{C} = \mathrm{Conv}\{\binom{1}{x}\binom{1}{x}^T \,|\, x \in \mathscr{P} \subset \Re^n\}$. Then $\mathscr{C} \subset \mathscr{D}_P$, and $\mathscr{C} = \mathscr{D}_P$ for $n \le 3$.*

Proof This follows from Corollary 1 and the fact that if $x \in \mathscr{P}$ then $x \in \mathscr{T}_i$ for some i. □

For an interesting application of Theorem 3 we consider $\mathscr{P} = \mathscr{B} \subset \Re^3$. As described at the end of the previous section, the QPB problem with data (9) shows that the inclusion $\mathscr{C} \subset \mathscr{D}_B$ is strict. However by triangulating the 3-cube we can obtain an exact, computable representation $\mathscr{C} = \mathscr{D}_P$. The simplest triangulation of $\mathscr{B} \subset \Re^3$ uses 6 tetrahedra of the form $\mathscr{T}_{ijk} = \{x \in \Re^3 \,|\, 0 \le x_i \le x_j \le x_k \le 1\}$ (a triangulation using 5 tetrahedra is also known). The corresponding matrices A_{ijk} have a very simple form, for example

$$A_{123} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \end{pmatrix}.$$

Although Theorem 3 gives a computable, disjunctive representation of $\mathscr{C}$ for $\mathscr{F} = \mathscr{B} \subset \Re^3$, it is natural to ask what additional constraints are required to restrict $\mathscr{D}_B$ to $\mathscr{C}$ exactly. While we have not been able to answer this question fully, we now describe some exploratory results.

The matrix Q in (9) was found by detailed examination of the sets $\mathscr{D}_{T_{ijk}}$, where each $\mathscr{T}_{ijk}$ is an element of the triangulation of $\mathscr{B} \subset \Re^3$ described above. This Q immediately yields the valid inequality $P_0 \bullet Y \ge 0$, where

$$P_0 := \begin{pmatrix} 2/3 & 0^T \\ 0 & \frac{1}{3}ee^T - I \end{pmatrix},$$

which cuts into $\mathscr{D}_B$. By also considering combinations of affine transformations of the form $x_j \to 1 - x_j$ that complement a variable, taking $\mathscr{B}$ to itself, one can propagate the constraint $P_0 \bullet Y \ge 0$ to form additional cuts. For $n = 3$, there are a total of $8 = 2^3$ combinations of original and complemented variables to consider. One can verify that the eight possibilities yield four distinct cuts, one of which is $P_0 \bullet Y \ge 0$. The remaining three are $P_j \bullet Y \ge 0$, $j = 1,2,3$, where

$$P_1 := \frac{1}{3}\begin{pmatrix} 0 & (e_1+e)^T \\ e_1+e & 2(e_2e_3^T + e_3e_2^T - I) - ee^T \end{pmatrix},$$
$$P_2 := \frac{1}{3}\begin{pmatrix} 0 & (e_2+e)^T \\ e_2+e & 2(e_1e_3^T + e_3e_1^T - I) - ee^T \end{pmatrix},$$
$$P_3 := \frac{1}{3}\begin{pmatrix} 0 & (e_3+e)^T \\ e_3+e & 2(e_1e_2^T + e_2e_1^T - I) - ee^T \end{pmatrix}.$$

We consider the effect of adding these four cuts to $\mathscr{D}_B$ to better approximate $\mathscr{C}$. Recall that the optimal value of (8) using the data (9) is $-3/4$. The corresponding optimal solution is

$$\bar{Y} := \begin{pmatrix} 1 & \frac{1}{2}e^T \\ \frac{1}{2}e & \frac{1}{4}ee^T + \frac{1}{4}I \end{pmatrix} \in \mathscr{D}_B.$$

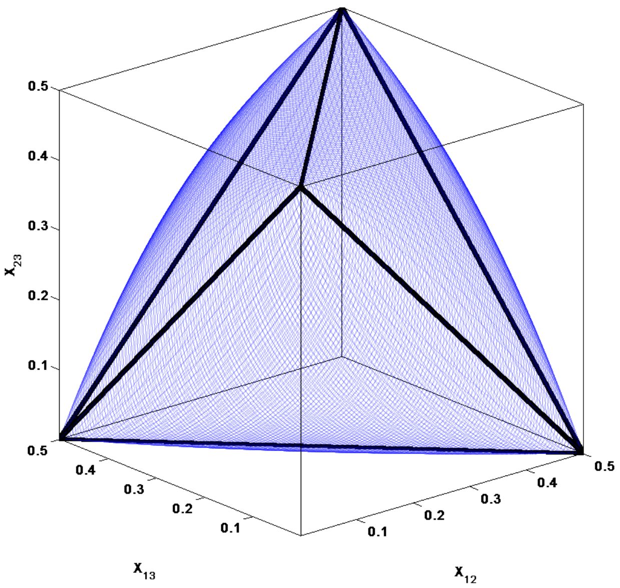

Fig. 1 Plot of the three-dimensional sets $\bar{R}^1$ and $\bar{R}^2$

By construction, $P_0 \bullet \bar{Y} < 0$, and so re-solving with the same objective over the restricted feasible set

$$\mathscr{D}_B \cap \{Y : P_j \bullet Y \geq 0, j = 0,1,2,3\} \tag{10}$$

eliminates $\bar{Y}$. In fact, the new optimal value is exactly $-2/3$, meaning that the constraint $P_0 \bullet Y \geq 0$ supports $\mathscr{C}$.

To visualize the effect of adding the cuts P_j, $j = 0,1,2,3$, we consider fixing values for x and $\mathrm{diag}(X)$ and plotting the feasible values of the remaining three variables X_{12}, X_{13} and X_{23}. In particular, define the sets

$$\begin{aligned} R^1 &:= \{Y : x = \mathrm{diag}(X) = e/2\} \cap \mathscr{D}_B, \\ R^2 &:= \{Y : x = \mathrm{diag}(X) = e/2\} \cap \mathscr{D}_B \cap \{Y : P_j \bullet Y \geq 0, j = 0,1,2,3\}. \end{aligned}$$

Note that the values $x = \mathrm{diag}(X) = e/2$ are "worst possible" in terms of the magnitude of the differences between x_i^2 and X_{ii}. Let $\bar{R}^1$ and $\bar{R}^2$ be the projections of R^1 and R^2, respectively, onto the variables (X_{12}, X_{13}, X_{23}). In Figure 1, $\bar{R}^1$ is shown as a translucent, curved convex body around $\bar{R}^2$, which itself is a tetradhedron with bold lines highlighting its edges. Since the boundaries of $\bar{R}^1$ and $\bar{R}^2$ were found numerically, one cannot be sure from the figure alone that R^2 is a tetrahedron, but this can be easily verified. In fact the vertices of $\bar{R}^2$ are all in $\mathscr{C}$, and the facets of $\bar{R}^2$ are precisely the four cuts added to $\mathscr{D}_B$. Since $\mathscr{C}$ is convex, this implies that the four constraints derived above generate the convex hull of $\mathscr{C}$ intersected with the affine subspace $\{Y : x = \mathrm{diag}(X) = e/2\}$

The above analysis demonstrates the strength of the cuts $P_i \bullet Y \geq 0$, $i = 0,1,2,3$ in certain portions of $\mathscr{C}$, and one might hope that these four cuts intersected with

$\mathscr{D}_B$ are strong enough to generate $\mathscr{C}$. We have determined that unfortunately this is not the case. For example the matrix

$$\hat{Y} := \begin{pmatrix} 1.00 & 0.50 & 0.50 & 0.50 \\ 0.50 & 0.45 & 0.35 & 0.30 \\ 0.50 & 0.35 & 0.45 & 0.11 \\ 0.50 & 0.30 & 0.11 & 0.45 \end{pmatrix}$$

satisfies

$$\hat{Y} \in (\mathscr{D}_B \cap \{Y : P_j \bullet Y \geq 0, y = 0,1,2,3\}) \setminus \mathscr{C}.$$

The fact that $\hat{Y} \notin \mathscr{C}$ has been established numerically using the disjunctive formulation for $\mathscr{C}$ given by Theorem 3. So, even though the four cuts derived above are very strong in certain portions of $\mathscr{C}$, they do not sufficiently tighten $\mathscr{D}_B$ to fully describe $\mathscr{C}$. Obtaining constraints on Y that fully characterize $\mathscr{C}$ for $\mathscr{F} = \mathscr{B} \subset \Re^3$ remains an interesting open problem.

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