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New bounds on the unconstrained quadratic integer programming problem

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Abstract We consider the maximization $\gamma = \max\{x^T Ax : x \in \{-1, 1\}^n\}$ for a given symmetric $A \in \mathcal{R}^{n\times n}$. It was shown recently, using properties of zonotopes and hyperplane arrangements, that in the special case that A has a small rank, so that $A = VV^T$ where $V \in \mathcal{R}^{n\times m}$ with $m < n$, then there exists a polynomial time algorithm (polynomial in n for a given m) to solve the problem $\max\{x^T VV^T x : x \in \{-1, 1\}^n\}$. In this paper, we use this result, as well as a spectral decomposition of A to obtain a sequence of non-increasing upper bounds on γ with no constraints on the rank of A. We also give easily computable necessary and sufficient conditions for the absence of a gap between the solution and its upper bound. Finally, we incorporate the semidefinite relaxation upper bound into our scheme and give an illustrative example.

Keywords Quadratic integer programming · Semidefinite relaxation · Zonotope · Hyperplane arrangements

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1 Notation

$\mathcal{R}$ denotes the set of real numbers. For integer n, $\mathcal{R}^n$ denotes the space of n-dimensional (column) vectors whose entries are in $\mathcal{R}$, and, for real a and b, $\{a, b\}^n$ denotes the set of all n-dimensional vectors whose entries are either a or b. For integers n and m, $\mathcal{R}^{n\times m}$ denotes the space of all $n \times m$ matrices whose entries are in $\mathcal{R}$. For $A \in \mathcal{R}^{n\times m}$, A^T denotes the transpose of A. If $A = A^T \in \mathcal{R}^{n\times n}$, $\underline{\lambda}(A)$ denotes the smallest and $\bar{\lambda}(A)$ the largest, eigenvalue of A and we write $A \succeq 0$ if $\underline{\lambda}(A) \geq 0$ and $A \succ 0$ if $\underline{\lambda}(A) > 0$. The m–dimensional identity matrix is denoted by I_m and the $m \times n$ null matrix is denoted by $0_{m,n}$ with the subscripts omitted if they can be inferred from the context. For $A = A^T \in \mathcal{R}^{n\times n}$ the spectral decomposition is the decomposition $A = U\Lambda U^T$, where $U \in \mathcal{R}^{n\times n}$ is orthogonal and $\Lambda \in \mathcal{R}^{n\times n}$ is a diagonal matrix of the eigenvalues of A.

2 Introduction

In this paper we consider the classical NP–hard unconstrained quadratic integer programming (QIP) problem in $(-1, 1)$ variables

$$\gamma := \max_{x \in \{-1,1\}^n} x^T A x,$$

for given $A = A^T \in \mathcal{R}^{n\times n}$ [11]. The QIP problem has many applications in combinatorial optimization. The form of the QIP considered here can be generalized to zero one problems using the simple linear transformation $y = (x + e)/2$ where $e \in \mathcal{R}^n$ is the vector of ones and to problems involving a linear term ($x^T A x + 2b^T x$ for given $b \in \mathcal{R}^n$) using the simple homogenization procedure

$$\begin{aligned}\max_{x \in \{-1,1\}^n} x^T A x + 2b^T x &= \max_{\substack{x \in \{-1,1\}^n \\ x_{n+1} \in \{-1,1\}}} x^T A x + 2b^T x x_{n+1} \\ &= \max_{x \in \{-1,1\}^{n+1}} x^T \begin{bmatrix} A & b \\ b^T & 0 \end{bmatrix} x.\end{aligned}$$

It is well known that other optimization problems, such as the Maximum-Cut Problem [6] can also be transformed to the QIP problem.

Since the QIP problem is NP hard, exact solutions of large-scale problems are normally impossible to obtain. However, in many practical applications bounds are often sufficient. These may help to identify sub-optimal solutions or to indicate infeasibility of the design objectives.

The original motivation of this work, and also of our related work in [19], arose from the attempt to develop systematic methods for breaching the convex relaxation upper bound of the structured singular value arising in robust control [12–16,18]. Our approach to both problems is similar: The solution of the dual (relaxation) problem is used to formulate an auxiliary optimization problem which is of the same form as the primal, but of reduced rank, and thus computationally tractable. The solution of the auxiliary problem is then shown to induce improved bounds on the original (primal) problem. We believe that this approach is general and can be applied to a large class of optimization problems where relaxations are employed. Apart from the similarity of the general approach, the QIP considered in this work appears to be directly relevant to the structured singular value problem in the case of real uncertainty [15].

For notational convenience in our subsequent analysis, we redefine the constraint set as

$$\mathcal{X} := \{-n^{-\frac{1}{2}}, n^{-\frac{1}{2}}\}^n = \frac{1}{\sqrt{n}}\{-1, 1\}^n, \tag{2.1}$$

so that the QIP we consider becomes

$$\gamma := \max_{x \in \mathcal{X}} f(x) = \frac{1}{n} \max_{y \in \{-1,1\}^n} f(y), \tag{2.2}$$

where

$$f(x) = x^T A x = \frac{1}{n} f(\sqrt{n}x), \quad y = \sqrt{n}x \in \{-1, 1\}^n. \tag{2.3}$$

The paper is organized as follows. In Sect. 3 we derive a sequence of non–increasing upper bounds on the QIP problem. Each successive bound can be obtained by solving a reduced rank QIP problem of increasing rank. Section 4 establishes a link between these reduced rank QIP problems and the problem of enumerating the vertices of a zonotope. Section 5 incorporates the semidefinite relaxation upper bound into our scheme. Section 6 gives an example that illustrates our bounds. Finally, we summarize our results in Sect. 7.

3 Upper bounds on the QIP problem

In this section we present our main results which generalize the technique in [19]. Our results can be formulated directly in the form of two algorithms. These involve a sequential procedure and a "one-shot" method, respectively, both of which can be solved in polynomial-time. In either case, the bounds on the original QIP problem are obtained by solving an auxiliary QIP problem of reduced rank, which determines the complexity of the resulting relaxation algorithm. Thus, it is possible to calculate the tightest possible bound which can be obtained with our method that is compatible with the available computational power.

Consider the QIP problem defined in Eqs. 2.2 and 2.3. If all the eigenvalues of A are equal (that is, if $A = \lambda I_n$ for some $\lambda \in \mathcal{R}$), then the solution of the QIP problem is trivial and we may therefore assume that A has at least two distinct eigenvalues. The next result defines a sequence of non–increasing upper bounds on γ, starting from the largest eigenvalue of A, which is known to be an upper bound on γ. The derivation of each bound requires the solution of a reduced rank QIP problem of the form $\max_{x\in\mathcal{X}} x^T V V^T x$ where V is a tall matrix. The result is given in a form that is readily implementable as an algorithm.

Lemma 3.1 *Let $A = A^T \in \mathcal{R}^{n\times n}$ be given and assume that A has at least two distinct eigenvalues. Let $\mathcal{X}$, γ and $f(x)$ be as defined in (2.1), (2.2) and (2.3), respectively. Let A have r distinct eigenvalues $\lambda_1 > \cdots > \lambda_r$ with multiplicities $m_1, \ldots, m_r$, respectively, where $2 \le r \le n$ and $\sum_{i=1}^r m_i = n$ so that A has an ordered spectral form*

$$A = U\Lambda U^T = \begin{bmatrix} U_1 \cdots U_r \end{bmatrix} \begin{bmatrix} \lambda_1 I_{m_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_r I_{m_r} \end{bmatrix} \begin{bmatrix} U_1{}^T \\ \vdots \\ U_r{}^T \end{bmatrix} = \sum_{j=1}^r U_j \lambda_j U_j{}^T,$$

where $U = [\, U_1 \ \cdots \ U_r \,] \in \mathcal{R}^{n\times n}$ is orthogonal, $\Lambda = diag(\lambda_1 I_{m_1}, \ldots, \lambda_r I_{m_r})$ is the diagonal matrix of the eigenvalues of A, with $U_i \in \mathcal{R}^{n\times m_i}$, $i = 1, \ldots, r$. Set

$$f_0(x) = 0, \qquad \phi_0 = 0, \qquad \gamma_0 = 0, \qquad \lambda_{r+1} = 0,$$

and for $i = 1, \ldots, r$, define

$$f_i(x) = \sum_{j=1}^{i} x^T U_j \frac{\lambda_j - \lambda_{i+1}}{\gamma_i - \lambda_{i+1}} U_j{}^T x \tag{3.1}$$

$$= x^T \begin{bmatrix} U_1 \cdots U_i \end{bmatrix} \begin{bmatrix} \frac{\lambda_1-\lambda_{i+1}}{\gamma_i-\lambda_{i+1}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{\lambda_i-\lambda_{i+1}}{\gamma_i-\lambda_{i+1}} \end{bmatrix} \begin{bmatrix} U_1{}^T \\ \vdots \\ U_i{}^T \end{bmatrix} x,$$

$$\phi_i = \max_{x \in \mathcal{X}} f_i(x), \tag{3.2}$$

$$\gamma_i = \phi_{i-1}\gamma_{i-1} + (1 - \phi_{i-1})\lambda_i. \tag{3.3}$$

Then for $i = 1, \ldots, r$,

$$0 \le \phi_i \le 1, \tag{3.4}$$

$$\lambda_i \le \gamma_i, \tag{3.5}$$

and

$$\gamma \le \gamma_i. \tag{3.6}$$

Furthermore,

$$\gamma = \gamma_i \Leftrightarrow \phi_i = 1 \Leftrightarrow \exists x \in \mathcal{X} \text{ such that } \phi_{i-1} = f_{i-1}(x) \text{ and } \sum_{j=1}^{i} x^T U_j U_j{}^T x = 1. \tag{3.7}$$

Hence,

$$\gamma = \gamma_r \le \cdots \le \gamma_2 \le \gamma_1 = \lambda_1. \tag{3.8}$$

Finally, suppose that $\phi_j < 1$ *for* $j = 1, \ldots, i-1$ *and* $\phi_i = 1$. *Then*

$$\gamma = \gamma_r = \cdots = \gamma_i < \gamma_{i-1} < \cdots < \gamma_1. \tag{3.9}$$

Proof First note that $f_1(x) = x^T U_1 U_1{}^T x$ and so $0 \le \phi_1 \le 1$ since $0 \preceq U_1 U_1{}^T \preceq I_n$. Next, we prove (3.4) and (3.5) by induction. Clearly, $\lambda_1 = \gamma_1$. Thus (3.4) and (3.5) are satisfied for $i = 1$. Suppose they are satisfied for $i < r$ and let γ_{i+1} be defined by (3.3). Then since $\gamma_i \ge \lambda_i > \lambda_{i+1}$ and $0 \le \phi_i \le 1$ it follows that $\gamma_{i+1} \ge \lambda_{i+1}$. An inspection of (3.1) (with i set to $i+1$) verifies that $f_{i+1}(x) \ge 0$. Furthermore, a simple calculation verifies that for all $x \in \mathcal{X}$ and $0 < i < r-1$,

$$f_{i+1}(x) = 1 - \frac{(\gamma_i - \lambda_{i+1})[\phi_i - f_i(x)] + (\lambda_{i+1} - \lambda_{i+2})\left[1 - \sum_{j=1}^{i+1} x^T U_j U_j{}^T x\right]}{(\gamma_{i+1} - \lambda_{i+2})},$$

and so $f_{i+1}(x)$ (and hence ϕ_{i+1}) is ≤ 1 since all terms in bracket in both numerator and denominator are non-negative. This proves (3.4) and (3.5).

Next we prove (3.6). A manipulation shows that (see Appendix A for a full derivation)

$$f(x) = \begin{cases} \gamma_1 - \sum_{j=2}^{r} x^T U_j (\lambda_1 - \lambda_j) U_j{}^T x - \lambda_1 (1 - x^T x), \\ \gamma_i - h_i(x), \ 1 < i < r, \\ \gamma_r - (\gamma_{r-1} - \lambda_r)(\phi_{r-1} - f_{r-1}(x)) - \lambda_r (1 - x^T x), \end{cases} \tag{3.10}$$

$$f_i(x) = \begin{cases} x^T U_1 U_1{}^T x, \ i = 1, \\ 1 - g_i(x), \ 1 < i < r, \\ \gamma_r^{-1} f(x), \ i = r, \end{cases} \tag{3.11}$$

where

$$h_i(x) = (\gamma_{i-1} - \lambda_i)\,(\phi_{i-1} - f_{i-1}(x)) - \sum_{j=i+1}^{r} x^T U_j(\lambda_i - \lambda_j)U_j{}^T x - \lambda_i(1 - x^T x)$$

$$g_i(x) = \frac{(\gamma_{i-1} - \lambda_i)\left[\phi_{i-1} - f_{i-1}(x)\right] + (\lambda_i - \lambda_{i+1})[1 - \sum_{j=1}^{i} x^T U_j U_j{}^T x]}{(\gamma_i - \lambda_{i+1})}.$$

The three expressions for $f(x)$ show that for each $i = 1, 2, \ldots, r$, $f(x) \leq \gamma_i$ for every $x \in \mathcal{X}$; using (3.2) this shows that $\gamma \leq \gamma_i$ for all $i = 1, 2, \ldots, r$; which is (3.6).

We prove (3.7) first when $i = 1$. Now using the definition of ϕ_i and the first expression of $f_i(x)$ in (3.11),

$$\phi_1 = \max_{x \in \mathcal{X}} f_1(x) = \max_{x \in \mathcal{X}} x^T U_1 U_1{}^T x.$$

It follows that $\phi_1 = 1$ if and only if there exists $x \in \mathcal{X}$ such that $x^T U_1 U_1{}^T x = 1$. Using the definition of γ and the first expression for $f(x)$ in (3.10),

$$\gamma = \max_{x \in \mathcal{X}} f(x) = \max_{x \in \mathcal{X}} \gamma_1 - \sum_{j=2}^{r} x^T U_j(\lambda_1 - \lambda_j)U_j{}^T x.$$

It follows that $\gamma = \gamma_1$ if and only if there exists $x \in \mathcal{X}$ such that $\sum_{j=2}^{r} x^T U_j(\lambda_1 - \lambda_j)U_j{}^T x = 0$, or equivalently, if $x^T U_1 U_1{}^T x = 1$ since $\lambda_1 > \lambda_j$ for all $j > 1$. Next, we prove (3.7) for i such that $1 < i < r$. Suppose first that $\gamma = \gamma_i$ for some i such that $1 < i < r$. Then there exists $\hat{x} \in \mathcal{X}$ such that $f(\hat{x}) = \gamma = \gamma_i$, i.e. $f_{i-1}(\hat{x}) = \phi_{i-1}$ and $U_j^T \hat{x} = 0$ for $j = i + 1, \ldots, r$. Thus

$$1 = \|\hat{x}\|^2 = \sum_{j=1}^{r} \hat{x}^T U_j U_j^T \hat{x} = \sum_{j=1}^{i} \hat{x}^T U_j U_j^T \hat{x},$$

and so $f_i(\hat{x}) = 1$ by (3.11). Since $f_i(x) \leq 1$ for every $x \in \mathcal{X}$ we have that $\phi_i = \max_{x \in \mathcal{X}} f_i(x) = f_i(\hat{x}) = 1$. Conversely, suppose that $\phi_i = 1$ $(1 < i < r)$. Then, since $f_i(x) \leq 1$ for every $x \in \mathcal{X}$, there exists $\hat{x} \in \mathcal{X}$ such that $f_i(\hat{x}) = 1$. Since $\gamma_{i-1} - \lambda_i > 0$, $\lambda_i - \lambda_{i-1} > 0$ and $\gamma_i - \lambda_{i+1} > 0$, this implies that $f_{i-1}(\hat{x}) = \phi_{i-1}$ and $\sum_{j=1}^{i} \hat{x}^T U_j U_j^T \hat{x} = 1$, hence $U_j^T \hat{x} = 0$ for $j = i + 1, \ldots, r$. Thus $\max_{x \in \mathcal{X}} f(x) = f(\hat{x}) = \gamma_i$ or $\gamma \geq \gamma_i$, which together with (3.6) proves that $\gamma = \gamma_i$. To prove (3.7) when $i = r$, note that

$$\phi_r = \max_{x \in \mathcal{X}} f_r(x) = \frac{1}{\gamma_r} \max_{x \in \mathcal{X}} f(x) = \frac{\gamma}{\gamma_r}.$$

It follows that $\gamma = \gamma_r$ if and only if $\phi_r = 1$. Furthermore, using the third expression of $f(x)$ in (3.10),

$$\gamma = \max_{x \in \mathcal{X}} f(x) = \max_{x \in \mathcal{X}} \gamma_r - (\gamma_{r-1} - \lambda_r)\,(\phi_{r-1} - f_{r-1}(x)).$$

It follows that $\gamma = \gamma_r$ if and only if there exists $x \in \mathcal{X}$ such that $\phi_{r-1} = f_{r-1}(x)$ as required (since $\sum_{j=1}^{r} x^T U_j U_j{}^T x = 1$ for all $x \in \mathcal{X}$ and $\gamma_{r-1} > \lambda_r$).

To prove (3.8) we need to show that $\{\gamma_i\}$ is a non-increasing sequence with $\gamma_r = \gamma$. The first property follows on noting that $\gamma_{i-1} - \gamma_i = (\gamma_{i-1} - \lambda_i)(1 - \phi_{i-1})$ using (3.3), since $0 \leq \phi_i \leq 1$ and $\gamma_{i-1} \geq \lambda_{i-1} > \lambda_i$. To show that $\gamma_r = \gamma$ note first that $\gamma \leq \gamma_r$ from (3.6). Let $\hat{x} \in \operatorname{argmax}\{f_{r-1}(x) : x \in \mathcal{X}\}$ so that $f_{r-1}(\hat{x}) = \phi_{r-1}$. Then using the third expression

for $f(x)$ in (3.10) we get $f(\hat{x}) = \gamma_r$ since $\hat{x}^T\hat{x} = 1$. Thus $\gamma \geq \gamma_r$ and so $\gamma = \gamma_r$. Note that in this case, we also have $\operatorname{argmax}\{f(x) : x \in \mathcal{X}\} = \operatorname{argmax}\{f_{r-1}(x) : x \in \mathcal{X}\}$.

Finally, suppose that $\phi_j < 1$ for $j = 1, \ldots, i-1$ and $\phi_i = 1$. Then, there exists $\hat{x} \in \mathcal{X}$ such that $f_i(\hat{x}) = 1$. This, together with the second expression for $f_i(x)$ in (3.11), implies that $f_{i-1}(\hat{x}) = \phi_{i-1}$ and that $U_j^T\hat{x} = 0$ for $j = i+1, \ldots r$. Thus the second expression for $f(x)$ in (3.10) implies that $f(\hat{x}) = \gamma_i$ so that $\gamma \geq \gamma_i$, and this in turn implies that $\gamma = \gamma_i$ from (3.6). Equation (3.8) now implies that

$$\gamma = \gamma_r = \cdots = \gamma_i \leq \gamma_{i-1} \leq \cdots \leq \gamma_1. \tag{3.12}$$

Next, suppose for contradiction that one of the above inequalities is actually an equality, i.e. that $\gamma_j = \gamma_{j-1} =: \hat{\gamma}$ for some $j \leq i$. Since $\gamma_j = \phi_{j-1}\gamma_{j-1} + (1-\phi_{j-1})\lambda_j$, this implies that $(1-\phi_{j-1})\hat{\gamma} = (1-\phi_{j-1})\lambda_j$ and hence that $\gamma_j = \gamma_{j-1} = \lambda_j$ since $\phi_{j-1} < 1$ by assumption; this however is a contradiction since $\gamma_{j-1} \geq \lambda_{j-1} > \lambda_j$, which establishes (3.9) and concludes the proof. □

The algorithm suggested by Lemma 3.1 iteratively calculates a non-increasing sequence γ_i, $i = 1, \ldots, r-1$, of upper bounds on γ. Each step requires the solution of the maximization problem in (3.2). Although, as shown in [2] (see Sect. 4 below), each of these optimizations can be solved in polynomial time in n, as i tends to r the cost becomes prohibitive and, as far as we are aware, the solution of (3.2) at level i does not help in the solution at level $i+1$.

Lemma 3.1 establishes monotonicity properties of our bounds, as well as necessary and sufficient conditions for $\gamma = \gamma_i$. The following corollary suggests a "one shot" algorithm and is a recasting of Lemma 3.1.

Corollary 3.2 *Let $A = A^T \in \mathcal{R}^{n\times n}$ be as given in Lemma 3.1. Choose the largest i such that $1 \leq i < r$ and such that the maximization in (3.13) below is tractable. Define*

$$\begin{aligned}
V_1 &= \begin{bmatrix} U_1 \cdots U_i \end{bmatrix}, & \Lambda_1 &= \begin{bmatrix} \lambda_1 I_{m_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & 0 & \lambda_i I_{m_i} \end{bmatrix}, \\
V_2 &= U_{i+1}, & \Lambda_2 &= \lambda_{i+1} I_{m_{i+1}}, \\
V_3 &= \begin{bmatrix} U_{i+2} \cdots U_r \end{bmatrix}, & \Lambda_3 &= \begin{bmatrix} \lambda_{i+2} I_{m_{i+2}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & 0 & \lambda_r I_{m_r} \end{bmatrix},
\end{aligned}$$

so that A has a spectral form given by

$$A = U\Lambda U^T = \begin{bmatrix} V_1 & V_2 & V_3 \end{bmatrix} \begin{bmatrix} \Lambda_1 & 0 & 0 \\ 0 & \Lambda_2 & 0 \\ 0 & 0 & \Lambda_3 \end{bmatrix} \begin{bmatrix} V_1{}^T \\ V_2{}^T \\ V_3{}^T \end{bmatrix}.$$

Let

$$S := \Lambda_1 - \Lambda_2 = \Lambda_1 - \lambda_{i+1} I_{m_{i+1}},$$

so that $S \succ 0$ and is diagonal, and define

$$V = V_1 S^{\frac{1}{2}} \in \mathcal{R}^{n\times m},$$

where $m = \sum_{j=1}^{i} m_j$. Let $\bar{\phi}_i$ be the maximum of the reduced rank quadratic integer program (RRQIP)

$$\text{(RRQIP)} \qquad \bar{\phi}_i = \max_{x\in\mathcal{X}} x^T V V^T x. \tag{3.13}$$

Then

$$\gamma := \max_{x \in \mathcal{X}} x^T A x \leq \lambda_{i+1} + \bar{\phi}_i =: \gamma_i.$$

Furthermore, $\gamma = \gamma_i$ if and only if there exists a maximizer $x_i \in \mathcal{X}$ for (3.13) such that $V_3{}^T x_i = 0$.

Proof The corollary follows from Lemma 3.1 since

$$\gamma_{i+1} = \phi_i \gamma_i + (1 - \phi_i)\lambda_{i+1} = \lambda_{i+1} + (\gamma_i - \lambda_{i+1})\phi_i = \lambda_{i+1} + \bar{\phi}_i,$$

from (3.3) and the definitions of ϕ_i in (3.2) and $\bar{\phi}_i$ in (3.13). However, since the result may be used directly to develop an algorithm for calculating our bounds, we give an independent proof.

Using $A = U \Lambda U^T$, $UU^T = V_1 V_1{}^T + V_2 V_2{}^T + V_3 V_3{}^T = I_n$, and $x^T x = 1$ for all $x \in \mathcal{X}$, a simple manipulation verifies the following equality valid for all $x \in \mathcal{X}$

$$x^T A x = \lambda_{i+1} + x^T V_1 (\Lambda_1 - \Lambda_2) V_1{}^T x - x^T V_3 (\Lambda_2 - \Lambda_3) V_3{}^T x.$$

The result now follows upon noting that $S = \Lambda_1 - \Lambda_2 \succ 0$ and $\Lambda_2 - \Lambda_3 \succ 0$ imply that $x^T A x \leq \lambda_{i+1} + \bar{\phi}_i$. □

4 A polynomial time solution to the RRQIP problem

The RRQIP problem in (3.13) has been considered in a slightly modified form ($x \in \{0, 1\}^n$) in [2]. In our notation, [2] argue that the solution of (3.13) reduces to the enumeration of the extreme points of the zonotope $\mathcal{Z} = \{V^T x : x \in \mathcal{X}\}$, where $m < n$ since

$$\bar{\phi}_i = \max_{x \in \mathcal{X}} x^T V V^T x = \max_{z \in \mathcal{Z}} z^T z,$$

and the last maximization is achieved at an extreme point of $\mathcal{Z}$ since $\mathcal{Z}$ is convex. The problem of enumerating the extreme points of $\mathcal{Z}$ is well known, see for example [5,7,8,20,24], although the treatment is given in the equivalent dual setting of finding arrangements of hyperplanes. It is shown in [2] that this identification gives the number of vertices of $\mathcal{Z}$ as $O(n^{m-1})$ and allows the enumeration of the vertices in an $O(n^{m-1})$ time algorithm for $m \geq 3$ and $O(n^m)$ time algorithm for $m \leq 2$.

The reverse-enumeration algorithm [3,9] is a systematic polynomial-time procedure for visiting all nodes of the adjacency-graph of the arrangement and thus identifying all extreme points of $\mathcal{Z}$. The algorithm was implemented in Matlab and was found to perform well for small and medium-size problems. See [19] for additional details of this algorithm and its implementation.

5 Incorporating the semidefinite relaxation

In this section we incorporate into our technique the semidefinite relaxation method for obtaining upper bounds on γ; see [1,4,17,22,23], and [21] and the references therein.

For any symmetric A, $D \in \mathcal{R}^{n \times n}$ and e, $x \in \mathcal{R}^n$ the following identity

$$x^T A x = -(e^T D e - x^T D x) - x^T (D - A) x + e^T D e, \tag{5.1}$$

can be easily verified. Set

$$e = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \in \mathcal{R}^n.$$

Then for all $x \in \mathcal{X}$ and diagonal D such that $D - A \succeq 0$ we have $x^T Ax \leq e^T De$ and so

$$\gamma = \max_{x \in \mathcal{X}} x^T Ax \leq \bar{\gamma},$$

where

$$\text{(SDR)} \qquad \bar{\gamma} := \min_{\substack{D \text{ is diagonal} \\ D - A \succeq 0}} e^T De,$$

so that $\bar{\gamma}$ is an upper bound on γ. Let $\bar{D}$ be a minimizer for the SDR problem so that $\bar{D}$ is diagonal, $e^T \bar{D} e = \bar{\gamma}$ and $\bar{D} - A \succeq 0$ with

$$\bar{\lambda}(A - \bar{D}) = 0. \tag{5.2}$$

(See [21]). Substituting $e^T \bar{D} e = \bar{\gamma}$ in (5.1) and noting that $e^T \bar{D} e = x^T \bar{D} x$ for all $x \in \mathcal{X}$,

$$\gamma = \max_{x \in \mathcal{X}} x^T Ax = \max_{x \in \mathcal{X}} -x^T (\bar{D} - A)x + \bar{\gamma} = \max_{x \in \mathcal{X}} x^T \bar{A} x,$$

where

$$\bar{A} = \bar{\gamma} I_n + A - \bar{D},$$

and we can use $\bar{A}$ instead of A in our algorithm. However, $\bar{\gamma} = \bar{\lambda}(\bar{A})$ from (5.2) and so the semidefinite relaxation upper bound becomes our first bound γ_1 (since $\gamma_1 = \bar{\lambda}(\bar{A}) = \bar{\gamma}$). Thus our subsequent bounds are, in general, tighter than the SDR bound.

6 Example

Consider the test problem (QIP2, p. 305) in [10]:

$$\gamma = \min_{x \in \{0,1\}^n} x^T Ax, \tag{6.1}$$

with

$$A = \begin{bmatrix} -1 & -2 & 2 & 8 & -5 & 1 & -4 & 0 & 0 & 8 \\ -2 & 2 & 0 & -5 & 4 & -4 & -4 & -5 & 0 & -5 \\ 2 & 0 & 2 & -3 & 7 & 0 & -3 & 7 & 5 & 0 \\ 8 & -5 & -3 & -1 & -3 & -1 & 7 & 1 & 7 & 2 \\ -5 & 4 & 7 & -3 & 1 & 0 & -4 & 2 & 4 & -2 \\ 1 & -4 & 0 & -1 & 0 & 1 & 9 & 5 & 2 & 0 \\ -4 & -4 & -3 & 7 & -4 & 9 & 3 & 1 & 2 & 0 \\ 0 & -5 & 7 & 1 & 2 & 5 & 1 & 0 & -3 & -2 \\ 0 & 0 & 5 & 7 & 4 & 2 & 2 & -3 & 2 & 3 \\ 8 & -5 & 0 & 2 & -2 & 0 & 0 & -2 & 3 & 3 \end{bmatrix},$$

where the optimal solution γ is known to be equal to -29. By transforming the minimization into maximization, (0,1) variables into $(-1, 1)$ variables, and incorporating the semidefinite relaxation bound as outlined in Sect. 5, Corollary 3.2 gives the bounds $\gamma_1, \cdots, \gamma_{10}$ shown in the graph below. Note that γ_1 is the SDR bound and $\gamma_{10} = \gamma = -29$ (Fig 1).

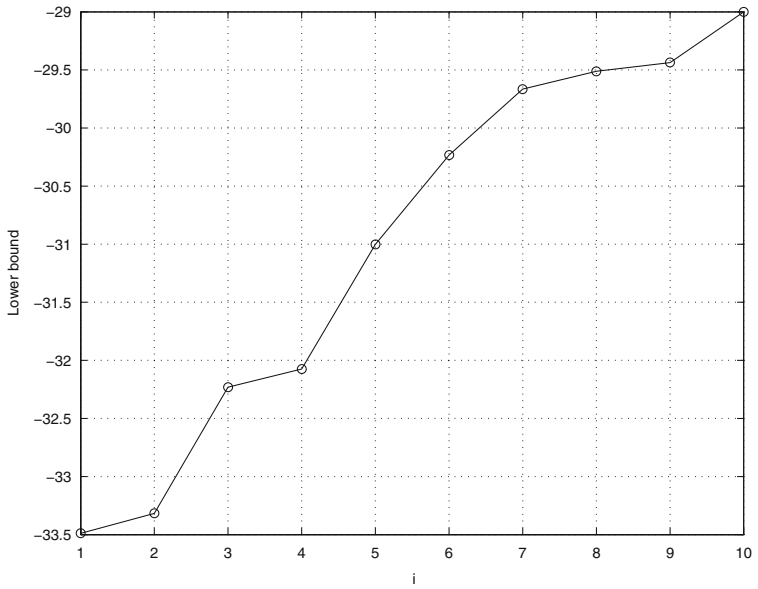

Fig. 1 Graph of the bounds γ_i for $i = 1, \ldots, 10$ for the problem in (6.1)

7 Summary

By way of summarizing our results, we list the contributions of this paper:

1. We have used the identification in [2] of the solution of the reduced rank QIP problem with the problem of enumerating the extreme points of a low dimensional zonotope to derive a sequence of non-increasing upper bounds on the QIP problem.
2. Our work generalizes the work in [2], which only deals with QIP problems where the data matrix A has a small rank, to the case where A has no rank restrictions.
3. Our bounds are given in two forms readily implementable as algorithms.
4. We have incorporated the semidefinite relaxation upper bound developed in [1,4,17,21–23] so that it is equal to our first bound γ_1.

Appendix A

Here we give a detailed derivation of the three expressions for $f(x)$ and $f_i(x)$ used in the proof of Lemma 3.1. This is summarized in the following lemma.

Lemma 8.1 *In previously defined notation, (3.10) and (3.11) hold.*

Proof We start by establishing the expressions for $f_i(x)$. The expressions for $f_1(x)$ and $f_r(x)$ are immediate. To establish the expression for $f_i(x)$ for $1 < i < r$, we start with the definition of $f_i(x)$ in (3.1). This gives

$$
\begin{aligned}
(\gamma_{i+1}-\lambda_{i+2})f_{i+1}(x) &= \sum_{j=1}^{i+1}(\lambda_j-\lambda_{i+2})x^TU_jU_j^Tx \\
&= \sum_{j=1}^{i}(\lambda_j-\lambda_{i+1})x^TU_jU_j^Tx + (\lambda_{i+1}-\lambda_{i+2})\sum_{j=1}^{i+1}x^TU_jU_j^Tx \\
&= (\gamma_i-\lambda_{i+1})f_i(x) + (\lambda_{i+1}-\lambda_{i+2})\sum_{j=1}^{i+1}x^TU_jU_j^Tx \\
&= (\gamma_i-\lambda_{i+1})(f_i(x)-\phi_i) + \phi_i(\gamma_i-\lambda_{i+1}) \\
&\quad +(\lambda_{i+1}-\lambda_{i+2})\sum_{j=1}^{i+1}x^TU_jU_j^Tx
\end{aligned}
$$

Using $\gamma_{i+1} = \phi_i(\gamma_i - \lambda_{i+1}) + \lambda_{i+1}$ gives

$$
\begin{aligned}
(\gamma_{i+1}-\lambda_{i+2})f_{i+1}(x) &= \gamma_{i+1}-\lambda_{i+2}+(\gamma_i-\lambda_{i+1})\,(f_i(x)-\phi_i) \\
&\quad -(\lambda_{i+1}-\lambda_{i+2})\left[1-\sum_{j=1}^{i+1}x^TU_jU_j^Tx\right]
\end{aligned}
$$

and hence

$$
f_{i+1}(x) = 1 - \frac{(\gamma_i-\lambda_{i+1})(\phi_i-f_i(x)) + (\lambda_{i+1}-\lambda_{i+2})\left[1-\sum_{j=1}^{i+1}x^TU_jU_j^Tx\right]}{\gamma_{i+1}-\lambda_{i+2}}
$$

as required.

The first expression for $f(x)$ can be established by writing

$$
\begin{aligned}
f(x) &= \sum_{j=1}^{r}\lambda_jx^TU_jU_j^Tx = \lambda_1x^TU_1U_1^Tx + \sum_{j=2}^{r}\lambda_jx^TU_jU_j^Tx \\
&= \gamma_1 - \sum_{j=2}^{r}(\lambda_1-\lambda_j)x^TU_jU_j^Tx - \lambda_1(1-x^Tx)
\end{aligned}
$$

since $\gamma_1 = \lambda_1$. To derive the second expression for $f(x)$, we first write

$$
\begin{aligned}
f(x) &= \sum_{j=1}^{r}\lambda_jx^TU_jU_j^Tx \\
&= \sum_{j=1,\,j\neq i}^{r}\lambda_jx^TU_jU_j^Tx - \lambda_i\sum_{j=1,\,j\neq i}^{r}x^TU_jU_j^Tx + \lambda_i\sum_{j=1}^{r}x^TU_jU_j^Tx \\
&= \sum_{j=1}^{i-1}(\lambda_j-\lambda_i)x^TU_jU_j^Tx - \lambda_i\sum_{j=i+1}^{r}x^TU_jU_j^Tx + \sum_{j=i+1}^{r}\lambda_jx^TU_jU_j^Tx + \lambda_ix^Tx.
\end{aligned}
$$

Thus, on using (3.1) and (3.3),

$$f(x) = (\gamma_{i-1} - \lambda_i) f_{i-1}(x) - \lambda_i \sum_{j=i+1}^{r} x^T U_j U_j^T x + \sum_{j=i+1}^{r} \lambda_j x^T U_j U_j^T x + \lambda_i x^T x$$

$$= \gamma_i - (\gamma_{i-1} - \lambda_i)(\phi_{i-1} - f_{i-1}(x)) - \sum_{j=i+1}^{r} (\lambda_i - \lambda_j) x^T U_j U_j^T x - \lambda_i (1 - x^T x).$$

Finally, the third expression for $f(x)$ follows by writing

$$f(x) = \sum_{j=1}^{r} \lambda_j x^T U_j U_j^T x = \sum_{j=1}^{r-1} \lambda_j x^T U_j U_j^T x + \lambda_r x^T U_r U_r^T x$$

$$= \sum_{j=1}^{r-1} (\lambda_j - \lambda_r) x^T U_j U_j^T x + \lambda_r \sum_{j=1}^{r-1} x^T U_j U_j^T x + \lambda_r x^T U_r U_r^T x$$

$$= (\gamma_{r-1} - \lambda_r) f_{r-1}(x) + \lambda_r x^T x$$

$$= \gamma_r - (\gamma_{r-1} - \lambda_r)(\phi_{r-1} - f_{r-1}(x)) - \lambda_r (1 - x^T x)$$

where again we have used (3.1) and (3.3). This completes the proof. □

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