

# A coordinate ascent method for solving semidefinite relaxations of non-convex quadratic integer programs

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**Abstract.** We present a coordinate ascent method for a class of semidefinite programming problems that arise in non-convex quadratic integer optimization. These semidefinite programs are characterized by a small total number of active constraints and by low-rank constraint matrices. We exploit this special structure by solving the dual problem, using a barrier method in combination with a coordinate-wise exact line search. The main ingredient of our algorithm is the computationally cheap update at each iteration and an easy computation of the exact step size. Compared to interior point methods, our approach is much faster in obtaining strong dual bounds. Moreover, no explicit separation and re-optimization is necessary even if the set of primal constraints is large, since in our dual approach this is covered by implicitly considering all primal constraints when selecting the next coordinate.

**Keywords:** Semidefinite programming, non-convex quadratic integer optimization, coordinate descent method

## 1 Introduction

The importance of Mixed-Integer Quadratic Programming (MIQP) lies in both theory and practice of mathematical optimization. On one hand, a wide range of problems arising in practical applications can be formulated as MIQP. On the other hand, it is the most natural generalization of Mixed-Integer Linear Programming (MILP). However, it is well known that MIQP is NP-hard, as it contains MILP as a special case. Moreover, contrarily to what happens in MILP, the hardness of MIQP is not resolved by relaxing the integrality requirement on the variables: while convex quadratic problems can be solved in polynomial time by either the ellipsoid method [6] or interior point methods [5,9], the general problem of minimizing a non-convex quadratic function over a box is NP-hard, even if only one eigenvalue of the Hessian is negative [8].

Buchheim and Wiegele [2] proposed the use of semidefinite relaxations and a specialized branching scheme (Q-MIST) for solving unconstrained non-convex quadratic minimization problems where the variable domains are arbitrary closed

subsets of  $\mathbb{R}$ . Their work is a generalization of the well-known semidefinite programming approach to the maximum cut problem or, equivalently, to unconstrained quadratic minimization over variables in the domain  $\{-1, 1\}$ . Q-MIST needs to solve a semidefinite program (SDP) at each node of the branch-and-bound tree, which can be done using any standard SDP solver. In [2], an interior point method was used for this task, namely the CSDP library [1]. It is well-known that interior point algorithms are theoretically efficient to solve SDPs, they are able to solve small to medium size problems with high accuracy, but they are memory and time consuming for large scale instances.

A related approach to solve the same kind of non-convex quadratic problems was presented by Dong [3]. A convex quadratic relaxation is produced by means of a cutting surface procedure, based on multiple diagonal perturbations. The separation problem is formulated as a semidefinite problem and is solved by coordinate-wise optimization methods. More precisely, the author defines a barrier problem and solves it using coordinate descent methods with exact line search. Due to the particular structure of the problem, the descent direction and the step length can be computed by closed formulae, and fast updates are possible using the Sherman-Morrison formula. Computational results show that this approach produces lower bounds as strong as the ones provided by Q-MIST and it runs much faster for instances of large size.

In this paper, we adapt and generalize the coordinate-wise approach of [3] in order to solve the dual of the SDP relaxation arising in the Q-MIST approach. In our setting, it is still true that an exact coordinate-wise line search can be performed efficiently by using a closed-form expression, based on the Sherman-Morrison formula. Essentially, each iteration of the algorithm involves the update of one coordinate of the vector of dual variables and the computation of an inverse of a matrix that changes by a rank-two constraint matrix when changing the value of the dual variable. Altogether, our approach fully exploits the specific structure of our problem, namely a small total number of (active) constraints and low-rank constraint matrices of the semidefinite relaxation. Furthermore, in our model the set of dual variables can be very large, so that the selection of the best coordinate requires more care than in [3]. However, our new approach is much more efficient than the corresponding separation approach for the primal problem described in [2].

## 2 Preliminaries

We consider non-convex quadratic mixed-integer optimization problems of the form

$$\begin{aligned} \min \quad & x^\top \hat{Q}x + \hat{l}^\top x + \hat{c} \\ \text{s.t.} \quad & x \in D_1 \times \cdots \times D_n, \end{aligned} \tag{1}$$

where  $\hat{Q} \in \mathbb{R}^{n \times n}$  is symmetric but not necessarily positive semidefinite,  $\hat{l} \in \mathbb{R}^n$ ,  $\hat{c} \in \mathbb{R}$ , and  $D_i = \{l_i, \dots, u_i\} \subseteq \mathbb{Z}$  is finite for all  $i = 1, \dots, n$ . Buchheim and

Wiegele [2] have studied the more general case where each  $D_i$  is an arbitrary closed subset of  $\mathbb{R}$ . The authors have implemented a branch-and-bound approach called Q-MIST, it mainly consists in reformulating Problem (1) as a semidefinite optimization problem and solving a relaxation of the transformed problem within a branch-and-bound framework. In this section, first we describe how to obtain a semidefinite relaxation of Problem (1), then we formulate it in a matrix form and compute the dual problem.

## 2.1 Semidefinite relaxation

Semidefinite relaxations for quadratic optimization problems can already be found in an early paper of Lovász in 1979 [7], but it was not until the work of Goemans and Williamson in 1995 [4] that they started to catch interest. The basic idea is as follows: given any vector  $x \in \mathbb{R}^n$ , the matrix  $xx^\top \in \mathbb{R}^{n \times n}$  is rank-one, symmetric and positive semidefinite. In particular, also the augmented matrix

$$\ell(x) := \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^\top = \begin{pmatrix} 1 & x^\top \\ x & xx^\top \end{pmatrix} \in \mathbb{R}^{(n+1) \times (n+1)}$$

is positive semidefinite. This well-known fact leads to semidefinite reformulations of various quadratic problems. Defining a matrix

$$Q := \begin{pmatrix} \hat{c} & \frac{1}{2}\hat{l}^\top \\ \frac{1}{2}\hat{l} & \hat{Q} \end{pmatrix},$$

Problem (1) can be rewritten as

$$\begin{aligned} \min \quad & \langle Q, X \rangle \\ \text{s.t.} \quad & X \in \ell(D_1 \times \cdots \times D_n), \end{aligned}$$

so that it remains to investigate the set  $\ell(D_1 \times \cdots \times D_n)$ . The following result was proven in [2].

**Theorem 1.** *Let  $X \in \mathbb{R}^{(n+1) \times (n+1)}$  be symmetric. Then  $X \in \ell(D_1 \times \cdots \times D_n)$  if and only if*

- (a)  $(x_{i0}, x_{ii}) \in P(D_i) := \text{conv}\{(u, u^2) \mid u \in D_i\}$  for all  $i = 1, \dots, n$ ,
- (b)  $x_{00} = 1$ ,
- (c)  $\text{rank}(X) = 1$ , and
- (d)  $X \succeq 0$ .

We derive that the following optimization problem is a convex relaxation of (1), obtained by dropping the rank-one constraint of Theorem 1 (c):

$$\begin{aligned} \min \quad & \langle Q, X \rangle \\ \text{s.t.} \quad & (x_{i0}, x_{ii}) \in P(D_i) \quad \forall i = 1, \dots, n \\ & x_{00} = 1 \\ & X \succeq 0 \end{aligned} \tag{2}$$

This is an SDP, since the constraints  $(x_{i0}, x_{ii}) \in P(D_i)$  can be replaced by a set of linear constraints, as discussed in the next section.

## 2.2 Matrix formulation

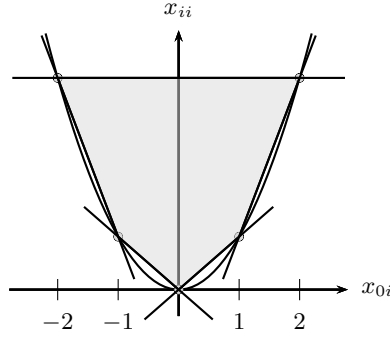
In the case of finite  $D_i$  considered here, the set  $P(D_i)$  is a polytope in  $\mathbb{R}^2$  with  $|D_i|$  many extreme points. It can thus be described equivalently by a set of  $|D_i|$  linear inequalities.

**Lemma 1.** *For  $D_i = \{l_i, \dots, u_i\}$ , the polytope  $P(D_i)$  is completely described by lower bounding facets  $-x_{ii} + (j + (j + 1))x_{0i} \leq j(j + 1)$  for  $j = l_i, l_i + 1, \dots, u_i - 1$  and one upper bounding facet  $x_{ii} - (l_i + u_i)x_{0i} \leq -l_i u_i$ .*

Exploiting  $x_{00} = 1$ , we may rewrite the polyhedral description of  $P(D_i)$  presented in the previous lemma as

$$\begin{aligned} (1 - j(j + 1))x_{00} - x_{ii} + (j + (j + 1))x_{0i} &\leq 1, \quad j = l_i, l_i + 1, \dots, u_i - 1 \\ (1 + l_i u_i)x_{00} + x_{ii} - (l_i + u_i)x_{0i} &\leq 1. \end{aligned}$$

We write the resulting inequalities in matrix form as  $\langle A_{ij}, X \rangle \leq 1$ . To keep analogy with the facets, the index  $ij$  represents the inequalities corresponding to lower bounding facets if  $j = l_i, l_i + 1, \dots, u_i - 1$  whereas  $j = u_i$  corresponds to the upper facet; see Figure 1.



**Fig. 1.** The polytope  $P(\{-2, -1, 0, 1, 2\})$ . Lower bounding facets are indexed, from left to right, by  $j = -2, -1, 0, 1$ , the upper bounding facet is indexed by 2.

Moreover, we write the constraint  $x_{00} = 1$  in matrix form as  $\langle A_0, X \rangle = 1$ , where  $A_0 := e_0 e_0^\top$ . In summary, Problem (2) can now be stated as

$$\begin{aligned} \min \quad & \langle Q, X \rangle \\ \text{s.t.} \quad & \langle A_0, X \rangle = 1 \\ & \langle A_{ij}, X \rangle \leq 1 \quad \forall j = l_i, \dots, u_i, \forall i = 1, \dots, n \\ & X \succeq 0. \end{aligned} \tag{3}$$

The following simple observation is crucial for our algorithm presented in the following section.

**Lemma 2.** *The constraint matrix  $A_0$  has rank one. All constraint matrices  $A_{ij}$  have rank one or two. The rank of  $A_{ij}$  is one if and only if  $j = u_i$  and  $u_i - l_i = 2$ .*

### 2.3 Dual problem

In order to derive the dual problem of (3), we define

$$\mathcal{A}(X) := \begin{pmatrix} \langle A_0, X \rangle \\ \langle A_{ij}, X \rangle_{j \in \{l_i, \dots, u_i\}, i \in \{1, \dots, n\}} \end{pmatrix}$$

and associate a dual variable  $y_0 \in \mathbb{R}$  with the constraint  $\langle A_0, X \rangle = 0$  as well as dual variables  $y_{ij} \leq 0$  with  $\langle A_{ij}, X \rangle \leq 1$ , for  $j \in \{l_i, \dots, u_i\}$  and  $i \in \{1, \dots, n\}$ . We then define  $y \in \mathbb{R}^{m+1}$  as

$$y := \begin{pmatrix} y_0 \\ (y_{ij})_{j \in \{l_i, \dots, u_i\}, i \in \{1, \dots, n\}} \end{pmatrix}.$$

The dual semidefinite program of Problem (3) is

$$\begin{aligned} \max \quad & \langle b, y \rangle \\ \text{s.t.} \quad & Q - \mathcal{A}^\top y \succeq 0 \\ & y_0 \in \mathbb{R} \\ & y_{ij} \leq 0 \quad \forall j = l_i, \dots, u_i, \forall i = 1, \dots, n, \end{aligned} \tag{4}$$

the vector  $b \in \mathbb{R}^{m+1}$  being the all-ones vector. It is easy to verify that the primal problem (3) is strictly feasible if  $|D_i| \geq 2$  for all  $i = 1, \dots, n$ , so that strong duality holds in all non-trivial cases.

We conclude this section by emphasizing some characteristics of any feasible solution of Problem (3).

**Lemma 3.** *Let  $X^*$  be a feasible solution of Problem (3). For  $i \in \{1, \dots, n\}$ , consider the active set*

$$\mathcal{A}_i = \{j \in \{l_i, \dots, u_i\} \mid \langle A_{ij}, X^* \rangle = 1\}$$

*corresponding to variable  $i$ . Then*

- (i) *for all  $i \in \{1, \dots, n\}$ ,  $|\mathcal{A}_i| \leq 2$ , and*
- (ii) *if  $|\mathcal{A}_i| = 2$ , then  $x_{ii}^* = x_{i0}^{*2}$  and  $x_{i0}^* \in D_i$ .*

*Proof.* The polytope  $P(D_i)$  is two-dimensional with non-degenerate vertices. Due to the way the inequalities  $\langle A_{ij}, X \rangle \leq 1$  are defined it is impossible to have more than two inequalities intersecting at one point. Therefore, a given point  $(x_{ii}, x_{i0}) \in P(D_i)$  satisfies zero, one, or two inequalities with equality. In the last case, we have  $x_{ii} = x_{i0}^2$  by construction, which implies  $x_{i0} \in D_i$ .  $\square$

For the dual problem (4), Lemma 3 (i) means that at most  $2n+1$  out of the  $m+1$  variables can be non-zero in an optimal solution. Clearly, such a small number of non-zero variables is beneficial in a coordinate-wise optimization method. Moreover, by Lemma 3 (ii), if two dual variables corresponding to the same primal variable are non-zero in an optimal dual solution, then this primal variable will obtain an integer feasible value in the optimal primal solution.

### 3 A coordinate ascent method

We aim at solving the dual problem (4) by coordinate-wise optimization, in order to obtain fast lower bounds to be used inside the branch-and-bound framework Q-MIST. Our approach is motivated by an algorithm proposed by Dong [3]. The author formulates Problem (1) as a convex quadratically constrained problem, and devises a cutting surface procedure based on diagonal perturbations to construct convex relaxations. The separation problem turns out to be a semidefinite problem with convex non-smooth objective function, and it is solved by a primal barrier coordinate minimization algorithm with exact line search.

The dual Problem (4) has a similar structure to the semidefinite problem solved in [3], therefore similar ideas can be applied. Our SDP is more general however, it contains more general constraints with matrices of rank two (instead of one) and most of our variables are constrained to be non-positive. Another difference is that we deal with a very large number of constraints, out of which only a few are non-zero however. On the other hand, our objective function is linear, which is not true for the problem considered in [3].

As a first step, we introduce a penalty term modelling the semidefinite constraint  $Q - \mathcal{A}^\top y \succeq 0$  of Problem (4) and obtain

$$\begin{aligned} \max \quad & f(y; \sigma) := \langle b, y \rangle + \sigma \log \det(Q - \mathcal{A}^\top y) \\ \text{s.t.} \quad & Q - \mathcal{A}^\top y \succ 0 \\ & y_0 \in \mathbb{R} \\ & y_{ij} \leq 0 \quad \forall j = l_i, \dots, u_i, \forall i = 1, \dots, n \end{aligned} \tag{5}$$

for  $\sigma > 0$ . The gradient of the objective function of Problem (5) is

$$\nabla_y f(y; \sigma) = b - \sigma \mathcal{A}((Q - \mathcal{A}^\top y)^{-1}).$$

For the following, we denote  $W := (Q - \mathcal{A}^\top y)^{-1}$ , so that

$$\nabla_y f(y; \sigma) = b - \sigma \mathcal{A}(W). \tag{6}$$

We will see later that, using the Sherman-Morrison formula, the matrix  $W$  can be updated quickly when changing the value of a dual variable, which is crucial for the performance of the algorithm proposed. We begin by describing a general algorithm to solve (5) in a coordinate maximization manner. In the following, we explain each step of this algorithm in detail.

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#### Outline of a barrier coordinate ascent algorithm for Problem (4)

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- 1 **Starting point:** choose any feasible solution  $y$  of (5);
  - 2 **Direction:** choose a coordinate direction  $e_{ij}$ ;
  - 3 **Step size:** using exact line search, determine the step length  $s$ ;
  - 4 **Move along chosen coordinate:**  $y \leftarrow y + se_{ij}$ ;
  - 5 **Update** the matrix  $W$  accordingly;
  - 6 **Decrease** the penalty parameter  $\sigma$ ;
  - 7 **Go to (2)**, unless some stopping criterion is satisfied;
-

### 3.1 Definition of a starting point

If  $Q \succ 0$ , we can safely choose  $y^{(0)} = 0$  as starting point. Otherwise, define  $a \in \mathbb{R}^n$  by  $a_i = (A_{iu_i})_{0i}$  for  $i = 1, \dots, n$ . Moreover, define

$$\begin{aligned}\tilde{y} &:= \min\{\lambda_{\min}(\hat{Q}) - 1, 0\}, \\ y_0 &:= \hat{c} - \tilde{y} \sum_{i=1}^n (1 + l_i u_i) - 1 - (\tfrac{1}{2}\hat{l} - \tilde{y}a)^\top (\tfrac{1}{2}\hat{l} - \tilde{y}a),\end{aligned}$$

and  $y^{(0)} \in \mathbb{R}^{m+1}$  as

$$y^{(0)} := \begin{pmatrix} y_0 \\ (y_{ij})_{j \in \{l_i, \dots, u_i\}, i \in \{1, \dots, n\}} \end{pmatrix}, \quad y_{ij} = \begin{cases} \tilde{y}, & j = u_i, i = 1, \dots, n \\ 0, & \text{otherwise.} \end{cases}$$

Then the following lemma holds; the proof can be found in Appendix A.

**Lemma 4.** *The vector  $y^{(0)}$  is feasible for (5).*

### 3.2 Choice of an ascent direction

We improve the objective function coordinate-wise: at each iteration  $k$  of the algorithm, we choose an ascent direction  $e_{ij^{(k)}} \in \mathbb{R}^m$  where  $ij^{(k)}$  is the coordinate of the gradient with maximum absolute value

$$ij^{(k)} := \arg \max_{ij} |\nabla_y f(y; \sigma)_{ij}|. \quad (7)$$

However, moving a coordinate  $ij$  to a positive direction is allowed only if  $y_{ij} < 0$ , so that the coordinate  $ij^{(k)}$  in (7) has to be chosen among those satisfying

$$(\nabla_y f(y; \sigma)_{ij} > 0 \text{ and } y_{ij} < 0) \quad \text{or} \quad \nabla_y f(y; \sigma)_{ij} < 0.$$

The entries of the gradient depend on the type of inequality. By (6), we have

$$\nabla_y f(y; \sigma)_{ij} = 1 - \sigma \langle W, A_{ij} \rangle.$$

The number of lower bounding facets for a single primal variable  $i$  is  $u_i - l_i$ , which is not polynomial in the input size from a theoretical point of view. From a practical point of view, a large domain  $D_i$  may slow down the coordinate selection if all potential coordinates have to be evaluated explicitly.

However, the regular structure of the gradient entries corresponding to lower bounding facets for variable  $i$  allows to limit the search to at most two candidates per variable. To this end, we define the function

$$\varphi_i(j) := 1 - \sigma \langle W, A_{ij} \rangle = 1 - \sigma((1 - j(j+1))W_{00} + (2j+1)W_{i0} - W_{ii})$$

and aim at finding a minimizer of  $|\varphi|$  over  $\{l_i, \dots, u_i - 1\}$ . As  $\varphi_i$  is a univariate quadratic function, we can restrict our search to at most three candidates,

namely the bounds  $l_i$  and  $u_i - 1$  and the rounded global minimizer of  $\varphi_i$ , if it belongs to  $l_i, \dots, u_i - 1$ ; the latter is

$$\left\lceil \frac{W_{i0}}{W_{00}} - \frac{1}{2} \right\rceil.$$

In summary, taking into account also the upper bounding facets and the coordinate zero, we need to test at most  $4n + 1$  candidates in order to solve (7), independently of the bounds  $l_i$  and  $u_i$ .

### 3.3 Computation of the step size

We compute the step size  $s^{(k)}$  by exact line search in the chosen direction. For this, we need to solve the following one-dimensional maximization problem

$$s^{(k)} = \arg \max_s \{f(y^{(k)} + se_{ij^{(k)}}; \sigma) \mid Q - \mathcal{A}^\top(y^{(k)} + se_{ij^{(k)}}) \succ 0, s \leq -y_{ij^{(k)}}\} \quad (8)$$

unless the chosen coordinate is zero, in which case the upper bound on  $s$  is dropped. Note that  $s \mapsto f(y^{(k)} + se_{ij^{(k)}}; \sigma)$  is strictly concave on

$$\{s \in \mathbb{R} \mid Q - \mathcal{A}^\top(y^{(k)} + se_{ij^{(k)}}) \succ 0\}.$$

By the first order optimality conditions, we thus need to find the unique  $s^{(k)} \in \mathbb{R}$  satisfying the semidefinite constraint  $Q - \mathcal{A}^\top(y^{(k)} + s^{(k)}e_{ij^{(k)}}) \succ 0$  such that either

$$\nabla_s f(y^{(k)} + s^{(k)}e_{ij^{(k)}}; \sigma) = 0 \quad \text{and} \quad y_{ij^{(k)}} + s^{(k)} \leq 0$$

or

$$\nabla_s f(y^{(k)} + s^{(k)}e_{ij^{(k)}}; \sigma) > 0 \quad \text{and} \quad s^{(k)} = -y_{ij^{(k)}}.$$

In order to simplify the notation, we omit the superindex  $(k)$  in the following. From the definition,

$$\begin{aligned} f(y + se_{ij}; \sigma) &= \langle b, y \rangle + s \langle b, e_{ij} \rangle + \sigma \log \det(Q - \mathcal{A}^\top y - s \mathcal{A}^\top(e_{ij})) \\ &= \langle b, y \rangle + s + \sigma \log \det(W^{-1} - s A_{ij}). \end{aligned}$$

Then, the gradient with respect to  $s$  is

$$\nabla_s f(y + se_{ij}; \sigma) = 1 - \sigma \langle A_{ij}, (W^{-1} - s A_{ij})^{-1} \rangle. \quad (9)$$

Now the crucial task is to compute the inverse of the matrix  $W^{-1} - s A_{ij}$ , which is of dimension  $n+1$ . For this purpose, notice that  $W^{-1}$  is changed by a rank-one or rank-two matrix  $s A_{ij}$ ; see Lemma 2. Therefore, we can compute both the inverse matrix  $(W^{-1} - s A_{ij})^{-1}$  and the optimal step length by means of the Sherman-Morrison formula for the rank-one or rank-two update; see Appendix B.1.

Finally, we have to point out that the zero coordinate can also be chosen as ascent direction, in that case the gradient is

$$\nabla_s f(y + se_0; \sigma) = 1 - \sigma \langle A_0, (W^{-1} - s A_0)^{-1} \rangle,$$

and the computation of the step size is analogous.



### 3.4 Algorithm overview

Our approach to solve Problem (4) is summarized in Algorithm CD.

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**Algorithm CD:** Barrier coordinate ascent algorithm for Problem (4)

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**Input:**  $Q \in \mathbb{R}^{(n+1) \times (n+1)}$   
**Output:** A lower bound on the optimal value of Problem (3)

- 1 Use Lemma 4 to compute  $y^{(0)}$  such that  $Q - \mathcal{A}^\top y^{(0)} \succ 0$
- 2 Compute  $W^{(0)} \leftarrow (Q - \mathcal{A}^\top y^{(0)})^{-1}$
- 3 **for**  $k \leftarrow 0$  **until** *max-iterations* **do**
- 4     Choose a coordinate direction  $e_{ij^{(k)}}$  as described in Section 3.2
- 5     Compute the step size  $s^{(k)}$  as described in Section 3.3
- 6     Update  $y^{(k+1)} \leftarrow y^{(k)} + s^{(k)} e_{ij^{(k)}}$
- 7     Update  $W^{(k)}$  using the Sherman-Morrison formula
- 8     Update  $\sigma$
- 9     Terminate if some stopping criterion is met
- 10 **return**  $\langle b, y^{(k)} \rangle$

---

Before entering the main loop, the running time of Algorithm CD is dominated by the computation of the minimum eigenvalue of  $\hat{Q}$  needed to compute  $y^{(0)}$  and by the computation of the inverse matrix of  $Q - \mathcal{A}^\top y^{(0)}$ . Both can be done in  $O(n^3)$  time. Each iteration of the algorithm can be performed in  $O(n^2)$ . Indeed, as discussed in Section 3.2, we need to consider  $O(n)$  candidates for the coordinate selection, so that this task can be performed in  $O(n^2)$  time. For calculating the step size and updating the matrix  $W^{(k)}$ , we also need  $O(n^2)$  time using the Sherman-Morrison formula.

Notice that the algorithm produces a feasible solution  $y^{(k)}$  of Problem (4) at every iteration and hence a valid lower bound  $\langle b, y^{(k)} \rangle$  for Problem (3). In particular, when used within a branch-and-bound algorithm, this means that Algorithm CD can be stopped as soon as  $\langle b, y^{(k)} \rangle$  exceeds a known upper bound for Problem (3). Otherwise, the algorithm can be stopped after a fixed number of iterations or when other criteria show that only a small further improvement of the bound can be expected.

The choice of an appropriate termination rule however is closely related to the update of  $\sigma$  performed in Step 8. The aim is to find a good balance between the convergence for fixed  $\sigma$  and the decrease of  $\sigma$ . In our implementation, we use the following rule: whenever the entry of the gradient corresponding to the chosen coordinate has an absolute value below 0.01, we multiply  $\sigma$  by 0.25. As soon as  $\sigma$  falls below  $10^{-5}$ , we fix it to this value.

### 3.5 Two-dimensional update

In Algorithm CD, we change only one coordinate in each iteration, as this allows to update the matrix  $W^{(k)}$  in  $O(n^2)$  time using the Sherman-Morrison formula. This was due to the fact that all constraint matrices in the primal SDP (3) have rank at most two. However, taking into account the special structure of

the constraint matrix  $A_0$ , one can see that every linear combination of any constraint matrix  $A_{ij}$  with  $A_0$  still has rank at most two. In other words, we can simultaneously update the dual variables  $y_0$  and  $y_{ij}$  and still recompute  $W^{(k)}$  in  $O(n^2)$  time.

In order to improve the convergence of Algorithm CD, we choose a coordinate  $ij$  as explained in Section 3.2 and then perform an exact plane-search in the two-dimensional space corresponding to the directions  $e_0$  and  $e_{ij}$ , i.e., we solve the bivariate problem

$$\arg \max_{(s_0, s)} \{f(y + s_0 e_0 + s e_{ij}; \sigma) \mid Q - \mathcal{A}^\top(y + s_0 e_0 + s e_{ij}) \succ 0, s \leq -y_{ij}\}, \quad (10)$$

where we again omit the superscript  $(k)$  for sake of readability. Similar to the one-dimensional case in (8), due to strict concavity of  $(s_0, s) \mapsto f(y + s_0 e_0 + s e_{ij}; \sigma)$  over  $\{(s_0, s) \in \mathbb{R}^2 \mid Q - \mathcal{A}^\top(y + s_0 e_0 + s e_{ij}) \succ 0\}$ , solving (10) is equivalent to finding the unique pair  $(s_0, s) \in \mathbb{R}^2$  such that

$$\nabla_{s_0} f(y + s_0 e_0 + s e_{ij}; \sigma) = 0$$

and either

$$\nabla_s f(y + s_0 e_0 + s e_{ij}; \sigma) = 0 \quad \text{and} \quad y_{ij} + s \leq 0$$

or

$$\nabla_s f(y + s_0 e_0 + s e_{ij}; \sigma) > 0 \quad \text{and} \quad s = -y_{ij}.$$

To determine  $(s_0, s)$ , it thus suffices to set both gradients to zero and solve the resulting two-dimensional system of equations. If it turns out that  $y_{ij} + s > 0$ , we fix  $s := -y_{ij}$  and recompute  $s_0$  by solving

$$\nabla_{s_0} f(y + s_0 e_0 + s e_{ij}; \sigma) = 0.$$

Proceeding as before, we have

$$f(y + s_0 e_0 + s e_{ij}; \sigma) = \langle b, y \rangle + s_0 + s + \sigma \log \det(W^{-1} - s_0 A_0 - s A_{ij}),$$

and the gradients with respect to  $s_0$  and  $s$  are

$$\begin{aligned} \nabla_{s_0} f(y + s_0 e_0 + s e_{ij}; \sigma) &= 1 - \sigma \langle A_0, (W^{-1} - s_0 A_0 - s A_{ij})^{-1} \rangle \\ \nabla_s f(y + s_0 e_0 + s e_{ij}; \sigma) &= 1 - \sigma \langle A_{ij}, (W^{-1} - s_0 A_0 - s A_{ij})^{-1} \rangle. \end{aligned}$$

The matrix  $s_0 A_0 + s A_{ij}$  is of rank two; replacing  $(W^{-1} - s_0 A_0 - s A_{ij})^{-1}$  by the Sherman-Morrison formula and setting the gradients to zero, we obtain a system of two quadratic equations. For details, see Appendix B.2. Using these ideas, a slightly different version of Algorithm CD is obtained by changing Steps 5 and 6 adequately, which we call Algorithm CD2D.

## 4 Experiments

For our experiments, we generate random instances in the same way as proposed in [2]: the objective matrix is  $\hat{Q} = \sum_{i=1}^n \mu_i v_i v_i^\top$ , where the  $n$  numbers  $\mu_i$  are chosen as follows: for a given value of  $p \in [0, 100]$ , the first  $pn/100$   $\mu_i$ 's are generated uniformly from  $[-1, 0]$  and the remaining ones from  $[0, 1]$ . Additionally, we generate  $n$  vectors of dimension  $n$ , with entries uniformly at random from  $[-1, 1]$ , and orthonormalize them to obtain the vectors  $v_i$ . The parameter  $p$  represents the percentage of negative eigenvalues, so that  $\hat{Q}$  is positive semidefinite for  $p = 0$ , negative semidefinite for  $p = 100$  and indefinite for any other value  $p \in (0, 100)$ . The entries of the vector  $\hat{l}$  are generated uniformly at random from  $[-1, 1]$ , and  $\hat{c} = 0$ . In this paper, we restrict our evaluation to ternary instances, i.e., instances with  $D_i = \{-1, 0, 1\}$ .

We evaluate the performance of both Algorithms CD and CD2D in the root node of the branch-and-bound tree and compare them with CSDP, the SDP solver used in [2]. Our experiments were performed on an Intel Xeon processor running at 2.5 GHz. Algorithms CD and CD2D were implemented in C++, using routines from the LAPACK package only in the initial phase for computing a starting point and the inverse matrix  $W^{(0)}$ .

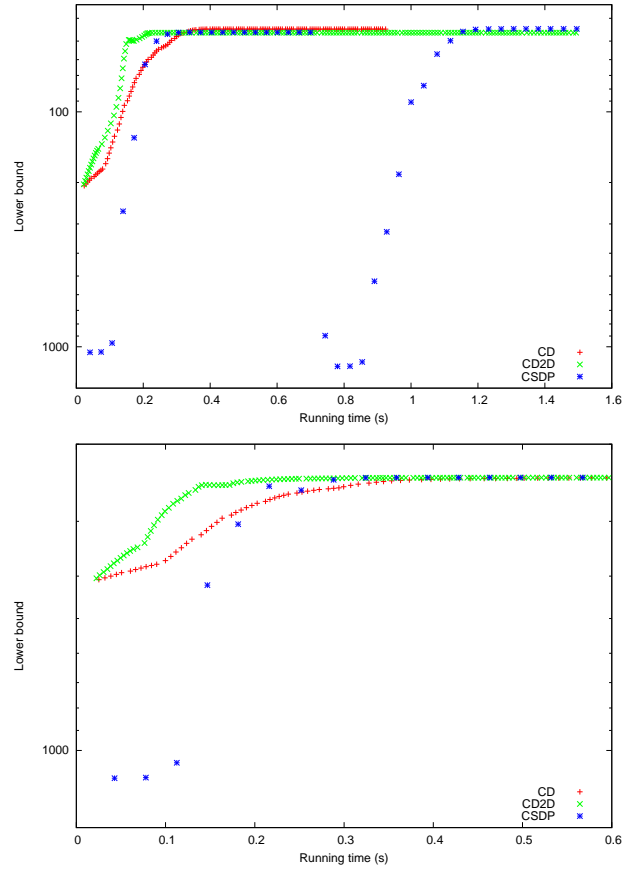
The main motivation to consider a fast coordinate ascent method was to obtain quick and good lower bounds for the quadratic integer problem (1). We are thus interested in the improvement of the lower bound over time. In Figure 2, we plotted the lower bounds obtained by CSDP and by the algorithms CD and CD2D in the root node for two ternary instances of size  $n = 100$ , for the two values  $p = 0$  and  $p = 100$ . Notice that we use a log scale for the  $y$ -axis.

From Figure 2, we see that Algorithm CD2D clearly dominates both other approaches: the lower bound it produces exceeds the other bounds until all approaches come close to the optimum of (2). This is true in particular for the instance with  $p = 100$ . Even Algorithm CD is stronger than CSDP in the beginning, but then CSDP takes over. Note that the computation of the root bound for the instance shown in Figure 2 (a) involves one re-optimization due to separation. For this reason, the lower bound given by CSDP has to restart with a very weak value.

As a next step, we will integrate the Algorithm CD2D into the branch-and-bound framework of Q-MIST. We are confident that this will improve the running times of Q-MIST significantly when choosing the stopping criteria carefully. This is left as future work.

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**Fig. 2.** Comparison of the lower bounds in the root node obtained by Q-MIST with CSDP, CD and CD2D; for  $p = 0$  (top) and  $p = 100$  (bottom)

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## A Feasible starting point

*Proof.* (of Lemma 4) We have  $y_{ij}^{(0)} \leq 0$  by construction, so it remains to show that  $Q - \mathcal{A}^\top y^{(0)} \succ 0$ . To this end, first note that

$$\tilde{c} := \hat{c} - y_0 - \tilde{y} \sum_{i=1}^n (1 + l_i u_i) = 1 + (\frac{1}{2}\hat{l} - \tilde{y}a)^\top (\frac{1}{2}\hat{l} - \tilde{y}a) > 0. \quad (11)$$

By definition,

$$\begin{aligned} Q - \mathcal{A}^\top y^{(0)} &= Q - y_0 A_0 - \tilde{y} \sum_{i=1}^n A_{iu_i} \\ &= Q - y_0 A_0 - \tilde{y} \begin{pmatrix} \sum_{i=1}^n (1 + l_i u_i) & a^\top \\ a & I_n \end{pmatrix} \\ &= \begin{pmatrix} \tilde{c} & (\frac{1}{2}\hat{l} - \tilde{y}a)^\top \\ \frac{1}{2}\hat{l} - \tilde{y}a & \hat{Q} - \tilde{y}I_n \end{pmatrix}, \end{aligned}$$

which by Schur complement and (11) is positive definite if

$$(\hat{Q} - \tilde{y}I) - \frac{1}{\tilde{c}}(\frac{1}{2}\hat{l} - \tilde{y}a)(\frac{1}{2}\hat{l} - \tilde{y}a)^\top \succ 0.$$

Denoting  $B := (\frac{1}{2}\hat{l} - \tilde{y}a)(\frac{1}{2}\hat{l} - \tilde{y}a)^\top$ , we have

$$\lambda_{\max}(B) = (\frac{1}{2}\hat{l} - \tilde{y}a)^\top (\frac{1}{2}\hat{l} - \tilde{y}a) \geq 0$$

and thus

$$\begin{aligned} \lambda_{\min} \left( (\hat{Q} - \tilde{y}I_n) - \frac{1}{\tilde{c}}B \right) &\geq \lambda_{\min}(\hat{Q} - \tilde{y}I_n) + \frac{1}{\tilde{c}}\lambda_{\min}(-B) \\ &= \lambda_{\min}(\hat{Q}) - \tilde{y} - \frac{\lambda_{\max}(B)}{1 + \lambda_{\max}(B)} > 0 \end{aligned}$$

by definition of  $\tilde{y}$ . □

## B Computation of the step size

### B.1 One-dimensional problem

We need to find the value of  $s$  such that the gradient in (9) is zero. For this we need to solve the following equation:

$$1 - \sigma \langle A_{ij}, (W^{-1} - sA_{ij})^{-1} \rangle = 0. \quad (12)$$

Notice that each constraint matrix  $A_{ij}$  can be factored as follows:

$$A_{ij} = E_{ij} I C_{ij},$$

where  $E_{ij} \in \mathbb{R}^{(n+1) \times 2}$ , defined by  $E_{ij} := (e_0 \ e_i)$ ,  $e_0, e_i \in \mathbb{R}^{n+1}$ ,  $C \in \mathbb{R}^{2 \times (n+1)}$  defined by  $C := (A_{ij})_{\{0,i\}, \{0, \dots, n\}}$  and  $I$  is the  $2 \times 2$ -identity matrix. As mentioned in Section 3.3, the inverse matrix  $(W^{-1} - sA_{ij})^{-1}$  can be computed using the Sherman-Morrison formula as follows:

$$(W^{-1} - sA_{ij})^{-1} = (W^{-1} - sE_{ij}IC_{ij})^{-1} = W + WE_{ij}(\frac{1}{s}I + C_{ij}WE_{ij})^{-1}C_{ij}W.$$

Notice that the matrix  $\frac{1}{s}I + C_{ij}WE_{ij}$  is a  $2 \times 2$ -matrix, so its inverse can be easily computed. Replacing the inverse in (12), we get

$$1 - \sigma\langle A_{ij}, W \rangle - \sigma\langle A_{ij}, WE_{ij}(\frac{1}{s}I + C_{ij}WE_{ij})^{-1}C_{ij}W \rangle = 0.$$

Due to the sparsity of the constraint matrices  $A_{ij}$ , the inner matrix product is simplified a lot, in fact we have to compute only the entries  $00$ ,  $0i$ ,  $0i$  and  $ii$  of the matrix product  $WE_{ij}(\frac{1}{s}I + C_{ij}WE_{ij})^{-1}C_{ij}W$ . We arrive at a quadratic equation in  $s$ , namely

$$as^2 + bs + c = 0,$$

where

$$\begin{aligned} a &= -(A_{ij})_{0i}^2 w_{0i}^2 + (A_{ij})_{00}(A_{ij})_{ii} w_{0i}^2 + (A_{ij})_{0i}(A_{ij})_{0i} w_{00} w_{ii} \\ &\quad - (A_{ij})_{00}(A_{ij})_{ii} w_{00} w_{ii}, \\ b &= (A_{ij})_{00} w_{00} + 2(A_{ij})_{0i} w_{0i} - 2\sigma(A_{ij})_{0i}^2 w_{0i}^2 + 2\sigma(A_{ij})_{00}(A_{ij})_{ii} w_{0i}^2 \\ &\quad + (A_{ij})_{ii} w_{ii} + 2\sigma(A_{ij})_{0i}^2 w_{00} w_{ii} - 2\sigma(A_{ij})_{00}(A_{ij})_{ii} w_{00} w_{ii}, \\ c &= -1 + \sigma(A_{ij})_{00} w_{00} + 2\sigma(A_{ij})_{0i} w_{0i} + \sigma(A_{ij})_{ii} w_{ii}. \end{aligned}$$

Finally,  $s$  is obtained using the well-known formula for the roots of a general quadratic equation.

The computation of the step size becomes simpler if the chosen coordinate direction corresponds to  $y_0$ . We then need to find a solution of the equation

$$1 - \sigma\langle A_0, (W^{-1} - sA_0)^{-1} \rangle = 0. \quad (13)$$

The inverse of  $W^{-1} - sA_0$  is represented using the Sherman-Morrison formula for rank-one,

$$(W^{-1} - sA_0)^{-1} = (W^{-1} - se_0 e_0^\top)^{-1} = W - \frac{s}{1 + sw_{ii}} (We_i)(We_i)^\top.$$

Using this to solve (13), we obtain the step size

$$s = \frac{1}{w_{ii}} - \sigma.$$

A similar formula for the step size is obtained for other cases when the constraint matrix  $A_{ij}$  has rank one.

## B.2 Two-dimensional problem

We write  $s_0 A_0 + s A_{ij} = E_{ij} I C_{ij}$ , where  $E_{ij} = (e_0 \ e_i) \in \mathbb{R}^{(n+1) \times 2}$ , and

$$C_{ij} = \begin{pmatrix} s_0 + s(A_{ij})_{00} & \dots & s(A_{ij})_{0i} & \dots \\ s(A_{ij})_{0i} & \dots & s(A_{ij})_{ii} & \dots \end{pmatrix} \in \mathbb{R}^{2 \times (n+1)}.$$

To compute the inverse matrix  $(W^{-1} - s_0 A_0 - s A_{ij})^{-1}$  we use the Sherman-Morrison formula again, obtaining

$$(W^{-1} - s_0 A_0 - s A_{ij})^{-1} = (W^{-1} - E_{ij} I C_{ij})^{-1} = W + W E_{ij} (I + C_{ij} W E_{ij})^{-1} C_{ij} W.$$

Substituting this in the gradients and setting them to zero, we obtain the following system of two quadratic equations

$$\begin{aligned} \sigma \langle A_0, (W^{-1} - s_0 A_0 - s A_{ij})^{-1} \rangle &= 1 \\ \sigma \langle A_{ij}, (W^{-1} - s_0 A_0 - s A_{ij})^{-1} \rangle &= 1, \end{aligned}$$

the solutions of which are  $(s'_0, s')$  and  $(s''_0, s'')$  given as follows:

$$\begin{aligned} s'_0 &= -(-4(A_{ij})_{0i}^3(A_{ij})_{ii}w_{0i}w - 4\alpha(A_{ij})_{0i}(A_{ij})_{ii}^2w_{0i}w - 4(A_{ij})_{0i}^4w_{00}w \\ &\quad + 2(A_{ij})_{0i}^2(3(A_{ij})_{00}(A_{ij})_{ii}w_{00}w - 2(A_{ij})_{ii}w_{00}w - (A_{ij})_{ii}^2w(w_{ii} + \sigma w) \\ &\quad + \rho) + (A_{ij})_{ii}(-2(A_{ij})_{00}(A_{ij})_{00}(A_{ij})_{ii}w_{00}w + 2(A_{ij})_{00}((A_{ij})_{ii}w_{00}w \\ &\quad - (A_{ij})_{ii}^2w(w_{ii} + \sigma w) + \rho) + (-(A_{ij})_{ii}^2w(2w_{ii} + \sigma w) + \rho))/\delta, \\ s' &= (2(A_{ij})_{0i}^2w_{00}w_{0i}^2 - 2(A_{ij})_{00}(A_{ij})_{ii}w_{00}w_{0i}^2 + 2(A_{ij})_{ii}w_{00}w_{0i}^2 + \sigma(A_{ij})_{ii}^2w_{0i}^4 \\ &\quad - 2(A_{ij})_{0i}^2w_{00}^2w_{ii} + 2(A_{ij})_{00}(A_{ij})_{ii}w_{00}^2w_{ii} - 2(A_{ij})_{ii}w_{00}^2w_{ii} \\ &\quad - 2\sigma(A_{ij})_{ii}^2w_{00}w_{0i}^2w_{ii}\sigma(A_{ij})_{ii}^2w_{00}^2w_{ii}^2 - \rho)/\delta, \\ s''_0 &= (4(A_{ij})_{0i}^4w_{00}w + 4(A_{ij})_{0i}^3(A_{ij})_{ii}w_{0i}w + 4\alpha(A_{ij})_{0i}(A_{ij})_{ii}^2w_{0i}w \\ &\quad + 2(A_{ij})_{0i}^2(2(A_{ij})_{ii}w_{00}w - 3(A_{ij})_{00}(A_{ij})_{ii}w_{00}w + (A_{ij})_{ii}^2w(w_{ii} + \sigma w) \\ &\quad + \rho) - (A_{ij})_{ii}(-2(A_{ij})_{00}(A_{ij})_{ii}w_{00}w + 2(A_{ij})_{00}((A_{ij})_{ii}w_{00}w \\ &\quad + (A_{ij})_{ii}^2w(w_{ii} + \sigma w) + \rho) - ((A_{ij})_{ii}^2w(2w_{ii} + \sigma w) + \rho))/\delta, \\ s'' &= (2(A_{ij})_{0i}^2w_{00}w_{0i}^2 - 2(A_{ij})_{00}(A_{ij})_{ii}w_{00}w_{0i}^2 + 2(A_{ij})_{ii}w_{00}w_{0i}^2 + \sigma(A_{ij})_{ii}^2w_{0i}^4 \\ &\quad - 2(A_{ij})_{0i}^2w_{00}^2w_{ii} + 2(A_{ij})_{00}(A_{ij})_{ii}w_{00}^2w_{ii} - 2(A_{ij})_{ii}w_{00}^2w_{ii} \\ &\quad - 2\sigma(A_{ij})_{ii}^2w_{00}w_{0i}^2w_{ii} + \sigma(A_{ij})_{ii}^2w_{00}^2w_{ii}^2 + \rho)/\delta. \end{aligned}$$

Here we set

$$\begin{aligned} w &= w_{0i}^2 - w_{00}w_{ii}, \\ \alpha &= -(A_{ij})_{00} + 1, \\ \rho^2 &= w^2(4(A_{ij})_{0i}^4w_{00}^2 + 8(A_{ij})_{0i}^3(A_{ij})_{ii}w_{00}w_{0i} + 8\alpha(A_{ij})_{0i}(A_{ij})_{ii}^2w_{00}w_{0i} \\ &\quad + 4(A_{ij})_{0i}^2(A_{ij})_{ii}(\alpha w_{00}^2 + (A_{ij})_{ii}w_{0i}^2) + (A_{ij})_{ii}^3(-4(A_{ij})_{00}w_{0i}^2 + 4w_{0i}^2 \\ &\quad + \sigma^2(A_{ij})_{ii}w^2)), \\ \delta &= -2(A_{ij})_{ii}^2((A_{ij})_{0i}^2 + \alpha(A_{ij})_{ii})w^2. \end{aligned}$$