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The sparse(st) optimization problem: reformulations, optimality, stationarity, and numerical results

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Abstract

We consider the sparse optimization problem with nonlinear constraints and an objective function, which is given by the sum of a general smooth mapping and an additional term defined by the ℓ_0-quasi-norm. This term is used to obtain sparse solutions, but difficult to handle due to its nonconvexity and nonsmoothness (the sparsity-improving term is even discontinuous). The aim of this paper is to present two reformulations of this program as a smooth nonlinear program with complementarity-type constraints. We show that these programs are equivalent in terms of local and global minima and introduce a problem-tailored stationarity concept, which turns out to coincide with the standard KKT conditions of the two reformulated problems. In addition, a suitable constraint qualification as well as second-order conditions for the sparse optimization problem are investigated. These are then used to show that three Lagrange–Newton-type methods are locally fast convergent. Numerical results on different classes of test problems indicate that these methods can be used to drastically improve sparse solutions obtained by some other (globally convergent) methods for sparse optimization problems.

Keywords Sparse optimization · Global minima · Local minima · Strong stationarity · Lagrange–Newton method · Quadratic convergence · B-subdifferential

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1 Introduction

The sparse(st) optimization problem considered in this paper is the constrained problem

$$\min_x f(x) + \rho\|x\|_0 \quad \text{s.t.} \quad x \in X, \tag{SPO}$$

with a parameter $\rho > 0$, a feasible set X (usually) given by

$$X = \{x \in \mathbb{R}^n \mid g(x) \leq 0,\ h(x) = 0\}$$

with (at least) continuous functions $f : \mathbb{R}^n \to \mathbb{R}$, $g : \mathbb{R}^n \to \mathbb{R}^m$, $h : \mathbb{R}^n \to \mathbb{R}^p$ and $\|x\|_0$ being the number of nonzero components x_i of the vector x. Following standard terminology, we call $\|x\|_0$ the ℓ_0-norm throughout this manuscript though it is not a norm. Typical applications, where sparse solutions of a given optimization problem are required, include compressed sensing for sparse representation of signals or image data, sparse portfolio selection problems, feature selection in classification learning, sparse regression or the sparse principal component analysis, see [34, Section 2] for an overview and references.

Following [23], the solution methods for problems like SPO can be divided into the following three categories: (a) convex approximations, (b) nonconvex approximations, and (c) nonconvex exact reformulations.

The most common convex approximation technique uses the ℓ_1-norm instead of the ℓ_0-norm in SPO. An overview on such ℓ_1-surrogate models, their advantages and solution approaches can be found in [34, Section 4.1]. Provided that f and X themselves are convex, the resulting optimization problem is convex (though nonsmooth) and can therefore be solved by a variety of methods for convex optimization, see [1]. This approach is very popular, for example, in solving compressed sensing problems. On the other hand, there exist prominent applications, where the ℓ_1-norm provides absolutely no sparsity (like the portfolio optimization problem used in our numerical section).

This drawback leads to other sparsity improving terms that result in nonconvex approximation schemes. A natural choice is to use the ℓ_p-quasi-norm for some $p \in (0, 1)$, which is no longer convex, but still continuous, see [19]. Despite its nonconvexity, if there are no constraints (i.e., $X = \mathbb{R}^n$), the resulting problem can still be solved relatively efficiently by a proximal-type method. For additional constraints, one can apply an augmented Lagrangian-type method and use the proximal-type approach to solve the resulting (unconstrained) subproblems, see [10, 26]. In principle, these techniques can also be used for the ℓ_0-norm, but the discontinuity still causes some trouble and typically leads to slowly convergent (proximal-type) gradient methods, see [26]. Another method belonging to the class of nonconvex approximations is the penalty decomposition method [25], which introduces an additional variable and solves the resulting problem by an alternating minimization technique. Also the DC-type methods (DC = difference of convex) described in [23] result in a nonconvex approximation which is shown to be exact under some additional assumptions, see also the DC-reformulation of the ℓ_0-norm from [20] (this reformulation, however, is

applied to cardinality-constrained problems where the ℓ_0-term is not in the objective function but in the constraints, see below for a more detailed discussion).

Finally, regarding the class (c) of exact nonconvex reformulations, there are, to the best of our knowledge, still just a very few papers providing such reformulations. A natural choice is to use a mixed-integer program, cf. reformulation MIP. This is useful for finding sparse solutions of – often quadratic – problems, whose dimension is not too large, and allows, in principle, to compute a global minimum, see e.g. [2]. By modifying the objective function with a suitable regularizing term, c.f. [3], also larger problem dimensions can be handled. For nonlinear programs or large-scale problems, however, this typically leads to an intractable reformulation. One alternative approach is the complementarity-type reformulation suggested in [16], see also [4] for a similar approach in the context of low-rank matrix recovery, which can be shown to be completely equivalent to the original sparse optimization problem SPO. The focus of the paper [16], however, is slightly different.

More precisely, in this paper, we present two reformulations of the general sparse optimization problem SPO. These reformulations are introduced in Sect. 2, and partially motivated by a related approach from [6, 8] for cardinality-constrained optimization problems, cf. the corresponding discussion in Sect. 2. One of the two reformulations is exactly the one from [16] that we already mentioned previously. Note that the subsequent results shown for our two reformulated problems are even new for the approach from [16]. In particular, we verify in Sect. 3 that problem SPO and our two reformulations are equivalent in terms of both local and global minima an observation not stated in [16]. We further stress that the related approaches for cardinality-constrained problems [6, 8] yield a complete equivalence with respect to global minima only, not with respect to local minima. The full equivalence between both global nad local minima in the case of SPO is therefore a quite surprising and impressive observation. Section 3 introduces a problem-tailored strong stationarity concept and a corresponding constraint qualification and shows that these correspond to the standard KKT conditions and a standard constraint qualification of the two reformulated problems. We then discuss suitably adapted second-order conditions in Sect. 5.

Though the main goal of this paper is to lay the foundations of two exact nonconvex reformulations of the sparse optimization problem SPO, the corresponding discussion leads, in a very natural way, to Lagrange–Newton-type methods for the solution of SPO, see Sect. 6. Like all Newton-type methods, this is primarily a locally (fast) convergent algorithm, whereas a central difficulty for the solution of sparse optimization problems is to design suitable globally convergent methods. Nevertheless, the corresponding numerical results in Sect. 7 indicate that the Lagrange–Newton-type methods can be used to obtain significant improvements over solutions calculated by other (globally convergent) sparse solvers. We close with some final remarks in Sect. 8.

Notation: Throughout this manuscript, $e_i \in \mathbb{R}^n$ denotes the i-th unit vector, whereas $e := (1, \ldots, 1)^T \in \mathbb{R}^n$ is the all-one vector. Given $x \in \mathbb{R}^n$ and $x^* \in X$, we define the index sets

$$I_0(x) := \{i \mid x_i = 0\} \quad \text{and} \quad I_g(x^*) := \{i \mid g_i(x^*) = 0\}$$

of zero components of x and active inequality constraints at x^*, respectively. For an arbitrary vector x, we write $\operatorname{diag}(x)$ for the corresponding diagonal matrix, whose diagonal entries are given by the elements of x. Given two vectors $x, y \in \mathbb{R}^n$, the Hadamard (elementwise) product is denoted by $x \circ y$, i.e., the elements of this vector are given by $x_i \cdot y_i$ for all $i = 1, \ldots, n$.

2 Two smooth reformulations of SPO

In this section we derive two smooth reformulations of SPO and show that the local and global minima of these reformulated problems coincide with the local and global minima of the original sparse optimization problem SPO. One of these reformulations is already known from [16], whereas the other one is new and will be more suited for our numerical experiments later on. Note that the results stated in this manuscript for the known formulation from [16] are still new and not contained in that reference. Throughout this section, we only require f, g, h to be continuous.

Let us consider the sparse optimization problem from SPO with an arbitrary set $X \subseteq \mathbb{R}^n$. For any $x \in \mathbb{R}^n$, define a corresponding binary variable $y \in \{0, 1\}^n$ by setting $y_i := 0$ for $x_i \neq 0$ and $y_i := 1$ for $x_i = 0$. Using this y, we can calculate the ℓ_0-norm of x as

$$\|x\|_0 = \sum_{x_i \neq 0} 1 = \sum_{i=1}^{n} (1 - y_i) = n - e^T y.$$

Thus, we could rewrite problem SPO by the following mixed-integer problem

$$\min_{x,y} f(x) + \rho(n - e^T y) \quad \text{s.t.} \quad x \in X, \; x \circ y = 0, \; y \in \{0, 1\}^n. \tag{MIP}$$

In order to move to a continuous optimization problem, we discard the binary constraints on y. We need to retain the constraint $y \leq e$, because otherwise the objective function of (MIP) does not admit a minimum. This leads us to the reformulation

$$\min_{(x,y)} f(x) + \rho(n - e^T y) \quad \text{s.t.} \quad x \in X, \; x \circ y = 0, \; y \leq e. \tag{SPOlin}$$

Since the auxiliary variable y enters the objective function linearly, we denote this problem SPOlin. This is in contrast to our second formulation

$$\min_{(x,y)} f(x) + \frac{\rho}{2} \sum_{i=1}^{n} y_i(y_i - 2) \quad \text{s.t.} \quad x \in X, \; x \circ y = 0 \tag{SPOsq}$$

called SPOsq, since we add a quadratic term to the objective function. Note that this quadratic term is designed in such a way that it vanishes, whenever $x_i \neq 0$ (due to the complementarity-type constraint), and that it attains its minimum at $y_i = 1$ whenever this variable is unconstrained, i.e., for all i with $x_i = 0.$, see Fig. 1.

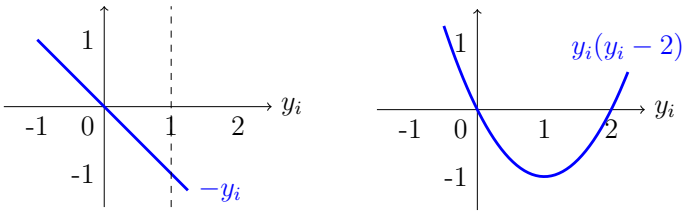


Fig. 1 Comparison of the terms $-y_i$ used in SPOlin and $y_i(y_i - 2)$ used in SPOsq

Problem SPOlin corresponds to the reformulation already introduced in [16], whereas SPOsq seems to be new. Observe that, if the feasible set X contains no inequality constraints, then the new formulation SPOsq boils down to an equality-constrained optimization problem, in contrast to SPOlin, which still includes the inequalities $y \leq e$. This observation is particularly useful in our setting since, later, we will apply a Lagrange–Newton-type method in order to solve the sparse optimization problem.

Before we take a closer look at the relaxed problems SPOlin and SPOsq, we would like to briefly discuss the relation of the sparse problem SPO and its relaxations to the two closely related problem classes of *cardinality-constrained problems*

$$\min_x \ f(x) \quad \text{s.t.} \quad x \in X, \ \|x\|_0 \leq \kappa$$

and *cardinality minimization problems*

$$\min_x \ \|x\|_0 \quad \text{s.t.} \quad x \in X, \ f(x) \leq \delta,$$

where $\kappa \in \mathbb{N}$ and $\delta \in \mathbb{R}$ are given constants. Using the same ideas as above, these problems can be relaxed to the continuous problems

$$\min_{x,y} \ f(x) \text{ s.t. } x \in X, \ x \circ y = 0, \ y \leq e, \ n - e^T y \leq \kappa,$$
$$\min_{x,y} \ n - e^T y \text{ s.t. } x \in X, \ x \circ y = 0, \ y \leq e, \ f(x) \leq \delta,$$

respectively. As we show below, for problem SPO the two relaxations are equivalent to the original problem in terms of global and local minima. Using the same arguments, it is also possible to show this equivalence for the cardinality minimization problem. However, for the cardinality-constrained problem it is known, see [6], that only the global minima of the original problem and its relaxation coincide, but the relaxation may have additional local minima.

Furthermore, one may be tempted to view problem SPO as a penalty reformulation of either of the other two problems. However, while a solution x^* of SPO is always a solution of the other two problems with $\kappa := \|x^*\|_0$ or $\delta := f(x^*)$, respectively, the opposite implication is in general not true. This means that solutions of the cardinality-constrained problem or cardinality minimization problem cannot always be recovered

as solutions of SPO. More details on these relations can be found in [34, Proposition 1.1].

3 Properties of reformulations

In the moment, it is not clear why we can view the programs SPOlin and SPOsq as reformulations of the given nonsmooth and discontinuous sparse optimization problem SPO. But, as we show below, these three programs are completely equivalent in terms of both global and local minima. Even their corresponding stationary points coincide, see Sect. 4 for details on this. Some of statements presented in Sect. 3 can be proven in an elementary and straightforward manner. For the sake of completion they have thus been moved to the appendix.

In order to verify these statements, we first need some preliminary results. Note that x is obviously feasible for the given problem SPO if and only if there exists a suitable vector $y \in \mathbb{R}^n$ such that (x, y) is feasible for SPOlin or SPOsq. Furthermore, we have the following relations for feasible points of these two programs.

Lemma 3.1 *The following statements hold:*

(i) Let (x, y) be feasible for SPOlin. Then $\|x\|_0 \leq n - e^T y$, with equality if and only if $y_i = 1$ for all $i \in I_0(x)$.
(ii) Let (x, y) be feasible for SPOsq. Then $\|x\|_0 - n \leq \sum_{i=1}^n y_i(y_i - 2)$, with equality if and only if $y_i = 1$ for all $i \in I_0(x)$.

Proof cf. appendix. □

The following result shows that the constellation $y_i = 1$ for $i \in I_0(x)$ is indeed the most preferable one.

Lemma 3.2 *Let (x^*, y^*) be a local minimum of SPOlin or SPOsq. Then we have $y_i^* = 1$ for all $i \in I_0(x^*)$.*

Proof cf. appendix. □

Next, we show that the set of local minima of the sparse optimization problem SPO is independent of the particular choice of the penalty parameter. Note that, this is due to the discontinuity of the ℓ_0-norm and that a similar result for sparse optimization problems involving the ℓ_1-norm, e.g., does not hold. This observation may actually be viewed as an advantage of the ℓ_0-norm, since this implies that a suitable choice of the penalty parameter is much less critical for the ℓ_0-formulation of the sparse optimization problem than other (continuous) formulations like the one based on the ℓ_1-norm or the ℓ_q-quasi-norm for $q \in (0, 1)$.

Proposition 3.3 *Let x^* be a local minimum of SPO with penalty parameter $\rho_1 > 0$. Then x^* is also a local minimum of SPO for any other penalty parameter $\rho_2 > 0$.*

Proof cf. appendix. □

The previous statement also holds for the two reformulated programs SPOlin and SPOsq. This is a consequence, e.g., of the following result, which states that x^* is a local minimum of the sparse optimization problem SPO if and only if there exists a vector y^* such that the pair (x^*, y^*) is a local minimum of either SPOlin or SPOsq.

Theorem 3.4 (Equivalence of Local Minima) *The following statements are equivalent:*

(i) x^* *is a local optimum of SPO.*
(ii) There exists y^* *such that* (x^*, y^*) *is a local optimum of SPOlin.*
(iii) There exists y^* *such that* (x^*, y^*) *is a local optimum of SPOsq.*

Proof Notice that, by Lemma 3.2, y^* has to be of the form

$$y_i^* = \begin{cases} 1 & \text{for } i \in I_0(x^*), \\ 0 & \text{otherwise,} \end{cases} \tag{*}$$

in order for (x^*, y^*) to be a local minimum of SPOlin or SPOsq.

$(i) \Longrightarrow (ii)$: Let x^* be a local minimum of SPO and let y^* be defined as in (*). Then

$$f(x^*) + \rho\big(n - e^T y^*\big) = f(x^*) + \rho \left\|x^*\right\|_0 \leq f(x) + \rho \left\|x\right\|_0 \leq f(x) + \rho\big(n - e^T y\big)$$

for all feasible (x, y) with x sufficiently close to x^*, where the first equality and the last inequality follow from Lemma 3.1(i).

$(ii) \Longrightarrow (i)$: Let (x^*, y^*) be the local minimum of SPOlin with y^* as in (*). Assume that x^* is not a local minimum of SPO. Then there exists a sequence $\{x^k\} \subseteq X$ such that $x^k \to x^*$ and

$$f(x^k) + \rho \left\|x^k\right\|_0 < f(x^*) + \rho \left\|x^*\right\|_0 \quad \forall k \in \mathbb{N}. \tag{1}$$

Recall that $\left\|x^k\right\|_0 \geq \|x^*\|_0$ holds for all k sufficiently large. Hence we either have a subsequence $\{x^k\}_K$ such that $\left\|x^k\right\|_0 = \|x^*\|_0$ holds for all $k \in K$, or $\|x^*\|_0 + 1 \leq \left\|x^k\right\|_0$ is true for almost all $k \in \mathbb{N}$. In the former case, it follows that (x^k, y^*) is feasible for SPOlin, hence we obtain from Lemma 3.1(i) and the minimality of (x^*, y^*) for SPOlin that

$$\begin{aligned} f(x^k) + \rho \left\|x^k\right\|_0 &= f(x^k) + \rho \left\|x^*\right\|_0 \\ &= f(x^k) + \rho(n - e^T y^*) \geq f(x^*) + \rho(n - e^T y^*) \\ &= f(x^*) + \rho \left\|x^*\right\|_0, \end{aligned}$$

which contradicts (1). Otherwise, we have $\|x^*\|_0 + 1 \leq \left\|x^k\right\|_0$ and, by continuity, also $f(x^*) \leq f(x^k) + \rho$ for all $k \in \mathbb{N}$ sufficiently large, which, in turn, gives

$$f(x^k) + \rho \left\|x^k\right\|_0 \geq f(x^k) + \rho + \rho \left\|x^*\right\|_0 \geq f(x^*) + \rho \left\|x^*\right\|_0.$$

Hence, also in this situation, we have a contradiction to (1).

$(i) \Longrightarrow (iii)$: Let x^* be a local minimum of SPO. Then x^* is also a local minimum of the optimization problem

$$\min \; f(x) + \frac{\rho}{2}\big(\|x\|_0 - n\big) \quad \text{s.t.} \quad x \in X, \tag{2}$$

since, by Proposition 3.3, we can modify the penalty parameter, and since adding a constant to the objective function does not change the location of the local minima. Now, let y^* be defined as in statement (*). Then

$$\begin{aligned} f(x^*) + \frac{\rho}{2}\sum_{i=1}^{n} y_i^*\big(y_i^* - 2\big) = f(x^*) + \frac{\rho}{2}\big(\|x^*\|_0 - n\big) &\le f(x) + \frac{\rho}{2}\big(\|x\|_0 - n\big) \\ &\le f(x) + \frac{\rho}{2}\sum_{i=1}^{n} y_i\big(y_i - 2\big), \end{aligned}$$

for all feasible (x, y) with x sufficiently close to x^*, where the first equality and the last inequality follow from Lemma 3.1(ii).

$(iii) \Longrightarrow (i)$: Let (x^*, y^*) be a local minimum of SPOsq with y^* as in (*). Assume that x^* is not a local minimum of SPO. Then x^* is not a local minimum of (2). Hence, there exists a sequence $\{x^k\} \subseteq X$ such that $x^k \to x^*$ and

$$f(x^k) + \frac{\rho}{2}\big(\|x^k\|_0 - n\big) < f(x^*) + \frac{\rho}{2}\big(\|x^*\|_0 - n\big) \quad \forall k \in \mathbb{N}. \tag{3}$$

Recall that $\|x^k\|_0 \ge \|x^*\|_0$ holds for all k sufficiently large. Thus, once again, we either have a subsequence $\{x^k\}_K$ such that $\|x^k\|_0 = \|x^*\|_0$ holds for all $k \in K$, or $\|x^*\|_0 + 1 \le \|x^k\|_0$ is true for almost all $k \in \mathbb{N}$. In the former case, it follows that (x^k, y^*) is feasible for SPOsq, hence we obtain from Lemma 3.1(ii) and the minimality of (x^*, y^*) for SPOsq that

$$\begin{aligned} f(x^k) + \frac{\rho}{2}\big(\|x^k\|_0 - n\big) = f(x^k) + \frac{\rho}{2}\big(\|x^*\|_0 - n\big) &= f(x^k) + \frac{\rho}{2}\sum_{k=1}^{n} y_i^*\big(y_i^* - 2\big) \\ &\ge f(x^*) + \frac{\rho}{2}\sum_{k=1}^{n} y_i^*\big(y_i^* - 2\big) = f(x^*) + \frac{\rho}{2}\big(\|x^*\|_0 - n\big), \end{aligned}$$

which contradicts (3). Otherwise, we have $\|x^*\|_0 + 1 \le \|x^k\|_0$ and, by continuity, also $f(x^*) \le f(x^k) + \frac{\rho}{2}$ for all $k \in \mathbb{N}$ sufficiently large, which, in turn, gives

$$f(x^k) + \frac{\rho}{2}\big(\|x^k\|_0 - n\big) \ge f(x^k) + \frac{\rho}{2} + \frac{\rho}{2}\big(\|x^*\|_0 - n\big) \ge f(x^*) + \frac{\rho}{2}\big(\|x^*\|_0 - n\big).$$

Hence, also in this situation, we have a contradiction to (3). □

Scaling the penalty parameter ρ as in the proof of the previous result has, of course, an impact on the global minima of SPO. We therefore do not obtain equivalence of the global minima in the above sense, i.e., independent of the choice of the penalty parameter. However, the following result holds.

Theorem 3.5 (Equivalence of Global Minima) *The following statements hold:*

(i) x^* *is a global minimum of SPO if and only if there exists* y^* *such that* (x^*, y^*) *is a global minimum of SPOlin.*
(ii) x^* *is a global minimum of SPO with penalty parameter* $\frac{\rho}{2}$ *if and only if there exists* y^* *such that* (x^*, y^*) *is a global minimum of SPOsq.*

Proof According to Lemma 3.1 (i), the inequality $f(x)+\rho(n-e^T y) \geq f(x)+\rho \|x\|_0$ holds for all (x, y) feasible for SPOlin, with equality if and only if $y_i = 1$ for all $i \in I_0(x)$. The pair (x^*, y^*) therefore solves SPOlin if and only if x^* solves SPO, with $y_i^* = 1$ for all $i \in I_0(x^*)$.

To prove part (ii), we recall that x^* is a global minimum of SPO with penalty parameter $\frac{\rho}{2}$ if and only if x^* is a solution of

$$\min_x \; f(x) + \frac{\rho}{2}\big(\|x\|_0 - n\big) \quad \text{s.t.} \quad x \in X.$$

Using Lemma 3.1 (ii), the claim follows analogously to the proof of part (i). □

Effectively, formulation SPOsq can be considered as a reformulation of the scaled problem

$$\min_x \; f(x) + \frac{\rho}{2}\|x\|_0 \quad \text{s.t.} \quad x \in X.$$

Nevertheless, invariance of the local minima to the chosen parameter ρ is also reflected in the stationary conditions, which we derive in the next section. We therefore neglect the scaling issue in our subsequent analysis of a local Newton-type method, as any solution found cannot guaranteed to be globally optimal.

4 Stationary conditions

This section introduces a stationarity concept for the nonsmooth and discontinuous sparse optimization problem SPO and relates it to the KKT conditions of the two smooth reformulations from SPOlin and SPOsq. Throughout this section, we assume that all functions f, g, h are continuously differentiable.

To this end, let us introduce the function

$$L^{SP}(x, \lambda, \mu) := f(x) + \lambda^T g(x) + \mu^T h(x),$$

which is exactly the Lagrangian of SPO except that we do not include the term with the ℓ_0-norm. In particular, L^{SP} is therefore a smooth function. Based on L^{SP}, the

ordinary Lagrangians of the smooth optimization problems SPOlin and SPOsq can be written as

$$L^{lin}(x, y, \lambda, \mu, \gamma, \sigma) := L^{SP}(x, \lambda, \mu) + \rho(n - e^T y) + \gamma^T(x \circ y) + \sigma^T(y - e)$$

and

$$L^{sq}(x, y, \lambda, \mu, \gamma) := L^{SP}(x, \lambda, \mu) + \frac{\rho}{2}\sum_{i=1}^{n} y_i(y_i - 2) + \gamma^T(x \circ y),$$

respectively. The standard KKT conditions of SPOlin are therefore given by

$$\nabla_x L^{lin}(x, y, \lambda, \mu, \gamma, \sigma) = \nabla_x L^{SP}(x, \lambda, \mu) + \gamma \circ y = 0, \tag{4}$$
$$\nabla_y L^{lin}(x, y, \lambda, \mu, \gamma, \sigma) = -\rho e + \gamma \circ x + \sigma = 0, \tag{5}$$
$$\lambda \geq 0, \quad g(x) \leq 0, \quad \lambda \circ g(x) = 0, \tag{6}$$
$$h(x) = 0, \tag{7}$$
$$x \circ y = 0, \tag{8}$$
$$\sigma \geq 0, \quad y \leq e, \quad \sigma \circ (y - e) = 0. \tag{9}$$

We take a closer look at system (5), (8), (9) componentwise for $i = 1, \ldots, n$

$$-\rho + \gamma_i x_i + \sigma_i = 0, \tag{10}$$
$$x_i \cdot y_i = 0, \tag{11}$$
$$\sigma_i \geq 0, \quad y_i \leq 1, \quad \sigma_i(y_i - 1) = 0, \tag{12}$$

and assume there is a solution $(x_i^*, y_i^*, \gamma_i^*, \sigma_i^*)$. We distinguish two cases. First, let $x_i^* = 0$, then clearly $\sigma_i^* = \rho$ and $y_i^* = 1$, whereas γ_i^* is arbitrary. In the second case, we have $x_i^* \neq 0$, which immediately implies $y_i^* = 0$, $\sigma_i^* = 0$ and further $\gamma_i^* = \rho / x_i^*$. Hence, $(x_i^*, y_i^*, \gamma_i^*)$ also solves

$$\rho(y_i - 1) + \gamma_i x_i = 0 \quad \text{and} \quad x_i \cdot y_i = 0. \tag{13}$$

Conversely, let $(x_i^*, y_i^*, \gamma_i^*)$ be a solution of equation (13). Then with $\sigma_i^* = \rho$, if $x_i^* = 0$ and $\sigma_i^* = 0$, if $x_i^* \neq 0$ the tuple $(x_i^*, y_i^*, \gamma_i^*, \sigma_i^*)$ is clearly a solution of system (10), (11), (12).

Using this reasoning, we can compress the system (4)–(9) by deleting the variable σ to the system

$$\nabla_x L^{SP}(x, \lambda, \mu) + \gamma \circ y = 0, \tag{14}$$
$$\rho(y - e) + \gamma \circ x = 0, \tag{15}$$
$$\lambda \geq 0, \quad g(x) \leq 0, \quad \lambda \circ g(x) = 0, \tag{16}$$
$$h(x) = 0, \tag{17}$$
$$x \circ y = 0, \tag{18}$$

Now, it is easy to see that (14)–(16) are precisely the KKT conditions of problem SPOsq. In summary, we have the following result.

Proposition 4.1 (Equivalence of KKT Points) *The vector* $(x^*, y^*, \lambda^*, \mu^*, \gamma^*)$ *is a KKT point of SPOsq if and only if there exists* σ^* *such that* $(x^*, y^*, \lambda^*, \mu^*, \gamma^*, \sigma^*)$ *is a KKT point of SPOlin. The multipliers* σ^*, γ^* *and the variable* y^* *depend uniquely on* (x^*, λ^*, μ^*) *with*

$$y_i^* = \begin{cases} 1, & i \in I_0(x^*), \\ 0, & i \notin I_0(x^*), \end{cases} \quad \gamma_i^* = \begin{cases} -\nabla_{x_i} L^{SP}(x^*, \lambda^*, \mu^*) & i \in I_0(x^*), \\ \frac{\rho}{x_i^*} & i \notin I_0(x^*), \end{cases}$$

$$\sigma_i^* = \begin{cases} \rho, & i \in I_0(x^*), \\ 0, & i \notin I_0(x^*). \end{cases}$$

Proof The equivalence of the two KKT systems is an immediate result by the equivalence of (5) and (9) to (15) under the condition (8) present in both systems, which we established componentwise. Additionally, we already verified the unique dependence of y^* and σ^* on x^*, as well as $\gamma_i^* = \rho / x_i^*$ for $i \notin I_0(x^*)$. The representation of γ_i^* for $i \in I_0(x^*)$, on the other hand, can be obtained by (4). □

For a fixed triple (x, λ, μ), the only possible choice of (y, γ, σ) with which a KKT point of either of the above systems could be obtained, is therefore already determined. This, in turn, tells us that the possibility to satisfy the KKT conditions depends on the values of (x, λ, μ) only. This motivates us to define a stationary concept for the original sparse optimization problem SPO in the following way.

Definition 4.2 We call a point x^* an *S-stationary point* (*strongly stationary point*) of SPO if there exist multipliers (λ^*, μ^*) such that the following conditions hold:

$$\begin{aligned} \nabla_{x_i} L^{SP}(x^*, \lambda^*, \mu^*) = 0, \quad \forall i \notin I_0(x^*), \\ \lambda^* \geq 0,\ g(x^*) \leq 0,\ \lambda^* \circ g(x^*) = 0, \\ h(x^*) = 0. \end{aligned} \tag{19}$$

Note that there exist a couple of different stationarity concepts like W-, C-, M-, and S-stationarity for a number of related problem classes, including mathematical programs with complementarity constraints [22], cardinality constraints [8], vanishing constraints [21], and switching constraints [28]. Similarly, it would be possible to state some of these other stationarity concepts for problem SPO as well. However, on the one hand, it turns out that suitable methods for the solution of sparse optimization problems can be shown to converge to S-stationary points, see [32] for some preliminary results in this direction, which is in contrast to the other classes of problems mentioned before and which indicates that there is no need to introduce these weaker stationarity concepts for sparse optimization problems, and, on the other hand, for the purpose of the approach presented here, we only require the S-stationarity from Definition 4.2. The system (19) can be understood as the KKT conditions of

$$\min_x \ f(x) \quad \text{s.t.} \quad x \in X,\ x_i = 0,\ i \in I_0(x^*).$$

To compute an S-stationary point, one may be tempted to simply restrict the feasible set to some subspace $U := \{x \mid x_i = 0,\ i \in I\}$ for an arbitrary I. Note, however, that $X \cap U$ might be empty or only contain stationary points, which are unfavourable for the initial problem SPO. From a computational standpoint it is therefore beneficial to vary the indexset I, which is exactly the task of auxiliary variable y.

S-stationarity turns out to be equivalent to the KKT conditions of the reformulated problems SPOlin and SPOsq.

Theorem 4.3 (Equivalence of S-Stationary and KKT Points) *The following are equivalent:*

(i) x^* *is S-stationary for SPO with some multipliers* (λ^*, μ^*).
(ii) There exists $(y^*, \gamma^*, \sigma^*)$*, depending on* (x^*, λ^*, μ^*) *only, such that* $(x^*, y^*, \lambda^*, \mu^*, \gamma^*, \sigma^*)$ *is a KKT point of SPOlin.*
(iii) There exists (y^*, γ^*)*, depending on* (x^*, λ^*, μ^*) *only, such that* $(x^*, y^*, \lambda^*, \mu^*, \gamma^*)$ *is a KKT point of SPOsq.*

Proof Assume x^* is S-stationary for SPO. Then there exists (λ^*, μ^*) such that (19) holds. Choosing y^* and γ^* as in Proposition 4.1, we obtain a KKT point of SPOsq. Conversely, let $(x^*, y^*, \lambda^*, \mu^*, \gamma^*)$ be a KKT point of SPOsq. Then (14) holds. Hence (19) is satisfied for (x^*, λ^*, μ^*), which implies that x^* is an S-stationary point of SPO. The remaining equivalence follows from Proposition 4.1. □

We next introduce a problem-tailored constraint qualification which, in particular, guarantees that a local minimum of SPO is an S-stationary point. This constraint qualification is relatively strong, and much weaker ones will be discussed in a forthcoming report. For the purpose of this paper, where we plan to consider a Lagrange–Newton-type method for the solution of sparse optimization problems, the following condition is the most suitable one.

Definition 4.4 A feasible point $x^* \in X$ of SPO satisfies the *sparse LICQ* (*SP-LICQ*, for short) if the vectors

$$\nabla g_i(x^*)\ (i \in I_g(x^*)), \quad \nabla h_i(x^*)\ (i = 1, \ldots, p), \quad e_i\ (i \in I_0(x^*))$$

are linearly independent.

The linear independence constraint qualification (LICQ) is well-known within nonlinear programming and is said to hold if all the gradients w.r.t. to active constraints are linearly independent [29]. As such, note that SP-LICQ corresponds to standard LICQ of the *tightened nonlinear program*

$$\min_x\ f(x) \quad \text{s.t.} \quad g(x) \le 0,\ h(x) = 0,\ x_i = 0\ (i \in I_0(x^*)) \tag{20}$$

depending on a feasible point $x^* \in X$. We establish the following connection between SP-LICQ for SPO with standard LICQ for SPOlin and SPOsq.

Theorem 4.5 (Equivalence of LICQ-type Conditions) *Let* (x^*, y^*) *be feasible for SPOlin and SPOsq, respectively and assume* $\{i \mid x_i^* = y_i^* = 0\} = \emptyset$. *Then the following are equivalent:*

(i) SP-LICQ is satisfied at x^*,
(ii) Standard LICQ holds at (x^*, y^*) *for SPOlin,*
(iii) Standard LICQ holds at (x^*, y^*) *for Problem SPOsq.*

Proof It is easy to see that SP-LICQ holds at x^* for SPO if and only if the following vectors are linearly independent:

$$\begin{pmatrix} \nabla g_i(x^*) \\ 0 \end{pmatrix} (i \in I_g(x^*)), \quad \begin{pmatrix} \nabla h_i(x^*) \\ 0 \end{pmatrix} (i = 1, \ldots, p), \quad \begin{pmatrix} \alpha_i e_i \\ 0 \end{pmatrix} (i \in I_0(x^*)),$$
$$\begin{pmatrix} 0 \\ \beta_i e_i \end{pmatrix} (i \notin I_0(x^*)) \quad \begin{pmatrix} 0 \\ \xi_i e_i \end{pmatrix} (i \in J), \tag{21}$$

for arbitrary $\alpha_i, \beta_i, \xi_i \in \mathbb{R} \setminus \{0\}$ and an arbitrary subset $J \subseteq I_0(x^*)$.
Case 1: Choose (x^*, y^*) feasible for SPOlin with $\{i \mid x_i^* = y_i^* = 0\} = \emptyset$. Now, set $\alpha_i := y_i^*$ for $i \in I_0(x^*)$, $\beta_i := x_i^*$ for $i \notin I_0(x^*)$. Furthermore, set $J := \{i \mid y_i^* = 1\} \subset I_0(x^*)$ and $\xi_i := 1$ for $i \in J$, respectively. Plugging our choices of α, β, ξ, and J into (21) yields the set of gradients of the equality and active inequality constraints of SPOlin. The claim follows.
Case 2: Let (x^*, y^*) feasible for SPOsq with $\{i \mid x_i^* = y_i^* = 0\} = \emptyset$. Choose $J := \emptyset$ and α, β as in case 1. Then system (21) collapses to the set of gradients of the equality and active inequality constraints of SPOsq. The claim follows. □

The central assumption in Theorem 4.5 is, of course, that the bi-active set $\{i \mid x_i^* = y_i^* = 0\}$ is empty. In the context of sparse optimization problems and our reformulations, however, this assumption turns out to be very weak and is automatically satisfied, for example, if x^* is a local minimum of SPO or at a KKT-point of either SPOlin or SPOsq. This is an immediate consequence of Lemma 3.2.

Therefore, if SP-LICQ holds at a local optimum x^* of SPO, it follows that there is a unique vector y^* with $y_i^* = 1$ for all $i \in I_0(x^*)$ such that the KKT conditions of SPOlin and SPOsq, respectively, have a unique solution guaranteed by standard LICQ, which holds for both of the smooth reformulations. In particular, local minima of x^* of SPO, where SP-LICQ holds, are thus S-stationary with uniquely defined multipliers. Nevertheless, SP-LICQ is a relatively strong constraint qualification, and we will come back to this point later.

5 Second-order conditions

The aim of this section is to introduce problem-tailored second-order conditions for the sparse optimization Problem SPO and to relate these conditions to standard second-order conditions associated with the two smooth reformulations SPOlin and SPOsq,

respectively. Naturally, these second-order conditions play a central role for our subsequent development of Lagrange–Newton-type methods for the solution of sparse optimization problems. Note that, throughout this section, we make the implicit assumption that all functions f, g, h are twice continuously differentiable.

Definition 5.1 Let x^* be an S-stationary point of SPO, with multipliers (λ^*, μ^*). We call

$$\begin{aligned} C^{SPO}(x^*, \lambda^*) := \{d \mid \nabla g_i(x^*)^T d = 0 \quad & \forall i \in I_g(x^*),\ \lambda_i^* > 0, \\ \nabla g_i(x^*)^T d \le 0 \quad & \forall i \in I_g(x^*),\ \lambda_i^* = 0, \\ \nabla h(x^*)^T d = 0, & \\ d_i = 0 \quad & \forall i \in I_0(x^*)\}, \end{aligned}$$

and

$$\begin{aligned} SC^{SPO}(x^*, \lambda^*) := \{d \mid \nabla g_i(x^*)^T d = 0 \quad & \forall i \in I_g(x^*),\ \lambda_i^* > 0, \\ \nabla h(x^*)^T d = 0, & \\ d_i = 0 \quad & \forall i \in I_0(x^*)\}, \end{aligned}$$

the *critical cone* and *critical subspace*, respectively, of SPO at x^* with multiplier λ^*.

Note that the critical cone and the critical subspace of problem SPO are problem-tailored definitions, which can also be interpreted as the standard critical cone and the standard critical subspace of the corresponding tightened nonlinear program from (20). The usual critical cone and critical subspace of problem SPO would not contain the condition that $e_i^T d = 0$ for $i \in I_0(x^*)$ and, hence, these standard sets would be larger than those from the previous definition.

Definition 5.1 allows the following formulation of sparse second-order sufficiency conditions.

Definition 5.2 Let x^* be an S-stationary point of SPO, with multipliers (λ^*, μ^*). Then we say that (x^*, λ^*, μ^*) satisfies

(i) *SP-SOSC (sparse second-order sufficiency condition)* if

$$d^T \nabla^2_{xx} L^{SP}(x^*, \lambda^*, \mu^*) d > 0, \quad \forall d \in C^{SPO}(x^*, \lambda^*) \setminus \{0\},$$

(ii) *strong SP-SOSC (strong sparse second-order sufficiency condition)* if

$$d^T \nabla^2_{xx} L^{SP}(x^*, \lambda^*, \mu^*) d > 0, \quad \forall d \in SC^{SPO}(x^*, \lambda^*) \setminus \{0\}.$$

Note that the Hessian $\nabla^2_{xx} L^{SP}(x^*, \lambda^*, \mu^*)$ depends only on f, g, h, whereas the sparsity term is encoded in the critical cone/subspace. We clarify the significance of SP-SOSC in the following result.

Theorem 5.3 (Second-Order Sufficiency Conditions) *Let* (x^*, λ^*, μ^*) *be an S-stationary point such that (strong) SP-SOSC holds in* x^**. Then the following statements hold:*

(i) (Strong) SOSC for SPOlin holds at $(x^*, y^*, \lambda^*, \mu^*, \gamma^*, \sigma^*)$ *with* $(y^*, \gamma^*, \sigma^*)$ *defined in Proposition 4.1.*
(ii) (Strong) SOSC for SPOsq holds at $(x^*, y^*, \lambda^*, \mu^*, \gamma^*)$ *with* (y^*, γ^*) *defined in Proposition 4.1.*
(iii) x^* *is a local minimizer of SPO.*

Proof For a given S-stationary point (x^*, λ^*, μ^*) let y^*, γ^*, and σ^* be chosen as in Proposition 4.1 and define $z := (x, y)$. The Hessian matrices of the Lagrangians of problems SPOlin and SPOsq with respect to z are given by

$$\nabla^2_{zz} L^{lin}(x^*, y^*, \lambda^*, \mu^*, \gamma^*, \sigma^*) = \begin{pmatrix} \nabla^2_{xx} L^{SP}(x^*, \lambda^*, \mu^*) & \operatorname{diag}(\gamma^*) \\ \operatorname{diag}(\gamma^*) & 0 \end{pmatrix} \quad \text{and}$$
$$\nabla^2_{zz} L^{sq}(x^*, y^*, \lambda^*, \mu^*, \gamma^*) = \begin{pmatrix} \nabla^2_{xx} L^{SP}(x^*, \lambda^*, \mu^*) & \operatorname{diag}(\gamma^*) \\ \operatorname{diag}(\gamma^*) & \rho I_n \end{pmatrix},$$

respectively, where I_n denotes the identity matrix in $\mathbb{R}^{n\times n}$. Since $y_i^* = 1$ and $\sigma_i^* = \rho > 0$ for all $i \in I_0(x^*)$, we obtain the following critical cones for the smooth problems SPOlin and SPOsq, respectively:

$$\begin{aligned} C^{lin}(z^*, \lambda^*) = \{d = (d_x, d_y)^T \mid\ & \nabla g_i(x^*)^T d_x = 0 \quad \forall i \in I_g(x^*),\ \lambda_i^* > 0, \\ & \nabla g_i(x^*)^T d_x \le 0 \quad \forall i \in I_g(x^*),\ \lambda_i^* = 0, \\ & \nabla h(x^*)^T d_x = 0, \\ & (d_x)_i = 0 \quad \forall i \in I_0(x^*), \\ & d_y = 0\}, \\ C^{sq}(z^*, \lambda^*) = \{d = (d_x, d_y)^T \mid\ & \nabla g_i(x^*)^T d_x = 0 \quad \forall i \in I_g(x^*),\ \lambda_i^* > 0, \\ & \nabla g_i(x^*)^T d_x \le 0 \quad \forall i \in I_g(x^*),\ \lambda_i^* = 0, \\ & \nabla h(x^*)^T d_x = 0, \\ & (d_x)_i = 0 \quad \forall i \in I_0(x^*), \\ & (d_y)_i = 0 \quad \forall i \notin I_0(x^*)\} \end{aligned}$$

and, similarly, the critical subspaces

$$\begin{aligned} SC^{lin}(z^*, \lambda^*) := \{d = (d_x, d_y)^T \mid\ & \nabla g_i(x^*)^T d_x = 0 \quad \forall i \in I_g(x^*),\ \lambda_i^* > 0, \\ & \nabla h(x^*)^T d_x = 0, \\ & (d_x)_i = 0 \quad \forall i \in I_0(x^*), \\ & d_y = 0\}, \end{aligned}$$

$$SC^{sq}(z^*, \lambda^*) := \{d = (d_x, d_y)^T \mid \nabla g_i(x^*)^T d_x = 0 \quad \forall i \in I_g(x^*),\ \lambda_i^* > 0,$$
$$\nabla h(x^*)^T d_x = 0,$$
$$(d_x)_i = 0 \quad \forall i \in I_0(x^*),$$
$$(d_y)_i = 0 \quad \forall i \notin I_0(x^*)\}.$$

For a vector $d = (d_x, d_y)^T$, we obtain

$$\begin{aligned}\begin{pmatrix} d_x \\ d_y \end{pmatrix}^T \nabla^2_{zz} L^{sq} \begin{pmatrix} d_x \\ d_y \end{pmatrix} &= \begin{pmatrix} d_x \\ d_y \end{pmatrix}^T \nabla^2_{zz} L^{lin} \begin{pmatrix} d_x \\ d_y \end{pmatrix} + \rho \left\| d_y \right\|_2^2 \\ &= {d_x}^T \nabla^2_{xx} L^{SP}(x^*, \lambda^*, \mu^*) d_x \\ &\quad + 2(\gamma^*)^T (d_x \circ d_y) + \rho \left\| d_y \right\|_2^2 . \end{aligned} \tag{22}$$

Assume $d = (d_x, d_y)^T \in C^{lin}(x^*, \lambda^*)$ is a nonzero vector. Then we have

$$d_x \in C^{SPO}(x^*, \lambda^*), \quad d_y = 0.$$

In particular, this implies $d_x \neq 0$. According to (22), the SP-SOSC immediately implies claim (i). The proof for strong SOSC is analogous.

Assume $d = (d_x, d_y)^T \in C^{sq}(x^*, \lambda^*)$ is a nontrivial vector. It holds

$$d_x \in C^{SPO}(x^*, \lambda^*), \quad (d_y)_i = 0,\ i \notin I_0(x^*).$$

At least one of the two vectors d_x, d_y is nonzero and we know $d_x \circ d_y = 0$. Hence SP-SOSC implies (ii), according to inequality (22). Strong SOSC can again be verified analogously.

Finally, the validity of SOSC for either SPOlin or SPOsq immediately yields (iii) due to the equivalence of local minima. □

We next state a second-order necessary optimality condition for the sparse optimization problem SPO, which can be derived via the relation to the corresponding second-order conditions of one of the two smooth reformulations SPOlin or SPOsq. Note that this necessary condition will not be used later, but is stated here for the sake of completeness.

Theorem 5.4 *(Second-Order Necessary Condition) Let x^* be a local minimum of SPO satisfying SP-LICQ. Then there exist unique multipliers (λ^*, μ^*) such that (x^*, λ^*, μ^*) is an S-stationary point of SPO satisfying the second-order necessary condition*

$$d^T \nabla_{xx} L^{SP}(x^*, \lambda^*, \mu^*) d \geq 0, \quad \forall\, d \in C^{SPO}(x^*, \lambda^*).$$

Proof The existence and uniqueness of the multipliers (λ^*, μ^*) such that the triple (x^*, λ^*, μ^*) satisfies the S-stationarity conditions is an immediate consequence of Theorems 4.3 and 4.5.

Furthermore, we know from these results that there exist (uniquely defined) vectors y^* and σ^* such that $(x^*, y^*, \lambda^*, \mu^*, \sigma^*)$ is a KKT point of SPOsq satisfying standard LICQ, and with (x^*, y^*) being a local minimizer of SPOsq, cf. Theorem 3.4. Hence the standard second-order necessary optimality condition holds for SPOsq, i.e., we have

$$\begin{pmatrix} d_x \\ d_y \end{pmatrix}^T \begin{pmatrix} \nabla^2_{xx} L^{SP}(x^*, \mu^*, \lambda^*) & \operatorname{diag}(\gamma^*) \\ \operatorname{diag}(\gamma^*) & \rho I_n \end{pmatrix} \begin{pmatrix} d_x \\ d_y \end{pmatrix} \geq 0, \quad \forall \begin{pmatrix} d_x \\ d_y \end{pmatrix} \in C^{sq}(x^*, \lambda^*).$$

This is equivalent to

$$(d_x)^T \nabla^2_{xx} L^{SP}(x^*, \mu^*, \lambda^*)\, d_x + \rho \left\| d_y \right\|_2^2 \geq 0, \quad \forall \begin{pmatrix} d_x \\ d_y \end{pmatrix} \in C^{sq}(x^*, \lambda^*), \tag{23}$$

where we used the fact that $(d_x)_i \cdot (d_y)_i = 0$, cf. the previous proof. Now it is easy to see that any vector $d = (d_x, d_y)^T$ with $d_x \in C^{SPO}(x^*, \lambda^*)$ and $d_y = 0$ is contained in $C^{sq}(x^*, \lambda^*)$. In view of (23), this directly yields

$$(d_x)^T \nabla^2_{xx} L^{SP}(x^*, \mu^*, \lambda^*)\, d_x \geq 0, \quad \forall d_x \in C^{SPO}(x^*, \lambda^*).$$

This completes the proof. □

Note that there exist more general second-order conditions for standard nonlinear programs, see, e.g., [5]. In principle, it is possible to translate these conditions also to problem-tailored second-order optimality conditions for the sparse optimization problem SPO due to its relation to the standard second-order optimality conditions to one of the reformulated smooth problems SPOlin or SPOsq. We omit the corresponding details.

6 Lagrange–Newton-type methods

The aim of this section is to present some Lagrange–Newton-type methods for the (local) solution of the sparse optimization problem SPO. The idea is to use one of our smooth reformulations and to apply a Newton-type method to the corresponding KKT conditions. In principle, we could take either the reformulation SPOlin or the one from SPOsq. Here we decide to consider the reformulation SPOsq which, in particular, has the advantage that the corresponding KKT conditions consist of nonlinear equations only, if the original problem SPO contains not inequalities. This observation might be useful for Lagrange–Newton-type approaches. Nevertheless, the theory also covers the case where inequality constraints are present.

More precisely, we consider three different Newton-type methods: First, we take the full KKT system of SPOsq and investigate the local convergence properties of a corresponding nonsmooth Newton method applied to this system. Second, we consider a reduced variant of this method which eliminates the y-variables and show that it converges under the same set of assumptions as the previous approach. Third, we deal

with a method which tries to overcome some singularity problems for some classes of sparse optimization problems, which include nonnegativity constraints.

But before we get into the details, let us briefly recall the central ideas behind a nonsmooth version of the Newton method.

Remark 6.1 *(Nonsmooth Newton's method in a nutshell)* Given a mapping $T : \mathbb{R}^n \to \mathbb{R}^n$, we can try to compute a root of T with a Newton-type iteration scheme

$$z^{k+1} = z^k - H_k^{-1} T(z^k) \qquad \forall k = 0, 1, 2, \ldots,$$

where $H_k \in \mathbb{R}^{n \times n}$ is a matrix typically related to the derivative of T at z^k.

If we want to apply this to the KKT system of SPOsq, we first have to reformulate the conditions

$$\lambda_i \geq 0, \quad g_i(x) \leq 0, \quad \lambda_i g_i(x) = 0 \qquad \forall i = 1, \ldots, m$$

into m equality constraints. This can be achieved by using a suitable *NCP-function* $\varphi : \mathbb{R}^2 \to \mathbb{R}$, which is defined by the property

$$\phi(a, b) = 0 \qquad \Longleftrightarrow \qquad a \geq 0,\ b \geq 0,\ ab = 0.$$

Two prominent examples are the *minimum function* and the *Fischer-Burmeister function*

$$\phi_m(a, b) := \min\{a, b\} \qquad \text{and} \qquad \phi_{FB}(a, b) := \sqrt{a^2 + b^2} - a - b.$$

Defining the function $\Phi_g : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^m$ componentwise as

$$(\Phi_g)_i(x, \lambda) = \phi(-g_i(x), \lambda_i),$$

we can thus replace the conditions on g and λ by the equation system $\Phi_g(x, \lambda) = 0$.

However, most NCP functions are (by design) nonsmooth at least in the origin. We thus cannot use the Jacobian $H_k = T'(z^k)$ as in the classical Newton's method, but instead need some tools from nonsmooth analysis. If the mapping T is a locally Lipschitz continuous mapping, then Rademacher's Theorem implies that T is almost everywhere differentiable. Hence the set

$$\partial_B T(z) := \left\{ H \;\middle|\; \exists \{z^k\} \subseteq D_T : z^k \to z \text{ and } T'(z^k) \to H \right\}$$

is nonempty and bounded, where D_T denotes the set of differentiable points of T. The set $\partial_B T(z)$ is called the *B-subdifferential* of T in z and its convex hull gives the *generalized Jacobian* $\partial T(z)$ by Clarke [11]. A point z is called *BD-regular*, if all elements in $\partial_B T(z)$ are nonsingular.

If we use a matrix $H_k \in \partial_B T(z^k)$ in the Newton-type iteration scheme, the resulting nonsmooth Newton's method is known to be locally superlinearly or even quadratically convergent to a root z^*, if this root z^* is BD-regular and T satisfies an additional

smoothness property called *semismoothness* and *strong semismoothness*, respectively. For the precise definitions and proofs of the previous statements, the interested reader is referred to the papers [30, 31] and the monograph [14].

Throughout this section, we assume that all functions f, g, h are twice continuously differentiable. Furthermore, ϕ denotes either the minimum or the Fischer-Burmeister function, unless we state something else explicitly. Then it is known that the three operators T used below are semismooth. They are strongly semismooth if, in addition, the second-order derivatives of f, g, h are locally Lipschitz continuous. In order to verify the local fast convergence of the nonsmooth Newton method applied to $T(z) = 0$, it thus suffices to prove BD-regularity in the root z^*. For more details on this, we refer the reader, for instance, to [15].

The first Newton-type method presented in this section uses the operator

$$T(x, y, \lambda, \mu, \gamma) := \begin{pmatrix} \nabla_x L^{SP}(x, \lambda, \mu) + \gamma \circ y \\ \rho(y - e) + \gamma \circ x \\ \Phi_g(x, \lambda) \\ h(x) \\ x \circ y \end{pmatrix},$$

where Φ_g is defined as in Remark 6.1. Due to the defining property of an NCP-function, it follows that $(x^*, y^*, \lambda^*, \mu^*, \gamma^*)$ is a KKT point of the reformulated problem SPOsq if and only if it solves the (in general nonsmooth) system of equations $T(x, y, \lambda, \mu, \gamma) = 0$.

In order to ensure fast local convergence of the nonsmooth Newton method applied to the system $T(z) = 0$, it suffices to show that a solution $z^* = (x^*, y^*, \lambda^*, \mu^*, \gamma^*)$ thereof is BD-regular under suitable assumptions.

Theorem 6.2 *Let $z^* = (x^*, y^*, \lambda^*, \mu^*, \gamma^*)$ be a solution of $T(z) = 0$ such that the following assumptions hold:*

(i) SP-LICQ is satisfied at x^*.
(ii) Strong SP-SOSC is satisfied at (x^*, λ^*, μ^*).

Then z^* is a BD-regular point of T.

Proof Based on our previous result, the statement can be traced back to existing results in the literature. Since z^* is a KKT point of SPOsq, we know that the bi-active set $\{i \mid x_i^* = 0 = y_i^*\}$ is empty. Therefore, it follows from assumption (i) and Theorem 4.5 that ordinary LICQ holds for SPOsq at z^*. Similarly, assumption (ii) and Theorem 5.3 imply that the strong second-order sufficiency conditions holds for SPOsq at z^*. Standard results on the local convergence of nonsmooth Newton methods then imply that all elements $H \in \partial_B T(z^*)$ are nonsingular, see, e.g., [13, 14, 17]. □

We next consider a reduced formulation of the system $T(z) = 0$. To this end, note that $T(z) = 0$ immediately gives

$$y = e - \frac{\gamma \circ x}{\rho}, \tag{24}$$

cf. (15). Hence, eliminating the variable y in the definition of T by replacing it with the above expression, we obtain the reduced operator

$$T_{red}(x,\lambda,\mu,\gamma) = \begin{pmatrix} \nabla_x L^{SP}(x,\lambda,\mu) + \gamma \circ (e - \frac{\gamma \circ x}{\rho}) \\ \Phi(-g(x),\lambda) \\ h(x) \\ x \circ (e - \frac{\gamma \circ x}{\rho}) \end{pmatrix},$$

which is independent of y. In view of its derivation, it still holds that any zero of T_{red} yields a KKT point of SPOsq and vice versa, whenever the variable y is defined as above. In order to locally solve the KKT system of SPOsq, we can therefore, alternatively, apply a nonsmooth Newton method to the system $T_{red}(w) = 0$, where $w = (x,\lambda,\mu,\gamma)$. The central point for the local fast convergence of this approach is again the BD-regularity of a solution w^*.

Theorem 6.3 *T is BD-regular in (x,y,λ,μ,γ) with $y = (e - \gamma \circ x/\rho)$ if and only if T_{red} is BD-regular in (x,λ,μ,γ).*

Proof Let $w = (x,\lambda,\mu,\gamma)$ and $z = (x,y,\lambda,\mu,\gamma)$ with $y = e - \gamma \circ x/\rho$. The definition of the B-subdifferential then yields

$$H \in \partial_B T(z) \iff H = \begin{pmatrix} \nabla^2_{xx} L^{SP}(x,\lambda,\mu) & \operatorname{diag}(\gamma) & g'(x)^T & h'(x)^T & \operatorname{diag}(y) \\ \operatorname{diag}(\gamma) & \rho I_n & 0 & 0 & \operatorname{diag}(x) \\ J_1\Phi_g & 0 & J_2\Phi_g & 0 & 0 \\ h'(x) & 0 & 0 & 0 & 0 \\ \operatorname{diag}(y) & \operatorname{diag}(x) & 0 & 0 & 0 \end{pmatrix},$$

and, similarly, $H_{red} \in \partial_B T_{red}(w)$ if and only if

$$H_{red} = \begin{pmatrix} \nabla^2_{xx} L^{SP}(x,\lambda,\mu) - \frac{\operatorname{diag}(\gamma)^2}{\rho} & g'(x)^T & h'(x)^T & \operatorname{diag}(e - \frac{2\gamma \circ x}{\rho}) \\ J_1\Phi_g & J_2\Phi_g & 0 & 0 \\ h'(x) & 0 & 0 & 0 \\ \operatorname{diag}(e - \frac{2\gamma \circ x}{\rho}) & 0 & 0 & -\frac{\operatorname{diag}(x)^2}{\rho} \end{pmatrix},$$

with $(J_1\Phi_g, J_2\Phi_g) \in \partial_B \Phi_g(x,\lambda)$. Assume w is BD-regular for T_{red}. Let $H \in \partial_B T(z)$ and consider the system

$$Hd = 0 \quad \text{with appropriately partitioned} \quad d = (d_x, d_y, d_\lambda, d_\mu, d_\gamma). \tag{25}$$

Solving for d_y explicitly and plugging in $y = e - \gamma \circ x/\rho$ yields

$$\frac{1}{\rho}(-\gamma \circ d_x - x \circ d_\gamma) - d_y = 0,$$

$$\begin{pmatrix} \nabla^2_{xx} L^{SP}(x,\lambda,\mu) - \frac{\operatorname{diag}(\gamma)^2}{\rho} & g'(x)^T & h'(x)^T & \operatorname{diag}(e - \frac{2\gamma\circ x}{\rho}) \\ J_1\Phi_g & J_2\Phi_g & 0 & 0 \\ h'(x) & 0 & 0 & 0 \\ \operatorname{diag}(e - \frac{2\gamma\circ x}{\rho}) & 0 & 0 & -\frac{\operatorname{diag}(x)^2}{\rho} \end{pmatrix} \begin{pmatrix} d_x \\ d_\lambda \\ d_\mu \\ d_\gamma \end{pmatrix} = 0\,. \tag{26}$$

BD-regularity of T_{red} implies $(d_x, d_\lambda, d_\mu, d_\gamma) = (0,0,0,0)$ and therefore also $d_y = 0$. Hence H is nonsingular. Since this holds for arbitrary $H \in \partial_B T(z)$, the BD-regularity of T in z follows.

The proof of the converse statement is similar: Assume T_{red} is not BD-regular in w. Then there is a singular matrix $H^*_{red} \in \partial_B T_{red}(w^*)$, i.e., there exists $(J_1\Phi^*_g, J_2\Phi^*_g) \in \partial_B \Phi_g(x^*, \lambda^*)$ such that the corresponding element H^*_{red} is singular. This means that there is a nontrivial element $d_0 = (d^1_0, d^3_0, d^4_0, d^5_0)^T \in \ker(H^*_{red})$. Setting $d^2_0 := \frac{1}{\rho}(-\gamma \circ d^1_0 - x \circ d^5_0)$ and reversing the previous arguments, we obtain a singular element in $\partial_B T(z)$. □

Note that the assumption $y = (e - \gamma \circ x/\rho)$ used in Theorem 6.3 holds automatically at any KKT point. Theorem 6.3 therefore allows to translate the result from Theorem 6.2 directly to the reduced operator T_{red}. A potential disadvantage of the reduced formulation is the fact that the replacement of the variable y by the expression (24) increases the nonlinearity of the resulting operator T_{red}.

Finally, we turn to a third Newton-type method for the solution of sparse optimization problems SPO, whose feasible set X contains nonnegativity constraints for some or all variables. For notational simplicity, we consider only the fully nonnegative case

$$x \geq 0.$$

In our general approach, we have to view these constraints as part of the inequalities $g(x) \leq 0$, which causes problems with the constraint qualification. SP-LICQ would require the linear independence of the gradient vectors $-e_i$ (resulting from the constraint $x_i \geq 0$ as an inequality) and e_i (resulting from the sparsity in the definition of SP-LICQ) for all $i \in I_0(x^*)$, which is obviously impossible.

We can overcome this situation in the following way: In any local minimum of SPOsq, we have $y \geq 0$ according to Lemma 3.2. Together with the constraint $x \circ y = 0$ and the nonnegativity constraint $x \geq 0$ we thus obtain the full complementarity conditions $x \geq 0, y \geq 0, x \circ y = 0$, which we can replace by an additional NCP-function $\Phi(x,y) = 0$ with $\Phi_i(x,y) = \phi(x_i, y_i)$ for all $i = 1, \ldots, n$. The constraints $x \geq 0$ then do not need to be considered as a part of the standard inequality constraints

$g(x) \leq 0$ any more. This motivates to consider the nonlinear system of equations

$$T_C(x, y, \lambda, \mu, \gamma) = 0 \quad \text{with} \quad T_C(x, y, \lambda, \mu, \gamma) := \begin{pmatrix} \nabla_x L^{SP}(x, \lambda, \mu) + \gamma \circ y \\ \rho(y - e) + \gamma \circ x \\ \Phi_g(x, \lambda) \\ h(x) \\ \Phi(x, y) \end{pmatrix},$$

with two NCP-functions Φ_g, Φ. Then SP-LICQ is a reasonable assumption for this reformulation, and the following result holds.

Theorem 6.4 *Let $z^* = (x^*, y^*, \lambda^*, \mu^*, \gamma^*)$ be a solution of $T_C(z) = 0$ such that the assumptions of Theorem 6.2 hold. Then z^* is a BD-regular point of T_C.*

Proof First observe that $T_C(z^*) = 0$ implies $T(z^*) = 0$, hence z^* is a KKT point of SPOsq. In view of Proposition 4.1, we therefore have that the bi-active set $\{i \mid x_i^* = y_i^* = 0\}$ is empty. This implies that Φ is continuously differentiable in a neighborhood of (x^*, y^*), with componentwise derivatives given by (recall that Φ is defined either by the Fischer-Burmeister function or by the minimum function)

$$\begin{aligned} \nabla \phi_{FB}(x_i^*, 0) &= (0, -1)^T \quad \text{and} \quad \nabla \phi_m(x_i^*, 0) = (0, 1)^T, \\ \nabla \phi_{FB}(0, y_i^*) &= (-1, 0)^T \quad \text{and} \quad \nabla \phi_m(0, y_i^*) = (1, 0)^T. \end{aligned}$$

Thus, each element $H_C \in \partial_B T_C(z^*)$ can be written as:

$$H_C = \begin{pmatrix} \nabla_{xx}^2 L^{SP}(x^*, \lambda^*, \mu^*) & \operatorname{diag}(\gamma^*) & g'(x^*)^T & h'(x^*)^T & \operatorname{diag}(y^*) \\ \operatorname{diag}(\gamma^*) & \rho I_n & 0 & 0 & \operatorname{diag}(x^*) \\ J_1 \Phi_g & 0 & J_2 \Phi_g & 0 & 0 \\ h'(x^*) & 0 & 0 & 0 & 0 \\ \operatorname{diag}(c_x) & \operatorname{diag}(c_y) & 0 & 0 & 0 \end{pmatrix},$$

with c_x, c_y such that

$$((c_x)_i, (c_y)_i) \in \begin{cases} \{-1, 1\} \times \{0\} & \text{if } i \in I_0(x^*), \\ \{0\} \times \{-1, 1\} & \text{otherwise,} \end{cases}$$

and arbitrary $(J_1 \Phi_g, J_2 \Phi_g) \in \partial_B \Phi_g(x^*, \lambda^*)$. Define

$$A := \begin{pmatrix} I_{2n+m+p} & 0 \\ 0 & \operatorname{diag}\big((c_x + c_y) \circ (x^* + y^*)\big) \end{pmatrix},$$

and observe that A is nonsingular. Then a simple calculation shows that $A \cdot H_C \in \partial_B T(z^*)$. Since A is nonsingular and all elements in $\partial_B T(z^*)$ are nonsingular by Theorem 6.2, it follows that H_C is nonsingular. This completes the proof. □

Though the third formulation using the operator T_C is mainly designed for problems having additional nonnegativity constraints, we can also apply this idea also to problems without these nonnegativity constraints, by splitting the variables $x = x^+ - x^-$ into their positive and negative parts $x^+x^- \geq 0$. Since this is a pretty standard approach also used in [16], we skip the corresponding details.

Some additional remarks on the choice of the NCP-function are in order. Assume that problem SPO has a feasible set described by inequality constraints and we choose

$$\Phi_g(x, \lambda) = \min\{-g(x), \lambda\},$$

to be understood componentwisely. Then the lower part of $\partial_B T(z)$ reads

$$\begin{pmatrix} -\mathrm{diag}(c_x)g'(x) & 0 & \mathrm{diag}(c_y) & 0 \\ \mathrm{diag}(y) & \mathrm{diag}(x) & 0 & 0 \end{pmatrix}$$

such that the matrix $\big(\mathrm{diag}(c_x),\ \mathrm{diag}(c_y)\big)$ belongs to the subdifferential $\partial_B\big(\min\{a, b\}\big)$. Then, in particular, if $g(x) > 0$, we always have $\mathrm{diag}(c_y) = 0$. Depending on the values of x, y and $g'(x)$ we may encounter a singularity. The situation is even worse for the operator T_C. To this end, consider the minimum-function $\min\{x, y\}$ as surrogate for $x \circ y$ and assume we have an iterate (x^k, y^k) with $y_i^k > x_i^k$ (which is, for instance, the case in the portfolio setting, since, in general, we initialize $y_i^0 = 1$ for all $i = 1, \ldots, n$). Then, with any equality constraints h in place, the lower part of $\partial_B T_C(z^k)$ reads

$$\begin{pmatrix} h'(x) & 0 & 0 & 0 \\ E_n & 0 & 0 & 0 \end{pmatrix},$$

and we immediately encounter a singularity. In our subsequent implementation, we therefore prefer to use the Fischer-Burmeister approach simply because the (generalized) partial derivatives of the minimum function have 0-1-entries, whereas the corresponding partial derivatives of the Fischer-Burmeister-function are usually both different from zero (unless we are in a KKT point).

7 Numerical results

In this section we present some numerical results obtained by applying the previously developed Lagrange–Newton-type methods to some commonly known fields of sparse optimization problems. We start with some preliminaries regarding our implementation.

7.1 Implementation

Initial values

Lagrange–Newton-type methods are mainly locally convergent approaches. Our aim is to show these methods can be used to improve solutions obtained by globally

convergent techniques. Therefore, we pre-process the problem by first solving the ℓ_1-surrogate problem

$$\min_x \; f(x) + \rho \, \|x\|_1 \quad \text{s.t.} \quad x \in X,$$

with f, X as in SPO. We then use the solution x_{ℓ_1} of the ℓ_1-surrogate problem as initial point x^0 for the Lagrange–Newton-type methods, which we consider post-processing of the ℓ_1-surrogate problem. Accumulation points x^* of our Lagrange–Newton-type methods should (hopefully) be preferable for SPO over the ℓ_1-solution.

Note that it is, in general, not useful to have $x^0 = 0$ as the initial guess. In fact, in cases where constraints do not exist, the initial guess $x^0 = 0$ does already yield an S-stationary point. The starting point $x^0 = x_{\ell_1}$, obtained by the pre-preprocessing phase, may also have many zero components, but should, nonetheless, be a much better choice than the zero vector. Furthermore, we found it beneficial to initialize $y^0 := e$ since we want to see a majority of 0-entries in the accumulation point x^* of the algorithm, which would correlate with a y^* consisting of mainly 1-entries. For any of the Lagrangian multipliers (λ, μ, γ) we worked with the canonical choice: $\lambda^0 = 0$, $\mu^0 = 0$, $\gamma^0 = 0$, in the respective dimensions. Note that any choice of γ^0 might be arbitrarily bad since, for an accumulation point x^* with an entry $10^{-4} \approx |x_i^*| \neq 0$, one has to expect $\gamma_i^* \approx \rho \, \operatorname{sign}(x^*) 10^4$.

In our numerical test, we were able to improve upon the ℓ_1-solution x^0 in terms of the target value of the respective SPO and also in terms of the initial sparsity.

Dealing with the B-subdifferential

We only consider the Fischer-Burmeister function, whenever an NCP-function is required in our computations. The method to obtain an element in the B-subdifferential of the Fischer-Burmeister function is widely known, compare [12]. We fix a point $z = (x, y, \lambda, \mu, \gamma)$ and consider the operator T_C with the components:

$$\phi_{FB}(x_i, y_i), \; (i = 1, \ldots, n), \quad \phi_{FB}(-g_j(x), \lambda_j), \; (j = 1, \ldots, m),$$

and

$$I^{xy} := \{i \mid x_i = y_i = 0\}, \quad I^{g\lambda} := \{j \mid g_j(x) = \lambda_j = 0\}.$$

Define:

$$(x^t, y^t, \lambda^t) := (x - te(n), y - te(n), \lambda - te(p)), \quad \text{for } t > 0,$$

with $e = (1, 1, \ldots, 1)^T$ of the appropriate dimension. Passing to the limit $t \searrow 0$ yields

$$\lim_{t \searrow 0} \nabla_{(x_i, y_i)} \phi_{FB}(x_i^t, y_i^t)^T = \begin{cases} \left(\frac{x_i}{\sqrt{x_i^2 + y_i^2}} - 1, \; \frac{y_i}{\sqrt{x_i^2 + y_i^2}} - 1 \right), & i \notin I^{xy}, \\ \left(-\frac{1}{\sqrt{2}} - 1, \; -\frac{1}{\sqrt{2}} - 1 \right), & i \in I^{xy}, \end{cases} \tag{27}$$

and by applying the mean-value theorem to g_j, we further have

$$\lim_{t \searrow 0} \nabla_{(x_j,\lambda_j)} \phi_{FB}(-g_j(x^t), \lambda_j^t)^T = \\ = \begin{cases} \left(\left(\frac{g_j(x)}{\sqrt{g_j(x)^2+\lambda_j^2}} + 1 \right) g_j'(x), \ \frac{\lambda_j}{\sqrt{g_j(x)^2+\lambda_j^2}} - 1 \right), & j \notin I^{g\lambda}, \\ \left(\left(-\frac{\nabla g_j(x)^T e}{\sqrt{(\nabla g(x)^T e)^2+1}} + 1 \right) g_j'(x), \ -\frac{1}{\sqrt{(\nabla g(x)^T e)^2+1}} - 1 \right), & j \in I^{g\lambda}, \end{cases} \tag{28}$$

which are elements of the B-subdifferential of the Fischer-Burmeister function.

Termination criterion

The canonical condition for terminating one of our Newton-type methods with operator T would be

$$\|T(x)\| \leq \varepsilon,$$

with some sufficiently small tolerance ε. Unfortunately, we occasionally observe the problematic behavior that in some components $x_i^k \to 0$, but at the same time $y_i^k \to 0$ and $\gamma_i^k \to \infty$. Recall that at a minimum or stationary point (x^*, y^*), we should instead have $y_i^* = 1$ for all i with $x_i^* = 0$. When we observe the behavior, typically the iterates x^k are nonetheless sufficiently feasible and the gradient of the Lagrangian to L^{SP} is sufficiently small in every component i with $x_i^k \not\approx 0$, which points to the fact that the accumulation point is S-stationary. We therefore terminate the algorithms, when the following check for S-stationarity is satisfied:

(S.1) Choose tolerances $\delta \geq 0$, $\varepsilon \geq 0$ and define the set of nonzero components as

$$I_{\neq 0} := \{i \mid |x_i^k| \geq \delta\}.$$

(S.2) Set $L := \nabla_x L^{SP}(x^k, \mu^k, \lambda^k) = \nabla f(x^k) + g'(x^k)^T \lambda^k + h'(x^k)^T \mu^k$ and compute

$$\text{res} = \left\| \begin{pmatrix} L_{I^{\neq 0}} \\ \Phi_g(x^k, \lambda^k) \\ h(x^k) \end{pmatrix} \right\|$$

$$\left(\text{or} \quad \text{res} = \left\| \begin{pmatrix} L_{I^{\neq 0}} \\ \Phi_g(x^k, \lambda^k) \\ h(x^k) \\ \max\{0, -x^k_{I^{\neq 0}}\} \end{pmatrix} \right\| \quad \text{in case } x \geq 0 \right).$$

(S.3) Terminate the iteration, if res $\leq \varepsilon$.

In our application, we set $\delta = 10^{-4}$ and $\varepsilon = 10^{-6}$.

7.2 Sparse portfolio selection

The portfolio optimization problem in the sense of Markowitz [27] can be represented as

$$\min_x \ \frac{1}{2} x^T Q x \quad \text{s.t.} \quad e^T x = 1, \ \alpha^T x \geq \beta, \ x \geq 0, \tag{29}$$

where x_i denotes the amount of asset i bought, α_i is the expected payout of asset i and $Q \in \mathbb{R}^{n \times n}$ is the covariance matrix of all payouts. If additionally an investor is interested in having only a few active assets, this can be formulated as a sparse optimization problem

$$\min_x \ \frac{1}{2} x^T Q x + \rho \, \|x\|_0 \quad \text{s.t.} \quad e^T x = 1, \ \alpha^T x \geq \beta, \ x \geq 0. \tag{30}$$

Pre-processing this sparse problem with the ℓ_1-norm does not yield any useful result, because for all $x \geq 0$ we have $\|x\|_1 = e^T x$, which is constant on the feasible set of (30). Therefore, solutions of the ℓ_1-surrogate problem for (30) coincide with solutions of (29). We thus solve (29) in our numerical tests to obtain an initial point x^0 minimizing $x^T Q x$ on the feasible set and then use Lagrange–Newton-type methods to search for a sparse value x^* in its vicinity.

We ran our tests in MATLAB[1] R2020b and used the set of synthetic portfolio selection test problems from Frangioni and Gentile[2] in Sect. 7.2.1 and some real-world financial data acquired via the python module `yfinance`[3] in Sect. 7.2.2.

7.2.1 Test examples by frangioni and gentile

In order to obtain the form (30), we neglected the upper and lower bounds on entries $i \notin I_0(x)$ of x given in the test collection. The initial point x^0 was obtained by applying the `quadprog`-function of MATLAB to problem (29). In the Lagrange–Newton-type methods, the restriction $x \geq 0$ was then only explicitly incorporated in the operator T_C. For T and T_{red} these sign constraints were only considered in the termination criterion, but not present in the Lagrange–Newton-step. Nonetheless, for all test instances and all operators T, T_{red}, T_C the algorithms terminated within 100 steps in an ε-feasible point.

The goals was to iterate from the x^0 to a point, which is still sufficiently good with regards to the objective $f(x)$, but is of much higher sparsity than x^0. For $\rho = 1$ and dimension $n = 400$, the resulting values of $f(x) + \|x\|_0$ for the initial value x^0 and the three Lagrange-Newton-type methods are given in Fig. 2. The average amount of necessary iterations, as well as the required (system-)time (including 0.02s on average to procure a solution by the call to `quadprog`) to obtain a stationary point for each of the three methods is shown in Table 1.

[1] https://de.mathworks.com/products/matlab.html.

[2] http://groups.di.unipi.it/optimize/Data/MV.html.

[3] https://pypi.org/project/yfinance/.

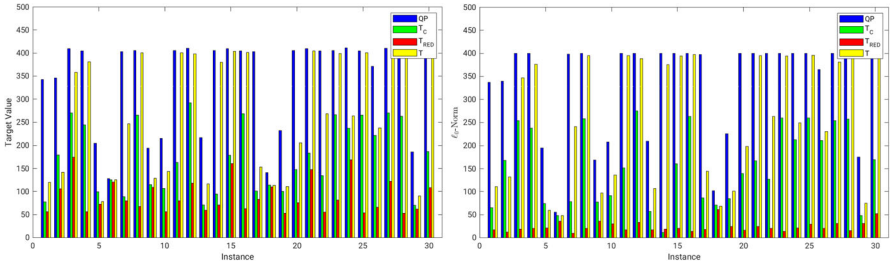


Fig. 2 Target value $f(x) + \|x\|_0$ and ℓ_0-norm for portfolio selection with dimension $n = 400$

Table 1 A comparison of runtime and number of iterations

	T_C	T_{red}	T
Average number of iterations	12.9	40.7	35.9
Average system-time	0.65s	0.93s	1.85s

In every instance we were able to improve on the initial point x^0, computed with `quadprog` applied to (29), with any of the solutions obtained by T, T_{red} and T_C. Almost always, T_{red} led to the best results followed by T_C and finally T. However, T_{red} as well as T have a much higher iteration count than anticipated for a Newton-type method, which could be caused by the difficult structure of the constraints $x \circ y = 0$ and $x \circ (1 - \gamma \circ x/\rho) = 0$, and the lack of a good initial guess x^0. Only T_C, where complementarity between x and y was handled by ϕ_{FB}, delivered a sufficiently low iteration count. To have an idea of the quality of the obtained stationary points, we applied the mixed-integer solver GUROBI[4] with a runtime of 300 seconds system-time to the 30 instances of dimension $n = 400$. We compared the results of GUROBI to the ones achieved by T_{red}, since the latter one performed the best amongst our proposed operators. The results are detailed in Fig. 3. We see that the solutions obtained by our approach are usually not too far away from those found by GUROBI, in some instances even better. Note that the average running time of T_{red} was at 0.93s, whereas GUROBI was set so 300s, which is by a factor of approximately 322.58 slower than the aforementioned Lagrange–Newton method.

7.2.2 Financial data

We picked 198 stocks with medium to mega cap in the US region among the top stock gainers as listed on yahoo finance on February 5th 2024. To generate the Markov risk model we acquired financial data for these 193 assets between January 1st 2015 and February 5th 2024 via the yahoo finance API. The covariance matrix Q and the vector α of expected returns were generated by the `pyoptportfolio`[5] package. The matrix Q was created with the `risk_matrix` function, where `ledoit_wolf` was chosen as the method and the annual expected returns α were estimated by a

[4] https://www.gurobi.com.

[5] https://pyportfolioopt.readthedocs.io/en/latest/.

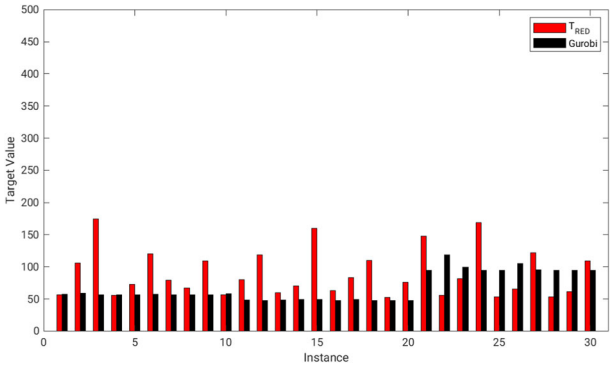


Fig. 3 Comparison of the target value $f(x) + \|x\|_0$ between T_{red} and GUROBI for $n = 400$

Table 2 Finance data overview

	$f(x) + \|x\|_0$	$f(x)$	$\|x\|_0$	CPU-time	#Iterations	(annual) exp. return	(annual) Sharpe ratio[1]
ℓ_1	196.03	0.03	196	0.16s	-	21.097	123.82
T	136.04	0.04	136	0.28s	57	23.22	118.76
T_{red}	5.28	4.28	1	0.19s	68	1174.9	568.24
T_C	31.19	0.19	31	0.08	11	46.73	107.37

[1] Introduced by William F. Sharpe. For reference see [33]

call to the `mean_historical_return` function. In order to construct a feasible problem, we chose

$$\beta = \frac{1}{n}\sum_{i=1}^{n} \alpha_i \quad (\approx 21.097).$$

The numerical test was carried out in exactly the same way as described in the previous subsection. We detail the results[6] in Table 2.

In a second test, arbitrary upper bounds $u \in [0, 1]^n$ were introduced to the set of constraints. The components u_i were drawn from a uniform distribution over the interval $[0, 1]$. We observed T_{red} sometimes generating negative entries in x, which has to be considered as a failed run. As we explicitly cannot add $x \geq 0$ to our set of constraints we instead augmented the target function with a penalty term

$$f(x) + \rho y^T (y - 2) + \alpha \, \|\min\{0, x\}\|_2^2 ,$$

[6] Newton's method failed to converge for T_{red} when starting at x_0 generated by the ℓ_1-solver. We instead applied the method directly to $x_0 = 0$, where the first iteration was taken as a least squares approximation. However, the initial point $x^0 = 0$ did not work for T and T_C as T failed entirely and T_C returned significantly worse values. For this reason, we started T and T_C as in the previous section with the initial point x^0 generated by the ℓ_1-solver and only started T_{red} with $x^0 = 0$. (Note that in general $x^0 = 0$ is not an ideal initial point, because the corresponding Jacobian of all there of the above operators are singular in $x = 0$.).

Table 3 Finance data with upper bounds overview

	$f(x)+\|x\|_0$	$f(x)$	$\|x\|_0$	CPU-time	#Iterations	(annual) exp. return	(annual) Sharpe ratio
ℓ_1	196.03	0.03	196	0.16s	–	21.097	123.82
T	136.24	0.04	136.2	2.58s	51.4	25.76	129.61
T_{red}	7.17	3.07	4.1	1.7s	55	811.32	481.36
T_C	82.09	0.09	82	0.55s	10	41.24	130.37

with an $\alpha > 0$. Notice that the new target function remains C^1, whereas its gradient is still semismooth. As the given covariance matrix Q was strictly positive definite and the newly added penalty term is convex, we may recover BD-regularity at zeros of the respective operators. For computational purposes we went with the somewhat canonical choice of setting $\alpha = 1/2$. In Table 3, we detail the average results over 10 indivdual runs.

7.3 Compressive sensing

In its essence, compressive sensing deals with reconstructing an n-dimensional vector $\overline{x}$ encoded by some sensing-matrix $A \in \mathbb{R}^{m\times n}$ with $m \ll n$ into a signal $A\overline{x} = b$ of much lower dimension. Assuming that the original signal $\overline{x}$ was sparse leads to the following formulation for compressive sensing

$$\min_x \ \|x\|_0 \quad \text{s.t.} \quad Ax = b, \tag{31}$$

which was studied by Tao and Candès [7]. Problem (31) can be seen as an instance of SPO with $f \equiv 0$. Since we need some second order information for our local Newton-type methods, instead of the noise-free problem (31) we are more interested in the problem

$$\min_x \ \|x\|_0 \quad \text{s.t.} \quad \left\|Ax - \overline{b}\right\|_2 \leq \delta,$$

with some tolerance $\delta > 0$. This problem is motivated by the assumption that the received signal is $\overline{b} = b + r$ with some noise r. However, this formulation requires that the noise level δ is known at least approximately. To avoid this problem, a penalty formulation

$$\min_x \ \frac{1}{2}\left\|Ax - \overline{b}\right\|_2^2 + \rho\,\|x\|_0 \tag{32}$$

as seen in [35] is often considered instead. Replacing the ℓ_0-norm with the convex, sparsity inducing ℓ_1-norm results in the *basis persuit denoising* problem, presented as in [9]:

$$\min_x \ \frac{1}{2}\left\|Ax - \overline{b}\right\|_2^2 + \rho\,\|x\|_1\,. \tag{33}$$

In our numerical test, we compute an initial point x^0 by solving the ℓ_1-surrogate problem (33) and then use x^0 together with the three Newton-type methods to solve (32).

We set up our examples as in [37]: Let $SA \in \mathbb{R}^{(m+p)\times n}$ be some sensing-matrix and $\overline{x} \in \mathbb{R}^n$ be some sparse vector. We set:

$$Sb := SA \cdot \overline{x},$$

and split SA and Sb into:

$$SA = \begin{pmatrix} A \\ C \end{pmatrix}, \quad A \in \mathbb{R}^{m\times n}, C \in \mathbb{R}^{p\times n}, \quad Sb = \begin{pmatrix} b \\ d \end{pmatrix}, \quad b \in \mathbb{R}^m, d \in \mathbb{R}^p.$$

We then consider the following problem

$$\min_x \; F_\rho(x) := \frac{1}{2}\|Ax - b\|_2^2 + \rho\,\|x\|_0 \quad \text{s.t.} \quad Cx = d, \tag{34}$$

where the linear constraints $Cx = d$ can be considered as noise-free information and exclude $x = 0$ from the feasible set. The dimensions were set to $n = 512$, $m = 128$ and $p = 8$, the sparsity of $\overline{x}$ was chosen as $s = \|\overline{x}\|_0 = 32$. The sensing-matrix SA was initialized as a Gauß-matrix as in [36], such that:

$$SA_j \sim \mathcal{N}(0, E_{p+m}/(p+m)), \quad \forall j = 1, \ldots, n.$$

Closely following [37], we initialized the components of (34) as

$$\begin{array}{lll} \bar{x} = \texttt{zeros}(n, 1), & \Gamma = \texttt{randperm}(n), & \bar{x}(\Gamma(1:s)) = \texttt{randn}(s, 1), \\ Sb = SA\bar{x}, & & \\ J = \texttt{randperm}(p+m), & J_1 = J(1:m), & J_2 = J(m+1:end), \\ A = SA(J_1), & b = Sb(J_1), & C = SA(J_2), \\ d = Sb(J_2). & & \end{array}$$

To obtain an initial guess x^0, we considered the ℓ_1-problem (33) as a quadratic program and applied MATLAB's `quadprog` as seen in [18], which required the split $x = x_+ - x_-$ with $x_+, x_- \geq 0$. From the solution (x_+^0, x_-^0) we could recover $x^0 = x_+^0 - x_-^0$. Note that in order to invoke the operator T_C, we now have to split x into positive and negative part, because otherwise we do not have any nonnegativity constraints. For T_C we thus used (x_+^0, x_-^0) as is to initialize the algorithm. Unfortunately, this split leads to a much higher computational cost for T_C, since in every Newton-step a system of $6n + m$ equations had to be solved.

This time we chose a discrete set $\{0.1, 0.5, 1, 2, 3, 4, 5\}$ of values for ρ and ran 100 test examples for each of those values. We were faced with some unsuccessful runs regarding T_C, where the algorithm failed to converge in 5.6% of all tests, since either the iteration number exceeded the maximum of 100 steps or we had to terminate

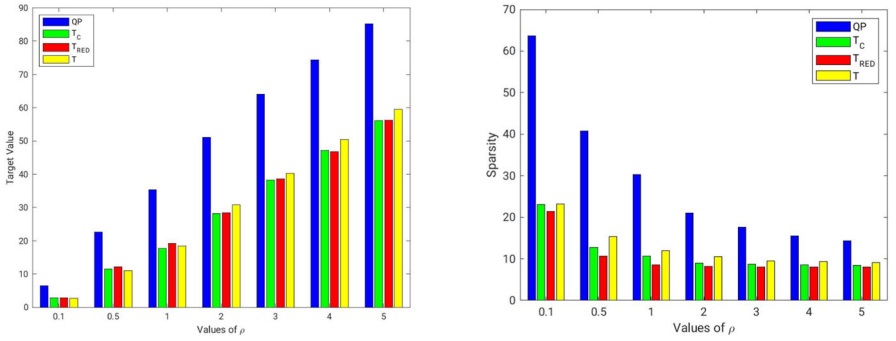


Fig. 4 Average target value of $f(x) + \rho \|x\|_0$ and ℓ_0-Norm for successful compressive sensing runs

early, as the error in the Newton-step with respect to the ℓ_2-norm went past the safety threshold of 100. For all values of ρ, the resulting average value $f(x) + \rho \|x\|_0$ of all successful runs is shown in Fig. 4. Again, we observe a significant improvement of the objective function value for all operators T, T_{red}, T_C, but now with less pronounced differences between the three operators.

7.4 Logistic regression

Consider the following sparse optimization problem

$$\min_w \sum_{i=1}^{m} \log(1 + \exp(-y_i \cdot w^T x_i)) + \rho \|w\|_0 , \tag{35}$$

which we refer to as the penalized maximum log-likelihood function. This estimator is applied to match a sigmoid-function to a set of measurements $x_1, \ldots, x_m$ and corresponding Bernoulli-variables $y_1, \ldots, y_n \in \{-1, 1\}^m$, where additionally sparsity is promoted in the parameters w_i. Replacing $\|\cdot\|_0$ by $\|\cdot\|_1$ in (35), we obtain a convex composite optimization problem, which can be tackled by FISTA or proximal BFGS methods, compare [24].

In our numerical test, we consider the problem *gisette* from the NIPS 2003 feature selection challenge, which was acquired from the *LIBSVM*-website.[7] The classification problem is high-dimensional ($n = 5000, m = 6000$) and was scaled to $[-1, 1]$. Recall that applying either of the Newton-type methods with T_C, T or T_{red} to the *gisette* problem leads to a drastic increase in the dimensionality (in the case of T_C: $n = 30{,}000$). Computation was therefore outsourced to a faster PC and handled in *Python*.

We computed an initial point x^0 by solving the ℓ_1-surrogate problem to (35) with FISTA. Running the three Newton-type methods with this initial point then lead to the results in Fig. 5. The abbreviations *TCx, Tx, Rx* show the solutions found by the respective operators T_C, T and T_{red}. As one can see, all three of the operators lead to

[7] https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/.

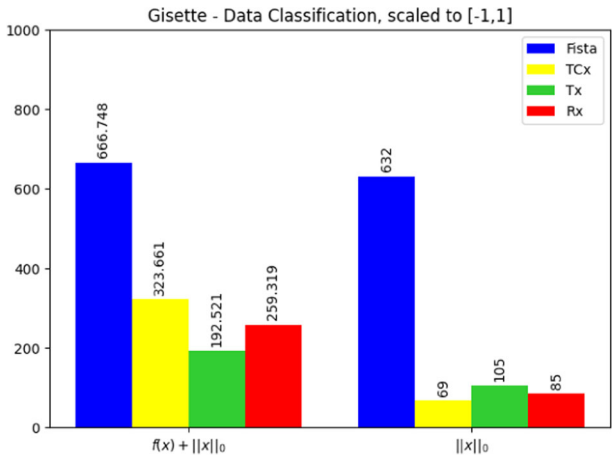


Fig. 5 Comparison of target value $f(x) + \|x\|_0$ and sparsity $\|x\|_0$ for logistic regression. TCx, Tx and Rx show the solutions found by the operators T_C, T and T_{red}, respectively

an improved sparsity $\|x\|_0$ and an improved function value $f(x) + \|x\|_0$, meaning a better solution of the original problem (35).

8 Final remarks

The aim of this paper was mainly to lay the theoretical foundation for two reformulations of the highly difficult sparse optimization problem SPO. In particular, it was shown that we get full equivalence of problem SPO with these two reformulations in terms of global and local minima. Moreover, the corresponding stationary conditions also coincide and corresponding second-order conditions are closely related. These results can be used to develop and investigate Lagrange–Newton-type methods for the numerical solution of problem SPO and the numerical results indicate that one can use these methods in order to get significant improvements of solutions obtained by some other techniques.

The Lagrange–Newton-type methods, of course, are local in nature, but result quite naturally as a direct consequence of our theoretical considerations.[8] Our future research, however, will concentrate on the development of globally convergent methods based on our reformulations. Some preliminary results in this direction can already be found in [32].

[8] https://pypi.org/project/yfinance/.

Appendix: Proofs for Section 3

Proof of Lemma 3.1 (i) The definition of the index set $I_0(x)$ and the assumed feasibility of (x, y) implies

$$n - e^T y = n - \sum_{i \in I_0(x)} y_i - \sum_{i \notin I_0(x)} y_i = n - \sum_{i \in I_0(x)} y_i \geq n - \sum_{i \in I_0(x)} 1 = \|x\|_0 .$$

This also shows that equality holds if and only if $y_i = 1$ for all $i \in I_0(x)$.

(ii) Recall that the function $y_i \mapsto y_i(y_i - 2)$ attains its (unique) minimum at $y_i = 1$ with corresponding minimal function value -1. The definition of the index set $I_0(x)$ and the feasibility of (x, y) therefore yield

$$\sum_{i=1}^{n} y_i(y_i - 2) = \sum_{i \in I_0(x)} y_i(y_i - 2) \geq \sum_{i \in I_0(x)} -1 = \Big(n - \sum_{i \in I_0(x)} 1\Big) - n = \|x\|_0 - n,$$

and equality holds if and only if $y_i = 1$ for all $i \in I_0(x)$.

□

Proof of Lemma 3.2 Let (x^*, y^*) be a local minimum of SPOlin. We can fix $x = x^*$ and know that y^* solves

$$\max_y \; e^T y \quad \text{s.t.} \quad y_i = 0, \; i \notin I_0(x^*), \; y \leq e.$$

Similarly, let (x^*, y^*) be a local minimum of SPOsq. We can fix $x = x^*$ and know that y^* solves

$$\min_y \sum_{i=1}^{n} y_i(y_i - 2) \quad \text{s.t.} \quad y_i = 0, \; i \notin I_0(x^*).$$

In both cases the statement follows. □

Proof of Proposition 3.3 Let ρ_1 and ρ_2 be two penalty parameters, and let x^* be a local minimum of

$$\min_x \; f(x) + \rho_1 \|x\|_0 \quad \text{s.t.} \quad x \in X. \tag{36}$$

Assume that x^* is not a local minimum of

$$\min_x \; f(x) + \rho_2 \|x\|_0 \quad \text{s.t.} \quad x \in X.$$

Then there exists a sequence $\{x^k\} \subseteq X$ with $x^k \to x^*$ such that

$$f(x^k) + \rho_2 \left\|x^k\right\|_0 < f(x^*) + \rho_2 \left\|x^*\right\|_0 \quad \forall k \in \mathbb{N}. \tag{37}$$

Note that $\left\|x^k\right\|_0 \geq \|x^*\|_0$ holds for all k sufficiently large. First consider the case that there exists a subsequence such that $\left\|x^k\right\|_0 = \|x^*\|_0$ holds for all $k \in K$. Then we obtain

$$\begin{aligned} f(x^k) + \rho_1 \left\|x^k\right\|_0 &= f(x^k) + \rho_2 \left\|x^k\right\|_0 + (\rho_1 - \rho_2) \left\|x^k\right\|_0 \\ &< f(x^*) + \rho_2 \left\|x^*\right\|_0 + (\rho_1 - \rho_2) \left\|x^k\right\|_0 \\ &= f(x^*) + \rho_2 \left\|x^*\right\|_0 + (\rho_1 - \rho_2) \left\|x^*\right\|_0 \;=\; f(x^*) + \rho_1 \left\|x^*\right\|_0 \end{aligned}$$

for all $k \in K$, contradicting the assumption that x^* is a local minimum of (36). In the other case, we have $\left\|x^k\right\|_0 > \|x^*\|_0$ and, therefore, $\|x^*\|_0 + 1 \leq \left\|x^k\right\|_0$ for almost all $k \in \mathbb{N}$. Furthermore, by continuity of f, it follows that $f(x^*) \leq f(x^k) + \rho_2$ for all k sufficiently large. This implies

$$\begin{aligned} f(x^*) + \rho_2 \left\|x^*\right\|_0 \leq f(x^k) + \rho_2 + \rho_2 \|x^*\|_0 = f(x^k) + \rho_2\big(1 + \|x^*\|_0\big) \\ \leq f(x^k) + \rho_2 \left\|x^k\right\|_0, \end{aligned}$$

a contradiction to (37). Altogether, this completes the proof. □

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Data availability The data which was used to create the results within this manuscript is composed of 1. mixed-integer portfolio optimization problems by Frangioni and Gentile. At the moment of writing, they are publicly available (c.f. page 22, footnote 2). To our knowledge, the test instance are randomly generated. The specific instance for this manuscript lies with the authors and is available on request. 2. financial data collected with the `yfinance` python-package[9]. The acquired data was solely used to create values for the numerical experiment in Sect. 7.2.2. The data lies with the authors and is available on request. 3. compressive sensing test sets, which have been generated procedurally and randomly by MATLAB from a random seed. 4. the *gisette* classification problem, which originates from the NIPS 2003 feature selection challenge. The specific data used in section 7.4 is publicly available with the *LIBSVM*-library (c.f. page 26, footnote 8).

Declarations

Conflict of interest There are no conflict of interest to report.

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