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Maximization of a PSD quadratic form and factorization

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Abstract
We consider the problem of maximization of a convex quadratic form on a convex polyhedral set, which is known to be NP-hard. In particular, we focus on upper bounds on the maximum value. We investigate utilization of different vector norms (estimating the Euclidean one) and different objective matrix factorizations. We arrive at some kind of duality with positive duality gap in general, but with possibly tight bounds. We discuss theoretical properties of these bounds and also extensions to generally preconditioned factors. We employ mainly the maximum vector norm since it yields efficiently computable bounds, however, we study other norms, too. Eventually, we leave many challenging open problems that arose during the research.

Keywords Convex quadratic form · Concave programming · NP-hardness · Upper bound · Maximum norm · Preconditioning

1 Introduction

This paper addresses the problem of maximizing a convex quadratic form on a convex polyhedral set. Formally, we consider the problem

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$$f^* = \max\ x^T Ax \text{ subject to } x \in \mathcal{M}, \tag{1}$$

where $\mathcal{M}$ is a convex polyhedral set and $A \in \mathbb{R}^{n\times n}$ is a symmetric positive definite matrix (an extension to singular A is discussed in Remark 1). This is a basic problem arising in the context of global optimization [4,9,16,17]. Computation of the maximum is NP-hard even when $\mathcal{M}$ is restricted to be a box (hypercube) [2,11,18]. This is underlined by the fact that the maximum is attained in a vertex of $\mathcal{M}$ provided $\mathcal{M}$ is bounded [9].

There are too many works in this area that we cannot give a thorough overview here. For a bibliographic survey, we refer to [5] for quadratic programming and to [14] for concave function minimization. Among the many methods to solve (1), one can identify approaches utilizing cutting plane methods [10], reformulation-linearization/convexification and branch and bound methods [1,16,21], polynomial time approximation methods [19], or extended Lagrange multiplier approach [20]. Theory and methods based on a global optimization perspective are presented in [12]. Most of these methods exploit the structure of the feasible set and the objective function simultaneously. In contrast, in this paper we propose bounds based on a finer overestimation of the objective function. Due to this difference, the proposed bound may outperform on some instances and vice versa; some instances are provided in [8].

Upper bound. This paper is an extension of [8], where we introduced the following problem (the theory presented here is new). Since the matrix A can be factorized as $A = G^T G$ we can write $x^T Ax = x^T G^T Gx = \|Gx\|_2^2$. Thus the problem (1) can be formulated as

$$\max\ \|Gx\|_2^2 \text{ subject to } x \in \mathcal{M}. \tag{2}$$

To derive an upper bound on f^* we can simply estimate the Euclidean norm by some other norm from above. The quality of the resulting upper bound will also depend on the particular factorization $A = G^T G$ employed. Therefore the main focus of this paper is to investigate the relation between the upper bounds and the factorization and the vector norm used. Throughout this paper, we assume that a certain factorization $A = G^T G$, $G \in \mathbb{R}^{n\times n}$, is provided and fixed; alternative factorizations are then denoted by $A = R^T R$.

Notation. The Hadamard product of matrices $A, B \in \mathbb{R}^{m\times n}$ is denoted by $A \circ B$. The ith row and jth column of a matrix M are denoted by M_{i*} and M_{*j}, respectively. Next, $e = (1, \ldots, 1)^T$ stands for the vector of ones, I_n for the identity matrix of size n, and $e_i = (I_n)_{*i}$ for the ith canonical unit vector. We use three specific vector norms, the Euclidean norm $\|x\|_2 = \sqrt{x^T x}$, the ℓ_1-norm $\|x\|_1 = \sum_i |x_i|$ and the maximum (Chebyshev) norm $\|x\|_\infty = \max_i |x_i|$. Whenever we use $\|\cdot\|$ without an index we understand it as a general vector norm. The sign of $r \in \mathbb{R}$ is defined as $\operatorname{sgn}(r) = 1$ if $r \geq 0$ and $\operatorname{sgn}(r) = -1$ otherwise. Inequalities, the sign and the absolute value are applied entry-wise for vectors and matrices.

2 Upper bounds by maximum norm

This section describes properties of upper bounds on f^* when applying the maximum norm. Denote by $\mathcal{H}$ the set of orthogonal matrices of size n and by

$$g^*:=\min_{R\in\mathbb{R}^{n\times n}:A=R^TR}\ \max_{x\in\mathcal{M}}\ \|Rx\|_\infty^2$$

the best upper bound obtained by a factorization of A.

Theorem 1 *We have*

$$f^*=n\cdot\max_{x\in\mathcal{M}}\ \min_{H\in\mathcal{H}}\ \|HGx\|_\infty^2\le n\cdot\min_{H\in\mathcal{H}}\ \max_{x\in\mathcal{M}}\ \|HGx\|_\infty^2=g^*. \tag{3}$$

Proof Let us prove the first equation in (3). For every $H\in\mathcal{H}$ and $x\in\mathcal{M}$, we have

$$\|Gx\|_2^2=\|HGx\|_2^2\le n\cdot\|HGx\|_\infty^2.$$

Taking the minimum over $H\in\mathcal{H}$,

$$\|Gx\|_2^2\le n\cdot\min_{H\in\mathcal{H}}\ \|HGx\|_\infty^2.$$

Taking the maximum over $x\in\mathcal{M}$,

$$f^*=\max_{x\in\mathcal{M}}\ \|Gx\|_2^2\le n\cdot\max_{x\in\mathcal{M}}\ \min_{H\in\mathcal{H}}\ \|HGx\|_\infty^2.$$

To show that the inequality is attained as equation, let $x\in\mathcal{M}$ and denote $y:=Gx$. Utilizing a Householder transformation, let $H\in\mathcal{H}$ be a Householder matrix transforming y to $\alpha\cdot e$, where $\alpha:=\frac{1}{\sqrt{n}}\|y\|_2$ (such a matrix always exists, see [13]). That is, $Hy=\alpha\cdot e$. Now, we have

$$n\cdot\|Hy\|_\infty^2=n\cdot\|\alpha\cdot e\|_\infty^2=n\cdot\alpha^2=\|y\|_2^2.$$

Therefore $\|Gx\|_2^2=n\cdot\min_{H\in\mathcal{H}}\ \|HGx\|_\infty^2$ for each $x\in\mathcal{M}$, which proves the equation.

Let us prove the right-hand side equation in (3), which takes the form

$$\min_{H\in\mathcal{H}}\ \max_{x\in\mathcal{M}}\ \|HGx\|_\infty^2=\min_{A=R^TR}\ \max_{x\in\mathcal{M}}\ \|Rx\|_\infty^2.$$

Let $H\in\mathcal{H}$ be arbitrary and put $R:=HG$. Then $R^TR=(HG)^THG=G^TH^THG=G^TG=A$ is a factorization of A. Conversely, let $A=G^TG=R^TR$ be two factorizations of A. Then $I_n=(G^T)^{-1}R^TRG^{-1}=(RG^{-1})^TRG^{-1}$, so $H:=RG^{-1}$ is an orthogonal matrix. Therefore we derived $R=HG$ for some $H\in\mathcal{H}$.

Eventually, the inequality $f^*\le g^*$ follows from the standard max–min inequality. □

In other words, the proposition says that the upper bound g^* overestimates f^* the same way as max–min inequality. The inequality holds as equation in certain cases, see Proposition 2. On the other hand, we can find examples of strict version of the inequality in (3); see Example 1.

Example 1 Let $\mathcal{M}$ be the convex hull of points $(0,0)^T$, $(1,0)^T$, $(\frac{\sqrt{3}}{2}, \frac{1}{2})^T$ and $(0,1)^T$, and let A be the identity matrix I_2. It is seen that $f^* = 1$. As each orthogonal matrix of size 2 has either the form

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}$$

for some $\theta \in [0, 2\pi)$, we have

$$\begin{aligned} &\min_{H\in\mathcal{H}} \max_{x\in\mathcal{M}} \|Hx\|_\infty^2 \\ &\quad = \min\nolimits_{\theta\in[0,2\pi)} \max\{|\cos\theta|, |\sin\theta|, |\cos(\theta - \tfrac{\pi}{6})|, |\cos(\theta + \tfrac{\pi}{3})|\}^2. \end{aligned}$$

The above equality is derived from the fact that convex functions attain their maximum at some vertices. Denote

$$f(\theta) = \max\{|\cos\theta|, |\sin\theta|, |\cos(\theta - \tfrac{\pi}{6})|, |\cos(\theta + \tfrac{\pi}{3})|\}.$$

It is seen that

$$f(\theta) = \begin{cases} \cos\theta & 0 \le \theta \le \frac{\pi}{12}, \\ \cos(\theta - \frac{\pi}{6}) & \frac{\pi}{12} \le \theta \le \frac{\pi}{3}, \\ \sin\theta & \frac{\pi}{3} \le \theta \le \frac{7\pi}{12}, \\ -\cos(\theta + \frac{\pi}{3}) & \frac{7\pi}{12} \le \theta \le \frac{5\pi}{6}, \\ -\cos\theta & \frac{5\pi}{6} \le \theta \le \pi. \end{cases}$$

Hence, $\min_{\theta\in[0,2\pi)} f(\theta) = \frac{\sqrt{3}}{2}$, which implies $g^* = \frac{3}{2} > f^* = 1$.

Proposition 1 *We have $g^* \le n \cdot f^*$.*

Proof. Write

$$\begin{aligned} g^* &= n \cdot \min_{H\in\mathcal{H}} \max_{x\in\mathcal{M}} \|HGx\|_\infty^2 \le n \cdot \min_{H\in\mathcal{H}} \max_{x\in\mathcal{M}} \|HGx\|_2^2 \\ &= n \cdot \min_{H\in\mathcal{H}} \max_{x\in\mathcal{M}} x^T A x = n \cdot f^*. \end{aligned}$$

□

Proposition 2 *Let $H^* \in \mathcal{H}$ and $x^* \in \mathcal{M}$ be optimal solutions for g^*. If $|H^*Gx^*|$ has all entries the same, then (3) holds as equation.*

Proof. The right-hand side of (3) reads

$$g^* = n\|H^*Gx^*\|_\infty^2 = \|H^*Gx^*\|_2^2 = \|Gx^*\|_2^2 \le f^*. \quad \square$$

Remark 1 (Extensions to singular A) The derived results can easily be extended to the case when A is singular. Let $m{:=}\operatorname{rank}(A)$ and $A = G^T G$ be a full rank factorization, that is, $G \in \mathbb{R}^{m\times n}$. Then (3) can be extended to

$$f^* = m \cdot \max_{x\in\mathcal{M}} \min_{H\in\mathcal{H}} \|HGx\|_\infty^2 \leq m \cdot \min_{H\in\mathcal{H}} \max_{x\in\mathcal{M}} \|HGx\|_\infty^2 = g^*, \tag{4}$$

where

$$g^*{:=} \min_{R\in\mathbb{R}^{m\times n}: A=R^T R} \max_{x\in\mathcal{M}} \|Rx\|_\infty^2.$$

The proof is analogous, only the proof of the right-hand side equation in (4) differs a bit because we cannot invert matrix G. The remedy is to consider the Moore–Penrose pseudoinverse $G^\dagger$ of G; see [13]. Let $A = G^T G = R^T R$ be two full rank factorizations of A. Then $I_m = (G^T)^\dagger G^T G G^\dagger = (G^T)^\dagger R^T R G^\dagger = (RG^\dagger)^T RG^\dagger$, so $H{:=}RG^\dagger$ is an orthogonal matrix. Now, $RG^\dagger G = HG$. Since the row spaces of R and G are the same and since $G^\dagger G$ is the projector to the row space of G, we have $R = RG^\dagger G = HG$. Therefore we again derived that $R = HG$ for some $H \in \mathcal{H}$.

2.1 Maximization on a box

In this section, we consider the case when the feasible set is a box. In contrast to numerical experiments from [8] for general polyhedral set $\mathcal{M}$, we will show that g^* is not tight in this case.

By a box we mean an interval vector

$$\boldsymbol{x} = [\underline{x}, \overline{x}] = \{x \in \mathbb{R}^n;\ \underline{x} \leq x \leq \overline{x}\},$$

where $\underline{x}, \overline{x} \in \mathbb{R}^n$, $\underline{x} \leq \overline{x}$. The center and the radius of $\boldsymbol{x}$ are respectively defined as

$$x_c = \frac{1}{2}(\underline{x} + \overline{x}), \quad x_\Delta = \frac{1}{2}(\overline{x} - \underline{x}).$$

Now, we can reformulate the original problem (1) for $\mathcal{M}$ being an interval box $\boldsymbol{x}$ as

$$f^* = \max\ x^T Ax \text{ subject to } x \in \boldsymbol{x}.$$

Assumptions. Without loss of generality assume that $x_c = 0$ and $x_\Delta = e$. The latter is obtained simply by a scaling. The former can be obtained as follows. Introduce an auxiliary variable z and consider the quadratic form

$$q(y, z){:=}(y^T, z) \begin{pmatrix} A & Ax_c \\ x_c^T A & x_c^T Ax_c \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = (y + zx_c)^T A(y + zx_c)$$

on the interval domain $y \in [-x_\Delta, x_\Delta]$, $z \in [-1, 1]$. The maximum value of the quadratic form is attained for $z \in \{\pm 1\}$. Since $q(y, z) = q(-y, -z)$, we can consider

only the value of $z = 1$. Thus we obtain that the quadratic form is the same as the original one by substitution $x{:=}y + x_c$.
Upper bound. The optimal upper bound based on (3) takes the form of

$$g^*{:=}n \cdot \min_{R\in\mathbb{R}^{n\times n}:A=R^TR} \max_{x\in\boldsymbol{x}} \|Rx\|_\infty^2. \tag{5}$$

Since

$$\max_{x\in\boldsymbol{x}} \|Rx\|_\infty^2 = \max_{x:\|x\|_\infty=1} \|Rx\|_\infty^2 = \||R|e\|_\infty^2 = \|R\|_\infty^2,$$

we can also reformulate (5) as

$$g^* = n \cdot \min_{R\in\mathbb{R}^{n\times n}:A=R^TR} \|R\|_\infty^2.$$

For the feasible set in the form of an interval box, the presented upper bound is not tight. As shown below, even a trivial upper bound $f^* \le e^T|A|e$ is never worse.

Proposition 3 *We have* $f^* \le e^T|A|e \le g^*$.

Proof For any factorization $A = R^TR$, we have

$$e^T|A|e = e^T|R^TR|e \le e^T|R^T||R|e = \||R|e\|_2^2 \le n\|R\|_\infty^2.$$

The factorization, for which g^* is attained then yields $e^T|A|e \le g^*$. □

On the other hand, there are cases when the upper bound is tight, as in the proposition below. Notice that condition $\mathrm{sgn}(G)\circ(es^T) \ge 0$ means that the entries of the column G_{*i} are nonnegative if $s_i = 1$ and nonpositive if $s_i = -1$.

Proposition 4 *If* $\mathrm{sgn}(G)\circ(es^T) \ge 0$ *and* $Gs = \alpha s$ *for some* $\alpha \ge 0$ *and* $s \in \{\pm 1\}^n$, *then* $f^* = g^*$.

Proof By the assumptions, each column of G has either nonnegative or nonpositive entries. Thus $f^* = \|Gs\|_2^2 = \|\alpha s\|_2^2 = n\alpha^2$. From (3), we have by putting $H{:=}I_n$

$$g^* \le n \cdot \max_{x\in\boldsymbol{x}} \|I_nGx\|_\infty^2 = n\|Gs\|_\infty^2 = n\|\alpha s\|_\infty^2 = n\alpha^2.$$

Therefore $f^* = g^*$. □

3 General preconditioning

In (3), we preconditioned matrix G by an orthogonal matrix H since orthogonal matrices have no effect on the quadratic form $x^TAx = x^TG^TGx$. In this section, we consider a general class of matrices that are suitable for upper bounds:

$$\begin{aligned}\mathcal{B}&:=\{B \in \mathbb{R}^{n\times n};\ \|x\|_2 \le \sqrt{n}\|Bx\|_\infty\ \forall x \in \mathbb{R}^n\}\\ &= \{B \in \mathbb{R}^{n\times n};\ 1 \le \sqrt{n}\|Bx\|_\infty\ \forall x \in \mathbb{R}^n : \|x\|_2 = 1\}.\end{aligned} \tag{6}$$

We immediately have the following:

Proposition 5 *We have* $f^* \le n \cdot \max_{x\in\mathcal{M}} \|BGx\|_\infty^2$ *for each* $B \in \mathcal{B}$.

Obviously, $\mathcal{H} \subseteq \mathcal{B}$. We will present some properties of the set $\mathcal{B}$ now. To this end, let $B = U\Sigma V^T$ be an SVD decomposition of a given $B \in \mathcal{B}$, where U, V are orthogonal matrices, and Σ is the diagonal matrix with singular values $\sigma_1 \ge \cdots \ge \sigma_n$ on the diagonal.

Proposition 6 *If* $\sigma_n(B) \ge 1$, *then* $B \in \mathcal{B}$.

Proof Since for the spectral norm $\|B^{-1}\|_2 = \sigma_n^{-1}(B) \le 1$, we have for each $y \in \mathbb{R}^n$

$$\|B^{-1}y\|_2 \le \|B^{-1}\|_2 \cdot \|y\|_2 \le \|y\|_2 \le \sqrt{n}\|y\|_\infty.$$

By substitution $x:=B^{-1}y$ the inequality $\|x\|_2 \le \sqrt{n}\|Bx\|_\infty$ follows. □

Proposition 7 *If* $B \in \mathcal{B}$, *then* $\sigma_n(B) > 1/\sqrt{n}$.

Proof Suppose to the contrary that $\sigma_n(B) \le 1/\sqrt{n}$. We distinguish two cases. First, suppose that $\sigma_n(B) < 1/\sqrt{n}$. Choose $x:=Ve_n = V_{*n}$, for which $\|x\|_2 = 1$ and

$$\sqrt{n}\|Bx\|_\infty = \sqrt{n}\|U\Sigma e_n\|_\infty = \sqrt{n}\sigma_n\|U_{*n}\|_\infty < \|U_{*n}\|_\infty \le 1;$$

a contradiction.

Suppose now that $\sigma_n(B) = 1/\sqrt{n}$ and choose $x:=V(\varepsilon, \ldots, \varepsilon, 1)^T$, where $\varepsilon > 0$ is sufficiently small. Then

$$\begin{aligned}\sqrt{n}\|Bx\|_\infty &= \sqrt{n}\|U\Sigma(\varepsilon, \ldots, \varepsilon, 1)^T\|_\infty\\ &= \sqrt{n}\left\|U \operatorname{diag}\left(\sigma_1\varepsilon, \ldots, \sigma_{n-1}\varepsilon, 1/\sqrt{n}\right)^T\right\|_\infty.\end{aligned}$$

If $|U_{nn}| = 1$, then $|U_{*n}| = e_n$ and

$$\|x\|_2 > 1 = \sqrt{n}\|Bx\|_\infty;$$

a contradiction. If $|U_{nn}| < 1$, then for sufficiently small $\varepsilon > 1$ we have $\sqrt{n}\|Bx\|_\infty < 1$, which is again a contradiction. □

The inequality in Proposition 7 is tight in the following sense.

Proposition 8 *For each* $\varepsilon > 0$ *there is* $B \in \mathcal{B}$ *such that* $\sigma_n(B) = (1 + \varepsilon)/\sqrt{n}$.

Proof We show that matrix $B:=\operatorname{diag}(\alpha,\ldots,\alpha,(1+\varepsilon)/\sqrt{n})$ works provided $\alpha>0$ is large enough. Let $x\in\mathbb{R}^n$ be arbitrary such that $\|x\|_2=1$ and we need to show that

$$1\le\left\|\left(\alpha\sqrt{n}\,x_1,\ldots,\alpha\sqrt{n}\,x_{n-1},(1+\varepsilon)x_n\right)\right\|_\infty. \tag{7}$$

This is obviously true when $|x|_n\ge 1/(1+\varepsilon)$. Otherwise, if $|x|_n<1/(1+\varepsilon)$, then in view of $\|x\|_2=1$ there is i such that

$$|x|_i\ge\sqrt{\frac{1}{n-1}\left(1-\frac{1}{(1+\varepsilon)^2}\right)}.$$

Therefore, the choice

$$\alpha:=\left(\frac{n}{n-1}\left(1-\frac{1}{(1+\varepsilon)^2}\right)\right)^{-1/2}$$

is sufficient to make (7) hold true. □

Notice that it is not true in general that the smaller singular values the better. Even orthogonal matrices need not be the best choice.

Example 2 Let $\mathcal{M}:=\{x^*\}=\{(1,9)^T\}$, $G=I_2$ and

$$B_1=\frac{1}{\sqrt{82}}\begin{pmatrix}-1&9\\9&1\end{pmatrix},\quad B_2=\frac{1}{\sqrt{82}}\begin{pmatrix}-1&9\\9&1\end{pmatrix}\begin{pmatrix}7&0\\0&1\end{pmatrix}.$$

We have $B_1,B_2\in\mathcal{B}$, matrix B_1 is orthogonal and matrix B_2 has singular values 7 and 1. Indeed, matrices B_1 and B_2 share the same orthogonal matrices from their SVD decomposition. However,

$$\|B_1x^*\|_\infty=8.8345>8.1719=\|B_2x^*\|_\infty,$$

so matrix B_2 provides tighter upper bound.

Lemma 1 *We have $B\in\mathcal{B}$ if and only if $\|B^{-1}y\|_2\le\sqrt{n}\ \forall y\in\mathbb{R}^n:|y|\le e$.*

Proof By substitution $y:=Bx$ (notice that B must be nonsingular) we have $B\in\mathcal{B}$ if and only if $\|B^{-1}y\|_2\le\sqrt{n}\|y\|_\infty$ for each $y\in\mathbb{R}^n$. It is sufficient to consider only y such that $|y|\le e$, giving rise to the equivalent condition $\|B^{-1}y\|_2\le\sqrt{n}$. □

Proposition 9 *Checking $B\in\mathcal{B}$ is a co-NP-hard problem.*

Proof By Lemma 1, we have to check $y^T(B^{-1})^TB^{-1}y\le n$ for each $y\in\mathbb{R}^n$ such that $|y|\le e$. In other words, we have to check if the optimal value of the quadratic programming problem

$$\max\ y^T(B^{-1})^TB^{-1}y \text{ subject to } -e\le y\le e$$

is at most n. However, maximization of a convex quadratic function on a hypercube is intractable [18]. □

Checking $B \in \mathcal{B}$ thus need not be an easy task. Thus we focus on some sufficient conditions and special cases.

Proposition 10 *If* $\||B^{-1}|e\|_2 \le \sqrt{n}$, *then* $B \in \mathcal{B}$.

Proof By Lemma 1, we have to check $\|B^{-1}y\|_2 \le \sqrt{n}$ for each $y \in \mathbb{R}^n$ such that $|y| \le e$. Since $\|B^{-1}y\|_2 \le \||B^{-1}|e\|_2$, the statement follows. □

The following proposition states when the above bound is tight.

Proposition 11 *Let* $B \in \mathbb{R}^{n\times n}$ *such that* $\operatorname{sgn}(B^{-1}) \circ (es^T) \ge 0$ *for some* $s \in \{\pm 1\}^n$. *Then* $B \in \mathcal{B}$ *if and only if* $\||B^{-1}|e\|_2 \le \sqrt{n}$.

Proof From the assumption we have $|B^{-1}| = B^{-1}\operatorname{diag}(s)$. Define

$$x^* := \frac{1}{\||B^{-1}|e\|_2}|B^{-1}|e = \frac{1}{\||B^{-1}|e\|_2}B^{-1}\operatorname{diag}(s)e > 0.$$

Recall that by definition we have $B \in \mathcal{B}$ if and only if $1 \le \sqrt{n}\|Bx\|_\infty$ for all $x \in \mathbb{R}^n$ such that $\|x\|_2 = 1$. We will show that the minimum of the right-hand side is attained for x^*.

In order that $B \in \mathcal{B}$, necessarily the condition for x^* must hold true

$$1 = \|x^*\|_2 \le \sqrt{n}\|Bx^*\|_\infty = \frac{\sqrt{n}}{\||B^{-1}|e\|_2}\|\operatorname{diag}(s)e\|_\infty = \frac{\sqrt{n}}{\||B^{-1}|e\|_2},$$

from which $\||B^{-1}|e\|_2 \le \sqrt{n}$.

Now, suppose to the contrary that there exists $x \in \mathbb{R}^n$ such that $\|x\|_2 = 1$ and $\|Bx\|_\infty < \|Bx^*\|_\infty$, which implies

$$|Bx| \le \|Bx\|_\infty e < \|Bx^*\|_\infty e = \frac{1}{\||B^{-1}|e\|_2}e.$$

From this we can derive two inequalities. First,

$$\operatorname{diag}(s)Bx < \frac{1}{\||B^{-1}|e\|_2}e,$$

from which

$$x < \frac{1}{\||B^{-1}|e\|_2}B^{-1}\operatorname{diag}(s)e = x^*.$$

Second,

$$-\operatorname{diag}(s)Bx < \frac{1}{\||B^{-1}|e\|_2}e,$$

from which

$$-x < \frac{1}{\||B^{-1}|e\|_2} B^{-1}\,\mathrm{diag}(s)e = x^*.$$

Therefore we have $|x| < x^*$, which contradicts the condition $1 = \|x\|_2 = \|x^*\|_2$. □

Obviously, the set $\mathcal{B}$ is not closed under addition. It is also not closed under multiplication as the following example shows: Let $B := \mathrm{diag}(10, 0.8)$; then $B \in \mathcal{B}$, but $B^2 \notin \mathcal{B}$ due to Proposition 7. The set $\mathcal{B}$ is, however, closed under multiplication by orthogonal matrices.

Proposition 12 *If $B \in \mathcal{B}$ and $H \in \mathcal{H}$, then $BH \in \mathcal{B}$.*

3.1 Nonnegative case

The definition of the set of preconditioning matrices $\mathcal{B}$ is very general. In this section, we suppose that $Gx \geq 0$ for every $x \in \mathcal{M}$; basically, this can be obtained by an appropriate shift. Now, the class of matrices that are suitable for upper bounds is defined as

$$\begin{aligned}\mathcal{B}^+ &:= \{B \in \mathbb{R}^{n\times n};\ \|x\|_2 \leq \sqrt{n}\|Bx\|_\infty\ \forall x \geq 0\}\\ &= \{B \in \mathbb{R}^{n\times n};\ 1 \leq \sqrt{n}\|Bx\|_\infty\ \forall x \geq 0,\ \|x\|_2 = 1\}.\end{aligned}$$

Obviously, $\mathcal{H} \subseteq \mathcal{B} \subseteq \mathcal{B}^+$. We conjecture that checking $B \in \mathcal{B}^+$ is co-NP-hard, too. It seems intractable even in the case $B \geq 0$. The condition from Proposition 6 is tight even for the class $\mathcal{B}^+$ since $(1-\varepsilon)I_n \notin \mathcal{B}^+$ for an arbitrarily small $\varepsilon > 0$.

Notice also that analogy of Proposition 7 does not hold for $\mathcal{B}^+$. For example, matrix $B = \frac{1}{\sqrt{n}} ee^T$ is singular, but it belongs to $\mathcal{B}^+$.

An analogy of Proposition 11 holds true even for class $\mathcal{B}^+$, however, it produces the same family of matrices.

Proposition 13 *Let $B \in \mathbb{R}^{n\times n}$ such that $\mathrm{sgn}(B^{-1}) = es^T$ for some $s \in \{\pm 1\}^n$. Then $B \in \mathcal{B}^+$ if and only if $\||B^{-1}|e\|_2 \leq \sqrt{n}$.*

Proof We have $B \in \mathcal{B}^+$ if and only if $1 \leq \sqrt{n}\|Bx\|_\infty$ for each $x \geq 0$, $\|x\|_2 = 1$. This brings us to the optimization problem

$$\min\ \|Bx\|_\infty \text{ subject to } x \geq 0,\ \|x\|_2 = 1.$$

We can reformulate it as

$$\min\ z \text{ subject to } \pm Bx \leq ez,\ x \geq 0,\ \|x\|_2 = 1.$$

Since $\mathrm{diag}(s)B^{-1} = |B^{-1}| \geq 0$, we can write

$$\min\ z \text{ subject to } \pm\,\mathrm{diag}(s)x \leq \mathrm{diag}(s)B^{-1}ez,\ x \geq 0,\ \|x\|_2 = 1,$$

or

$$\min\ z \text{ subject to } \pm x \le |B^{-1}|ez,\ x \ge 0,\ \|x\|_2 = 1.$$

Condition $-x \le |B^{-1}|ez$ is redundant. Condition $x \le |B^{-1}|ez$ will be satisfied as equality for the optimal solution since otherwise we can define $x' := |B^{-1}|ez$, and $x'' := x'/\|x'\|$ then gives smaller objective value $z'' := \|Bx''\|_\infty$. Hence the problem reduces to

$$\min\ z \text{ subject to } \||B^{-1}|ez\|_2 = 1,\ z \ge 0,$$

from which the optimal value is $z = 1/\||B^{-1}|e\|_2$. Therefore $B \in \mathcal{B}^+$ if and only if $1 \le \sqrt{n}z$, which yields the condition from the statement. □

Now, we present several sufficient conditions for matrix B to belong to class $\mathcal{B}^+$.

Proposition 14 *Let $B \in \mathbb{R}^{n\times n}$ such that $B_{i*} \ge \frac{1}{\sqrt{n}}e^T$ for some $i \in \{1,\dots,n\}$. Then $B \in \mathcal{B}^+$.*

Proof For each $x \ge 0$, $\|x\|_2 = 1$, we have $\|Bx\|_\infty \ge |Bx|_i \ge B_{i*}e^T x \ge 1$. □

Proposition 15 *Let $B \in \mathbb{R}^{n\times n}$, $B \ge 0$. Define $c_j := \max_i B_{ij}$ for $j = 1,\dots,n$. Let I be the row index set of these maxima. For each $i \in I$, choose the minimum value of all maxima being in ith row of B, and put the corresponding column index to the set J. If $\sum_{j\in J} c_j^{-2} \le n$, then $B \in \mathcal{B}^+$.*

***Proof*.** Define $\gamma := \sqrt{\sum_{j\in J} c_j^{-2}}$ and B_{IJ} to be the submatrix indexed by rows I and columns J. Let $x \ge 0$, $\|x\|_2 = 1$. Define $\tilde{x}$ to be restriction of x to the index set J, and moreover each removed entry $x_{j'}$ is added to the entry x_j, $j \in J$, that caused that $j' \notin J$ by the definition of J. Now we have $\|\tilde{x}\|_2 \ge 1$ and $\|Bx\|_\infty \ge \|B_{IJ}\tilde{x}\|_\infty$. Next, there is $j \in J$ such that $\tilde{x}_j \ge (c_j\gamma)^{-1}$. Let $i \in I$ be the index corresponding to j. Then $B_{ij}\tilde{x}_j = c_j\tilde{x}_j \ge \gamma^{-1}$. Therefore

$$\sqrt{n}\|Bx\|_\infty \ge \sqrt{n}\|B_{IJ}\tilde{x}\|_\infty \ge \sqrt{n}B_{ij}\tilde{x}_j \ge \sqrt{n}\gamma^{-1} \ge 1. \quad □$$

Corollary 1 *Let $B \in \mathbb{R}^{n\times n}$, $B \ge 0$. Then $B \in \mathcal{B}^+$ as long as each column of B contains at least one entry greater than or equal to* 1.

4 Upper bounds by other vector norms

Besides the maximum norm, we can use also other norms in (2) to obtain an upper bound on f^*. Let $\|\cdot\|$ be any vector norm. Since all vector norms are equivalent, there is $\beta > 0$ such that $\|x\|_2 \le \beta\|x\|$ for each $x \in \mathbb{R}^n$. Let $\tilde{e} \in \mathbb{R}^n$ be a vector, for which this bound is tight, that is, $\|\tilde{e}\|_2 = \beta\|\tilde{e}\|$. An adaptation of (2) reads

$$f^* = \max_{x\in\mathcal{M}} \|Gx\|_2^2 \le \beta^2 \cdot \max_{x\in\mathcal{M}} \|Gx\|^2. \tag{8}$$

By

$$h^* := \beta^2 \cdot \min_{R \in \mathbb{R}^{n\times n}: A = R^T R} \ \max_{x \in \mathcal{M}} \|Rx\|^2 \tag{9}$$

we denote the optimal upper bound based on factorization of A. We can extend Theorem 1 to general vector norms.

Theorem 2 *We have*

$$f^* = \beta^2 \cdot \max_{x\in\mathcal{M}} \min_{H\in\mathcal{H}} \|HGx\|^2 \le \beta^2 \cdot \min_{H\in\mathcal{H}} \max_{x\in\mathcal{M}} \|HGx\|^2 = h^*. \tag{10}$$

Proof Let us prove the first equation in (10). For every $H \in \mathcal{H}$ and $x \in \mathcal{M}$, we have

$$\|Gx\|_2^2 = \|HGx\|_2^2 \le \beta^2 \|HGx\|^2.$$

Taking the minimum over $H \in \mathcal{H}$,

$$\|Gx\|_2^2 \le \beta^2 \cdot \min_{H\in\mathcal{H}} \|HGx\|^2.$$

Taking the maximum over $x \in \mathcal{M}$,

$$f^* = \max_{x\in\mathcal{M}} \|Gx\|_2^2 \le \beta^2 \cdot \max_{x\in\mathcal{M}} \min_{H\in\mathcal{H}} \|HGx\|^2.$$

To show that the inequality is attained as equation, let $x \in \mathcal{M}$ denote $y := Gx$. Then

$$\|y\|_2^2 \le \beta^2 \cdot \min_{H\in\mathcal{H}} \|Hy\|^2.$$

Utilizing a Householder transformation, let $H \in \mathcal{H}$ be a Householder matrix transforming y to $\alpha \cdot \tilde{e}$, where $\alpha := \|y\|_2 / \|\tilde{e}\|_2$. That is, $Hy = \alpha \cdot \tilde{e}$. Now, we have

$$\beta^2 \|Hy\|^2 = \beta^2 \|\alpha \cdot \tilde{e}\|^2 = \beta^2 \|\tilde{e}\|^2 \frac{\|y\|_2^2}{\|\tilde{e}\|_2^2} = \beta^2 \|\tilde{e}\|^2 \frac{\|y\|_2^2}{\beta^2 \|\tilde{e}\|^2} = \|y\|_2^2.$$

Therefore $\|Gx\|_2^2 = \beta^2 \cdot \min_{H\in\mathcal{H}} \|HGx\|^2$ for each $x \in \mathcal{M}$, which proves the equation.

The proof of the right-hand side equation in (10) is the same as for (3).

The inequality follows from $f^* \le h^*$ or from the standard max–min inequality. □

4.1 Upper bounds on a box by ℓ_1-norm

It is natural to use the ℓ_1-norm as an alternative norm, which is discussed in this section. Here, we have $\beta = 1$ since $\|x\|_2 \le \|x\|_1$ for each $x \in \mathbb{R}^n$. In this section we assume that the feasible set is an interval box, that is, $\mathcal{M} = \boldsymbol{x} = [-e, e]$.

Proposition 16 *If G has nonzero entries in one row only, then $f^* = h^*$.*

Proof From the assumption, $Gs = e_i y^T$ for some i, where $y \in \mathbb{R}^n$. Denoting $s := \operatorname{sgn}(y) \in \{\pm 1\}^n$ and $\alpha := y^T s = |y|^T e$, we have $Gs = \alpha e_i$. Next, $f^* = \|Gs\|_2^2 = \|\alpha e_i\|_2^2 = \alpha^2$. From (10), we have by putting $H := I_n$

$$h^* \leq \max_{x \in \boldsymbol{x}} \|I_n Gx\|_1^2 = \|Gs\|_1^2 = \|\alpha e_i\|_1^2 = \alpha^2.$$

Therefore $f^* = h^*$. □

Unfortunately, ℓ_1-norm is not suitable for a computationally cheap upper bound because even the inner optimization problem in (9) is hard. The value

$$\max_{x \in \boldsymbol{x}} \|Rx\|_1 = \max_{x : \|x\|_\infty = 1} \|Rx\|_1 = \|R\|_{\infty,1}$$

is the so called subordinate matrix norm of R. Rohn [15] proved that, in contrast to many other norms, this one is NP-hard to compute (cf. also [3]). Tight bounds can be calculated by means of semidefinite programming [6]. Some other bounds and not apriori exponential algorithm were presented in [7].

5 Conclusion

In this paper, we discussed upper bounds on the maximum of a convex quadratic function on a convex polyhedral set. In particular, we focused on the objective matrix factorization and estimations of the Euclidean norm by another vector norms. We presented some kind of duality (utilizing min–max inequality) and derived the related theoretical properties.

The preliminary numerical experiments from [8] indicate a potential of obtaining tight bounds, however, there are still many obstacles and challenging problems remaining.

First, the value of g^* needs to be inspected more from the point of view of both theory and methods. Computational complexity of determining g^* is unknown, as well as any characterization of optimality. The heuristic methods from [8] are promising, but there is an open space for other, too.

Second, we showed that our approach (with maximum norm) is not convenient when $\mathcal{M}$ has the form of a box. On the other hand, for general convex polyhedra the experiments from [8] were favorable. Thus identifying the classes of sets for which our approach is suitable is another open problem.

Third, we proposed a more general preconditioning of the factors than just by orthogonal matrices. It would be interesting to determine the gap and quality of the upper bounds. Also, some (heuristic) method employing the preconditioning would be of interest. From the theoretical perspective, we stated a conjecture on intractability of recognizing matrices belonging to $\mathcal{B}^+$.

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References

1. Bazaraa, M.S., Sherali, H.D., Shetty, C.M.: Nonlinear Programming. Theory and Algorithms, 3rd edn. Wiley, New York (2006)
2. Černý, M., Hladík, M.: The complexity of computation and approximation of the t-ratio over one-dimensional interval data. Comput. Stat. Data Anal. **80**, 26–43 (2014)
3. Fiedler, M., Nedoma, J., Ramík, J., Rohn, J., Zimmermann, K.: Linear Optimization Problems with Inexact Data. Springer, New York (2006)
4. Floudas, C.A., Visweswaran, V.: Quadratic optimization. In: Horst, R., Pardalos, P.M. (eds.) Handbook of Global Optimization, pp. 217–269. Springer, Boston, MA (1995)
5. Gould, N.I.M., Toint, P.L.: A quadratic programming bibliography. RAL Internal Report 2000-1, Science and Technology Facilities Council, Scientific Computing Department, Numerical Analysis Group (2012). ftp://ftp.numerical.rl.ac.uk/pub/qpbook/qp.pdf. Accessed 24 Nov 2019
6. Hartman, D., Hladík, M.: Tight bounds on the radius of nonsingularity. In: Nehmeier, Mm, et al. (eds.) Scientific Computing, Computer Arithmetic, and Validated Numerics: 16th International Symposium, SCAN 2014, Würzburg, Germany, September 21–26, LNCS, vol. 9553, pp. 109–115. Springer (2016)
7. Hartman, D., Hladík, M.: Regularity radius: properties, approximation and a not a priori exponential algorithm. Electron. J. Linear Algebra **33**, 122–136 (2018)
8. Hladík, M., Hartman, D.: Maximization of a convex quadratic form on a polytope: factorization and the Chebyshev norm bounds. In: Le Thi, H.A., et al. (eds.) Optimization of Complex Systems: Theory, Models, Algorithms and Applications, AISC, vol. 991, pp. 119–127. Springer, Cham (2020)
9. Horst, R., Tuy, H.: Global Optimization. Deterministic Approaches. Springer, Berlin (1990)
10. Konno, H.: Maximizing a convex quadratic function over a hypercube. J. Oper. Res. Soc. Jpn. **23**(2), 171–188 (1980)
11. Kreinovich, V., Lakeyev, A., Rohn, J., Kahl, P.: Computational Complexity and Feasibility of Data Processing and Interval Computations. Kluwer, Dordrecht (1998)
12. Locatelli, M., Schoen, F.: Global optimization: Theory, Algorithms, and Applications, MOS-SIAM Series on Optimization, vol. 15. SIAM, Philadelphia, PA (2013)
13. Meyer, C.D.: Matrix Analysis and Applied Linear Algebra. SIAM, Philadelphia (2000)
14. Pardalos, P., Rosen, J.: Methods for global concave minimization: a bibliographic survey. SIAM Rev. **28**(3), 367–79 (1986)
15. Rohn, J.: Computing the norm $\|A\|_{\infty,1}$ is NP-hard. Linear Multilinear Algebra **47**(3), 195–204 (2000)
16. Sherali, H.D., Adams, W.P.: A Reformulation-Linearization Technique for Solving Discrete and Continuous Nonconvex Problems. Kluwer, Boston (1999)
17. Tuy, H.: Convex Analysis and Global Optimization, Springer Optimization and Its Applications, vol. 110, 2nd edn. Springer, Cham (2016)
18. Vavasis, S.A.: Nonlinear Optimization: Complexity Issues. Oxford University Press, New York (1991)
19. Vavasis, S.A.: Polynomial time weak approximation algorithms for quadratic programming. In: Pardalos, P.M. (ed.) Complexity in Numerical Optimization, pp. 490–500. World Scientific Publishing, Singapore (1993)
20. Zamani, M.: A new algorithm for concave quadratic programming. J. Glob. Optim. **75**(3), 655–681 (2019)
21. Zamani, M.: New bounds for nonconvex quadratically constrained quadratic programming. arXiv preprint arXiv:1902.08861 (2019)