Merit functions for semi-definite complementarity problems¹

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Abstract

Merit functions such as the gap function, the regularized gap function, the implicit Lagrangian, and the norm squared of the Fischer-Burmeister function have played an important role in the solution of complementarity problems defined over the cone of nonnegative real vectors. We study the extension of these merit functions to complementarity problems defined over the cone of block-diagonal symmetric positive semi-definite real matrices. The extension suggests new solution methods for the latter problems. © 1998 The Mathematical Programming Society, Inc. Published by Elsevier Science B.V.

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1. Introduction

There recently has been very active research on semi-definite linear programs (SDLP) and, more generally, semi-definite linear complementarity problems (SDLCP), which are extensions of LP and LCP, respectively, whereby the cone of nonnegative real vectors is replaced by the cone of symmetric positive semi-definite real matrices. These problems have important applications in engineering [5] and in combinatorial optimization [1,23,25], where the SDLP relaxation can yield a much better approximation of the original problem than does the LP relaxation [23]. Although SDLP are special cases of convex programs, difficulties with representing the positive semi-definiteness constraint algebraically and with the possible presence of a duality gap have thus far rendered conventional solution methods for convex programs ineffective for SDLP. Instead, research efforts have focussed on interior-point methods, for SDLP (see [1,2,27,35,46,47,54,62] and references therein) and,

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to a lesser extent, for SDLCP [35,60] and for semi-definite (nonlinear) complementarity problems (SDCP) [57]. There have also been preliminary efforts to develop simplex type methods for SDLP [51]. While interior-point methods have been successful at solving SDLP, it is worthwhile to explore other solution approaches for SDLP and for the more general problems of SDLCP and SDCP. In particular, there recently has been active research on the use of *merit functions* to solve LCP and NCP [8,10,13–16,18,20,29,30,32,44,50] and the solution methods thus developed, such as the Newton-type methods based on the Fischer–Burmeister function, appear to be more effective than interior-point methods. Motivated by these developments, we study in this paper the extension of merit functions for LCP/NCP to its semi-definite counterpart, SDCP. As we shall see, this extension is easy for some merit functions, namely the gap function, the regularized gap function, and the implicit Lagrangian, but is highly nontrivial for other merit functions, namely those based on the Fischer– Burmeister function (see Sections 6 and 7).

We formally describe the semi-definite complementarity problem (SDCP) below. Let \mathscr{X} denote the space of $n \times n$ block-diagonal real matrices with *m* blocks of sizes n_1, \ldots, n_m , respectively (the blocks are fixed). Thus, \mathscr{X} is closed under matrix addition x + y, multiplication xy, transposition x^T , and inversion x^{-1} , where $x, y \in \mathscr{X}$. We endow \mathscr{X} with the inner product and norm.

$$\langle x, y \rangle := \operatorname{tr}[x^{\mathrm{T}}y], \qquad ||x|| := \sqrt{\langle x, x \rangle},$$

where $x, y \in \mathcal{X}$ and $tr[\cdot]$ denotes the matrix trace (i.e., $tr[x] = \sum_{i=1}^{n} x_{ii}$). (||x|| is the Frobenius-norm of x and := means "define".) Let \mathscr{S} denote the subspace comprising those $x \in \mathscr{X}$ that are symmetric, i.e., $x^{T} = x$. Let \mathscr{K} denote the closed convex cone comprising those elements of \mathscr{S} that are positive semi-definite (abbreviated as "psd"). Our problem is to find, for given mappings $F : \mathscr{S} \mapsto \mathscr{S}$ and $G : \mathscr{S} \mapsto \mathscr{S}$, an $x \in \mathscr{S}$ satisfying

$$F(x) \in \mathscr{K}, \qquad G(x) \in \mathscr{K}, \qquad \langle F(x), G(x) \rangle = 0.$$
 (1)

This problem contains as special cases the SDLP (for which $n_2 = \cdots = n_m = 1$, $G \equiv I$ and F is affine and skew-symmetric in the sense that $\langle x - x', F(x) - F(x') \rangle = 0$ for all $x, x' \in \mathscr{S}$) and LCP/NCP (for which $n_1 = \cdots = n_m = 1$ and $G \equiv I$). Notice that $(\mathscr{S}, \langle \cdot, \cdot \rangle, || \cdot ||)$ forms a Hilbert space. In fact, each matrix $x \in \mathscr{S}$ may be associated with the vector $\hat{x} := (\cdots, x_{ij}, \cdots)_{i \leq j}^T \in \mathfrak{R}^v$, where $v := \sum_{k=1}^m n_k (n_k + 1)/2$. Accordingly, the inner product on \mathscr{S} is associated with the weighted Euclidean inner product on \mathfrak{R}^v : $\langle \hat{x}, \hat{y} \rangle_{\mathfrak{R}^v} := \sum_{k=1}^m \sum_{i=n_1+\cdots+n_{k-1}+1}^{n_1+\cdots+n_k} (x_{ii}y_{ii} + \sum_{j=i+1}^{n_1+\cdots+n_k} 2x_{ij}y_{ij})$, and \mathscr{K} corresponds to a certain closed convex cone in \mathfrak{R}^v . While \mathscr{K} has a complicated geometrical structure compared to the nonnegative orthant in \mathfrak{R}^v , it does share the property that $\mathscr{K}^\circ = -\mathscr{K}$, where $\mathscr{K}^\circ := \{y \in \mathscr{S} : \langle x, y \rangle \leq 0 \ \forall x \in \mathscr{K}\}$.

We say that a function $f: \mathscr{C} \mapsto [0, \infty)$ is a merit function (for the SDCP) on a set $\mathscr{C} \subset \mathscr{S}$ (typically $\mathscr{C} = \mathscr{S}$ or $\mathscr{C} = G^{-1}(\mathscr{K})$), provided that x satisfies Eq. (1) if and only if f(x) = 0. Then we may reformulate the SDCP as the following minimization problem:

minimize f(x) subject to $x \in \mathscr{C}$,

and apply a feasible descent method to solve this minimization problem. There are many choices for a merit function. The earliest choices is the gap function

$$f(x) := \max_{\zeta \in \mathscr{K}} \{ \langle F(x), G(x) - \zeta \rangle \}$$
(2)

proposed by Auslender [4] and Hearn [24], which is a merit function on $G^{-1}(\mathcal{K})$ (see Proposition 3.1). There is also a "dual" version of this gap function, given by

$$f(x) := \max_{\zeta \in \mathscr{K}} \{ \langle F(G^{-1}(\zeta)), G(x) - \zeta \rangle \},\tag{3}$$

which is a merit function on $G^{-1}(\mathscr{K})$ provided that F and G are relatively pseudomonotone on $G^{-1}(\mathscr{K})$ and F is continuous on $G^{-1}(\mathscr{K})$ and G^{-1} is defined and continuous on \mathscr{K} (see Proposition 3.2). A second choice is the regularized gap function, parameterized by a scalar $\alpha > 0$,

$$f_{\alpha}(x) := \max_{\zeta \in \mathscr{K}} \left\{ \langle F(x), G(x) - \zeta \rangle - \frac{1}{2\alpha} \| G(x) - \zeta \|^2 \right\}$$
(4)

proposed independently by Fukushima [20] and Auchmuty [3], which is a merit function on $G^{-1}(\mathscr{K})$ (see Proposition 4.1). (See [21,36] and references therein for surveys and extensions of gap and regularized gap functions.) A third choice is the implicit Lagrangian function, parameterized by a scalar $\alpha > 1$,

$$f_{\alpha}(x) := \max_{\xi,\zeta\in\mathscr{X}} \left\{ \langle F(x), G(x) - \zeta \rangle - \langle \xi, G(x) \rangle - \frac{1}{2\alpha} (\|F(x) - \xi\|^2 + \|G(x) - \zeta\|^2) \right\}$$
(5)

proposed by Mangasarian and Solodov [44] in the context of NCP and further studied in [11,28,38,52,53,61,64,65], which is a merit function on \mathscr{S} (see Proposition 5.1). A fourth choice is the function

$$f(x) := \|G(x) - [G(x) - F(x)]_{+}\|^{2}$$
(6)

studied in [7,37,39,41,45,48,50], which is a merit function on \mathscr{S} (see Proposition 2.1). (Here $[\cdot]_+$ denotes orthogonal projection onto \mathscr{K} : $[x]_+ = \arg \min_{\xi \in \mathscr{K}} ||x - \xi||$.) A fifth choice is

$$f(x) := \frac{1}{2} \|\phi(F(x), G(x))\|^2, \tag{7}$$

where $\phi \colon \mathscr{S} \times \mathscr{S} \mapsto \mathscr{S}$ is the function

$$\phi(a,b) := (a^2 + b^2)^{1/2} - (a+b) \tag{8}$$

attributed by Fischer to Burmeister (see [15,17,18]). This choice of f, which is a merit function on \mathscr{S} (see Proposition 6.1), has been much studied in the context of NCP (see [8,12–14,19,22,28,29,31–34,59]; also see [16] for a survey). In the case of NCP, other choices of the function ϕ in Eq. (7) have been proposed, with the earliest one given by Mangasarian [43], followed by other proposals [9,30–32,59]. However, it is unclear whether these other choices can be extended to SDCP (see the discussion following Lemma 2.1). A sixth choice is

$$f(x) := \psi_0(\langle F(x), G(x) \rangle) + \psi(F(x), G(x)), \tag{9}$$

where $\psi_0: \mathfrak{R} \mapsto [0, \infty)$ satisfies $\psi_0(t) = 0$ if and only if $t \leq 0$ and $\psi: \mathscr{S} \times \mathscr{S} \mapsto [0, \infty)$ satisfies

$$\psi(a,b) = 0, \quad \langle a,b \rangle \leqslant 0 \text{ if and only if } (a,b) \in \mathscr{K} \times \mathscr{K}, \quad \langle a,b \rangle = 0.$$
(10)

This function, studied by Luo and the author [42] in the context of NCP, is a merit function on \mathscr{S} (see Proposition 7.1). For each of the above six choices of f, we will derive conditions for f to be convex and/or differentiable, and for the stationary point of f to be a solution of SDCP. We will also study, to a lesser extent, growth properties of f and the generation of feasible descent directions for f.

In what follows, we denote by \mathcal{O} the set of orthogonal $p \in \mathcal{X}$ (i.e., $p^{T} = p^{-1}$). We say that F and G are relatively pseudo-monotone on $\mathcal{C} \subset \mathcal{S}$ if

$$\langle F(x), G(x) - G(x') \rangle \leq 0 \Rightarrow \langle F(x'), G(x) - G(x') \rangle \leq 0 \quad \forall x, x' \in \mathscr{C}.$$

More restrictively, F and G are relatively monotone on \mathscr{C} if

$$\langle F(x) - F(x'), G(x) - G(x') \rangle \ge 0 \quad \forall x, x' \in \mathscr{C}$$

and F and G are relatively strongly monotone on \mathscr{C} if there exists a $\gamma \in (0,\infty)$ such that

$$\langle F(x) - F(x'), G(x) - G(x') \rangle \ge \gamma ||x - x'||^2 \quad \forall x, x' \in \mathscr{C}.$$

(In the case where $G \equiv I$, the above three conditions reduce to F being, respectively, pseudo-monotone, monotone, and strongly monotone.) When F is differentiable (in the Fréchet sense) on \mathscr{C} , we denote by $\nabla F(x)$ the Jacobian of F at each $x \in \mathscr{C}$, viewed as a linear mapping from \mathscr{G} to \mathscr{G} . When a function $f: \mathscr{C} \mapsto \mathfrak{R}$ is differentiable (in the Fréchet sense) on \mathscr{C} , we denote by ∇f the gradient of f, viewed as a mapping from \mathscr{C} to \mathscr{S} . We say that a linear mapping $M: \mathscr{S} \mapsto \mathscr{S}$ is positive semi-definite (respectively, positive definite) if $\langle x, Mx \rangle \ge 0$ (respectively, $\langle x, Mx \rangle > 0$) for all $x \in \mathcal{S}$ with $x \ne 0$, and we denote the adjoint of M by M^* (i.e., $\langle y, Mx \rangle = \langle M^*y, x \rangle$ for all $x, y \in \mathcal{S}$). For any $x \in \mathcal{S}$, we denote by x_{ij} the (i, j)th entry of x and, for any $I, J \subset \{1, \ldots, n\}$, we denote by x_{IJ} the submatrix of x with rows $i \notin I$ and columns $j \notin J$ removed. For any $\lambda_1, \ldots, \lambda_n \in \mathfrak{R}$, we denote by diag $[\lambda_1, \ldots, \lambda_n]$ the $n \times n$ diagonal matrix with diagonal entries $\lambda_1, \ldots, \lambda_n$. We will freely use the following facts about trace [26]: For any $x, y \in \mathscr{X}$ and any $p \in \mathscr{O}$, $tr[x] = tr[x^T] = tr[pxp^T]$, tr[xy] = tr[yx], and tr[x+y] = tr[yx]tr[x] + tr[y]. Also, $\|\cdot\|$ is a norm on \mathscr{X} and, in particular, the triangle inequality and the Cauchy-Schwarz inequality hold for $\|\cdot\|$. Lastly, we have from $\mathscr{K}^{\circ} = -\mathscr{K}$ that, for any $a \in \mathscr{S}$,

$$a \in \mathscr{K} \iff \langle a, b \rangle \ge 0 \quad \forall b \in \mathscr{K}$$

$$\tag{11}$$

and (see Lemma 2.1(a) and [66], Lemma 2.2)

$$a = [a]_{+} + [a]_{-}, \qquad [a]_{+}[a]_{-} = 0, \qquad [a]_{-} = -[-a]_{+},$$

$$a[a]_{+} = [a]_{+}a = ([a]_{+})^{2}, \qquad (12)$$

where $[\cdot]_{-}$ denotes the orthogonal projection on to \mathscr{K}° .

2. Projection residual function

In this section, we study the merit function f given by Eq. (6), which has a relatively simple structure and is related to the growth rate of many other merit functions. We begin with the following lemma, part (a) of which gives a way to compute the projection $[a]_+$ via the spectral decomposition of a.

Lemma 2.1. (a) For any $a \in \mathcal{S}$, we have $[a]_+ = p^T \operatorname{diag}[\max\{0, \lambda_1\}, \dots, \max\{0, \lambda_n\}]p$, where $p \in \mathcal{O}$ and $\lambda_1, \dots, \lambda_n \in \mathfrak{R}$ satisfy $a = p^T \operatorname{diag}[\lambda_1, \dots, \lambda_n]p$.

(b) For any $(a,b) \in \mathscr{S} \times \mathscr{S}$, we have $a, b \in \mathscr{K}$, $\langle a, b \rangle = 0$ if and only if $a = [a - b]_+$.

Proof. (a). We have, for any $c \in \mathscr{K}$ that

$$\|a - c\|^{2} = \|pap^{\mathsf{T}} - pcp^{\mathsf{T}}\|^{2} = \|\text{diag}[\lambda_{1}, \dots, \lambda_{n}] - pcp^{\mathsf{T}}\|^{2}$$
$$= \sum_{i=1}^{n} \left((\lambda_{i} - [pcp^{\mathsf{T}}]_{ii})^{2} + \sum_{j \neq i} ([pcp^{\mathsf{T}}]_{ij})^{2} \right),$$

where the third equality also uses the symmetry of pcp^{T} . Since $pcp^{T} \in \mathcal{H}$ so that $[pcp^{T}]_{ii} \ge 0$ for all *i*, the right-hand side is minimized by the *c* with $[pcp^{T}]_{ii} = \max\{0, \lambda_i\}$ and $[pcp^{T}]_{ij} = 0$ for all $i \ne j$, i.e., $c = p^{T} \operatorname{diag}[\max\{0, \lambda_1\}, \ldots, \max\{0, \lambda_n\}]p$.

(b). This result is well known [66] and the proof is included for completeness. Consider any $(a,b) \in \mathscr{K} \times \mathscr{K}$ satisfying $\langle a,b \rangle = 0$. For any $c \in \mathscr{K}$,

$$||(a-b)-c||^{2} = ||a-c||^{2} + 2\langle c-a,b\rangle + ||b||^{2} = ||a-c||^{2} + 2\langle c,b\rangle + ||b||^{2}.$$

Since $b \in \mathscr{K}$ so, by Eq. (11), $\langle c, b \rangle \ge 0$, the right-hand side attains its minimum at c = a so $a = [a - b]_+$. Conversely, consider any $(a, b) \in \mathscr{S} \times \mathscr{S}$ satisfying $a = [a - b]_+$. Then $a \in \mathscr{K}$ and

$$0 \le ||(a-b) - c||^2 - ||b||^2 = ||a-c||^2 + 2\langle c-a, b\rangle \quad \forall c \in \mathscr{K}.$$
(13)

For any $z \in \mathscr{K}$ and any $t \in (0, \infty)$, we have $c := a + tz \in \mathscr{K}$ and so Eq. (13) yields $0 \leq t^2 ||z||^2 + 2t\langle z, b \rangle$. Dividing both sides by t and letting $t \to 0$ yields $0 \leq \langle z, b \rangle$ for all $z \in \mathscr{K}$. By Eq. (11), $b \in \mathscr{K}$. Similarly, for any $t \in (0, 1]$, we have $c := (1 - t)a \in \mathscr{K}$ and so Eq. (13) yields $0 \leq t^2 ||a||^2 - 2t\langle a, b \rangle$. Dividing both sides by t and letting $t \to 0$ yields $0 \leq -\langle a, b \rangle$. Since $a, b \in \mathscr{K}$ so $\langle a, b \rangle \ge 0$ by Eq. (11), this implies $\langle a, b \rangle = 0$. \Box

Just as in the NCP case, the residual $[a - b]_+ - a$ may be written equivalently in Mangasarian's framework [43] as $\frac{1}{2}(|a - b| - a - b)$, where $|x| := (x^2)^{1/2}$ for any

 $x \in \mathscr{S}$. This is because $|a - b| = p^{\mathrm{T}} \mathrm{diag}[|\lambda_1|, \dots, |\lambda_n|]p$, where $p \in \mathscr{O}$ and $\lambda_1, \dots, \lambda_n \in \Re$ satisfy $a - b = p^{\mathrm{T}} \mathrm{diag}[\lambda_1, \dots, \lambda_n]p$, so that

$$|a - b| - a - b = |a - b| + (a - b) - 2a = p^{T} \operatorname{diag}[|\lambda_{1}| + \lambda_{1}, \dots, |\lambda_{n}| + \lambda_{n}]$$

$$p - 2a = 2p^{T} \operatorname{diag}[\max\{0, \lambda_{1}\}, \dots, \max\{0, \lambda_{n}\}]p - 2a = 2[a - b]_{+} - 2a,$$

where the last equality uses Lemma 2.1(a). Thus, there is some hope that perhaps Mangasarian's general formula of $\theta(|a-b|) - \theta(a) - \theta(b)$ can also be extended to SDCP (assuming $\theta: \mathcal{G} \mapsto \mathcal{G}$ is strictly monotone and satisfies $\theta(0) = 0$?)

It follows from Lemma 2.1(b) that an $x \in \mathcal{S}$ satisfies Eq. (1) if and only if

 $G(x) - [G(x) - F(x)]_{+} = 0.$

The left-hand side, which, by Eq. (12), is equal to $F(x) - [F(x) - G(x)]_+$, is sometimes called the "projection residual". Thus f given by Eq. (6) is a merit function on \mathscr{S} , which we state formally in the following proposition along with a condition for f to have a quadratic growth rate.

Proposition 2.1. Let $f: \mathcal{S} \mapsto \mathfrak{R}$ be given by Eq. (6). Then the following hold: (a) $f(x) \ge 0$ for all $x \in \mathcal{S}$, and f(x) = 0 if and only if x satisfies Eq. (1). (b) If F and G are Lipschitz continuous and relatively strongly monotone on \mathcal{S} , then there exists a constant c > 0 such that $f(x) \ge c ||x - x^*||^2$ for all $x \in \mathcal{S}$, where x^* denotes the unique solution to Eq. (1).

Proof. (a) follows from Lemma 2.1(b). (b) follows from an argument similar to the proof of [48], Theorem. 3.1. \Box

A drawback of f given by Eq. (6), due in part to its nondifferentiability, is the difficulty of finding descent directions for it. In the case of NCP, the NE/SQP approach of Pang and Gabriel [50] finds descent directions, but this approach does not appear to extend to SDCP since the computation of each direction uses the Cartesian product structure of the nonnegative orthant as well as the solution of a certain convex quadratic program. Nonetheless, the projection residual motivates iterative methods of the form

 $G(x^{\text{new}}) \approx [G(x) - \alpha F(x)]_+,$

where $\alpha \in (0, \infty)$ is some suitably chosen stepsize. Although such methods are not descent methods for f given by Eq. (6), in the case where $G \equiv I$ and F is continuous and monotone, it has been shown that these methods are convergent (see [58] and references therein) and, in particular, are descent methods for the square of the distance (measured in the norm $\|\cdot\|$) to the solution set. However, these methods are first-order methods and, as such, are better suited for large-scale problems where second-order methods have difficulty.

3. Gap functions

In this section, we study the merit function f given by Eq. (2) and Eq. (3). Due to the correspondence between $(\mathscr{S}, \langle \cdot, \cdot \rangle)$ and $(\mathfrak{R}^{\nu}, \langle \cdot, \cdot \rangle_{\mathfrak{R}^{\nu}})$ with $\nu := \sum_{k=1}^{m} n_k (n_k + 1)/2$

(see the discussion in Section 1), most of the results are easy extensions of known results [4,24]. For completeness, we have included the proofs, which are short.

Proposition 3.1. Let $f: G^{-1}(\mathscr{K}) \mapsto \mathfrak{R} \cup \{\infty\}$ be given by Eq. (2). Then the following hold:

(a) For any $x \in G^{-1}(\mathcal{K})$, we have $f(x) \ge 0$ with f(x) = 0 if and only if x satisfies Eq. (1).

(b) If F and G are affine and relatively monotone on $G^{-1}(\mathcal{K})$, then f is convex on $G^{-1}(\mathcal{K})$.

Proof. (a). Fix any $x \in G^{-1}(\mathscr{K})$. By Eq. (11), if $F(x) \in \mathscr{K}$, then $\langle F(x), \zeta \rangle \ge 0$ for all $\zeta \in \mathscr{K}$, implying $f(x) = \langle F(x), G(x) \rangle \ge 0$ (the nonnegativity follows from $F(x), G(x) \in \mathscr{K}$); otherwise, there exists a $\zeta \in \mathscr{K}$ with $\langle F(x), \zeta \rangle < 0$, implying $f(x) = \infty$. Thus, $f(x) \ge 0$ and f(x) = 0 if and only if $F(x) \in \mathscr{K}$ and $\langle F(x), G(x) \rangle = 0$.

(b). Consider any $\zeta \in \mathscr{K}$ and let $f_{\zeta}(x) := \langle F(x), G(x) - \zeta \rangle$. For any $x, x' \in G^{-1}(\mathscr{K})$ and any $t \in [0, 1]$, by using the affine property of F and G, we obtain $f_{\zeta}(tx + (1 - t)x') = tf_{\zeta}(x) + (1 - t)f_{\zeta}(x') + t(1 - t)\langle F(x) - F(x'), G(x') - G(x) \rangle$. Then the relative monotonicity of F and G yields that f_{ζ} is convex on $G^{-1}(\mathscr{K})$, so f, being the pointwise maximum of $f_{\zeta}, \zeta \in \mathscr{K}$, is also convex on $G^{-1}(\mathscr{K})$. \Box

Proposition 3.2. Assume F and G are relatively pseudo-monotone on $G^{-1}(\mathcal{K})$, F is continuous on $G^{-1}(\mathcal{K})$, and G^{-1} is defined and continuous on \mathcal{K} . Let $f: G^{-1}(\mathcal{K}) \mapsto \mathfrak{R} \cup \{\infty\}$ be given by Eq. (3). Then the following hold:

(a) For any $x \in G^{-1}(\mathcal{K})$, we have $f(x) \ge 0$ with f(x) = 0 if and only if x satisfies Eq. (1).

(b) If in addition G is affine on $G^{-1}(\mathscr{K})$, then f is convex on $G^{-1}(\mathscr{K})$.

Proof. (a). Fix any $x \in G^{-1}(\mathscr{K})$. Then, $\zeta = G(x)$ is included in the max of Eq. (3), so $f(x) \ge 0$. If $F(x) \in \mathscr{K}$ and $\langle F(x), G(x) \rangle = 0$ so, by Eq. (11), $\langle F(x), G(x) - \zeta \rangle \le 0$ for all $\zeta \in \mathscr{K}$, the relative pseudo-monotonicity of F and G would imply $\langle F(G^{-1}(\zeta)), G(x) - \zeta \rangle \le 0$ for all $\zeta \in \mathscr{K}$ and hence f(x) = 0. Conversely, if f(x) = 0 so that $\langle F(G^{-1}(\zeta)), G(x) - \zeta \rangle \le 0$ for all $\zeta \in \mathscr{K}$, then, for any $\zeta' \in \mathscr{K}$, we would have, upon letting $x(t) := G^{-1}(t\zeta' + (1-t)G(x))$ for all $t \in (0, 1)$, that

$$\langle F(x(t)), G(x) - \zeta' \rangle = \frac{1}{t} \langle F(x(t)), G(x) - (t\zeta' + (1-t)G(x)) \rangle \leq 0$$

and, upon letting $t \to 0$ and using the continuity of F and G^{-1} , that $\langle F(x), G(x) - \zeta' \rangle \leq 0$. Then, Eq. (11) would imply that $F(x) \in \mathscr{K}$ and $\langle F(x), G(x) \rangle = 0$.

(b). Since G is affine on $G^{-1}(\mathscr{K})$, then, for each $\zeta \in \mathscr{K}$, the function $f_{\zeta}(x) := \langle F(G^{-1}(\zeta)), G(x) - \zeta \rangle$ is affine on $G^{-1}(\mathscr{K})$, so f, being the pointwise maximum of $f_{\zeta}, \zeta \in \mathscr{K}$, is convex on $G^{-1}(\mathscr{K})$. \Box

Under the hypothesis of Proposition 3.2, the SDCP is equivalent to the variational inequality problem of finding an $z^* \in \mathcal{K}$ satisfying

 $\langle F(G^{-1}(z^*)), z - z^* \rangle \ge 0 \quad \forall z \in \mathscr{K},$

and, moreover, $F \circ G^{-1}$ is pseudo-monotone and continuous on \mathscr{K} . Accordingly, Proposition 3.2 may alternatively be proven by suitably applying the results in [4], p. 121 or [24]. It should be noted that the two gap functions Eq. (2) and Eq. (3) are mainly of theoretical interest since, due in part to their nondifferentiability, there is no efficient method for minimizing them. For further discussions of these functions, see [21,36].

4. Regularized gap function

In this section, we study the merit function f_{α} given by Eq. (4). As with the gap functions of Section 3, most of the results are easy extensions of known results [3,20,61]. We begin with the following lemma based on [61], Proposition 2.1.

Lemma 4.1. For any $\alpha \in (0, \infty)$, define the function $\psi_{\alpha} \colon \mathscr{G} \times \mathscr{G} \mapsto \Re$ by

$$\psi_{\alpha}(a,b) := \max_{\zeta \in \mathscr{K}} \left\{ \langle a, b - \zeta \rangle - \frac{1}{2\alpha} \| b - \zeta \|^2 \right\}.$$

Then the following hold:

(a) For all $(a,b) \in \mathscr{S} \times \mathscr{K}$, we have

$$\psi_{\alpha}(a,b) \ge \frac{1}{2\alpha} \|b - [b - \alpha a]_{+}\|^{2},$$

and $\psi_{\alpha}(a,b) = 0$ if and only if in addition $a \in \mathcal{K}$ and $\langle a,b \rangle = 0$.

(b) ψ_{α} is differentiable at every $(a,b) \in \mathscr{G} \times \mathscr{G}$, with

$$abla_a\psi_{\alpha}(a,b)=b-[b-\alpha a]_+,\qquad
abla_b\psi_{\alpha}(a,b)=a-rac{1}{lpha}(b-[b-\alpha a]_+).$$

Proof. This can be seen by following the proof of [61], Proposition 2.1, with u = b, v = -a and with α replaced by $1/\alpha$. Also, we use the correspondence between $(\mathscr{S}, \langle \cdot, \cdot \rangle)$ and $(\mathfrak{R}^{\nu}, \langle \cdot, \cdot \rangle_{\mathfrak{R}^{\nu}})$ with $v := \sum_{k=1}^{m} n_k (n_k + 1)/2$, as discussed in Section 1. \Box

Following [61], we will relate f_{α} to the norm of the projection residual functions $R_{\alpha} \colon \mathscr{S} \mapsto \mathscr{S} \ (\alpha \in (0, \infty))$ defined by

$$R_{\alpha}(x) := G(x) - [G(x) - \alpha F(x)]_{+}.$$

By Lemma 2.1(b), we have that x satisfies Eq. (1) if and only if $R_{\alpha}(x) = 0$. By using Lemma 4.1; we obtain the following proposition which estimates the growth rate of f_{α} in terms of $||R_{\alpha}||$, and gives formulas for ∇f_{α} and a certain descent direction for f_{α} at any nonglobal minimum $x \in G^{-1}(\mathscr{K})$ with $\nabla G(x)^{-1} \nabla F(x)$ positive definite. These results are similar to [61], Theorem 3.1, and [20], Theorem 3.2, Proposition 4.1.

Proposition 4.1. Fix any $\alpha \in (0, \infty)$ and let $f_{\alpha}: G^{-1}(\mathscr{X}) \mapsto \mathfrak{R}$ be given by Eq. (4). Then the following hold:

(a) For all $x \in G^{-1}(\mathscr{K})$, we have

$$f_{\alpha}(x) \geq \frac{1}{2\alpha} \|R_{\alpha}(x)\|^2,$$

and $f_{\alpha}(x) = 0$ if and only if x satisfies Eq. (1). (b) If F and G are differentiable on $G^{-1}(\mathcal{K})$, then so is f_{α} and

$$\nabla f_{\alpha}(x) = \nabla F(x)R_{\alpha}(x) + \nabla G(x)\left(F(x) - \frac{1}{\alpha}R_{\alpha}(x)\right)$$

for all $x \in G^{-1}(\mathscr{K})$.

(c) Assume F and G are differentiable on $G^{-1}(\mathscr{K})$. Then, for every $x \in G^{-1}(\mathscr{K})$ where $\nabla G(x)$ is invertible and $\nabla G(x)^{-1} \nabla F(x)$ is positive definite, either (i) $f_{\alpha}(x) = 0$ or (ii) $\nabla f_{\alpha}(x) \neq 0$ with $\langle d(x), \nabla f_{\alpha}(x) \rangle < 0$, where

$$d(x) := -(\nabla G(x)^{-1})^* R_{\alpha}(x)$$

Proof. (a) and (b) follow from Lemma 4.1 (also see [61], Theorem. 3.1 for essentially the same result). The proof of (c) is similar that of [20], Proposition 4.1, for the case $G \equiv I$: Fix any $x \in G^{-1}(\mathscr{K})$ with $\nabla G(x)$ invertible and $\nabla G(x)^{-1} \nabla F(x)$ positive definite. Then

$$\begin{aligned} \langle d(x), \nabla f_{\alpha}(x) \rangle &= -\langle R_{\alpha}(x), \nabla G(x)^{-1} \nabla F(x) R_{\alpha}(x) + F(x) - \frac{1}{\alpha} R_{\alpha}(x) \rangle \\ &\leqslant - \langle R_{\alpha}(x), \nabla G(x)^{-1} \nabla F(x) R_{\alpha}(x) \rangle, \end{aligned}$$

where the inequality follows from the fact that $\langle \zeta - [a]_+, a - [a]_+ \rangle \leq 0$ for all $a \in \mathscr{S}$ and $\zeta \in \mathscr{K}$ (and, in particularly, for $a = G(x) - \alpha F(x)$ and $\zeta = G(x)$). Since $\nabla G(x)^{-1} \nabla F(x)$ is positive definite, then either $R_x(x) = 0$ or $\langle d(x), \nabla f_x(x) \rangle < 0$. The former is equivalent to $f_x(x) = 0$. \Box

In the further special case where G is affine, it can be seen that $x + d(x) \in G^{-1}(\mathscr{K})$ so that, by Proposition 4.1(c), d(x) is a feasible descent direction for f_{α} over $G^{-1}(\mathscr{K})$ at x (cf. [20], Proposition 4.1) whenever $f_{\alpha}(x) > 0$ and $\nabla G(x)^{-1} \nabla F(x)$ is positive definite. In general, we can use a gradient projection method

$$x^{\text{new}} \approx [x - t \nabla f_{\alpha}(x)]_{+}$$

with $t \in (0, \infty)$ a stepsize, to minimize f_{α} . A drawback of f_{α} is that, without an assumption such as $\nabla G(x)^{-1} \nabla F(x)$ be positive definite for all $x \in G^{-1}(\mathscr{K})$, finding a global minimum of f_{α} is difficult. Additional growth properties of f_{α} are discussed in [63], Lemma 4.1.

5. Implicit Lagrangian function

In this section, we study the merit function f_{α} given by Eq. (5). As with the gap functions and the regularized gap function of Sections 3 and 4, most of the results are easy extensions of known results, particularly [61,64]. We begin with the following lemma based on [61], Proposition 2.2.

Lemma 5.1. For any $\alpha \in (0, \infty)$, define the function $\psi_{\alpha} \colon \mathscr{G} \times \mathscr{G} \mapsto \Re$ by

$$\psi_{\alpha}(a,b) := \max_{\xi \in \mathscr{K}, \xi \in \mathscr{K}} \left\{ \langle a, b - \zeta \rangle - \langle \xi, b \rangle - \frac{1}{2\alpha} (\|a - \xi\|^2 + \|b - \zeta\|^2) \right\}.$$

Then the following hold:

(a) Fix any $\alpha \in (1, \infty)$. For all $(a, b) \in \mathscr{S} \times \mathscr{S}$, we have

$$(\alpha - 1) \|b - [b - a]_{+}\|^{2} \ge \psi_{\alpha}(a, b) = -\psi_{1/\alpha}(a, b) \ge (1 - 1/\alpha) \|b - [b - a]_{+}\|^{2}$$

and $\psi_{\alpha}(a,b) = 0$ if and only if in addition $a, b \in \mathscr{K}$ and $\langle a, b \rangle = 0$.

(b) Fix any $\alpha \in (0,\infty)$. ψ_{α} is differentiable at every $(a,b) \in \mathscr{G} \times \mathscr{G}$, with

$$\nabla_a \psi_\alpha(a,b) = b - [b - \alpha a]_+ - \frac{1}{\alpha}(a - [a - \alpha b]_+),$$

$$\nabla_b \psi_\alpha(a,b) = a - [a - \alpha b]_+ - \frac{1}{\alpha}(b - [b - \alpha a]_+).$$

Proof. Apply [61], Proposition 2.2 with the correspondence $\tilde{\pi} \equiv -\psi_{\alpha}$, u = a, v = -b, and use the fact $\mathscr{K}^{\circ} = -\mathscr{K}$ and the third identity in Eq. (12). Also, we use the correspondence between $(\mathscr{S}, \langle \cdot, \cdot \rangle)$ and $(\mathfrak{R}^{v}, \langle \cdot, \cdot \rangle_{\mathfrak{R}^{v}})$ with $v := \sum_{k=1}^{m} n_{k}(n_{k} + 1)/2$, as discussed in Section 1. (Correction Note: The term $1/(\alpha - 1)$ appearing in [61] Eq. (5) should be $1/(\alpha - 1)$. \Box

Following [61], we define the projection residual function $S_{\alpha} \colon \mathscr{S} \mapsto \mathscr{S} \ (\alpha \in (0, \infty))$ by

$$S_{\alpha}(x) := F(x) - [F(x) - \alpha G(x)]_+.$$

Since, by the first and the third identity in Eq. (12), we have $b - [b - a]_{+} = a - [a - b]_{+}$ for any $(a, b) \in \mathscr{S} \times \mathscr{S}$, it follows that $R_1 \equiv S_1$ on \mathscr{S} . However, in general $R_{\alpha} \neq S_{\alpha}$ for $\alpha \neq 1$. By using Lemma 5.1, we obtain the following proposition which estimates the growth rate of f_{α} in terms of $||R_1||$, and gives formulas for ∇f_{α} and a certain descent direction for f_{α} at any nonglobal minimum x with $\nabla G(x)^{-1} \nabla F(x)$ positive definite. These results are based on [61], Theorem. 3.2 and [64], Theorem. 2.2 and Lemma 3.1.

Proposition 5.1. Fix any $\alpha \in (1, \infty)$ and let $f_{\alpha} \colon \mathscr{S} \mapsto \mathfrak{R}$ be given by Eq. (5). Then the following hold:

(a) For all $x \in \mathcal{S}$, we have

$$(\alpha - 1) \|R_1(x)\|^2 \ge f_{\alpha}(x) = -f_{1/\alpha}(x) \ge (1 - 1/\alpha) \|R_1(x)\|^2$$

and $f_{\alpha}(x) = 0$ if and only if x satisfies Eq. (1).

(b) If F is differentiable on \mathcal{S} , then so is f_{α} and

$$\nabla f_{\alpha}(x) = \nabla F(x) \left(R_{\alpha}(x) - \frac{1}{\alpha} S_{\alpha}(x) \right) + \nabla G(x) \left(S_{\alpha}(x) - \frac{1}{\alpha} R_{\alpha}(x) \right)$$

for all $x \in \mathcal{G}$.

(c) Assume F and G are differentiable on \mathscr{S} . Then, for every $x \in \mathscr{S}$ where $\nabla G(x)$ is invertible and $\nabla G(x)^{-1} \nabla F(x)$ is positive definite, either (i) $f_{\alpha}(x) = 0$ or (ii) $\nabla f_{\alpha}(x) \neq 0$ with $\langle d(x), \nabla f_{\alpha}(x) \rangle \leq - \langle d(x), \nabla G(x)^{-1} \nabla F(x) d(x) \rangle$, where

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$$d(x) := -(\nabla G(x)^{-1})^* \left(R_x(x) - \frac{1}{\alpha} S_x(x) \right).$$

Proof. (a) and (b) follow from Lemma 5.1 (also see [61], Theorem. 3.2). The proof of (c) is somewhat different than that given in [64] for the NCP case: Fix any $x \in \mathscr{S}$ with $\nabla G(x)$ invertible and $\nabla G(x)^{-1} \nabla F(x)$ positive definite. (We will drop (x) for simplicity.) By the first identity in Eq. (12), we have $R_x - (1/\alpha)S_x = G - [G - \alpha F]_+ - 1/\alpha$ $(F - [F - \alpha G]_+) = -[G - \alpha F]_+ + (1/\alpha)[F - \alpha G]_-$ and, similarly, $S_x - (1/\alpha)R_x = -[F - \alpha G]_+ + (1/\alpha)[G - \alpha F]_-$. Thus

$$\left\langle R_{\alpha} - \frac{1}{\alpha} S_{\alpha}, S_{\alpha} - \frac{1}{\alpha} R_{\alpha} \right\rangle = \left\langle -[G - \alpha F]_{+} + \frac{1}{\alpha} [F - \alpha G]_{-}, -[F - \alpha G]_{+} + \frac{1}{\alpha} [G - \alpha F]_{-} \right\rangle$$
$$= \left\langle [G - \alpha F]_{+}, [F - \alpha G]_{+} \right\rangle + \frac{1}{\alpha^{2}} \left\langle [F - \alpha G]_{-}, [G - \alpha F]_{-} \right\rangle \ge 0,$$

where the second equality uses the second identity in Eq. (12) and the inequality uses Eq. (11) and the third identity in Eq. (12). Thus,

$$\langle d, \nabla f_{\alpha} \rangle = - \left\langle R_{\alpha} - \frac{1}{\alpha} S_{\alpha}, \nabla G^{-1} \nabla F \left(R_{\alpha} - \frac{1}{\alpha} S_{\alpha} \right) + S_{\alpha} - \frac{1}{\alpha} R_{\alpha} \right\rangle$$

$$\leq - \left\langle R_{\alpha} - \frac{1}{\alpha} S_{\alpha}, \nabla G^{-1} \nabla F \left(R_{\alpha} - \frac{1}{\alpha} S_{\alpha} \right) \right\rangle = - \left\langle d, \nabla G^{-1} \nabla F d \right\rangle.$$

If $\nabla f_{\alpha}(x) = 0$, then d(x) = 0 or, equivalently, $R_{\alpha}(x) - \frac{1}{\alpha}S_{\alpha}(x) = 0$, which together with $\nabla f_{\alpha}(x) = 0$ and the formula for $\nabla f_{\alpha}(x)$ in (b) and the nonsingularity of $\nabla G(x)$ would imply $S_{\alpha}(x) - (1/\alpha)R_{\alpha}(x) = 0$. Since $\alpha \neq 1$, the latter two equations would yield $R_{\alpha}(x) = S_{\alpha}(x) = 0$ or, equivalently, $f_{\alpha}(x) = 0$. \Box

The implicit Lagrangian f_x given by Eq. (5), in contrast to the gap functions and the regularized gap function, is a merit function on all of \mathscr{S} and has nice differentiability properties. However, it suffers the same drawback as the regularized gap function in that, without an assumption such as $\nabla G(x)^{-1} \nabla F(x)$ be positive definite for all $x \in G^{-1}(\mathscr{K})$, finding a global minimum of f_x is difficult.

6. Norm squared of the Fischer-Burmeister function

In this section, we study the merit function f given by Eq. (6), with ϕ given by Eq. (8). In contrast to the merit function of Sections 3-5, it is not easy to extend the analysis of this merit function from the NCP case [8,14,16,22,29,32,33,59] to SDCP. In particular, ϕ involves taking the square root of the sum of two symmetric psd matrices, which significantly complicates the analysis and necessitates the development of new arguments. In fact, it is surprising that many properties of f in the NCP case do indeed extend to SDCP. We begin with the following lemma stating some key properties of ϕ and of matrix square root.

Lemma 6.1. (a) For any $(a,b) \in \mathcal{K} \times \mathcal{K}$, $\langle a,b \rangle = 0$ if and only if, for $p \in \mathcal{O}$ and $\lambda_k, \ldots, \lambda_n \in (0,\infty)$ satisfying $pap^{\mathrm{T}} = \mathrm{diag}[0,\ldots,0,\lambda_k,\ldots,\lambda_n]$, we have $[pbp^{\mathrm{T}}]_{ij} = 0$ for all $i \geq k$ or $j \geq k$.

(b) For ϕ given by Eq. (8) and any $(a,b) \in \mathscr{S} \times \mathscr{S}$, we have $\phi(a,b) = 0$ if and only if $a, b \in \mathscr{K}$ and $\langle a, b \rangle = 0$.

(c) For any $a \in \mathscr{K}$ and $b \in \mathscr{S}$, if $a^2 - b^2 \in \mathscr{K}$, then $a - b \in \mathscr{K}$.

Proof. (a). Fix any $(a,b) \in \mathscr{K} \times \mathscr{K}$ and let $p \in \mathcal{O}$ and $\lambda_k, \ldots, \lambda_n \in (0,\infty)$ satisfy $pap^{\mathrm{T}} = \text{diag}[0, \ldots, 0, \lambda_k, \ldots, \lambda_n]$. Then

$$\langle a, b \rangle = \operatorname{tr}[ab] = \operatorname{tr}[pap^{\mathsf{T}}pbp^{\mathsf{T}}]$$

= $\operatorname{tr}[\operatorname{diag}[0, \dots, 0, \lambda_k, \dots, \lambda_n]pbp^{\mathsf{T}}] = \sum_{i=k}^n \lambda_i [pbp^{\mathsf{T}}]_{ii}.$

Since $pbp^{T} \in \mathcal{H}$ so $[pbp^{T}]_{ii} \ge 0$ for i = k, ..., n, then $\langle a, b \rangle = 0$ if and only if $[pbp^{T}]_{ii} = 0$ for all $i \ge k$. Since pbp^{T} is symmetric and psd, the latter holds if and only if $[pbp^{T}]_{ij} = 0$ for $i \ge k$ or $j \ge k$.

(b). Fix any $(a, b) \in \mathscr{P} \times \mathscr{P}$. If $a, b \in \mathscr{H}$ and $\langle a, b \rangle = 0$, then, by part (a), for $p \in \mathscr{O}$ and $\lambda_k, \ldots, \lambda_n \in (0, \infty)$ satisfying $pap^{\mathrm{T}} = \operatorname{diag}[0, \ldots, 0, \lambda_k, \ldots, \lambda_n]$, we have $[pbp^{\mathrm{T}}]_{ij} = 0$ for $i \ge k$ or $j \ge k$. Thus, $pabp^{\mathrm{T}} = pap^{\mathrm{T}}pbp^{\mathrm{T}} = \operatorname{diag}[0, \ldots, 0, \lambda_k, \ldots, \lambda_n]$ $pbp^{\mathrm{T}} = 0$, implying ab = 0. Similarly, ba = 0. Hence $a^2 + b^2 = (a + b)^2$ or, equivalently, $(a^2 + b^2)^{1/2} = a + b$, i.e., $\phi(a, b) = 0$. Conversely, if $\phi(a, b) = 0$, then $a + b = (a^2 + b^2)^{1/2} \in \mathscr{H}$ and $(a + b)^2 = a^2 + b^2$ or, equivalently, ab + ba = 0. For $p \in \mathscr{O}$ and $\lambda_1, \ldots, \lambda_n \in \mathfrak{R}$ (ordered so $\lambda_1, \ldots, \lambda_{k-1}$ are zero, $\lambda_k, \ldots, \lambda_{l-1}$ are positive, and $\lambda_l, \ldots, \lambda_n$ are negative for some $1 \le k \le l \le n+1$) satisfying $pap^{\mathrm{T}} = \operatorname{diag}[\lambda_1, \ldots, \lambda_n]$, we have $0 = p(ab + ba)p^{\mathrm{T}} = pap^{\mathrm{T}}pbp^{\mathrm{T}} + pbp^{\mathrm{T}} \quad pap^{\mathrm{T}} = \operatorname{diag}[\lambda_1, \ldots, \lambda_n]$, implying $(\lambda_i + \lambda_j)[pbp^{\mathrm{T}}]_{ij} = 0$ for all i and j. Thus, $[pbp^{\mathrm{T}}]_{ij} = 0$ except possibly when $\lambda_i = \lambda_j = 0$ or $\lambda_i \lambda_j < 0$, so that

$$p(a+b)p^{\mathrm{T}} = pap^{\mathrm{T}} + pbp^{\mathrm{T}} = \begin{bmatrix} [pbp^{\mathrm{T}}]_{\substack{i < k, \\ j < k}} & 0 & 0 \\ 0 & \mathrm{diag}[\lambda_k, \dots, \lambda_{l-1}] & [pbp^{\mathrm{T}}]_{\substack{k \leq i < l, \\ j \geq l}} \\ 0 & [pbp^{\mathrm{T}}]_{\substack{i > l, \\ k \leq j < l}} & \mathrm{diag}[\lambda_l, \dots, \lambda_n] \end{bmatrix}.$$

Since this matrix is in \mathscr{K} so its diagonal entries are all nonnegative, we must have l = n + 1 and the submatrix $[pbp^T]_{\substack{i \leq k, \ j \leq k}}$ must be psd. Hence, pap^T and pbp^T are both in \mathscr{K} , implying a and b are both in \mathscr{K} . Moreover, a and b satisfy the condition following "if and only if" in (a), so, by part (a), $\langle a, b \rangle = 0$.

(c). Fix any $a \in \mathscr{H}$ and $b \in \mathscr{S}$ with $a^2 - b^2 \in \mathscr{H}$. We will show that a - |b| is psd (recall $|b| := (b^2)^{1/2}$), which would imply a - b is psd (since |b| - b is psd). Suppose a - |b| is not psd so there exists nonzero $v \in \mathfrak{R}^n$ and $\lambda \in (-\infty, 0)$ with $(a - |b|)v = \lambda v$. Since $a \in \mathscr{H}$, then

$$pap^{\mathsf{T}} = \begin{bmatrix} \tilde{a}_{II} & 0\\ 0 & 0 \end{bmatrix}$$

for some $p \in \mathcal{O}$, some $I \subset \{1, ..., n\}$, and some positive definite (abbreviated as pd) submatrix \tilde{a}_{II} . Since $a^2 - b^2$ is psd, we must also have

$$p|b|p^{\mathrm{T}} = \begin{bmatrix} \tilde{b}_{II} & 0\\ 0 & 0 \end{bmatrix}$$

for some psd submatrix \tilde{b}_{II} . Thus,

$$\begin{bmatrix} (\tilde{a}_{II} - \tilde{b}_{II})[pv]_I \\ 0 \end{bmatrix} = p(a - |b|)p^{\mathsf{T}}pv = p(a - |b|)v = \lambda pv$$

implying $[pv]_I \neq 0$. Since $(a + |b|)(a - |b|) + (a - |b|)(a + |b|) = 2a^2 - 2b^2 \in \mathcal{K}$, we obtain

$$0 \leq v^{\mathsf{T}}((a+|b|)(a-|b|) + (a-|b|)(a+|b|))v = 2\lambda v^{\mathsf{T}}(a+|b|)v$$

= $2\lambda (pv)^{\mathsf{T}}p(a+|b|)p^{\mathsf{T}}pv = 2\lambda [pv]_{I}^{\mathsf{T}}(\tilde{a}_{II} + \tilde{b}_{II})[pv]_{I} < 0,$

where the last inequality follows from $\tilde{a}_{II} + \tilde{b}_{II}$ being pd, $[pv]_I \neq 0$ and $\lambda < 0$. This is clearly a contradiction.

For any $c \in \mathcal{K}$, let \mathcal{S}_c denote the subspace of \mathcal{S} comprising those $x \in \mathcal{S}$ whose nullspace contains the nullspace of c. It is readily seen that

$$\mathscr{S}_{c} = \left\{ x \in \mathscr{S}: pxp^{\mathsf{T}} = \begin{bmatrix} \tilde{x}_{II} & 0\\ 0 & 0 \end{bmatrix} \text{for some submatrix } \tilde{x}_{II} \right\}$$
(14)

for any $p \in \mathcal{O}$ and $I \subset \{1, \ldots, n\}$ such that

$$pcp^{\mathrm{T}} = \begin{bmatrix} \tilde{c}_{II} & 0\\ 0 & 0 \end{bmatrix}$$
(15)

for some pd submatrix \hat{c}_{II} . Define the linear mapping $L_c: \mathscr{G}_c \mapsto \mathscr{G}_c$ by

$$L_c[x] := cx + xc.$$

It can be seen that L_c is positive definite (i.e., $\langle x, L_c[x] \rangle = 2 \operatorname{tr}[\tilde{c}_{II}\tilde{x}_{II}^2] > 0$ whenever $\tilde{x}_{II} \neq 0$) and so has an inverse L_c^{-1} , i.e., for any $x \in \mathscr{S}_c$, $L_c^{-1}[x]$ is the unique $d \in \mathscr{S}_c$ satisfying cd + dc = x. $[L_c^{-1}$ can be obtained in closed form by choosing p so \tilde{c}_{II} is diagonal, so that

$$L_{c}^{-1}[x] = p^{\mathsf{T}} \begin{bmatrix} [\tilde{x}_{ij}/(\tilde{c}_{ii} + \tilde{c}_{jj})]_{j \in I}^{i \in I} & 0\\ 0 & 0 \end{bmatrix} p_{j \in I}$$

where \tilde{x}_{II} is given by Eq. (14).] Moreover, for any $x, y \in \mathscr{S}_c$, we have

$$\langle y, L_c[x] \rangle = \langle L_c[y], x \rangle, \qquad x L_c^{-1}[c] = L_c^{-1}[c] x = x/2,$$

 $x L_c^{-1}[x] = 0 \Rightarrow x = 0.$ (16)

By replacing x and y in the first identity of Eq. (16) with $L_c^{-1}[x]$ and $L_c^{-1}[y]$ respectively, we see that this identity also holds when L_c is replaced with L_c^{-1} .

Lemma 6.2 derives a formula for the first-order term in perturbing $c \in \mathscr{H}$ to $(c^2 + w)^{1/2}$. A key part of the formula involves the mapping $L_{\tilde{c}_{\mathcal{H}}}^{-1}$. In what follows, we will use "O(t)" (respectively, "o(t)") as a shorthand to denote an element of \mathscr{S} that depends on t and whose norm tends to 0 at least as fast as (respectively, faster than) t, i.e., $\limsup_{t\to 0} ||O(t)||/t < \infty$ (respectively, $\limsup_{t\to 0} ||O(t)||/t = 0$).

Lemma 6.2. Fix any $c \in \mathcal{K}$ and any $p \in \mathcal{O}$ such that Eq. (15) holds for some $I \subset \{1, \ldots, n\}$ and some pd submatrix \tilde{c}_{II} . For each $w \in \mathcal{S}$ with $c^2 + w \in \mathcal{K}$, upon letting $z := (c^2 + w)^{1/2} - c$ and

$$\tilde{w} = \begin{bmatrix} \tilde{w}_{II} & \tilde{w}_{IJ} \\ \tilde{w}_{IJ}^{\mathsf{T}} & \tilde{w}_{JJ} \end{bmatrix} := pwp^{\mathsf{T}}, \qquad \tilde{z} = \begin{bmatrix} \tilde{z}_{II} & \tilde{z}_{IJ} \\ \tilde{z}_{IJ}^{\mathsf{T}} & \tilde{z}_{JJ} \end{bmatrix} := pzp^{\mathsf{T}}, \tag{17}$$

where $J := \{1, ..., n\} \setminus I$, we have $\|\tilde{z}_{JJ}\| \leq n^{1/4} \|\tilde{w}_{JJ}\|^{1/2}$, $\tilde{z}_{IJ} = \tilde{c}_{II}^{-1} \tilde{w}_{IJ} + o(\|w\|)$, and $\tilde{z}_{II} = L_{\tilde{c}_{II}}^{-1} [\tilde{w}_{IJ}] + o(\|w\|)$.

Proof. Squaring both sides of $(c^2 + w)^{1/2} = c + z$ and multiplying left and right by p and p^T (also using Eqs. (15) and (17)) gives

$$\begin{bmatrix} \tilde{c}_{II}^2 + \tilde{w}_{II} & \tilde{w}_{IJ} \\ \tilde{w}_{IJ}^{\mathsf{T}} & \tilde{w}_{JJ} \end{bmatrix} = p(c^2 + w)p^{\mathsf{T}} = p(c+z)^2 p^{\mathsf{T}} = \begin{bmatrix} \tilde{c}_{II} + \tilde{z}_{II} & \tilde{z}_{IJ} \\ \tilde{z}_{IJ}^{\mathsf{T}} & \tilde{z}_{JJ} \end{bmatrix}^2$$

or, equivalently:

$$\begin{split} \tilde{w}_{II} &= \tilde{z}_{II}\tilde{c}_{II} + \tilde{c}_{II}\tilde{z}_{II} + \tilde{z}_{II}^2 + \tilde{z}_{IJ}\tilde{z}_{IJ}^{\mathsf{T}},\\ \tilde{w}_{IJ} &= \tilde{c}_{II}\tilde{z}_{IJ} + \tilde{z}_{II}\tilde{z}_{IJ} + \tilde{z}_{IJ}\tilde{z}_{JJ},\\ \tilde{w}_{JJ} &= \tilde{z}_{IJ}^{\mathsf{T}}\tilde{z}_{IJ} + \tilde{z}_{JJ}^2. \end{split}$$
(18)

The last equation in Eq. (18) yields $\|\tilde{z}_{IJ}\|^2 + \|\tilde{z}_{JJ}\|^2 = \operatorname{tr}[\tilde{w}_{JJ}] \leq \sqrt{n} \|\tilde{w}_{JJ}\|$ [26], p. 43. We claim that, as $\|\tilde{w}_{II}\| \to 0$ and $\|\tilde{w}_{JJ}\| \to 0$, we must have $\|\tilde{z}_{II}\| \to 0$. If not, then the first equation in Eq. (18) together with $\|\tilde{z}_{IJ}\| \to 0$ would yield in the limit (and using the continuity of matrix multiplication) that $0 = \tilde{z}_{II}\tilde{c}_{II} + \tilde{c}_{II}\tilde{z}_{II} + \tilde{z}_{II}^2$ has a nonzero solution \tilde{z}_{II} . Adding \tilde{c}_{II}^2 to both sides gives $\tilde{c}_{II}^2 = (\tilde{c}_{II} + \tilde{z}_{II})^2$ and, since \tilde{c}_{II} and $\tilde{c}_{II} + \tilde{z}_{II}$ are both psd, this implies $\tilde{z}_{II} = 0$, a contradiction. Now, the second equation in Eq. (18) yields

$$\tilde{w}_{IJ} = (\tilde{c}_{II} + \tilde{z}_{II})\tilde{z}_{IJ} + \tilde{z}_{IJ}O(\|\tilde{w}_{JJ}\|^{1/2})$$

and since \tilde{c}_{II} is pd and $\|\tilde{z}_{II}\| \to 0$ as $\|w\| \to 0$, the implicit function theorem yields that $\tilde{z}_{IJ} = \tilde{c}_{II}^{-1} \tilde{w}_{IJ} + o(\|w\|)$. Then the first equation yields

$$\tilde{w}_{II} = L_{\tilde{c}_{II}}[\tilde{z}_{II}] + \tilde{z}_{II}^2 + O(||w||^2).$$

Since \tilde{c}_{II} is pd so that $L_{\tilde{c}_{II}}$ is an invertible linear mapping and $\|\tilde{z}_{II}\| \to 0$ as $\|w\| \to 0$, we obtain from the implicit function theorem that

$$\tilde{z}_{II} = L_{\tilde{c}_{II}}^{-1}[\tilde{w}_{II}] + o(||w||) + O(||w||^2) = L_{\tilde{c}_{II}}^{-1}[\tilde{w}_{II}] + o(||w||). \quad \Box$$

By using Lemmas 6.1 and 6.2, we obtain the following lemma which extends some results of Kanzow [32] and Geiger and Kanzow [22] for the NCP case and is the key to analyzing f given by Eq. (6), with ϕ given by Eq. (8). In what follows, we define, for any $x \in \mathscr{X}$,

$$sym[x] := x + x^{\mathrm{T}}.$$

Lemma 6.3. Let ϕ be given by Eq. (8) and define the function $\psi \colon \mathscr{G} \times \mathscr{G} \mapsto \Re$ by

$$\psi(a,b) := \frac{1}{2} \|\phi(a,b)\|^2.$$

Then the following hold:

(a) For all $(a,b) \in \mathscr{S} \times \mathscr{S}$, we have $\psi(a,b) \ge 0$ and $\psi(a,b) = 0$ if and only if in addition $a, b \in \mathscr{K}$ and $\langle a, b \rangle = 0$.

(b) ψ is differentiable at every $(a, b) \in \mathscr{S} \times \mathscr{S}$, with

$$\nabla_a \psi(a,b) = \operatorname{sym} \left[L_c^{-1} [c-a-b](a-c) \right],$$

$$\nabla_b \psi(a,b) = \operatorname{sym} \left[L_c^{-1} [c-a-b](b-c) \right]$$

where $c := (a^2 + b^2)^{1/2}$.

(c) For every $(a,b) \in \mathscr{S} \times \mathscr{S}$, we have $\langle \nabla_a \psi(a,b), \nabla_b \psi(a,b) \rangle \ge ||(c-a-b)g||^2$, where $c := (a^2 + b^2)^{1/2}$ and $g := L_c^{-1}[c-a-b]$.

Proof. (a) follows from Lemma 6.1(b). To show (b), we note that

$$\psi(a,b) = \frac{1}{2} ||(a^2 + b^2)^{1/2} - a - b||^2 = \frac{1}{2} \operatorname{tr} \left[\left((a^2 + b^2)^{1/2} - a - b \right)^2 \right]$$
$$= \operatorname{tr} \left[a^2 + ab + b^2 - (a^2 + b^2)^{1/2} (a + b) \right].$$
(19)

Fix any $(a,b) \in \mathscr{S} \times \mathscr{S}$ and let $c := (a^2 + b^2)^{1/2}$. Since $c \in \mathscr{K}$, we have that Eq. (15) holds for some $p \in \mathcal{O}$, some $I \subset \{1, \ldots, n\}$ and some pd submatrix \tilde{c}_{II} . Then

$$(pap^{\mathrm{T}})^{2} + (pbp^{\mathrm{T}})^{2} = pc^{2}p^{\mathrm{T}} = \begin{bmatrix} \tilde{c}_{II}^{2} & 0\\ 0 & 0 \end{bmatrix}$$

Since both $(pap^{T})^{2}$ and $(pbp^{T})^{2}$ are psd, it is readily seen that

$$pap^{\mathrm{T}} = \begin{bmatrix} \tilde{a}_{II} & 0\\ 0 & 0 \end{bmatrix}, \qquad pbp^{\mathrm{T}} = \begin{bmatrix} \tilde{b}_{II} & 0\\ 0 & 0 \end{bmatrix}$$
 (20)

for some submatrices \tilde{a}_{II} and \tilde{b}_{II} . Thus, $a, b \in \mathscr{S}_c$ (see Eq. (14)). Fix any $u \in \mathscr{S}$ and let $w := au + ua + u^2$ and $z := (c^2 + w)^{1/2} - c$. By Lemma 6.2, we have $\tilde{z}_{II} = L_{\tilde{c}_{II}}^{-1}[\tilde{w}_{II}] + o(||w||)$, where \tilde{w}_{II} and \tilde{z}_{II} (as well as \tilde{z}_{IJ} and \tilde{z}_{JJ}) are given by Eq. (17). Thus,

$$\operatorname{tr}\left[\left((c^{2}+w)^{1/2}-c\right)(a+b)\right] = \operatorname{tr}\left[p((c^{2}+w)^{1/2}-c)p^{\mathrm{T}}(pap^{\mathrm{T}}+pbp^{\mathrm{T}})\right]$$
$$= \operatorname{tr}\left[\begin{bmatrix}\tilde{z}_{II} & \tilde{z}_{IJ}\\\tilde{z}_{IJ}^{\mathrm{T}} & \tilde{z}_{JJ}\end{bmatrix}\begin{bmatrix}\tilde{a}_{II}+\tilde{b}_{II} & 0\\0 & 0\end{bmatrix}\right]$$

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$$= \operatorname{tr}\left[\tilde{z}_{II}(\tilde{a}_{II} + \tilde{b}_{II})\right] = \operatorname{tr}\left[\left(L_{\tilde{c}_{II}}^{-1}[\tilde{w}_{II}] + o(||w||)\right)(\tilde{a}_{II} + \tilde{b}_{II})\right]$$

$$= \operatorname{tr}\left[L_{\tilde{c}_{II}}^{-1}[[p(au + ua)p^{\mathsf{T}}]_{II}](\tilde{a}_{II} + \tilde{b}_{II})\right] + o(||u||)$$

$$= \operatorname{tr}\left[L_{\tilde{c}_{II}}^{-1}[\tilde{a}_{II} + \tilde{b}_{II}][p(au + ua)p^{\mathsf{T}}]_{II}\right] + o(||u||)$$

$$= \operatorname{tr}\left[\left[\frac{\tilde{d}_{II} \quad 0}{0 \quad 0}\right]p(au + ua)p^{\mathsf{T}}\right] + o(||u||) = \operatorname{tr}[d(au + ua)] + o(||u||)$$

$$= \operatorname{tr}\left[L_{c}^{-1}[a + b](au + ua)] + o(||u||), \qquad (21)$$

where the sixth equality uses the first identity in Eq. (16) (see the remark below it), the seventh and eighth equalities follow from letting

$$\tilde{d}_{II} := L_{\tilde{c}_{II}}^{-1} [\tilde{a}_{II} + \tilde{b}_{II}] \text{ and } d := p^{\mathsf{T}} \begin{bmatrix} \tilde{d}_{II} & 0\\ 0 & 0 \end{bmatrix} p \in \mathscr{S}_{c};$$

the last equality follows from $\tilde{c}_{II}\tilde{d}_{II} + \tilde{d}_{II}\tilde{c}_{II} = \tilde{a}_{II} + \tilde{b}_{II}$ or, equivalently,

$$cd + dc = p^{\mathsf{T}} \begin{bmatrix} \tilde{c}_{II} & 0\\ 0 & 0 \end{bmatrix} p p^{\mathsf{T}} \begin{bmatrix} \tilde{d}_{II} & 0\\ 0 & 0 \end{bmatrix} p + p^{\mathsf{T}} \begin{bmatrix} \tilde{d}_{II} & 0\\ 0 & 0 \end{bmatrix} p p^{\mathsf{T}} \begin{bmatrix} \tilde{c}_{II} & 0\\ 0 & 0 \end{bmatrix} p$$
$$= p^{\mathsf{T}} \begin{bmatrix} \tilde{a}_{II} + \tilde{b}_{II} & 0\\ 0 & 0 \end{bmatrix} p = a + b,$$

so $d = L_c^{-1}[a + b]$. Thus, Eq. (19) and Eq. (21) yield

$$\begin{split} \psi(a+u,b) &- \psi(a,b) \\ &= \operatorname{tr} \left[(a+u)^2 + (a+u)b + b^2 - ((a+u)^2 + b^2)^{1/2}(a+b+u) \right. \\ &- a^2 - ab - b^2 + c(a+b) \right] \\ &= \operatorname{tr} \left[2au + ub - cu - \left((c^2 + w)^{1/2} - c \right)(a+b+u) \right] \\ &= \operatorname{tr} \left[2au + ub - cu - L_c^{-1}[a+b](au+ua) \right] + \operatorname{o}(||u||) \\ &= \langle 2a + b - c - L_c^{-1}[a+b]a - aL_c^{-1}[a+b], u \rangle + \operatorname{o}(||u||), \end{split}$$

where the first and second equalities also use $a^2 + b^2 = c^2$, so that

$$\begin{aligned} \nabla_a \psi(a,b) &= 2a + b - c - L_c^{-1}[a+b]a - aL_c^{-1}[a+b] \\ &= (L_c^{-1}[c] - L_c^{-1}[a+b])(a-c) + (a-c)(L_c^{-1}[c] - L_c^{-1}[a+b]) \\ &= L_c^{-1}[c-a-b](a-c) + (a-c)L_c^{-1}[c-a-b], \end{aligned}$$

where the second equality uses the fact $x = L_c^{-1}[x]c + cL_c^{-1}[x]$ with x = a + b and the fact $x/2 = L_c^{-1}[c]x = xL_c^{-1}[c]$ (see Eq. (16)) with x = a - c; the last equality uses the linearity of L_c^{-1} . A similar argument gives the formula for $\nabla_b \psi(a, b)$. For any $u, v \in \mathcal{S}$, a similar argument as the one above (with $w := au + ua + u^2 + bv + vb + v^2$ instead, etc.) yields

$$\psi(a+u,b+v) - \psi(a,b) = \langle \nabla_a \psi(a,b), u \rangle + \langle \nabla_b \psi(a,b), v \rangle + o(||u||) + o(||v||),$$

so ψ is differentiable at (a, b).

(c). Fix any $(a,b) \in \mathscr{G} \times \mathscr{G}$. Upon letting x := c - a, y := c - b, $g := L_c^{-1}[c - a - b]$, we have

$$\begin{aligned} \langle \nabla_a \psi(a,b), \nabla_b \psi(a,b) \rangle \\ &= \operatorname{tr}[(gx + xg)(gy + yg)] = 2\operatorname{tr}[xgyg + gxyg] \\ &= 2\operatorname{tr}[x^{1/2}gy^{1/2}y^{1/2}gx^{1/2} + g(c-a)(c-b)g] \\ &= 2||y^{1/2}gx^{1/2}||^2 + \operatorname{tr}[g(2ab - 2ac - 2cb + c^2 + a^2 + b^2)g] \\ &= 2||y^{1/2}gx^{1/2}||^2 + \operatorname{tr}[g(ab + ba - ac - ca - cb - bc + c^2 + a^2 + b^2)g] \\ &= 2||y^{1/2}gx^{1/2}||^2 + \operatorname{tr}[g(c-a-b)^2g] = 2||y^{1/2}gx^{1/2}||^2 + ||(c-a-b)g||^2, \end{aligned}$$

where the third equality uses the fact $c^2 - a^2$ and $c^2 - b^2$ and c are all in \mathscr{K} so that, by Lemma 6.1(c), x = c - a and y = c - b are both in \mathscr{K} ; the fourth equality uses $c^2 = a^2 + b^2$; the fifth equality uses $tr[w] = tr[w^T]$ for any $w \in \mathscr{X}$.

The function ψ defined in Lemma 6.3 is not twice differentiable everywhere on $\mathscr{S} \times \mathscr{S}$ but, analogous to the NCP case, ψ is twice differentiable at every $(a,b) \in \mathscr{S} \times \mathscr{S}$ with $a^2 + b^2$ pd. Moreover, we can compute the Hessian explicitly: For any $(u,v) \in \mathscr{S} \times \mathscr{S}$, we have

$$\nabla_{aa}^{2}\psi(a,b)u = \operatorname{sym}\left[L_{c}^{-1}[Z_{a}[u] - u - Z_{a}[u]g - gZ_{a}[u]](a-c) - g(Z_{a}[u] - u)\right],$$

$$\nabla_{ab}^{2}\psi(a,b)u = \operatorname{sym}\left[L_{c}^{-1}[Z_{a}[u] - u - Z_{a}[u]g - gZ_{a}[u]](b-c) - gZ_{a}[u]\right],$$

$$\nabla_{ba}^{2}\psi(a,b)v = \operatorname{sym}\left[L_{c}^{-1}[Z_{b}[v] - v - Z_{b}[v]g - gZ_{b}[v]](a-c) - gZ_{b}[v]\right],$$

$$\nabla_{bb}^{2}\psi(a,b)v = \operatorname{sym}\left[L_{c}^{-1}[Z_{b}[v] - v - Z_{b}[v]g - gZ_{b}[v]](b-c) - g(Z_{b}[v] - v)\right], \quad (22)$$

where $c := (a^2 + b^2)^{1/2}$, $g := L_c^{-1}[c - a - b]$ and $Z_a[u] := L_c^{-1}[au + ua]$, $Z_b[v] := L_c^{-1}[bv + vb]$. To see this, note that when we perturb a by some $u \in \mathcal{S}$ to a + u, both c and g are perturbed accordingly by some $z, h \in \mathcal{S}$ to c + z and g + h, respectively. Since c is pd, Lemma 6.2 with $w := au + ua + u^2$ yields

$$z = L_c^{-1}[au + ua] + o(||u||) = Z_a[u] + o(||u||).$$

Also, g and h satisfy the equations cg + gc = c - a - b and (c + z)(g + h) + (g + h))(c + z) = (c + z) - (a + u) - b which together yield ch + hc + zh + hz = z - u - zg - gz so

$$h = L_c^{-1}[z - u - zg - gz] + o(||z||).$$

Using the above two equations for z and h and the formula for $\nabla_a \psi$ given in Lemma 6.3(b), we find

$$\nabla_a \psi(a+u,b) - \nabla_a \psi(a,b) = \operatorname{sym} \left[L_c^{-1} [Z_a[u] - u - Z_a[u]g - gZ_a[u]](a-c) - g(Z_a[u] - u) \right] + o(||u||),$$

and the first formula in Eq. (22) follows. The other formulas follow by similar arguments. In the case when c is not pd, the formulas (22) still hold, provided that $u, v \in \mathscr{G}_c$.

By using Lemma 6.3, we readily obtain the following proposition which shows f given by Eqs. (7) and (8) to be a merit function on \mathscr{S} , and gives formulas for ∇f and a certain descent direction for f at any nonglobal minimum x with $\nabla G(x)^{-1} \nabla F(x)$ positive semi-definite. This proposition is motivated by analogous results for the NCP case obtained by Geiger and Kanzow [22], Theorem 2.5, Lemma 4.1 and others [8,14,29].

Proposition 6.1. Let $f : \mathscr{S} \mapsto \mathfrak{R}$ be given by Eq. (7) with ϕ given by Eq. (8). Then the following hold:

(a) For all $x \in \mathcal{S}$, we have $f(x) \ge 0$ and f(x) = 0 if and only if x satisfies Eq. (1).

(b) If F and G are differentiable on \mathcal{S} , then so is f and

$$\nabla f(x) = \nabla F(x) \nabla_a \psi(F(x), G(x)) + \nabla G(x) \nabla_b \psi(F(x), G(x))$$

for all $x \in \mathcal{S}$, where ψ is defined as in Lemma 6.3.

(c) Assume F and G are differentiable on \mathscr{S} . Then, for every $x \in \mathscr{S}$ where $\nabla G(x)$ is invertible and $\nabla G(x)^{-1} \nabla F(x)$ is positive semi-definite, either (i) f(x) = 0 or (ii) $\nabla f(x) \neq 0$ with $\langle d(x), \nabla f(x) \rangle < 0$, where

$$d(x) := -(\nabla G(x)^{-1})^* \nabla_a \psi(F(x), G(x)).$$

Proof. (a) and (b) follow from Lemma 6.3(a) and (b). To see (c), fix any $x \in \mathscr{S}$ with $\nabla G(x)$ invertible and $\nabla G(x)^{-1} \nabla F(x)$ positive semi-definite. We have, upon using Lemma 6.3(c) (and dropping (x) for simplicity),

$$\begin{aligned} \langle d, \nabla f \rangle &= - \langle \nabla_a \psi(F, G), \nabla G^{-1} \nabla F \nabla_a \psi(F, G) + \nabla_b \psi(F, G) \rangle \\ &\leqslant - \| (c - a - b)g \|^2, \end{aligned}$$

where $a := F(x), b := G(x), c := (a^2 + b^2)^{1/2}, g := L_c^{-1}[c - a - b]$. Thus, $\langle d(x), \nabla f(x) \rangle < 0$ unless $(c - a - b)L_c^{-1}[c - a - b] = 0$ or, by (6.3), c - a - b = 0. The latter, by Lemma 6.1(b), implies x satisfies Eq. (1) or, equivalently, f(x) = 0.

By using the chain rule, we can find explicit formula for the Hessian $\nabla^2 f(x)$ at every $x \in \mathscr{S}$ with $F(x)^2 + G(x)^2$ pd. For example (and simplicity), suppose F and G are affine so that F(x) = Ax + a and G(x) = Bx + b for some linear mappings Aand B from \mathscr{S} to \mathscr{S} and some $a, b \in \mathscr{S}$ (so $\nabla F(x) = A^*$, $\nabla G(x) = B^*$ for all $x \in \mathscr{S}$). Then straightforward calculation yields that, for any $d \in \mathscr{S}$,

$$\nabla f(x+d) - \nabla f(x) = A^* (\nabla^2_{aa} \psi(F(x), G(x)) A d + \nabla^2_{ba} \psi(F(x), G(x)) B d) + B^* (\nabla^2_{ab} \psi(F(x), G(x)) A d + \nabla^2_{bb} \psi(F(x), G(x)) B d) + o(||d||) = \nabla^2 f(x) d + o(||d||),$$

where $\nabla_{aa}^2 \psi, \ldots, \nabla_{bb}^2 \psi$ are given by Eq. (22). To solve an equation of the form $\nabla^2 f(x)d = r$, with $r \in \mathscr{S}$ given, as is needed by Newton-type methods for minimizing f (see, e.g., [14,16,29,30]), we can either seek to develop special factorization schemes or, more directly, express d as a linear combination of some basis vectors for \mathscr{S} and solve for the coefficients in the combination. If $F(x)^2 + G(x)^2$ is not pd, then we can

replace $\nabla^2 f(x)$ in the Newton-type methods by either a generalized Hessian or a positive definite linear mapping.

7. A function of Luo and Tseng

In this section, we study the merit function f given by Eq. (9) with ψ_0 satisfying $\psi_0(t) = 0$ if and only if $t \leq 0$ and ψ satisfying Eq. (10). For much of our analysis, we will further restrict the choice of ψ . Let Ψ_+ denote the collection of $\psi : \mathscr{S} \times \mathscr{S} \mapsto [0, \infty)$ satisfying Eq. (10) that are differentiable and satisfy the following conditions:

$$\langle \nabla_a \psi(a,b), \nabla_b \psi(a,b) \rangle \ge 0, \qquad \langle a, \nabla_a \psi(a,b) \rangle + \langle b, \nabla_b \psi(a,b) \rangle \ge 0$$

$$\forall (a,b) \in \mathscr{S} \times \mathscr{S}.$$
 (23)

(See [42], Eq. (13) for related conditions in the context of NCP.) The lemma below provides one choice of ψ belonging to Ψ_+ . Moreover, this choice of ψ is convex.

Lemma 7.1. Let $\psi: \mathscr{S} \times \mathscr{S} \mapsto [0, \infty)$ be given by

$$\psi(a,b) := \frac{1}{2} (\|[a]_{-}\|^{2} + \|[b]_{-}\|^{2}).$$
(24)

Then the following hold:

- (a) ψ satisfies Eq. (10).
- (b) ψ is convex and differentiable at every $(a, b) \in \mathscr{S} \times \mathscr{S}$ with $\nabla_a \psi(a, b) = [a]_-$ and $\nabla_b \psi(a, b) = [b]_-$.
- (c) For every $(a,b) \in \mathscr{S} \times \mathscr{S}$, we have $\langle \nabla_a \psi(a,b), \nabla_b \psi(a,b) \rangle \ge 0$.
- (d) For every $(a,b) \in \mathscr{S} \times \mathscr{S}$, we have $\langle a, \nabla_a \psi(a,b) \rangle + \langle b, \nabla_b \psi(a,b) \rangle = \|[a]_-\|^2 + \|[b]_-\|^2$.

Proof. (a) and (b). By the decomposition $a = [a]_{-} + [a]_{+}$ (see Eq. (12)), we have $||[a]_{-}||^{2} = ||a - [a]_{+}||^{2} = \min_{w \in \mathscr{K}} ||a - w||^{2}$ which is differentiable convex in a with $\nabla_{a}\psi(a,b) = [a]_{-}$ [56], p. 255 and equals 0 if and only if $a \in \mathscr{K}$. Similarly for $||[b]_{-}||^{2}$. Thus, $\psi(a,b)$ is differentiable convex in (a,b) and equals 0 if and only if $a, b \in \mathscr{K}$. Since $a, b \in \mathscr{K}$ implies $\langle a, b \rangle \ge 0$, it follows that Eq. (10) holds.

(c) and (d). We have from (b) that $\langle \nabla_a \psi(a,b), \nabla_b \psi(a,b) \rangle = \langle [a]_-, [b]_- \rangle \ge 0$, where the inequality uses Eq. (11) and the third identity in Eq. (12). Also, we have $\langle a, \nabla_a \psi(a,b) \rangle = \langle a, [a]_- \rangle = \text{tr}[a[a]_-] = \text{tr}[([a]_-)^2] = ||[a]_-||^2$, where the third equality uses Eq. (12). A similar argument shows $\langle b, \nabla_b \psi(a,b) \rangle = ||[b]_-||^2$. \Box

Next, we consider a further restriction on ψ . Let Ψ_{++} denote the collection of $\psi \in \Psi_+$ satisfying the following condition:

$$\psi(a,b) = 0 \quad \forall (a,b) \in \mathscr{S} \times \mathscr{S} \text{ with } \langle \nabla_a \psi(a,b), \nabla_b \psi(a,b) \rangle = 0.$$
(25)

(See [42], Eq. (14) for a related condition in the context of NCP.) The lemma below provides one choice of a ψ , based on the Fischer-Burmeister function Eq. (8), belonging to Ψ_{++} . Note that the choice (24) does not belong to Ψ_{++} .

Lemma 7.2. Let ψ be given by

$$\psi(a,b) := \frac{1}{2} \| [\phi(a,b)]_+ \|^2$$
(26)

with ϕ given by Eq. (8). Then the following hold:

- (a) ψ satisfies Eq. (10).
- (b) ψ is differentiable at every $(a,b) \in \mathscr{S} \times \mathscr{S}$, with

$$\nabla_a \psi(a,b) = \operatorname{sym} \left[L_c^{-1} \left[[c-a-b]_+ \right] (a-c) \right],$$

$$\nabla_b \psi(a,b) = \operatorname{sym} \left[L_c^{-1} \left[[c-a-b]_+ \right] (b-c) \right],$$

where $c := (a^2 + b^2)^{1/2}.$

- (c) For every $(a,b) \in \mathscr{G} \times \mathscr{G}$, we have $\langle \nabla_a \psi(a,b), \nabla_b \psi(a,b) \rangle \ge ||(c-a-b)g||^2$, where $c := (a^2 + b^2)^{1/2}$ and $g := L_c^{-1}[[c-a-b]_+]$. Consequently, ψ satisfies Eq. (25).
- (d) For every $(a,b) \in \mathscr{G} \times \mathscr{G}$, we have $\langle a, \nabla_a \psi(a,b) \rangle + \langle b, \nabla_b \psi(a,b) \rangle =$ $\|[c-a-b]_+\|^2$, where $c := (a^2+b^2)^{1/2}$.

Proof. (a). Fix any $(a, b) \in \mathscr{S} \times \mathscr{S}$ with $\psi(a, b) = 0$ and $\langle a, b \rangle \leq 0$. Let $z := -\phi(a, b)$. Then $[-z]_+ = [\phi(a, b)]_+ = 0$, so $z \in \mathscr{K}$. Since $a + b = (a^2 + b^2)^{1/2} + z$, squaring both sides and simplifying yields

$$ab + ba = (a^{2} + b^{2})^{1/2}z + z(a^{2} + b^{2})^{1/2} + z^{2}$$

Taking the trace of both sides gives

$$2\langle a,b\rangle = 2\operatorname{tr}[z^{1/2}(a^2+b^2)^{1/2}z^{1/2}] + ||z||^2.$$

Since $z^{1/2}(a^2 + b^2)^{1/2}z^{1/2}$ is in \mathscr{K} so its trace is nonnegative, the right-hand side is nonnegative, which together with $\langle a, b \rangle \leq 0$ implies z = 0. Then $\phi(a, b) = 0$ and Lemma 6.1(b) yields $a, b \in \mathscr{K}$, $\langle a, b \rangle = 0$. Conversely, if $a, b \in \mathscr{K}$ and $\langle a, b \rangle = 0$, then Lemma 6.1(b) yields $\phi(a, b) = 0$, so $\psi(a, b) = 0$ and $\langle a, b \rangle \leq 0$.

(b). Fix any $(a,b) \in \mathscr{G} \times \mathscr{G}$ and let $c := (a^2 + b^2)^{1/2}$ and r := c - a - b. For any $u \in \mathscr{G}$, we have upon letting $w := au + ua + u^2$ and $r' := (c^2 + w)^{1/2} - a - b - u$ that

$$\begin{aligned} \left| \psi(a+u,b) - \psi(a,b) - \langle [r]_{+}, r' - r \rangle \right| &= \left| \frac{1}{2} \| [r']_{+} \|^{2} - \frac{1}{2} \| [r]_{+} \|^{2} - \langle [r]_{+}, r' - r \rangle \right| \\ &= \left| \langle [r'']_{+} - [r]_{+}, r' - r \rangle \right| \\ &\leq \| [r'']_{+} - [r]_{+} \| \| r' - r \| \\ &\leq \| [r' - r \|^{2}, \end{aligned}$$
(27)

where r'' = (1-t)r + tr' for some $t \in [0, 1]$ and the second equality follows from the differentiability of $\|[\cdot]_+\|^2$ and the mean-value theorem; the last inequality uses the nonexpansive property of $[\cdot]_+$ [66]. We now bound the right-hand side. We have that Eq. (15) holds for some $p \in \mathcal{O}$, some $I \subset \{1, \ldots, n\}$ and some pd submatrix \tilde{c}_{II} , which implies that Eq. (20) holds for some submatrices \tilde{a}_{II} and \tilde{b}_{II} . Then

$$prp^{\mathrm{T}} = \begin{bmatrix} \tilde{c}_{II} - \tilde{a}_{II} - \tilde{b}_{II} & 0\\ 0 & 0 \end{bmatrix}$$

and it is readily seen that

$$p[r]_{+}p^{\mathrm{T}} = \begin{bmatrix} [\tilde{c}_{II} - \tilde{a}_{II} - \tilde{b}_{II}]_{+} & 0\\ 0 & 0 \end{bmatrix}.$$

Thus, $[r]_+ \in \mathscr{G}_c$ (see Eq. (14)). Also, upon defining \tilde{w} and \tilde{z} by Eq. (17), with $z := (c^2 + w)^{1/2} - c$, Lemma 6.2 yields

$$\langle [r]_{+}, r' - r \rangle = \langle [r]_{+}, z - u \rangle = \operatorname{tr} \left[p[r]_{+} p^{\mathrm{T}} p z p^{\mathrm{T}} - [r]_{+} u \right]$$

$$= \operatorname{tr} \left[[\tilde{c}_{II} - \tilde{a}_{II} - \tilde{b}_{II}]_{+} \tilde{z}_{II} - [r]_{+} u \right]$$

$$= \operatorname{tr} \left[[\tilde{c}_{II} - \tilde{a}_{II} - \tilde{b}_{II}]_{+} L_{\tilde{c}_{II}}^{-1} \left[[p(au + ua + u^{2})p^{\mathrm{T}}]_{II} \right] - [r]_{+} u \right] + \operatorname{o}(||u||)$$

$$= \operatorname{tr} \left[L_{\tilde{c}_{II}}^{-1} \left[[\tilde{c}_{II} - \tilde{a}_{II} - \tilde{b}_{II}]_{+} \right] \left[p(au + ua)p^{\mathrm{T}}]_{II} - [r]_{+} u \right] + \operatorname{o}(||u||)$$

$$= \operatorname{tr} \left[L_{c}^{-1} \left[[r]_{+} \right] (au + ua) - [r]_{+} u \right] + \operatorname{o}(||u||), \qquad (28)$$

where the fourth equality uses $\tilde{w} = pwp^{T} = p(au + ua + u^{2})p^{T}$; the last two equalities follow by the same argument as in the proof of Eq. (21). Also, by letting $\tilde{u} := pup^{T}$, we have from Eqs. (17) and (20) that

$$\begin{bmatrix} \tilde{w}_{II} & \tilde{w}_{IJ} \\ \tilde{w}_{IJ}^{\mathsf{T}} & \tilde{w}_{JJ} \end{bmatrix} = pwp^{\mathsf{T}} = p(au + ua + u^{2})p^{\mathsf{T}}$$

$$= \begin{bmatrix} \tilde{a}_{II} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \tilde{u}_{II} & \tilde{u}_{IJ} \\ \tilde{u}_{IJ}^{\mathsf{T}} & \tilde{u}_{JJ} \end{bmatrix} + \begin{bmatrix} \tilde{u}_{II} & \tilde{u}_{IJ} \\ \tilde{u}_{IJ}^{\mathsf{T}} & \tilde{u}_{JJ} \end{bmatrix} \begin{bmatrix} \tilde{a}_{II} & 0 \\ 0 & 0 \end{bmatrix} + pu^{2}p^{\mathsf{T}}$$

$$= \begin{bmatrix} \tilde{a}_{II}\tilde{u}_{II} + \tilde{u}_{II}\tilde{a}_{II} & \tilde{a}_{II}\tilde{u}_{IJ} \\ \tilde{u}_{IJ}^{\mathsf{T}}\tilde{a}_{II} & 0 \end{bmatrix} + pu^{2}p^{\mathsf{T}},$$

where $J := \{1, \ldots, n\} \setminus I$. Thus, $\tilde{w}_{II} = O(||u||)$, $\tilde{w}_{IJ} = O(||u||)$, $\tilde{w}_{JJ} = O(||u||^2)$, so Lemma 6.2 yields that $\tilde{z}_{II}, \tilde{z}_{IJ}$, and \tilde{z}_{JJ} are all O(||u||) or, equivalently, z = O(||u||). This implies

$$r' - r = z - u = O(||u||).$$
 (29)

(This fact can alternatively be shown by using Lemma 6.3(b).) Using Eqs. (28) and (29) to bound the right-hand side of Eq. (27) yields

$$\psi(a+u,b) - \psi(a,b) = \langle L_c^{-1}[[r]_+]a + aL_c^{-1}[[r]_+] - [r]_+, u \rangle + o(||u||)$$

implying

$$\begin{aligned} \nabla_a \psi(a,b) &= L_c^{-1} \big[[r]_+ \big] a + a L_c^{-1} \big[[r]_+ \big] - [r]_+ \\ &= L_c^{-1} \big[[r]_+ \big] a + a L_c^{-1} \big[[r]_+ \big] - \big(L_c^{-1} \big[[r]_+ \big] c + c L_c^{-1} \big[[r]_+ \big] \big) \\ &= L_c^{-1} \big[[r]_+ \big] (a-c) + (a-c) L_c^{-1} \big[[r]_+ \big], \end{aligned}$$

where the second equality uses the definition of L_c ; the last equality uses the linearity of L_c^{-1} . An analogous argument yields the formula for $\nabla_b \psi(a, b)$ and shows that $\psi(a + u, b + v) - \psi(a, b) = \langle \nabla_a \psi(a, b), u \rangle + \langle \nabla_b \psi(a, b), v \rangle + o(||u||) + o(||v||)$ for any $u, v \in \mathcal{S}$, so ψ is differentiable at (a, b). (c). The proof of the first part is identical to that of Lemma 6.3(c) but with $g := L_c^{-1}[[c-a-b]_+]$ instead. To see that ψ satisfies Eq. (25), suppose $\langle \nabla_a \psi(a,b), \nabla_b \psi(a,b) \rangle = 0$. Then the first part implies (c-a-b)g = 0 or, equivalently, $rL_c^{-1}[[r]_+] = 0$, where r := c - a - b. Thus,

$$0 = \operatorname{tr} \left[L_c^{-1} \left[[r]_+ \right] [r]_+ r L_c^{-1} \left[[r]_+ \right] \right] = \operatorname{tr} \left[L_c^{-1} \left[[r]_+ \right] ([r]_+)^2 L_c^{-1} \left[[r]_+ \right] \right] \\ = \left\| [r]_+ L_c^{-1} \left[[r]_+ \right] \right\|,$$

where the second equality uses the fourth identity in Eq. (12). Thus, $[r]_+L_c^{-1}[[r]_+] = 0$ which, by the third identity in Eq. (16), implies $[r]_+ = 0$ and hence $\psi(a,b) = \frac{1}{2} ||[r]_+||^2 = 0$.

(d). By (b), we have

$$\begin{aligned} \langle a, \nabla_a \psi(a, b) \rangle + \langle b, \nabla_b \psi(a, b) \rangle \\ &= \operatorname{tr} \left[L_c^{-1} \left[[c - a - b]_+ \right] ((a - c)a + a(a - c) + (b - c)b + b(b - c)) \right] \\ &= \operatorname{tr} \left[L_c^{-1} \left[[c - a - b]_+ \right] L_c [c - a - b] \right] \\ &= \operatorname{tr} \left[[c - a - b]_+ (c - a - b) \right] \\ &= \| [c - a - b]_+ \|^2, \end{aligned}$$

where the second equality uses $a^2 + b^2 = c^2$; the third equality uses the first identity in Eq. (16); and the last equality uses the fourth identity in Eq. (12).

The following proposition, patterned after [42], Theorem 2.3 for the NCP case, shows f given by Eqs. (9) and (10) to be a merit function on \mathscr{S} , and gives formulas for ∇f and, assuming $\psi \in \Psi_+$ (respectively, $\psi \in \Psi_{++}$), a certain descent direction for f at any non global minimum x with $\nabla G(x)^{-1} \nabla F(x)$ positive definite (respectively, positive semi-definite).

Proposition 7.1. Let $f: \mathscr{G} \mapsto \Re$ be given by Eq. (9) with $\psi_0: \Re \mapsto [0, \infty)$ satisfying $\psi_0(t) = 0$ if and only if $t \leq 0$ and $\psi: \mathscr{G} \times \mathscr{G} \mapsto [0, \infty)$ satisfying Eq. (10). Then the following hold:

(a) For all $x \in \mathcal{S}$, we have $f(x) \ge 0$ and f(x) = 0 if and only if x satisfies Eq. (1).

(b) If ψ_0, ψ and F, G are differentiable, then so is f and

$$\nabla f(x) = \nabla \psi_0(\langle F(x), G(x) \rangle)(\nabla F(x)G(x) + \nabla G(x)F(x)) + \nabla F(x)\nabla_a \psi(F(x), G(x)) + \nabla G(x)\nabla_b \psi(F(x), G(x))$$

for all $x \in \mathcal{G}$.

(c) If ψ_0, ψ are convex and F and G are affine and relatively monotone, then f is convex.

(d) Assume F and G are differentiable on \mathscr{S} and ψ belongs to Ψ_+ (respectively, Ψ_{++}) and ψ_0 is differentiable and strictly increasing on $[0, \infty)$. Then, for every $x \in \mathscr{S}$ where $\nabla G(x)$ is invertible and $\nabla G(x)^{-1} \nabla F(x)$ is positive definite (respectively, positive semidefinite), either (i) f(x) = 0 or (ii) $\nabla f(x) \neq 0$ with $\langle d(x), \nabla f(x) \rangle < 0$, where

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$$d(x) := -(\nabla G(x)^{-1})^* (\nabla \psi_0(\langle F(x), G(x) \rangle) G(x) + \nabla_a \psi(F(x), G(x))).$$

Proof. (a) follows from the Eq. (9) and the assumptions on ψ_0, ψ . (b) follows from the chain rule. (c) follows from the observations that, under the given hypothesis, $x \mapsto \langle F(x), G(x) \rangle$ is convex (see the proof of Proposition 3.1(b)) and ψ_0 is convex nondecreasing, so their composition is convex. Also, $x \mapsto \psi(F(x), G(x))$, being the composition of the affine mapping $x \mapsto (F(x), G(x))$ with the convex function ψ , is convex. To prove (d), consider the case $\psi \in \Psi_{++}$ and fix any $x \in \mathscr{S}$ with $\nabla G(x)$ invertible and $\nabla G(x)^{-1} \nabla F(x)$ positive semi-definite. We have upon letting $\alpha := \nabla \psi_0(\langle F(x), G(x) \rangle)$ (and dropping (x) for simplicity) that

$$\begin{split} \langle d, \nabla f \rangle &= -\langle \alpha G + \nabla_a \psi(F, G), \nabla G^{-1} \nabla F(\alpha G + \nabla_a \psi(F, G)) + \alpha F + \nabla_b \psi(F, G) \rangle \\ &\leqslant - \langle \alpha G + \nabla_a \psi(F, G), \alpha F + \nabla_b \psi(F, G) \rangle \\ &= -\alpha^2 \langle F, G \rangle - \alpha (\langle G, \nabla_b \psi(F, G) \rangle + \langle F, \nabla_a \psi(F, G) \rangle) \\ &- \langle \nabla_a \psi(F, G), \nabla_b \psi(F, G) \rangle \\ &\leqslant - \alpha^2 \langle F, G \rangle - \langle \nabla_a \psi(F, G), \nabla_b \psi(F, G) \rangle, \end{split}$$

where the last inequality follows from $\alpha \ge 0$ (since ψ_0 is increasing) and Eq. (23). Since ψ_0 is strictly increasing on $[0, \infty)$ so that $t\nabla\psi_0(t) > 0$ if and only if t > 0, the first term on the right-hand side is nonpositive and equals zero only if $\langle F, G \rangle \le 0$. By Eqs. (23) and (25), the second term on the right-hand side is nonpositive and equals zero only if $\psi(F, G) = 0$. Thus, $\langle d(x), \nabla f(x) \rangle < 0$ unless $\langle F(x), G(x) \rangle \le 0$ and $\psi(F(x), G(x)) = 0$, in which case Eq. (10) implies x satisfies Eq. (1) or, equivalently, f(x) = 0. The case of $\psi \in \Psi_+$ and $\nabla G(x)^{-1} \nabla F(x)$ being positive definite may be treated similarly. \Box

As in the case of the merit function Eqs. (7) and (8), f given by Eqs. (9) and (10) is typically not twice differentiable everywhere on \mathscr{S} . Still, in the case where ψ is given by either Eq. (24) or Eq. (26) and $\nabla^2 \psi^0$ is known, we can find explicit formula for $\nabla^2 f(x)$ at every $x \in \mathscr{S}$ where f is twice differentiable, and use this formula to develop Newton-type methods for minimizing f.

8. Topics for future research

The results of the previous sections in a sense only begin the study of merit functions for SDCP, with many topics remaining to be studied. On the numerical side, one major topic is the implementation and testing of merit-function-based methods for solving SDLP and SDCP. On the theoretical side, some specific open questions are:

Q1: In the NCP case, it is known that $\nabla G(x)^{-1} \nabla F(x)$ being a *P*-matrix (respectively, P_0 -matrix) is sufficient to ensure that a stationary point x of f given by Eq. (5) (respectively, Eqs. (7) and (8)) satisfies Eq. (1) [8,14,28]. For SDCP, we have shown

analogous results with $\nabla G(x)^{-1} \nabla F(x)$ being positive definite (respectively, positive semi-definite). Can this be extended to involve some notion of *P*-matrix and P_0 -matrix in the semi-definite setting? (Although \mathcal{K} does not have a Cartesian product structure, it may still be possible to work with the eigenvalues.)

Q2: In the NCP case, it is known that f(x) given by Eqs. (7) and (8), like the implicit Lagrangian (5), is bounded above and below by a constant multiple of $||R_1(x)||^2$ [59], Lemma 3.2. Also, ∇f is 1-order semi-smooth [14,29]. Are these still true for SDCP?

Q3: In the NCP case, it is known that ψ given by Eq. (26) is convex [42]. Is this still true for SDCP?

(A recent work by Qi and Chen [55] answers Q1 in the positive and Q3 in the negative.) There are also issues such as the boundedness of level sets for a merit function f and regularity conditions that characterize when a stationary point of f is a solution of the SDCP, etc. For some of these issues, the analysis readily extend from the NCP case while, for others, the extension appears to be more difficult. Lastly, we note that, in addition to the interior-point and the merit-function approach, there exist other approaches such as those based on the generalized-equation formulation, as studied by Robinson and others (see [49] for a survey), and that based on smoothing the complementarity conditions, as studied by Chen and Mangasarian [6]. Can these approaches be extended to SDCP?

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