RANK-ONE CONVEXIFICATION FOR SPARSE REGRESSION

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ABSTRACT. Sparse regression models are increasingly prevalent due to their ease of interpretability and superior out-of-sample performance. However, the exact model of sparse regression with an ℓ_0 constraint restricting the support of the estimators is a challenging non-convex optimization problem. In this paper, we derive new strong convex relaxations for sparse regression. These relaxations are based on the ideal (convex-hull) formulations for rank-one quadratic terms with indicator variables. The new relaxations can be formulated as semidefinite optimization problems in an extended space and are stronger and more general than the state-of-the-art formulations, including the perspective reformulation and formulations with the reverse Huber penalty and the minimax concave penalty functions. Furthermore, the proposed rank-one strengthening can be interpreted as a non-separable, non-convex sparsity-inducing regularizer, which dynamically adjusts its penalty according to the shape of the error function. In our computational experiments with benchmark datasets, the proposed conic formulations are solved within seconds and result in near-optimal solutions (with 0.4% optimality gap) for non-convex ℓ_0-problems. Moreover, the resulting estimators also outperform alternative convex approaches from a statistical viewpoint, achieving high prediction accuracy and good interpretability.

Keywords Sparse regression, best subset selection, lasso, elastic net, conic formulations, non-convex regularization
1. Introduction

Given a model matrix $X = [x_1, \ldots, x_p] \in \mathbb{R}^{n \times p}$ of explanatory variables, a vector $y \in \mathbb{R}^n$ of response variables, regularization parameters $\lambda, \mu \geq 0$ and a desired sparsity $k \in \mathbb{Z}^+$, we consider the least squares regression problem

$$\min_{\beta \in \mathbb{R}^p} \|y - X\beta\|^2 + \lambda \|\beta\|^2 + \mu \|\beta\|_1 \text{ s.t. } \|\beta\|_0 \leq k,$$

where $\|\beta\|_0$ denotes the support of $\beta$. Problem (1) encompasses a broad range of the regression models. It includes as special cases: ridge regression [22], when $\lambda > 0$, $\mu = 0$ and $k \geq p$; lasso [34], when $\lambda = 0$, $\mu \geq 0$ and $k \geq p$; elastic net [44] when $\lambda, \mu > 0$ and $k \geq p$; best subset selection [29], when $\lambda = \mu = 0$ and $k < p$. Additionally, Bertsimas and Van Parys [7] propose to solve (1) with $\lambda > 0$, $\mu = 0$ and $k < p$ for high-dimensional regression problems, while Mazumder et al. [28] study (1) with $\lambda = 0$, $\mu > 0$ and $k < p$ for problems with low Signal-to-Noise Ratios (SNR). The results in this paper cover all versions of (1) with $k < p$; moreover, they can be extended to problems with non-separable regularizations of the form $\lambda \|A\beta\|^2 + \mu \|C\beta\|_1$, resulting in sparse variants of the fused lasso [35], generalized lasso [36] and smooth lasso [21], among others.

Regularization techniques. The motivation and effects of the regularization are well-documented in the literature. Hastie et al. [18] coined the bet on sparsity principle, i.e., using an inference procedure that performs well in sparse problems since no procedure can do well in dense problems. Best subset selection with $k < p$ and $\lambda = \mu = 0$ is the direct approach to enforce sparsity without incurring bias. In contrast, ridge regression with $\lambda > 0$ (Tikhonov regularization) is known to induce shrinkage and bias, which can be desirable, for example, when $X$ is not orthogonal, but it does not result in sparsity. On the other hand, lasso, the $\ell_1$ regularization with $\mu > 0$ simultaneously causes shrinkage and induces sparsity, but the inability to separately control for shrinkage and sparsity may result in subpar performance in some cases [29, 40, 41, 42, 43]. Moreover, achieving a target sparsity level $k$ with lasso requires significant experimentation with the penalty parameter $\mu$. When $k \geq p$, the cardinality constraint on $\ell_0$ is redundant and (1) reduces to a convex optimization problem and can be solved easily. On the other hand, when $k < p$, problem (1) is non-convex and NP-hard [31], and finding an optimal solution may require excessive computational effort. Therefore, due to the perceived difficulties of tackling the non-convex $\ell_0$ constraint in (1), lasso-type simple approaches are still preferred for inference problems with sparsity [20].

Nonetheless, there has been a substantial effort to develop sparsity-inducing methodologies that do not incur as much shrinkage and bias as lasso does. The resulting techniques often result in optimization problems of the form

$$\min_{\beta \in \mathbb{R}^p} \|y - X\beta\|^2 + \sum_{i=1}^p \rho_i(\beta_i)$$

where $\rho_i : \mathbb{R} \to \mathbb{R}$ are non-convex regularization functions. Examples of such regularization functions include $\ell_q$ penalties with $0 < q < 1$ [14] and SCAD [13]. Although optimal solutions of (2) with non-convex regularizations may substantially improve upon the estimators obtained by lasso, solving (2) to optimality is still a difficult task [23, 27, 45], and suboptimal solutions may not benefit from
Table 1. Diagonal dominance of $X^T X$ for benchmark datasets.

| dataset          | $p$ | $n$  | $dd \times 100\%$ |
|------------------|-----|------|-------------------|
| housing          | 13  | 506  | 26.7%             |
| servo            | 19  | 167  | 0.0%              |
| auto MPG         | 25  | 392  | 1.5%              |
| solar flare      | 26  | 1,066| 8.8%              |
| breast cancer    | 37  | 196  | 3.6%              |
| diabetes         | 64  | 442  | 0.0%              |

the improved statistical properties. To address such difficulties, Zhang et al. [39] propose the minimax concave penalty (MC+), a class of sparsity-inducing penalty functions where the non-convexity of $\rho$ is offset by the convexity of $||y - X\beta||^2_2$ for sufficiently sparse solutions, so that (2) remains convex –Zhang et al. [39] refer to this property as sparse convexity. Thus, in the ideal scenario (and with proper tuning of the parameter controlling the concavity of $\rho$), the MC+ penalty is able to retain the sparsity and unbiasedness of best subset selection while preserving convexity, resulting in the best of both worlds. However, due to the separable form of the regularization term, the effectiveness of MC+ greatly depends on the diagonal dominance of the matrix $X^T X$ (this statement will be made more precise in §3), and may result in poor performance when the diagonal dominance is low.

Unfortunately, in many practical applications, the matrix $X^T X$ has low eigenvalues and is not diagonally dominant at all. To illustrate, Table 1 presents the diagonal dominance of five datasets from the UCI Machine Learning Repository [10] used in [16, 30], as well as the diabetes dataset with all second interactions used in [6, 12]. The diagonal dominance of a positive semidefinite matrix $A$ is computed as

$$dd(A) := (1/\text{tr}(A)) \max_{d \in \mathbb{R}_+^p} e^T d \text{ s.t. } A - \text{diag}(d) \succeq 0,$$

where $e$ is $p$-dimensional vector of ones, diag($d$) is the diagonal matrix such that diag($d$)$_i = d_i$ and tr($A$) denotes the trace of $A$. Accordingly, the diagonal dominance is the trace of the largest diagonal matrix that can be extracted from $A$ without violating positive semidefiniteness, divided by the trace of $A$. Observe in Table 1 that the diagonal dominance of $X^T X$ is very low or even 0%, and MC+ struggles for these datasets as we demonstrate in §5.

Mixed-integer optimization formulations. An alternative to utilizing non-convex regularizations is to leverage recent advances in mixed-integer optimization (MIO) to tackle (1) exactly [5,6,9]. By introducing indicator variables $z \in \{0,1\}^p$,
where \( z_i = \mathbb{I}_{\beta_i \neq 0} \), problem (1) can be reformulated as

\[
y^T y + \min -2y^T X \beta + \beta^T (X^T X + \lambda I) \beta + \mu \sum_{i=1}^p u_i \tag{3a}
\]

s.t.

\[
\sum_{i=1}^p z_i \leq k \tag{3b}
\]

\[
\beta_i \leq u_i, \quad -\beta_i \leq u_i \quad i = 1, \ldots, p \tag{3c}
\]

\[
\beta_i (1 - z_i) = 0 \quad i = 1, \ldots, p \tag{3d}
\]

\[
\beta \in \mathbb{R}^p, \quad z \in \{0, 1\}^p, \quad u \in \mathbb{R}^p_+. \tag{3e}
\]

The non-convexity of (1) is captured by the complementary constraints (3d) and the integrality constraints \( z \in \{0, 1\}^p \). In fact, one of the main challenges for solving (3) is handling constraints (3d). A standard approach in the MIO literature is to use the so-called big-M constraints and replace (3d) with

\[
-M z_i \leq \beta_i \leq M z_i \tag{4}
\]

for a sufficiently large number \( M \) to bound the variables \( \beta_i \). However, big-M constraints are known to be poor approximations of constraints (3d), especially in the case of regression where no natural big-M value is available. Bertsimas et al. [6] propose approaches to compute provable big-M values, but such values often result in prohibitively large computational times even in problems with a few dozens variables (or, even worse, may lead to numerical instabilities and cause convex solvers to crash). Alternatively, heuristic values for the big-M values can be estimated, e.g., setting \( M = \tau \|\hat{\beta}\|_\infty \) where \( \tau \in \mathbb{R}_+ \) and \( \hat{\beta} \) is a feasible solution of (1) found via a heuristic. While using such heuristic values yield reasonable performance for small enough values of \( \tau \), it may eliminate optimal solutions.

Branch-and-bound algorithms for MIO leverage strong convex relaxations of problems to prune the search space and reduce the number of sub-problems to be enumerated (and, in some cases, eliminate the need for enumeration altogether). Thus, a critical step to speed-up the solution times for (3) is to derive convex relaxations that approximate the non-convex problem well. Such strong relaxations can also be used directly to find good estimators for the inference problems (without branch-and-bound); in fact, it is well-known than the natural convex relaxation of (3) with \( \lambda = \mu = 0 \) and big-M constraints is precisely lasso, see [11] for example. Therefore, sparsity-inducing techniques that more accurately capture the properties of the non-convex constraint \( \|\beta\|_0 \leq k \) can be found by deriving tighter convex relaxations of (1). Pilanci et al. [32] exploit the Tikhonov regularization term and convex analysis to construct an improved convex relaxation using the reverse Huber penalty. In a similar vein, Bertsimas and Van Parys [7] leverage the Tikhonov regularization and duality to propose an efficient algorithm for high-dimensional sparse regression.

The perspective relaxation. Problem (3) is a mixed-integer convex quadratic optimization problem with indicator variables, a class of problems which has received a fair amount of attention in the optimization literature. In particular, the perspective relaxation [2, 13, 17] is, by now, a standard technique that can be

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1This method with \( \tau = 2 \) was used in the computations in [6].
used to substantially strengthen the convex relaxations by exploiting \textit{separable} quadratic terms. Specifically, consider the mixed-integer epigraph of a one-dimensional quadratic function with an indicator constraint,

\[
Q_1 = \left\{ z \in \{0,1\}, \beta \in \mathbb{R}, t \in \mathbb{R}_+ : \beta^2_i \leq t, \beta_i(1 - z_i) = 0 \right\}.
\]

The convex hull of \( Q_1 \) is obtained by relaxing the integrality constraint to bound constraints and using the closure of the perspective function\(^2\) of \( \beta^2_i \), expressed as a rotated cone constraint:

\[
\text{conv}(Q_1) = \left\{ z \in [0,1], \beta \in \mathbb{R}, t \in \mathbb{R}_+ : \frac{\beta^2_i}{z_i} \leq t \right\}.
\]

Xie and Deng \cite{XieDeng2016} apply the \textit{perspective relaxation} to the separable quadratic regularization term \( \lambda \| \beta \|^2 \), i.e., reformulate \eqref{eq:reg} as

\[
y^\top y + \min_{\beta} -2y^\top X \beta + \beta^\top (X^\top X) \beta + \lambda \sum_{i=1}^p \frac{\beta^2_i}{z_i} + \mu \sum_{i=1}^p u_i \tag{5a}
\]
\[
\text{s.t. } \sum_{i=1}^p z_i \leq k \tag{5b}
\]
\[
\beta_i \leq u_i, \ -\beta_i \leq u_i \quad i = 1, \ldots, p \tag{5c}
\]
\[
\beta \in \mathbb{R}^p, \ z \in \{0,1\}^p, \ u \in \mathbb{R}^p_+. \tag{5d}
\]

Moreover, they show that the continuous relaxation of \eqref{eq:reg} is equivalent to the continuous relaxation of the formulation used by Bertsimas and Van Parys \cite{BertsimasVanParys2011}. Dong et al. \cite{DongYang2016} also study the \textit{perspective relaxation} in the context of regression: first, they show that using the \textit{reverse Huber penalty} \cite{ZouHastie2005} is, in fact, equivalent to just solving the convex relaxation of \eqref{eq:reg} — thus the relaxations of \cite{BertsimasVanParys2011, ZouHastie2005, XieDeng2016} all coincide; second, they propose to use an \textit{optimal perspective relaxation}, i.e., by applying the perspective relaxation to a separable quadratic function \( \beta^\top D \beta \), where \( D \) is a nonnegative diagonal matrix such that \( X^\top X + \lambda I - D \succeq 0 \); finally, they show that solving this stronger convex relaxation of the optimal \textit{perspective relaxation} is, in fact, equivalent to using the \textit{MC+} penalty \cite{Mairal2010}.

Among these approaches the optimal \textit{perspective relaxation} of Dong et al. \cite{DongYang2016} is the only one that does not explicitly require the use of the Tikhonov regularization \( \lambda \| \beta \|^2 \). Nonetheless, as the authors point out, if \( \lambda = 0 \) then the method is effective only when the matrix \( X^\top X \) is sufficiently diagonally dominant, which, as illustrated in Table \ref{tab:results}, is not necessarily the case in practice. As a consequence, \textit{perspective relaxation} techniques may be insufficient to tackle problems when large shrinkage is undesirable and, hence, \( \lambda \) is small.

Our contributions. In this paper we derive tighter convex relaxations of \eqref{eq:reg} than the optimal \textit{perspective relaxation}. The relaxations are obtained from the study of ideal (convex-hull) formulations of the mixed-integer epigraphs of \textit{non-separable rank-one quadratic functions with indicators}. Since the \textit{perspective relaxation} corresponds to the ideal formulation of a \textit{one-dimensional} rank-one quadratic function, the proposed relaxations generalize and strengthen the existing results. In particular, they \textit{dominate} \textit{perspective relaxation} approaches for all

\footnote{We use the convention that \( \frac{\beta^2_i}{z_i} = 0 \) when \( \beta_i = z_i = 0 \) and \( \frac{\beta^2_i}{z_i} = \infty \) if \( z_i = 0 \) and \( \beta_i \neq 0 \).}
values of the regularization parameter $\lambda$ and, critically, are able to achieve high-quality approximations of even in low diagonal dominance settings with $\lambda = 0$. Alternatively, our results can also be interpreted as a new non-separable, non-convex regularization penalty $\rho_{R1}(\beta)$ which: (i) imposes larger penalties than the separable minimax concave penalty $\rho_{MC+}(\beta)$ to dense estimators, thus achieving better sparsity-inducing properties; and (ii) the nonconvexity of the penalty function is offset by the convexity of the term $\|y - X\beta\|_2^2$, and the resulting continuous problem can be solved to global optimality using convex optimization tools. In fact, they can be formulated as semidefinite optimization and, in certain special cases, as conic quadratic optimization.

To illustrate the regularization point of view for the proposed relaxations, consider a two-predictor regression problem in Lagrangean form:

$$\min_{\beta \in \mathbb{R}^2} \|y - X\beta\|_2^2 + \lambda \|\beta\|_2^2 + \mu \|\beta\|_1 + \kappa \|\beta\|_0, \quad (6)$$

where $X^\top X = \begin{pmatrix} 1 + \delta & 1 \\ 1 & 1 + \delta \end{pmatrix}$ and $\delta \geq 0$ is a parameter controlling the diagonal dominance. Figure 1 depicts the level sets of well-known regularizations including lasso ($\lambda = \kappa = 0$, $\mu = 1$), ridge ($\mu = \kappa = 0$, $\lambda = 1$), elastic net ($\kappa = 0$, $\lambda = \mu = 0.5$), the $MC+$ penalty for different values of $\delta$ and the proposed rank-one $R1$ regularization. The level sets of $MC+$ and $R1$ are obtained by setting $\lambda = \mu = 0$ and $\kappa = 1$, and using the appropriate convex strengthening, see §3 for details. Observe that the $R1$ regularization results in larger penalties than $MC+$ for all values of $\delta$, and the improvement increases as $\delta \to 0$. In addition, Figure 2 shows the effect of using constraints $\rho_{MC+}(\beta) \leq k$ and $\rho_{R1}(\beta) \leq k$ in a two-dimensional problem to achieve sparse solutions satisfying $\|\beta\|_0 \leq 1$. We see that the “natural” constraint $\rho_{MC+}(\beta) \leq 1$ yields dense solutions (for $\delta = 0.1$ the resulting solution corresponds to the ordinary least squares estimator), while tighter constraints $\rho_{MC+}(\beta) \leq k$ for $k < 1$ result in shrinkage and are not able to recover the sparse solutions corresponding to $\|\beta\|_0 \leq 1$. In contrast, we observe that constraints $\rho_{R1}(\beta) \leq k$ adapt to the curvature of the error function $\|y - X\beta\|_2^2$ to induce higher sparsity: in particular, the constraint $\rho_{R1}(\beta) \leq 1$, with the target sparsity $k = 1$, results in exact recovery without shrinkage in all cases.

**Outline.** The rest of the paper is organized as follows. In §2 we derive the proposed convex relaxations based on ideal formulations for rank-one quadratic terms with indicator variables. We also give an explicit semidefinite optimization (SDP) formulation in an extended space, which can be implemented with off-the-shelf conic optimization solvers. In §3 we study the links between the resulting convex relaxation and regularization penalties. In §4 we discuss the implementation of the proposed relaxation in a conic quadratic framework. In §5 we present computational experiments with synthetic as well as benchmark datasets, demonstrating that (i) the proposed formulation delivers near-optimal solutions (with provable optimality gaps) of (1) in most cases, (ii) using the proposed convex relaxation results in superior statistical performance when compared with usual estimators obtained from convex optimization approaches. In §6 we conclude the paper with a few final remarks.
Figure 1. Level sets of regularization penalties for the two-predictor case, where darker shades correspond to larger penalties. The top row regularizations do not depend on the diagonal dominance, but induce substantial bias. The $\mathcal{MC}_+$ regularization (second row) does not induce much bias, but depends on the diagonal dominance. The new $R_1$ regularization (bottom row) induces larger penalties than $\mathcal{MC}_+$ for all diagonal-dominances and is a better approximation to the $\ell_0$ penalty.
Figure 2. The axes correspond to the sparse solutions for $\|\beta\|_0 \leq 1$. In blue: feasible region given by $\rho_{MC}\beta \leq k$; in red: feasible region given by $\rho_{R1}\beta \leq k$; in gray: contours of the error function.
Notation. Define $P = \{1, \ldots, p\}$ and $e \in \mathbb{R}^p$ be the vector of ones. Given $T \subseteq P$ and a vector $a \in \mathbb{R}^p$, define $a_T$ as the subvector of $a$ induced by $T$, $a_i = a_{\{i\}}$ as the $i$-th element of $a$, and define $a(T) = \sum_{i \in T} a_i$. Given a symmetric matrix $A \in \mathbb{R}^{p \times p}$, let $A_T$ be the submatrix of $A$ induced by $T \subseteq P$, and let $S^+_T$ be set of $T \times T$ symmetric positive semidefinite matrices, i.e., $A_T \succeq 0 \iff A_T \in S^+_T$. We use $a_T$ or $A_T$ to make explicit that a given vector or matrix belongs to $T$.

Proposition 1.

The inequality \( \beta^T A_T \beta \leq t \) is valid for $Q_T$. \[(7)\]

Proof. Let $(z, \beta, t) \in Q_T$, and we verify that inequality (7) is satisfied. First observe that if $z = 0$, then $\beta = 0$ and inequality (7) reduces to $0 \leq t$, which is satisfied. Otherwise, if $z_i = 1$ for some $i \in T$, then $z(T) \geq 1$ and we find that $\frac{\beta^T A_T \beta}{z(T)} \leq \beta^T A_T \beta \leq t$, and inequality (7) is satisfied again. \(\square\)

Observe that if $T$ is a singleton, i.e., $T = \{i\}$, then (7) reduces to the well-known perspective inequality $A_{ii} \beta_i^2 \leq z_i$. Moreover, if $T = \{i, j\}$ and $A_T$ is rank-one, i.e., $\beta^T A_T \beta = |A_{ij}| (a \beta_i^2 + 2 \beta_i \beta_j + (1/a) \beta_j^2)$ for $A_{ij} \neq 0$ and scalar $a > 0$, then (7) reduces to

\[ |A_{ij}| (a \beta_i^2 + 2 \beta_i \beta_j + (1/a) \beta_j^2) \leq t(z_i + z_j), \quad (8) \]

one of the inequalities proposed in [24] in the context of quadratic optimization with indicators and bounded continuous variables. Note that inequality (8) is in general weak for bounded continuous variables (as non-negativity or other bounds can be used to strengthen the inequalities, see [3] for additional discussion), and inequality (7) is in general weak for arbitrary matrices $A_T \in S^+_T$. Nonetheless, as
we now show, inequality (7) gives the ideal description for $Q_T$ if $A_T$ is a rank-one matrix. Define

$$Q^1_T = \{(z, \beta, t) \in [0, 1]^T \times \mathbb{R}^T \times \mathbb{R}_+ : (a^T_T \beta)^2 \leq t, \beta_i (1 - z_i) = 0, \forall i \in T\}.$$  

**Theorem 1.** If $a_i \neq 0$ for all $i \in T$, then

$$\text{conv}(Q^1_T) = \{(z, \beta, t) \in [0, 1]^T \times \mathbb{R}^T \times \mathbb{R}_+ : (a^T_T \beta)^2 \leq t, \frac{(a^T_T \beta)^2}{z(T)} \leq t \}.$$  

**Proof.** Consider the optimization of an arbitrary linear function over $Q^1_T$ and $\bar{Q}_T := \{(z, \beta, t) \in [0, 1]^T \times \mathbb{R}^T \times \mathbb{R}_+ : (a^T_T \beta)^2 \leq t, \frac{(a^T_T \beta)^2}{z(T)} \leq t \}$:

$$\min_{(z, \beta, t) \in Q^1_T} u^T_T z + v^T_T \beta + \kappa t,$$

(9)

$$\min_{(z, \beta, t) \in \bar{Q}_T} u^T_T z + v^T_T \beta + \kappa t,$$

(10)

where $u_T, v_T \in \mathbb{R}^T$ and $\kappa \in \mathbb{R}$. We now show that either there exists an optimal solution of (10) that is feasible for (9), hence also optimal for (9) as $\bar{Q}_T$ is a relaxation of $Q^1_T$, or that (9) and (10) are both unbounded.

Observe that if $\kappa < 0$, then letting $z = \beta = 0$ and $t \to \infty$ we see that both problems are unbounded. If $\kappa = 0$ and $v_T = 0$, then (10) reduces to $\min_{z \in [0, 1]^T} u^T_T z$, which has an optimal integral solution $z^*$, and $(z^*, 0, 0)$ is optimal for (9) and (10). If $\kappa = 0$ and $v_i \neq 0$ for some $i \in T$, then letting $\beta_i \to \pm \infty$, $z_i \to 1$, and $\beta_j = z_j = t = 0$ for $j \neq i$, we find that both problems are unbounded. Thus, we may assume, without loss of generality that $\kappa > 0$, and, by scaling, $\kappa = 1$.

Additionally, as $a_T$ has no zero entry, we may assume, without loss of generality, that $a_T = e_T$, since otherwise $\beta$ and $v_T$ can be scaled by letting $\tilde{\beta}_i = a_i \beta_i$ and $\tilde{v}_i = v_i / a_i$ to arrive at an equivalent problem. Moreover, a necessary condition for (9)–(10) to be bounded is that

$$-\infty < \min_{\beta \in \mathbb{R}^T} v^T_T \beta \text{ s.t. } \beta(T) = \zeta$$

(11)

for any fixed $\zeta \in \mathbb{R}$. It is easily seen that (11) has an optimal solution if and only if $v_i = v_j$ for all $i \neq j$. Thus, we may also assume without loss of generality that $v^T_T \beta = v_0 \beta(T)$ for some scalar $v_0$. Performing the above simplifications, we find that (10) reduces to

$$\min_{z \in [0, 1]^P, \beta \in \mathbb{R}^P, t \in \mathbb{R}} u^T_T z + v_0 \beta(T) + t \text{ s.t. } \beta(T)^2 \leq t, \beta(T)^2 \leq t z(T).$$

(12)

Since the one-dimensional optimization $\min_{\beta \in \mathbb{R}^T} \{v_0 \beta + \beta^2\}$ has an optimal solution, it follows that (12) is bounded and has an optimal solution. We now prove that (12) has an optimal solution that is integral in $z$ and satisfies $\beta \circ (e - z) = 0$.

Let $(z^*, \beta^*, t^*)$ be an optimal solution of (12). First note that if $0 < z^*(T) < 1$, then $(\gamma z^*, \gamma \beta^*, \gamma t^*)$ is feasible for (10) for $\gamma$ sufficiently close to 1, with objective value $\gamma \left( u^T_T z^* + v_0 \beta^*(T) + t^* \right)$. If $u^T_T z^* + v_0 \beta^*(T) + t^* \geq 0$, then for $\gamma = 0$, $(\gamma z^*, \gamma \beta^*, \gamma t^*)$ has an objective value equal or lower. Otherwise, for $\gamma = 1/z^*(T)$, $(\gamma z^*, \gamma \beta^*, \gamma t^*)$ is feasible and has a lower objective value. Thus, we find that either 0 is optimal for (12) (and the proof is complete), or there exists an optimal solution with $z^*(T) \geq 1$. In the later case, observe that any $(\bar{z}, \beta^*, t^*)$ with $\bar{z} \in
arg min\{u^Tz : z^*(T) \geq 1, z \in [0,1]^n\} is also optimal for (12), an in particular there exists an optimal solution with \(\bar{z}\) integral.

Finally, let \(i \in T\) be any index with \(\bar{z}_i = 1\). Setting \(\beta_i = \beta^*(T)\) and \(\beta_j = 0\) for \(i \neq j\), we find another optimal solution \((\bar{z}, \beta^*, t^*)\) for (12) that satisfies the complementary constraints, and thus is feasible and optimal for (9). \(\square\)

Remark 1. Observe that describing \(\text{conv}(Q^1_T)\) requires two nonlinear inequalities in the original space of variables. More compactly, we can specify \(\text{conv}(Q^1_T)\) using a single convex inequality, as

\[
\text{conv}(Q^1_T) = \left\{(z, \beta, t) \in [0,1]^T \times \mathbb{R}^T \times \mathbb{R}_+ : \frac{(a^T_T \beta)^2}{\min\{1, z(T)\}} \leq t \right\}.
\]

Finally, we point out that \(\text{conv}(Q^1_T)\) is conic quadratic representable, as \((z, \beta, t) \in \text{conv}(Q^1_T)\) if and only if there exists \(w\) such that the system

\[
z \in [0,1]^T, \quad \beta \in \mathbb{R}^P, \quad t \in \mathbb{R}_+, \quad w \in \mathbb{R}_+, \quad w \leq 1, \quad w \leq z(T), \quad (a^T_T \beta)^2 \leq tw
\]

is feasible, where the last constraint is a rotated conic quadratic constraint and all other constraints are linear. \(\square\)

2.2. General case. Now consider again the mixed-integer optimization (8)

\[
y^T y + \min -2y^T X \beta + e^T u + t \tag{13a}
\]

s.t. \(\beta^T (X^T X + \lambda I) \beta \leq t \tag{13b}\)

\[e^T z \leq k\tag{13c}\]

\[\beta \leq u, \quad -\beta \leq u\tag{13d}\]

\[\beta \diamond (e - z) = 0\tag{13e}\]

\[\beta \in \mathbb{R}^P, \quad z \in \{0,1\}^P, \quad u \in \mathbb{R}^P_+, \quad t \in \mathbb{R}\tag{13f}\]

where the nonlinear terms of the objective is moved to constraint (13b). A direct application of (7) yields the inequality \(\beta^T (X^T X + \lambda I) \beta \leq tz(P)\), which is very weak and has no effect whenever \(z(P) \geq 1\).

Instead, let \(P \subseteq 2^T\) be a subset of the power set of \(P\), and for \(A_T \in \mathbb{R}^{T \times T}\) define \(\tilde{A}_T\) as the \(P \times P\) matrix obtained by filling the missing entries by zeros. Consider the valid inequality \(\phi_P(z, \beta) \leq t\), where \(\phi_P : [0,1]^P \times \mathbb{R}^P \to \mathbb{R}\) is defined as

\[
\phi_P(z, \beta) := \max_{A_T, R} \beta^T R \beta + \sum_{T \in P} \frac{\beta^T A_T \beta_T}{\min\{1, z(T)\}} \tag{14a}
\]

s.t. \(\sum_{T \in P} \tilde{A}_T + R = X^T X + \lambda I\) \(\forall T \in P\) \quad (14b) \quad A_T \in S^+_T, \quad R \in S^+_P, \quad (14c)

where strengthening (7) is applied to each low-dimensional quadratic term \(\beta^T A_T \beta\).

For a fixed value of \((z, \beta)\), problem (14) finds the best decomposition of the matrix \(X^T X + \lambda I\) as a sum of positive semidefinite matrices \(\tilde{A}_T, \quad T \in P\), and a remainder positive semidefinite matrix \(R\) to maximize the strengthening.
For a given decomposition, the objective (14a) is convex in \((z, \beta)\), thus \(\phi_P\) is a supremum of convex functions and is convex on its domain. Observe that the inclusion or omission of the empty set does not affect function \(\phi_P\), and we assume for simplicity that \(\emptyset \in P\).

Since inequalities (7) are ideal for rank-one matrices, one would expect inequality \(\phi_P(z, \beta) \leq t\) to be particularly strong if matrices \(A_T\) are rank-one in optimal solutions of (14). As we now show, this is indeed the case if \(P\) is downward closed.

**Proposition 2.** Let \(T \in P\). If \(U \in P\) for all \(U \subseteq T\), then there exists an optimal solution to (14) where \(A_T\) is a rank-one matrix.

**Proof.** Suppose \(A_T\) is not rank-one in an optimal solution to (14), also suppose for simplicity that \(T = \{1, \ldots, p_0\}\) for some \(p_0 \leq p\), and let \(T_i = \{i, \ldots, p_0\}\) for \(i = 1, \ldots, p_0\). Since \(A_T\) is positive semidefinite, there exists a Cholesky decomposition \(A_T = LL^T\) where \(L\) is a lower triangular matrix (possibly with zeros on the diagonal if \(A_T\) is not positive definite). Let \(L_i\) denote the \(i\)-th column of \(L\). Since \(A_T\) is not a rank-one matrix, there exist at least two non-zero columns of \(L\). Let \(L_j\) with \(j > 1\) be the second non-zero column. Then

\[
\frac{\beta_T^T A_T \beta_T}{\min \{1, z(T)\}} = \frac{\beta_T^T \left( \sum_{i \neq j} (L_i L_i^T) \right) \beta_T}{\min \{1, z(T)\}} + \frac{\beta_T^T (L_j L_j^T) \beta_T}{\min \{1, z(T)\}}
\]

Finally, since \(T_j \in P\), the (better) decomposition (15) is feasible for (14), and the proposition is proven. \(\square\)

By dropping the complementary constraints (13c), replacing the integrality constraints \(z \in \{0,1\}^P\) with bound constraints \(z \in \{0,1\}^P\), and utilizing the convex function \(\phi_P\) to reformulate (13b), we obtain the convex relaxation of (1)

\[
y^T y + \min -2y^T X \beta + e^T u + \phi_P(z, \beta) = (16a)
\]

\[
e^T z \leq k
\]

\[
\beta \leq u, -\beta \leq u
\]

\[
\beta \in \mathbb{R}^P, z \in \{0,1\}^P, u \in \mathbb{R}^P
\]

for a given \(P \subseteq 2^P\). Formulation (16) can be unwieldy, as function \(\phi_P\) is not given in closed form, is not differentiable, and each function evaluation requires solving the optimization problem (14). However, problem (16) can be explicitly reformulated in an extended space as an SDP as shown in the next section.

### 2.3. Extended SDP formulation
To state the extended SDP formulation, in addition to variables \(z \in \{0,1\}^P\) and \(\beta \in \mathbb{R}^P\), we introduce variables \(w \in [0,1]^P\) corresponding to terms \(w_T := \min \{1, z(T)\}\) and \(B \in \mathbb{R}^{P \times P}\) corresponding to terms \(B_{ij} = \beta_i \beta_j\). Observe that for \(T \in P\), \(\beta_T\) and \(B_T\) represent the subvector of \(\beta\) and submatrix of \(B\) induced by \(T\), whereas \(w_T\) is a scalar corresponding to the \(T\)-th coordinate of the \(|P|\)-dimensional vector \(w\).
Theorem 2. Problem \( (16) \) is equivalent to the SDP
\[
y^T y + \min \left( -2y^T X \beta + e^T u + \langle X^T X + \lambda I, B \rangle \right) \quad (17a)
s.t. \ e^T z \leq k \quad (17b)
\beta \leq u, \ -\beta \leq u \quad (17c)
w_T \leq e^T z_T \quad \forall T \in \mathcal{P} \quad (17d)
w_T B_T - \beta T \beta_T^T \in S_+^T \quad \forall T \in \mathcal{P} \quad (17e)
B - \beta \beta^T \in S_+^P \quad (17f)
\beta \in \mathbb{R}^P, \ z \in [0,1]^P, \ u \in \mathbb{R}^P, \ w \in [0,1]^P, \ B \in \mathbb{R}^{P \times P}. \quad (17g)
\]
Observe that \( (17) \) is indeed an SDP, as
\[
(w_T B_T - \beta T \beta_T^T) \in S_+^P \iff (w_T \beta_T^T) \geq 0;
\]
thus constraints \( (17e) \) and \( (17f) \) are indeed SDP-representable and the remaining constraints and objective are linear.

Proof of Theorem 2. It is easy to check that \( (17) \) is strictly feasible (set \( \beta = 0, z = e, w > 0 \) and \( B = I \)). Adding surplus variables \( \Gamma, \Gamma_T \) write \( (17) \) as
\[
y^T y + \min_{(\beta,z,u,w) \in C} \left\{ -2y^T X \beta + e^T u + \min_{B,T} \langle X^T X + \lambda I, B \rangle \right\}
\text{s.t.} \ w_T B_T - \Gamma T = \beta T \beta_T^T \quad \forall T \in \mathcal{P} \quad (A_T)
B - \Gamma = \beta \beta^T \quad (R)
\Gamma_T \in S_+^T \quad \forall T \in \mathcal{P}
\Gamma \in S_+^P
B \in \mathbb{R}^{P \times P},
\]
where \( C = \{ \beta \in \mathbb{R}^P, z \in [0,1]^P, u \in \mathbb{R}_+^P, w \in [0,1]^P : (17b), (17c), (17d) \} \). Using conic duality for the inner minimization problem, we find the dual
\[
y^T y + \min_{(\beta,z,u,w) \in C} \left\{ -2y^T X \beta + e^T u + \max_{A_T:R} \langle \beta \beta_T^T, R \rangle + \sum_{T \in \mathcal{P}} \langle \beta_T \beta_T^T, A_T \rangle \right\}
\text{s.t.} \ \sum_{T \in \mathcal{P}} w_T A_T + R = X^T X + \lambda I
A_T \in S_+^T \quad \forall T \in \mathcal{P}
R \in S_+^P.
\]
After substituting \( \bar{A}_T = w_T A_T \) and noting that there exists an optimal solution with \( w_T = \min \{ 1, z(T) \} \), we obtain formulation \( (14) \).

Note that if \( \mathcal{P} = \{ \emptyset \} \), there is no strengthening and \( (17) \) is equivalent to elastic net \((\lambda, \mu > 0)\), lasso \((\lambda = 0, \mu > 0)\), ridge regression \((\lambda > 0, \mu = 0)\) or ordinary least squares \((\lambda = \mu = 0)\). As \(|\mathcal{P}|\) increases, the quality of the conic relaxation \( (17) \) for the non-convex \( \ell_0 \)-problem \( (1) \) improves, but the computational burden required to solve the resulting SDP also increases. In particular, the full
rank-one strengthening with $\mathcal{P} = 2^P$ requires $2^{\lvert P \rvert}$ semidefinite constraints and is impractical. Proposition\(^2\) suggests using down-monotone sets $\mathcal{P}$ with limited size

\[
y^T y + \min -2y^T X \beta + e^T u + \langle X^T X + \lambda I, B \rangle
\]

\[\text{s.t. } e^T z \leq k\]

\[
\beta \leq u, -\beta \leq u
\]

\[(\text{sdp}_r)\]

\[
0 \leq w_T \leq \min\{1, e_T^T z_T\} \quad \forall T: |T| \leq r
\]

\[
w_T B_T - \beta_T \beta_T^T \in S^P_+ \quad \forall T: |T| \leq r
\]

\[
B - \beta \beta^T \in S^P_+
\]

\[\beta \in \mathbb{R}^P, z \in [0,1]^P, u \in \mathbb{R}^P, B \in \mathbb{R}^{P \times P}\]

for some $r \in \mathbb{Z}_+$. In fact, if $r = 1$, then $\text{sdp}_1$ reduces to the formulation of the optimal perspective relaxation proposed in [11], which is equivalent to using $\mathcal{MC}$ regularization. Our computations experiments show that whereas $\text{sdp}_1$ may be a weak convex relaxation for problems with low diagonal dominance, $\text{sdp}_2$ and $\text{sdp}_3$ achieve excellent relaxation bounds even for in the case of low diagonal-dominance within reasonable compute times.

3. REGULARIZATION

To better understand the properties of the proposed conic relaxations, in this section, we study them from a regularization perspective. Consider formulation\(^{[16,1]}\) in Lagrangean form with multiplier $\kappa$:

\[
y^T y + \min -2y^T X \beta + e^T u + \phi_P(z, \beta) + \kappa e^T z
\]

\[
\beta \leq u, -\beta \leq u
\]

\[
\beta \in \mathbb{R}^P, z \in [0,1]^P, u \in \mathbb{R}^P,
\]

where $p = 2$, and

\[
X^T X + \lambda I = \begin{pmatrix} 1 + \delta_1 & 1 \\ 1 & 1 + \delta_2 \end{pmatrix}
\]

(20)

Observe that assumption\(^{[20]}\) is without loss of generality, provided that $X^T X$ is not diagonal: given a two-dimensional convex quadratic function $a_1 \beta_1^2 + 2a_{12} \beta_1 \beta_2 + a_2 \beta_2^2$ (with $a_{12} \neq 0$), the substitution $\beta_1 = \alpha \beta_1$ and $\beta_2 = (a_{12}/\alpha) \beta_2$ with $|a_{12}|/a_2 \leq \alpha \leq a_1$ yields a quadratic form satisfying\(^{[20]}\).

If $\mathcal{P} = \{\emptyset, \{1\}, \{2\}\}$, then\(^{[10]}\) reduces to a perspective strengthening of the form

\[
y^T y + \min_{\beta \in \mathbb{R}^2, \beta \in \mathbb{R}^2} -2y^T X \beta + (\beta_1 + \beta_2)^2 + \delta_1 \frac{\beta_1^2}{z_1} + \delta_2 \frac{\beta_2^2}{z_2} + \mu \|\beta\|_1 + \kappa \|z\|_1.
\]

(21)

The links between\(^{[21]}\) and regularization were studied\(^{[9]}\) in [11].

**Proposition 3** (Dong et al. [11]). Problem\(^{[21]}\) is equivalent to the regularization problem

\[
\min_{\beta \in \mathbb{R}^2} \|y - X \beta\|^2_2 + \lambda \|\beta\|^2_2 + \mu \|\beta\|_1 + \rho_{\mathcal{MC}}(\beta; \lambda, \delta)
\]

\(^3\)The case with $\mu = 0$ is explicitly considered in Dong et al. [11], but the results extend straightforwardly to the case with $\mu > 0$. The results presented here differ slightly from those in [11] to account for a different scaling in the objective function.
where

$$\rho_{\text{HC}}(\beta; \kappa, \delta) = \begin{cases} \sum_{i=1}^2 \left( 2\sqrt{\kappa \delta_i} |\beta_i| - \delta_i \beta_i^2 \right) & \text{if } \delta_i \beta_i^2 \leq \kappa, \ i = 1, 2 \\ \kappa + 2\sqrt{\kappa \delta_i} |\beta_i| - \delta_i \beta_i^2 & \text{if } \delta_i \beta_i^2 \leq \kappa \text{ and } \delta_j \beta_j^2 > \kappa \\ 2\kappa & \text{if } \delta_i \beta_i^2 > \kappa, \ i = 1, 2. \end{cases}$$

Regularization $\rho_{\text{HC}}$ is non-convex and separable. Moreover, as pointed out in [11], the regularization given in Proposition 3 is the same as the Minimax Concave Penalty given in [39]; and, if $\lambda = \delta_1 = \delta_2$, then the regularization given in Proposition 3 reduces to the reverse Huber penalty derived in [32]. Observe that the regularization function $\rho_{\text{HC}}$ is highly dependent on the diagonal dominance $\delta$: specifically, in the low diagonal dominance setting with $\delta = 0$, we find that $\rho_{\text{HC}}(\beta; \kappa, 0) = 0$.

We now consider conic formulation (19) for the case $\mathcal{P} = \{\emptyset, \{1\}, \{2\}, \{1, 2\}\}$, corresponding to the full rank-one strengthening:

$$\min_{\beta \in \mathbb{R}^2} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1 + \mu \|\beta\|_1 + \rho_{\text{HC}}(\beta; \kappa, \delta). \tag{22}$$

**Proposition 4.** Problem (22) is equivalent to the regularization problem

$$\min_{\beta \in \mathbb{R}^2} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1 + \rho_{\text{HL}}(\beta; \kappa, \delta)$$

where

$$\rho_{\text{HL}}(\beta; \kappa, \delta) = \begin{cases} 2\sqrt{\kappa} \sqrt{\beta'(X^\top X + \lambda I)\beta + 2\sqrt{\delta_1 \delta_2} \beta_1 \beta_2 - \beta'(X^\top X + \lambda I)\beta} & \text{if } \beta'(X^\top X + \lambda I)\beta + 2\sqrt{\delta_1 \delta_2} \beta_1 \beta_2 < \kappa \\ \kappa + 2\sqrt{\delta_1 \delta_2} |\beta_1 \beta_2| & \text{if } (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)^2 \leq \kappa \leq (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)^2 \\ \sum_{i=1}^2 \left( 2\sqrt{\delta_i} |\beta_i| - \delta_i \beta_i^2 \right) & \text{if } (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)^2 > \kappa \\ \kappa + \sqrt{\delta_1} |\beta_1| - \delta_1 \beta_1^2 & \text{if } \delta_1 \beta_1^2 \leq \kappa \text{ and } \delta_j \beta_j^2 > \kappa \\ 2\kappa & \text{if } \delta_1 \beta_1^2 > \kappa, \ i = 1, 2. \end{cases}$$

Observe that, unlike $\rho_{\text{HC}}$, the function $\rho_{\text{HL}}$ is not separable in $\beta_1$ and $\beta_2$ and does not vanish when $\delta = 0$: indeed, for $\delta = 0$ we find that

$$\rho_{\text{HL}}(\beta; \kappa, 0) = \begin{cases} 2\sqrt{\kappa} \sqrt{\beta'(X^\top X + \lambda I)\beta - \beta'(X^\top X + \lambda I)\beta} & \text{if } \beta'(X^\top X + \lambda I)\beta < \kappa \\ \kappa & \text{if } 0 \leq \kappa \leq \beta'(X^\top X + \lambda I)\beta. \end{cases}$$

**Proof of Proposition 4.** We prove the result by projecting out the $z$ variables in (22), i.e., giving closed form solutions for them. There are three cases to consider, depending on the optimal value for $z_1 + z_2$.

- Case 1: $z_1 + z_2 < 1$. In this case, we find by setting the derivatives of the objective in (22) with respect to $z_1$ and $z_2$ that

$$\begin{align*}
\kappa - \delta_1 \beta_1^2 - \frac{(\beta_1 + \beta_2)^2}{(z_1 + z_2)^2} &= 0 \\
\kappa - \delta_2 \beta_2^2 - \frac{(\beta_1 + \beta_2)^2}{(z_1 + z_2)^2} &= 0
\end{align*}$$

$$\implies z_2 = \sqrt{\frac{\delta_2}{\delta_1} |\beta_2|} z_1.$$
Define \( \tilde{z} := \frac{z_1}{\sqrt{\delta_1} |\beta_1|} \), so \( z_2 = \sqrt{\delta_2} |\beta_2| \tilde{z} \), and \( z_1 + z_2 = (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|) \tilde{z} \). Moreover, we find that (22) reduces to

\[
y^\top y + \min_{z > 0, \beta \in \mathbb{R}^2} -2y^\top X \beta + \mu \|\beta\|_1 + \frac{(\beta_1 + \beta_2)^2 + (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)^2}{\kappa (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)} z \tilde{z}
\]

An optimal solution of (23) is attained at

\[
z^* = \frac{(\beta_1 + \beta_2)^2 + (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)^2}{\kappa (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)} \quad = \sqrt{\frac{(\beta_1 + \beta_2)^2 + (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)^2}{\kappa (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)}} \!
\]

with objective value

\[
y^\top y + \min_{\beta \in \mathbb{R}^2} -2y^\top X \beta + \mu \|\beta\|_1 + 2\sqrt{\kappa} \sqrt{(\beta_1 + \beta_2)^2 + (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)^2} \frac{z_1 + z_2}{\kappa (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)} \frac{z}{\sqrt{\delta_1} \sqrt{\delta_2}} \!
\]

Finally, this case happens when \( z_1 + z_2 < 1 \Leftrightarrow (\beta_1 + \beta_2)^2 + (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)^2 < \kappa \).

- Case 2: \( z_1 + z_2 > 1 \). In this case, we find by setting the derivatives of the objective in (22) with respect to \( z_1 \) and \( z_2 \) that \( \tilde{z}_i = \sqrt{\frac{2}{\delta_i}} |\beta_i| \) for \( i = 1, 2 \). Thus, in this case, for an optimal solution \( z^* \) of (22), we have \( z^*_i = \min \{ \tilde{z}_i, 1 \} \), and problem (22) reduces to

\[
y^\top y + \min_{\beta \in \mathbb{R}^2} -2y^\top X \beta + (\beta_1 + \beta_2)^2 + \sum_{i=1}^2 \max \left\{ \delta_i \beta_i^2, \sqrt{\delta_i} |\beta_i| \right\} + \mu \|\beta\|_1 + \frac{2}{\kappa} \left( \sum_{i=1}^2 (2\sqrt{\kappa} |\beta_i| - \delta_i \beta_i^2) \right) \!
\]

Finally, this case happens when \( z_1 + z_2 > 1 \Leftrightarrow (\sqrt{\delta_1} |\beta_1| + \sqrt{\delta_2} |\beta_2|)^2 > \kappa \). Observe that, in this case, the penalty function is precisely the one given in Proposition 3.

- Case 3: \( z_1 + z_2 = 1 \). In this case, problem (22) reduces to

\[
y^\top y + \min_{0 \leq z_1 \leq 1, \beta \in \mathbb{R}^2} -2y^\top X \beta + (\beta_1 + \beta_2)^2 + \frac{\delta_1 \beta_1^2}{z_1} + \frac{\delta_2 \beta_2^2}{1 - z_1} + \mu \|\beta\|_1 + \kappa. \quad (24)
\]
Setting derivative with respect to $z_1$ in (24) to 0, we have

$$0 = \delta_1 \beta_1^2 (1 - z_1)^2 - \delta_2 \beta_2^2 z_1^2$$

$$= \delta_1 \beta_1^2 - 2 \delta_1 \beta_2^2 z_1 + (\delta_1 \beta_1^2 - \delta_2 \beta_2^2) z_1^2.$$ 

Thus, we find that

$$z_1 = \frac{2 \delta_1 \beta_1^2 \pm \sqrt{4 \delta_1^2 \beta_1^4 - 4 \delta_1 \beta_1^2 (\delta_1 \beta_1^2 - \delta_2 \beta_2^2)}}{2 (\delta_1 \beta_1^2 - \delta_2 \beta_2^2)} = \frac{\sqrt{\delta_1 \beta_1^2 (\sqrt{\delta_1 \beta_1^2} \pm \sqrt{\delta_2 \beta_2^2})}}{\sqrt{\delta_1 \beta_1^2 (\sqrt{\delta_1 \beta_1^2} \pm \sqrt{\delta_2 \beta_2^2})}}.$$

Moreover, since $0 \leq z_1 \leq 1$, we have $z_1 = \frac{\sqrt{\delta_1 \beta_1^2} \pm \sqrt{\delta_2 \beta_2^2}}{\sqrt{\delta_1 \beta_1^2} \pm \sqrt{\delta_2 \beta_2^2}}$ and $1 - z_1 = \frac{\sqrt{\delta_1 \beta_1^2} \mp \sqrt{\delta_2 \beta_2^2}}{\sqrt{\delta_1 \beta_1^2} \pm \sqrt{\delta_2 \beta_2^2}}$.

Substituting in (24), we find the equivalent form

$$y^T y + \min_{\beta \in \mathbb{R}^2} -2y^T X \beta + (\beta_1 + \beta_2)^2 + (\sqrt{\delta_1 \beta_1^2} + \sqrt{\delta_2 \beta_2^2})^2 + \mu \|\beta\|_1 + \kappa$$

$$= \min_{\beta \in \mathbb{R}^2} \|y - X \beta\|^2 + \lambda \|\beta\|^2_2 + \mu \|\beta\|_1 + \kappa + 2 \sqrt{\delta_1 \beta_1^2} \beta_1 \beta_2.$$ 

This final case occurs when neither case 1 or 2 does, i.e., when $(\sqrt{\delta_1 \beta_1^2} + \sqrt{\delta_2 \beta_2^2})^2 \leq \kappa \leq (\beta_1 + \beta_2)^2 + (\sqrt{\delta_1 \beta_1^2} + \sqrt{\delta_2 \beta_2^2})^2$. 

Figure 1 compares usual regularization penalties with $\rho_{MC}$ and $\rho_{s.t.}$ (shown for $\kappa = 1$). Additionally, Figure 2 illustrates the better sparsity inducing properties of regularization $\rho_{s.t.}$ with respect to $\rho_{MC}$. Note that for the general $p$-dimensional case, the conic relaxation (16) can be rewritten as:

$$\min \|y - X \beta\|^2 + \lambda \|\beta\|^2_2 + e^T u + \rho_{s.t.}(\beta; k)$$

subject to $\beta \leq u$, $-\beta \leq u$,

$$\beta \in \mathbb{R}^p$$,

$$u \in \mathbb{R}^p,$$

with

$$\rho_{s.t.}(\beta; k) := \min_{z \in [0, 1]^p} \phi_P(z, \beta) - \beta^T (X^T X + \lambda I) \beta$$

subject to $e^T z \leq k$.

Explicit forms of such regularization penalties are difficult to derive for $p > 2$.

4. Conic quadratic relaxations

As mentioned in [1], strong convex relaxations of problem (1), such as $\text{sdp}_p$, can either be directly used to obtain good estimators via conic optimization, which is the approach we use in our computations, or can be embedded in a branch-and-bound algorithm to solve (1) to optimality. However, using SDP formulations such as (17) in branch-and-bound may be daunting since, to date, efficient branch-and-bound algorithms with SDP relaxations are not available. In contrast, off-the-shelf conic quadratic mixed-integer optimization solvers are successful in solving a broad class of practical problems, and are actively maintained and improved by numerous
software vendors. In this section, to facilitate the integration with branch-and-bound solvers, we show how the proposed conic relaxations, and specifically $\text{sdp}_2$, can be implemented in a conic quadratic framework.

### 4.1. Constraints with $S_T^+$ and $|T| = 1$

If $T = \{i\}$, then constraint \((18e)\), $\beta_i^2 \leq w_i B_{ii}$, is a rotated cone constraint as $w_i \geq 0$ and $B_{ii} \geq 0$ in any feasible solution of \((18)\), and thus conic quadratic representable. Moreover, observe that the variable $w_i$ can be dropped from the formulation, resulting in the constraint $\beta_i^2 \leq z_i B_{ii}$.

### 4.2. Constraints with $S_T^+$ and $|T| = 2$

As we now show, constraints \((18e)\) with $|T| = 2$ can be accurately approximated using conic quadratic constraints.

**Proposition 5.** Problem $\text{sdp}_2$ is equivalent to the optimization problem

\[
\begin{align*}
\min & \quad y^T y + \min & -2y^T X \beta + e^T u + \langle X^T X + \lambda I, B \rangle \\
\text{s.t.} & \quad e^T z \leq k \\
& \quad \beta \leq u, \quad -\beta \leq u \\
& \quad z_i B_{ii} \geq \beta_i^2 \quad \forall i \in P \quad \text{(25d)} \\
& \quad 0 \leq w_{ij} \leq 1, \quad w_{ij} \leq z_i + z_j \quad \forall i \neq j \quad \text{(25e)} \\
& \quad 0 \geq \max_{\alpha \geq 0} \left\{ \alpha \beta_i^2 + 2\beta_i \beta_j + \beta_j^2 / \alpha \right\} - 2B_{ij} - \alpha B_{ii} - B_{jj} / \alpha \quad \forall i \neq j \quad \text{(25f)} \\
& \quad 0 \geq \max_{\alpha \geq 0} \left\{ \alpha \beta_i^2 - 2\beta_i \beta_j + \beta_j^2 / \alpha \right\} + 2B_{ij} - \alpha B_{ii} - B_{jj} / \alpha \quad \forall i \neq j \quad \text{(25g)} \\
& \quad B - \beta' \in S_+^P \\
& \quad \beta \in \mathbb{R}^P, \quad z \in [0, 1]^P, \quad u \in \mathbb{R}^P, \quad B \in \mathbb{R}^{P \times P}. \quad \text{(25i)}
\end{align*}
\]

**Proof.** It suffices to compute the optimal value of $\alpha$ in \((25f)-(25g)\). Observe that the rhs of \((25f)\) can be written as

\[
v = \frac{2\beta_i \beta_j}{w_{ij}} - 2B_{ij} - \min_{\alpha \geq 0} \left\{ \alpha \left( B_{ii} - \frac{\beta_i^2}{w_{ij}} \right) + \frac{1}{\alpha} \left( B_{jj} - \frac{\beta_j^2}{w_{ij}} \right) \right\}. \quad \text{(26)}
\]

Moreover, in an optimal solution of \((25f)\), we have that $w_{ij} = \min\{1, z_i + z_j\}$. Thus, due to constraints \((25d)\), we find that $B_{ii} - \beta_i^2 / w_{ij} \geq 0$ in optimal solutions of \((25)\), and equality only occurs if either $z_i = 1$ or $z_j = 0$. If either $B_{ii} = \beta_i^2 / \min\{1, z_i + z_j\}$ or $B_{jj} = \beta_j^2 / \min\{1, z_i + z_j\}$, then the optimal value of \((26)\) is $v = 2\beta_i \beta_j / \min\{1, z_i + z_j\} - 2B_{ij}$, by setting $\alpha \to \infty$ or $\alpha = 0$, respectively. Otherwise, the optimal $\alpha$ equals

\[
\alpha = \sqrt{\frac{B_{jj} w_{ij} - \beta_j^2}{B_{ii} w_{ij} - \beta_i^2}}. \quad \text{(27)}
\]

\footnote{An effective implementation would require careful constraint management strategies and integration with the different aspects of branch-and-bound solvers, e.g., branching strategies and heuristics. Such an implementation is beyond the scope of the paper.}
Similarly, it can be shown that constraint (25g) reduces to
\( \beta \) with the objective value
\[ B \]
subsets of \( R \) interpretation, discussed next.

of the main reasons of the dramatic improvements of MIO software [8].

improve the continuous relaxations of mixed-integer optimization problems is one
resulting in tighter relaxations. Observe that the use of cuts (as described here) to
\( V \) to (27) (resulting in most violated constraints) can be added to sets
\( \alpha \)
where
\( V \)
dynamically: given an optimal solution of (31), new values of \( \alpha \) generated according
to (27) (resulting in most violated constraints) can be added to sets \( V^{+}_{ij} \) and \( V^{-}_{ij} \),
resulting in tighter relaxations. Observe that the use of cuts (as described here) to
improve the continuous relaxations of mixed-integer optimization problems is one
of the main reasons of the dramatic improvements of MIO software [8].

More compactly, constraints (28)–(29) are equivalent to
\[ (w_{ij}B_{ii} - \beta^2_i) (w_{ij}B_{jj} - \beta^2_j) \geq (w_{ij}B_{ij} - \beta_i\beta_j)^2. \]  

Moreover, note that constraints (18c) with \( T = \{ i, j \} \) are equivalent to
\( w_{ij}B_{ii} - \beta^2_i \)
\( w_{ij}B_{ij} - \beta_i\beta_j \)
\( w_{ij}B_{jj} - \beta^2_j \)
\( S_i^2 \)
\[ \iff \]
\( w_{ij}B_{ii} - \beta^2_i \geq 0, \ w_{ij}B_{jj} - \beta^2_j \geq 0, \text{ and } (30). \]

Since the first two constraints are implied by (25d) and \( w_{ij} = \min\{1, z_i + z_j\} \) in
optimal solutions, the proof is complete. \( \square \)

Observe that, for any fixed value of \( \alpha \), constraints (25f)–(25g) are conic quadratic
representable. Thus, we can obtain relaxations of (25) of the form
\[ y^T y + \min -2y^T X \beta + e^T u + \langle X^T X + \lambda I, B \rangle \] s.t. (25a), (25c), (25d), (25e), (25f), (25g)
(28), (29)
(31a)
(31b)
(31c)
(31d)

where \( V^{+}_{ij} \) and \( V^{-}_{ij} \) are any finite subsets of \( R_+ \). Relaxation (31) can be refined
dynamically: given an optimal solution of (31), new values of \( \alpha \) generated according
to (27) (resulting in most violated constraints) can be added to sets \( V^{+}_{ij} \) and \( V^{-}_{ij} \),
resulting in tighter relaxations. Observe that the use of cuts (as described here) to
improve the continuous relaxations of mixed-integer optimization problems is one
of the main reasons of the dramatic improvements of MIO software [8].

In relaxation (31), \( V^{+}_{ij} \) and \( V^{-}_{ij} \) can be initialized with any (possibly empty)
subsets of \( R_+ \). However, setting \( V^{+}_{ij} = V^{-}_{ij} = \{1\} \) yields a relaxation with a simple
interpretation, discussed next.
4.3. Diagonally dominant matrix relaxation. Let $\Lambda \in \mathcal{S}_+^P$ be diagonally dominant matrix. Observe that for any $(z, \beta) \in \{0, 1\}^P \times \mathbb{R}^P$ such that $\beta \circ (e - z) = 0$,
\[
t \geq \beta^T \Lambda \beta \quad \Leftrightarrow \quad t \geq \sum_{i=1}^{p} \left( \Lambda_{ii} - \sum_{j \neq i} |\Lambda_{ij}| \right) \beta_i^2 + \sum_{i=1}^{p} \sum_{j=i+1}^{p} |\Lambda_{ij}| \left( \beta_i + \text{sign}(\Lambda_{ij}) \beta_j \right)^2
\]
\[
\Leftrightarrow \quad t \geq \sum_{i=1}^{p} \left( \Lambda_{ii} - \sum_{j \neq i} |\Lambda_{ij}| \right) \frac{\beta_i^2}{z_i} + \sum_{i=1}^{p} \sum_{j=i+1}^{p} |\Lambda_{ij}| \frac{(\beta_i + \text{sign}(\Lambda_{ij}) \beta_j)^2}{\min\{1, z_i + z_j\}}.
\]
(32)
where the last line follows from using perspective strengthening for the separable quadratic terms, and using [4] for the non-separable, rank-one terms. See [4] for a similar strengthening for signal estimation based on nonnegative pairwise quadratic terms.

We now consider using decompositions of the form $\Lambda + R = X^T X + \lambda I$, where $\Lambda$ is a diagonally dominant matrix and $R \in \mathcal{S}_+^P$. Given such a decomposition, inequalities (32) can be used to strengthen the formulations. Specifically, we consider relaxations of (3) of the form
\[
y^T y + \min_{\beta} -2y^T X \beta + e^T u + \hat{\phi}(z, \beta)
\]
(33a)
where
\[
\hat{\phi}(z, \beta) := \max_{\Lambda, R} \beta^T R \beta + \sum_{i=1}^{p} \left( \Lambda_{ii} - \sum_{j \neq i} |\Lambda_{ij}| \right) \frac{\beta_i^2}{z_i} + \sum_{i=1}^{p} \sum_{j=i+1}^{p} |\Lambda_{ij}| \frac{(\beta_i + \text{sign}(\Lambda_{ij}) \beta_j)^2}{\min\{1, z_i + z_j\}}
\]
(34a)
s.t. $\Lambda + R = X^T X + \lambda I$
(34b)
$\Lambda_{ii} \geq \sum_{j=i} |\Lambda_{ij}| + \sum_{j \neq i} |\Lambda_{ij}| \quad \forall i \in P$
(34c)
$R \in \mathcal{S}_+^P$.
(34d)

Proposition 6. Problem (33) is equivalent to
\[
y^T y + \min_{\beta} -2y^T X \beta + e^T u + \langle X^T X + \lambda I, B \rangle
\]
(35a)
s.t. $e^T z \leq k$
(35b)
$\beta \leq u, -\beta \leq u$
(35c)
$z_i B_{ii} \geq \beta_i^2 \quad \forall i \in P$
(35d)
$sdp_{2-}$
(35e)
$0 \leq w_{ij} \leq 1, w_{ij} \leq z_i + z_j \quad \forall i \neq j$
(35f)
$0 \geq \frac{\beta_i^2 + 2\beta_i \beta_j + \beta_j^2}{w_{ij}} - 2B_{ij} - B_{ii} - B_{jj} \quad \forall i \neq j$
(35g)
$0 \geq \frac{\beta_i^2 - 2\beta_i \beta_j + \beta_j^2}{w_{ij}} + 2B_{ij} - B_{ii} - B_{jj} \quad \forall i \neq j$
(35h)
$B - \beta \beta' \in \mathcal{S}_+^P$
(35i)
$\beta \in \mathbb{R}^P, \ z \in [0, 1]^P, \ u \in \mathbb{R}^P, \ B \in \mathbb{R}^{P \times P}$.  
(35j)
Proof. Let $\Gamma, \Gamma^+, \Gamma^-$ be nonnegative $p \times p$ matrices such that: $\Gamma_{ii} = \Lambda_{ii}$ and $\Gamma_{ij} = 0$ for $i \neq j$; $\Gamma^+_{ii} = \Gamma^-_{ii} = 0$ and $\Gamma^+_{ij} - \Gamma^-_{ij} = \Lambda_{ij}$ for $i \neq j$. Problem (34) can be written as

$$\hat{\phi}(z, \beta) := \max_{\Gamma, \Gamma^+, \Gamma^-} \beta^T R \beta + \sum_{i=1}^{p} \left( \Gamma_{ii} - \sum_{j \neq i} (\Gamma^+_{ij} + \Gamma^-_{ij}) \right) \frac{\beta_i^2}{z_i}$$

$$+ \sum_{i=1}^{p} \sum_{j=i+1}^{p} \left( \Gamma^+_{ij} \frac{(\beta_i + \beta_j)^2}{\min\{1, z_i + z_j\}} + \Gamma^-_{ij} \frac{(\beta_i - \beta_j)^2}{\min\{1, z_i + z_j\}} \right)$$

(36a)

s.t. $\Gamma + \Gamma^+ + \Gamma^- + R = X^T X + \lambda I$

$$\Gamma_{ii} \geq \sum_{j<i} (\Gamma^+_{ji} + \Gamma^-_{ji}) + \sum_{j>i} (\Gamma^+_{ij} + \Gamma^-_{ij}) \quad \forall i \in P$$

$$R \in S_+^p.$$  

(36b)

(36c)

(36d)

(36e)

Then, similarly to the proof of Theorem 2, it is easy to show that the dual of (36) is precisely (35). □

4.4. Relaxing the constraint with $S_+^p$. We now discuss a relaxation of the $p$-dimensional semidefinite constraint $B - \beta \beta^T \in S_+^p$, present in all formulations. Consider the optimization problem

$$\bar{\phi}_P(z, \beta) := \max_{A_T, R, \pi} \beta^T R \beta + \sum_{T \in P} \frac{\beta_T^T A_T \beta_T}{\min\{1, z(T)\}}$$

(37a)

s.t. $\sum_{T \in P} A_T + R = X^T X + \lambda I$

$$A_T \in S_+^T \quad \forall T \in P$$

(37b)

(37c)

$$R = X^T \text{diag}(\pi) X$$

(37d)

$$\pi \in \mathbb{R}^n_+.$$  

(37e)

Observe that the objective and constraints (37a)-(37c) are identical to (14). However, instead of (14d), we have $R = \sum_{j=1}^{n} \pi_j X_j X_j^T$, where $X_j$ is the $j$-th row of $X$ (as a column vector). Moreover, since $\pi \geq 0$, $R \in S_+^p$ in any feasible solution of (37), thus (14) is a relaxation of (37), and, hence, $\bar{\phi}_P$ is indeed a lower bound on $\phi_P$. Therefore, instead of (16), one may use the simpler convex relaxation

$$y^T y + \min \left\{-2y^T X \beta + e^T u + \hat{\phi}_P(z, \beta) \right\}$$

(38a)

$$e^T z \leq k$$

(38b)

$$\beta \leq u, -\beta \leq u$$

(38c)

$$\beta \in \mathbb{R}^p, \ z \in [0, 1]^p, \ u \in \mathbb{R}^p_+$$

(38d)

for (1).
Proposition 7. Problem (38) is equivalent to the SDP
\[
y^\top y + \min -2y^\top X\beta + e^\top u + (X^\top X + \lambda I, B)
\]
s.t.
\[
e^\top z \leq k
\]
\[
\beta \leq u, \ -\beta \leq u
\]
\[
w^\top \beta \leq e^\top u, \ \beta \leq u\]
\[
B^\top \beta \beta^\top B \in S^+_P, \ \forall T \in P
\]
\[
X^\top _j (B - \beta \beta^\top ) X_j \geq 0 \quad \forall j = 1, \ldots, n
\]
\[
\beta \in \mathbb{R}^P, \ z \in [0, 1]^P, \ u \in \mathbb{R}^P_+, \ w \in [0, 1]^P, \ B \in \mathbb{R}^{P \times P}.
\]

Proof. The proof is based on conic duality similar to the proof of Theorem 2.

Observe that in formulation (39), the \((p+1)\)-dimensional semidefinite constraint (17f) is replaced with \(n\) rank-one quadratic constraints (39f). We denote by \(cqp_r\) the relaxation of \(sdp_r\) obtained by replacing (18f) with (39f). In general, \(cqp_r\) is still an SDP due to constraints (39e); however, note that special cases \(cqp_1\) and \(cqp_2\) are conic quadratic formulations, and \(cqp_2\) can be implemented in a conic quadratic framework by using cuts, as described in §4.2. Moreover, constraints (39) could also be dynamically refined to better approximate the SDP constraint, or formulation (39) could be improved with ongoing research on approximating SDP via mixed-integer conic quadratic optimization, e.g., see [25, 26].

Remark 2 (Further rank-one strengthening). Since constraints (39f) are rank-one quadratic constraints, additional strengthening can be achieved using the inequalities given in [2,1]. Specifically, let \(T_j = \{i \in P : X_{ji} \neq 0\}\), and inequalities (39f) may be replaced with stronger versions
\[
\langle B, X_j X_j^\top \rangle - \frac{(X_j^\top \beta)^2}{\min\{1, z(T_j)\}} \geq 0 \quad \forall j \in N.
\]
This strengthening is particularly effective when \(X\) is sparse.

5. Computations

In this section we report computational experiments with the proposed conic relaxations on synthetic as well as benchmark datasets. The convex optimization problems are solved with MOSEK 8.1 solver on a laptop with a 1.80GHz Intel\textsuperscript{\textregistered} Core\textsuperscript{TM} i7-8550U CPU and 16 GB main memory. All solver parameters were set to their default values. We divide our discussion in two parts: first, in §5.1 we test \(sdp_r\) on benchmark instances previously used in the literature, and focus on the relaxation quality and ability to approximate the exact \(\ell_0\)-problem \([1]\); then, in §5.2 we adopt the same experimental framework used in \([6,19]\) to generate synthetic instances and evaluate the proposed conic formulations from an inference perspective. In both cases, our results compare favorably with the results reported in previous works using the same instances.

5.1. Approximation study on benchmark instances. In this section we focus on the ability of \(sdp_r\) to provide near-optimal solutions to problem \([1]\).
5.1.1. Computing optimality gaps. Observe that the optimal objective value $\nu^*_r$ of $\text{sdp}_r$ provides a lower bound on the optimal objective value of (1). To obtain an upper bound, we use a simple heuristic to retrieve a feasible solution of (1): given an optimal solution vector $\hat{\beta}'$ for $\text{sdp}_r$, let $\hat{\beta}^*_k$ denote the $k$-th largest absolute value, let $T = \{i \in P : |\hat{\beta}^*_i| \geq \hat{\beta}^*_k\}$, let $\hat{\beta}_T$ be the $T$-dimensional $\text{ols/ridge}$ estimator using only predictors in $T$, i.e.,
$$
\hat{\beta}_T = (X^*_T X_T + \lambda I_T)^{-1} X^*_T y,
$$
where $X_T$ denotes the $n \times |T|$ matrix obtained by removing the columns with indexes not in $T$, and let $\hat{\beta}$ be the $P$-dimensional vector obtained by filling the missing entries in $\hat{\beta}_T$ with zeros. Since $\|\hat{\beta}\|_0 \leq k$ by construction, $\hat{\beta}$ is feasible for (1), and its objective value $\nu_u$ is an upper bound on the optimal objective value of (1). Moreover, the optimality gap can be computed as
$$
gap = \frac{\nu_u - \nu^*_r}{\nu^*_r} \times 100. \quad (40)
$$
Note that while stronger relaxations always result in improved lower bounds $\nu^*_r$, the corresponding heuristic upper bounds $\nu_u$ are not necessarily better, thus the optimality gaps are not guaranteed to improve with stronger relaxations. Nevertheless, as shown next, stronger relaxation do in general yield much better gaps in practice.

5.1.2. Datasets. For these experiments, we use the benchmark datasets in Table 1. The first five were first used in [30] in the context of MIO algorithms for best subset selection, and later used in [16]. The diabetes dataset with all second interactions was introduced in [12] in the context of lasso, and later used in [6]. A few datasets require some manipulation to eliminate missing values and handle categorical variables. The processed datasets before standardization can be downloaded from http://atamturk.ieor.berkeley.edu/data/sparse.regression.

5.1.3. Results. For each dataset, $\lambda \in \{0, 0.05, 0.1\}$ and $\mu = 0$, we solve the conic relaxations of (1) for $k = 3, 4, \ldots, \lfloor p/3 \rfloor$. Specifically, we solve $\text{sdp}_r$ for $r = 1, 2, 3$, we also solve $\text{cqp}_2$ (which, as pointed in [4] can be implemented as conic quadratic optimization) and we also present results for the natural convex relaxation of (1), that is, for $r = 0$, corresponding to ordinary least squares ($\text{ols}$) if $\lambda = 0$ and $\text{ridge}$ if $\lambda > 0$. Figure 3 presents, for each dataset and value of $\lambda$, the average optimality gap produced by each method (by averaging over all values of $k$ used).

We see that in large diagonal dominance settings ($\lambda > 0$ and the housing dataset) all proposed relaxations are able to achieve significant gap improvements over $\text{ols/ridge}$. In particular, in the large diagonal dominance setting, $\text{sdp}_2$ and $\text{sdp}_3$ achieve average optimality gaps of at most 0.7% in all cases, which in most cases is an order of magnitude less than $\text{sdp}_1$ and $\text{cqp}_2$, and two orders-of-magnitude less than $\text{ols/ridge}$. Specifically, for $\lambda = 0.05$, the average gaps (across all datasets) are 0.4% for $\text{sdp}_2$ and 0.3% for $\text{sdp}_3$; for $\lambda = 0.1$, the average gap is 0.2% for both $\text{sdp}_2$ and $\text{sdp}_3$. In contrast, achieving small optimality gaps in the

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5 In our experiments, the datasets were standardized first.

6 Since the data is standardized, $\lambda = 0.05$ and $\lambda = 0.1$ correspond to increasing the magnitude of the diagonal elements of $X^\top X$ by 5% and 10%, respectively.
low diagonal dominance setting $\lambda = 0$ is much more difficult: formulation $\text{sdp}_1$, proposed in [11] and corresponding to $\text{MC}_+$, is barely able to improve over $\text{ols}$, and other existing perspective-based relaxations [7, 32, 38] cannot be used in this setting. Formulation $\text{cqp}_2$ is equally ineffective in this setting. Nonetheless, formulations $\text{sdp}_2$ and $\text{sdp}_3$ are able to reduce the optimality gaps by an order-of-magnitude, and result in optimality gaps of 4% or less in all instances except for $\text{diabetes}$: the average optimality gaps with $\lambda = 0$ (excluding the $\text{housing}$ dataset) is 3.9% for $\text{sdp}_2$ and 3.5% for $\text{sdp}_3$, which are much lower than 27.6% for $\text{sdp}_1$ or 37.3% for $\text{ols}$. In summary, $\text{cqp}_2$ is competitive with $\text{sdp}_1$, with neither formulation consistently outperforming the other, $\text{sdp}_2$ results in considerable improvements over $\text{sdp}_1$ and $\text{cqp}_2$, and $\text{sdp}_3$ results in a small improvement over $\text{sdp}_2$.

To illustrate the effect of the sparsity parameter $k$ in the optimality gaps, we show in Figure 4 the optimality gaps of $\text{ols}$, $\text{sdp}_1$, $\text{sdp}_2$, and $\text{sdp}_3$ as a function of $k$ for the $\text{breast cancer}$ and $\text{diabetes}$ datasets. Observe that, in general, optimality gaps decrease as the cardinality increases (note that if $k = p$, the optimality gaps of all relaxations are 0%). Formulations $\text{ols}$ and $\text{sdp}_1$ are particularly poor for low values of $k$, while formulations $\text{sdp}_2$ and $\text{sdp}_3$ perform consistently well across all values of $k$. The results suggest that the stronger relaxations $\text{sdp}_2$ and $\text{sdp}_3$ are especially beneficial for low values of the sparsity parameter $k$.

5.1.4. Computation times. Table 2 presents, for each dataset and method, the average time required to solve the relaxations. While the new relaxations are certainly more expensive to solve than the simple relaxations such as $\text{ols}$/$\text{ridge}$, with the exception of $\text{sdp}_3$, they can still be solved efficiently, under ten seconds in all cases. Formulation $\text{sdp}_3$, which has $\binom{p}{3}$ additional 4-dimensional SDP constraints, requires substantially more time, although the computation time under two minutes is still quite reasonable for many practical applications. Formulation $\text{sdp}_2$ seems to achieve the best balance between quality and efficiency, resulting in excellent relaxation quality without incurring in excessive computational costs.

We now compare these solution times with the computation times required to solve to optimality the MIO problems, as reported in other papers. Gómez and Prokopyev [16] use CPLEX solver with provable big-M constraints on the same datasets: while the first four instances can be solved to optimality in seconds, problems with the $\text{breast cancer}$ dataset require around 80 seconds to solve to optimality, and problems with the $\text{diabetes}$ dataset cannot be solved to optimality within one hour of branch-and-bound. Bertsimas et al. [6] use Gurobi solver coupled with tailored warm-start methods and heuristic big-M constraints on the $\text{diabetes}$
Figure 3. Average optimality gaps for the convex formulations.
dataset: in general, the optimization problems are not solved within one hour of branch-and-bound due to the difficulty of improving the lower bounds of the algorithm, although the solver reports gaps\footnote{Since Bertsimas et al. \cite{Bertsimas2015} use heuristic big-M constraints, the convex formulations used in their method are not guaranteed to be relaxations of \eqref{eq:original_problem}, thus the reported gaps do not have the same interpretation as \eqref{eq:relaxed_problem}.} of the order of 0.3% after an hour of branch-and-bound. In conclusion, we see that sdp\textsubscript{2} runs much faster than branch-and-bound methods, although it does not attempt to solve \eqref{eq:original_problem} to optimality, and is able to report guaranteed optimality gaps without resorting to big-M constraints.

5.2. Inference study on synthetic instances. We now present inference results on synthetic data, using the same simulation setup as in \cite{Bertsimas2015, Pakman2015}. Here we present a summary of the simulation setup and refer the readers to \cite{Pakman2015} for an extended description.

5.2.1. Instance generation. For given dimensions $n, p$, sparsity $s$, predictor auto-correlation $\rho$, and signal-to-noise ratio SNR, the instances are generated as follows:

1. The (true) coefficients $\beta_0$ have the first $s$ components equal to one, and the rest equal to zero.
2. The rows of the predictor matrix $X \in \mathbb{R}^{n \times p}$ are drawn from i.i.d. distributions $\mathcal{N}_p(0, \Sigma)$, where $\Sigma \in \mathbb{R}^{p \times p}$ has entry $(i, j)$ equal to $\rho^{|i-j|}$.
3. The response vector $y \in \mathbb{R}^n$ is drawn from $\mathcal{N}_p(X \beta_0, \sigma^2 I)$, where $\sigma^2 = \beta_0^T X \beta_0 / \text{SNR}$.

In each experiment ten instances are generated with the same parameters and the averages are reported. We use the same SNR values as \cite{Pakman2015}, i.e., SNR = 0.05, 0.09, 0.14, 0.25, 0.42, 0.71, 1.22, 2.07, 3.52, 6.0. We use $n = 500$, $p = 100$ and $s = 5$, also corresponding to experiments presented in \cite{Pakman2015}.

5.2.2. Evaluation metrics. Let $x_0$ denote the test predictor drawn from $\mathcal{N}_p(0, \Sigma)$ and let $y_0$ denote its associated response value drawn from $\mathcal{N}(x_0^T \beta_0, \sigma^2)$. Given an estimator $\hat{\beta}$ of $\beta_0$, the following metrics are reported:
Relative risk:
\[
RR(\hat{\beta}) = \frac{\mathbb{E} (x_0^T \hat{\beta} - x_0^T \beta_0)^2}{\mathbb{E} (x_0^T \beta_0)^2}
\]
with a perfect score 0 and null score of 1.

Relative test error:
\[
RTE(\hat{\beta}) = \frac{\mathbb{E} (x_0^T \hat{\beta} - y_0)^2}{\sigma^2}
\]
with a perfect score of 1 and null score of SNR+1.

Proportion of variance explained:
\[
1 - \frac{\mathbb{E} (x_0^T \hat{\beta} - y_0)^2}{\text{Var}(y_0)}
\]
with perfect score of SNR/(1+SNR) and null score of 0.

**Sparsity:** We record the number of nonzeros \(\|\hat{\beta}\|_0\), as done in [19]. Additionally, we also report the number of variables correctly identified, given by \(\sum_{i=1}^{p} \mathbb{I}\{\hat{\beta}_i \neq 0 \text{ and } (\beta_0)_i \neq 0\}\).

5.2.3. Procedures. In addition to the training set of size \(n\), a validation set of size \(n\) is generated with the same parameters, matching the precision of leave-one-out cross-validation. We use the following procedures to obtain estimators \(\hat{\beta}\).

- **elastic net:** The elastic net procedure was tuned by generating 10 values of \(\lambda\) ranging from \(\lambda_{\text{max}} = \|X^T y\|_{\infty}\) to \(\lambda_{\text{max}}/200\) on a log scale, generating 10 values of \(\mu\) on the same interval, and using the pair \((\lambda, \mu)\) that results in the best prediction error on the validation set. A total of 100 tuning parameters values are used.

- **sdp\(_2\) cross:** The estimator obtained from solving sdp\(_2\) \((\lambda = \mu = 0)\) for all values of \(k = 0, \ldots, 7\) and choosing the one that results in the best prediction error on the validation set.

- **sdp\(_2\) \(k = s\):** The estimator obtained from solving sdp\(_2\) with \(k = s\) and \(\lambda = \mu = 0\) on the training set. Corresponds to a method with perfect insight on the true sparsity \(s\).

- **sdp\(_2\) \(k = s\):** The estimator obtained from solving sdp\(_2\) with \(k = s\) and \(\lambda = \mu = 0\) on the dataset obtained from merging the training and validation sets. The intuition is that, since cross-validation is not used at all, there is no reason to discard half of the data.

The elastic net procedure approximately corresponds to the lasso procedure with 100 tuning parameters used in [19]. Similarly, sdp\(_2\) with cross-validation approximately corresponds to the best subset procedure with 51 tuning parameters used in [19]; nonetheless, the estimators from [19] are obtained by running a MIO.

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8An entry \(\hat{\beta}_i\) is deemed to be non-zero if \(|\hat{\beta}_i| > 10^{-5}\). This is the default integrality precision in commercial MIO solvers.

9Hastie et al. [19] use values of \(k = 0, \ldots, 50\). Nonetheless, in our computations with the same tuning parameters, we found that values of \(k \geq 8\) are never selected after cross-validation. Thus our procedure with 8 tuning parameters results in the same results as the one with 51 parameters from a statistical viewpoint, but requires only a fraction of the computational effort.
solver for 3 minutes, while ours are obtained from solving to optimality a strong convex relaxation. The last two procedures are included to illustrate what is, in our opinion, one of the main advantages of solving (3) to optimality or using a strong convex relaxation: the interpretability of parameter $k$, and the ability to enforce a sparsity prior without a need for cross-validation. In these experiments we use $\text{sdp}_2$ since, as pointed out in §5.1, it achieves the best balance between relaxation accuracy and efficiency.

5.2.4. **Optimality gaps and computation times.** Before describing the statistical results, we briefly comment on the relaxation quality and computation time of $\text{sdp}_2$.

Table 3 shows, for instances with $n = 500$, $p = 100$, and $s = 5$, the optimality gap and relaxation quality of $\text{sdp}_2$ — each column represents the average over ten instances generated with the same parameters. In all cases, $\text{sdp}_2$ produces optimal or near-optimal estimators, with optimality gap at most $0.3\%$. In fact, with $\text{sdp}_2$, we find that $97\%$ of the estimators for $\rho = 0.00$ and $68\%$ of the estimators with $\rho = 0.35$ are provably optimal for (1). For a comparison, Hastie et al. [19] report that, in their experiments, the MIO solver (with a time limit of three minutes) is able to prove optimality for only $35\%$ of the instances generated with similar parameters. Although Hastie et al. [19] do not report optimality gaps for the instances where optimality is not proven, we conjecture that such gaps are significantly larger than those reported in Table 3 due to weak relaxations with big-$M$ formulations. In summary, for this class of instances, $\text{sdp}_2$ is able to produce optimal or practically optimal estimators of (1) in about 30 seconds.

![Table 3](image)

5.2.5. **Results: accuracy metrics.** Figure 5 plots the relative risk, relative test error, proportion of variance explained and sparsity results as a function of the SNR for instances with $n = 500$, $p = 100$, $s = 5$ and $\lambda = \mu = 0$. Figure 6 plots the same results for instances with $\rho = 0.35$. The setting with $\rho = 0.35$ was also presented in [19].

We see that **elastic net** outperforms $\text{sdp}_2$ with cross-validation in low SNR settings, i.e., in SNR $= 0.05$ for $\rho = 0$ and SNR $\leq 0.14$ for $\rho = 0.35$, but results in worse predictive performance for all other SNRs. Moreover, $\text{sdp}_2$ is able to recover the true sparsity pattern of $\beta_0$ for sufficiently large SNR, while **elastic net** is unable to do so. We also see that $\text{sdp}_2$ performs comparatively better than **elastic net** in instances with $\rho = 0$. Indeed, for large autocorrelations $\rho$, features where $(\beta_0)_i = 0$ still have predictive value, thus the dense estimator obtained by **elastic net** retains a relatively good predictive performance (however, such dense solutions

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10A solution is deemed optimal if $\text{gap} < 10^{-4}$, which is the default parameter in MIO solvers.
Figure 5. Relative risk, relative test error, proportion of variance explained and sparsity as a function of SNR, with \( n = 500, p = 100, s = 5 \) and \( \rho = 0.00 \).
Figure 6. Relative risk, relative test error, proportion of variance explained and sparsity as a function of SNR, with $n = 500$, $p = 100$, $s = 5$ and $\rho = 0.35$. 
are undesirable from an interpretability perspective). In contrast, when \( \rho = 0 \), such features are simply noise and elastic net results in overfitting, while methods that deliver sparse solution such as \( \text{sdp}_2 \) perform much better in comparison. We also note that \( \text{sdp}_2 \) with cross-validations selects model corresponding to sparsities \( k < s \) in low SNRs, while it consistently selects models with \( k \approx s \) in high SNRs. We point out that, as suggested in [28], the results for low SNR could potentially be improved by fitting models with \( \mu > 0 \).

We now compare the performance of \( \text{sdp}_2 \) with cross-validation with the methods that use the prior \( k = s \). When the validation set is discarded by the method that enforces the prior, we see that using cross-validation yields much better results in low SNRs, as values with \( k < s \) result in better performance; in contrast, simply enforcing the prior results in (slightly) better results for large SNRs. However, when the prior is enforced and the validation set is also used for training the model, the resulting method \( \text{sdp}_2 + \) outperforms all other methods for all SNRs. Note that, in general, it is not possible for \( \ell_1 \)-based methods to obtain a model with a desired sparsity without cross-validation, as the sparsity-inducing properties of parameter \( \mu \) cannot be interpreted naturally.

Note that the “true” parameter \( s \) is rarely known in practice (although in some applications it may be possible to narrow down \( s \) to a small interval using prior knowledge). However, independently of the “true” value of \( s \) (or whether the data-generating process is sparse at all), it may be desirable to restrict the search to parsimonious models of size at most \( k \) for interpretability, especially when the estimators \( \hat{\beta} \) are meant to be analyzed by human experts. In such situations, methods like \( \text{sdp}_2 \) may be preferred to \( \ell_1 \) methods that require extensive cross-validation to achieve a desired sparsity level. Finally, even if \( s \) is unknown and interpretability is not a concern, the ability to accurately approximate \( (1) \) through relaxations \( \text{sdp}_r \) allows the decision-maker to use information criteria such as AIC [1] and BIC [33], which do not require cross-validation, to select \( k \), see also [16, 37].

6. Conclusions

In this paper we derive strong convex relaxations for sparse regression. The relaxations are based on the ideal formulations for rank-one quadratic terms with indicator variables. The new relaxations are formulated as semidefinite optimization problems in an extended space and are stronger and more general than the state-of-the-art formulations. In our computational experiments, the proposed conic formulations outperform the existing approaches, both in terms of accurately approximating the best subset selection problems and of achieving desirable estimation properties in statistical inference problems with sparsity.

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