A Scalable Algorithm for Sparse Portfolio Selection

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Abstract: The sparse portfolio selection problem is one of the most famous and frequently-studied problems in the optimization and financial economics literatures. In a universe of risky assets, the goal is to construct a portfolio with maximal expected return and minimum variance, subject to an upper bound on the number of positions, linear inequalities and minimum investment constraints. Existing certifiably optimal approaches to this problem do not converge within a practical amount of time at real-world problem sizes with more than 400 securities. In this paper, we propose a more scalable approach. By imposing a ridge regularization term, we reformulate the problem as a convex binary optimization problem, which is solvable via an efficient outer-approximation procedure. We propose various techniques for improving the performance of the procedure, including a heuristic which supplies high-quality warm-starts, a preprocessing technique for decreasing the gap at the root node, and an analytic technique for strengthening our cuts. We also study the problem's Boolean relaxation, establish that it is second-order-cone representable, and supply a sufficient condition for its tightness. In numerical experiments, we establish that the outer-approximation procedure gives rise to dramatic speedups for sparse portfolio selection problems.

Key words: Sparse Portfolio Selection, Binary Convex Optimization, Outer Approximation.

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1. Introduction

Since the Nobel-prize winning work of Markowitz (1952), the problem of selecting an optimal portfolio of securities has received an enormous amount of attention from practitioners and academics alike. In a universe containing n distinct securities with expected marginal returns $\boldsymbol{\mu} \in \mathbb{R}^n$ and variance-covariance matrix of the returns $\boldsymbol{\Sigma} \in \mathbb{R}^{n \times n}$, the Markowitz model selects a portfolio which provides the highest expected return for a given amount of variance, by solving:

$$\min_{\boldsymbol{x} \in \mathbb{R}^n_+} \ \frac{\sigma}{2} \boldsymbol{x}^\top \boldsymbol{\Sigma} \boldsymbol{x} - \boldsymbol{\mu}^\top \boldsymbol{x} \text{ s.t. } \boldsymbol{e}^\top \boldsymbol{x} = 1. \tag{1}$$

To improve its realism, many authors have proposed augmenting Problem (1) with minimum investment, maximum investment, and cardinality constraints (see, e.g., Jacob 1974, Perold 1984, Chang et al. 2000). Unfortunately, these constraints are disparate and sometimes imply each other, which makes defining a cannonical portfolio selection model challenging. We refer the reader to (Jin et al. 2016) (see also Mencarelli and D'Ambrosio 2019) for a survey of real-life constraints.

Bienstock (1996) (see also Bertsimas et al. 1999) defined a realistic portfolio selection model by augmenting Problem (1) with two sets of inequalities. The first inequality allocates an appropriate amount of capital to each market sector, by requiring that the constraints $\boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u}$ holds. The second inequality controls the number of non-zero positions held, by requiring that the portfolio is sparse, i.e., $\|\boldsymbol{x}\|_0 \leq k$. The sparsity constraint is important because (a) managers incur monitoring costs for each non-zero position, and (b) investors believe that portfolio managers who do not control the number of positions held perform index-tracking while charging active management fees. Imposing the real-world constraints yields the following NP-hard (even without linear inequalities; see Appendix B for a proof) portfolio selection model:

$$\min_{\boldsymbol{x} \in \mathbb{R}^n_+} \ \frac{\sigma}{2}\boldsymbol{x}^\top \boldsymbol{\Sigma}\boldsymbol{x} - \boldsymbol{\mu}^\top \boldsymbol{x} \text{ s.t. } \boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u},\ \boldsymbol{e}^\top \boldsymbol{x} = 1,\ \|\boldsymbol{x}\|_0 \leq k. \tag{2}$$

By introducing binary variables $z_i \in \{0, 1\}$ which model whether $x_i = 0$, we can rewrite the above problem as a mixed-integer quadratic optimization problem:

$$\min_{\boldsymbol{z} \in \{0,1\}^n: \boldsymbol{e}^\top \boldsymbol{z} \leq k,\ \boldsymbol{x} \in \mathbb{R}^n_+} \ \frac{\sigma}{2}\boldsymbol{x}^\top \boldsymbol{\Sigma}\boldsymbol{x} - \boldsymbol{\mu}^\top \boldsymbol{x} \text{ s.t. } \boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u},\ \boldsymbol{e}^\top \boldsymbol{x} = 1,\ x_i = 0 \text{ if } z_i = 0,\ \forall i \in [n]. \tag{3}$$

In the past 20 years, a number of authors have proposed approaches for solving Problem (2) to certifiable optimality. However, no known method scales to real-world problem sizes[1] where $20 \leq k \leq 50$ and $500 \leq n \leq 3,200$. This lack of scalability presents a challenge for practitioners and academics alike, because a scalable algorithm for Problem (2) has numerous financial applications, while algorithms which do not scale to this problem size are less practically useful.

1.1. Problem Formulation and Main Contributions

In this paper, we provide two main contributions. Our first contribution is augmenting Problem (2) with a ridge regularization term, namely $1/2\gamma \cdot \|\boldsymbol{x}\|_2^2$, to yield:

$$\min_{\boldsymbol{x} \in \mathbb{R}^n_+} \ \frac{\sigma}{2}\boldsymbol{x}^\top \boldsymbol{\Sigma}\boldsymbol{x} + \frac{1}{2\gamma}\|\boldsymbol{x}\|_2^2 - \boldsymbol{\mu}^\top \boldsymbol{x} \text{ s.t. } \boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u},\ \boldsymbol{e}^\top \boldsymbol{x} = 1,\ \|\boldsymbol{x}\|_0 \leq k. \tag{4}$$

Imposing the regularizer is related to robustifying Problem (2) (see Appendix A, for a discussion).

Our second main contribution is a scalable outer-approximation algorithm for Problem (4). By exploiting Problem (4)'s regularization term, we challenge the long-standing modeling practice of writing the logical constraint "$x_i = 0$ if $z_i = 0$" as $x_i \leq z_i$ in Problem (4), by substituting the equivalent but non-convex term $x_i z_i$ for x_i, and invoking strong duality to alleviate the resulting non-convexity. This allows us to propose a new outer-approximation algorithm which solves large-scale sparse portfolio selection problems with up to $3,200$ securities to certifiable optimality.

1.2. The Scalability of State-of-the-Art Approaches

We now justify our claim that no existing method scales to real-world problem sizes where $500 \leq n \leq 3,200$ and $20 \leq k \leq 50$, by summarizing the scalability of existing approaches. To this end, Table 1 depicts the largest problem solved by each approach, as reported by its authors[2].

Table 1 Largest sparse portfolio instance solved during benchmarking, by approach. "$k_{\max}$" denotes the largest cardinality-constraint right-hand-side imposed when benchmarking an approach. "n/a" indicates that a cardinality constraint was not imposed.

Reference	Solution method	Largest instance solved (no. securities)	$k_{\max}$
Vielma et al. (2008)	Nonlinear Branch-and-Bound	100	10
Bonami and Lejeune (2009)	Nonlinear Branch-and-Bound	200	20
Frangioni and Gentile (2009)	Branch-and-Cut+SDP	400	n/a
Gao and Li (2013)	Nonlinear Branch-and-Bound	300	20
Cui et al. (2013)	Nonlinear Branch-and-Bound	300	10
Zheng et al. (2014)	Branch-and-Cut+SDP	400	12
Frangioni et al. (2016)	Branch-and-Cut+SDP	400	10
Frangioni et al. (2017)	Branch-and-Cut+SDP	400	10

To supplement Table 1's comparison, Table 2 depicts the constraints imposed by each approach.

1.3. Background and Literature Review

Our work touches on three different strands of the mixed-integer non-linear optimization literature, each of which propose certifiably optimal methods for solving Problem (2): (a) branch-and-bound methods which solve a sequence of relaxations, (b) decomposition methods which separate the discrete and continuous variables in Problem (2), and (c) perspective reformulation methods which obtain tight relaxations by linking the discrete and the continuous in a non-linear manner.

Branch-and-bound algorithms: A variety of branch-and-bound algorithms have been proposed for solving Mixed-Integer Nonlinear Optimization problems (MINLOs) to certifiable optimality, since the work of Glover (1975), who proposed linearizing logical constraints "$x=0$ if $z=0$" by rewriting them as $-Mz \leq x \leq Mz$ for some $M>0$. This approach is known as the big-M method.

The first branch-and-bound algorithm for solving Problem (2) to certifiable optimality was proposed by Bienstock (1996). This algorithm reformulates the sparsity constraint $\|\boldsymbol{x}\|_0 \leq k$ in a linear way, by introducing binary variables z_i which model whether the optimizer holds a non-zero position in the ith security, and requiring that $x_i \leq z_i$ for each security i. Similar but more efficient branch-and-bound schemes are studied in Bertsimas and Shioda (2009), Bonami and Lejeune

Table 2 Constraints imposed and solver used, by reference; see also (Mencarelli and D'Ambrosio 2019, Table 1). We use the following notation to refer to the constraints imposed: **C**: A Cardinality constraint $\|\boldsymbol{x}\|_0 \leq k$; **MR**: A Minimum Return constraint $\boldsymbol{\mu}^\top \boldsymbol{x} \geq \bar{r}$; **SC**: A Semi-Continuous, or minimum investment, constraint $x_i \in \{0\} \cup [l_i, u_i],\ \forall i \in [n]$; **SOC**: A Second-Order-Cone approximation of a chance constraint: $\boldsymbol{\mu}^\top \boldsymbol{x} + F_{\boldsymbol{x}}^{-1}(1-p)\sqrt{\boldsymbol{x}^\top \boldsymbol{\Sigma} \boldsymbol{x}} \geq R$; **LS**: A Lot-sizing constraint $x_i = M\rho_i : \rho_i \in \mathbb{Z}$.

Reference	Solver	C	MR	SC	SOC	LS	Data Source
Vielma et al. (2008)	`CPLEX` 10.0	✓	✗	✗	✓	✗	20 instances generated using S&P 500 daily returns
Bonami and Lejeune (2009)	`CPLEX` 10.1, `Bonmin`	✓	✗	✓	✓	✓	36 instances generated using S&P 500 daily returns
Frangioni and Gentile (2009)	`CPLEX` 11	✗	✓	✓	✗	✗	Frangioni and Gentile (2006)
Cui et al. (2013)	`CPLEX` 12.1	✓	✓	✓	✗	✗	20 self-generated instances
Gao and Li (2013)	`CPLEX` 12.3, `MOSEK`	✓	✓	✗	✗	✗	58 instances generated using S&P 500 daily returns
Zheng et al. (2014)	`CPLEX` 12.4	✓	✓	✓	✗	✗	Frangioni and Gentile (2006) OR-library (Beasley 1990)
Frangioni et al. (2016)	`CPLEX` 12.6	✓	✓	✓	✗	✗	Frangioni and Gentile (2006)
Frangioni et al. (2017)	`Gurobi` 5.6 `CPLEX` 12.7	✓	✓	✓	✗	✗	Vielma et al. (2008) Frangioni and Gentile (2006)

(2009), who solve instances of Problem (2) with up to 50 (resp. 200) securities to certifiable optimality. Unfortunately, these methods do not scale well, because reformulating a sparsity constraint via the big-M method often yields weak relaxations in practice[3] (Bienstock 2010).

Motivated by the need to obtain tighter relaxations, more sophisticated branch-and-bound schemes have since been proposed, which obtain higher-quality bounds by lifting the problem to a higher-dimensional space. The first lifted approach was proposed by Vielma et al. (2008), who successfully solved instances of Problem (2) with up to 200 securities to certifiable optimality, by taking efficient polyhedral relaxations of second order cone constraints. This approach has since been improved by Gao and Li (2013), Cui et al. (2013), who derive non-linear branch-and-bound schemes which use even tighter second order cone and semi-definite relaxations to solve problems with up to 450 securities to certifiable optimality.

In the present paper, we propose a different approach for obtaining high-quality relaxations. By writing the sparsity constraint in a non-linear way, we obtain high-quality relaxations in the problem's original space. This idea appears to some extent in the work of Cui et al. (2013) (as well as the perspective function approaches mentioned below). Cui et al. (2013) obtain a somewhat similar formulation (with n additional variables/constraints) by lifting, using semidefinite techniques, taking the dual twice, and eliminating variables. However, we obtain our formulation *directly*, and the simplicity of this approach allows us to derive a computationally efficient decomposition scheme.

Decomposition algorithms: A well-known method for solving MINLOs such as Problem (2) is called outer approximation (OA), which was first proposed by Duran and Grossmann (1986) (building on the work of Kelley (1960), Benders (1962), Geoffrion (1972)), who prove its finite termination; see also Leyffer (1993), Fletcher and Leyffer (1994), who supply a simpler proof of OA's convergence. OA separates a difficult MINLO into a finite sequence of *master* mixed-integer linear problems and non-linear *subproblems* (NLOs). This is often a good strategy, because linear integer and continuous conic solvers are usually much more powerful than MINLO solvers.

Unfortunately, OA has not yet been successfully applied to Problem (2), because it requires informative gradient inequalities from each subproblem to attain a fast rate of convergence. Among others, Borchers and Mitchell (1997), Fletcher and Leyffer (1998) have compared OA to branch-and-bound, and found that branch-and-bound outperforms OA for Problem (2). In our opinion, OA's poor performance in existing implementations is due to the way cardinality constraints are traditionally formulated. Indeed, imposing a cardinality constraint $\|\boldsymbol{x}\|_0 \leq k$ via $\boldsymbol{x} \leq \boldsymbol{z}, \boldsymbol{e}^\top \boldsymbol{z} \leq k, \boldsymbol{z} \in \{0,1\}^n$, as was done in the aforementioned works, yields weak relaxations, induces degeneracy, and supplies low-quality gradient inequalities[4].

In the present paper, by invoking strong duality, we derive a new gradient inequality, redesign OA using this inequality, and solve Problem (2) to certifiable optimality via OA. The numerical success of our decomposition scheme can be explained by three ingredients: (a) the strength of the gradient inequality, (b) our ability to sidestep degeneracy and generate *Pareto optimal* cuts at no additional cost, as discussed directly below, and (c) the tightness of our non-linear reformulation of a sparsity constraint, as further investigated in a more general setting in Bertsimas et al. (2019a).

Another important aspect of decomposition algorithms is the strength of the cuts generated. In general, OA selects one of multiple valid inequalities at each iteration, and some of these inequalities are weak and implied by other inequalities. To accelerate the convergence of decomposition methods such as OA, Magnanti and Wong (1981) proposed a method for cut generation which is widely regarded as the gold-standard: selecting *Pareto optimal* cuts, which are implied by no other available cut. Unfortunately, existing *Pareto optimal* schemes comprise solving two subproblems at each iteration. The first subproblem selects a *core point* (see Magnanti and Wong 1981, for a definition), and the second subproblem selects a *Pareto optimal* cut. Due to the additional cost of performing each iteration, this method is often slower than OA in practice (see Papadakos 2008).

In this paper, we exploit problem structure to sidestep degeneracy. When $\boldsymbol{z}$ is on the relative interior of $\{\boldsymbol{z} \in [0,1]^n : \boldsymbol{e}^\top \boldsymbol{z} \leq k\}$, i.e., $\boldsymbol{z} \in \{\boldsymbol{z} \in (0,1)^n : \boldsymbol{e}^\top \boldsymbol{z} < k\}$, the regularizer breaks degeneracy, which allows us to generate Pareto-optimal cuts after solving a single subproblem. Moreover, at binary points, we obtain the tightest cut for a given set of dual variables (see Section 3.2).

Perspective reformulation algorithms: An important aspect of solving Problem (2) is understanding its objective's convex envelope, since approaches which exploit the envelope perform better than approaches which use looser approximations of the objective. An important step in this direction was taken by Frangioni and Gentile (2006), who built on the work of Ceria and Soares (1999) to derive Problem (2)'s convex envelope under an assumption that $\boldsymbol{\Sigma}$ is diagonal, and reformulated the envelope as a semi-infinite piecewise linear function. By splitting a generic covariance matrix into a diagonal matrix plus a positive semidefinite matrix, they subsequently derived a class of perspective cuts which provide bound gaps of $< 1\%$ for instances of Problem (2) with up to 200 securities. This approach was subsequently refined by Frangioni and Gentile (2009), who solved auxilliary semidefinite optimization problems to extract larger diagonal matrices (see Frangioni and Gentile 2007), and thereby solve instances of Problem (2) with up to 400 securities.

The perspective reformulation approach has also been extended by other authors. An important work in the area is Aktürk et al. (2009) (see also Günlük and Linderoth 2012), who prove that if $\boldsymbol{\Sigma}$ is positive definite, i.e., $\boldsymbol{\Sigma} \succ \mathbf{0}$, then after extracting a diagonal matrix $\boldsymbol{D} \succ \mathbf{0}$ such that $\boldsymbol{\Sigma} - \boldsymbol{D} \succeq \mathbf{0}$, Problem (2) is equivalent to the following mixed-integer second order cone problem (MISOCP):

$$\begin{aligned} \min_{\boldsymbol{z} \in \mathcal{Z}_k^n,\ \boldsymbol{x} \in \mathbb{R}_+^n,\ \boldsymbol{\theta} \in \mathbb{R}_+^n} \quad & \frac{\sigma}{2} \boldsymbol{x}^\top \boldsymbol{\Sigma} \boldsymbol{x} + \frac{1}{2} \sum_{i=1}^n D_{i,i} \theta_i - \boldsymbol{\mu}^\top \boldsymbol{x} \\ \text{s.t.} \quad & \boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u},\ \boldsymbol{e}^\top \boldsymbol{x} = 1,\ \left\| \begin{pmatrix} 2x_i \\ \theta_i - z_i \end{pmatrix} \right\|_2 \leq \theta_i + z_i, \forall i \in [n]. \end{aligned} \tag{5}$$

In light of the above MISOCP, a natural question to ask is *what is the best matrix* $\boldsymbol{D}$ *to use?* This question was partially[5] answered by Zheng et al. (2014), who demonstrated that the matrix $\boldsymbol{D}$ which yields the tightest continuous relaxation is computable via semidefinite optimization, and invoked this observation to solve problems with up to 400 securities to optimality (see also Dong et al. 2015, who derive a similar perspective reformulation of sparse regression problems). We refer the reader to Günlük and Linderoth (2012) for a survey of perspective reformulation approaches.

Our approach: An unchallenged assumption in *all* perspective reformulation approaches is that Problem (2) *must not be modified.* Under this assumption, perspective reformulation approaches separate $\boldsymbol{\Sigma}$ into a diagonal matrix $\boldsymbol{D} \succeq \mathbf{0}$ plus a positive semidefinite matrix $\boldsymbol{H}$, such that $\boldsymbol{D}$ is as diagonally dominant as possible. Recently, this approach was challenged by Bertsimas and Van Parys (2019) (see also Bertsimas et al. 2019b). Following a standard statistical learning theory paradigm, they imposed a ridge regularizer and set $\boldsymbol{D}$ equal to $1/\gamma \cdot \mathbb{I}$. Subsequently, they derived a cutting-plane method which exploits the regularizer to solve large-scale sparse regression problems to certifiable optimality. In the present paper, we join Bertsimas and Van Parys (2019) in imposing a ridge regularizer, and derive a cutting-plane method which solves convex MIQOs *with constraints.* We also unify both approaches, by noting that Bertsimas and Van Parys (2019)'s algorithm can be improved by setting $\boldsymbol{D}$ equal to $1/\gamma \cdot \mathbb{I}$ *plus* a perspective reformulation's diagonal matrix, and this is particularly effective when $\boldsymbol{\Sigma}$ is diagonally dominant (see Section 3.2, 5.2).

1.4. Structure

The rest of this paper is laid out as follows:

- In Section 2, we lay the groundwork for our approach, by taking the dual of (4)'s relaxation.
- In Section 3, we propose an efficient numerical strategy for solving Problem (4). By observing that Problem (4)'s inner dual problem supplies subgradients with respect to the positions held, we design an outer-approximation procedure which solves Problem (4) to provable optimality. We also discuss practical aspects of the procedure, including a computationally efficient subproblem strategy, a prepossessing technique for decreasing the bound gap at the root node, and a method for strengthening our cuts at no additional cost.
- In Section 4, we propose techniques for obtaining certifiably near-optimal solutions quickly. First, we introduce a heuristic which supplies high-quality warm-starts. Second, we observe that Problem (4)'s continuous relaxation supplies a near-exact Second Order Cone representable lower bound, and exploit this observation by deriving a sufficient condition for the bound to be exact.
- In Section 5, we apply the cutting-plane method to the problems described in Chang et al. (2000), Frangioni and Gentile (2006), and three larger scale data sets: the S&P 500, Russell 1000, and Wilshire 5000. We also explore Problem (4)'s sensitivity to its hyperparameters, and establish empirically that optimal support indices tend to be stable for reasonable hyperparameter choices.

Notation

We let nonbold face characters denote scalars, lowercase bold faced characters such as $\boldsymbol{x} \in \mathbb{R}^n$ denote vectors, uppercase bold faced characters such as $\boldsymbol{X} \in \mathbb{R}^{n \times r}$ denote matrices, and calligraphic uppercase characters such as $\mathcal{X}$ denote sets. We let $\mathbf{e}$ denote a vector of all 1's, $\mathbf{0}$ denote a vector of all 0's, and $\mathbb{I}$ denote the identity matrix, with dimension implied by the context. If $\boldsymbol{x}$ is a n-dimensional vector then $\mathrm{Diag}(\boldsymbol{x})$ denotes the $n \times n$ diagonal matrix whose diagonal entries are given by $\boldsymbol{x}$. We let $[n]$ denote the set of running indices $\{1, ..., n\}$, $\boldsymbol{x} \circ \boldsymbol{y}$ denote the elementwise, or Hadamard, product between two vectors $\boldsymbol{x}$ and $\boldsymbol{y}$, and $\mathbb{R}^n_+$ denote the n-dimensional non-negative orthant. We let $\mathrm{relint}(\mathcal{X})$ denote the relative interior of a convex set $\mathcal{X}$, i.e., the set of points on the interior of the affine hull of $\mathcal{X}$ (see Boyd and Vandenberghe 2004, Section 2.1.3). Finally, we let $\mathcal{Z}^n_k$ denote the set of k-sparse binary vectors, i.e, $\mathcal{Z}^n_k := \{\boldsymbol{z} \in \{0,1\}^n : \ \boldsymbol{e}^\top \boldsymbol{z} \leq k\}$.

2. A Dual Perspective on Markowitz Portfolio Optimization

In this section, we lay the groundwork for our overall outer-approximation procedure, by taking the dual of Problem (4)'s continuous relaxation. While outer-approximation schemes for Problem

(4) have previously been proposed, existing implementations do not perform as well as branch-and-bound schemes (Fletcher and Leyffer 1998), because there is no known way to obtain accurate gradient information efficiently. However, as will be made clear in Section 3, the dual of Problem (4)'s relaxation allows us to do precisely this. To obtain the dual, in Section 2.1 we rewrite the problem as a constrained regression problem, and in Section 2.2 we take the Lagrangian dual.

2.1. Equivalence Between Portfolio Selection and Regression

In this section, we rewrite Problem (4) as a constrained regression problem, by taking the square root of $\boldsymbol{\Sigma}$ and completing the square. This step is justified, because $\boldsymbol{\Sigma}$ is positive semidefinite and of rank r, meaning there exists some $\boldsymbol{X} \in \mathbb{R}^{r \times n}$ such that $\boldsymbol{\Sigma} = \boldsymbol{X}^\top \boldsymbol{X}$ (see Boyd and Vandenberghe 2004, Section A.5.2). Therefore, by scaling $\boldsymbol{\Sigma} \hookleftarrow \sigma \boldsymbol{\Sigma}$ and letting:

$$\boldsymbol{y} := \left(\boldsymbol{X}\boldsymbol{X}^\top\right)^{-1} \boldsymbol{X}\boldsymbol{\mu}, \tag{6}$$

$$\boldsymbol{d} := \left(\boldsymbol{X}^\top \left(\boldsymbol{X}\boldsymbol{X}^\top\right)^{-1} \boldsymbol{X} - \mathbb{I}\right) \boldsymbol{\mu}, \tag{7}$$

be the projection of the return vector $\boldsymbol{\mu}$ onto the span and nullspace of $\boldsymbol{X}$, completing the square yields the following equivalent problem, where we add the constant $\frac{1}{2}\boldsymbol{y}^\top \boldsymbol{y}$ without loss of generality:

$$\min_{\boldsymbol{x} \in \mathbb{R}^n_+} \quad \frac{1}{2\gamma} \|\boldsymbol{x}\|_2^2 + \frac{1}{2} \|\boldsymbol{X}\boldsymbol{x} - \boldsymbol{y}\|_2^2 + \boldsymbol{d}^\top \boldsymbol{x} \text{ s.t. } \boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u},\ \boldsymbol{e}^\top \boldsymbol{x} = 1,\ \|\boldsymbol{x}\|_0 \leq k. \tag{8}$$

2.2. The Dual Problem

We now take the dual of Problem (8)'s continuous relaxation, as a first step towards rewriting Problem (8) as a saddle-point problem. The continuous relaxation is:

$$\min_{\boldsymbol{x} \in \mathbb{R}^n_+} \quad \frac{1}{2\gamma} \|\boldsymbol{x}\|_2^2 + \frac{1}{2} \|\boldsymbol{X}\boldsymbol{x} - \boldsymbol{y}\|_2^2 + \boldsymbol{d}^\top \boldsymbol{x} \text{ s.t. } \boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u},\ \boldsymbol{e}^\top \boldsymbol{x} = 1. \tag{9}$$

By introducing a vector of auxiliary variables $\boldsymbol{r}$ to avoid taking the pseudoinverse of $\boldsymbol{\Sigma}$, and matching each constraint with a vector of dual variables in square brackets, this problem becomes:

$$\begin{aligned}
\min_{\boldsymbol{x} \in \mathbb{R}^n,\ \boldsymbol{r} \in \mathbb{R}^r} \quad & \frac{1}{2\gamma} \|\boldsymbol{x}\|_2^2 + \frac{1}{2} \|\boldsymbol{r}\|_2^2 + \boldsymbol{d}^\top \boldsymbol{x} && \\
\text{s.t.} \quad & \boldsymbol{y} - \boldsymbol{X}\boldsymbol{x} = \boldsymbol{r}, && [\boldsymbol{\alpha}], \\
& \boldsymbol{A}\boldsymbol{x} \geq \boldsymbol{l}, && [\boldsymbol{\beta}_l], \\
& \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u}, && [\boldsymbol{\beta}_u], \\
& \boldsymbol{e}^\top \boldsymbol{x} = 1, && [\lambda], \\
& \boldsymbol{x} \geq \boldsymbol{0}, && [\boldsymbol{\pi}].
\end{aligned} \tag{10}$$

We now have the following theorem:

THEOREM 1. *Suppose that Problem (10) is feasible. Then, strong duality holds between Problem (10) and its dual problem, which is:*

$$\begin{aligned} \max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^r,\ \boldsymbol{w}\in\mathbb{R}^n,\\ \boldsymbol{\beta}_l,\ \boldsymbol{\beta}_u\in\mathbb{R}^m_+,\ \lambda\in\mathbb{R}}} \quad & -\frac{1}{2}\boldsymbol{\alpha}^\top\boldsymbol{\alpha}-\frac{\gamma}{2}\boldsymbol{w}^\top\boldsymbol{w}+\boldsymbol{y}^\top\boldsymbol{\alpha}+\boldsymbol{\beta}_l^\top\boldsymbol{l}-\boldsymbol{\beta}_u^\top\boldsymbol{u}+\lambda \\ s.t. \quad & \boldsymbol{w}\geq\boldsymbol{X}^\top\boldsymbol{\alpha}+\boldsymbol{A}^\top(\boldsymbol{\beta}_l-\boldsymbol{\beta}_u)+\lambda\boldsymbol{e}-\boldsymbol{d}. \end{aligned} \tag{11}$$

Proof of Theorem 1 Problem (10) is a feasible convex quadratic optimization problem with linear constraints. Therefore, strong duality holds between Problem (10) and its dual (Boyd and Vandenberghe 2004, Section 5.2.3), and we need only establish that Problem (11) is Problem (10)'s dual. To establish this, we invoke Lagrangian duality. Problem (10)'s Lagrangian is:

$$\mathcal{L}=\frac{1}{2\gamma}\boldsymbol{x}^\top\boldsymbol{x}+\frac{1}{2}\boldsymbol{r}^\top\boldsymbol{r}+\boldsymbol{d}^\top\boldsymbol{x}+\boldsymbol{\alpha}^\top(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{x}-\boldsymbol{r})-\boldsymbol{\pi}^\top\boldsymbol{x}-\lambda(\boldsymbol{e}^\top\boldsymbol{x}-1)-\boldsymbol{\beta}_l^\top(\boldsymbol{A}\boldsymbol{x}-\boldsymbol{l})+\boldsymbol{\beta}_u^\top(\boldsymbol{A}\boldsymbol{x}-\boldsymbol{u}).$$

Moreover, minimizing the Lagrangian $\mathcal{L}$ is equivalent to solving the following KKT conditions:

$$\begin{aligned} \nabla_{\boldsymbol{x}}\mathcal{L}=\boldsymbol{0} &\implies \frac{1}{\gamma}\boldsymbol{x}+\boldsymbol{d}-\boldsymbol{X}^\top\boldsymbol{\alpha}-\boldsymbol{\pi}-\lambda\boldsymbol{e}-\boldsymbol{A}^\top(\boldsymbol{\beta}_l-\boldsymbol{\beta}_u)=0, \\ &\implies \boldsymbol{x}=\gamma\left(\boldsymbol{X}^\top\boldsymbol{\alpha}+\boldsymbol{\pi}+\lambda\boldsymbol{e}+\boldsymbol{A}^\top(\boldsymbol{\beta}_l-\boldsymbol{\beta}_u)-\boldsymbol{d}\right), \\ \nabla_{\boldsymbol{r}}\mathcal{L}=\boldsymbol{0} &\implies \boldsymbol{r}-\boldsymbol{\alpha}=0 \implies \boldsymbol{r}=\boldsymbol{\alpha}. \end{aligned}$$

Substituting the above expressions for $\boldsymbol{x},\boldsymbol{r}$ into $\mathcal{L}$ defines the Lagrangian dual, where we eliminate $\boldsymbol{\pi}$, introduce $\boldsymbol{w}$ for brevity. □

The derivation of Problem (11) reveals that each optimal allocation $\boldsymbol{x}^\star$ in Problem (10) satisfies the following relationship for some set of optimal dual variables in Problem (11):

$$\boldsymbol{x}^\star=\gamma\boldsymbol{w}^\star. \tag{12}$$

Equation (12) permits recovery of an optimal primal solution from a set of optimal dual variables.

In the next section, we reintroduce the sparsity constraint and rewrite Problem (8) as a saddle-point problem, to develop a cutting-plane method which solves the problem to certifiable optimality.

3. A Cutting-Plane Method

In this section, we present an efficient outer-approximation method for solving Problem (4). The key step in deriving this method is enforcing the logical constraint $x_i=0$ *if* $z_i=0$ in a tractable fashion. While traditionally the logical constraint is enforced by writing $x_i\leq z_i$, this yields weak relaxations (see Section 1.3). Instead, we replace x_i with $z_i x_i$, and rewrite Problem (4) as:

$$\min_{\boldsymbol{z}\in\mathcal{Z}^n_k}\Big[f(\boldsymbol{z})\Big], \tag{13}$$

where:

$$f(\boldsymbol{z}) := \min_{\boldsymbol{x}\in\mathbb{R}^n} \quad \frac{1}{2\gamma}\boldsymbol{x}^\top\boldsymbol{x} + \frac{1}{2}\|\boldsymbol{X}\boldsymbol{Z}\boldsymbol{x}-\boldsymbol{y}\|_2^2 + \boldsymbol{d}^\top\boldsymbol{Z}\boldsymbol{x} \quad \text{s.t.} \quad \boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{Z}\boldsymbol{x} \leq \boldsymbol{u},\ \boldsymbol{e}^\top\boldsymbol{Z}\boldsymbol{x} = 1,\ \boldsymbol{Z}\boldsymbol{x} \geq \boldsymbol{0}, \quad (14)$$

and $\boldsymbol{Z}$ is a diagonal matrix such that $Z_{i,i} = z_i$. Note that we do not associate a $\boldsymbol{Z}$ term with $\frac{1}{2\gamma}\boldsymbol{x}^\top\boldsymbol{x}$, as the subproblem generated by $f(\boldsymbol{z})$ attains its minimum by setting $x_i = 0$ whenever $z_i = 0$.

We now justify this modeling choice via the following lemmas (proofs deferred to Appendix C):

Lemma 1. *The following two optimization problems have the same optimal value:*

$$\min_{\boldsymbol{z}\in\mathcal{Z}_k^n} \min_{\boldsymbol{x}\in\mathbb{R}^n} \quad \frac{1}{2\gamma}\boldsymbol{x}^\top\boldsymbol{Z}\boldsymbol{x} + \frac{1}{2}\|\boldsymbol{X}\boldsymbol{Z}\boldsymbol{x}-\boldsymbol{y}\|_2^2 + \boldsymbol{d}^\top\boldsymbol{Z}\boldsymbol{x} \quad \textit{s.t.} \quad \boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{Z}\boldsymbol{x} \leq \boldsymbol{u},\ \boldsymbol{e}^\top\boldsymbol{Z}\boldsymbol{x} = 1,\ \boldsymbol{Z}\boldsymbol{x} \geq \boldsymbol{0}, \quad (15)$$

$$\min_{\boldsymbol{z}\in\mathcal{Z}_k^n} \min_{\boldsymbol{x}\in\mathbb{R}^n} \quad \frac{1}{2\gamma}\boldsymbol{x}^\top\boldsymbol{x} + \frac{1}{2}\|\boldsymbol{X}\boldsymbol{Z}\boldsymbol{x}-\boldsymbol{y}\|_2^2 + \boldsymbol{d}^\top\boldsymbol{Z}\boldsymbol{x} \quad \textit{s.t.} \quad \boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{Z}\boldsymbol{x} \leq \boldsymbol{u},\ \boldsymbol{e}^\top\boldsymbol{Z}\boldsymbol{x} = 1,\ \boldsymbol{Z}\boldsymbol{x} \geq \boldsymbol{0}. \quad (16)$$

Lemma 2. *Let* $(\boldsymbol{x}^\star, \boldsymbol{z}^\star)$ *solve Problem* (15)*. Then,* $(\boldsymbol{x}^\star \circ \boldsymbol{z}^\star, \boldsymbol{z}^\star)$ *solves Problem* (16)*. Moreover, let* $(\boldsymbol{x}^\star, \boldsymbol{z}^\star)$ *solve Problem* (16)*. Then,* $(\boldsymbol{x}^\star \circ \boldsymbol{z}^\star, \boldsymbol{z}^\star) = (\boldsymbol{x}^\star, \boldsymbol{z}^\star)$ *solves Problem* (15)*.*

We have established that writing $\boldsymbol{x}^\top\boldsymbol{x}$, rather than $\boldsymbol{x}^\top\boldsymbol{Z}\boldsymbol{x}$, does not alter Problem (13)'s optimal objective value, and, up to pathological cases where the cardinality constraint is not binding and $x_i^\star = 0$ for some index i such that $z_i^\star = 1$, does not alter the set of optimal solutions. Therefore, we work with Problem (13) for the rest of this paper, and do not consider Problem (15) any further.

Problem (13)'s formulation might appear to be intractable, because it appears to be non-convex. However, it is actually convex. Indeed, in Section 3.1, we invoke duality to demonstrate that $f(\boldsymbol{z})$ can be rewritten as the supremum of functions which are linear in $\boldsymbol{z}$.

As $f(\boldsymbol{z})$ is convex in $\boldsymbol{z}$, a natural strategy for solving (13) is to iteratively minimize and refine a piecewise linear underestimator of $f(\boldsymbol{z})$. This strategy is called outer-approximation (OA), and was originally proposed by Duran and Grossmann (1986) (building on the work of Benders 1962, Geoffrion 1972). OA works as follows: by assuming that at each iteration t we have access to $f(\boldsymbol{z}_i)$ and a subgradient $\boldsymbol{g}_{\boldsymbol{z}_i}$ at the points $\boldsymbol{z}_i : i \in [t]$, we construct the following underestimator of $f(\boldsymbol{z})$:

$$f_t(\boldsymbol{z}) = \max_{1\leq i\leq t} \left\{ f(\boldsymbol{z}_i) + \boldsymbol{g}_{\boldsymbol{z}_i}^\top(\boldsymbol{z}-\boldsymbol{z}_i) \right\}.$$

By iteratively minimizing $f_t(\boldsymbol{z})$ over $\mathcal{Z}_n^k$ to obtain $\boldsymbol{z}_t$, and evaluating $f(\cdot)$ and its subgradient at $\boldsymbol{z}_t$, we obtain a non-decreasing sequence of underestimators $f_t(\boldsymbol{z}_t)$ which converge to the optimal value of $f(\boldsymbol{z})$ within a finite number of iterations, since $\mathcal{Z}_n^k$ is a finite set and OA never visits a point twice (see also Fletcher and Leyffer 1994, Theorem 2). Additionally, we can avoid solving a different MILO at each OA iteration by integrating the entire algorithm within a single branch-and-bound tree, as first proposed by Padberg and Rinald (1991), Quesada and Grossmann (1992), using `lazy constraint callbacks`. Lazy constraint callbacks are now standard components of modern MILO solvers such as `Gurobi`, `CPLEX` and `GLPK`, and substantially speed-up OA.

As we mentioned in Section 1.3, OA is a widely known procedure. However, it has not yet been successfully applied to Problem (4). In our opinion, the main bottleneck inhibiting efficient OA implementations is a lack of an efficient separation oracle which provides both zeroth and first order information. To our knowledge, there are two existing oracles, but neither oracle is both computationally efficient and accurate. The first oracle exploits the convexity of $f(\boldsymbol{z})$ to obtain a valid subgradient for $f(\boldsymbol{z})$ via a finite difference scheme, namely setting the jth entry of $\boldsymbol{g_z}$ to

$$g_{t,j} = \begin{cases} f(\boldsymbol{z}_t + \boldsymbol{e}_j) - f(\boldsymbol{z}_t), \text{ if } \boldsymbol{z}_{t,i} = 1, \\ f(\boldsymbol{z}_t) - f(\boldsymbol{z}_t - \boldsymbol{e}_j), \text{ if } \boldsymbol{z}_{t,i} = 1. \end{cases}$$

This method clearly provides the tightest possible subgradient. However, it requires $n+1$ function evaluations of $f(\cdot)$ to obtain one subgradient $\boldsymbol{g}_t$, which is not computationally efficient.

The second oracle enforces the sparsity constraint by writing $x_i \leq z_i, \forall i \in [n]$, and using the dual multiplier associated with each constraint as a subgradient. This is a valid approach, as the dual multipliers associated with the constraint $\boldsymbol{x} \leq \boldsymbol{z}$ are indeed valid subgradients. Unfortunately, they are often very weak, and usually degenerate, meaning OA converges very slowly when it uses these subgradients. Indeed, as discussed in Section 1.3, OA is dominated by branch-and-bound when subgradients are obtained in this fashion (Fletcher and Leyffer 1998).

We now outline a procedure which obtains stronger valid subgradients of $f(\cdot)$ using a single function evaluation, before outlining our overall outer-approximation approach.

3.1. Efficient Subgradient Evaluations

We now rewrite Problem (13) as a saddle-point problem, in the following theorem:

Theorem 2. *Suppose that Problem* (13) *is feasible. Then, it is equivalent to the following problem:*

$$\begin{aligned} \min_{\boldsymbol{z} \in \mathcal{Z}_k^n} \max_{\substack{\boldsymbol{\alpha} \in \mathbb{R}^r,\ \boldsymbol{w} \in \mathbb{R}^n, \\ \boldsymbol{\beta}_l,\ \boldsymbol{\beta}_u \in \mathbb{R}_+^m,\ \lambda \in \mathbb{R}}} \quad & -\frac{1}{2}\boldsymbol{\alpha}^\top \boldsymbol{\alpha} - \frac{\gamma}{2}\sum_i z_i w_i^2 + \boldsymbol{y}^\top \boldsymbol{\alpha} + \boldsymbol{\beta}_l^\top \boldsymbol{l} - \boldsymbol{\beta}_u^\top \boldsymbol{u} + \lambda \\ \text{s.t.} \quad & \boldsymbol{w} \geq \boldsymbol{X}^\top \boldsymbol{\alpha} + \boldsymbol{A}^\top (\boldsymbol{\beta}_l - \boldsymbol{\beta}_u) + \lambda \boldsymbol{e} - \boldsymbol{d}. \end{aligned} \tag{17}$$

Proof of Theorem 2 We prove this result in essentially the same manner as Theorem 1. Note that, by Theorem 1, for each fixed $\boldsymbol{z} \in \mathcal{Z}_n^k$, either the problem of minimizing over $\boldsymbol{x}, \boldsymbol{r}$ is infeasible or strong duality holds.

Let us first introduce an auxiliary vector of variables $\boldsymbol{r}$ such that $\boldsymbol{r}=\boldsymbol{y}-\boldsymbol{X}\boldsymbol{Z}\boldsymbol{x}$, as was done in Section 2. This allows us to rewrite Problem (13) as:

$$
\begin{aligned}
\min_{\boldsymbol{z}\in\mathcal{Z}_n^k,\ \boldsymbol{x}\in\mathbb{R}^n,\ \boldsymbol{r}\in\mathbb{R}^r} \quad & \frac{1}{2\gamma}\|\boldsymbol{x}\|_2^2+\frac{1}{2}\|\boldsymbol{r}\|_2^2+\boldsymbol{d}^\top\boldsymbol{Z}\boldsymbol{x} \\
\text{s.t.} \quad & \boldsymbol{y}-\boldsymbol{X}\boldsymbol{Z}\boldsymbol{x}=\boldsymbol{r}, && [\boldsymbol{\alpha}],\\
& \boldsymbol{A}\boldsymbol{Z}\boldsymbol{x}\geq\boldsymbol{l}, && [\boldsymbol{\beta}_l],\\
& \boldsymbol{A}\boldsymbol{Z}\boldsymbol{x}\leq\boldsymbol{u}, && [\boldsymbol{\beta}_u],\\
& \boldsymbol{e}^\top\boldsymbol{Z}\boldsymbol{x}=1, && [\lambda],\\
& \boldsymbol{Z}\boldsymbol{x}\geq\boldsymbol{0}, && [\boldsymbol{\pi}].
\end{aligned}
\tag{18}
$$

This problem has the following Lagrangian:

$$
\begin{aligned}
\mathcal{L} \quad =& \frac{1}{2\gamma}\boldsymbol{x}^\top\boldsymbol{x}+\frac{1}{2}\boldsymbol{r}^\top\boldsymbol{r}+\boldsymbol{d}^\top\boldsymbol{Z}\boldsymbol{x}+\boldsymbol{\alpha}^\top\left(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{Z}\boldsymbol{x}-\boldsymbol{r}\right)-\boldsymbol{\pi}^\top\boldsymbol{Z}\boldsymbol{x}\\
&-\lambda(\boldsymbol{e}^\top\boldsymbol{Z}\boldsymbol{x}-1)-\boldsymbol{\beta}_l^\top(\boldsymbol{A}\boldsymbol{Z}\boldsymbol{x}-\boldsymbol{l})+\boldsymbol{\beta}_u^\top(\boldsymbol{A}\boldsymbol{Z}\boldsymbol{x}-\boldsymbol{u}).
\end{aligned}
$$

For a fixed $\boldsymbol{z}$, minimizing this Lagrangian is equivalent to solving the following KKT conditions:

$$
\begin{aligned}
\nabla_{\boldsymbol{x}}\mathcal{L}=\boldsymbol{0} &\implies \frac{1}{\gamma}\boldsymbol{x}+\boldsymbol{Z}\left(\boldsymbol{d}-\boldsymbol{X}^\top\boldsymbol{\alpha}-\boldsymbol{\pi}-\lambda\boldsymbol{e}-\boldsymbol{A}^\top(\boldsymbol{\beta}_l-\boldsymbol{\beta}_u)\right)=\boldsymbol{0},\\
&\implies \boldsymbol{x}=\gamma\boldsymbol{Z}\left(\boldsymbol{X}^\top\boldsymbol{\alpha}+\boldsymbol{\pi}+\lambda\boldsymbol{e}+\boldsymbol{A}^\top(\boldsymbol{\beta}_l-\boldsymbol{\beta}_u)-\boldsymbol{d}\right),\\
\nabla_{\boldsymbol{r}}\mathcal{L}=\boldsymbol{0} &\implies \boldsymbol{r}-\boldsymbol{\alpha}=0\implies \boldsymbol{r}=\boldsymbol{\alpha}.
\end{aligned}
$$

Substituting the above expressions for $\boldsymbol{x}$, $\boldsymbol{r}$ into $\mathcal{L}$ then defines the Lagrangian dual, where we eliminate $\boldsymbol{\pi}$ and introduce $\boldsymbol{w}$ such that $\boldsymbol{x}:=\gamma\boldsymbol{Z}\boldsymbol{w}$ for brevity. The Lagrangian dual reveals that for any $\boldsymbol{z}$ such that Problem (14) is feasible:

$$
\begin{aligned}
f(\boldsymbol{z})=\max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^r,\ \boldsymbol{w}\in\mathbb{R}^n,\\ \boldsymbol{\beta}_l,\ \boldsymbol{\beta}_u\in\mathbb{R}^m_+,\ \lambda\in\mathbb{R}}} \quad & -\frac{1}{2}\boldsymbol{\alpha}^\top\boldsymbol{\alpha}-\frac{\gamma}{2}\boldsymbol{w}^\top\boldsymbol{Z}^2\boldsymbol{w}+\boldsymbol{y}^\top\boldsymbol{\alpha}+\boldsymbol{\beta}_l^\top\boldsymbol{l}-\boldsymbol{\beta}_u^\top\boldsymbol{u}+\lambda\\
\text{s.t.} \quad & \boldsymbol{w}\geq\boldsymbol{X}^\top\boldsymbol{\alpha}+\boldsymbol{A}^\top\left(\boldsymbol{\beta}_l-\boldsymbol{\beta}_u\right)+\lambda\boldsymbol{e}-\boldsymbol{d}.
\end{aligned}
$$

Moreover, at binary points $\boldsymbol{z}$, $z_i^2=z_i$ and therefore the above problem is equivalent to solving:

$$
\begin{aligned}
f(\boldsymbol{z})=\max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^r,\ \boldsymbol{w}\in\mathbb{R}^n,\\ \boldsymbol{\beta}_l,\ \boldsymbol{\beta}_u\in\mathbb{R}^m_+,\ \lambda\in\mathbb{R}}} \quad & -\frac{1}{2}\boldsymbol{\alpha}^\top\boldsymbol{\alpha}-\frac{\gamma}{2}\sum_i z_i w_i^2+\boldsymbol{y}^\top\boldsymbol{\alpha}+\boldsymbol{\beta}_l^\top\boldsymbol{l}-\boldsymbol{\beta}_u^\top\boldsymbol{u}+\lambda\\
\text{s.t.} \quad & \boldsymbol{w}\geq\boldsymbol{X}^\top\boldsymbol{\alpha}+\boldsymbol{A}^\top\left(\boldsymbol{\beta}_l-\boldsymbol{\beta}_u\right)+\lambda\boldsymbol{e}-\boldsymbol{d},
\end{aligned}
$$

where we strengthen the formulation by associating z_i, rather than z_i^2, with w_i^2.

Minimizing $\boldsymbol{z}$ over $\mathcal{Z}_k^n$ then yields the result, where we ignore choices of $\boldsymbol{z}$ which yield infeasible primal subproblems without loss of generality, as their dual problems are feasible and therefore unbounded by weak duality, and a choice of $\boldsymbol{z}$ such that $f(\boldsymbol{z})=+\infty$ is certainly suboptimal. □

Remark 1. Theorem 2 proves that $f(\boldsymbol{z})$ is convex in $\boldsymbol{z}$, by rewriting $f(\boldsymbol{z})$ as the pointwise maximum of functions which are linear in $\boldsymbol{z}$ (Boyd and Vandenberghe 2004, Section 3.2.3). This justifies our application of OA, which converges under a convexity assumption over finite sets such as $\mathcal{Z}_k^n$.

In the above proof, the relationship between the optimal primal and dual variables became:

$$\boldsymbol{x}^* = \gamma \mathrm{Diag}(\boldsymbol{z}^\star)\boldsymbol{w}^\star. \tag{19}$$

This relationship is equivalent to Equation (12) at binary points $\boldsymbol{z}$, but is also valid on $\mathrm{int}(\mathcal{Z}_k^n)$.

Theorem 2 supplies objective function evaluations $f(\boldsymbol{z}_t)$ and subgradients $\boldsymbol{g}_t$ after solving a single convex quadratic optimization problem. We formalize this observation in the following corollaries:

Corollary 1. *Let $\boldsymbol{w}^\star$, $\boldsymbol{\beta}_l^\star$, $\boldsymbol{\beta}_u^\star$, $\lambda^\star$, $\boldsymbol{\alpha}^\star$ be optimal dual multipliers for a given subset of securities $\hat{\boldsymbol{z}}$. Then, the value of $f(\hat{\boldsymbol{z}})$ is given by the following expression:*

$$f(\hat{\boldsymbol{z}}) = -\frac{\gamma}{2}\sum_i \hat{z}_i w_i^{\star 2} - \frac{1}{2}\|\boldsymbol{\alpha}^\star\|_2^2 + \boldsymbol{y}^\top\boldsymbol{\alpha}^\star + \lambda^\star + \boldsymbol{l}^\top\boldsymbol{\beta}_l^\star - \boldsymbol{u}^\top\boldsymbol{\beta}_u^\star. \tag{20}$$

Corollary 2. *Let $\boldsymbol{w}^\star(\boldsymbol{z})$ be an optimal choice of $\boldsymbol{w}$ for a particular subset of securities $\boldsymbol{z}$. Then, valid subgradients $\boldsymbol{g}_{\boldsymbol{z}} \in \partial f(\boldsymbol{z})$ with respect to each security i are given by the following expression:*

$$g_{\boldsymbol{z},i} = -\frac{\gamma}{2} w_i^\star(\boldsymbol{z})^2. \tag{21}$$

In later sections of this paper, we design aspects of our numerical strategy by assuming that $f(\boldsymbol{z})$ is Lipschitz continuous in $\boldsymbol{z}$. It turns out that this assumption is valid whenever we can bound $|\boldsymbol{w}_i^\star(\boldsymbol{z})|$ for each $\boldsymbol{z}$, as we now establish in the following corollary (proof deferred to Appendix C):

Corollary 3. *Let $\boldsymbol{w}^\star(\boldsymbol{z})$ be an optimal choice of $\boldsymbol{w}$ for a given subset of securities $\boldsymbol{z}$. Then:*

$$f(\boldsymbol{z}) - f(\hat{\boldsymbol{z}}) \leq \frac{\gamma}{2}\sum_i (\hat{z}_i - z_i) w_i^\star(\boldsymbol{z})^2.$$

3.2. A Cutting-Plane Method-Continued

Corollary 2 shows that evaluating $f(\hat{\boldsymbol{z}})$ yields a first-order underestimator of $f(\boldsymbol{z})$, namely

$$f(\boldsymbol{z}) \geq f(\hat{\boldsymbol{z}}) + \boldsymbol{g}_{\hat{\boldsymbol{z}}}^\top(\boldsymbol{z} - \hat{\boldsymbol{z}})$$

at no additional cost. Consequently, a numerically efficient strategy for minimizing $f(\boldsymbol{z})$ is the previously discussed OA method. We formalize this procedure in Algorithm 1. Note that we add the OA cuts via `lazy constraint callbacks` to maintain a single tree of partial solutions throughout the entire process, and avoid the cost otherwise incurred in rebuilding the tree whenever a cut is added, as proposed by Quesada and Grossmann (1992).

As Algorithm 1's rate of convergence depends heavily upon its implementation, we now discuss some practical aspects of the method:

Algorithm 1 An outer-approximation method for Problem (4)

Require: Initial solution $\boldsymbol{z}_1$

$t \leftarrow 1$

repeat

Compute $\boldsymbol{z}_{t+1}, \theta_{t+1}$ solution of

$$\min_{\boldsymbol{z} \in \mathcal{Z}_k^n, \theta} \theta \quad \text{s.t. } \theta \geq f(\boldsymbol{z}_i) + \boldsymbol{g}_{\boldsymbol{z}_i}^\top (\boldsymbol{z} - \boldsymbol{z}_i), \ \forall i \in [t],$$

Compute $f(\boldsymbol{z}_{t+1})$ and $\boldsymbol{g}_{\boldsymbol{z}_{t+1}} \in \partial f(\boldsymbol{z}_{t+1})$

$t \leftarrow t+1$

until $f(\boldsymbol{z}_t) - \theta_t \leq \varepsilon$

return $\boldsymbol{z}_t$

- **A computationally efficient subproblem strategy:** For computational efficiency purposes, we would like to solve subproblems which only involve active indices, i.e., indices where $z_i = 1$, since $k \ll n$. At a first glance, this does not appear to be possible, because we must supply an optimal choice of w_i for all n indices in order to obtain valid subgradients. Fortunately, we can in fact supply a full OA cut after solving a subproblem in $O(k)$ variables, by exploiting the structure of the saddle-point reformulation. Specifically, we optimize over the k indices i where $z_i = 1$ and set $w_i = \max(\boldsymbol{X}_i^\top \boldsymbol{\alpha}^\star + \boldsymbol{A}_i^\top (\boldsymbol{\beta}_l^\star - \boldsymbol{\beta}_u^\star) + \lambda^\star - d_i, 0)$ for the remaining $n-k$ w_i's. This procedure yields an optimal choice of w_i for each index i, because it is a feasible choice and the remaining w_i's have weight 0 in the objective function.

It turns out that this procedure yields the strongest possible cuts which can be generated at $\boldsymbol{z}$ *for this set of dual variables*, because (a) the procedure yields the minimum feasible absolute magnitude of w_i whenever $z_i = 0$, and (b) there is a unique optimal choice of w_i for the remaining indices, since Problem (17) is strongly concave in w_i when $z_i > 0$. In fact, if $w_i = 0$ is feasible for some security i such that $z_i = 0$, then we cannot improve upon the current iterate $\boldsymbol{z}$ by setting $z_i = 1$ and $z_j = 0$ for some active index j, as our lower approximation gives

$$f(\boldsymbol{z} + \boldsymbol{e}_i - \boldsymbol{e}_j) \geq f(\boldsymbol{z}) + \boldsymbol{g}_{\boldsymbol{z}}^\top (\boldsymbol{z} + \boldsymbol{e}_j - \boldsymbol{e}_i - \boldsymbol{z}) = f(\boldsymbol{z}) + \boldsymbol{g}_{\boldsymbol{z}}^\top (\boldsymbol{e}_j - \boldsymbol{e}_i) \geq f(\boldsymbol{z}).$$

Additionally, if $\boldsymbol{z} \in \text{Relint}(\mathcal{Z})$ then there is a unique optimal choice of $\boldsymbol{w}^\star$ and indeed the resulting cut is Pareto-optimal in the sense of Magnanti and Wong (1981) (see Proposition 1).

- **Cut generation at the root node:** Another important aspect of efficiently implementing decomposition methods is supplying as much information as possible to the solver before commencing branching, as discussed in Fischetti et al. (2016, Section 4.2). One effective way to achieve this is to relax the integrality constraint $\boldsymbol{z} \in \{0,1\}^n$ to $\boldsymbol{z} \in [0,1]^n$ in Problem (17), run a cutting-plane method on this continuous relaxation and apply the resulting cuts at the root node before solving the binary problem. Traditionally, this relaxation is solved using Kelley (1960)'s cutting-plane method. However, as Kelley (1960)'s method often converges slowly in practice, we instead solve the relaxation using an `in-out` bundle method (Ben-Ameur and Neto 2007, Fischetti et al. 2016). We supply pseudocode for our implementation of the `in-out` method in Appendix E.

In order to further accelerate OA, a variant of the root node processing technique which is often effective is to also run the `in-out` method at some leaf nodes, as proposed in (Fischetti et al. 2016, Section 4.3). This can be implemented via a `user cut callback`, by using the current LO solution $\boldsymbol{z}^\star$ as a stabilization point for the `in-out` method, and adding the cuts generated via the callback.

To avoid generating too many cuts at continuous points, we impose a limit of 200 cuts at the root node, 20 cuts at all other nodes, and do not run the `in-out` method at more than 50 nodes. One point of difference in our implementation of the `in-out` method (compared to Ben-Ameur and Neto 2007, Fischetti et al. 2016) is that we use the optimal solution to Problem (17)'s continuous relaxation as a stabilization point at the root node-this speeds up convergence greatly, and comes at the low price of solving an SOCP to elicit the stabilization point (we obtain the point by solving Problem (28); see Section 4.2). Cut purging mechanisms, as discussed in (Fischetti et al. 2016, Section 4.2) could also be useful, although we do not implement them in the present paper.

- **Feasibility cuts:** The linear inequality constraints $\boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u}$ may render some binary vectors $\hat{\boldsymbol{z}}$ infeasible. In this case, rather than adding an optimality cut, we add the following feasibility cut which bans $\hat{\boldsymbol{z}}$ from appearing in future iterations of OA[6]:

$$\sum_i \hat{z}_i(1-z_i) + \sum_i (1-\hat{z}_i) z_i \geq 1. \tag{22}$$

An alternative approach is to derive constraints on $\boldsymbol{z}$ which ensure that OA never selects an infeasible $\boldsymbol{z}$. For instance, if the only constraint on $\boldsymbol{x}$ is a minimum return constraint $\boldsymbol{\mu}^\top \boldsymbol{x} \geq r$ then imposing $\sum_{i:\mu_i \geq r} z_i \geq 1$ ensures that only feasible $\boldsymbol{z}$'s are selected. Whenever eliciting these constraints is possible, we recommend imposing them, to avoid infeasible subproblems entirely.

- **Extracting Diagonal Dominance:** In problems where $\boldsymbol{\Sigma}$ is diagonally dominant (i.e., $\Sigma_{i,i} \gg |\Sigma_{i,j}|$ for $i \neq j$), the performance of Algorithm 1 can often be substantially improved by *boosting* the regularizer, i.e., selecting a diagonal matrix $\boldsymbol{D} \succeq \boldsymbol{0}$ such that $\boldsymbol{\Sigma} - \boldsymbol{D} \succeq \boldsymbol{0}$, replacing $\boldsymbol{\Sigma}$ with $\boldsymbol{\Sigma} - \boldsymbol{D}$, and using a different regularizer $\gamma_i := \left(\frac{1}{\gamma} + D_{i,i}\right)^{-1}$ for each index i. In general, selecting such a $\boldsymbol{D}$ involves solving an SDO (Frangioni and Gentile 2007, Zheng et al. 2014), which is fast when $n = 100$s but requires a prohibitive amount of memory for $n = 1000$s. In the later case, we recommend taking a SOCP-representable inner approximation of the SD cone and improving the approximation via column generation (see Ahmadi et al. 2017, Bertsimas and Cory-Wright 2019).

- **Copy of variables:** In problems with multiple complicating constraints, many feasibility cuts may be generated, which can hinder convergence greatly. When this occurs, we recommend introducing a copy of $\boldsymbol{x}$ in the master problem (with appropriate constraints on $\boldsymbol{x}$) and relating the discrete and the continuous via $\boldsymbol{x} \leq \boldsymbol{z}$ (or $\boldsymbol{x} \leq \boldsymbol{x}_{\max} \circ \boldsymbol{z}$ when explicit upper bounds on $\boldsymbol{x}$ are known). This approach performs well on the highly constrained problems studied in Section 5.2.

We now remind the reader of the definition of a Pareto-optimal cut, in preparation for establishing that our proposed cut generation technique is indeed Pareto-optimal.

Definition 1. (c.f. Papadakos 2008, Definition 2) A cut $\theta \geq f(\boldsymbol{z}_i) + \boldsymbol{g}_{\boldsymbol{z}_i}^\top(\boldsymbol{z} - \boldsymbol{z}_i)$ is dominated on a set $\mathcal{Z}$ if there exists some other cut $\theta \geq f(\boldsymbol{z}_j) + \boldsymbol{g}_{\boldsymbol{z}_j}^\top(\boldsymbol{z} - \boldsymbol{z}_j)$ such that

$$f(\boldsymbol{z}_i) + \boldsymbol{g}_{\boldsymbol{z}_i}^\top(\boldsymbol{z} - \boldsymbol{z}_i) \leq f(\boldsymbol{z}_j) + \boldsymbol{g}_{\boldsymbol{z}_j}^\top(\boldsymbol{z} - \boldsymbol{z}_j), \quad \forall \boldsymbol{z} \in \mathcal{Z},$$

with inequality holding strictly at some $\boldsymbol{z} \in \mathcal{Z}$. A cut is *Pareto-optimal* if it is not non-dominated.

Proposition 1. *Let $\boldsymbol{w}^\star(\boldsymbol{z})$ be the optimal choice of $\boldsymbol{w}$ for a fixed $\boldsymbol{z} \in \mathrm{Relint}(\mathcal{Z}_k^n)$. Then, setting $g_{\boldsymbol{z},i} = \frac{-\gamma}{2} w_i^\star(\boldsymbol{z})^2,\ \forall i \in [n]$ yields a Pareto-optimal cut.*

Proof of Proposition 1 Almost identical to (Magnanti and Wong 1981, Theorem 1). □

By combining the above discussion on efficient cut generation with Corollary 3, we now supply a sufficient condition for a single outer-approximation cut to certify optimality:

Proposition 2. *Let an optimal set of dual multipliers for some $\boldsymbol{z} \in \mathcal{Z}_k^n$ be such that*

$$\boldsymbol{X}_i^\top \boldsymbol{\alpha}^\star + \boldsymbol{A}_i^\top(\boldsymbol{\beta}_l^\star - \boldsymbol{\beta}_u^\star) + \lambda^\star \leq d_i, \forall i \in [n] : z_i = 0$$

Then, $\boldsymbol{z}$ solves Problem (4).

Proof of Proposition 2 By assumption, we can set $w_i^\star(\boldsymbol{z}) = 0$ for each index i such that $z_i = 0$. Therefore, Corollary 3 implies that:

$$f(\boldsymbol{z}) - f(\hat{\boldsymbol{z}}) \leq \frac{\gamma}{2} \sum_{i: z_i = 1} (\hat{z}_i - z_i) w_i^\star(\boldsymbol{z})^2,\ \forall \hat{\boldsymbol{z}} \in \mathcal{Z}_n^k.$$

But $\hat{z}_i \leq z_i$ at indices where $z_i = 1$, so this inequality implies that $f(\boldsymbol{z}) \leq f(\hat{\boldsymbol{z}}),\ \forall \hat{\boldsymbol{z}} \in \mathcal{Z}_k^n$. □

Observe that this condition is automatically checked by branch-and-cut codes each time we add an outer-approximation cut. Indeed, as will see in Section 5, we sometimes certify optimality after adding a very small number of cuts, so this condition is sometimes satisfied in practice.

3.3. Modelling Minimum Investment Constraints

A frequently-studied extension to Problem (4) is to impose minimum investment constraints (see, e.g., Chang et al. 2000), which control transaction fees by requiring that $x_i \geq x_{i,\min}$ for each index i such that $x_i > 0$. We now extend our saddle-point reformulation to cope with them.

By letting z_i be a binary indicator variable which denotes whether we hold a non-zero position in the ith asset, we model these constraints via $x_i \geq z_i x_{i,\min},\ \forall i \in [n]$.

Moreover, by letting ρ_i be the dual multiplier associated with the ith minimum investment constraint, and repeating the steps of our saddle-point reformulation *mutatis mutandis*, we retain efficient objective function and subgradient evaluations in the presence of these constraints. Specifically, including the constraints is equivalent to adding the term $\sum_{i=1}^n \rho_i (z_i x_{i,\min} - x_i)$ to Problem (4)'s Lagrangian, which implies the saddle-point problem becomes:

$$\begin{aligned} \min_{\boldsymbol{z} \in \mathcal{Z}_k^n} \max_{\substack{\boldsymbol{\alpha} \in \mathbb{R}^r,\ \boldsymbol{w} \in \mathbb{R}^n, \boldsymbol{\rho} \in \mathbb{R}_n^+ \\ \boldsymbol{\beta}_l,\ \boldsymbol{\beta}_u \in \mathbb{R}_+^m,\ \lambda \in \mathbb{R}}} \quad & -\frac{1}{2}\boldsymbol{\alpha}^\top \boldsymbol{\alpha} - \frac{\gamma}{2}\sum_i z_i w_i^2 + \boldsymbol{y}^\top \boldsymbol{\alpha} + \boldsymbol{\beta}_l^\top \boldsymbol{l} - \boldsymbol{\beta}_u^\top \boldsymbol{u} + \lambda + \sum_i \rho_i z_i x_{i,\min} \\ \text{s.t.} \quad & \boldsymbol{w} \geq \boldsymbol{X}^\top \boldsymbol{\alpha} + \boldsymbol{A}^\top (\boldsymbol{\beta}_l - \boldsymbol{\beta}_u) + \lambda \boldsymbol{e} + \boldsymbol{\rho} - \boldsymbol{d}. \end{aligned} \tag{23}$$

Moreover, the subgradient with respect to each index i becomes

$$g_{\boldsymbol{z},i} = -\frac{\gamma}{2} w_i^\star(\boldsymbol{z})^2 + \rho_i x_{i,\min}. \tag{24}$$

We close this section by noting that if $z_i = 0$ then we can set $\rho_i = 0$ without loss of optimality. Therefore, we recommend solving a subproblem in the k variables such that $z_i > 0$ and subsequently setting $\rho_i = 0$ for the remaining variables, in the manner discussed in the previous subsection. Indeed, setting $w_i = \max\left(\boldsymbol{X}_i^\top \boldsymbol{\alpha}^\star + \boldsymbol{A}_i^\top (\boldsymbol{\beta}_l^\star - \boldsymbol{\beta}_u^\star) + \lambda^\star + \rho_i^\star - d_i, 0\right)$ for each index i where $z_i = 0$, as discussed in the previous subsection, supplies the minimum absolute value of w_i for these indices.

4. Improving the Performance of the Cutting-Plane Method

In portfolio rebalancing applications, practitioners often require a high-quality solution to Problem (4) within a fixed time budget. Unfortunately, Algorithm 1 is ill-suited to this task: while it always identifies a certifiably optimal solution, it does not always do so within a time budget. In this section, we propose alternative techniques which sacrifice some optimality for speed, and discuss how they can be applied to improve the performance of Algorithm 1. In Section 4.1 we propose a warm-start heuristic which supplies a high-quality solution to Problem (4) *apriori*, and in Section 4.2 we derive a second order cone representable lower bound which is often very tight in practice. Taken together, these techniques supply a certifiably near optimal solution very quickly, which can often be further improved by running Algorithm 1 for a short amount of time.

4.1. Improving the Upper Bound: A Warm-Start Heuristic

In branch-and-cut methods, a frequently observed source of inefficiency is that optimization engines explore highly-suboptimal regions of the search space in considerable depth. To discourage this behaviour, optimizers frequently supply a high-quality feasible solution (i.e., a warm-start), which is installed as an incumbent by the optimization engine. Warm-starts are beneficial for two reasons. First, they improve Algorithm 1's upper bound. Second, they allow Algorithm 1 to prune vectors of partial solutions which are provably worse than the warm-start, which in turn improves Algorithm 1's bound quality, by reducing the set of feasible $\boldsymbol{z}$ which can be selected at each subsequent iteration. Indeed, by pruning suboptimal solutions, warm-starts encourage branch-and-cut methods to focus on regions of the search space which contain near-optimal solutions.

We now describe a custom heuristic method which supplies high-quality feasible solutions for Problem (4). The heuristic is inspired by Bertsimas et al. (2016, Algorithm 1) and works under the assumption that $f(\boldsymbol{z})$ is Lipschitz continuous in $\boldsymbol{z}$, with Lipschitz constant L (this is justified whenever the optimal dual variables are bounded; see Corollary 3). Under this assumption, the heuristic approximately minimizes $f(\boldsymbol{z})$ by iteratively minimizing a quadratic approximation of $f(\boldsymbol{z})$ at $\hat{\boldsymbol{z}}$, namely $f(\boldsymbol{z}) \approx \|\boldsymbol{z} - \boldsymbol{l}_{\hat{\boldsymbol{z}}}\|_2^2$.

This idea is algorithmized as follows: given a sparsity pattern $\boldsymbol{z} \in \mathcal{Z}_k^n$ and an optimal sparse portfolio $\boldsymbol{x}^\star(\boldsymbol{z})$, the method iteratively solve the following problem, which ranks the differences between each securities contribution to the portfolio, $x_i^\star(\boldsymbol{z})$, and its gradient $g_{\boldsymbol{z},i}$:

$$\boldsymbol{z}_{\text{new}} := \arg\min_{\boldsymbol{z} \in \mathcal{Z}_k^n} \left\| \boldsymbol{z} - \boldsymbol{x}^\star(\boldsymbol{z}_{\text{old}}) + \frac{1}{L}\boldsymbol{g}_{\boldsymbol{z}_{\text{old}}} \right\|_2^2. \tag{25}$$

Note that, given $\boldsymbol{z}_{\text{old}}$, $\boldsymbol{z}_{\text{new}}$ can be obtained by simply setting $z_i = 1$ for the k indices where $\left|x_i^\star(\boldsymbol{z}_{\text{old}}) + \frac{1}{L} g_{\boldsymbol{z}_{\text{old}}}\right|$ is largest. We formalize this warm-start procedure in Algorithm 2.

Some remarks on the algorithm are now in order:

- In our numerical experiments, we run Algorithm 2 from five different randomly generated k-sparse binary vectors, to increase the probability that it identifies a high-quality solution.
- Averaging the dual multipliers across iterations, as suggested in the pseudocode, improves the method's performance; note that the contribution of each $\boldsymbol{w}_t$ to $\boldsymbol{w}^\star$ is $\frac{1}{t}\prod_{i=t+1}^{r}\frac{i-1}{i} = \frac{1}{r}$.
- In our numerical experiments, we pass Algorithm 2's output to `CPLEX`, which does not check whether there exists a feasible $\boldsymbol{x}_t$ associated with $\boldsymbol{z}_t$, or whether $\boldsymbol{z}_t$ is infeasible. As injecting an infeasible warm-start may cause `CPLEX` to fail to converge, we test feasibility by generating a cut at $\boldsymbol{z}_t$ before commencing outer-approximation. If the corresponding dual subproblem is unbounded then $\boldsymbol{z}_t$ is infeasible by weak duality and we refrain from injecting the warm-start.

Algorithm 2 A discrete ADMM heuristic (see Bertsekas 1999, Bertsimas et al. 2016).

$t \leftarrow 1$

$\boldsymbol{z}_1 \leftarrow$ randomly generated k-sparse binary vector.

while $\boldsymbol{z}_t != \boldsymbol{z}_{t-1}$ **and** $t < T$ **do**

Set $\boldsymbol{w}_t^\star$ optimal solution to:

$$\max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^r,\ \boldsymbol{w}\in\mathbb{R}^n,\\ \boldsymbol{\beta}_l,\ \boldsymbol{\beta}_u\in\mathbb{R}^m_+,\ \lambda\in\mathbb{R}}} \quad -\frac{1}{2}\boldsymbol{\alpha}^\top\boldsymbol{\alpha} - \frac{\gamma}{2}\sum_i z_{i,t} w_i^2 + \boldsymbol{y}^\top\boldsymbol{\alpha} + \boldsymbol{\beta}_l^\top \boldsymbol{l} - \boldsymbol{\beta}_u^\top \boldsymbol{u} + \lambda$$
$$\text{s.t.} \quad \boldsymbol{w} \geq \boldsymbol{X}^\top\boldsymbol{\alpha} + \boldsymbol{A}^\top(\boldsymbol{\beta}_l - \boldsymbol{\beta}_u) + \lambda\boldsymbol{e} - \boldsymbol{d}.$$

Average multipliers via $\boldsymbol{w}^\star \leftarrow \frac{1}{t}\boldsymbol{w}_t^\star + \frac{t-1}{t}\boldsymbol{w}^\star$.

Set $g_{\boldsymbol{z},i} = \frac{-\gamma}{2} w_i^{\star 2},\ \forall i \in [n]$.

Set $x_{i,t} = \gamma w_i^\star,\ \forall i \in [n] : z_i = 1$.

Set $\boldsymbol{z}_{t+1}$ optimal solution to

$$\min_{\boldsymbol{z}\in\mathcal{Z}_k^n} \left\| \boldsymbol{z} - \boldsymbol{x}_t + \frac{1}{L}\boldsymbol{g}_{\boldsymbol{z}_t} \right\|_2^2$$

$t \leftarrow t+1$

end while

return $\boldsymbol{z}_t$

4.2. Improving the Lower Bound: A Second Order Cone Relaxation

In financial applications, we sometimes require a certifiably near-optimal solution quickly but do not have time to verify optimality. Therefore, we now turn our attention to deriving near-exact polynomial-time lower bounds. Immediately, we see that we obtain a valid lower bound by relaxing the constraint $\boldsymbol{z} \in \mathcal{Z}_k^n$ to $\boldsymbol{z} \in \text{Conv}(\mathcal{Z}_k^n)$ in Problem (4). By invoking strong duality, we now demonstrate that this lower bound can be obtained by solving a single second order cone problem[7].

Theorem 3. *Suppose that Problem* (4) *is feasible. Then, the following three optimization problems attain the same optimal value:*

$$\min_{\boldsymbol{z}\in\text{Conv}\left(\mathcal{Z}_k^n\right)} \max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^r,\ \boldsymbol{w}\in\mathbb{R}^n,\\ \boldsymbol{\beta}_l,\ \boldsymbol{\beta}_u\in\mathbb{R}^m_+,\ \lambda\in\mathbb{R}}} \quad -\frac{1}{2}\boldsymbol{\alpha}^\top\boldsymbol{\alpha} - \frac{\gamma}{2}\sum_i z_i w_i^2 + \boldsymbol{y}^\top\boldsymbol{\alpha} + \boldsymbol{\beta}_l^\top \boldsymbol{l} - \boldsymbol{\beta}_u^\top \boldsymbol{u} + \lambda$$
$$s.t. \quad \boldsymbol{w} \geq \boldsymbol{X}^\top\boldsymbol{\alpha} + \lambda\boldsymbol{e} + \boldsymbol{A}^\top(\boldsymbol{\beta}_l - \boldsymbol{\beta}_u) - \boldsymbol{d}. \tag{26}$$

$$\max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^r,\ \boldsymbol{v}\in\mathbb{R}^n_+,\ \boldsymbol{w}\in\mathbb{R}^n,\\ \boldsymbol{\beta}_l,\ \boldsymbol{\beta}_u\in\mathbb{R}^m_+,\ \lambda\in\mathbb{R},\ t\in\mathbb{R}_+}} \quad -\frac{1}{2}\boldsymbol{\alpha}^\top\boldsymbol{\alpha} + \boldsymbol{y}^\top\boldsymbol{\alpha} + \boldsymbol{\beta}_l^\top \boldsymbol{l} - \boldsymbol{\beta}_u^\top \boldsymbol{u} + \lambda - \boldsymbol{e}^\top\boldsymbol{v} - kt$$
$$s.t. \quad \boldsymbol{w} \geq \boldsymbol{X}^\top\boldsymbol{\alpha} + \lambda\boldsymbol{e} + \boldsymbol{A}^\top(\boldsymbol{\beta}_l - \boldsymbol{\beta}_u) - \boldsymbol{d}, \tag{27}$$
$$v_i \geq \frac{\gamma}{2} w_i^2 - t, \quad \forall i \in [n].$$

$$\begin{aligned}\min_{\boldsymbol{z}\in \mathrm{Conv}\left(\mathcal{Z}_k^n\right)} \min_{\boldsymbol{x}\in\mathbb{R}_+^n, \boldsymbol{\theta}\in\mathbb{R}_+^n} \quad & \frac{1}{2}\|\boldsymbol{X}\boldsymbol{x}-\boldsymbol{y}\|_2^2+\frac{1}{2\gamma}\boldsymbol{e}^\top\boldsymbol{\theta}+\boldsymbol{d}^\top\boldsymbol{x} \\ s.t. \quad & \boldsymbol{l}\le \boldsymbol{A}\boldsymbol{x}\le \boldsymbol{u},\ \boldsymbol{e}^\top\boldsymbol{x}=1,\ \left\|\begin{pmatrix}2x_i\\ \theta_i-z_i\end{pmatrix}\right\|_2 \le \theta_i+z_i, \forall i\in[n].\end{aligned} \tag{28}$$

Proof of Theorem 3 Problem (26) is strictly feasible, since the interior of $\mathrm{Conv}(\mathcal{Z}_k^n)$ is non-empty and $\boldsymbol{w}$ can be increased without bound. Therefore, the Sion-Kakutani minimax theorem (Ben-Tal and Nemirovski 2001, Appendix D.4.) holds, and we can exchange the minimum and maximum operators in Problem (26), to yield:

$$\begin{aligned}\max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^r,\ \boldsymbol{w}\in\mathbb{R}^n,\\ \boldsymbol{\beta}_l,\ \boldsymbol{\beta}_u\in\mathbb{R}_+^m,\ \lambda\in\mathbb{R}}} \quad & -\frac{1}{2}\boldsymbol{\alpha}^\top\boldsymbol{\alpha}+\boldsymbol{y}^\top\boldsymbol{\alpha}+\boldsymbol{\beta}_l^\top\boldsymbol{l}-\boldsymbol{\beta}_u^\top\boldsymbol{u}+\lambda-\frac{\gamma}{2}\max_{\boldsymbol{z}\in\mathrm{Conv}\left(\mathcal{Z}_k^n\right)}\sum_i z_i w_i^2 \\ \text{s.t.} \quad & \boldsymbol{w}\ge \boldsymbol{X}^\top\boldsymbol{\alpha}+\lambda\boldsymbol{e}+\boldsymbol{A}^\top(\boldsymbol{\beta}_l-\boldsymbol{\beta}_u)-\boldsymbol{d}.\end{aligned} \tag{29}$$

Next, fixing $\boldsymbol{w}$ and applying strong duality between the inner primal problem:

$$\max_{\boldsymbol{z}\in\mathrm{Conv}\left(\mathcal{Z}_k^n\right)}\sum_i \frac{\gamma}{2}z_i w_i^2 = \max_{\boldsymbol{z}} \sum_i \frac{\gamma}{2}z_i w_i^2 \quad \text{s.t. } \boldsymbol{0}\le\boldsymbol{z}\le\boldsymbol{e},\ \boldsymbol{e}^\top\boldsymbol{z}\le k,$$

and its dual problem:

$$\min_{\boldsymbol{v}\in\mathbb{R}_+^n, t\in\mathbb{R}_+} \boldsymbol{e}^\top\boldsymbol{v}+kt \text{ s.t. } v_i+t\ge\frac{\gamma}{2}w_i^2, \forall i\in[n]$$

proves that strong duality holds between Problems (26)-(27).

Next, we observe that Problems (27)-(28) are dual, as can be seen by applying the relation

$$bc\ge a^2, b, c\ge 0 \iff \left\|\begin{pmatrix}2a\\ b-c\end{pmatrix}\right\|\le b+c$$

to rewrite Problem (27) as an SOCP in standard form, and applying SOCP duality (see, e.g., Boyd and Vandenberghe 2004, Exercise 5.43). Moreover, since Problem (27) is strictly feasible (as $\boldsymbol{v}$, $\boldsymbol{w}$ are unbounded from above) strong duality must hold between these problems. □

REMARK 2. We recognize Problem (28) as a perspective relaxation of Problem (4) (see Günlük and Linderoth 2012, for a survey). As perspective relaxations are often near-exact in practice (Frangioni and Gentile 2006, 2009) this explains why the SOCP bound is high-quality.

We now derive conditions under which Problem (27) provides an optimal solution to Problem (4) apriori (proof deferred to Appendix C). A similar condition for sparse regression problems has previously been derived in (Pilanci et al. 2015, Proposition 1) (see also Bertsimas et al. 2019b).

COROLLARY 4. **A sufficient condition for support recovery**

Let there exist some $\boldsymbol{z}\in\mathcal{Z}_k^n$ and set of dual multipliers $(\boldsymbol{v}^\star, \boldsymbol{w}^\star, \boldsymbol{\alpha}^\star, \boldsymbol{\beta}_l^\star, \boldsymbol{\beta}_u^\star, \lambda^\star)$ which solve Problem (27)*, such that these two quantities collectively satisfy the following conditions:*

$$\begin{aligned} \gamma \sum_i z_i w_i^\star &= 1, \\ \boldsymbol{l} \leq \gamma \sum_i \boldsymbol{A}_i w_i^\star z_i &\leq \boldsymbol{u}, \\ z_i w_i &\geq 0, \ \forall i \in [n], \\ v_i^\star = 0, \ \forall i \in [n] \ s.t. \ z_i &= 0. \end{aligned} \tag{30}$$

Then, Problem (27)*'s lower bound is exact. Moreover, let* $|w^\star|_{[k]}$ *denote the kth largest entry in* $\boldsymbol{w}^\star$ by absolute magnitude*. If* $|w^\star|_{[k]} > |w^\star|_{[k+1]}$ *in Problem* (27) *then setting*

$$z_i = 1, \ \forall i : |w_i^\star| \geq |w^\star|_{[k]},$$

$$z_i = 0, \ \forall i : |w_i^\star| < |w^\star|_{[k]}$$

supplies a $\boldsymbol{z} \in \mathcal{Z}_k^n$ *which satisfies the above condition and hence solves Problem* (4)*.*

When $\boldsymbol{\Sigma}$ is a diagonal matrix, $\boldsymbol{\mu}$ is a multiple of $\boldsymbol{e}$ and the system $\boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u}$ is empty, Theorem 3 can be applied to solve Problem (4) in closed form (proof deferred to Appendix C.5).

After the first iteration of this work, Bertsimas et al. (2019a) established a similar result for a general class of mixed-integer optimization problems with logical constraints, and demonstrated that randomly rounding solutions to Problem (28) according to $z_i^\star \sim \text{Bernoulli}(z_i)$ supplies certifiably near-optimal warm-starts. By invoking the probabilistic method, their result can be used to bound the size of the SOCP gap between Problem (4) and Problem (28) in terms of the problem data and the number of strictly fractional entries in Problem (28).

4.3. An Improved Cutting-Plane Method

We close this section by combining Algorithm 1 with the improvements discussed in this section, to obtain an efficient numerical approach to Problem (4), which we present in Algorithm 3. Note that we use the larger of θ_t and the SOCP lower bound in our termination criterion, as the SOCP gap is sometimes less than ϵ.

Figure 1 depicts the method's convergence on the problem *port2* with a cardinality value $k = 5$ and a minimum return constraint, as described in Section 5.1. Note that we did not use the SOCP lower bound when generating this plot; the SOCP lower bound is 0.009288 in this plot, and Algorithm 3 requires $1,225$ cuts to improve upon this bound.

5. Computational Experiments on Real-World Data

In this section, we evaluate our outer-approximation method, implemented in `Julia` 1.1 using the `JuMP.jl` package version 0.18.5 (Dunning et al. 2017) and solved using `CPLEX` version 12.8.0

Algorithm 3 A refined cutting-plane method for Problem (4).

Require: Initial warm-start solution $\boldsymbol{z}_1$

$t \leftarrow 1$

Set θ_{SOCP} optimal objective value of Problem (27)

repeat

Compute $\boldsymbol{z}_{t+1}, \theta_{t+1}$ solution of

$$\min_{\boldsymbol{z} \in \mathcal{Z}_k^n, \theta} \theta \quad \text{s.t. } \theta \geq f(\boldsymbol{z}_i) + g_{\boldsymbol{z}_i}^\top (\boldsymbol{z} - \boldsymbol{z}_i), \ \forall i \in [t].$$

Compute $f(\boldsymbol{z}_{t+1})$ and $g_{\boldsymbol{z}_{t+1}} \in \partial f(\boldsymbol{z}_{t+1})$

$t \leftarrow t+1$

until $f(\boldsymbol{z}_t) - \max(\theta_t, \theta_{\text{SOCP}}) \leq \varepsilon$

return $\boldsymbol{z}_t$

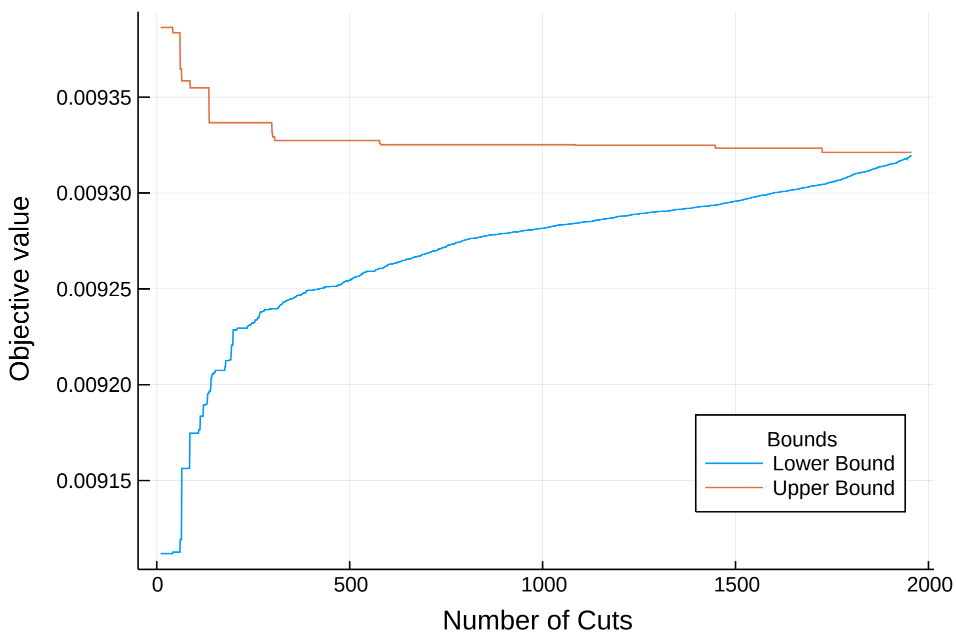


Figure 1 Convergence of Algorithm 3 on the OR-library problem *port2* with a minimum return constraint and a cardinality constraint $\|\boldsymbol{x}\|_0 \leq 5$. The behaviour shown here is typical.

for the master problems, and `Mosek` version 9.0 for the continuous quadratic subproblems. We compare the method against big-M and MISOCP formulations of Problem (4), solved in `CPLEX`.

All experiments were performed on a MacBook Pro with a 2.9GHz i9 CPU and 16GB 2400 MHz DDR4 Memory. As `JuMP.jl` is currently not thread-safe and `CPLEX` cannot combine multiple threads with `lazy constraint callbacks` when using `JuMP.jl`, we run all methods on one thread. We use default `CPLEX` parameters.

In the following numerical experiments, we solve the following optimization problem, which places a multiplier κ on the return term but is mathematically equivalent to Problem (4):

$$\min_{\boldsymbol{x}\in\mathbb{R}^n_+} \ \frac{1}{2}\boldsymbol{x}^\top\boldsymbol{\Sigma}\boldsymbol{x}+\frac{1}{2\gamma}\|\boldsymbol{x}\|_2^2-\kappa\boldsymbol{\mu}^\top\boldsymbol{x} \text{ s.t. } \boldsymbol{l}\leq\boldsymbol{A}\boldsymbol{x}\leq\boldsymbol{u},\ \boldsymbol{e}^\top\boldsymbol{x}=1,\ \|\boldsymbol{x}\|_0\leq k. \tag{31}$$

We either take $\kappa=0$ or $\kappa=1$, depending on whether we are penalizing low expected return portfolios in the objective or constraining the portfolios expected return.

We aim to answer the following questions:

1. How does Algorithm 3 compare to existing state-of-the-art solution methods?
2. How do constraints affect Algorithm 3's scalability?
3. How does Algorithm 3 scale as a function of the number of securities in the buyable universe?
4. How sensitive are optimal solutions to Problem (4) to the hyperparameters κ,γ,k?

5.1. A Comparison Between Algorithm 3 and State-of-the-Art Methods

We now present a direct comparison of Algorithm 3 with `CPLEX` version 12.8.0, where `CPLEX` uses both big-M and MISOCP formulations of Problem (4). Note that the MISOCP formulation which we pass directly to `CPLEX` is (c.f. Aktürk et al. 2009, Günlük and Linderoth 2012):

$$\min_{\boldsymbol{z}\in\mathcal{Z}^n_k,\boldsymbol{x}\in\mathbb{R}^n_+,\boldsymbol{\theta}\in\mathbb{R}^n_+} \ \frac{1}{2}\boldsymbol{x}^\top\boldsymbol{\Sigma}\boldsymbol{x}+\frac{1}{2\gamma}\boldsymbol{e}^\top\boldsymbol{\theta}-\boldsymbol{\mu}^\top\boldsymbol{x} \text{ s.t. } \boldsymbol{l}\leq\boldsymbol{A}\boldsymbol{x}\leq\boldsymbol{u},\ \boldsymbol{e}^\top\boldsymbol{x}=1,\ \left\|\begin{pmatrix}2x_i\\ \theta_i-z_i\end{pmatrix}\right\|_2\leq\theta_i+z_i,\forall i\in[n]. \tag{32}$$

We compare the three approaches in two distinct situations. First, when no constraints are applied and the system $\boldsymbol{l}\leq\boldsymbol{A}\boldsymbol{x}\leq\boldsymbol{u}$ is empty, and second when a minimum return constraint is applied, i.e., $\boldsymbol{\mu}^\top\boldsymbol{x}\geq\bar{r}$. In the former case we set $\kappa=1$, while in the later case we set $\kappa=0$ and similarly to Zheng et al. (2014) we set $\bar{r}$ in the following manner: Let

$$r_{\min}=\boldsymbol{\mu}^\top\boldsymbol{x}_{\min} \text{ where } \boldsymbol{x}_{\min}=\arg\min_{\boldsymbol{x}}\frac{1}{2}\boldsymbol{x}^\top(\frac{1}{\gamma}+\boldsymbol{\Sigma})\boldsymbol{x} \text{ s.t. } \boldsymbol{e}^\top\boldsymbol{x}=1,\boldsymbol{x}\geq\boldsymbol{0},$$

$$r_{\max}=\boldsymbol{\mu}^\top\boldsymbol{x}_{\max} \text{ where } \boldsymbol{x}_{\max}=\arg\max_{\boldsymbol{x}}\boldsymbol{\mu}^\top\boldsymbol{x}-\frac{1}{2\gamma}\boldsymbol{x}^\top\boldsymbol{x} \text{ s.t. } \boldsymbol{e}^\top\boldsymbol{x}=1,\boldsymbol{x}\geq\boldsymbol{0}$$

and set $\bar{r}=r_{\min}+0.3(r_{\max}-r_{\min})$.

Table 3 (resp. Table 4) depicts the time required for all 3 approaches to determine an optimal allocation of funds without (resp. with) the minimum return constraint. The problem data is taken from the 5 mean-variance portfolio optimization problems described by Chang et al. (2000) and subsequently included in the OR-library test set (Beasley 1990). Note that we turned off the SOCP lower bound for these tests, and ensured feasibility in the master problem by imposing

$$\sum_{i\in[n]:\mu_i\geq\bar{r}} z_i\geq 1$$

when running Algorithm 3 on the instances with a minimum return constraint (see Section 3.2). Furthermore, as Algorithm 3 is slow to converge for some instances with a return constraint, we also run the method after applying 50 cuts at the root node, generated using the `in-out` method (see Appendix E, for the relevant pseudocode).

Table 3 Runtime in seconds per approach with $\kappa = 1$, $\gamma = \frac{100}{\sqrt{n}}$ and no constraints in the system $\boldsymbol{l} \leq \boldsymbol{Ax} \leq \boldsymbol{u}$. We impose a time limit of 300s and run all approaches on one thread. If a solver fails to converge, we report the number of explored nodes at the time limit.

Problem	n	k	Algorithm 3			CPLEX Big-M		CPLEX MISOCP	
			Time	Nodes	Cuts	Time	Nodes	Time	Nodes
port 1	31	5	0.17	0	4	1.98	31,640	**0.03**	0
		10	0.16	0	4	1.11	16,890	**0.01**	0
		20	0.14	0	4	**0.01**	108	0.03	0
port 2	85	5	**0.01**	0	4	>300	1,968,000	0.11	0
		10	**0.01**	0	4	>300	2,818,000	0.12	0
		20	**0.01**	0	4	>300	3,152,000	0.29	0
port 3	89	5	**0.01**	0	8	>300	2,113,000	0.38	0
		10	**0.01**	0	4	>300	2,873,000	0.41	0
		20	**0.02**	0	4	>300	2,998,000	0.11	0
port 4	98	5	**0.03**	0	8	>300	1,888,000	0.41	0
		10	**0.02**	0	8	>300	2,457,000	2.74	3
		20	**0.03**	0	9	>300	2,454,000	0.38	0
port 5	225	5	**0.15**	0	9	>300	676,300	11.17	9
		10	**0.02**	0	4	>300	926,600	3.04	0
		20	**0.03**	0	7	>300	902,100	2.88	0

Table 4 indicates that some instances of *port2-port4* cannot be solved to certifiable optimality by any approach within an hour, in the presence of a minimum return constraint. Nonetheless, both Algorithm 3 and `CPLEX`'s MISOCP method obtain solutions which are certifiably within 1% of optimality very quickly. Indeed, Table 5 depicts the bound gaps of all 3 approaches at 120s on these problems; Algorithm 3 never has a bound gap larger than 0.5%.

The experimental results illustrate that our approach is several orders of magnitude more efficient than the big-M approach on all problems considered, and is typically more efficient than the MISOCP approach. Moreover, our approach's edge over `CPLEX` increases with the problem size.

Our main findings from this set of experiments are as follows:

1. For problems with unit simplex constraints, big-M approaches do not scale to real-world problem sizes in the presence of ridge regularization, because they cannot exploit the ridge regularizer and therefore obtain low-quality lower bounds, even after expanding a large number of nodes. This poor performance is due to the ridge regularizer; the big-M approach typically exhibits better performance than this in numerical studies done without a regularizer.

Table 4 Runtime in seconds per approach with $\kappa = 0$, $\gamma = \frac{100}{\sqrt{n}}$ and a minimum return constraint $\boldsymbol{\mu}^\top \boldsymbol{x} \geq \bar{r}$. We impose a time limit of 3600s and run all approaches on one thread. If a solver fails to converge, we report the number of explored nodes at the time limit.

Problem	n	k	Algorithm 3			Algorithm 3+in-out			CPLEX Big-M		CPLEX MISOCP	
			Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes	Time	Nodes
port 1	31	5	**0.22**	161	32	0.23	113	19	9.32	119,200	0.83	47
		10	**0.20**	159	28	0.25	86	25	1970	30,430,000	0.84	44
		20	0.16	0	7	0.16	0	4	258.4	4,966,000	**0.05**	0
port 2	85	5	48.29	73,850	1,961	**31.47**	42,950	1,272	$>3,600$	15,020,000	91.98	1,163
		10	807.3	243,500	6,433	891.97	255,200	6,019	$>3,600$	20,890,000	**82.44**	902
		20	**10.52**	12,260	1,224	13.0	13,650	1,350	$>3,600$	21,060,000	24.54	210
port 3	89	5	175.2	132,700	3,187	**151.1**	96,010	2,345	$>3,600$	14,680,000	213.3	2,528
		10	$>3,600$	439,400	9,851	$>3,600$	490,400	11,310	$>3,600$	20,710,000	**531.3**	5,776
		20	119.5	65,180	4,473	60.03	40,240	3,275	$>3,600$	22,240,000	**21.32**	170
port 4	98	5	2,690	479,700	11,320	**2,475**	499,700	11,040	$>3,600$	12,426,000	2779	25,180
		10	$>3,600$	311,200	12,400	$>3,600$	320,700	14,790	$>3,600$	20,950,000	$>3,600$	30,190
		20	1,638	241,600	10,710	2,067	279,500	12,760	$>3,600$	21,470,000	**148.9**	1,115
port 5	225	5	0.85	1,489	202	**0.40**	560	74	$>3,600$	5,000,000	28.3	22
		10	0.60	73	41	**0.03**	2	5	$>3,600$	8,989,000	3.33	0
		20	0.39	63	52	**0.08**	0	11	$>3,600$	10,960,000	115.02	90

Table 5 Bound gap at 120s per approach with $\kappa = 0$, $\gamma = \frac{100}{\sqrt{n}}$ and a minimum return constraint $\boldsymbol{\mu}^\top \boldsymbol{x} \geq \bar{r}$. We run all approaches on one thread.

Problem	n	k	Algorithm 3			Algorithm 3+in-out			CPLEX Big-M		CPLEX MISOCP	
			Gap (%)	Nodes	Cuts	Gap (%)	Nodes	Cuts	Gap (%)	Nodes	Gap (%)	Nodes
port 2	85	5	0	73,850	1,961	0	42,950	1,272	84.36	611,500	0	1,163
		10	0.26	90,670	3,463	0.15	72,240	3,366	425.2	1,057,000	0	902
		20	0	12,260	1,224	0	13,650	1,350	65.96	1,367,000	0	210
port 3	89	5	0.1	123,100	2,308	0.08	78,950	2,137	88.48	634,300	0.27	1,247
		10	0.29	65,180	4,473	0.21	62,840	3,503	452.4	1,073,000	0.19	1,246
		20	0	60,090	3,237	0	40,240	3,275	67.55	1,280,000	0	170
port 4	98	5	0.18	55,460	3,419	0.37	53,780	3,648	87.67	541,800	0.60	888
		10	0.46	51,500	3,704	0.29	46,700	3,241	84.22	1,018,000	0.29	977
		20	0.17	57,990	3,393	0.13	59,820	3,886	71.42	1,163,000	0.05	846

2. MISOCP approaches perform competitively, and are often a computationally reasonable approach for small to medium sized instances of Problem (4), as they are easy to implement and typically have bound gaps of $< 1\%$ in instances where they fail to converge within the time budget.

3. Varying the cardinality of the optimal portfolio does not affect solve times substantially without a minimum return constraint, although it has a nonlinear effect with this constraint.

For the rest of the paper, we do not consider big-M formulations of Problem (4), as they do not scale to larger problems with 200 or more securities in the universe of buyable assets.

5.2. Benchmarking Algorithm 3 in the Presence of Minimum Investment Constraints

In this section, we explore Algorithm 3's scalability in the presence of minimum investment constraints, by solving the problems generated by Frangioni and Gentile (2006) and subsequently solved by Frangioni and Gentile (2007, 2009), Zheng et al. (2014) among others[8]. These problems have minimum investment, maximum investment, and minimum return constraints, which render many entries in $\mathcal{Z}_k^n$ infeasible. Therefore, to avoid generating an excessive number of feasibility cuts, we use the copy of variables technique suggested in Section 3.2.

Additionally, as the covariance matrices in these problems are highly diagonally dominant (with much larger on-diagonal entries than off-diagonal entries), the method does not converge quickly if we do not extract any diagonal dominance. Indeed, Appendix D.1 shows that the method often fails to converge within 600s for the problems studied in this section when we do not extract a diagonally dominant term. Therefore, we first preprocess the covariance matrices to extract more diagonal dominance, as discussed in Section 3.2. Note that we need not actually solve any SDOs to preprocess the data, as high quality diagonal matrices for this problem data have been made publicly available by Frangioni et al. (2017) at http://www.di.unipi.it/optimize/Data/MV/diagonals.tgz (specifically, we use the entries in the "s" folder of this repository). After reading in their diagonal matrix $\boldsymbol{D}$, we replace $\boldsymbol{\Sigma}$ with $\boldsymbol{\Sigma}-\boldsymbol{D}$ and use the regularizer γ_i for each index i, where

$$\gamma_i = \left(\frac{1}{\gamma} + D_{i,i}\right)^{-1}.$$

We now compare the times for Algorithm 3 and `CPLEX`'s MISOCP routines to solve the diagonally dominant instances in the dataset generated by Frangioni and Gentile (2006), along with a variant of Algorithm 3 where we use the `in-out` method at the root node, and another variant where we apply the `in-out` method at both the root node and 50 leaf nodes. In all cases, we take $\gamma = \frac{1000}{\sqrt{n}}$, which ensures that $\gamma_i \approx \frac{1}{D_{i,i}}$. Table 6 depicts the average time taken by each approach, and demonstrates that Algorithm 3 substantially outperforms `CPLEX`, particularly for problems without a cardinality constraint. We provide the full instance-wise results pertaining to this dataset in Appendix D.1.

Our main findings from this experiment are as follows:

- Algorithm 3 outperforms `CPLEX` in the presence of minimum investment constraints, possibly because the master problems solved by Algorithm 3 are cardinality constrained LOs, rather than SOCPs, and therefore the method can quickly expand larger branch-and-bound trees.
- Running the `in-out` method at the root node improves solve times when $k \geq 10$, but does more harm than good when $k < 10$, because in the later case Algorithm 3 already performs well.
- Running the `in-out` method at leaf nodes does more harm than good for easy problems, but improves solve times for larger problems (400+ with $k \in \{8, 10\}$), as reported in Appendix D.1.

Table 6 Average runtime in seconds per approach with $\kappa = 0$, $\gamma = \frac{1000}{\sqrt{n}}$ for the problems generated by Frangioni and Gentile (2006). We impose a time limit of 600s and run all approaches on one thread. If a solver fails to converge, we report the number of explored nodes at the time limit, use 600s in lieu of the solve time, and report the number of failed instances (out of 10) next to the solve time in brackets.

Problem	k	Algorithm 3			Algorithm 3 + in-out			Algorithm 3 in-out + 50			CPLEX MISOCP	
		Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes
200+	6	**1.55**	1,298	236.3	1.77	1,262	209.4	7.4	910.4	118	87.74 (0)	95.3
200+	8	**1.95**	1,968	260.3	2.30	1,626	217	7.97	949.1	97.3	73.42 (0)	79.8
200+	10	7.74	7,606	509.7	**4.33**	3,686	298.9	10.35	2,066	175.5	161.9 (0)	184
200+	12	25.57	28,830	203.8	**2.06**	1,764	71.6	9.04	1,000	33.9	353.1 (4)	398.1
200+	200	18.71	23,190	208.4	**2.79**	2,288	92	10	1,394	56.1	599.3 (9)	735.1
300+	6	**16.83**	9,141	974.2	23.59	8,025	864.1	29.92	5,738	565.9	434.5 (3)	157.6
300+	8	**44.68**	21,050	1,577	64.46	19,682	1457.8	61.0	14,236	1,036	489.5 (5)	174.0
300+	10	88.57	44,160	1,901	**78.05**	33,253	1438.4	110.2	24,487	971.5	472.0 (5)	171.9
300+	12	16.16	13,880	262.7	**4.65**	3,181	127.4	15.94	1475	66.7	401.5 (4)	158.2
300+	300	21.36	18,140	262.1	**9.24**	6,288	191.9	24.33	5,971	168.4	600.0 (10)	219.2
400+	6	**54.47**	13,330	1,717	66.52	12,160	1,619	85.51	11,070	1,402	531.7 (8)	84.0
400+	8	173.8	35,390	2,828	**160.9**	32,930	2,709	163.3	28,020	2,363	534.0 (8)	80.8
400+	10	158.0	55,490	1,669	104.5	32,314	1369.7	**81.48**	22,130	824.9	517.9 (8)	74.8
400+	12	3.97	4,324	116.6	**1.9**	1,214	48.6	15.67	627.4	29.8	478.0 (4)	75.3
400+	400	8.68	7,540	120.5	**5.19**	3,539	88.8	21.31	3,210	79.4	600.0 (10)	74.2

- With a cardinality constraint, Algorithm 3's solve times are comparable to those reported by Zheng et al. (2014). Without a cardinality constraint, our solve times are an order of magnitude faster than Zheng et al. (2014)'s, and comparable to those reported by Frangioni et al. (2016).
- As shown in Appendix D.1, applying the diagonal dominance preprocessing technique proposed by Frangioni and Gentile (2007) yields faster solve times than applying the technique proposed by Zheng et al. (2014), even though the later technique yields tighter continuous relaxations (Zheng et al. 2014). This might occur because Frangioni and Gentile (2007)'s technique prompts our approach to make better branching decisions and/or Zheng et al. (2014)'s approach is only guaranteed to yield tighter continuous relaxations before (i.e. not after) branching.

5.3. Exploring the Scalability of Algorithm 3

In this section, we explore Algorithm 3's scalability with respect to the number of securities in the buyable universe, by measuring the time required to solve several large-scale sparse portfolio selection problems to provable optimality: the S&P 500, the Russell 1000, and the Wilshire 5000. In all three cases, the problem data is taken from daily closing prices from January 3 2007 to December 29 2017, which are obtained from Yahoo! Finance via the R package *quantmod* (see Ryan and Ulrich (2018)), and rescaled to correspond to a holding period of one month. We apply Singular Value Decomposition to obtain low-rank estimates of the correlation matrix, and rescale the low-rank correlation matrix by each asset's variance to obtain a low-rank covariance matrix $\boldsymbol{\Sigma}$. We also omit days with a greater than 20% change in closing prices when computing the mean and covariance for the Russell 1000 and Wilshire 5000, since these changes occur on low-volume trading and typically reverse the next day.

Tables 7—9 depict the times required for Algorithm 3 and `CPLEX MISOCP` to solve the problem to provable optimality for different choices of γ, k, and $\text{Rank}(\boldsymbol{\Sigma})$. In particular, they depict the time taken to solve (a) an unconstrained problems where $\kappa = 1$ and (b) a constrained problem where $\kappa = 0$ containing a minimum return constraint computed in the same fashion as in Section 5.1.

Table 7 Runtimes in seconds per approach for the S&P 500 with $\kappa = 1$ (left); $\kappa = 0$ and a minimum return constraint (right), a one-month holding period and a runtime limit of 600s. For instances with a minimum return constraint where $\gamma = \frac{100}{\sqrt{n}}$, we run the in-out method at the root node before running Algorithm 3. We run all approaches on one thread. When a method fails to converge, we report the bound gap at 600s.

γ	$\text{Rank}(\boldsymbol{\Sigma})$	k	Algorithm 3			CPLEX MISOCP		Algorithm 3			CPLEX MISOCP	
			Time	Nodes	Cuts	Time	Nodes	Time	Nodes	Cuts	Time	Nodes
$\frac{1}{\sqrt{n}}$	50	10	0.01	0	4	0.54	0	0.01	0	3	73.28	210
		50	0.02	0	4	0.49	0	0.28	108	45	78.59	499
		100	0.03	0	4	1.00	0	0.05	7	7	0.97	0
		200	0.06	0	4	0.86	0	0.08	1	5	53.53	300
$\frac{1}{\sqrt{n}}$	100	10	0.01	0	4	1.49	0	2.01	972	344	339.8	420
		50	0.02	0	4	1.36	0	0.32	104	41	283.8	410
		100	0.04	0	4	1.30	0	0.06	5	7	286.2	520
		200	0.09	0	4	3.10	0	0.06	0	3	472.7	990
$\frac{1}{\sqrt{n}}$	150	10	0.01	0	4	2.61	0	3.96	1,633	410	268.3	157
		50	0.03	0	4	2.23	0	0.29	62	33	265.6	200
		100	0.06	0	4	4.71	0	0.07	0	6	394.9	340
		200	0.14	0	4	4.80	0	0.13	0	3	6.20	0
$\frac{1}{\sqrt{n}}$	200	10	0.01	0	4	2.74	0	5.20	2,804	450	345.0	171
		50	0.03	0	4	3.14	0	0.49	86	47	337.7	210
		100	0.06	0	4	17.27	3	0.15	5	8	104.2	40
		200	0.13	0	4	105.2	60	0.10	0	3	46.18	10
$\frac{100}{\sqrt{n}}$	50	10	0.01	0	4	0.51	0	0.09%	70,200	3,855	0.10%	1,600
		50	0.02	0	4	1.14	0	0.77	309	113	268.5	841
		100	0.03	0	4	0.68	0	0.09	0	8	1.66	0
		200	0.07	0	4	1.04	0	0.16	0	4	15.26	10
$\frac{100}{\sqrt{n}}$	100	10	0.01	0	4	1.30	0	0.26%	54,000	4,721	0.24%	598
		50	0.03	0	4	3.48	0	0.07	1	7	0.28%	291
		100	0.06	0	5	5.93	0	0.11	0	4	0.29%	352
		200	0.13	0	5	2.16	0	0.14	0	5	301.3	380
$\frac{100}{\sqrt{n}}$	150	10	0.02	0	4	2.00	0	0.33%	46,720	4,437	0.28%	345
		50	0.04	0	4	34.57	20	0.09	0	6	0.28%	291
		100	0.06	0	4	27.76	20	0.11	0	4	0.29%	352
		200	0.10	0	4	26.93	20	0.35	0	6	344.3	270
$\frac{100}{\sqrt{n}}$	200	10	0.02	0	4	7.77	0	0.45%	56,100	4,336	0.36%	280
		50	0.04	0	4	48.75	20	0.20	1	19	0.35%	256
		100	0.10	0	5	44.02	20	0.15	0	5	0.0	0
		200	0.16	0	4	36.57	20	0.18	0	4	76.80	10

Table 8 Runtimes in seconds per approach for the Russell 1000 with $\kappa = 1$ (left); $\kappa = 0$ and a minimum return constraint (right), a one-month holding period and a runtime limit of 600s. For instances with a minimum return constraint, we run the in-out method at the root node before running Algorithm 3. We run all approaches on one thread. When a method fails to converge, we report the bound gap at 600s.

γ	Rank($\boldsymbol{\Sigma}$)	k	Algorithm 3			CPLEX MISOCP		Algorithm 3			CPLEX MISOCP	
			Time	Nodes	Cuts	Time	Nodes	Time	Nodes	Cuts	Time	Nodes
$\frac{1}{\sqrt{n}}$	50	10	0.02	0	6	7.77	3	12.38	2467	316	0.01%	545
		50	0.06	0	12	9.19	7	0.32	0	7	0.01%	900
		100	0.04	0	5	0.92	0	0.81	10	14	0.01%	1,048
		200	0.07	0	5	1.83	0	0.46	1	14	0.01%	1,043
$\frac{1}{\sqrt{n}}$	100	10	0.03	3	7	13.27	5	272.3	49,200	1,266	0.01%	400
		50	0.09	2	12	154.0	90	1.32	10	13	0.01%	400
		100	0.05	0	5	2.83	0	15.52	5,271	250	0.01%	599
		200	0.14	0	8	335.9	260	2.12	111	64	0.01%	399
$\frac{1}{\sqrt{n}}$	200	10	0.05	2	10	41.08	7	24.14	8,200	318	31.20%	138
		50	0.16	8	14	344.0	60	0.01%	86,020	1,433	0.02%	100
		100	0.08	0	5	60.54	10	4.88	131	41	0.01%	100
		200	0.16	0	5	6.79	0	0.01%	64,600	1,049	4.00%	100
$\frac{1}{\sqrt{n}}$	300	10	0.06	1	10	175.9	15	9.00	1,200	246	0.01%	70
		50	0.16	2	13	323.3	31	0.02%	61,100	1,227	63.35%	78
		100	0.16	0	8	260.4	30	0.02%	48,550	856	3.01%	64
		200	0.31	0	8	0.01%	464	0.01%	29,480	786	6.00%	75
$\frac{100}{\sqrt{n}}$	50	10	0.04	1	11	7.58	3	0.59%	62,050	2,553	0.39%	700
		50	0.04	0	9	2.34	0	0.61%	114,000	1,531	0.32%	837
		100	0.36	0	4	2.57	0	112.1	42,661	787	0.12%	993
		200	0.09	0	5	1.25	0	0.40	0	19	135.4	220
$\frac{100}{\sqrt{n}}$	100	10	0.03	2	9	11.50	5	0.77%	69,800	2,599	0.55%	400
		50	0.06	0	8	65.82	40	0.68%	93,580	1,472	0.38%	400
		100	0.06	0	5	22.82	10	0.43%	82,500	1,359	0.46%	470
		200	0.11	0	5	42.68	30	0.34	0	13	0.37%	400
$\frac{100}{\sqrt{n}}$	200	10	0.06	1	10	31.33	0	0.84%	84,617	2,183	1.23%	126
		50	0.10	1	10	164.4	30	1.55%	99,600	1,576	1.31%	100
		100	0.08	0	4	71.91	10	0.92%	69,850	1,279	9.36%	118
		200	0.16	0	5	50.98	10	0.35	1	10	2.20%	123
$\frac{100}{\sqrt{n}}$	300	10	0.06	1	12	134.1	15	0.94%	72,400	2,759	1.00%	65
		50	0.10	0	8	207.7	20	1.78%	58,740	1,363	48.31%	62
		100	0.10	0	4	544.3	50	1.16%	55,810	1,027	14.40%	61
		200	0.20	0	5	221.4	30	1.04%	61,410	1,122	2.92%	61

Our main finding from this set of experiments is that Algorithm 3 is substantially faster than `CPLEX`'s MISOCP routine, particularly as the rank of $\boldsymbol{\Sigma}$ increases. The relative numerical success of Algorithm 3 in this section, compared to the previous section, can be explained by the differences in the problems solved: (a) in this section, we optimize over a sparse unit simplex, while in the previous section we optimized over minimum-return and minimum-investment constraints, (b) in this section, we use data taken directly from stock markets, while in the previous section we used less realistic synthetic data, which evidently made the problem harder.

Table 9 Runtimes in seconds per approach for the Wilshire 5000 with $\kappa = 1$ (left); $\kappa = 0$ and a minimum return constraint (right), a one-month holding period and a runtime limit of 600s. For instances with a minimum return constraint where $\gamma = \frac{100}{\sqrt{n}}$, we run the in-out method at the root node before running Algorithm 3. We run all approaches on one thread. When a method fails to converge, we report the bound gap at 600s (using the symbol "-" to denote that a method failed to produce a feasible solution).

γ	Rank($\boldsymbol{\Sigma}$)	k	Algorithm 3			CPLEX MISOCP		Algorithm 3			CPLEX MISOCP	
			Time	Nodes	Cuts	Time	Nodes	Time	Nodes	Cuts	Time	Nodes
$\frac{1}{\sqrt{n}}$	100	10	0.04	0	4	15.07	0	1.95	0	2	50.0%	122
		50	0.07	0	10	244.8	29	2.32	0	2	32.0%	132
		100	0.22	0	4	30.08	2	0.59	10	9	62.0%	127
		200	0.24	0	4	40.54	3	0.27	0	6	44.5%	100
$\frac{1}{\sqrt{n}}$	200	10	0.07	0	6	70.12	2	2.34	0	8	30.0%	43
		50	0.08	0	8	392.5	25	5.54	31	17	74.0%	40
		100	0.08	0	5	0.01%	91	1.70	0	12	62.0%	44
		200	0.25	0	4	49.26	0	0.01%	8,451	361	41.5%	40
$\frac{1}{\sqrt{n}}$	500	10	0.15	10	11	0.01%	13	10.53	300	66	–	5
		50	0.54	0	8	0.01%	30	0.01%	49,000	805	–	6
		100	0.20	0	6	492.7	3	0.01%	36,670	1,068	–	5
		200	0.57	0	5	0.01%	20	3.41	0	14	–	5
$\frac{1}{\sqrt{n}}$	1,000	10	0.48	35	28	0.01%	9	0.01%	40,500	1,130	–	2
		50	1.08	20	29	0.01%	9	0.02%	56,800	937	–	2
		100	0.44	0	7	0.01%	11	0.02%	25,040	523	–	2
		200	0.56	0	4	0.01%	10	2.61	1	12	–	2
$\frac{100}{\sqrt{n}}$	100	10	0.03	0	5	29.30	2	0.28%	24,870	1,178	50.1%	91
		50	0.04	0	5	39.08	3	0.38%	45,810	636	62.1%	82
		100	0.07	0	5	200.0	11	0.12%	55,700	912	45.1%	80
		200	0.10	0	10	99.07	10	0.49	0	10	22.1%	91
$\frac{100}{\sqrt{n}}$	200	10	0.06	0	8	56.48	2	0.38%	34,100	1,071	–	29
		50	0.08	0	7	78.00	3	0.47%	40,340	1,034	66.1%	30
		100	0.20	0	5	0.01%	20	0.43%	15,010	325	45.1%	33
		200	0.14	0	4	224.4	10	0.98	6	10	20.1%	30
$\frac{100}{\sqrt{n}}$	500	10	0.15	5	13	0.01%	16	0.52%	32,920	1,235	–	4
		50	0.08	0	4	0.01%	6	1.11%	65,560	771	–	3
		100	0.27	0	8	0.01%	10	0.79%	23,540	651	–	2
		200	0.30	0	4	0.01%	10	0.52	0	6	–	2
$\frac{100}{\sqrt{n}}$	1,000	10	0.48	29	32	0.17%	10	1.02%	6,7600	1,108	–	2
		50	0.26	0	8	0.01%	9	1.74%	33,930	1,122	–	0
		100	0.56	0	8	0.01%	9	1.85%	53,500	804	–	2
		200	0.66	0	4	0.01%	9	1.28	1	7	–	2

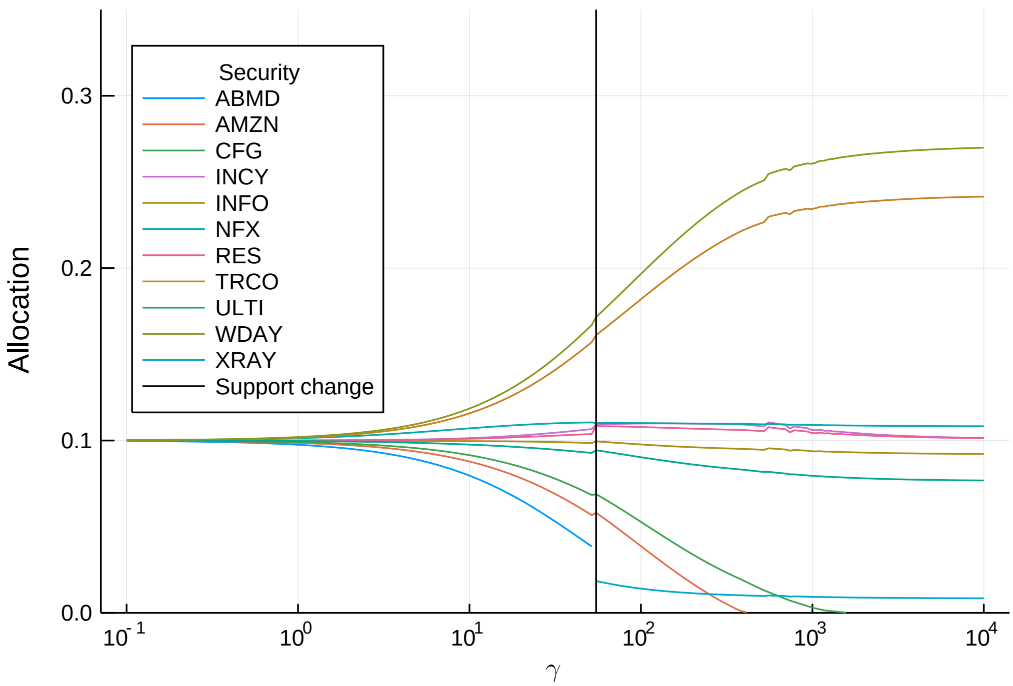
5.4. Exploring Sensitivity to Hyperparameters

Our next experiment explores Problem (4)'s stability to changes in its hyperparameters γ and k. The first experiment studies $\boldsymbol{x}^\star$'s sensitivity to γ for a rank-300 approximation of the Russell 1000 with a one month holding period, a sparsity budget $k = 10$ and a weight $\kappa = 1$.

Figure 2 depicts the relationship between $\boldsymbol{x}^\star$ and γ for this set of hyperparameters, and indicates that $\boldsymbol{x}^\star$ is stable with respect to small changes in γ. Moreover, the optimal support indices when

γ is small are near-optimal when γ is large. This suggests that a good strategy for cross-validating γ could be to solve Problem (4) to certifiable optimality for one value of γ, find the best value of γ conditional on using these support indices, and finally resolve Problem (4) with the optimal γ.

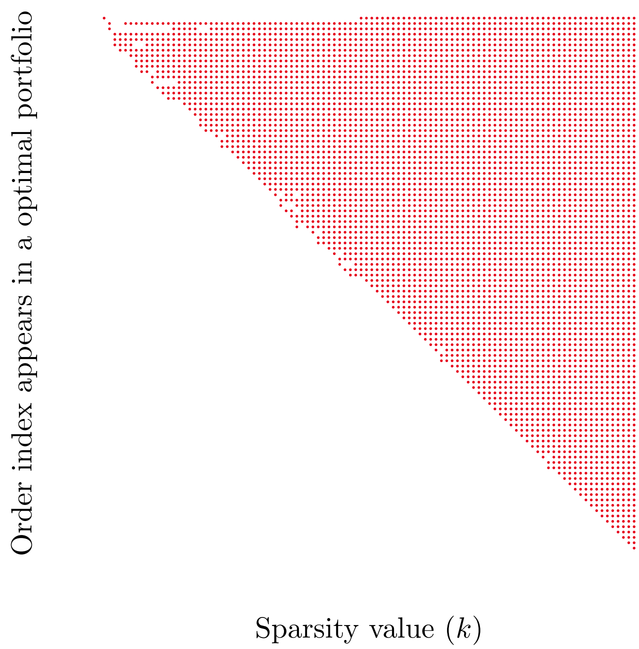
Figure 2 Sensitivity to γ for the Russell 1000 with $\kappa = 1$ and $k = 10$. The optimal security indices $\boldsymbol{z}^\star$ changed once over the entire range of γ.



Our second experiment studies Problem (4)'s sensitivity to changes in the sparsity budget k with $\gamma = \frac{1}{\sqrt{n}}$, $\kappa = 1/5$ and the same problem data as the previous experiment. In this experiment, incrementing the sparsity constraint results in the optimal allocation of funds $\boldsymbol{x}^\star$ changing whenever the sparsity constraint is binding. Therefore, we consider changes in $\boldsymbol{z}^\star$ rather than $\boldsymbol{x}^\star$ when performing the sensitivity analysis, and take the view that Problem (4) is stable with respect to changes in k if $\boldsymbol{z}^\star$ does not change too much. This is a reasonable perspective when changes in k correspond to investing funds from a new investor.

To this end, we compute the optimal security indices $i : z_i^\star = 1$ for each $k \in [100]$ and plot the sparsity patterns against the order in which security indices are first selected in an optimal solution as we increase k. In the resulting plot, an upper diagonal matrix would indicate that incrementing k by 1 results in the same securities selected as for an optimal k-sparse portfolio, plus one new security. Figure 3 depicts the resulting sparsity pattern, and suggests that the heuristic of ranking securities by the order in which they first appear in a sparsity pattern is near-optimal (since the matrix is very nearly upper triangular).

Figure 3 Sparsity pattern by k for the Russell 1000 with $\kappa = 1/5$, $\gamma = \frac{1}{\sqrt{n}}$, sorted by the order the indices first appear in an optimal solution.



5.5. Summary of Findings From Numerical Experiments

We are now in a position to answer the four questions introduced at the start of this section. Our findings are as follows:

1. In the absence of complicating constraints, Algorithm 3 is substantially more efficient than state-of-the-art MIQO solvers such as `CPLEX`. This efficiency improvement can be explained by (a) our ability to generate stronger and more informative lower bounds via dual subproblems, and (b) our dual representation of the problems subgradients. Indeed, the method did not require more than one second to solve any of the constraint-free problems considered here, although this phenomenon can be partially attributed to the problem data used.

2. Although imposing complicating constraints, such as minimum investment constraints, slows Algorithm 3, the method performs competitively in the presence of these constraints. Moreover, running the `in-out` cutting-plane method at the root node substantially reduces the initial bound gap, and allows the method to supply a certifiably near-optimal (if not optimal) solution in seconds.

3. Algorithm 3 scales to solve real-world problem instances which comprise selecting assets from universes with 1,000s of securities, such as the Russell 1000 and the Wilshire 5000, while existing state-of-the-art approaches such as `CPLEX` either solve these problems much more slowly or do not successfully solve them, because they cannot attain sufficiently strong lower bounds quickly.

4. Solutions to Problem (4) are stable with respect to the hyperparameters κ and γ. Moreover, while for small values of k optimal solutions are unstable to changes in the sparsity budget, for

$k \geq 20$ the optimal indices for a $(k+1)$-sparse portfolio typically correspond to those for a k-sparse portfolio, plus one additional security.

6. Conclusion and Extensions

This paper describes a scalable algorithm for solving quadratic optimization problems subject to sparsity constraints, and applies it to the problem of sparse portfolio selection. Although sparse portfolio selection is NP-hard, and therefore considered to be intractable, our algorithm provides provably optimal portfolios even when the number of securities is in the $1,000$s.

After this paper was first submitted, Atamturk and Gomez (2019) derived a family of convex relaxations for sparse regression problems which are provably at least as tight as, and often strictly tighter than, the Boolean relaxation derived by Bertsimas and Van Parys (2019) for sparse regression problems, which corresponds to Problem (27) here (see Atamturk and Gomez 2019, pp. 17). A very interesting extension to this paper would be to combine the scalability of our approach with the tightness of the aforementioned work. Unfortunately, we cannot directly develop a scalable outer-approximation approach from Atamturk and Gomez (2019)'s formulation, because (a) the resulting continuous relaxations are SDOs and intractable when $n > 100$ with current technology and (b) it is optimization folklore that MISDO branch-and-cut schemes are notoriously difficult to implement efficiently, because interior point methods currently cannot benefit from warm-starts. Nonetheless, it seems possible that most of the tightness of their relaxation could be retained by taking an appropriate SOCP outer-approximation of their formulation (see, e.g. Ahmadi and Majumdar 2019, Bertsimas and Cory-Wright 2019) and re-imposing integrality *ex-post*.

Endnotes

1. To our knowledge, the Wilshire 5000 index, which contains around $3,200$ frequently traded securities, is the largest index by number of securities. As portfolio optimization problems generally involve optimizing over securities within an index, we have written $3,200$ here as an upper bound, although one could conceivably also optimize over securities from multiple stock indices.

2. As Bonami and Lejeune (2009) constrain the minimum number of sectors invested in, we report this in lieu of a cardinality constraint.

3. Indeed, if all securities are i.i.d. then investing $\frac{1}{k}$ in k randomly selected securities constitutes an optimal solution to Problem (2), but, as proven in Bienstock (2010), branch-and-bound must expand $2^{\frac{n}{10}}$ nodes to improve upon a naive sparsity-constraint free bound by 10%, and expand all 2^n nodes to certify optimality.

4. To see this, observe that applying OA with this formulation comprises using the dual multipliers on the constraint $\boldsymbol{x} \leq \boldsymbol{z}$ as subgradients. From the primal-dual KKT conditions, we can see that if $z_i = 0$ then, in general, there are multiple optimal choices of the ith multiplier. Moreover, as we

usually have $\boldsymbol{e}^\top \boldsymbol{z} = k$ and $\boldsymbol{e}^\top \boldsymbol{x} = 1$ at optimality, each non-zero x_i is usually strictly less than z_i, and dual multipliers are usually 0 at active indices. The resulting degeneracy often causes OA to converge extremely slowly.

5. Note that weaker continuous relaxations may in fact perform better after branching.

6. An alternative approach which could also be useful is to observe that if a dual subproblem is unbounded then there exists some set of dual variables which give a certificate of unboundedness

$$-\frac{1}{2}\hat{\boldsymbol{\alpha}}^\top \hat{\boldsymbol{\alpha}} - \frac{\gamma}{2}\sum_i z_i \hat{w}_i^2 + \boldsymbol{y}^\top \hat{\boldsymbol{\alpha}} + \hat{\boldsymbol{\beta}}_l^\top \boldsymbol{l} - \hat{\boldsymbol{\beta}}_u^\top \boldsymbol{u} + \hat{\lambda} > 0.$$

Therefore, a valid feasibility cut is

$$-\frac{1}{2}\hat{\boldsymbol{\alpha}}^\top \hat{\boldsymbol{\alpha}} + \boldsymbol{y}^\top \hat{\boldsymbol{\alpha}} + \hat{\boldsymbol{\beta}}_l^\top \boldsymbol{l} - \hat{\boldsymbol{\beta}}_u^\top \boldsymbol{u} + \hat{\lambda} \leq \frac{\gamma}{2}\sum_i z_i \hat{w}_i^2.$$

This is essentially the feasibility cut generated by a Generalized Benders approach (Geoffrion 1972).

7. Strictly speaking, Problem (27) is actually a convex QCQP rather than a SOCP. However, by exploiting the well-known relationship (see, e.g., Boyd and Vandenberghe 2004, Exercise 4.26)

$$bc \geq a^2, b, c \geq 0 \iff \left\| \begin{pmatrix} 2a \\ b-c \end{pmatrix} \right\| \leq b + c$$

we can see that Problem (27) can be rewritten as an equivalent SOCP.

8. This problem data is available at www.di.unipi.it/optimize/Data/MV.html

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Appendix A: Robustness Properties of the Model

In this Appendix, we demonstrate that Problem (4) is highly related to a robust optimization problem, by demonstrating that augmenting Problem (4) with an l_2, rather than l_2^2 regularizer, is equivalent to robustifying Problem (4) with an ellipsoidal uncertainty set:

Theorem 4. *The following two optimization problems are equivalent:*

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \max_{\boldsymbol{\Delta}:\|\boldsymbol{\Delta\mu}\|_2\leq\frac{1}{2\gamma}} \quad \frac{\sigma}{2}\boldsymbol{x}^\top\boldsymbol{\Sigma x}-(\boldsymbol{\mu}+\Delta\boldsymbol{\mu})^\top\boldsymbol{x} \text{ s.t. } \boldsymbol{l}\leq\boldsymbol{Ax}\leq\boldsymbol{u},\ \boldsymbol{e}^\top\boldsymbol{x}=1,\ \boldsymbol{x}\geq\boldsymbol{0},\ \|\boldsymbol{x}\|_0\leq k, \tag{33a}$$

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \quad \frac{\sigma}{2}\boldsymbol{x}^\top\boldsymbol{\Sigma x}+\frac{1}{2\gamma}\|\boldsymbol{x}\|_2-\boldsymbol{\mu}^\top\boldsymbol{x} \text{ s.t. } \boldsymbol{l}\leq\boldsymbol{Ax}\leq\boldsymbol{u},\ \boldsymbol{e}^\top\boldsymbol{x}=1,\ \boldsymbol{x}\geq\boldsymbol{0},\ \|\boldsymbol{x}\|_0\leq k. \tag{33b}$$

Proof of Theorem 4 This result follows from applying Lagrangian duality and manipulating Problem (33a)'s KKT conditions. □

Theorem 4 demonstrates that the ridge-regularized Markowitz portfolio model is almost a robust optimization problem (but not quite, for ridge regularization involves an l_2^2 norm, not an l_2 norm).

Appendix B: NP-Hardness Properties of the Model

In this Appendix, we provide a more general set of conditions under which Problem 2 is NP-hard than is, to our knowledge, currently available in the literature. As our results are-to a large extent-direct corollaries of (Gao and Li 2013, Lemma 1), it could be argued that these results are already known. However, as they have not yet been explicitly stated, we now state them for completeness.

Our first result demonstrates that eliciting a sparse minimum variance portfolio is NP-hard, both with and without a non-negativity constraint:

LEMMA 3. *Let $\mathbf{\Sigma} \succ \mathbf{0}$ be a positive definite matrix. Then, the following two optimization problems are NP-hard:*

$$\min_{\boldsymbol{x} \in \mathbb{R}^n} \quad \boldsymbol{x}^\top \mathbf{\Sigma} \boldsymbol{x} \ s.t.\ \boldsymbol{e}^\top \boldsymbol{x} = 1,\ \|\boldsymbol{x}\|_0 \leq k. \tag{34}$$

$$\min_{\boldsymbol{x} \in \mathbb{R}^n_+} \quad \boldsymbol{x}^\top \mathbf{\Sigma} \boldsymbol{x} \ s.t.\ \boldsymbol{e}^\top \boldsymbol{x} = 1,\ \|\boldsymbol{x}\|_0 \leq k. \tag{35}$$

Proof of Lemma 3 The NP-hardness of Problem (34) is explicitly shown in (Gao and Li 2013, Section E.C.1), who reduce the K-SUBSET VECTOR-PROBLEM (see Garey and Johnson 2002) to Problem (34). Moreover, as the reduction of K-SUBSET VECTOR-SUM to Problem (34) in (Gao and Li 2013, Section E.C.1) uses binary variables, the reduction holds when Problem (34) is augmented with a non-negativity constraint. Therefore, Problem (35) is also NP-hard. □

REMARK 3. Lemma 3 demonstrates that Problem (4)'s difficulty is due to both minimizing a quadratic form under a sparsity constraint, and the constraints $\boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u}$. This situation is quite different to the results given in (Gao and Li 2013, Lemma 1) and (Bienstock 1996, Theorem 1), which *only* establish that the constraints $\boldsymbol{l} \leq \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{u}$ are a source of NP-hardness, by respectively establishing that Problem (4) is NP-hard under a constraint on the Portfolio's expected return, and when $\boldsymbol{A}$ has at least 3 rows.

In retrospect, the NP-hardness of minimizing a quadratic form over a sparsity-constrained simplex should not be surprising. Indeed, sparse regression (i.e., a special case of Problems (34)-(35) without constraints), is strongly NP-hard (see Chen et al. 2019, Theorem 1), and therefore we should anticipate that convex quadratic optimization over a sparse unit simplex is also NP-hard. $\triangleleft$

Appendix C: Omitted Proofs

In this section, we supply the omitted proofs of results stated in the manuscript, in the order in which the results were stated.

C.1. Proof of Lemma 1

Proof of Lemma 1 It suffices to show that for each solution to (15) there exists a feasible solution to Problem (16) with an equal or lower cost, and vice versa.

Let $(\boldsymbol{x}, \boldsymbol{z})$ be a feasible solution to Problem (15), and let us set $\hat{\boldsymbol{x}} := \boldsymbol{x} \circ \boldsymbol{z}$. Then $(\hat{\boldsymbol{x}}, \boldsymbol{z})$ is feasible in Problem (16), because $z_i^2 = z_i$ implies $\boldsymbol{Z}^2 \boldsymbol{x} = \boldsymbol{Z}\boldsymbol{x}$. Moreover, $(\hat{\boldsymbol{x}}, \boldsymbol{z})$ has the same cost in Problem (16) as $(\boldsymbol{x}, \boldsymbol{z})$ does in Problem (15), because $\boldsymbol{x}^\top \boldsymbol{Z} \boldsymbol{x} = \boldsymbol{x}^\top \boldsymbol{Z}^2 \boldsymbol{x} = \hat{\boldsymbol{x}}^\top \hat{\boldsymbol{x}}$.

Alternatively, let $(\boldsymbol{x}, \boldsymbol{z})$ be a feasible solution to Problem (15). Then, $(\boldsymbol{x}, \boldsymbol{z})$ is feasible in (16), and takes an equal or lower cost, since $\boldsymbol{z} \leq \boldsymbol{e}$ implies $\boldsymbol{x}^\top \boldsymbol{Z} \boldsymbol{x} \leq \boldsymbol{x}^\top \boldsymbol{x}$. □

C.2. Proof of Lemma 2

Proof of Lemma 2 By Lemma 1, both problems attain the same optimal value. Moreover, the feasible regions for both problems are identical, and invariant under the transformation $\boldsymbol{x} \leftarrow \boldsymbol{x} \circ \boldsymbol{z}$. Therefore, given an optimal solution to one problem, it suffices to show that the candidate solution attains the same cost in the second problem.

Let $(\boldsymbol{x}^\star, \boldsymbol{z}^\star)$ solve Problem (15). Then, $(\boldsymbol{x}^\star \circ \boldsymbol{z}^\star, \boldsymbol{z}^\star)$ solves Problem (16), because $\boldsymbol{x}^\top \boldsymbol{Z} \boldsymbol{x} = \boldsymbol{x}^\top \boldsymbol{Z}^2 \boldsymbol{x}$ and therefore both solutions have the same cost.

Alternatively, let $(\boldsymbol{x}^\star, \boldsymbol{z}^\star)$ solve Problem (16). Then, $\boldsymbol{x}_i^\star = 0$ for each index i such that $\boldsymbol{z}_i^\star = 0$, as otherwise $(\boldsymbol{x}^\star \circ \boldsymbol{z}^\star, \boldsymbol{z}^\star)$ is a feasible solution with a strictly lower cost, which contradicts the optimality of $(\boldsymbol{x}^\star, \boldsymbol{z}^\star)$. As $\boldsymbol{z}^\star$ is binary, this implies that $\boldsymbol{x}^\star = \boldsymbol{x}^\star \circ \boldsymbol{z}^\star$, which in turn implies $\boldsymbol{x}^{\star\top} \boldsymbol{x}^\star = \boldsymbol{x}^{\star\top} \boldsymbol{Z}^\star \boldsymbol{x}^\star$. Therefore, $(\boldsymbol{x}^\star, \boldsymbol{z}^\star)$ has the same cost in Problem (15), and hence is optimal.

$\square$

C.3. Proof of Corollary 3

Proof of Corollary 3 This result follows from applying the lower approximation

$$f(\hat{\boldsymbol{z}}) \geq f(\boldsymbol{z}) + \boldsymbol{g}_{\boldsymbol{z}}^\top (\hat{\boldsymbol{z}} - \boldsymbol{z}),$$

re-arranging to yield

$$f(\boldsymbol{z}) - f(\hat{\boldsymbol{z}}) \leq -\boldsymbol{g}_{\boldsymbol{z}}^\top (\hat{\boldsymbol{z}} - \boldsymbol{z})$$

and invoking Corollary 2 to rewrite the right-hand-side in the desired form. $\square$

C.4. Proof of Corollary 4

Proof of Corollary 4 Let there exist some $(\boldsymbol{v}^\star, \boldsymbol{w}^\star, \boldsymbol{\alpha}^\star, \boldsymbol{\beta}_l^\star, \boldsymbol{\beta}_u^\star, \lambda^\star)$ which solve Problem (27), and binary vector $\boldsymbol{z} \in \mathcal{Z}_k^n$, such that these two quantities collectively satisfy the conditions encapsulated in Expression (30). Then, this optimal solution to Problem (27) provides the following lower bound for Problem (4):

$$-\frac{1}{2}\boldsymbol{\alpha}^{*\top}\boldsymbol{\alpha}^\star + \boldsymbol{y}^\top \boldsymbol{\alpha}^\star + \boldsymbol{\beta}_l^{*\top} \boldsymbol{l} - \boldsymbol{\beta}_u^{*\top} \boldsymbol{u} + \lambda^\star - \boldsymbol{e}^\top \boldsymbol{v}^\star - kt^\star.$$

Moreover, let $\hat{\boldsymbol{x}}$ be a candidate solution to Problem (4) defined by $\hat{x}_i := \gamma w_i z_i$. Then, $\hat{\boldsymbol{x}}$ is feasible for Problem (4), since $\boldsymbol{l} \leq A\hat{\boldsymbol{x}} \leq \boldsymbol{u}$, $\boldsymbol{e}^\top \hat{\boldsymbol{x}} = 1$, $\hat{\boldsymbol{x}} \geq \boldsymbol{0}$ and $\|\hat{\boldsymbol{x}}\|_0 \leq k$ by Expression (30) and the definition of $\boldsymbol{z}$. Moreover, the construction of $\hat{\boldsymbol{x}}$ via the dual problem's KKT conditions imply that Problem (4)'s objective when $\boldsymbol{x} = \hat{\boldsymbol{x}}$ is given by:

$$-\frac{1}{2}\boldsymbol{\alpha}^{*\top}\boldsymbol{\alpha}^\star + \boldsymbol{y}^\top \boldsymbol{\alpha}^\star + \boldsymbol{\beta}_l^{*\top} \boldsymbol{l} - \boldsymbol{\beta}_u^{*\top} \boldsymbol{u} + \lambda^\star - \frac{1}{2\gamma}\hat{\boldsymbol{x}}^\top \hat{\boldsymbol{x}},$$

which is less than or equal to Problem (27)'s objective, since $v_i^\star = 0 \ \forall i \in [n]$ s.t. $z_i = 0$.

Finally, let $|w^\star|_{[k]} > |w^\star|_{[k+1]}$ and let S denote the set of indices such that $|w_i^\star| \geq |w^\star|_{[k]}$. Then, as the primal-dual KKT conditions for max-k norms (see, e.g., Zakeri et al. 2014, Lemma 1) imply that an optimal choice of t is given by $t^\star = \frac{\gamma}{2} w_{[k]}^{\star 2}$, we can set $t^\star = \frac{\gamma}{2} w_{[k]}^{\star 2}$ without loss of generality (after adjusting $v^\star$ appropriately). Note that, in general, this choice is not unique. Indeed, any $t \in [\frac{\gamma}{2} w_{[k+1]}^\star, \frac{\gamma}{2} w_{[k]}^\star]$ constitutes an optimal choice (Zakeri et al. 2014).

We then have that $v_i^\star = 0, \forall i \notin S$, which implies that the constraint $v_i + t \geq \frac{\gamma}{2} w_i^2$ holds strictly for any $i \notin S$. Therefore, the dual multipliers associated with these constraints must take value 0. But this constraints dual multipliers are precisely $\boldsymbol{z} \in \mathrm{Conv}(\mathcal{Z}_k^n)$, which implies that $z_i = 1, \forall i \in S$ gives a valid set of dual multipliers. Moreover, by Equation (19), setting $\boldsymbol{x}_i = \gamma z_i w_i^\star$ supplies an optimal (and thus feasible) choice of $\boldsymbol{x}$ for this fixed $\boldsymbol{z}$. Therefore, this primal-dual pair satisfies Equation (30). $\square$

C.5. An Application of Theorem 3

We now apply Theorem 3 to prove that if $\boldsymbol{\Sigma}$ is a diagonal matrix, $\boldsymbol{\mu}$ is a multiple of the vector of all 1's and the matrix $\boldsymbol{A}$ is empty then Problem (4) is solvable in closed-form. Let us first observe that under these conditions Problem (4) is equivalent to

$$\min \quad \sum_i \frac{1}{2\gamma_i} x_i^2 \text{ s.t. } \boldsymbol{e}^\top \boldsymbol{x} = 1, \boldsymbol{x} \geq \boldsymbol{0}, \|\boldsymbol{x}\|_0 \leq k.$$

We now have the following result:

Corollary 5. *Let $0 < \gamma_1 \leq \gamma_2 \leq ... \gamma_n$. Then, strong duality holds between the problem*

$$\min \quad \sum_i \frac{1}{2\gamma_i} x_i^2 \textit{ s.t. } \boldsymbol{e}^\top \boldsymbol{x} = 1, \boldsymbol{x} \geq \boldsymbol{0}, \|\boldsymbol{x}\|_0 \leq k \tag{36}$$

and its SOCP relaxation:

$$\begin{aligned} \max_{\substack{\boldsymbol{v} \in \mathbb{R}_n^+,\ \boldsymbol{w} \in \mathbb{R}^n, \\ \lambda \in \mathbb{R},\ t \in \mathbb{R}_+}} \quad & \lambda - \boldsymbol{e}^\top \boldsymbol{v} - kt \\ \textit{s.t.} \quad & \boldsymbol{w} \geq \lambda \boldsymbol{e}, \\ & v_i \geq \frac{\gamma_i}{2} w_i^2 - t, \quad \forall i \in [n]. \end{aligned} \tag{37}$$

Moreover, an optimal solution to Problem (36) *is $x_i = \frac{\gamma_i}{\sum_{i=1}^k \gamma_i}$ for $i \leq k$, $x_i = 0$ for $i > k$.*

Proof of Corollary 5 By Theorem 3, a valid lower bound to Problem (36) is given by the SOCP:

$$\begin{aligned} \max_{\substack{\boldsymbol{v} \in \mathbb{R}_n^+,\ \boldsymbol{w} \in \mathbb{R}^n, \\ \lambda \in \mathbb{R},\ t \in \mathbb{R}_+}} \quad & \lambda - \boldsymbol{e}^\top \boldsymbol{v} - kt \\ \text{s.t.} \quad & \boldsymbol{w} \geq \lambda \boldsymbol{e}, \\ & v_i \geq \frac{\gamma_i}{2} w_i^2 - t, \quad \forall i \in [n]. \end{aligned} \tag{38}$$

Let us assume that $\lambda^\star \geq 0$ (otherwise the objective value cannot exceed 0, which is certainly suboptimal). Then, we can let the constraint $w_i \geq \lambda$ be binding without loss of optimality. This allows us to simplify this problem to:

$$\begin{aligned} \max_{\substack{\boldsymbol{v}\in\mathbb{R}^+_n,\ \boldsymbol{w}\in\mathbb{R}^n,\\ \lambda\in\mathbb{R},\ t\in\mathbb{R}+}} \quad & \lambda - \boldsymbol{e}^\top \boldsymbol{v} - kt \\ \text{s.t.} \quad & v_i \geq \frac{\gamma_i}{2}\lambda^2 - t, \quad \forall i \in [n]. \end{aligned} \tag{39}$$

The KKT conditions for max-k norms (see, e.g., Zakeri et al. 2014, Lemma 1) then reveal that an optimal choice of t is given by the kth largest value of $\frac{\gamma_i}{2}\lambda^2$, i.e., $t^\star = \frac{\gamma_k}{2}\lambda^2$ and an optimal choice of v_i is given by $v_i = \max\left(\frac{\gamma_i}{2}\lambda^2 - t, 0\right)$, i.e.,

$$v_i^\star = \begin{cases} \frac{\gamma_i - \gamma_k}{2}\lambda^2, & \forall i \leq k, \\ v_i = 0, & \forall i > k. \end{cases}$$

Substituting these terms into the objective function gives an objective of

$$\lambda - \sum_{i=1}^k \frac{\gamma_i}{2}\lambda^2,$$

which implies that an optimal choice of λ is $\lambda = \frac{1}{\sum_{i=1}^k \gamma_i}$. Next, substituting the expression $\lambda = \frac{1}{\sum_{i=1}^k \gamma_i}$ into the objective function gives an objective value of $\frac{\lambda}{2}$, which implies that a lower bound on Problem (36)'s objective is $\frac{1}{2\sum_{i=1}^k \gamma_i}$.

Finally, we construct a primal solution via $z_i = 1, \forall i \leq k$, and the primal-dual KKT condition $x_i = \gamma_i z_i w_i = \gamma_i z_i \lambda = \frac{\gamma_i z_i}{\sum_{i=1}^k \gamma_i}$. This is feasible, by inspection. Moreover, it has an objective value of

$$\sum_{i=1}^k \frac{1}{2\gamma_i}\left(\gamma_i \lambda\right)^2 = \frac{\lambda}{2}\sum_{i=1}^k \gamma_i \lambda = \frac{\lambda}{2},$$

and therefore is optimal.

□

Appendix D: Supplementary Experimental Results

D.1. Supplementary Results on Problems With Minimum Investment Constraints

We now present the instance-wise runtimes (in seconds) for all instances generated by Frangioni and Gentile (2006), in Tables 10-12.

Table 10 Performance of the outer-approximation method vs. CPLEX's MISOCP method on the 200^{+} instances generated by Frangioni and Gentile (2006), with a time budget of 600s per approach, $\kappa=0$, $\gamma=\frac{1000}{\sqrt{n}}$. We run all approaches on one thread.

Problem	k	Algorithm 3			Algorithm 3 + in-out			Algorithm 3 + in-out + 50			CPLEX MISOCP	
		Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes
pard200-1	6	0.74	674	126	1.61	832	162	10.80	248	36	28.54	33
pard200-1	8	1.10	1,038	188	2.00	1,140	220	12.95	488	60	30.63	33
pard200-1	10	8.73	8,844	654	8.58	6,582	494	12.44	2,838	180	65.04	69
pard200-1	12	1.37	1,902	136	1.05	1,079	74	7.84	532	29	130.9	122
pard200-1	nc	1.66	3,026	123	1.58	1,182	101	9.68	928	79	>600	624
pard200-2	6	0.13	141	24	0.16	81	10	3.21	42	5	33.26	37
pard200-2	8	0.36	327	59	0.28	117	23	5.19	64	11	35.90	29
pard200-2	10	4.19	6,313	317	4.07	4,449	243	10.62	2,530	144	278.6	331
pard200-2	12	0.65	1,953	20	0.42	187	8	7.94	182	7	>600	775
pard200-2	nc	0.7	1,716	24	0.53	233	11	7.37	184	10	>600	800
pard200-3	6	0.87	904	158	0.81	740	96	6.55	413	40	103.7	103
pard200-3	8	0.67	818	98	0.82	671	84	6.54	343	40	85.76	81
pard200-3	10	2.45	4,584	189	1.45	1,444	90	8.28	840	42	210.9	215
pard200-3	12	1.71	3,034	42	0.78	923	23	7.75	461	9	>600	648
pard200-3	nc	1.21	2,803	38	0.65	781	21	8.68	416	9	>600	688
pard200-4	6	1.53	2,096	262	2.31	1,740	227	8.34	1,529	193	230.3	248
pard200-4	8	2.73	3,820	343	2.82	3,055	260	9.50	1,740	139	176.1	194
pard200-4	10	10.83	14,200	647	10.82	11,380	522	17.9	7,912	446	527.5	617
pard200-4	12	0.98	2,332	22	0.32	272	12	7.83	226	11	581.4	643
pard200-4	nc	0.86	2,315	22	0.39	251	12	7.65	206	11	592.7	648
pard200-5	6	0.44	225	79	0.41	147	49	5.06	69	15	33.6	31
pard200-5	8	0.66	407	112	0.53	253	65	5.71	93	16	36.0	34
pard200-5	10	2.86	3,577	322	1.76	1,644	149	7.62	453	48	84.98	79
pard200-5	12	135.9	171,500	722	12.13	10,700	294	18.45	6,098	171	>600	686
pard200-5	nc	120.4	131,100	777	15.16	11,960	285	17.06	5,866	142	>600	818
pard200-6	6	7.15	4,635	933	7.44	5,148	902	16.1	4,875	675	172.2	199
pard200-6	8	6.05	5,985	777	8.38	5,885	733	12.25	4,120	349	112.6	135
pard200-6	10	2.64	2,305	283	2.05	1,172	206	7.48	514	107	82.61	103
pard200-6	12	1.08	1,934	81	0.54	461	37	7.18	409	23	189.0	211
pard200-6	nc	1.1	1,737	76	0.74	799	48	8.22	483	32	>600	700
pard200-7	6	0.64	687	122	0.74	602	97	6.77	291	54	112.7	119
pard200-7	8	0.36	431	59	0.32	207	31	7.12	88	16	59.57	65
pard200-7	10	2.21	3,570	216	1.15	1,205	105	8.13	640	46	83.51	75
pard200-7	12	12.03	15,000	76	1.17	1,185	20	9.17	725	13	>600	648
pard200-7	nc	8.77	12,930	72	1.32	1,464	23	9.39	841	16	>600	802
pard200-8	6	0.2	97	43	0.19	75	25	2.57	41	11	20.55	19
pard200-8	8	0.36	199	68	0.51	124	36	3.37	47	12	32.90	30
pard200-8	10	3.21	3,635	295	0.78	442	88	7.26	151	20	40.55	37
pard200-8	12	96.29	82,400	581	3.09	2,237	171	8.71	1,080	56	185.2	200
pard200-8	nc	45.68	66,790	574	2.96	2,455	160	10.21	1,999	67	>600	964
pard200-9	6	2.6	2,404	390	2.62	2,262	338	7.75	1,211	110	79.61	91
pard200-9	8	5.62	5,052	657	5.83	3,814	540	10.19	2,093	289	108.1	136
pard200-9	10	3.76	3,582	403	3.09	1,817	259	9.53	754	125	65.21	82
pard200-9	12	1.98	2,535	147	0.52	296	42	7.76	134	10	23.70	23
pard200-9	nc	1.96	2,473	148	1.65	1,675	95	9.89	899	78	>600	675
pard200-10	6	1.2	1,122	226	1.42	992	188	6.86	385	41	63.01	73
pard200-10	8	1.62	1,599	242	1.48	992	178	6.91	415	41	56.54	61
pard200-10	10	36.51	25,450	1,771	9.51	6,730	833	14.27	4,025	597	178.0	232
pard200-10	12	3.8	5,711	211	0.58	300	35	7.78	152	10	20.48	25
pard200-10	nc	4.75	7,010	230	2.93	2,085	164	11.84	2115	117	>600	632

Table 11 Performance of the outer-approximation method vs. CPLEX's MISOCP method on the 300^+ instances generated by Frangioni and Gentile (2006), with a time budget of 600s per approach, with $\kappa = 0$, $\gamma = \frac{1000}{\sqrt{n}}$. We run all approaches on one thread.

Problem	k	Algorithm 3			Algorithm 3 + in-out			Algorithm 3 + in-out + 50			CPLEX MISOCP	
		Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes
pard300-1	6	36.56	15,870	1,974	68.44	14,130	1,864	67.68	10,920	1,295	> 600	210
pard300-1	8	158.8	39,650	3,412	238.9	37,830	3,320	193.8	29,560	2,508	> 600	190
pard300-1	10	108.3	60,560	2,593	94.63	46,350	2,053	59.74	23,270	1,243	> 600	230
pard300-1	12	17.93	17,070	523	8.23	5,390	219	16.30	1,567	73	261.3	101
pard300-1	nc	33.85	29,030	483	26.44	15,490	419	44.41	15,060	418	> 600	206
pard300-2	6	13.87	7,583	935	22.34	6,805	819	28.03	4,563	496	346.5	117
pard300-2	8	37.76	28,910	1,962	68.53	21,470	1,753	66.81	16,060	1,254	583.0	233
pard300-2	10	64.51	41,320	2,247	44.76	30,230	1,237	439.9	15,460	658	562.7	216
pard300-2	12	2.76	4,355	115	0.77	532	26	12.22	194	4	172.3	57
pard300-2	nc	4.91	7,423	123	1.91	1,440	63	13.29	739	38	> 600	250
pard300-3	6	33.24	21,540	1,205	47.62	20,050	1,137	52.85	13,420	793	> 600	210
pard300-3	8	34.00	37,920	1,410	52.85	35,640	1,293	38.12	21,620	668	> 600	206
pard300-3	10	254.3	128,500	3,526	283.2	103,700	3,114	288.0	112,000	2,502	> 600	210
pard300-3	12	81.05	59,470	342	4.5	3,607	84	18.83	1,144	47	> 600	295
pard300-3	nc	77.34	58,550	328	8.26	5,867	116	25.16	5,137	74	> 600	206
pard300-4	6	51.46	18,810	2,255	55.49	18,400	1,849	64.77	15,930	1,539	> 600	225
pard300-4	8	75.72	39,830	3,192	161.3	45,040	3,108	154.5	36,930	2,611	> 600	224
pard300-4	10	168.0	58,710	3,968	195.2	58,490	3,672	168.2	44,360	3,048	> 600	238
pard300-4	12	19.98	18,650	267	8.93	5,509	187	22.75	3,707	127	> 600	229
pard300-4	nc	27.19	22,010	284	16.06	12,240	215	31.03	9,941	199	> 600	257
pard300-5	6	3.99	2,670	425	5.49	2,295	351	12.05	934	104	358.1	131
pard300-5	8	6.88	5,509	491	6.53	4,227	357	11.90	1,100	73	192.5	68
pard300-5	10	13.5	11,890	790	6.86	4,610	385	14.23	1,419	140	330.3	123
pard300-5	12	1.07	1,141	81	0.43	174	30	10.71	120	18	247.7	92
pard300-5	nc	1.05	813	82	1.03	511	50	12.24	360	31	> 600	224
pard300-6	6	3.66	2,478	420	4.00	2,341	353	11.47	1,089	101	155.5	55
pard300-6	8	10.35	8,220	771	9.71	6,503	635	15.40	3,518	295	307.6	110
pard300-6	10	26.95	15,450	1,151	19.09	12,090	927	21.74	6,265	402	> 600	209
pard300-6	12	6.62	7,094	275	3.74	1,118	136	19.10	794	79	121.4	47
pard300-6	nc	7.65	9,391	257	5.17	3,233	195	19.06	3,056	158	> 600	214
pard300-7	6	2.82	2,009	323	3.89	1,413	285	12.86	1,120	195	551.5	227
pard300-7	8	4.08	4,395	337	3.3	1,996	250	13.68	1,182	168	> 600	210
pard300-7	10	5.08	5,494	334	1.77	1,716	107	11.13	464	26	199.0	63
pard300-7	12	0.71	1,278	37	0.56	455	18	11.94	373	14	577.8	208
pard300-7	nc	1.43	2,940	37	0.59	615	13	11.53	374	12	> 600	200
pard300-8	6	5.28	3,174	589	6.05	3,052	549	13.53	2,232	282	331.9	113
pard300-8	8	11.74	7,725	1,034	15.13	7,912	983	20.73	5,125	658	523.2	185
pard300-8	10	23.65	18,550	1,174	12.02	8,273	602	18.47	3,646	354	368.3	130
pard300-8	12	7.02	8,034	331	4.33	2,786	171	14.83	1,447	104	234.7	89
pard300-8	nc	8.88	9,420	333	7.09	6,558	287	19.36	4,719	239	> 600	220
pard300-9	6	12.26	13,400	1,033	15.08	8,177	931	20.94	4,948	620	538.5	195
pard300-9	8	97.90	31,670	2,356	76.99	30,940	2,192	77.93	24,080	1,823	> 600	207
pard300-9	10	215.2	97,800	2,741	118.1	64,980	1,907	66.37	36,790	1,113	> 600	201
pard300-9	12	11.08	11,750	268	9.68	8,423	196	18.18	3,710	117	> 600	269
pard300-9	nc	24.51	25,400	284	10.65	8,604	225	31.34	10,640	196	> 600	240
pard300-10	6	5.13	3,884	583	7.5	3,589	503	15.05	2,227	234	262.5	93
pard300-10	8	9.54	6,685	803	11.44	5,257	687	17.12	3,190	300	289.0	107
pard300-10	10	6.02	3,417	486	4.96	2,097	380	14.25	1,215	229	259.5	99
pard300-10	12	13.33	9,969	388	5.35	3,815	207	14.56	1,690	84	> 600	195
pard300-10	nc	26.77	16,430	410	15.2	8,326	336	35.89	9,676	319	> 600	175

Table 12 Performance of the outer-approximation method vs. CPLEX's MISOCP method on the 400^+ instances generated by Frangioni and Gentile (2006), with a time budget of 600s per approach, with $\kappa = 0$, $\gamma = \frac{1000}{\sqrt{n}}$. We run all approaches on one thread.

Problem	k	Algorithm 3			Algorithm 3 + in-out			Algorithm 3 + in-out + 50			CPLEX MISOCP	
		Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes
pard400-1	6	64.88	18,730	2,963	69.91	17,430	2,670	86.00	17,793	2,320	> 600	95
pard400-1	8	364.5	54,420	5,400	283.6	66,130	4,734	232.7	41,000	4,086	> 600	94
pard400-1	10	36.33	24,850	980	13.25	8,578	554	24.45	3,740	318	> 600	97
pard400-1	12	14.19	11,480	328	9.40	6,732	214	24.06	4,030	144	> 600	100
pard400-1	nc	49.56	35,030	336	17.41	11,580	261	44.27	16,000	238	> 600	74
pard400-2	6	0.18	71	21	0.12	24	8	3.31	18	6	160.9	17
pard400-2	8	0.31	227	24	0.13	12	8	2.17	14	8	350.9	53
pard400-2	10	0.14	87	10	0.05	0	2	0.05	0	2	178.2	23
pard400-2	12	0.12	54	6	0.24	10	3	1.13	5	3	> 600	69
pard400-2	nc	0.12	52	5	0.25	9	2	2.57	12	2	> 600	70
pard400-3	6	1.38	1,335	149	1.70	895	121	16.37	534	84	> 600	100
pard400-3	8	3.22	2,458	271	3.24	1,862	206	18.40	1,353	133	> 600	80
pard400-3	10	8.81	9,924	347	3.22	2,500	146	19.15	1,351	55	> 600	82
pard400-3	12	0.45	838	12	0.26	102	2	13.71	59	2	582.0	92
pard400-3	nc	0.56	1,259	10	0.22	130	2	15.34	74	2	> 600	100
pard400-4	6	53.04	18,490	1,712	54.56	14,360	1,677	57.55	10,890	1,237	> 600	99
pard400-4	8	183.9	47,460	3,660	179.0	42,140	3,522	166.1	37,070	2,923	> 600	90
pard400-4	10	259.1	76,390	2,153	516.5	81,900	5,782	439.3	96,750	3,614	> 600	90
pard400-4	12	1.88	2,428	98	0.64	311	21	15.56	220	12	407.6	67
pard400-4	nc	3.76	4,738	105	2.14	1,795	66	18.33	1,008	53	> 600	90
pard400-5	6	11.07	5,100	658	11.41	4,793	586	23.78	3,363	363	> 600	94
pard400-5	8	17.42	12,060	939	20.97	9,459	811	35.33	6,300	507	> 600	94
pard400-5	10	213.7	74,590	2,312	175.9	73,740	1,933	100.6	42,380	1,184	> 600	89
pard400-5	12	9.29	9,720	272	4.13	2,538	105	19.9	765	59	485.4	95
pard400-5	nc	17.16	15,750	306	19.33	12,320	235	38.46	9,137	244	> 600	70
pard400-6	6	0.27	116	30	0.25	32	9	6.34	37	6	356.2	61
pard400-6	8	0.17	92	15	0.06	0	2	0.08	0	2	208.4	33
pard400-6	10	0.42	317	36	0.18	44	9	4.81	18	2	200.9	33
pard400-6	12	4.8	7,491	76	0.91	545	22	19.21	324	15	> 600	97
pard400-6	nc	5.4	8,154	82	1.36	654	17	19.44	372	15	> 600	83
pard400-7	6	48.05	16,100	2,514	90.72	12,480	2,376	122.5	14,130	2,233	> 600	98
pard400-7	8	114.0	39,650	3,412	178.3	30,110	3,224	194.2	27,800	2,819	> 600	86
pard400-7	10	31.51	21,060	1,304	35.49	19,670	985	32.94	8,230	497	> 600	86
pard400-7	12	1.38	1,567	70	0.42	164	13	12.63	60	5	169.5	25
pard400-7	nc	1.77	2,063	83	2.09	1,410	64	17.73	893	42	> 600	61
pard400-8	6	118.1	27,150	3,187	165.0	28,200	3,025	185.1	24,550	2,753	> 600	98
pard400-8	8	342.8	91,060	5,120	335.7	62,250	5,377	356.2	58,570	4,889	> 600	97
pard400-8	10	229.3	113,200	2,704	105.9	60,640	1,546	86.51	36,100	1,100	> 600	91
pard400-8	12	3.14	3,999	100	1.31	948	31	19.45	248	16	375.6	55
pard400-8	nc	3.14	3,717	92	4.26	3,786	78	22.05	1,974	63	> 600	57
pard400-9	6	77.79	22,580	2,345	103.5	20,500	2,242	107.7	17,480	1,788	> 600	88
pard400-9	8	466.0	60,570	4,064	227.1	63,950	3,900	217.7	54,390	3,298	> 600	89
pard400-9	10	409.0	126,200	3,610	16.71	8,440	448	34.38	6,406	315	> 600	77
pard400-9	12	0.69	747	52	0.72	238	33	14.43	212	20	> 600	96
pard400-9	nc	0.61	629	43	0.77	458	33	14.5	379	22	> 600	100
pard400-10	6	170.0	23,610	3,587	168.1	22,860	3,473	227.1	21,270	3,172	> 600	90
pard400-10	8	245.2	45,870	5,375	380.3	53,370	5,307	410.4	53,740	4,974	> 600	92
pard400-10	10	391.6	108,400	3,236	177.5	67,620	2,292	72.6	26,350	1,162	> 600	80
pard400-10	12	3.79	4,910	152	1.01	557	42	16.65	351	22	360.0	57
pard400-10	nc	4.70	4,035	143	4.08	3253	130	20.43	2,239	113	> 600	37

We now present the instance-wise runtimes (in seconds) for the smallest instances generated by Frangioni and Gentile (2006), without any diagonal matrix extraction, and $k \in \{6, 8, 10, 12, n\}$. Table 13 demonstrates that not using any diagonal matrix extraction technique substantially slows our approach.

Finally, we present the instance-wise runtimes (in seconds) for the smallest instances generated by Frangioni and Gentile (2006), with the diagonal matrix extraction technique proposed by Zheng et al. (2014), and $k \in \{10, n\}$ (we restrict the values k can take to use the diagonal matrices pre-computed by Frangioni et al. (2017)). Table 14 demonstrates that using the diagonal matrix extraction technique proposed by Zheng et al. (2014) substantially slows our approach; the results for $n \in \{300, 400\}$ are similar. Indeed, this technique is only faster for the pard200-1 problem with $k = 10$, and is slower in the other 95% of instances (sometimes substantially so).

Table 13 Performance of the outer-approximation method on the 200^{+} instances generated by Frangioni and Gentile (2006), with a time budget of 600s per approach, $\kappa=0$, $\gamma=\frac{1000}{\sqrt{n}}$, and no diagonal matrix extraction. We run all approaches on one thread.

Problem	k	Algorithm 3			Algorithm 3+in-out			Algorithm 3 + in-out + 50			CPLEX MISOCP	
		Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes
pard200-1	6	>600	143,800	10,650	>600	217,200	9,671	>600	120,900	7,530	>600	700
pard200-1	8	>600	94,900	11,830	400.6	118,300	6,461	>600	106,900	7,822	>600	600
pard200-1	10	>600	173,000	10,020	>600	71,050	10,340	>600	63,470	5,422	>600	700
pard200-1	12	>600	223,700	6,852	>600	68,600	10,500	>600	42,450	6,632	>600	686
pard200-1	nc	>600	286,600	8,236	>600	59,070	12,560	>600	53,580	8,221	>600	800
pard200-2	6	>600	243,600	10,930	239.9	47,180	8,305	>600	90,460	8,538	>600	500
pard200-2	8	>600	328,100	9,365	>600	234,100	8,547	>600	207,800	2,011	>600	242
pard200-2	10	>600	468,400	9,134	0.2	47	12	5.32	28	16	>600	700
pard200-2	12	>600	273,300	7,406	0.47	3	18	1.12	3	18	>600	700
pard200-2	nc	>600	505,000	8,497	0.21	65	12	9.95	69	12	>600	600
pard200-3	6	>600	112,800	12,020	1.36	236	32	43.69	515	32	>600	505
pard200-3	8	>600	235,000	10,150	1.24	385	24	59.49	750	24	>600	500
pard200-3	10	>600	245,500	6,940	3.56	6,937	12	136.5	44,310	18	>600	510
pard200-3	12	>600	292,360	7,016	57.13	63,850	944	>600	139,800	935	>600	346
pard200-3	nc	>600	334,300	8,382	42.01	77,870	2,384	285.73	120,900	3,660	>600	600
pard200-4	6	>600	86,780	13,660	0.3	0	14	0.49	0	14	>600	500
pard200-4	8	>600	272,600	10,700	0.4	642	20	50.41	620	20	>600	561
pard200-4	10	>600	289,900	8,193	0.61	516	30	46.85	879	32	>600	498
pard200-4	12	>600	303,600	6,790	0.9	228	16	51.31	216	16	>600	294
pard200-4	nc	>600	366,100	7,999	0.38	86	22	13.87	80	22	>600	587
pard200-5	6	>600	112,000	9,616	>600	141,200	9,208	>600	127,100	7,060	>600	700
pard200-5	8	>600	132,600	11,370	135.0	52,970	4,089	>600	93,390	7,365	>600	600
pard200-5	10	>600	183,100	9,788	>600	51,300	10,010	>600	68,410	6,456	>600	700
pard200-5	12	>600	203,500	5,519	>600	53,730	9,813	>600	39,300	5,365	>600	600
pard200-5	nc	>600	315,400	9,270	>600	59,070	12,680	>600	86,240	7,025	>600	800
pard200-6	6	>600	116,700	11,260	>600	181,500	8,698	>600	131,200	6,758	>600	691
pard200-6	8	>600	161,100	10,700	>600	202,060	9,698	>600	105,400	8,449	>600	700
pard200-6	10	>600	141,200	11,370	>600	80,800	11,170	>600	56,700	7,828	>600	700
pard200-6	12	>600	236,600	7,586	>600	52,560	11,000	>600	41,630	5,415	>600	400
pard200-6	nc	>600	338,100	9,120	>600	71,790	13,850	>600	50,980	8,922	>600	800
pard200-7	6	>600	106,000	8,527	3.66	4,736	392	72.66	6,080	391	>600	500
pard200-7	8	>600	149,800	12,640	>600	193,900	10,840	>600	222,800	3,503	>600	500
pard200-7	10	>600	214,200	9,858	>600	139,000	8,465	>600	154,300	5,859	>600	485
pard200-7	12	>600	313,000	7,902	>600	206,900	9,568	>600	215,100	3,773	>600	500
pard200-7	nc	>600	220,800	6,976	>600	194,500	8,507	>600	209,600	4,971	>600	700
pard200-8	6	>600	167,600	11,200	>600	217,700	9,307	>600	173,200	7,609	>600	650
pard200-8	8	>600	183,200	11,140	>600	213,900	10,100	>600	103,100	5,954	>600	700
pard200-8	10	>600	182,400	10,190	>600	115,600	9,215	>600	35,700	4,307	>600	360
pard200-8	12	>600	217,000	6,149	>600	52,420	10,550	>600	52,300	9,066	>600	700
pard200-8	nc	>600	241,600	6,751	>600	56,070	11,820	>600	50,590	7,702	>600	471
pard200-9	6	>600	126,500	11,140	>600	128,500	9,437	>600	106,200	7,029	>600	600
pard200-9	8	>600	130,300	10,580	>600	135,700	8,579	>600	88,600	6,653	>600	700
pard200-9	10	>600	186,500	11,160	>600	63,560	10,570	>600	57,800	5,646	>600	600
pard200-9	12	>600	266,100	7,433	>600	61,000	10,700	>600	42,550	6,381	>600	689
pard200-9	nc	>600	256,100	7,535	>600	57,280	10,540	>600	38,560	6,376	>600	800
pard200-10	6	>600	179,600	12,700	>600	245,900	7,980	>600	155,100	7,300	>600	600
pard200-10	8	>600	123,600	10,060	>600	198,370	8,670	>600	36,770	2,414	>600	680
pard200-10	10	>600	164,800	8,273	>600	46,100	9,375	>600	29,000	4,824	>600	393
pard200-10	12	>600	193,300	5,776	>600	52,820	9,616	>600	37,900	5,834	>600	364
pard200-10	nc	>600	193,700	5,523	>600	40,770	8,887	>600	34,300	6,096	>600	432

Table 14 Performance of the outer-approximation method on the 200^+ instances generated by Frangioni and Gentile (2006), with a time budget of 600s per approach, $\kappa = 0$, $\gamma = \frac{1000}{\sqrt{n}}$, and the diagonal matrix extraction technique proposed by Zheng et al. (2014). We run all approaches on one thread.

Problem	k	Algorithm 3			Algorithm 3 + in-out			Algorithm 3 + in-out + 50		
		Time	Nodes	Cuts	Time	Nodes	Cuts	Time	Nodes	Cuts
pard200-1	10	0.74	130	30	0.03	0	4	0.03	0	4
pard200-1	nc	>600	887,400	1,386	>600	539,900	1,070	>600	369,500	675
pard200-2	10	234.3	239,500	875	57.14	45,230	193	78.88	39,000	196
pard200-2	nc	>600	995,900	823	>600	157,100	135	>600	226,100	66
pard200-3	10	245.1	207,200	1,195	71.95	55,050	365	76.64	30,910	249
pard200-3	nc	>600	903,500	888	>600	357,200	246	>600	268,400	259
pard200-4	10	>600	442,500	1,967	344.7	223,700	1,053	228.9	135,500	760
pard200-4	nc	535.1	913,500	1,092	>600	297,600	94	529.8	212,600	94
pard200-5	10	>600	439,900	4,965	48.87	70,200	206	69.71	52,300	204
pard200-5	nc	>600	1,340,000	1,314	>600	531,400	1,408	>600	573,200	1,358
pard200-6	10	>600	311,800	4,922	6.54	6,382	116	36.29	12,370	107
pard200-6	nc	>600	1,280,000	1,016	>600	479,900	789	>600	557,600	580
pard200-7	10	549.8	389,000	2,542	515.6	228,100	1,336	292.4	105,900	743
pard200-7	nc	>600	1,245,000	522	>600	496,200	183	>600	502,600	119
pard200-8	10	>600	399,200	3,419	2.32	1,638	46	20.19	1,716	45
pard200-8	nc	>600	1,337,000	862	>600	674,300	552	>600	507,900	420
pard200-9	10	589.7	576,100	1,756	6.31	8,746	122	26.53	8,290	143
pard200-9	nc	>600	1,264,000	1,941	>600	703,900	1,977	>600	498,000	1,970
pard200-10	10	>600	416,200	3,798	288.4	160,300	1,070	422.0	192,800	1,002
pard200-10	nc	>600	974,400	1,584	>600	498,100	1,513	>600	313,400	1482

Appendix E: Additional Pseudocode

In this appendix, we provide auxiliary pseudocode pertaining to the experiments run in Section 5. Specifically, we provide pseudocode pertaining to our implementation of the `in-out` method of Ben-Ameur and Neto (2007), which we have applied before running Algorithm 3 in some problems in Section 5.

Algorithm 4 The in-out method of Ben-Ameur and Neto (2007), as applied at the root node.

Require: Optimal solution to Problem (28) $\boldsymbol{z}^\star$, objective value θ_{socp}

$\epsilon \leftarrow 10^{-10}, \lambda \leftarrow 0.1, \delta \leftarrow 2\epsilon$

$t \leftarrow 1$

repeat

Compute $\boldsymbol{z}_0, \theta_0$ solution of

$$\min_{\boldsymbol{z} \in \text{Conv}\left(\mathcal{Z}_k^n\right), \theta} \theta \quad \text{s.t. } \theta \geq f(\boldsymbol{z}_i) + g_{\boldsymbol{z}_i}^\top (\boldsymbol{z} - \boldsymbol{z}_i), \ \forall i \in [t].$$

if z_0 has not improved for 5 consecutive iterations **then**

Set $\lambda = 1$

if z_0 has not improved for 10 consecutive iterations **then**

Set $\delta = 0$

end if

end if

Set $z_{t+1} \leftarrow \lambda z_0 + (1-\lambda) z_{\text{socp}} + \delta \boldsymbol{e}$.

Round $\boldsymbol{z}_{t+1}$ coordinate-wise so that $\boldsymbol{z}_{t+1} \in [0,1]^n$.

Compute $f(\boldsymbol{z}_{t+1})$ and $g_{\boldsymbol{z}_{t+1}} \in \partial f(\boldsymbol{z}_{t+1})$.

Apply cut $\theta \geq f(\boldsymbol{z}_{t+1}) + g_{\boldsymbol{z}_{t+1}}^\top (\boldsymbol{z} - \boldsymbol{z}_{t+1})$ at root node of integer model.

$t \leftarrow t+1$

until $f(\boldsymbol{z}_0) - \theta_0 \leq \varepsilon$ or $t > 200$

return $\boldsymbol{z}_t$