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Computable representations for convex hulls of low-dimensional quadratic forms

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Abstract

Let $\mathcal{C}$ be the convex hull of points $\{\binom{1}{x}\binom{1}{x}^T \mid x \in \mathcal{F} \subset \Re^n\}$. Representing or approximating $\mathcal{C}$ is a fundamental problem for global optimization algorithms based on convex relaxations of products of variables. If $n \le 4$ and $\mathcal{F}$ is a simplex then $\mathcal{C}$ has a computable representation in terms of matrices X that are doubly nonnegative (positive semidefinite and componentwise nonnegative). If $n = 2$ and $\mathcal{F}$ is a box, then $\mathcal{C}$ 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 $\{(x_1, x_2, x_1x_2) \mid x \in \mathcal{F}\}$ when $\mathcal{F} \subset \Re^2$ 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 $\{(x_1, x_2, x_1x_2) \mid x \in \mathcal{F}\}$. When $n = 3$ and $\mathcal{F}$ is a box, a representation for $\mathcal{C}$ can be obtained by utilizing the simplex result for $n = 4$ in conjunction with a triangulation of the 3-cube.

Keywords: Reformulation-linearization technique, semidefinite programming, convex envelope.

AMS subject classification: 90C26, 90C22

1 Introduction

Let $\mathcal{C}$ be the convex hull of $\{\binom{1}{x}\binom{1}{x}^T \,|\, x \in \mathcal{F} \subset \Re^n\}$. Representing or approximating $\mathcal{C}$ is a fundamental problem for global optimization methods based on convex relaxations of products of variables, for example the popular BARON algorithm [12]. Typically the set $\mathcal{F}$ 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 $\mathcal{F}$, a simplex and a box, and obtain computable representations for $\mathcal{C}$ in low dimensions.

For the case where $\mathcal{F}$ is a regular simplex and $n \le 4$, $\mathcal{C}$ 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 $\mathcal{C}$ does not hold when $n > 4$. As a corollary of the result for a simplex we obtain a representation for the case where $\mathcal{F}$ is a triangle in $\Re^2$ or tetrahedron in $\Re^3$. The problem of representing the convex hull of $\{(x_1, x_2, x_1x_2) \,|\, x \in \mathcal{F}\}$, where $\mathcal{F} \subset \Re^2$ is a triangle was considered in [9]. Our result both generalizes and simplifies the analysis in [9], which itself extends the earlier work of [14].

A well-known result in the global optimization literature is that when $\mathcal{F} \subset \Re^2$ 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 $\{(x_1, x_2, x_1x_2) \,|\, x \in \mathcal{F}\}$ (see for example [13] or [9] and references therein). We extend this result by showing that when $\mathcal{F} \subset \Re^2$ is a box, $\mathcal{C}$ 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 $\mathcal{C}$ does not hold when $n > 2$.

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

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 ($X \in \text{DNN} \iff X \succeq 0,\ X \geq 0$), and CP to denote the cone of $m \times m$ completely positive matrices ($X \in \text{CP} \iff X = \sum_{i=1}^k x_i x_i^T,\ x_i \in \Re^m_+,\ i = 1, \ldots, k$). 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 Conv$\{\cdot\}$ to denote the convex hull.

2 Simplex constraint

In this section we consider a feasible set of the form $\mathcal{F} = \mathcal{S} = \{x \geq 0 \,|\, e^T x = 1\}$. The problem of minimizing a general quadratic $x^T Q x + c^T x$ over $x \in \mathcal{S}$ is often referred to as standard quadratic programming (QPS) [2, 3, 4]. 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 [10]. In [4] a 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 $X \in$ CP and $E \bullet X = 1$. Moreover one can assume without loss of generality that $c = 0$ since for $x \in \mathcal{S}$, $c^T x$ 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 [4, Lemma 4.5] *The extreme points of the set* $\{X \in \text{CP} \,|\, E \bullet X = 1\}$ *are exactly the rank-one matrices* $X = xx^T$, $x \in \mathcal{S}$.

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 $n \le 4$ the following result implies that $\mathrm{CP} = \mathrm{DNN}$ and $\mathrm{CP}^* = \mathrm{DNN}^*$. Approximation results for QPS with $n > 4$ based on a hierarchy of cones between DNN^* and CP^* are given in [3].

Proposition 2 [8] *To any symmetric matrix X associate an undirected graph $G(X)$ with edge set $\{(i,j) \,|\, i \ne j, X_{ij} \ne 0\}$, and call a loopless graph G* completely positive *if any matrix $X \in \mathrm{DNN}$ with $G(X) = G$ also has $X \in \mathrm{CP}$. 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 $\mathcal{C}$ for $n \le 4$. Define

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

Theorem 3 *Let $\mathcal{C} = \mathrm{Conv}\{\binom{1}{x}\binom{1}{x}^T \,|\, x \in \mathcal{S}\}$. Then $\mathcal{C} \subset \mathcal{D}_S$, and $\mathcal{C} = \mathcal{D}_S$ for $n \le 4$.*

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

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

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

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

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

In [3, Example 5.1] it is shown that this equivalence may not hold when $n > 4$, implying that the inclusion $\mathcal{C} \subset \mathcal{D}_S$ can be strict when $n > 4$.

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

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

Corollary 4 *Let* $\mathcal{C} = \text{Conv}\{\binom{1}{x}\binom{1}{x}^T \,|\, x \in \mathcal{T}\}$. *Then* $\mathcal{C} \subset \mathcal{D}_T$, *and* $\mathcal{C} = \mathcal{D}_T$ *for* $n \leq 3$.

3 Box constraints

In this section we consider a feasible set of the form $\mathcal{F} = \mathcal{B} = \{x \,|\, 0 \leq x \leq e\}$. Minimization of a quadratic function over $\mathcal{B}$ is commonly referred to as box-constrained quadratic programming (QPB). QPB has been heavily studied in the global optimization literature; see for example [16] and references therein. For $x \in \mathcal{B}$ 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

$$\begin{aligned} X_{ij} &\leq x_i, && \text{(4a)} \\ X_{ij} &\leq x_j, && \text{(4b)} \\ X_{ij} &\geq 0, && \text{(4c)} \\ X_{ij} &\geq x_i + x_j - 1. && \text{(4d)} \end{aligned}$$

The constraints (4) arise when applying the reformulation-linearization technique [13] 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 [15]). It is also easy to see that the

RLT constraints imply that $0 \le x \le e$; this is a special case of a general result for RLT [13, Proposition 8.1].

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

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

where $s = e - x$, $Z = xe^T - X$ and $S = ee^T - xe^T - ex^T + X$. 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 $Z \ge 0$, while the lower bounds (4d) are equivalent to $S \ge 0$. Consequently $Y \in \text{PSD} \cap \text{RLT}$ if and only if $Y^+ \in \text{DNN}$, where Y^+ is given by (5).

A matrix of the form

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

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

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

The main result of [5] gives a representation of $\mathcal{C}^+$ 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 Y^+.

Proposition 5 [5] $\mathcal{C}^+ = \{Y^+ \in \text{CP} \,|\, x + s = e, \text{diag}(X + 2Z + S) = e\}$.

Using Propositions 2 and 5, we can obtain a computable representation of $\mathcal{C}$ for $n = 2$. Define

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

Theorem 6 *Let* $\mathcal{C} = \text{Conv}\{\binom{1}{x}\binom{1}{x}^T \,|\, x \in \mathcal{B}\}$. *Then* $\mathcal{C} \subset \mathcal{D}_B$, *and* $\mathcal{C} = \mathcal{D}_B$ *for* $n = 2$.

Proof: It is obvious that if $x \in \mathcal{B}$ then $\binom{1}{x}\binom{1}{x}^T \in \mathcal{D}_B$, and since $\mathcal{D}_B$ is convex we immediately have $\mathcal{C} \subset \mathcal{D}_B$. Next suppose that $Y \in \text{PSD} \cap \text{RLT}$. Then $Y^+ \in \text{DNN}$, where Y^+ is defined as in (5). For $n = 2$, Proposition 2 then implies that

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

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 $s = \frac{1}{2}(Se + Z^Te)$. Defining $\lambda_i = \frac{1}{2}e^T(x_i + s_i)$, $i = 1, \ldots, k$ it follows that

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

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

In addition to the proof above based on Propositions 2 and 5, it is also possible to prove Theorem 6 using the theory for extreme points of semidefinite programs from [11]. We prefer the proof given since it is both simpler and more closely related to the analysis for the case $\mathcal{F} = \mathcal{S}$ given in the previous section.

In many cases of interest, the constraint $x \in \mathcal{B} = \{x \,|\, 0 \leq x \leq e\}$ is replaced by the constraint that x lie in a hyper-rectangle; $x \in \mathcal{R} = \{x \,|\, l \leq x \leq u\}$. Since there is an invertible affine transformation between $\mathcal{B}$ and $\mathcal{R}$ it is easy to write a version of Theorem 6 for $x \in \mathcal{R}$. In fact it can be shown that for $x \in \mathcal{R}$, Theorem 6 holds exactly as stated if the condition $Y \in \text{RLT}$, 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 $\mathcal{R} = \{x \,|\, -e \leq x \leq e\}$ that uses $Y \succeq 0$ and simple upper bounds on $\text{diag}(X)$ is given in [17].) It is also possible to generalize Theorem 6 to the case where $\mathcal{F}$ is a parallelepiped, but since this case does not commonly occur in practice we omit the details.

It follows from Theorem 6 that for $n = 2$ and a quadratic objective $c^T x + x^T Qx$, the solution value of QPB is equal to

$$\min \; \tilde{Q} \bullet Y, \quad Y \in \text{PSD} \cap \text{RLT}, \tag{7}$$

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 6 were true for $n > 2$, then (7) 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

$$c = \begin{pmatrix} 18 \\ -62 \\ 42 \end{pmatrix}, \qquad Q = \begin{pmatrix} -44 & 23 & 33 \\ 23 & 9 & 28 \\ 33 & 28 & -90 \end{pmatrix} \tag{8}$$

has solution value -53 (obtained using the finite branch-and-bound algorithm of [6]), while the problem (7) has a solution value of approximately -53.004. Although (7) 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 (7). (In the next section we show that an exact representation for $\mathcal{C}$ when $\mathcal{F} = \mathcal{B} \subset \Re^3$ can be obtained by applying Corollary 4 to a triangulation of $\mathcal{B}$.) For larger n we have found that the lower bound from (7) is often quite sharp. For example, in 15 problems of size $n = 30$ from [16], the percentage gap between the exact solution value and the value from (7) has a maximum of 3.06%, is 0.00% on 8 instances and averages 0.41% [1].

4 Triangulated polytopes

In this section we consider the case where $\mathcal{F} \subset \Re^n$ is a triangulated polytope. In particular we assume that $\mathcal{F} = \mathcal{P} = \cup_{i=1}^k \mathcal{T}_i$, where each $\mathcal{T}_i$ 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 $\mathcal{T}_i = \{y \in \Re^n \,|\, y = A_i x, \; x \in \mathcal{S} \subset \Re^{n+1}\}$ 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 $\mathcal{F}$ has a simple enough structure so that a triangulation can be explicitly given. Define

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

Theorem 7 *Let* $\mathcal{C} = \text{Conv}\{\binom{1}{x}\binom{1}{x}^T \,|\, x \in \mathcal{P}\}$. *Then* $\mathcal{C} \subset \mathcal{D}_P$, *and* $\mathcal{C} = \mathcal{D}_P$ *for* $n \leq 3$.

Proof: This follows from Corollary 4 and the fact that if $x \in \mathcal{P}$ then $x \in \mathcal{T}_i$ for some i. □

For an interesting application of Theorem 7 we consider $\mathcal{P} = \mathcal{B} \subset \Re^3$. As described at the end of the previous section, the QPB problem with data (8) shows that the inclusion $\mathcal{C} \subset \mathcal{D}_B$ is strict. However by triangulating the 3-cube we can obtain an exact, computable representation $\mathcal{C} = \mathcal{D}_P$. The simplest triangulation of $\mathcal{B} \subset \Re^3$ uses 6 tetrahedra of the form $\mathcal{T}_{ijk} = \{x \in \Re^3 \,|\, 0 \leq x_i \leq x_j \leq x_k \leq 1\}$ (a triangulation using 5 tetrahedra is also known). The corresponding matrices A_{ijk} have a very simple form, for example

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

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