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STRONG FORMULATIONS FOR QUADRATIC OPTIMIZATION WITH M-MATRICES AND SEMI-CONTINUOUS VARIABLES

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ABSTRACT. We study quadratic optimization with semi-continuous variables and an M-matrix, i.e., PSD with non-positive off-diagonal entries. This structure arises in image segmentation, portfolio optimization, as well as a substructure of general quadratic optimization problems. We prove, under mild assumptions, that the minimization problem is solvable in polynomial time by showing its equivalence to a submodular minimization problem. To strengthen the formulation, we decompose the quadratic function into a sum of simple quadratic functions with at most two semi-continuous variables and provide the convex-hull descriptions of these sets. We also describe strong conic quadratic valid inequalities. Preliminary computational experiments indicate that the proposed inequalities can substantially improve the strength of the continuous relaxations with respect to the standard perspective reformulation.

Keywords Quadratic optimization, submodularity, perspective formulation, conic quadratic cuts

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1. INTRODUCTION

Consider the mixed-integer quadratic set

$$S = \left\{(x,y,t) \in \{0,1\}^N \times \mathbb{R}_+^N \times \mathbb{R} : y'Qy \leq t,\ y_i \leq x_i \text{ for all } i \in N\right\},$$

where $N = \{1,\dots,n\}$, and Q is an M-matrix [28], i.e., $Q \succeq 0$ and $Q_{ij} \leq 0$ if $i \neq j$. Set S arises directly in a variety of applications including portfolio optimization [7, 20] and image segmentation [16]. It is also a substructure of general quadratic optimization with semi-continuous variables, which includes the best subset selection [6], control [13], and sparse filter design [30] problems, among others. M-matrices arise in the analysis of Markov chains [18]. Convex quadratic programming with an M-matrix is also studied on its own right [23].

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For the special case where the matrix Q is diagonal, the quadratic function is separable and the convex hull of S can be described using the *perspective reformulation* [9, 12]. This perspective formulation has a compact conic quadratic representation [2, 14] and is now a standard technique for mixed-integer nonlinear optimization [24, 31]. In particular, a convex quadratic function $y'Ay$ is decomposed as $y'Dy+y'Ry$, where $A=D+R$, $D,R \succeq 0$ and D is diagonal and then each diagonal term $D_{ii}y_i^2 \leq t_i$, $i \in N$, is reformulated as $y_i^2 \leq t_i x_i$. Such a decomposition and strengthening of the diagonal terms are also standard for the binary restriction, where $y_i = x_i$, $i \in N$, in which case $x'Ax \Leftrightarrow \sum_{i\in N} D_{ii}x_i + x'Rx$ [e.g. 3, 29].

The binary restriction of S, where $y_i = x_i$ and $Q_{ij} \leq 0$ is also well-understood, since in that case the quadratic function $x'Qx$ is submodular [26] and min $\{a'x + x'Qx : x \in \{0,1\}^n\}$ is a minimum cut problem [e.g., 25] and, thus, is solvable in poynomial time. Although, for the diagonal case and the binary restriction, the convex hull of S is known, few results are available for S. In particular, the quadratic function $y'Qy$ is nonseparable, and convex envelopes of multilinear functions are not well-understood, even in the bilinear case [22].

Whereas the set S with an M-matrix is interesting on its own, the convexification results on S can also be used to strengthen a general quadratic $y'Ay$ by decomposing A as $A = Q+R$, where Q is an M-matrix, generalizing the perspective reformulation approach above.

The key idea for deriving strong formulations for S is decompose the quadratic function in the definition of S as the sum of quadratic functions involving one or two variables:

$$y'Qy = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} Q_{ij} \right) y_i^2 - \sum_{i=1}^{n} \sum_{j=i+1}^{n} Q_{ij}(y_i - y_j)^2. \tag{1}$$

Since a quadratic function with the single semi-continuous variable is well-understood, we turn our attention to studying the mixed-integer set with two semi-continuous variables:

$$X = \left\{ (x,y,t) \in \{0,1\}^2 \times \mathbb{R}_+^2 \times \mathbb{R} : (y_1 - y_2)^2 \leq t,\ y_i \leq x_i,\ i = 1,2 \right\}.$$

The set X is a special case of the mixed-integer set

$$\hat{X} = \left\{ (x,y,t) \in \{0,1\}^2 \times \mathbb{R}_+^2 \times \mathbb{R} : q(y) \leq t,\ y_i \leq x_i,\ i = 1,2 \right\},$$

studied by Jeon et al. [17], where $q(y)$ is a general convex quadratic function. Jeon et al. give conic quadratic valid inequalities for $\hat{X}$ and demonstrate their effectiveness via computational experiments, but the convex hull description of $\hat{X}$ is unknown. In this paper, we improve upon the results of Jeon et al. for the set X. In particular, our main contributions are (*i*) showing under mild assumptions that the minimization of the quadratic function with an M-matrix and semi-continuous variables is equivalent to a submodular minimization problem and, hence, solvable in polynomial time; (*ii*) the convex hull description of X; (*iii*) conic quadratic inequalities amenable to use with conic quadratic MIP solvers — the proposed inequalities dominate the ones given by Jeon et al.; (*iv*) the demonstration of the strength of the inequalities for solving quadratic optimization problems with semi-continuous variables.

Outline The rest of the paper is organized as follows. In Section 2 we review the previous results for S and X. In Section 3 we study the relaxations of S and X, where the semi-continuous variables are unbounded and the related optimization problem. In Section 4 we give the convex hull description of X with bounded semi-continuous variables. The convex hulls obtained in Sections 3 and 4 cannot be immediately implemented with off-the-shelf solvers. Thus, in Section 5 we propose valid conic quadratic inequalities and discuss their strength. In Section 6 we provide a summary computational experiments and in Section 7 we conclude the paper. In Appendix B we give extensions to quadratic functions with positive off-diagonal entries and semi-continuous variables unrestricted in sign.

Notation. Throughout the paper, we use the following convention for division by 0: ${}^0\!/_0 = 0$ and ${}^a\!/_0 = \infty$ if $a > 0$. In particular, the function $p : [0,1] \times \mathbb{R}_+ \to \mathbb{R}_+$ given by $p(x,y) = {}^{y^2}\!/_x$ is the closure of the perspective function of the quadratic function $q(y) = y^2$, and is convex [e.g. 15, p. 160]. For a set $X \subseteq \mathbb{R}^N$, $\text{conv}(X)$ denotes the convex hull of X. Throughout, Q denotes an $n \times n$ M-matrix, i.e., $Q \succeq 0$ and $Q_{ij} \leq 0$ for $i \neq j$.

2. Preliminaries

In this section we briefly review the relevant results on the binary restriction of S and the previous results on set X.

2.1. The binary restriction of S.

Let S_B be the binary restriction of S, i.e. $y = x \in \{0,1\}^n$. In this case, the decomposition

$$x'Qx = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} Q_{ij} \right) x_i^2 - \sum_{i=1}^{n} \sum_{j=i+1}^{n} Q_{ij}(x_i - x_j)^2 \leq t \tag{2}$$

leads to $\text{conv}(S_B)$, by simply taking the convex hull of each term. Indeed, the quadratic problem $\min \left\{ x'Qx : x \in \{0,1\}^n \right\}$ is equivalent to an undirected min-cut problem [e.g. 25] and can be formulated as

$$\min \sum_{i=1}^{n} \left(\sum_{j=1}^{n} Q_{ij} \right) x_i - \sum_{i=1}^{n} \sum_{j=i+1}^{n} Q_{ij} t_{ij} : x_i - x_j \leq t_{ij},\ x_j - x_i \leq t_{ij},\ 0 \leq x \leq 1.$$

Decomposition (2) leading to a simple convex hull description of S_B in the binary case is the main motivation for studying decomposition (1) with the semi-continuous variables.

2.2. Previous results for set X.

Here we review the valid inequalities of Jeon et al. [17] for X. Although their construction is not directly applicable, one can utilize it to obtain limiting inequalities. For $q(y) = y'Ay$ the inequalities of Jeon et al. are described via the inverse of the Cholesky factor of A. However, for X, we have $q(y) = (y_1 - y_2)^2$ or $q(y) = y'Ay$, where $A = \left[\begin{smallmatrix} 1 & -1 \\ -1 & 1 \end{smallmatrix}\right]$ is a singular matrix and the Cholesky factor is not invertible.

However, if the quadratic matrix is given by $A = \begin{bmatrix} d_1 & -1 \\ -1 & d_2 \end{bmatrix}$ with $d_1, d_2 > 1$, then their approach yields three valid inequalities:

$$d_2 \frac{y_2^2}{x_2} - \frac{1}{d_1} x_1 + \left(\frac{d_1 d_2 - 1}{d_1} \right) \frac{y_2^2}{x_2} \leq t$$

$$(d_2 - 1) \frac{y_2^2}{x_2} + d_1 \frac{y_1^2}{x_1} + \frac{x_2}{d_1} - 2x_2 \leq t$$

$$\left(\frac{d_1 d_2 - 1}{d_1} \right) \frac{y_2^2}{x_2} + \frac{\left(\sqrt{d_1} y_1 - \sqrt{\frac{1}{d_1}} y_2 \right)^2}{x_1 + x_2} \leq t.$$

As $d_1, d_2 \to 1$, we arrive at three limiting valid inequalities for X.

Proposition 1 (Jeon at al. [17]). *The following convex inequalities are valid for X:*

$$\frac{y_2^2}{x_2} - x_1 \leq t, \tag{3}$$

$$\frac{y_1^2}{x_1} - x_2 \leq t, \tag{4}$$

$$\frac{(y_1 - y_2)^2}{x_1 + x_2} \leq t. \tag{5}$$

Inequalities (3)–(5) are not sufficient to describe conv(X). In the next two sections we describe conv(X) and give new conic quadratic valid inequalities dominating (3)–(5) for X.

3. The unbounded semi-continuous relaxation

In this section we study the unbounded relaxations of S and X obtained by dropping the upper bound on the continuous variables:

$$S^\infty = \left\{ (x,y,t) \in \{0,1\}^N \times \mathbb{R}_+^N \times \mathbb{R} : y'Qy \leq t,\ y_i(1-x_i) = 0 \text{ for all } i \in N \right\},$$

$$X^\infty = \left\{ (x,y,t) \in \{0,1\}^2 \times \mathbb{R}_+^2 \times \mathbb{R} : (y_1 - y_2)^2 \leq t : y_i(1-x_i) = 0,\ i = 1,2 \right\}.$$

In Section 3.1 we show that the minimization of a linear function over S^∞ is equivalent to a submodular minimization problem. In Section 3.2, we describe conv(X^∞) and in Section 3.3 we use the results in Section 3.2 to derive valid inequalities for S^∞.

3.1. Optimization over S^∞.

We now show that the optimization of a linear function over S^∞ can be solved in polynomial time under a mild assumption on the objective function. Consider the problem

$$\text{(P)} \quad \min \left\{ a'x + b'y + t : (x,y,t) \in S^\infty \right\},$$

where Q is a positive definite M-matrix and $b \leq 0$. We will show that (QP) is a submodular minimization problem. The positive definiteness assumption on Q ensures that an optimal solution exists. Otherwise, if there is $y \geq 0$ with $y'Qy = 0$, the problem may be unbounded. The assumption $b \leq 0$ is satisfied in most applications (e.g., see Sections 6.1 and 6.3). If $b > 0$, then $y = 0$ in any optimal solution.

Proposition 2 (Characterization 15 [28])**.** *A positive definite M-matrix Q is* inverse-positive*, i.e., its inverse satisfies $Q^{-1}_{ij} \geq 0$ for all i, j.*

Proposition 3. *Problem (P) can be solved in polynomial time.*

Proof. We assume that $a \geq 0$ (otherwise $x = 1$ in any optimal solution) and that an optimal solution exists. Given an optimal solution (x^*, y^*) to (QP), let $T = \{i \in N : y_i^* > 0\}$, b_T the subvector of b induced by T, and by Q_T the submatrix of Q induced by T. Then, from KKT conditions, we find $b_T + 2Q_T y_T = 0 \Leftrightarrow y_T = -Q_T^{-1} b_T / 2$. Thus, an optimal solution satisfies $b'y^* + y^{*\prime} Q y^* = -\frac{b_T' Q_T^{-1} b_T}{4}$.

Defining $\theta_{ij} : 2^N \to \mathbb{R}$ for $i, j \in N$ as $\theta_{ij}(T) = (Q_T^{-1})_{ij}$ if $i, j \in T$ and 0 otherwise, observe that (P) is equivalent to the binary minimization problem

$$\min_{T \subseteq N} \ a(T) - \frac{1}{4} \sum_{i \in N} \sum_{j \in N} b_i b_j \theta_{ij}(T).$$

Note that since Q_T is a positive definite M-matrix for any $T \subseteq N$, $Q_T = \mu I_T - P_T$, where P_T is a nonnegative matrix and the largest eigenvalue of P_T is less than μ. By scaling, we may assume that $\mu = 1$. Moreover, $Q_T^{-1} = (I - P_T)^{-1} = \sum_{\ell=0}^{\infty} P_T^{\ell}$ [e.g. 32]. For $\ell \in \mathbb{Z}_+$ and all $i, j \in N$ let $\bar{\theta}^{\ell}_{ij}(T) = (P_T^{\ell})_{ij}$ if $i, j \in T$, and 0 otherwise. Note that $\theta_{ij}(T) = \sum_{\ell=0}^{\infty} \bar{\theta}^{\ell}_{ij}(T)$. Finally, define for $k \in N$ and $T \subseteq N \setminus \{k\}$ the function $\rho^{\ell}_{ij}(k, T) = \bar{\theta}^{\ell}_{ij}(T \cup \{k\}) - \bar{\theta}^{\ell}_{ij}(T)$.

Claim 1. *For all $i, j \in N$ and $\ell \in \mathbb{Z}_+$, $\bar{\theta}^{\ell}_{ij}$ is a monotone supermodular function.*

Proof. The claim is proved by induction on ℓ.

- Base case, $\ell = 0$: Let $k \in N$ and $T \subseteq N \setminus \{k\}$. Note that $P_T^0 = I_T$. Thus $\rho^0_{kk}(k, T) = 1$, and $\rho^0_{ij}(k, T) = 0$ for all cases except $i = j = k$. Thus, the marginal contributions are constant and $\bar{\theta}^0_{ij}$ is supermodular. Monotonicity can be checked easily.
- Induction step: Suppose $\bar{\theta}^{\ell}_{ij}$ is supermodular and monotone for all $i, j \in N$. Observe that $\bar{\theta}^{\ell+1}_{ij}(T) = \sum_{t \in N} \bar{\theta}^{\ell}_{it}(T) P_{tj}$ if $i, j \in T$ and $\bar{\theta}^{\ell+1}_{ij}(T) = 0$ otherwise. Monotonocity of $\bar{\theta}^{\ell+1}_{ij}$ follows immediately from the monotonicity of the functions $\bar{\theta}^{\ell}_{it}$. Now let $k \in N$ and $T_1 \subseteq T_2 \subseteq N \setminus \{k\}$. To prove supermodularity, we check that $\rho^{\ell+1}_{ij}(k, T_2) - \rho^{\ell+1}_{ij}(k, T_1) \geq 0$ by considering all cases:

$k \notin \{i, j\}$:: If $\{i, j\} \subseteq T_1$ then $\rho^{\ell+1}_{ij}(k, T_2) - \rho^{\ell+1}_{ij}(k, T_1) = \sum_{t \in N} (\rho^{\ell}_{it}(k, T_2) - \rho^{\ell}_{it}(k, T_1)) P_{tj} \geq 0$ by supermodularity of functions $\bar{\theta}^{\ell}_{it}$; if $\{i, j\} \not\subseteq T_1$ and $\{i, j\} \subseteq T_2$ then $\rho^{\ell+1}_{ij}(k, T_2) - \rho^{\ell+1}_{ij}(k, T_1) = \rho^{\ell+1}_{ij}(k, T_2) \geq 0$ by monotonicity; finally, if $\{i, j\} \not\subseteq T_2$ then $\rho^{\ell+1}_{ij}(k, T_2) - \rho^{\ell+1}_{ij}(k, T_1) = 0$.

$k = i$: : If $j \in T_1$ then $\rho^{\ell+1}_{kj}(k, T_2) - \rho^{\ell+1}_{kj}(k, T_1) = \sum_{t \in N} (\rho^{\ell}_{kt}(k, T_2) - \rho^{\ell}_{kt}(k, T_1)) P_{tj} \geq 0$ by supermodularity of functions $\bar{\theta}^{\ell}_{kt}$; if $j \notin T_1$ and $j \in T_2$ then $\rho^{\ell+1}_{kj}(k, T_2) - \rho^{\ell+1}_{kj}(k, T_1) = \bar{\theta}^{\ell+1}_{kj}(T_2 \cup \{k\}) \geq 0$; finally, if $j \notin T_2$ then $\rho^{\ell+1}_{kj}(k, T_2) - \rho^{\ell+1}_{kj}(k, T_1) = 0$. The case $k = j$ is identical.

□

As $\theta_{ij}(T) = \sum_{\ell=0}^{\infty} \bar{\theta}_{ij}^{\ell}(T)$ is a sum of supermodular functions, it is supermodular. Consequently, $1/4 \sum_{i\in N}\sum_{j\in N} b_i b_j \theta_{ij}(T)$ is a supermodular function and (P) is a submodular minimization problem, solvable in polynomial time [e.g. 27]. □

3.2. **Convex hull of X^{∞}.** Consider the function $f : [0,1]^2 \times \mathbb{R}_+^2 \to \mathbb{R}_+$ defined as

$$f(x,y) = \begin{cases} \frac{(y_1-y_2)^2}{x_1} & \text{if } y_1 \geq y_2 \\ \frac{(y_2-y_1)^2}{x_2} & \text{if } y_1 \leq y_2 \end{cases} \tag{6}$$

and the corresponding nonlinear inequality

$$f(x,y) \leq t. \tag{7}$$

Remark 1. Observe that that inequality (7) dominates inequality (5) since

$$\frac{(y_1-y_2)^2}{x_1+x_2} \leq \frac{(y_1-y_2)^2}{\max\{x_1,x_2\}} \leq f(x,y).$$

Inequalities (3)–(4) are not valid for the unbounded relaxation X^{∞}.

Proposition 4. *Inequality* (7) *is valid for* X^{∞}.

Proof. There are four cases to consider. If $x_1 = x_2 = 1$, then $f(x,y)$ reduces to the original quadratic inequality $(y_1-y_2)^2$, thus the inequality is valid. If $x_1 = x_2 = 0$, then the points in X^{∞} satisfy $y_1 = y_2 = 0$ and $t \geq 0$; since $f(0,0) = 0$, none of these points are cut off by (7). If $x_1 = 1$ and $x_2 = 0$, then $y_2 = 0$ in any point in X^{∞} and, in particular, $y_1 \geq y_2$; thus $f(x,y)$ reduces to the original inequality. The case where $x_1 = 0$ and $x_2 = 1$ is similar. □

Proposition 5. *The function f is convex on its domain.*

Proof. Let $(\bar{x},\bar{y}),(\hat{x},\hat{y}) \in [0,1]^2 \times \mathbb{R}_+^2$ and let $(x^*,y^*) = (1-\lambda)(\bar{x},\bar{y}) + \lambda(\hat{x},\hat{y})$ for $0 \leq \lambda \leq 1$ be a convex combination of $(\bar{x},\bar{y})$ and $(\hat{x},\hat{y})$. We need to prove that

$$f(x^*,y^*) \leq (1-\lambda)f(\bar{x},\bar{y}) + \lambda f(\hat{x},\hat{y}). \tag{8}$$

If $\bar{y}_1 \geq \bar{y}_2$ and $\hat{y}_1 \geq \hat{y}_2$, or $\bar{y}_1 \leq \bar{y}_2$ and $\hat{y}_1 \leq \hat{y}_2$, inequality (8) holds by convexity of the individual functions in the definition of f. Otherwise, assume, without loss of generality, that $\bar{y}_1 \geq \bar{y}_2$, $\hat{y}_1 \leq \hat{y}_2$, and $y_1^* \leq y_2^*$. Letting $\gamma = \lambda - (1-\lambda)\frac{\bar{y}_1-\bar{y}_2}{\hat{y}_2-\hat{y}_1}$, observe that

- $\gamma \leq \lambda \leq 1$.
- $\gamma \geq 0$, which is equivalent to $y_2^* - y_1^* \geq 0$.
- $y_2^* - y_1^* = \gamma(\hat{y}_2 - \hat{y}_1)$.
- $\gamma\hat{x}_2 \leq \lambda\hat{x}_2 \leq x_2^*$.

Then, we find

$$f(x^*,y^*) = \frac{(y_2^*-y_1^*)^2}{x_2^*} \leq \frac{(y_2^*-y_1^*)^2}{\gamma\hat{x}_2} = \gamma\frac{(\hat{y}_2-\hat{y}_1)^2}{\hat{x}_2} \leq \lambda f(\hat{x},\hat{y}) + (1-\lambda)f(\bar{x},\bar{y}).$$

□

As Theorem 1 below states, inequality (7) and bound constraints for the binary variables describe the convex hull of X^∞.

Theorem 1 (Convex hull of X^∞)**.**

$$conv(X^\infty) = \left\{(x,y,t) \in [0,1]^2 \times \mathbb{R}^2_+ \times \mathbb{R} : f(x,y) \le t\right\}.$$

Proof. Consider the optimization problems

$$(P_0) \qquad \min_{(x,y,t)\in X^\infty} a'x + b'y + ct;$$
$$(P_1) \qquad \min_{(x,y,t)\in[0,1]^2\times\mathbb{R}^2_+\times\mathbb{R}} a'x + b'y + ct \text{ s.t. } f(x,y) \le t.$$

To prove the result we show that for any value of a,b,c, either (P_0) and (P_1) are both unbounded, or there exists a solution integral in x that is optimal for both problems. If $c<0$, then (P_0) and (P_1) are both unbounded, and if $c=0$ then (P_1) corresponds to an optimization problem over an integral polyhedron and it is easily checked that (P_0) and (P_1) are equivalent. Thus, the interesting case is $c>0$ or, by scaling, $c=1$. Note that $t=(y_1-y_2)^2$ in any optimal solution of (P_0), and $t=f(x,y)$ in any optimal solution of (P_1). If $b_1,b_2 \ge 0$, then $y_1=y_2=0$ is optimal with corresponding integer x optimal for both (P_0) and (P_1). Moreover, if $b_1+b_2<0$, then both problems are unbounded: $x_1=x_2=1$, $y_1=y_2=\lambda$ is feasible for any $\lambda>0$ for both problems. Thus, one needs to consider only the case where $b_1+b_2 \ge 0$ and $b_1<0$ or $b_2<0$. Without loss of generality, let $b_1<0$ and $b_2>0$.

Optimal solutions of (P_0). There exists an optimal solution with $y_2=0$ (if $0<y_2\le y_1$, subtracting $\varepsilon>0$ from both y_1 and y_2 does not increase the objective – and if $y_2>y_1$, then swapping the values of y_1 and y_2 reduces the objective). Thus, $y_2=0$, $x_2=0$ if $a_2\ge 0$ and $x_2=1$ otherwise, and either $x_1=y_1=0$ or $x_1=1$ and $y_1=-\frac{b_1}{2}$, which is the stationary point of $b_1y_1+y_1^2$.

Optimal solutions of (P_1). Note that there exists an optimal solution of (P_1) where at least one of the continuous variables is 0 (if $0<y_1,y_2$, subtracting $\varepsilon>0$ from both variables does not increase the objective value — this operation does not change the relative order of y_1 and y_2). Then, we conclude that $y_2=0$ in an optimal solution (if $y_1=0$ and $y_2>0$, then setting $y_2=0$ reduces the objective value). Moreover, when $y_2=0$, then $f(x,y)=y_1^2/x_1$. Thus, in the optimal solution $y_1=-b_1x_1/2$. Substituting in the objective, we see that (P_1) simplifies to $\min_{0\le x_1,x_2\le 1} a_2x_2 + \left(a_1 - b_1^2/4\right)x_1$. For an optimal solution, $x_2=0$ if $a_2\ge 0$ and $x_2=1$ otherwise, and $x_1=0$ if $a_1-b_1^2/4\ge 0$ and $x_1=1$ otherwise. And, if $x_1=1$, then $y_1=-b_1/2$. Hence, the optimal solutions coincide. □

3.3. **Valid inequalities for S^∞.**

Inequalities in an extended formulation. Let $\bar{Q}_i=\sum_{j=1}^n Q_{ij}$ and $P=\{i\in N:\bar{Q}_i>0\}$ and $\bar{P}=N\setminus P$. Using decomposition (1) and introducing t_{ij}, $1\le i\le j\le n$, one can write a convex relaxation of S^∞ as

$$\sum_{i\in\bar{P}} \bar{Q}_i y_i + \sum_{i\in P} \bar{Q}_i y_i^2/x_i - \sum_{i=1}^{n}\sum_{j=i+1}^{n} Q_{ij} t_{ij} \le t$$
$$f(x_i,x_j,y_i,y_j) \le t_{ij}, \;\; 1 \le i \le j \le n.$$

Inequalities in the original space of variables. By projecting out the auxiliary variables t_{ij} one obtains valid inequalities in the original space of variables. If the variables are indexed such that $y_1 \ge y_2 \ge \ldots \ge y_n$, we obtain the inequality

$$\sum_{i\in\bar{P}} \bar{Q}_i y_i + \sum_{i\in P} \bar{Q}_i y_i^2/x_i - \sum_{i=1}^{n}\sum_{j=i+1}^{n} Q_{ij} (y_i - y_j)^2/x_i \le t. \tag{9}$$

Observe that the nonlinear inequality (9) is valid only if $y_1 \ge \ldots \ge y_n$ holds. However, utilizing convexity, we can obtain linear inequalities that are valid for S^∞ by underestimating (9) via its gradient at a differentiable point. Let $(\bar{x},\bar{y}) \in [0,1]^N \times \mathbb{R}^N_+$ such that $\bar{y}_1 \ge \ldots \ge \bar{y}_n$ and $\bar{x} > 0$. Then the linear inequality

$$-\sum_{i\in P} \bar{Q}_i \left(\frac{\bar{y}_i}{\bar{x}_i}\right)^2 x_i + \sum_{i=1}^{n}\left(\sum_{j=i+1}^{n} \frac{Q_{ij}(\bar{y}_i - \bar{y}_j)^2}{\bar{x}_i^2}\right) x_i$$
$$+2\sum_{i\in P} \bar{Q}_i \frac{\bar{y}_i}{\bar{x}_i} y_i + \sum_{i\in\bar{P}} \bar{Q}_i y_i + 2\sum_{i=1}^{n}\left(\sum_{j=1}^{i-1} \frac{Q_{ij}(\bar{y}_j - \bar{y}_i)}{\bar{x}_j} - \sum_{j=i+1}^{n} \frac{Q_{ij}(\bar{y}_i - \bar{y}_j)}{\bar{x}_i}\right) y_i \le t,$$

corresponding to a first order approximation of (9) around $(\bar{x},\bar{y})$, is valid for S^∞ (regardless of the ordering of the variables).

4. The bounded set X

Let $g : [0,1]^2 \times \mathbb{R}^2_+ \to \mathbb{R}_+$ be defined as

$$g(x,y) = \begin{cases} \frac{(y_1-x_2)^2}{x_1-x_2} + \frac{(x_2-y_2)^2}{x_2} & \text{if } y_2 \le x_2 \le y_1 \text{ and } x_2(x_1-y_1) \le y_2(x_1-x_2) \\ \frac{(y_2-x_1)^2}{x_2-x_1} + \frac{(x_1-y_1)^2}{x_1} & \text{if } y_1 \le x_1 \le y_2 \text{ and } x_1(x_2-y_2) \le y_1(x_2-x_1) \\ f(x,y) & \text{otherwise,} \end{cases} \tag{10}$$

where f is the function defined in (6). This section is devoted to proving the main result:

Theorem 2 (Convex hull of X)**.**

$$conv(X) = \left\{(x,y,t) \in [0,1]^2 \times \mathbb{R}^3_+ : g(x,y) \le t, \; y_i \le x_i, \; i = 1,2\right\}.$$

Remark 2. For the binary restriction X_B with $y_i = x_i$, $i = 1,2$, $g(x,y) \le t$ reduces to $|x_1 - x_2| \le t$, which together with the bound constraints describe the convex hull of X_B.

The rest of this section is organized as follows. In Section 4.1 we give the convex hull description of the intermediate set with one semi-continuous variables and one bounded continuous variable:

$$X_1 = \left\{(x,y,t) \in \{0,1\} \times \mathbb{R}^2_+ \times \mathbb{R} : (y_1 - y_2)^2 \le t, \; y_1 \le x, \; y_2 \le 1\right\}.$$

In Section 4.2 we use this results to prove Theorem 2. Finally, in Section 4.3 we give valid inequalities for S. Unlike in Section 3, the convex hull proofs in this section are constructive.

4.1. **Convex hull description of X_1.** Let $g_1 : [0,1]\times\mathbb{R}^2_+ \to \mathbb{R}_+$ be given by

$$g_1(x,y_1,y_2) = \begin{cases} \frac{(y_2-x)^2}{1-x} + \frac{(x-y_1)^2}{x} & \text{if } x-y_1 \le x(y_2-y_1) \\ \frac{(y_1-y_2)^2}{x} & \text{if } y_2 \le y_1 \\ (y_2-y_1)^2 & \text{otherwise.} \end{cases}$$

Proposition 6. *conv*$(X_1) = \left\{(x,y,t)\in[0,1]\times\mathbb{R}^2_+\times\mathbb{R} : g_1(x,y_1,y_2)\le t,\ y_1\le x,\ y_2\le 1\right\}$.

Proof. Note that a point (x,y,t) belongs to conv(X_1) if and only if there exists $(\bar{x},\bar{y},\bar{t})$, $(\hat{x},\hat{y},\hat{t})$ and $0\le\lambda\le 1$ such that

$$t = (1-\lambda)\bar{t}+\lambda\hat{t} \tag{11}$$
$$x = (1-\lambda)\bar{x}+\lambda\hat{x} \tag{12}$$
$$y_1 = (1-\lambda)\bar{y}_1+\lambda\hat{y}_1 \tag{13}$$
$$y_2 = (1-\lambda)\bar{y}_2+\lambda\hat{y}_2 \tag{14}$$
$$\bar{x}=0,\ \hat{x}=1 \tag{15}$$
$$\bar{y}_1=0,\ 0\le\hat{y}_1\le 1 \tag{16}$$
$$0\le\bar{y}_2,\ \hat{y}_2\le 1 \tag{17}$$
$$\bar{t}\ge\bar{y}_2^2 \tag{18}$$
$$\hat{t}\ge(\hat{y}_1-\hat{y}_2)^2. \tag{19}$$

From constraints (12) and (15) we see $\lambda = x$, from constraint (13) $\hat{y}_1=\frac{y_1}{x}$, from (16) $y_1\le x$, from (14) we find $\bar{y}_2=\frac{y_2-x\hat{y}_2}{1-x}$, and from (17) we get $0\le\hat{y}_2\le 1$ and $0\le\frac{y_2-x\hat{y}_2}{1-x}\le 1$. Thus, (11)–(19) is feasible if and only if $0\le y_1\le x$, $0\le y_2\le 1$ and there exists $\hat{y}_2$ such that

$$t\ge\frac{(y_2-x\hat{y}_2)^2}{1-x}+\frac{(x\hat{y}_2-y_1)^2}{x},\ \ 0\le\hat{y}_2\le 1,\ \ \frac{y_2}{x}-\frac{1-x}{x}\le\hat{y}_2\le\frac{y_2}{x}.$$

The existence of such $\hat{y}_2$ can be checked by solving the convex optimization problem

$$\text{(M1)}\qquad \begin{aligned} &\min\varphi(\hat{y}_2) := \frac{(y_2-x\hat{y}_2)^2}{1-x}+\frac{(x\hat{y}_2-y_1)^2}{x} \\ &\text{s.t. } \max\left\{0,\frac{y_2}{x}-\frac{1-x}{x}\right\}\le\hat{y}_2\le\min\left\{1,\frac{y_2}{x}\right\}. \end{aligned}$$

The equation $\varphi'(\hat{y}_2)=0$ yields

$$\begin{aligned} &-\frac{(y_2-x\hat{y}_2)}{1-x}+\frac{(x\hat{y}_2-y_1)}{x}=0 \\ \Leftrightarrow &\hat{y}_2 = y_2+y_1\frac{1-x}{x} := \eta(x,y). \end{aligned}$$

Let $\hat{y}_2^*$ be an optimal solution to (M1). Note that $\hat{y}_2^* > 0$ whenever $\eta(x,y) > 0$. Moreover, $\eta(x,y) \le \frac{y_2}{x} - \frac{1-x}{x} \implies y_1 + 1 \le y_2$, which can only happen if $y_1 = 0$ and $y_2 = 1$, in which case $\frac{y_2}{x} - \frac{1-x}{x} = 1$. Thus, we may assume that $\hat{y}_2^*$ is not equal to one of its lower bounds.

Now observe that $\frac{y_2}{x} \le \eta(x,y) \Leftrightarrow y_2 \le y_1$, in which case $\eta(x,y) \le \frac{y_1}{x} \le 1$. Additionally, if $1 \le \eta(x,y)$, then $x \le y_2$ and in particular $y_1 \le y_2$. Therefore, the cases $\eta(x,y) \le \min\{1, \frac{y_2}{x}\}$, $\eta(x,y) \ge 1$, and $\eta(x,y) \ge \frac{y_2}{x}$ are mutually exclusive if $\frac{y_2}{x} \ne x$, and the optimal solution of (M1) corresponds to setting $\hat{y}_2^* = \eta(x,y)$, $\hat{y}_2^* = 1$, or $\hat{y}_2^* = \frac{y_2}{x}$, respectively. By calculating the objective function of (M1) with the appropriate value of $\hat{y}_2^*$, we find $\varphi(\hat{y}_2^*) = g_1(x,y_1,y_2)$. Hence, $(x,y,t) \in \text{conv}(X_1)$ if and only if $t \ge g_1(x,y_1,y_2)$ and $0 \le y_1 \le x \le 1$, $0 \le y_2 \le 1$. □

4.2. **Convex hull description of X.** We use a similar argument as in the proof of Proposition 6 to prove Theorem 2. Let (x,y,t) be a point such that $0 \le y_i \le x_i \le 1$ and *we additionally assume that* $y_1 \ge y_2$. A point (x,y,t) belongs to conv(X) if and only if there exists $(\bar{x},\bar{y},\bar{t})$, $(\hat{x},\hat{y},\hat{t})$, and $0 \le \lambda \le 1$ such that

$$t = (1-\lambda)\bar{t} + \lambda\hat{t} \tag{20}$$
$$x_1 = (1-\lambda)\bar{x}_1 + \lambda\hat{x}_1 \tag{21}$$
$$x_2 = (1-\lambda)\bar{x}_2 + \lambda\hat{x}_2 \tag{22}$$
$$y_1 = (1-\lambda)\bar{y}_1 + \lambda\hat{y}_1 \tag{23}$$
$$y_2 = (1-\lambda)\bar{y}_2 + \lambda\hat{y}_2 \tag{24}$$
$$\bar{x}_2 = 0,\ \hat{x}_2 = 1 \tag{25}$$
$$\bar{y}_2 = 0,\ 0 \le \hat{y}_2 \le 1 \tag{26}$$
$$0 \le \bar{y}_1 \le \bar{x}_1 \le 1,\ 0 \le \hat{y}_1 \le \hat{x}_1 \le 1 \tag{27}$$
$$\bar{t} \ge \bar{y}_1^2/\bar{x}_1 \tag{28}$$
$$\hat{t} \ge g_1(\hat{x}_1,\hat{y}_1,\hat{y}_2). \tag{29}$$

Using a similar reasoning as in the proof of Proposition 6, we find $\lambda = x_2$, $\hat{y}_2 = \frac{y_2}{x_2}$, $\bar{x}_1 = \frac{x_1 - x_2\hat{x}_1}{1-x_2}$, $\bar{y}_1 = \frac{y_1 - x_2\hat{y}_1}{1-x_2}$, and

$$\text{(M2)} \qquad t \ge \min_{\hat{x}_1,\hat{y}_1} \psi(\hat{x}_1,\hat{y}_1)$$
$$\text{s.t. } 0 \le \hat{y}_1 \le \hat{x}_1 \le 1 \tag{30}$$
$$\hat{y}_1 \le \frac{y_1}{x_2},\ \hat{x}_1 - \hat{y}_1 \le \frac{x_1 - y_1}{x_2},\ \frac{x_1}{x_2} - \frac{1-x_2}{x_2} \le \hat{x}_1, \tag{31}$$

where

$$\psi(\hat{x}_1,\hat{y}_1) := \frac{(y_1 - x_2\hat{y}_1)^2}{x_1 - x_2\hat{x}_1} + x_2 g_1(\hat{x}_1,\hat{y}_1,y_2/x_2).$$

Thus, to find the convex hull of X, we need to compute in closed form the solutions of the optimization problem (M2).

Lemma 1. *There exists an optimal solution* $(\hat{x}_1^*,\hat{y}_1^*)$ *to (M2) such that* $\hat{y}_1^* \ge \frac{y_2}{x_2}$.

Proof. Note that if $\hat{y}_1 < \frac{y_2}{x_2}$, the function ψ is non-increasing in $\hat{y}_1$ for any value of $\hat{x}_1$. Thus there exists an optimal solution where $\hat{y}_1$ is set to one of its upper bounds, i.e., either $\hat{y}_1^* = y_1/x_2$ or $\hat{y}_1^* = \hat{x}_1^*$. Since we assume $y_1 \geq y_2$ and $\hat{y}_1 < y_2/x_2$, the case $\hat{y}_1^* = y_1/x_2$ is not possible.

Now suppose that $\hat{y}_1 = \hat{x}_1$. Then observe that $1 \leq \frac{y_2}{x_2} + \hat{y}_1 \frac{1-\hat{x}_1}{\hat{x}_1} \Leftrightarrow \hat{x}_1 \leq \frac{y_2}{x_2}$. Thus

$$\psi(\hat{x}_1) = \frac{(y_1 - x_2\hat{x}_1)^2}{x_1 - x_2\hat{x}_1} + \frac{(y_2 - x_2\hat{x}_1)^2}{x_2 - x_2\hat{x}_1}$$

in this case (substituting $\hat{y}_1 = \hat{x}_1$). Taking the derivative, we find

$$\psi'(\hat{x}_1) = x_2 \frac{y_1 - x_2\hat{x}_1}{(x_1 - x_2\hat{x}_1)^2}(-2x_1 + x_2\hat{x}_1 + y_1) + x_2 \frac{(y_2 - x_2\hat{x}_1)}{(x_2 - x_2\hat{x}_1)^2}(-2x_2 + x_2\hat{x}_1 + y_2) \cdot$$

Note that $y_1 - x_2\hat{x}_1 \geq 0$ since $\hat{x}_1 = \hat{y}_1 \leq y_1/x_2$ in any feasible solution, and $y_2 - x_2\hat{x}_1 \geq 0$, by assumption. Additionally

- since $y_1 \leq x_1$ and $\hat{x}_1 = \hat{y}_1 \leq y_1/x_2 \leq x_1/x_2$, we find that $-2x_1 + x_2\hat{x}_1 + y_1 \leq 0$,
- since $y_2 \leq x_2$ and $\hat{x}_1 \leq 1$, we find that $-2x_2 + x_2\hat{x}_1 + y_2 \leq 0$.

Therefore, $\psi'(x_1)$ is non-positive, i.e., ψ is non-increasing. Then, increasing $\hat{y}_1 = \hat{x}_1$ another optimal solution can be found. In particular, an optimal solution with $\hat{y}_1^* \geq y_2/x_2$ exits. □

From Lemma 1 we can assume, without loss of generality, that

$$\psi(\hat{x}_1, \hat{y}_1) = \frac{(y_1 - x_2\hat{y}_1)^2}{x_1 - x_2\hat{x}_1} + \frac{(x_2\hat{y}_1 - y_2)^2}{x_2\hat{x}_1} \cdot \tag{32}$$

Taking partial derivatives, we find that

$$\begin{aligned}
\frac{\partial \psi}{\partial \hat{y}_1}(\hat{x}_1, \hat{y}_1) &= 2x_2 \left(-\frac{y_1 - x_2\hat{y}_1}{x_1 - x_2\hat{x}_1} + \frac{x_2\hat{y}_1 - y_2}{x_2\hat{x}_1} \right), \\
\frac{\partial \psi}{\partial \hat{x}_1}(\hat{x}_1, \hat{y}_1) &= x_2 \left(\frac{y_1 - x_2\hat{y}_1}{x_1 - x_2\hat{x}_1} \right)^2 - x_2 \left(\frac{x_2\hat{y}_1 - y_2}{x_2\hat{x}_1} \right)^2.
\end{aligned}$$

Lemmas 2–4 characterize the optimal solutions of (M2), depending on the values of (x, y). Note that if

$$\hat{y}_1 = \frac{y_2}{x_2} + \frac{\hat{x}_1}{x_1}(y_1 - y_2), \tag{33}$$

then $\frac{\partial \psi}{\partial \hat{y}_1}(\hat{x}_1, \hat{y}_1) = \frac{\partial \psi}{\partial \hat{x}_1}(\hat{x}_1, \hat{y}_1) = 0$, independently of the values of $\hat{x}_1$ and $\hat{y}_1$. Thus, any feasible point that satisfies (33) is an optimal solution of (M2), as is the case for Lemmas 2 and 3. In contrast, under the conditions of Lemma 4, no feasible point satisfies (33) as it would violate upper bound constraints. The proofs are given in Appendix A.

Lemma 2. *If $x_1 \leq x_2$ then $\hat{x}_1^* = \frac{x_1 - \varepsilon}{x_2}$, where $\varepsilon > 0$ is a sufficiently small number, and $\hat{y}_1^* = \frac{y_2}{x_2} + \frac{\hat{x}_1^*}{x_1}(y_1 - y_2)$ is an optimal solution to $(M2)$ with objective $\psi(\hat{x}_2^*, \hat{y}_2^*) = \frac{(y_1 - y_2)^2}{x_1}$.*

Lemma 3. *If $x_1 > x_2$ and $y_2(x_1-x_2)+y_1x_2 \leq x_2x_1$, then $\hat{x}_1^* = 1$ and $\hat{y}_1^* = \frac{y_2}{x_2} + \frac{\hat{x}_1^*}{x_1}(y_1-y_2)$ is an optimal solution to $(M2)$ with objective $\psi(\hat{x}_2^*, \hat{y}_2^*) = \frac{(y_1-y_2)^2}{x_1}$.*

Lemma 4. *If $x_1 > x_2$ and $y_2(x_1-x_2)+y_1x_2 \geq x_2x_1$, then $\hat{x}_1^* = 1$ and $\hat{y}_1^* = 1$ is an optimal solution to $(M2)$ with objective $\psi(\hat{x}_2^*, \hat{y}_2^*) = \frac{(y_1-x_2)^2}{x_1-x_2} + \frac{(x_2-y_2)^2}{x_2}$.*

Note that Lemmas 2, 3 and 4 cover all cases with $y_1 \geq y_2$. We can now prove the main result.

Theorem 2. If $y_1 \geq y_2$, the description of the convex hull follows directly from Lemmas 2, 3 and 4. If $y_1 \leq y_2$, the result follows from symmetry. □

4.3. **Valid inequalities for** S. Similar to the discussion in Section 3.3, the description of $\text{conv}(X)$ can be used to derive strong extended convex relaxations for S. In order to obtain inequalities in the original space of variables to find nonlinear inequalities we project out the auxiliary variables for a given ordering $y_1 \geq \ldots \geq y_n$ of the semi-continuous variables with additional restrictions corresponding to conditions $x_j(x_i - y_i) \leq y_j(x_i - x_j)$ in (10). Finally, to obtain linear inequalities valid independent of the conditions, we derive the first order approximations.

Suppose $y_1 \geq \ldots \geq y_n$ and $x_j(x_i-y_i) \leq y_j(x_i-x_j)$ for $j > i$, which holds, in particular, if $x = y$. By eliminating the auxiliary variables under these conditions we obtain the inequality

$$\phi(x,y) = \sum_{i \in \bar{P}} \bar{Q}_i y_i + \sum_{i \in P} \bar{Q}_i y_i^2/x_i - \sum_{i=1}^{n} \sum_{j=i+1}^{n} Q_{ij} \left(\frac{(y_1-x_2)^2}{x_1-x_2} + \frac{(x_2-y_2)^2}{x_2} \right) \leq t. \tag{34}$$

Let $\pi_i = Q_{ii} + 2\sum_{j=i}^{i-1} Q_{ij}$ and $\alpha_i = 2\sum_{j=1}^{i} Q_{ij}$, and recall $\bar{Q}_i = \sum_{j=1}^{n} Q_{ij}$. The partial derivatives of ϕ evaluated at a point $(\bar{x}, \bar{y})$ where $\bar{x} = \bar{y}$ are as follows:

$$\frac{\partial \phi}{\partial x_i}(\bar{x},\bar{y}) = \sum_{j=i+1}^{n} Q_{ij} + \sum_{j=i+1}^{i-1} Q_{ij} - \bar{Q}_i = -Q_{ii} = \pi - \alpha_i, \qquad i \in P$$

$$\frac{\partial \phi}{\partial x_i}(\bar{x},\bar{y}) = \sum_{j=i+1}^{n} Q_{ij} + \sum_{j=i+1}^{i-1} Q_{ij} = \pi - \alpha_i + \bar{Q}_i, \qquad i \in \bar{P}$$

$$\frac{\partial \phi}{\partial y_i}(\bar{x},\bar{y}) = -2\sum_{j=i+1}^{n} Q_{ij} + 2\bar{Q}_i = -\alpha_i, \qquad i \in P$$

$$\frac{\partial \phi}{\partial y_i}(\bar{x},\bar{y}) = -2\sum_{j=i+1}^{n} Q_{ij} + \bar{Q}_i = -\alpha_i - \bar{Q}_i, \qquad i \in \bar{P}.$$

Thus, since $\phi(\bar{x},\bar{y}) + \nabla\phi(\bar{x},\bar{y})(x-\bar{x}, y-\bar{y}) \leq g(x,y) \leq t$, we obtain the linear inequality

$$\sum_{i=1}^{n} \pi_i x_i \leq t + \sum_{i=1}^{n} \alpha_i (x_i - y_i) - \sum_{i \in \bar{P}} \bar{Q}_i (x_i - y_i). \tag{35}$$

Observe that inequality (35) depends only on the ordering of $\bar{x}$, but not on the actual values.

Remark 3. Consider the submodular function given by $q(x) = x'Qx$. The extreme points of the extended polymatroid [11] associated with q, Π, correspond to the vectors π in inequality (35); thus, the convex lower envelope of q is described by the function $\bar{q}(x) = \max_{\pi \in \Pi} \pi' x$ [21]. Atamtürk and Bhardwaj [4] employ these polymatroid inequalities for the binary case. For the semi-continuous case, the inequality (35) is tight for the binary restriction $x = y$, and the right hand side is relaxed as the distance between x and y increases.

Remark 4. The values α_i in inequality (35) corresponds to the value of derivative of $q(x)$ with respect to x_i when $x_j = 1$ for all $j \leq i$ and $x_j = 0$ for $j > i$. Atamtürk and Jeon [5] use lifting to derive similar inequalities for another class of nonlinear functions with semi-continuous variables and submodular binary restriction.

5. Valid inequalities for X

The inequalities $f(x,y) \leq t$ and $g(x,y) \leq t$ derived in Sections 3 and 4 for X^∞ and X, respectively, cannot be directly used within off-the-shelf solvers as they are piecewise functions. However, since they are convex, they can be implemented using gradient outer-approximations at differentiable points (as discussed in Sections 3.3 and 4.3): given a fractional point $(\bar{x}, \bar{y})$ with $\bar{x} > 0$, the inequality

$$g(\bar{x},\bar{y}) + \nabla g(\bar{x},\bar{y})'(x - \bar{x}, y - \bar{y}) \leq t \tag{36}$$

can be used as a cutting plane to improve the continuous relaxation. However, such an approach may require adding too many inequalities (36) to the formulation, possibly resulting in poor performance (see also Sections 6.1 and 6.3 for additional discussion on computations). Therefore, in this section we give valid conic quadratic inequalities that provide a strong approximation of $\text{conv}(X)$ and can be readily used within conic quadratic solvers.

5.1. Derivation of the inequalities.

For the restriction $L_2 = \{(x,y,t) \in X : x_2 = 0\}$ observe that

$$\text{conv}(L_2) = \left\{ (x,y,t) \in [0,1]^2 \times \mathbb{R}^2_+ \times \mathbb{R} : \frac{y_1^2}{x_1} \leq t,\ y_1 \leq x_1,\ x_2 = y_2 = 0 \right\}.$$

We now consider inequalities obtained by lifting the valid inequality $\frac{y_1^2}{x_1} \leq t$ for $\text{conv}(L_2)$, i.e., inequalities of the form

$$\frac{y_1^2}{x_1} + h(x_2, y_2) \leq t \tag{37}$$

for X, where $h : [0,1] \times \mathbb{R}_+ \to \mathbb{R}$. We additionally require the left hand side of (37) to be convex, which is the case if and only if h is convex.

Proposition 7. *Inequality*

$$\frac{y_1^2}{x_1} + \frac{y_2^2}{x_2} - 2y_2 \leq t \tag{38}$$

is valid for X and is the strongest convex inequality of the form (37).

Proof. Any valid inequality of the form (37) needs to satisfy

$$h(x_2,y_2) \leq \alpha = \min \left\{ (y_1-y_2)^2 - \frac{y_1^2}{x_1} \ : \ 0 \leq y_1 \leq x_1, \ x_1 \in \{0,1\} \right\}.$$

If $x_1 = 0$, then $\alpha = y_2^2$; else, $\alpha = -2y_1y_2 + y_2^2$. Thus, $y_1 = x_1 = 1$ is a minimizer. We also find that $h(x_2,y_2) \leq y_2^2 - 2y_2$ for $x_2 \in \{0,1\}$. To find the strongest convex inequality, we compute $\text{conv}(W)$, where

$$W = \left\{ (x_2,y_2,t_2) \in \{0,1\} \times \mathbb{R}_+^2 : y_2^2 - 2y_2 \leq t_2, \ y_2 \leq x_2 \right\}.$$

Using the perspective reformulation, one sees that

$$\text{conv}(W) = \left\{ (x_2,y_2,t_2) \in [0,1] \times \mathbb{R}_+^2 : \frac{y_2^2}{x_2} - 2y_2 \leq t_2, \ y_2 \leq x_2 \right\},$$

and we get inequality (38). □

By changing the lifting order, we also get that valid inequality $\frac{y_1^2}{x_1} + \frac{y_2^2}{x_2} - 2y_1 \leq t$, or, writing the inequalities more compactly, we arrive at the convex valid inequality

$$\frac{y_1^2}{x_1} + \frac{y_2^2}{x_2} - 2\min\{y_1,y_2\} \leq t. \tag{39}$$

Remark 5. Observe that inequality (39) dominates inequality (4) since

$$\frac{y_1^2}{x_1} - x_2 = \frac{y_1^2}{x_1} - y_2 - (x_2 - y_2) \leq \frac{y_1^2}{x_1} - y_2 - (x_2 - y_2)\frac{y_2}{x_2} = \frac{y_1^2}{x_1} + \frac{y_2^2}{x_2} - 2y_2.$$

Similarly, we find that (39) dominates inequality (3).

Remark 6. For the binary case, $y_i = x_i$, $i = 1,2$, inequality (39) reduces to $|x_1 - x_2| \leq t$.

5.2. **Strength of the inequalities.** In order to assess the strength of inequality (39), we consider the optimization problem

$$\begin{aligned} \text{(SR)} \qquad & \min a_1x_1 + a_2x_2 + b_1y_1 + b_2y_2 + t \\ & \text{s.t. } (y_1 - y_2)^2 \leq t \\ & \quad \frac{y_1^2}{x_1} + \frac{y_2^2}{x_2} - 2\min\{y_1,y_2\} \leq t \\ & \quad 0 \leq y_1 \leq x_1 \leq 1 \\ & \quad 0 \leq y_2 \leq x_2 \leq 1. \end{aligned}$$

and show that the solution of (SR) are integral in x under mild assumptions on the coefficients a and b. First, we prove an auxiliary lemma.

Lemma 5. *If there exists an optimal solution to (SR) with $y_i \in \{0,1\}$ for some $i \in \{1,2\}$, then there exists an optimal solution that is integral in x.*

Proof. If $y_1 = 0$, then clearly there is an optimal solution with $x_1 \in \{0,1\}$, depending on the sign of a_1. Moreover, (SR) reduces to $\min_{0\leq y_2 \leq x_2 \leq 1} \left\{ a_2x_2 + b_2y_2 + y_2^2/x_2 \right\}$, which has an optimal integral solution in x_2. On the other hand, if $y_1 = x_1 = 1$, then (SR) reduces to $\min_{0\leq y_2\leq x_2\leq 1}\left\{a_2x_2+(b_2-2)y_2+y_2^2/x_2\right\}$, which, again, has an optimal integral solution in x_2. The case with $y_2\in\{0,1\}$ is symmetric. $\square$

Proposition 8. *If a_1,a_2 have the same sign and b_1,b_2 have the same sign, then (SR) has an optimal solution that is integral in x.*

Proof. Note that if $a_1,a_2\leq 0$, then $x_1=x_2=1$ for an optimal solution of (SR). Also, if $b_1,b_2\geq 0$, then $y_1=y_2=0$ in an optimal solution of (SR), in which case x is integral in extreme point solutions. It remains to show that if $a_1,a_2\geq 0$ and $b_1,b_2\leq 0$, then there exists an optimal solution of (SR) that is integral in x.

Suppose that $y_1=y_2=y$ in an optimal solution. Then $(y_1-y_2)^2=0$ and $\frac{y^2}{x_1}+\frac{y^2}{x_2}-2y\leq 0$. Thus, $t=0$ and (SR) reduces to

$$\min\left\{a_1x_1+a_2x_2+(b_1+b_2)y : 0\leq y\leq \min\{x_1,x_2\}\leq 1\right\},$$

which has an optimal solution integral in x.

Now suppose, without loss of generality, there is an optimal solution with $1>y_1>y_2>0$ (if $y_1=1$ or $y_2=0$ then by Lemma 5 the solution is integral in x). Then observe that, in this case, the functions $(y_1-y_2)^2$ and y_2^2/x_2-2y_2 are non-increasing in y_2. Since $b_2\leq 0$, there exists a solution where y_2 is at its upper bound, i.e., $y_2=x_2$. Thus problem (SR) reduces to

$$(\mathrm{SR}')\ \ \min\left\{a_1x_1+b_1y_1+(a_2+b_2)y_2+t : (y_1-y_2)^2\leq t, \frac{y_1^2}{x_1}-y_2\leq t, y_1\leq x_1\leq 1\right\}.$$

Let $(\lambda,\mu,\alpha,\beta)$ be the dual variables associated with the $\leq$ constraints displayed in the order above. and consider the dual feasibility conditions of problem (SR′)

$$\begin{aligned}
-a_1 &= -\mu_1\frac{y_1^2}{x_1^2}-\alpha+\beta\\
-b_1 &= 2\lambda(y_1-y_2)+2\mu\frac{y_1}{x_1}+\alpha\\
-(a_2+b_2) &= -2\lambda(y_1-y_2)-\mu\\
1 &= \lambda+\mu\\
0 &\leq \lambda,\mu,\alpha,\beta.
\end{aligned}$$

Let $(\bar{x_1},\bar{y_1},\bar{y_2},\bar{t})$ be a KKT point with multipliers $(\bar{\lambda},\bar{\mu},\bar{\alpha},\bar{\beta})$ and suppose that $\bar{x}_1<1$. Then observe that for small $\varepsilon>0$, $(\frac{\bar{y}_1+\varepsilon}{\bar{y}_1}\bar{x_1},\bar{y_1}+\varepsilon,\bar{y_2}+\varepsilon,\bar{t})$ is also a KKT point with the same multipliers. In particular, by choosing ε so that $1=\frac{\bar{y}+\varepsilon}{\bar{y}}\bar{x}$, we see that there is an optimal solution with $x_1=1$. Then, problem (SR′) further simplifies to

$$(\mathrm{SR}'')\quad \min\{b_1y_1+(a_2+b_2)y_2+t : (y_1-y_2)^2\leq t, y_1^2-y_2\leq t\}.$$

It remains to show that $y_2=x_2$ is integral. Note that

$$y_1^2-2y_1y_2+y_2^2=y_1^2-y_2(2y_1-1)\geq y_1^2-y_2,$$

and, therefore, constraint $y_1^2-y_2\leq t$ is not binding when $y_1<1$. So, (SR′′) is equivalent to $\min b_1y_1+(a_2+b_2)y_2+(y_1-y_2)^2$. However, by increasing or decreasing

y_1 and y_2 by the same amount it is easy to check that there exists an optimal solution where either $y_1 = 1$ or $y_2 = 0$, and from Lemma 5 there exists an optimal integral solution. □

6. Computations

In this section we report a summary of computational experiments performed to test the effectiveness of the proposed inequalities in a branch-and-bound algorithm. All experiments are conducted using Gurobi 7.5 solver on a workstation with a 3.60GHz Intel® Xeon® E5-1650 CPU and 32 GB main memory with a single thread. The time limit is set to one hour and Gurobi's default settings are used. Cuts (if used) are added only at the root node using the callback features of Gurobi, and the reported times include the time used to add cuts.

6.1. **Image segmentation with ℓ-0 penalty.** Given a finite set N, functions $d_i : \mathbb{R} \to \mathbb{R}_+$ for $i \in N$ and $s_{ij} : \mathbb{R} \to \mathbb{R}_+$ for $i \neq j$, consider

$$(D) \qquad \min_{y \in Y} \sum_{i \in N} d_i(y_i) + \sum_{i \neq j} s_{ij}(y_i - y_j),$$

where $Y \subseteq \mathbb{R}^N_+$. Problem (D) arises as the Markov Random Fields (MRF) problem for image segmentation, see [8, 19]. In the MRF context, d_i are the *deviation* penalty functions, used to model the cost of changing the value of a pixel from the observed value p_i to y_i, e.g., $d_i(y_i) = c_i(p_i - y_i)^2$ with $c_i \in \mathbb{R}_+$; functions s_{ij} are the *separation* penalty functions, used to model the cost of having adjacent pixels with different values, e.g., $s_{ij}(y_i - y_j) = c_{ij}(y_i - y_j)^2$ with $c_{ij} > 0$ if pixels i and j are adjacent, and $s_{ij}(y_i - y_j) = 0$ otherwise. Often, $Y = [0,1]^N$ or is given by a suitable discretization, i.e., y is a vector of integer multiples of a parameter ε. We consider in our computations the case $Y = [0,1]^N$, but the proposed approach can be used with any Y.

Problem (D) can be cast as the nonlinear dual of the undirected minimum cost network flow problem [1] and efficient algorithms exist when all functions are convex [16]. In contrast, we consider here the case where the deviation functions involve a non-convex ℓ-0 penalty, which is often used to induce sparsity, e.g., restricting the number of pixels that can have a color different from the background color. In particular, $d_i(y_i) = a_i\|y_i\|_0 + \bar{d}_i(y_i)$ with $\bar{d}_i = c_i(p_i - y_i)^2$. Thus, the problem can be formulated as

$$\min \sum_{i \in N} a_i x_i + \sum_{i \in N} c_i(p_i - y_i)^2 + \sum_{i \neq j} c_{ij} t_{ij} \text{ s. t. } (x_i, x_j, y_i, y_j, t_{ij}) \in X, \ \forall i \neq j. \quad (40)$$

Instances. The instances are constructed as follows. The elements of N correspond to points in a $k \times k$ grid, thus $n = k^2$, and separation functions s_{ij} are non-zero whenever the corresponding points are adjacent in the grid. The parameters p_i for $i \in N$, and c_{ij} for each pair of adjacent points $i, j \in N$ are drawn uniformly between 0 and 1. We set $a_i = c_i$, where c_i is generated as follows: first we draw $\tilde{c}_i$ uniformly between 0 and 1 for all $i \in N$, let $C_1 = \sum_{i \in N} \tilde{c}_i$ and $C_2 = \sum_{i: p_i \geq 0.5}(2p_i - 1)$; then we set $c_i = \tilde{c}_i \frac{C_1}{C_2}$. Instances generated with these parameters are observed to have large integrality gaps.

Formulations. We test the following formulations for solving problem (40):

- `Continuous`**:** The natural convex relaxation.
- `Perspective`**:** Variables $z_i \geq 0$ and rotated cone constraints $y_i^2 \leq z_i x_i$ are added for $i \in N$, and the deviation penalty functions in the objective are rewritten as $c_i p_i^2 - 2c_i p_i y_i + c_i z_i$.
- `Conic`**:** In addition to the perspective reformulation, the conic quadratic inequalities (39) are also added in an extended formulation.

Furthermore, we also test models `Perspective+cuts` and `Conic+cuts`, where the gradient inequalities (36) are used as cutting planes to strengthen the `Perspective` and `Conic` formulations, respectively. If $\bar{x}_i = 0$ for some $i \in N$ then we use the gradient expansion around $\bar{x}_i = 10^{-5}$ instead.

Results. Table 1 shows a comparison of the performance of the algorithm for each formulation for varying grid sizes. Each row in the table represents the average for five instances for a grid size. Table 1 displays the initial gap (`igap`), the root gap improvement (`rimp`), the number of branch and bound nodes (`nodes`), the elapsed time in seconds (`time`), and the end gap at termination (`egap`) (in brackets, we report the number of instances solved to optimality within the time limit). The initial gap is computed as $\texttt{igap} = \frac{\texttt{obj}_{\texttt{best}} - \texttt{obj}_{\texttt{cont}}}{|\texttt{obj}_{\texttt{best}}|}$, where $\texttt{obj}_{\texttt{best}}$ is the objective value of the best feasible solution found and $\texttt{obj}_{\texttt{cont}}$ is the objective of the relaxation `Continuous`. The root improvement is computed as $\texttt{rimp} = \frac{\texttt{obj}_{\texttt{relax}} - \texttt{obj}_{\texttt{cont}}}{\texttt{obj}_{\texttt{best}} - \texttt{obj}_{\texttt{cont}}}$, where $\texttt{obj}_{\texttt{relax}}$ is the objective value of the relaxation obtained after processing the first node of the branch-and-bound tree for a given formulation.

We observe that the `Continuous` formulation requires a substantial amount of branching before proving optimality, resulting in long solution times. The `Perspective` formulation results in a root gap improvement close to 50% and better times and end gaps than the `Continuous` formulation. However, even with the `Perspective` formulation, instances with $k \times k = 400$ and larger cannot be solved to optimality leaving end gaps 15.3% or more. In contrast, formulation `Conic` results in root gap improvements close to 100%, and the performance of the branch-and-bound algorithm is orders-of-magnitude better than with the `Continuous` and `Perspective` formulations: instances with $k \times k = 400$ that are not close to being solved after one hour of computation with `Continuous` and `Perspective` are solved to optimality in one second; while formulation `Continuous` is able to solve in five minutes instances with 100 variables, formulation `Conic` is able to solve in the same amount of time formulations with $2,500$ variables, i.e., instances 250 times larger.

Note that formulation `Conic+cuts` results in very modest improvement in the strength of the continuous relaxation when compared with `Conic` (less than 0.3% additional root gap improvement) and almost no difference in terms of nodes, times or end gaps. Observe that in (40) the coefficients of the linear objective terms corresponding to the discrete and continuous variables have the same sign, and the experimental results are consistent with Proposition 8 — `Conic` indeed is a very close approximation of inequalites (36) in this case.

Finally, note that if cuts are added without the approximation given by inequalities (39) (formulation `Perspective+cuts`), the root improvement is substantial for small instances but it degrades as the size increases. We conjecture that the required number of cuts to obtain an adequate relaxation increases with the size of the instances. Thus, for larger instances, Gurobi may stop adding cuts before obtaining a strong relaxation. Additionally, to solve second-order conic subproblems in branch-and-bound, solvers like Gurobi construct a linear outer approximation of the convex sets; adding a large number of cuts may interfere with the construction of the outer approximation, leading to weak relaxations of the convex set, which is observed for instances with $k \times k = 10,000$. Using the approximation of the convex hull derived in Section 5 as a starting point appears to circumvent such numerical difficulties.

6.2. **Portfolio optimization with transaction costs.** Consider a simple portfolio optimization problem with transaction costs similar to the one discussed in [10, p.146]. However, in our case, transactions have a fixed cost and there is a restricted number of transactions. For simplicity, we consider assets with uncorrelated returns (see Section 6.3 for computations with general quadratic functions).

Let N be the set of assets, $\mu, \sigma \in \mathbb{R}^N_+$ be the vectors of expected returns and standard deviations of returns. Let $w \in \mathbb{R}^N_+$ denote the current holdings in each asset, let $a^+, a^- \in \mathbb{R}^N_+$ be the fixed transaction costs associated with buying and selling any quantity, $c^+, c^- \in \mathbb{R}^N$ be the variable transaction costs and profits of buying and selling each asset, let $u^+, u^- \in \mathbb{R}^N_+$ be the upper bounds on the transactions, and let k be the maximum number of transactions. Then the problem of finding a minimum risk portfolio that satisfies a given expected return $b \in \mathbb{R}$ with at most k transactions can be formulated as the mixed-integer quadratic problem:

$$
\begin{aligned}
\min\ & v(y) = \sum_{i \in N} \sigma_i^2 (w_i + y_i^+ - y_i^-)^2 \\
\text{s.t.}\ & \sum_{i \in N} \left(\mu_i w_i + y_i^+ (\mu_i - c_i^+) - y_i^- (\mu_i - c_i^-) - a_i^+ x_i^+ - a_i^- x_i^- \right) \geq b \\
& \sum_{i \in N} (x_i^+ + x_i^-) \leq k \\
& 0 \leq y_i^+ \leq u_i^+ x_i^+,\ 0 \leq y_i^- \leq u_i^- x_i^-, \quad \forall i \in N \\
& (x^+, x^-, y^+, y^-) \in \{0,1\}^N \times \{0,1\}^N \times \mathbb{R}^N_+ \times \mathbb{R}^N_+,
\end{aligned}
$$

where $v(y)$ is the variance of the new portfolio, the decision variables y_i^+ (y_i^-) indicate the amount bought (sold) in asset i and the variables x_i^+ (x_i^-) indicate whether asset i is bought (sold). Note that the quadratic objective function is nonseparable and the corresponding quadratic matrix is positive semi-definite but not positive definite; therefore, the classical perspective reformulation cannot be used. Additionally, observe that the portfolio optimization problem can be reformulated by adding continuous variables $t \in \mathbb{R}^N_+$, constraints $(x_i^+, x_i^-, y_i^+, y_i^-, t_i) \in X$ for all $i \in N$

to minimize the linear objective

$$\sum_{i\in N} \sigma_i^2(2w_i(y_i^+ - y_i^-) + t_i)\cdot \tag{41}$$

Note that since each continuous variable is involved in exactly one term in the objective, the extended formulation given by (41) and constraints $(x_i^+, x_i^-, y_i^+, y_i^-, t_i) \in \text{conv}(X)$ results in the convex envelope of $v(y)$.

Instances. The instances are constructed as follows. We set $w_i = u_i^+ = u_i^- = 1$ for all $i \in N$. Coefficients σ_i are drawn uniformly between 0 and 1, μ_i are drawn uniformly between 0 and $2\sigma_i$, the transactions costs and profits c_i^+ and c_i^- are drawn uniformly between 0 and μ_i, the fixed costs a_i^+ and a_i^- are drawn uniformly between 0 and $u_i^+(\mu_i - c_i^+)$ and $u_i^-(\mu_i - c_i^-)$, respectively. The target return is set to $\beta \sum_{i\in N} \mu_i$ where $\beta > 0$ is a parameter; k is set to $n/10$.

Formulations. We test the formulations `Continuous`, `Continuous+cuts`, `Conic`, and `Conic+cuts`, as defined in Section 6.1. As mentioned above, the perspective reformulation cannot be used for these instances. Also note that when using formulations `Conic` and `Conic+cuts`, the additional variables and rotated cone constraints usually used with the perspective reformulation are still added to the formulation, resulting in a mixed-integer conic quadratic optimization problem. However, for formulation `Continuous+cuts` such variables are not required, resulting in a mixed-integer quadratic optimization problem.

Results. Table 2 shows the results for varying number of assets n and values of the expected return β. Observe that instances with lower values of β are more difficult to solve for the `Continuous` formulation: low β results in more feasible solutions, and more branch-and-bound nodes need to be explored before proving optimality. We also see that the `Continuous` formulation is not effective for instances with 250 or more assets, where most instances (27 out of 30) are not solved to optimality within the time limit and leaving large end gaps at termination. On the other hand, the other three formulations achieve root improvements of over 90% in most cases, and lead to much lower solution times and end gaps.

Observe that for the portfolio problem, the coefficients of y_i^+ and y_i^- in the objective and return constraints have opposite signs. Thus, we expect the approximation given by `Conic` not to be as effective as in Section 6.1 and, therefore, the cuts to have a larger impact in closing the root gaps. Indeed, we see in these experiments that adding cuts leads to an additional 2% to 4% root improvement (compared to the 0.3% improvement observed in Section 6.1)[1]. In particular, formulation `Continuous+cuts` is able to solve all instances in seconds, even instances with low values of β where all other formulations struggle.

[1]The root gap improvements of 95% achieved by `Conic` indicate that the approximation given in Section 5 is strong and considerably better than the natural continuous relaxation.

6.3. **General convex quadratic functions.** The quadratic matrices used in the previous computations had specific structures, given by the applications considered. Although our results are M-matrices, in this section, we test the strength of the formulations for more general problems, with dense matrices having positive and negative off-diagonal entries. To employ the results developed for M-matrices, we simply apply the strengthening on the pairs of variables with a negative off-diagonal entry. Toward this end, we consider the mean-variance portfolio optimization

$$
(MV) \quad \begin{aligned} \min\ & y'Ay \\ \text{s.t. } & b'y \geq r \\ & 1'x \leq k \\ & 0 \leq y \leq x \\ & x \in \{0,1\}^n. \end{aligned}
$$

where the objective is to minimize the portfolio variance $y'Ay$, where A is a covariance matrix, subject to meeting a target return and satisfying sparsity constraints.

Instances. In order test the effect of positive off-diagonal elements and diagonal dominance, the matrix A is constructed as follows: Let $\rho \geq 0$ be a parameter that controls the magnitude of the positive off-diagonal entries of A, and $\delta \geq 0$ be a parameter that controls the diagonal dominance of A. First, we construct a factor matrix $F = GG'$, where each entry in $G_{20\times 20}$ in drawn uniformly from $[-1,1]$, and an exposure matrix $X_{n\times 20}$ such that $X_{ij} = 0$ with probability 0.8, and X_{ij} is drawn uniformly from $[0,1]$, otherwise. Then we construct an auxiliary matrix $\bar{A} = XFX'$. Then, for $i \neq j$, we set $A_{ij} = \bar{A}_{ij}$ if $\bar{A}_{ij} \leq 0$, and we set $A_{ij} = \rho\bar{A}_{ij}$ otherwise[2]. Finally, υ_i is drawn uniformly from $[0, \delta\bar{\sigma}]$, where $\bar{\sigma} = \frac{1}{n}\sum_{i\neq j}|A_{ij}|$, and $A_{ii} = \sum_{j\in N}|A_{ij}| + \upsilon_i$. Additionally, b_i is drawn uniformly between $0.5U_{ii}$ and $1.5U_{ii}$, $r = 0.25\sum_{i\in N} b_i$ and $k = n/5$.

Formulations. We test the same formulations as in Section 6.1. In this case, the diagonal matrix $\text{diag}(\upsilon)$ is used for the `Perspective` formulation.

Results. Table 3 presents the results for matrices with non-positive off diagonal entries (i.e., $\rho = 0$) and varying diagonal dominance δ. Table 4 presents the results for matrices with fixed diagonal dominance and varying magnitudes for positive off-diagonal entries ρ. We see that, in all cases formulation `Conic` results in better root gap improvements than `Perspective` and `Continuous`. The gap improvements depend on the parameters δ and ρ. In Table 3 we see that `Conic` formulation closes an additional 30% to 40% gap with respect to `Perspective` (independent of the diagonal dominance δ). In Table 4 we observe that, as expected, `Conic`

[2]The matrices generated this way have only 20.1% of the off-diagonal entries negative on average – the rest are positive if $\rho > 0$ and 0 if $\rho = 0$. The ratio of the magnitude of the negative entries vs. the total, i.e., $\frac{\sum_{i\neq j: A_{ij}<0}|A_{ij}|}{\sum_{i\neq j}|A_{ij}|}$, is on average 0.72 if $\rho = 0.1$, 0.57 if $\rho = 0.2$ and 0.34 if $\rho = 0.5$.

formulation is more effective at closing root gaps when the magnitude ρ for the positive off-diagonal entries is small. Nevertheless, for all instances formulations `Conic` and `Conic+cuts` result in significantly stronger root improvements than `Perspective` (at least 15%, and often much more) and the number of nodes required to solve the instances is decreased by at least an order of magnitude.

Observe that the stronger formulations of `Conic` and `Conic+cuts` do not necessarily lead to better solution times for small instances. Nevertheless, for the larger instances ($n = 100$), using the `Conic` formulation leads to faster solution times, lower end gaps and more instances solved to optimality for all values of δ and ρ. As in Section 6.1, we observe little difference between `Conic` and `Conic+cuts` — consistent with Proposition 8— and that `Perspective+cuts` is not effective in closing the root gap. Approximating the nonlinear function with gradient inequalities appears to cause numerical issues as adding cuts weakens the relaxation contrary to expectations. Please see our comments at the end of Section 6.1.

7. Conclusions

In this paper we show, under mild assumptions, that minimization of a quadratic function with an M-matrix over semi-continuous variables is a submodular minimization problem, hence, solvable in polynomial time. We derive strong formulations using the convex hull description of non-separable quadratic terms with two semi-continuous variables arising from a decomposition of the quadratic function. Additionally, we provide strong conic quadratic valid inequalities approximating the convex hulls. The derived formulations generalize previous results in the binary case and separable semi-continuous case, and the inequalities dominate valid inequalities given in the literature. Computational experiments indicate that the proposed conic formulations may be significantly more effective compared to the natural convex relaxation and the perspective reformulation.

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TABLE 1. Experiments with image segmentation with ℓ-0 penalty.

$k \times k$	igap	Continuous			Perspective				Perspective+cuts				Conic				Conic+cuts			
		nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap
100	51.0	2,065,285	301	0.0[5]	47.9	70,898	17	0.0[5]	99.6	27,006	601	0.0[5]	99.4	7	0	0.0[5]	99.7	7	0	0.0[5]
400	47.7	9,520,774	3,600	34.0[0]	48.6	5,277,876	3,600	15.3[0]	93.2	305	2	0.0[5]	99.5	59	1	0.0[5]	99.5	58	1	0.0[5]
2,500	47.9	1,091,872	3,600	46.3[0]	45.6	682,406	3,600	25.6[0]	47.2	38,989	2,235	9.9[2]	99.3	17,561	393	0.0[5]	99.6	9,220	210	0.0[5]
10,000	47.4	167,529	3,600	47.2[0]	45.9	131,986	3,600	25.9[0]	32.4	25,992	3,600	0.2[0]	99.5	25,842	3,600	0.1[0]	99.6	26,695	3,600	0.1[0]

TABLE 2. Experiments with portfolio optimization with fixed transaction costs.

n	β	igap	Continuous				Continuous+cuts				Conic				Conic+cuts			
			rimp	nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap
	0.95	30.8	0.0	40,595	10	0.0[5]	98.1	57	0	0.0[5]	87.0	1,962	10	0.0[5]	92.8	1,507	6	0.0[5]
100	0.98	27.2	0.0	8,252	2	0.0[5]	97.9	342	3	0.0[5]	98.9	30	0	0.0[5]	95.1	168	1	0.0[5]
	1.00	31.6	0.0	3,547	1	0.0[5]	96.4	54	0	0.0[5]	95.3	78	0	0.0[5]	98.5	27	0	0.0[5]
Average			**0.0**	**17,465**	**5**	**0.0[15]**	**97.5**	**151**	**1**	**0.0[15]**	**93.7**	**690**	**3**	**0.0[15]**	**95.5**	**567**	**2**	**0.0[15]**
	0.95	32.4	0.0	5,785,770	3,600	14.9[0]	99.1	169	1	0.0[5]	92.3	198,879	3,600	2.4[0]	95.4	287,237	3,600	1.5[0]
250	0.98	26.1	0.0	5,231,252	3,190	6.8[1]	97.2	317	1	0.0[5]	97.2	125	0	0.0[5]	98.1	52,860	720	0.3[4]
	1.00	26.9	0.0	4,934,387	2,884	2.7[2]	98.2	226	0	0.0[5]	97.1	7,491	87	0.0[5]	98.0	20,363	689	0.0[5]
Average			**0.0**	**5,317,136**	**3,224**	**8.1[3]**	**98.2**	**238**	**1**	**0.0[15]**	**95.5**	**68,832**	**1,229**	**0.8[10]**	**97.2**	**120,153**	**1,670**	**0.6[9]**
	0.95	32.3	0.0	3,079,780	3,600	24.5[0]	97.9	391	3	0.0[5]	94.5	49,749	2,161	0.8[2]	97.1	114,302	2,880	0.6[1]
500	0.98	26.1	0.0	3,220,896	3,600	17.3[0]	97.3	362	3	0.0[5]	94.1	296	2	0.0[5]	98.5	236	1	0.0[5]
	1.00	27.4	0.0	3,396,448	3,600	16.3[0]	98.8	348	1	0.0[5]	97.2	275	1	0.0[5]	99.4	265	1	0.0[5]
Average			**0.0**	**3,232,375**	**3,600**	**19.4[0]**	**98.0**	**367**	**2**	**0.0[15]**	**95.3**	**16,773**	**721**	**0.3[12]**	**98.3**	**38,268**	**961**	**0.2[11]**

TABLE 3. Experiments with non-positive off diagonal entries and varying diagonal dominance.

n	δ	igap	Continuous			Perspective				Perspective+cuts				Conic				Conic+cuts			
			nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap
	0.1	88.2	$4 \cdot 10^5$	86	0.0[5]	7.2	$4 \cdot 10^5$	99	0.0[5]	19.2	15,230	544	0.0[5]	43.6	3,704	107	0.0[5]	43.9	4,653	154	0.0[5]
60	0.5	80.2	$5 \cdot 10^5$	103	0.0[5]	28.0	$2 \cdot 10^5$	47	0.0[5]	38.9	3,243	92	0.0[5]	66.1	1,783	44	0.0[5]	66.6	1,567	49	0.0[5]
	1.0	74.0	$6 \cdot 10^5$	121	0.0[5]	44.4	$6 \cdot 10^4$	18	0.0[5]	52.8	1,335	35	0.0[5]	81.5	863	14	0.0[5]	82.3	709	19	0.0[5]
Average			$\mathbf{5 \cdot 10^5}$	**103**	**0.0[15]**	**26.5**	$\mathbf{2 \cdot 10^5}$	**55**	**0.0[15]**	**37.0**	**6,603**	**224**	**0.0[15]**	**63.7**	**2,117**	**55**	**0.0[15]**	**64.3**	**2,310**	**74**	**0.0[15]**
	0.1	90.3	$1 \cdot 10^7$	3,600	9.7[0]	7.2	$9 \cdot 10^6$	3,600	10.1[0]	4.0	31,194	3,600	16.1[0]	37.0	26,657	2,758	5.7[2]	37.3	36,998	2,776	4.6[2]
80	0.5	82.8	$1 \cdot 10^7$	3,600	10.5[0]	28.2	$6 \cdot 10^6$	2,902	2.8[3]	16.8	29,220	3,017	4.0[2]	60.2	11,367	1,108	0.0[5]	60.4	13,898	1,208	0.0[5]
	1.0	77.0	$1 \cdot 10^7$	3,600	9.5[0]	44.1	$2 \cdot 10^6$	988	0.0[5]	27.2	4,889	566	0.0[5]	78.4	2,689	183	0.0[5]	79.0	3,395	233	0.0[5]
Average			$\mathbf{1 \cdot 10^7}$	**3,600**	**9.9[0]**	**26.5**	$\mathbf{5 \cdot 10^6}$	**2,496**	**4.3[8]**	**16.0**	**21,768**	**2,394**	**6.7[7]**	**58.5**	**13,571**	**1,350**	**1.9[12]**	**58.9**	**18,097**	**1,406**	**1.5[12]**
	0.1	90.2	$1 \cdot 10^7$	3,600	30.0[0]	6.4	$6 \cdot 10^6$	3,600	29.3[0]	2.8	14,855	3,600	35.8[0]	37.1	19,660	3,600	19.6[0]	37.0	17,047	3,600	21.6[2]
100	0.5	83.0	$1 \cdot 10^7$	3,600	27.5[0]	25.2	$5 \cdot 10^6$	3,600	18.7[0]	12.8	11,912	3,600	16.4[0]	58.6	16,398	3,432	7.7[1]	58.7	18,645	3,600	7.9[0]
	1.0	77.3	$1 \cdot 10^7$	3,600	25.0[0]	39.9	$6 \cdot 10^6$	3,600	10.0[0]	19.7	16,144	3,236	4.8[1]	75.0	11,376	1,824	2.1[3]	75.4	10,588	1,822	2.5[3]
Average			$\mathbf{1 \cdot 10^7}$	**3,600**	**27.5[0]**	**23.8**	$\mathbf{6 \cdot 10^6}$	**3,600**	**19.3[0]**	**11.8**	**14,304**	**3,479**	**19.0[1]**	**56.9**	**15,811**	**2,952**	**9.8[4]**	**57.1**	**15,426**	**3,007**	**10.7[3]**

TABLE 4. Experiments with constant diagonal dominance & varying positive off-diagonal entries.

n	ρ	igap	Continuous			Perspective				Perspective+cuts				Conic				Conic+cuts			
			nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap	rimp	nodes	time	egap
	0.1	62.4	$7 \cdot 10^5$	153	0.0[5]	46.0	$7 \cdot 10^4$	22	0.0[5]	56.1	10,165	62	0.0[5]	77.6	2,141	19	0.0[5]	78.1	2,065	23	0.0[5]
60	0.2	57.3	$7 \cdot 10^5$	144	0.0[5]	46.8	$7 \cdot 10^4$	22	0.0[5]	56.4	16,642	89	0.0[5]	73.5	3,314	20	0.0[5]	73.9	3,261	24	0.0[5]
	0.5	51.2	$6 \cdot 10^5$	128	0.0[5]	48.0	$6 \cdot 10^4$	19	0.0[5]	53.6	22,526	137	0.0[5]	65.1	8,635	36	0.0[5]	65.5	8,742	60	0.0[5]
Average			$\mathbf{7 \cdot 10^5}$	**142**	**0.0[15]**	**46.9**	$\mathbf{6 \cdot 10^5}$	**21**	**0.0[15]**	**55.4**	**16,444**	**96**	**0.0[15]**	**72.1**	**4,696**	**25**	**0.0[15]**	**72.5**	**4,689**	**36**	**0.0[15]**
	0.1	64.4	$1 \cdot 10^7$	3,600	7.6[0]	46.9	$2 \cdot 10^6$	852	0.0[5]	32.8	53,774	1,401	0.4[4]	77.4	8,979	244	0.0[5]	78.2	8,551	183	0.0[5]
80	0.2	58.8	$1 \cdot 10^7$	3,600	5.9[0]	48.1	$2 \cdot 10^6$	881	0.0[5]	37.8	98,151	1,997	0.6[4]	74.3	25,152	349	0.0[5]	75.4	22,630	327	0.0[5]
	0.5	51.8	$1 \cdot 10^7$	3,255	3.2[1]	49.7	$8 \cdot 10^5$	391	0.0[5]	43.7	185,839	2,462	0.4[4]	67.8	66,779	482	0.0[5]	68.5	64,512	535	0.0[5]
Average			$\mathbf{1 \cdot 10^7}$	**3,485**	**5.5[1]**	**48.2**	$\mathbf{1 \cdot 10^6}$	**708**	**0.0[15]**	**38.1**	**112,588**	**1,953**	**0.5[12]**	**73.2**	**33,637**	**358**	**0.0[15]**	**74.0**	**31,898**	**349**	**0.0[15]**
	0.1	65.0	$9 \cdot 10^6$	3,600	23.1[0]	42.3	$5 \cdot 10^6$	3,600	9.1[0]	28.8	65,628	3,600	6.4[0]	73.0	83,300	2,667	2.5[2]	73.8	67,074	2,904	2.6[2]
100	0.2	59.4	$9 \cdot 10^6$	3,600	20.9[0]	43.9	$5 \cdot 10^6$	3,600	7.8[0]	32.9	72,439	3,600	9.0[0]	70.6	122,553	3,031	2.8[2]	71.2	116,173	3,033	3.3[1]
	0.5	52.5	$9 \cdot 10^6$	3,600	17.2[0]	46.2	$5 \cdot 10^6$	3,600	5.4[0]	39.1	136,082	3,600	7.7[0]	64.4	261,440	3,327	3.8[1]	64.8	270,701	3,396	3.7[1]
Average			$\mathbf{9 \cdot 10^6}$	**3,600**	**20.4[0]**	**44.2**	$\mathbf{5 \cdot 10^6}$	**3,600**	**7.4[0]**	**33.6**	**91,383**	**3,600**	**7.4[0]**	**69.3**	**155,764**	**3,008**	**3.0[5]**	**69.9**	**151,316**	**3,111**	**3.2[4]**

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APPENDIX A. PROOFS OF AUXILIARY LEMMAS

Lemma 2. We have $\frac{\partial\psi}{\partial\hat{y}_1}(\hat{x}_1^*,\hat{y}_1^*)=\frac{\partial\psi}{\partial\hat{x}_1}(\hat{x}_1^*,\hat{y}_1^*)=0$ and (x_1^*,y_1^*) satisfies all constraints (30)–(31). Thus, (x_1^*,y_1^*) is a KKT point and, by convexity, is an optimal solution. Substituting in (32), we get the result. □

Lemma 3. Observe that $(\hat{x}_1^*,\hat{y}_1^*)$ is feasible as $\hat{y}_1^*=\frac{y_2}{x_2}+\frac{y_1-y_2}{x_1}\leq\frac{y_2}{x_2}+\frac{y_1-y_2}{x_2}=\frac{y_1}{x_2}$; $\hat{y}_1^*=\frac{y_2}{x_2}+\frac{y_1-y_2}{x_1}=\frac{y_2x_1+y_1x_2-y_2x_2}{x_1x_2}\leq 1=\hat{x}_1^*$; $\hat{x}_1^*-\hat{y}_1^*=1-\frac{y_2}{x_2}-\frac{y_1-y_2}{x_1}\leq 1-\frac{y_2}{x_1}-\frac{y_1-y_2}{x_1}=\frac{x_1-y_1}{x_1}\leq\frac{x_1-y_1}{x_2}$; $\frac{x_1}{x_2}-\frac{1-x_2}{x_2}=\frac{x_1-1}{x_2}+1\leq 1=\hat{x}_1^*$. Additionally, note that $\frac{\partial\psi}{\partial\hat{y}_1}(\hat{x}_1^*,\hat{y}_1^*)=\frac{\partial\psi}{\partial\hat{x}_1}(\hat{x}_1^*,\hat{y}_1^*)=0$. Thus, (x_1^*,y_1^*) is a KKT point and, by convexity, is an optimal solution. Substituting in (32), we find the result. □

Lemma 4. Note that since $x_2\geq y_2$ and $y_2(x_1-x_2)+y_1x_2\geq x_2x_1$, we have $x_2(x_1-x_2)+y_1x_2\geq x_2x_1\Leftrightarrow y_1\geq x_2$ and, in particular, $\hat{y}_1^*\leq\frac{y_1}{x_2}$. Additionally, it is easy to check that all other constraints (30)–(31) are satisfied. Moreover, from $y_2(x_1-x_2)+y_1x_2\geq x_2x_1$ we find that $\frac{x_2-y_2}{x_2}\leq\frac{y_1-x_2}{x_1-x_2}$. Now let μ_1 and μ_2 be the dual variables associated with constraints $\hat{y}_1\leq\hat{x}_1$ and $\hat{x}_1\leq 1$, respectively. Since both constraints are satisfied at equality at $(\hat{x}_1^*,\hat{y}_1^*)$, then we see that the dual variables μ_1 and μ_2 may take positive values without violating complementary slackness. In particular, let $\mu_1^*=2x_2\left(\frac{y_1-x_2}{x_1-x_2}-\frac{x_2-y_2}{x_2}\right)\geq 0$ and $\mu_2^*=x_2\left(\frac{y_1-x_2}{x_1-x_2}-\frac{x_2-y_2}{x_2}\right)\left(\frac{x_1-y_1}{x_1-x_2}+\frac{y_2}{x_2}\right)\geq 0$. Then, $\frac{\partial\psi}{\partial\hat{y}_1}(\hat{x}_1^*,\hat{y}_1^*)=\mu_1^*$ and $\frac{\partial\psi}{\partial\hat{x}_1}(\hat{x}_1^*,\hat{y}_1^*)=-\mu_1^*+\mu_2^*$. Thus $(\hat{x}_1^*,\hat{y}_1^*)$ corresponds to a KKT point and, by convexity, is optimal. Substituting in (32) gives the result. □

APPENDIX B. EXTENSIONS TO OTHER QUADRATIC FUNCTIONS WITH TWO SEMI-CONTINUOUS VARIABLES

In this paper we focus on the set X, i.e., a set with non-negative semi-continuous variables and non-positive off-diagonal entries in the quadratic matrix. Although an in-depth study of more general quadratic functions is outside the scope of this paper, the approach used in Section 5 can be naturally extended to other quadratic functions. We briefly discuss two such extensions.

B.1. **General quadratic functions.** Observe that a general quadratic function $y'Ay$ can be decomposed as

$$y'Ay=\sum_{i=1}^{n}\left(\left(A_{ii}-\sum_{j\neq i}|A_{ij}|\right)y_i^2-\sum_{j>i:A_{ij}<0}A_{ij}(y_i-y_j)^2+\sum_{j>i:A_{ij}>0}A_{ij}(y_i+y_j)^2\right).$$

Thus, stronger formulations for general quadratic functions may be obtained by studying the set with two semi-continuous variables and positive off-diagonal term

$$X_+=\left\{(x,y,t)\in\{0,1\}^2\times\mathbb{R}_+^2\times\mathbb{R}:(y_1+y_2)^2\leq t,\ y_i\leq x_i,\ i=1,2\right\}.$$

Proposition 9. *Inequality*

$$\frac{y_1^2}{x_1}+\frac{y_2^2}{x_2}\leq t \tag{42}$$

is valid for X_+ and is the strongest among inequalities of the form (37).

The proof is analogous the the proof of Proposition 7 as is omitted for brevity. Despite that inequality (42) is similar in spirit to (38), and that it is the strongest among inequalities of the form (37), it does not seem to be as strong as (38) for X. In particular, although inequality (42) is very effective in some case, it may be ineffective in others, and an integrality result similar to Proposition 8 does not hold for (42).

B.2. **Quadratic functions with semi-continuous variables unrestricted in sign.** Consider the set with two semi-continuous variables

$$X_{\pm} = \left\{(x,y,t) \in \{0,1\}^2 \times \mathbb{R}^2 \times \mathbb{R} : (y_1 \pm y_2)^2 \leq t,\ -x_i \leq y_i \leq x_i \text{ for } i=1,2\right\}.$$

Observe that, since the continuous variables can be positive or negative, the sign inside the quadratic expression does not matter (e.g., it can be flipped via the transformation $\bar{y}_2 = -y_2$). Thus we assume, without loss of generality, that it is a minus sign.

Proposition 10. *Inequality* (4)*, originally proposed by Jeon et al. [17], is valid for* $X_{\pm}$ *and is the strongest among inequalities of the form* (37)*.*

Proof. Any valid inequality for $X_{\pm}$ of the form (37) needs to satisfy

$$h(x_2,y_2) \leq \alpha = \min\left\{(y_1-y_2)^2 - \frac{y_1^2}{x_1}\ :\ -x_1 \leq y_1 \leq x_1,\ x_1 \in \{0,1\}\right\}.$$

If $x_1 = 0$, then $\alpha = y_2^2$. Else, $\alpha = -2y_1y_2 + y_2^2$; in this case, the minimum is attained at $y_1^* = 1$ if $y_2 \geq 0$ and at $y_1^* = -1$ otherwise. Thus, we find that $h(x_2,y_2) \leq y_2^2 - 2|y_2|$ for $x_2 \in \{0,1\}$. To find the strongest convex inequality, we compute $\text{conv}(W_{\pm})$, where $W_{\pm} = \left\{(y_2,x_2,t_2) \in \{0,1\} \times \mathbb{R} \times \mathbb{R} : y_2^2 - 2|y_2| \leq t_2,\ -x_2 \leq y_2 \leq x_2\right\}$. The convex lower envelope corresponding to the one-dimensional non-convex function $h_1(y_2) = y_2^2 - 2|y_2|$ for $y_2 \in [-1,1]$ is the constant function equal to -1. Moreover, it can be shown that

$$\text{conv}(W_{\pm}) = \left\{(y_2,x_2,t_2) \in [0,1] \times \mathbb{R}_+^2 : -x_2 \leq t_2,\ -x_2 \leq y_2 \leq x_2\right\}$$

and we get the convex valid inequality $\frac{y_1^2}{x_1} - x_2 \leq t$ for $X_{\pm}$. □

In light of Proposition 10, inequalities (38) can be interpreted as inequalities that additionally account for the non-negativity of the semi-continuous variables, with respect to the valid inequalities proposed by Jeon et al. [17]. Moreover, although not explicitly considered by Jeon et al., their inequalities may be particularly effective for quadratic optimization problems with semi-continuous variables unrestricted in sign.