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Continuous Optimization

Spectral bounds for unconstrained (−1,1)-quadratic optimization problems

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ABSTRACT

Given an unconstrained quadratic optimization problem in the following form:

$(QP)\min\{x^tQx \mid x \in \{-1,1\}^n\}$,

with $Q \in \mathbb{R}^{n\times n}$, we present different methods for computing bounds on its optimal objective value. Some of the lower bounds introduced are shown to generally improve over the one given by a classical semidefinite relaxation. We report on theoretical results on these new bounds and provide preliminary computational experiments on small instances of the maximum cut problem illustrating their performance.

1. Introduction

Consider a quadratic function $q : \mathbb{R}^n \to \mathbb{R}$ given by: $q(x) = x^tQx$, where Q denotes a $n \times n$ rational matrix.

An unconstrained (−1,1)-quadratic optimization problem can be expressed as follows:

$$(QP)Z^* = \min\{q(x)|x \in \{-1,1\}^n\},$$

where $\{-1,1\}^n$ denotes the set of n-dimensional vectors with entries either equal to 1 or −1. Without loss of generality we assume that the matrix Q is symmetric.

Problem (QP) is a classical combinatorial optimization problem with many applications, e.g. in statistical physics and circuit design (Barahona et al., 1988; Grötschel et al., 1989; Pinter, 1984). It is well-known that any (0,1)-quadratic problem expressed as: $\min\{x^tAx + c^tx|x \in \{0,1\}^n\}$, $A \in \mathbb{R}^{n\times n}$, $c \in \mathbb{R}^n$, can be formulated in the form of problem (QP) (with dimension $n+1$ instead of n) and conversely (Hammer, 1965; De Simone, 1990).

Problem (QP) is known to be NP-hard in general (Karp, 1972). Some polynomially solvable cases have been identified from among the following (Allemand et al., 2001; Ben-Ameur and Neto, 2008b; Çela et al., 2006).

Proposition 1.1. *For a fixed integer p, if the matrix Q (given by its nonzero eigenvalues and associated eigenvectors) has rank at most p and negative diagonal entries only, then problem* (QP) *can be solved in polynomial time.*

Note also the following extension of the last Proposition given in Ben-Ameur and Neto (2008b).

Proposition 1.2. *For fixed integers* $p \geqslant 2$ *and* $q \geqslant 0$, *if the matrix Q (given by its nonzero eigenvalues and associated eigenvectors) has rank at most p and at most q positive diagonal entries, then problem* (QP) *can be solved in polynomial time.*

Different methods for computing bounds for problems such as (QP) have been proposed in the literature. An early reference is Hammer and Rubin (1970), in which the authors proposed a method convexifying the objective function by making use of the smallest eigenvalue of the matrix Q. This approach has then been generalized and improved by many people (see e.g. Delorme and Poljak, 1993a,b; Poljak and Rendl, 1995; Billionnet and Elloumi, 2007) leading to bounds equivalent to the ones obtained by a semidefinite formulation presented in Goemans and Williamson (1995). More recently further improvements over the latter have been introduced, e.g. in Malik et al. (2006) and Ben-Ameur and Neto (2008a).

Let us introduce some notation. The eigenvalues of the matrix Q will be noted $\lambda_1(Q) \leqslant \lambda_2(Q) \leqslant \ldots \leqslant \lambda_n(Q)$ (or more simply $\lambda_1 \leqslant \lambda_2 \leqslant \ldots \leqslant \lambda_n$ when clear from the context) and corresponding unit (in Euclidean norm) and pairwise orthogonal eigenvectors: $v_1, \ldots, v_n$. The jth entry of vector v_i is noted v_{ij}. Given some set of vectors $a_1, \ldots, a_q \in \mathbb{R}^n$, $q \in \mathbb{N}$, we note $Lin(a_1, \ldots, a_q)$ the subspace spanned by these vectors. Given some vector $y \in \{-1,1\}^n$, $dist(y, Lin(v_1, \ldots, v_p))$ stands for the Euclidean distance between the vector y and $Lin(v_1, \ldots, v_p)$, i.e. $dist(y, Lin(v_1, \ldots, v_p)) = \|y - y_p\|_2$ where y_p stands for the orthogonal projection of y onto $Lin(v_1, \ldots, v_p)$ and $\|\cdot\|_2$ represents the Euclidean norm. Given some index $j \in \{1, \ldots, n\}$, d_j will denote the distance between the set $\{-1,1\}^n$ and the subspace that is spanned by the eigenvectors $v_1, \ldots, v_j$, i.e. $\min\{dist(y, Lin(v_1, \ldots, v_j))|y \in \{-1,1\}^n\}$. Notice that d_j depends on a particular spectral decomposition of the matrix Q when there is an eigenvalue with multiplicity greater than

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one: considering different orders for the eigenvectors associated with the same eigenvalue generally leads to different values of d_j. Analogously, $\bar{d}_j$ will denote the distance between the set $\{-1,1\}^n$ and $Lin(v_j,\ldots,v_n)$.

By using the property $x_i^2 = 1,\ \forall i \in \{1,\ldots,n\}$ for any vector $x \in \{-1,1\}^n$, we notice that the set of optimal solutions of the problem (QP) remains unchanged if diagonal entries of the matrix Q are modified. More precisely, let $u \in \mathbb{R}^n, Diag(u) \in \mathbb{R}^{n\times n}$ stand for the matrix with diagonal u and all the other entries set equal to zero, and denote with $(QP)_u$ the $(-1,1)$-quadratic problem: $\overline{Z} = \min\{x^t(Q + Diag(u))x | x \in \{-1,1\}^n\}$. Then, trivially we have: $Z^* = \overline{Z} - \sum_{i=1}^n u_i$. However altering the diagonal entries of the matrix Q generally changes its spectrum, i.e. eigenvalues and eigenvectors. The bounds that we introduce rely on the spectrum of the matrix Q. And applying them to the matrix $Q + Diag(u)$ instead of Q, we can still derive bounds that are valid for the original problem but they depend on the vector u that is used.

To simplify the presentation we consider Q (rather than $Q + Diag(u)$) as an input matrix for which we compute bounds for the corresponding problem (QP), since for the case we use $Q + Diag(u)$ it is then trivial to derive bounds for the original problem.

The present paper is organized as follows. In Section 2 we present three methods for computing bounds for problem (QP). The basic spectral bounds of Section 2.1 have an expression involving the eigenvalues $(\lambda_i)_{i=1}^n$ and distances $(d_i)_{i=1}^{n-1}$. They were originally introduced in Ben-Ameur and Neto (2008a) for the maximum cut problem. Another method for computing bounds from a substitution of the matrix Q by a sum of particular matrices is proposed in Section 2.2. Basic idea here is to replace the original problem (QP) by several instances each satisfying Proposition 1.1. A different approach is undertaken in Section 2.3 where the original matrix Q is replaced by a single matrix satisfying Proposition 1.1 and whose spectrum differs from Q in some subset of eigenvalues. Then in Section 3 we draw a comparison between some of these bounds with the one from a classical semidefinite relaxation. The bounds introduced are then evaluated on instances of the maximum cut problem in Sections 4 and 5, before we draw some conclusions and perspectives in Section 6.

2. Computing bounds for problem (*QP*)

In this section we introduce three different ways of computing bounds for problem (QP), all using the eigenvalues and eigenvectors of the matrix Q (possibly with modified diagonal entries). The basic spectral bounds of Section 2.1 have been firstly introduced in Ben-Ameur and Neto (2008a) and are reminded here for completeness, whereas the bounds introduced in Sections 2.2 and 2.3 are – up to the authors' knowledge – completely new.

2.1. Basic spectral bounds

Using the smallest eigenvalue of the matrix Q the following lower bound trivially holds: $Z^* \geqslant \lambda_1 n$. This bound can be strengthened by using the whole spectrum of the matrix Q.

Proposition 2.1. *The following inequality holds:* $Z^* \geqslant \lambda_1 n + \sum_{j=1}^{n-1} d_j^2(\lambda_{j+1} - \lambda_j)$.

Proof. Consider a vector $y \in \{-1,1\}^n$, and its expression in a basis of eigenvectors: $y = \sum_{i=1}^n \alpha_i v_i$. Then we namely have: $y^t y = n = \sum_i \alpha_i^2$. Also from the definition of the distances $d_j,\ j \in \{1,\ldots,n\}$, the following inequality holds: $d_j^2 \leqslant \sum_{i=j+1}^n \alpha_i^2$.

We have $y^t Q y = \sum_{i=1}^n \alpha_i^2 \lambda_i = \lambda_1 n + \sum_{i=2}^n (\lambda_i - \lambda_1)\alpha_i^2$. Now, from the last inequality mentioned above with $j = 1$ we get: $\alpha_2^2 \geqslant d_1^2 - \sum_{i=3}^n \alpha_i^2$. Hence we have:

$$y^t Q y \geqslant \lambda_1 n + (\lambda_2 - \lambda_1)d_1^2 - (\lambda_2 - \lambda_1)\sum_{i=3}^n \alpha_i^2 + \sum_{i=3}^n (\lambda_i - \lambda_1)\alpha_i^2,$$

$$\iff y^t Q y \geqslant \lambda_1 n + (\lambda_2 - \lambda_1)d_1^2 + \sum_{i=3}^n (\lambda_i - \lambda_2)\alpha_i^2,$$

and, inductively (by using analogously the inequality $\alpha_j^2 \geqslant d_{j-1}^2 - \sum_{i=j+1}^n \alpha_i^2$), we get:

$$y^t Q y \geqslant \lambda_1 n + \sum_{i=1}^{n-1} (\lambda_{i+1} - \lambda_i) d_i^2. \qquad \square$$

In the same way that we derived lower bounds on the optimal objective value, upper bounds can be obtained. Using the largest eigenvalue λ_n of the matrix Q we get: $Z^* \leqslant n\lambda_n$. A better upper bound using the whole spectrum is as follows.

Proposition 2.2. *The following inequality holds:* $Z^* \leqslant \lambda_n n + \sum_{j=1}^{n-1} \bar{d}_{j+1}^2(\lambda_j - \lambda_{j+1})$.

Proof. Analogous to the proof of Proposition 2.1. $\square$

Thus the results from Propositions 2.2 and 2.1 lead to the "spectral gap":

$$(\lambda_n - \lambda_1)n - \sum_{j=1}^{n-1} (\lambda_{j+1} - \lambda_j)\left(d_j^2 + \bar{d}_{j+1}^2\right). \tag{1}$$

Let Z_c^* stand for the optimal objective value of the following relaxation of problem $(QP) : \min\{x^t Q x | x \in [-1,1]^n\}$ denoted (QPC) in what follows. In the particular case when the matrix Q has at least one negative eigenvalue, then by computing the objective value of a properly scaled eigenvector associated with a negative eigenvalue, we get the simple upper bound given hereafter.

Proposition 2.3. *If the matrix Q has at least one negative eigenvalue then this upper bound holds:*

$$Z_c^* \leqslant \min\left\{\frac{\lambda_q}{\|v_q\|_\infty^2} | \lambda_q < 0\right\}, \tag{2}$$

with $\|v_q\|_\infty = \max_{i\in\{1,\ldots,n\}} v_{qi}$.

An upper bound for problem (QP) can be obtained similarly.

Proposition 2.4. *The following upper bound holds for problem* (QP)*:*

$$Z^* \leqslant \min\left\{\frac{\lambda'_q}{\|v'_q\|_\infty^2} | \lambda'_q < 0\right\} + \sum_{i=1}^n \bar{q}_i, \tag{3}$$

where $\lambda'_1, \lambda'_2, \ldots, \lambda'_n$ *denote the eigenvalues of the matrix* $Q - Diag(\bar{q}), v'_1, v'_2, \ldots, v'_n$ *are corresponding unit eigenvectors and* $\bar{q} = (\bar{q}_1, \ldots, \bar{q}_n)$ *stands for the diagonal of the matrix Q.*

Proof. It follows from a result by Rosenberg (see Proposition 1 in Rosenberg (1972)) that the optimal objective values of problems (QP) and (QPC) are identical if the matrix Q has zero diagonal entries only. Applying this property and Proposition 2.3 to the matrix $Q - Diag(\bar{q})$ leads to the result. $\square$

A "geometric view" to the spectral bound of Proposition 2.1 is provided by the following result.

Proposition 2.5. *If a vector* $y \in \{-1,1\}^n$ *satisfies:* $dist(y, Lin(v_1,\ldots,v_k)) = d_k$ *for all indices* $k \in \{1,\ldots,n-1\}$ *such that* $\lambda_{k+1} > \lambda_k$ *then y is an optimal solution of problem* (QP).

Proof. Let y verify the assumptions of the proposition. Let d'_i stand for the distance $dist(y, Lin(v_1,\ldots,v_i))$ and I denotes the set of indices k for which the strict inequality holds: $\lambda_{k+1} > \lambda_k$. Then we have $d'_i = d_i,\ \forall i \in I$ and $d'_i \geqslant d_i$ otherwise. Also, $\sum_{j=1}^n d_j^2(\lambda_{j+1} - \lambda_j) =$