SIAM J. MATRIX ANAL. APPL.
Vol. 28, No. 2, pp. 360–385

A QUADRATICALLY CONVERGENT NEWTON METHOD FOR COMPUTING THE NEAREST CORRELATION MATRIX*

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Abstract. The nearest correlation matrix problem is to find a correlation matrix which is closest to a given symmetric matrix in the Frobenius norm. The well-studied dual approach is to reformulate this problem as an unconstrained continuously differentiable convex optimization problem. Gradient methods and quasi-Newton methods such as BFGS have been used directly to obtain globally convergent methods. Since the objective function in the dual approach is not twice continuously differentiable, these methods converge at best linearly. In this paper, we investigate a Newton-type method for the nearest correlation matrix problem. Based on recent developments on strongly semismooth matrix valued functions, we prove the quadratic convergence of the proposed Newton method. Numerical experiments confirm the fast convergence and the high efficiency of the method.

Key words. correlation matrix, semismooth matrix equation, Newton method, quadratic convergence

AMS subject classifications. 49M45, 90C25, 90C33

DOI. 10.1137/050624509

1. Introduction.

Given a symmetric matrix $G \in \mathcal{S}^n$, computing its nearest correlation matrix, a problem from finance, is recently studied by Higham [25] and is given by

$$\begin{array}{ll} \min & \frac{1}{2}\| G - X \|^2 \\ \text{s.t.} & X_{ii} = 1, \quad i = 1, \ldots, n, \\ & X \in \mathcal{S}^n_+, \end{array} \tag{1}$$

where $\mathcal{S}^n$ and $\mathcal{S}^n_+$ are, respectively, the space of $n \times n$ symmetric matrices and the cone of positive semidefinite matrices in $\mathcal{S}^n$, and $\| \cdot \|$ is the Frobenius norm. It is noted that by introducing auxiliary variables, one may reformulate problem (1) as semidefinite programs or second-order cone programs, which may be solved by the well-developed modern interior point methods. However, when n is reasonably large, the direct use of interior point methods seems infeasible [25].[1] In tackling this difficulty, an alternating projection method of Dykstra [20] was proposed by Higham [25]. The projection method converges at best linearly. The latest study on problem (1) includes a dual approach proposed by Malick [35] and Boyd and Xiao [7]. This dual approach falls within the framework suggested by Rockafellar [43, p. 4] for general convex optimization problems.

Problem (1) is a special case of the following convex optimization problem:

*Received by the editors February 16, 2005; accepted for publication (in revised form) by N. J. Higham January 4, 2006; published electronically May 5, 2006.
http://www.siam.org/journals/simax/28-2/62450.html

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[1] By using preconditioned conjugate gradient methods to solve the linear system resulting from the interior point method, one may expect the interior point method to work well in practice [48].

$$\begin{array}{ll} \min & \frac{1}{2}\| x^0 - x \|^2 \\ \text{s.t.} & \mathcal{A}x = b \\ & x \in K\,, \end{array} \tag{2}$$

where $K \subseteq \mathcal{X}$ is a closed convex subset in a Hilbert space $\mathcal{X}$ endowed with an inner product $\langle \cdot, \cdot \rangle$ and its induced norm $\| \cdot \|$, $\mathcal{A} : \mathcal{X} \mapsto \mathbb{R}^n$ is a bounded linear operator, $b \in \mathbb{R}^n$ and $x^0 \in \mathcal{X}$ are given data (for problem (1), $\mathcal{X} = \mathcal{S}^n$, $K = \mathcal{S}^n_+$, $b = e$, the vector of all ones, $x^0 = G$, and $\mathcal{A}X = \mathrm{diag}[X]$, the vector formed by all diagonal elements of $X \in \mathcal{S}^n$). Problem (2) is also known as the best approximation from a closed convex set in a Hilbert space. See the recent book by Deutsch [13] and the references therein for details on this topic.

It has now become well known [14] that the (unique) solution x^* of (2) has the representation

$$x^* = \Pi_K(x^0 + \mathcal{A}^* y^*) \tag{3}$$

if and only if the set $\{K, \mathcal{A}^{-1}(b)\}$ has the so-called strong conical hull intersection property (CHIP), where $\Pi_K(\cdot)$ denotes the metric projection operator onto K under the inner product $\langle \cdot, \cdot \rangle$, y^* is a solution of the equation

$$\mathcal{A}\Pi_K(x^0 + \mathcal{A}^* y) = b, \tag{4}$$

and $\mathcal{A}^*$ denotes the adjoint of $\mathcal{A}$ (when $\mathcal{A} = \mathrm{diag}$, $\mathcal{A}^* y = \mathrm{Diag}[y]$, the diagonal matrix whose ith diagonal element is given by y_i). The property CHIP was initially characterized by Chui, Deutsch, and Ward [9] and was refined by Deutsch, Li, and Ward [14] to strong CHIP, which turns out to be a necessary and sufficient condition for the solution of (2) to have representation (3). In practice, however, strong CHIP is often difficult to verify for many interesting cases. Fortunately, there is an easy-to-verify sufficient condition:

$$b \in \mathrm{ri}\ (\mathcal{A}(K))\ . \tag{5}$$

$\mathcal{A}(K)$ is often called the data cone when K is a cone in $\mathcal{X}$ [9] and ri denotes the relative interior. We refer the reader to [2, 3, 5, 6, 10, 15, 36, 37] for related developments.

One well-studied concrete example of problem (2) is the convex best interpolation problem studied in [22, 27, 28, 36], where K is a closed convex cone given by

$$K := \{x \in L_2[0,1] \,|\, x \geq 0 \text{ a.e. on } [0,1]\}.$$

Newton's method for the dual of the convex best interpolation problem has been known to be the most efficient algorithm since [29, 1, 17]. The effectiveness of Newton's method was successfully explained very recently by Dontchev, Qi, and Qi [18, 19], where the authors established the superlinear (quadratic) convergence of Newton's method. The success of Newton's method for solving the convex best interpolation problem motivates us to study Newton's method for matrix nearness problem (1).

Coming to problem (1), we see $b = e$ and $\mathcal{A}(\mathcal{S}^n_+) = \mathbb{R}^n_+$, the nonnegative orthant of $\mathbb{R}^n$. Obviously, $e \in \mathrm{int}\mathbb{R}^n_+ = \mathrm{ri}\ \mathbb{R}^n_+$. Hence, (3) and (4) imply that there exists $y^* \in \mathbb{R}^n$ such that the unique solution X^* of (1) has the representation

$$X^* = (G + \mathcal{A}^* y^*)_+ \tag{6}$$

and y^* is a solution of the equation

$$\mathcal{A}\left(G + \mathcal{A}^* y\right)_+ = b, \quad y \in \mathbb{R}^n, \tag{7}$$

where X_+ denotes the metric projection of X onto $\mathcal{S}^n_+$, i.e., $X_+ := \Pi_{\mathcal{S}^n_+}(X)$. In fact, (7) is just the optimality condition of the following unconstrained and differentiable convex optimization problem [43]:

$$\min_{y \in \mathbb{R}^n} \theta(y) := \frac{1}{2} \| \left(G + \mathcal{A}^* y\right)_+ \|^2 - b^T y. \tag{8}$$

This is the dual problem of (1) studied in [35, 7]. The function $\theta(\cdot)$ is continuously differentiable, and its gradient mapping $\nabla\theta(\cdot)$ is globally Lipschitz continuous with the Lipschitz constant 1. Moreover, since Slater's condition is satisfied, $\theta(\cdot)$ is coercive; i.e., $\theta(y) \to +\infty$ as $\|y\| \to +\infty$ [43]. These nice properties allow one to apply either gradient-type methods or quasi-Newton methods to problem (8) directly [25, 35, 7]. However, since $\theta(\cdot)$ is not twice continuously differentiable, the convergence rate of these methods is at best linear. In this paper, we will show that Newton's method for solving problem (8) can achieve quadratic convergence by using the fact that the metric projection operator $\Pi_{\mathcal{S}^n_+}(\cdot)$ is strongly semismooth [46, 8]. We refer the interested reader to [47] for the strong semismoothness of the metric projection operator over the symmetric cones which include the nonnegative orthant, the second-order cone, and the positive semidefinite cone $\mathcal{S}^n_+$.

The paper is organized as follows. In section 2, we review some basic concepts and results concerning semismooth functions, especially in association with the projection X_+. In section 3, we develop Newton's method and show that it is quadratically convergent. As by-products of our analysis, we prove that the solution y^* is unique for any $G \in \mathcal{S}^n$ and $b > 0$ and is strongly semismooth as a function of G and b. This further implies that the solution X^* is also strongly semismooth as a function of G and b. Section 4 discusses some extensions which cover the W-weighted version of (1), a case with lower bounds, and a nonsymmetric case. We demonstrate that the developed Newton method applies to all those extensions under mild conditions. In section 5, we discuss the implementation issues and report our preliminary numerical results, which show that the Newton method is very efficient compared to existing methods. The conjugate gradient (CG) method is employed to solve the linear system obtained by Newton's method. We conclude our paper in section 6.

We use $\circ$ to denote the Hardmard product of matrices; i.e., for any $B, C \in \mathcal{S}^n$

$$B \circ C = [B_{ij} C_{ij}]^n_{i,j=1}.$$

We let E denote the matrix of all ones in $\mathcal{S}^n$. For subsets α, β of $\{1, 2, \ldots, n\}$, we denote $B_{\alpha\beta}$ as the submatrix of B indexed by α and β. Let e denote the vector of all ones.

2. Preliminaries. In this section, we review some basic concepts such as semismooth functions and generalized Jacobian of Lipschitz functions. These concepts will be used to define Newton's method for solving (7) and play an important role in our convergence analysis. We also review a perturbation result on eigenvalues of symmetric matrices.

Let $\Phi : \mathbb{R}^m \mapsto \mathbb{R}^\ell$ be a (locally) Lipschitz function. According to Redemacher's theorem (see [44, Sect. 9.J] for a proof), Φ is differentiable almost everywhere. We let

$$D_\Phi := \{x \in \mathbb{R}^m | \ \Phi \text{ is differentiable at } x\}.$$

Let $\Phi'(x)$ denote the Jacobian of Φ at $x \in D_\Phi$. The Bouligand subdifferential of Φ at $x \in \mathbb{R}^n$ is then defined by

$$\partial_B \Phi(x) := \left\{ V \in \mathbb{R}^{\ell \times m} \,|\, V \text{ is an accumulation point of } \Phi'(x^k),\ x^k \to x,\ x^k \in D_\Phi \right\}.$$

The generalized Jacobian in the sense of Clarke [11] is the convex hull of $\partial_B \Phi(x)$, i.e.,

$$\partial \Phi(x) = \operatorname{co} \partial_B \Phi(x).$$

Note that $\partial \Phi(x)$ is compact and upper-semicontinuous.

When $\ell = m$, a direct generalization of classical Newton's method for a system of smooth equations to $\Phi(x) = 0$ with a Lipschitz function Φ is given by [32, 42]

$$x^{k+1} = x^k - V_k^{-1} \Phi(x^k), \qquad V_k \in \partial \Phi(x^k), \quad k = 0, 1, 2, \ldots, \tag{9}$$

with x^0 as an initial guess. In general, the above iterative method does not converge. For a counterexample, see Kummer [32]. In extending Kojima and Shindo's condition for superlinear (quadratic) convergence of Newton's method for piecewise smooth equations [30], Kummer [32] proposed a general condition for guaranteeing the superlinear convergence of (9). However, Qi and Sun [42] popularized (9) by showing that the iterate sequence generated by (9) converges superlinearly if Φ belongs to an important subclass of Lipschitz functions—semismooth functions.

We say that Φ is semismooth at x if (i) Φ is directionally differentiable at x and (ii) for any $V \in \partial \Phi(x + h)$,

$$\Phi(x + h) - \Phi(x) - Vh = o(\|h\|).$$

Φ is said to be strongly semismooth at x if Φ is semismooth at x and for any $V \in \partial \Phi(x + h)$,

$$\Phi(x + h) - \Phi(x) - Vh = O(\|h\|^2).$$

The concept of semismoothness was introduced by Mifflin [38] for functionals. In order to study the convergence of (9), Qi and Sun [42] extended the definition of semismoothness to vector-valued functions and established the following convergence result.

THEOREM 2.1 (see [42, Thm. 3.2]). *Let x^* be a solution of the equation $\Phi(x) = 0$ and let Φ be a locally Lipschitz function which is semismooth at x^*. Assume that all $V \in \partial \Phi(x^*)$ are nonsingular matrices. Then every sequence generated by* (9) *is superlinearly convergent to x^*, provided that the starting point x^0 is sufficiently close to x^*. Moreover, if Φ is strongly semismooth at x^*, the convergence rate is quadratic.*

A similar result to the above theorem on the superlinear convergence of (9) can be found in [32, Prop. 3]. Theorem 2.1 gave the rates of convergence of (9) once the starting point x^0 is within the convergence region. The next theorem provides an estimate on how large the region of convergence can be.

THEOREM 2.2 (see [42, Thm. 3.3]). *Suppose that Φ is locally Lipschitz continuous and semismooth on $S := \{x \in \mathbb{R}^m \,|\, \|x - x^0\| \le r\}$. Also suppose that for any $V \in \partial \Phi(x)$, x, $y \in S$, V is nonsingular,*

$$\|V^{-1}\| \le \beta, \quad \|V(y - x) - \Phi'(x; y - x)\| \le \gamma \|y - x\|,$$

and

$$\|\Phi(y) - \Phi(x) - \Phi'(x; y - x)\| \le \delta \|y - x\|,$$

where $\beta\|\Phi(x^0)\| \le r(1-\alpha)$ *and* $\alpha := \beta(\gamma+\delta) < 1$. *Then the iterates* (9) *remain in* S *and converges to the unique solution of* $\Phi(x) = 0$ *in* S. *Moreover, the error estimate*

$$\|x^k - x^*\| \le [\alpha/(1-\alpha)]\|x^k - x^{k-1}\|$$

holds for $k = 1, 2, \ldots$.

Theorem 2.2 is an extension of the classical Newton–Kantorovich convergence theorem of Newton's method for solving smooth equations [40, Sect. 12.6]. Now we return our attention to problem (1). To facilitate our analysis, we define $F : \mathbb{R}^n \mapsto \mathbb{R}^n$ by

$$F(y) := \mathcal{A}(G + \mathcal{A}^* y)_+.$$

Then (7) becomes

$$F(y) = b \tag{10}$$

with $b = e$. It has been proved recently that $(\cdot)_+$ is strongly semismooth everywhere on $\mathcal{S}^n$ [46, 8]. Since the composite of strongly semismooth functions is still strongly semismooth, F is strongly semismooth everywhere on $\mathbb{R}^n$. So, in order to apply Theorem 2.1 to get a quadratically convergent Newton method, we need only to address the nonsingularity of $\partial F(y^*)$. It turns out to be the most difficult part in the analysis of Newton's method for solving (10). We will devote the whole next section to this issue.

We will also need the following perturbation result of Weyl for eigenvalues of symmetric matrices; see [4, p. 63] and [26, p. 367].

LEMMA 2.3. *Let* $\lambda_1 \ge \cdots \ge \lambda_n$ *be the eigenvalues of any* $X \in \mathcal{S}^n$ *and* $\mu_1 \ge \cdots \ge \mu_n$ *be the eigenvalues of any* $Y \in \mathcal{S}^n$. *Then*

$$|\lambda_i - \mu_i| \le \|X - Y\| \qquad \forall i = 1, \ldots, n.$$

3. Newton's method. In this section, we consider the nonsmooth Newton method for (10):

$$y^{k+1} = y^k - V_k^{-1}(F(y^k) - b), \qquad V_k \in \partial F(y^k), \quad k = 0, 1, 2, \ldots . \tag{11}$$

As we briefly discussed in section 2, the core issue for (11) is the nonsingularity of $\partial F(y)$ when y is near y^*, which is a solution of (10). Our main result in this section is that every element in $\partial F(y^*)$ is positive definite. Since F is already known to be strongly semismooth, Theorem 2.1 implies that method (11) is quadratically convergent if the initial point y^0 is sufficiently near y^*.

To facilitate our proofs for the positive definiteness of $\partial F(y^*)$ we need a few more notions. For any given $X \in \mathcal{S}^n$, let $\lambda(X)$ denote the eigenvalue vector of X arranged in the nonincreasing order, i.e., $\lambda_1(X) \ge \lambda_2(X) \ge \cdots \ge \lambda_n(X)$. Let $\mathcal{O}$ denote the set of all orthogonal matrices in $\mathbb{R}^{n\times n}$ and $\mathcal{O}_X$ be the set of orthonormal eigenvectors of X defined by

$$\mathcal{O}_X := \left\{ P \in \mathcal{O} |\ X = P\mathrm{Diag}[\lambda(X)]P^T \right\}.$$

Let $f : \mathbb{R} \to \mathbb{R}$ be a continuous function. Then one can define Löwner's function $f : \mathcal{S}^n \to \mathcal{S}^n$ (we adopt the convention of using f to denote both the scalar-valued and matrix-valued functions) by

$$f(X) := P\mathrm{Diag}[f(\lambda_1(X)), f(\lambda_2(X)), \ldots, f(\lambda_n(X))]P^T, \quad P \in \mathcal{O}_X. \tag{12}$$

The study on the matrix-valued function $f(X)$ defined in (12) was initiated by Löwner in his landmark paper [33]. See Donoghue [16] and Bhatia [4] for detailed discussions on (12).

For any $\mu = (\mu_1, \ldots, \mu_n)^T \in \mathbb{R}^n$ such that f is differentiable at $\mu_1, \ldots, \mu_n$, we denote by $f^{[1]}(\mu)$ the $n \times n$ symmetric matrix whose (i,j)th entry is

$$\left(f^{[1]}(\mu)\right)_{ij} = \begin{cases} \dfrac{f(\mu_i) - f(\mu_j)}{\mu_i - \mu_j} & \text{if } \mu_i \neq \mu_j, \\ f'(\mu_i) & \text{if } \mu_i = \mu_j. \end{cases}$$

The matrix $f^{[1]}(\mu)$ is called the first divided difference of f at μ. The following result of Löwner is well known. For a proof, see Donoghue [16, Chap. VIII] or [4, Chap. V.3.3].

LEMMA 3.1. *Let $P \in \mathcal{O}$ be such that $X = P\mathrm{Diag}[\lambda_1(X), \ldots, \lambda_n(X)]P^T$. Let (a_1, a_2) be an open interval in $\mathbb{R}$ that contains $\lambda_j(X)$, $j = 1, \ldots, n$. If f is continuously differentiable on (a_1, a_2), then f is differentiable at X and its derivative, for any $H \in \mathcal{S}^n$, is given by*

$$f'(X)H = P\left(f^{[1]}(\lambda(X)) \circ (P^T H P)\right) P^T. \tag{13}$$

Throughout the remainder of the paper, we let $f(t) = t_+ := \max(0, t)$, $t \in \mathbb{R}$. It is easy to derive from Moreau's theorem on the characterization of the metric projection operator over closed convex cones that (see [24, 50] for a proof)

$$X_+ = f(X) = P\mathrm{Diag}[\max\{\lambda_1(X), 0\}, \max\{\lambda_2(X), 0\}, \ldots, \max\{\lambda_n(X), 0\}]P^T.$$

By using Lemma 3.1 (by considering any continuously differentiable scalar-valued function with value one on an open set containing all the nonnegative eigenvalues of X and zero on an open set containing all negative eigenvalues of X) and the fact that $(\cdot)_+$ is (continuously) differentiable at $X \in \mathcal{S}^n$ if and only if X is nonsingular, we obtain the following useful result.

PROPOSITION 3.2. *Let $P \in \mathcal{O}$ be such that $X = P\mathrm{Diag}[\lambda_1(X), \ldots, \lambda_n(X)]P^T$. Then $\Pi_{\mathcal{S}^n_+}(\cdot)$ is (continuously) differentiable at an $X \in \mathcal{S}^n$ with eigenvalues $\lambda_1(X), \ldots, \lambda_n(X)$ if and only if $\lambda_i(X) \neq 0$, $i = 1, \ldots, n$. Moreover, if $\lambda_i(X) \neq 0$, $i = 1, \ldots, n$, then the derivative of $\Pi_{\mathcal{S}^n_+}(\cdot)$ at X, for any $H \in \mathcal{S}^n$, is given by (13) with $f(t) = t_+$, $t \in \mathbb{R}$.*

See [8, Props. 4.3, 4.4] for a generalization on Proposition 3.2. We further let

$$C(y) := G + \mathcal{A}^* y \quad \text{and} \quad \lambda(y) := \lambda(C(y)).$$

We define three index sets associated with $\lambda(y)$:

$$\alpha(y) := \{i |\ \lambda_i(y) > 0\}, \quad \beta(y) := \{i |\ \lambda_i(y) = 0\}, \text{ and } \gamma(y) := \{i |\ \lambda_i(y) < 0\}.$$

We also let $\Lambda(y) := \mathrm{Diag}[\lambda(y)]$. When no confusion is involved, we often omit y for brevity. Let y^* be a solution of (4) throughout this section. For simplicity, we let

$$\lambda^* := \lambda(y^*), \ \alpha^* := \alpha(y^*), \ \gamma^* := \gamma(y^*), \text{ and } \Lambda^* := \Lambda(y^*).$$

Now we present our first technical result which is a direct consequence of the positiveness of b.

LEMMA 3.3. *Suppose that $b > 0$ in (10). Then $\alpha^* \neq \emptyset$. Moreover, for any $P \in \mathcal{O}_{C(y^*)}$ we have*

$$\sum_{\ell \in \alpha^*} P_{i\ell}^2 > 0 \qquad \forall i = 1, \ldots, n.$$

Proof. Suppose that $P \in \mathcal{O}_{C(y^*)}$ is arbitrarily given. Then

$$(C(y^*))_+ = P \begin{pmatrix} \Lambda_\alpha^* & & \\ & 0 & \\ & & 0 \end{pmatrix} P^T$$

and (10) implies

$$\mathcal{A}P \begin{pmatrix} \Lambda_\alpha^* & & \\ & 0 & \\ & & 0 \end{pmatrix} P^T = b\,,$$

where Λ_α^* is a diagonal matrix of $|\alpha^*| \times |\alpha^*|$ with its diagonal elements given by $\lambda_i^*, i \in \alpha^*$. The fact that $b \neq 0$ implies that α^* is not empty. Equivalently, we have

$$\left(\sum_{\ell \in \alpha^*} \lambda_\ell^* P_{1\ell}^2, \sum_{\ell \in \alpha^*} \lambda_\ell^* P_{2\ell}^2, \ldots, \sum_{\ell \in \alpha^*} \lambda_\ell^* P_{n\ell}^2 \right) = (b_1, b_2, \ldots, b_n).$$

Since $\lambda_\ell^* > 0$ for all $\ell \in \alpha^*$, the lemma is proved to be true. □

Let

$$\delta^* := \frac{1}{2} \min_{i \in \alpha^* \cup \gamma^*} |\lambda_i^*|$$

and

$$\mathcal{B}(y^*, \delta^*) := \{y \in \mathbb{R}^n \mid \|y - y^*\| \leq \delta^*\}.$$

Then the perturbation result in Lemma 2.3 implies that for all $y \in \mathcal{B}(y^*, \delta^*)$,

$$|\lambda_i(y) - \lambda_i^*| \leq \|C(y) - C(y^*)\| \leq \|y - y^*\| \leq \delta^* \qquad \forall\, i = 1, \ldots, n.$$

LEMMA 3.4. *F is differentiable at y if and only if f is differentiable at $C(y)$. And in this case*

$$F'(y)h = \mathcal{A}f'(C(y))H \qquad \forall\, h \in \mathbb{R}^n\,,$$

where $H := \mathcal{A}^* h = \mathrm{Diag}[h]$ and

$$f'(C(y))H = P\left(f^{[1]}(\lambda(y)) \circ (P^T H P)\right) P^T \qquad \forall\, P \in \mathcal{O}_{C(y)}.$$

Moreover, when $y \in \mathcal{B}(y^*, \delta^*)$, we have

$$\left(f^{[1]}(\lambda(y))\right)_{ij} = 1 \qquad \forall\, i, j \in \alpha^*$$

and

$$\left(f^{[1]}(\lambda(y))\right)_{ij} = 0 \qquad \forall\, i, j \in \gamma^*,$$

i.e.,

$$\left(f^{[1]}(\lambda(y))\right)_{\alpha^*\alpha^*} = E_{\alpha^*\alpha^*}, \qquad \left(f^{[1]}(\lambda(y))\right)_{\gamma^*\gamma^*} = 0_{\gamma^*\gamma^*}. \tag{14}$$

Proof. It is obvious that if f is differentiable at $C(y)$, then F is differentiable at y because it is composed of f with linear transformations.

Suppose f is not differentiable at $C(y)$. Then Proposition 3.2 implies that f is not differentiable at $\lambda_i(y)$ for some $i \in \{1,\dots,n\}$. The special structure of $f(t) = \max\{0,t\}$ yields that $\lambda_i(y) = 0$. Since $f(t)$ is directionally differentiable and nondecreasing, it holds that

$$f'(x;1) \geq f'(x;-1) \qquad \forall\, x \in \mathbb{R}.$$

In particular,

$$f'(\lambda_i;1) = 1 > 0 = f'(\lambda_i;-1).$$

We let $d, \hat{d} \in \mathbb{R}^n$ be defined, respectively, by

$$d_\ell = f'(\lambda_\ell;1) \;\text{ and }\; \hat{d}_\ell = f'(\lambda_\ell;-1), \quad \ell = 1,\dots,n.$$

Since $d_i = 1 > \hat{d}_i = 0$, we see that $d \neq \hat{d}$ and $d \geq \hat{d}$. Consider two sequences, respectively, specified by $\{y + te\}_{t>0}$ and $\{y - te\}_{t>0}$. We have

$$C(y+te) = P\mathrm{Diag}[\lambda + te]P^T \;\text{ and }\; C(y-te) = P\mathrm{Diag}[\lambda - te]P^T, \quad P \in \mathcal{O}_{C(y)}.$$

Hence,

$$\lim_{t\downarrow 0} \frac{F(y+te)-F(y)}{t} = \mathcal{A}P\mathrm{Diag}[d]P^T \;\text{ and }\; \lim_{t\downarrow 0} \frac{F(y-te)-F(y)}{-t} = \mathcal{A}P\mathrm{Diag}[\hat{d}]P^T.$$

With a bit of further calculation, we see by noticing $d_\ell \geq \hat{d}_\ell$ for $\ell = 1,\dots,n$ and $d_i > \hat{d}_i$ that

$$\mathcal{A}P\mathrm{Diag}[d]P^T - \mathcal{A}P\mathrm{Diag}[\hat{d}]P^T = \begin{pmatrix} \sum_{\ell=1}^n (d_\ell - \hat{d}_\ell)P_{1\ell}^2 \\ \vdots \\ \sum_{\ell=1}^n (d_\ell - \hat{d}_\ell)P_{n\ell}^2 \end{pmatrix} \neq 0.$$

This means that

$$\lim_{t\downarrow 0} \frac{F(y+te)-F(y)}{t} \neq \lim_{t\downarrow 0} \frac{F(y-te)-F(y)}{-t},$$

implying that F is not differentiable at y. This establishes the first part of the lemma.

The formula for F' follows just from the chain rule and Proposition 3.2. The relation in (14) follows from the definition of $f^{[1]}$ and the fact that for any $y \in \mathcal{B}(y^*,\delta^*)$, $\lambda_i(y) > 0$ for all $i \in \alpha^*$ and $\lambda_i(y) < 0$ for all $i \in \gamma^*$. ∎

We now define a collection of matrices in relation to λ^*:

$$\mathcal{M} := \left\{ M \in \mathbb{R}^{n\times n} \mid\; M = \begin{pmatrix} E_{\alpha^*\alpha^*} & E_{\alpha^*\beta^*} & (\tau_{ij})_{\substack{i\in\alpha^* \\ j\in\gamma^*}} \\ E_{\beta^*\alpha^*} & (\omega_{ij})_{\substack{i\in\beta^* \\ j\in\beta^*}} & 0 \\ (\tau_{ji})_{\substack{i\in\alpha^* \\ j\in\gamma^*}} & 0 & 0 \end{pmatrix} \;\begin{array}{l} \omega_{ij} = \omega_{ji} \in [0,1], \\ \text{for } i,j \in \beta^*, \\ \tau_{ij} = \lambda_i^*/(\lambda_i^* - \lambda_j^*), \\ \text{for } i \in \alpha^*, j \in \gamma^*. \end{array} \right\}$$

We note that $\mathcal{M}$ is a compact set and $1 > \tau_{ij} > 0$ for any $M \in \mathcal{M}$.

LEMMA 3.5. *For any $h \in \mathbb{R}^n$ we have*

$$\partial_B F(y^*)h \subseteq \{\mathcal{A}WH : \ W \in \mathcal{W}\} ,$$

*where $H := \mathcal{A}^*h =$*Diag$[h]$ *and*

$$\mathcal{W} := \left\{W |\ WH = P\left(M \circ (P^T HP)\right)P^T,\ P \in \mathcal{O}_{C(y^*)},\ M \in \mathcal{M} \text{ and } h \in \mathbb{R}^n\right\} .$$

Proof. Let $V \in \partial_B F(y^*)$. By the very definition of $\partial_B F$ we have a sequence $\{y^k\}$ converging to y^* such that F is differentiable at each y^k and $F'(y^k) \to V$. Equivalently, we have

$$\lim_{k\to\infty} F'(y^k)h = Vh \qquad \forall h \in \mathbb{R}^n. \tag{15}$$

Then it follows from Lemma 3.4 that there exists $P^k \in \mathcal{O}_{C(y^k)}$ such that

$$F'(y^k)h = \mathcal{A}f'(C(y^k))H,$$

where $H = \mathcal{A}^*h =$ Diag$[h]$ and

$$f'(C(y^k))H = P^k\left(f^{[1]}(\lambda(y^k)) \circ ((P^k)^T HP^k)\right)(P^k)^T.$$

Denoting $\lambda^k := \lambda(y^k)$ for simplicity, when $y^k \in \mathcal{B}(y^*, \delta^*)$,

$$\lambda_i^k > 0 \text{ for } i \in \alpha^* \ \text{ and } \ \lambda_i^k < 0 \text{ for } i \in \gamma^*,$$

and λ_i^k for $i \in \beta^*$ could be positive or nonpositive but converges to $\lambda_i^* = 0$. Hence, the definition of $f^{[1]}$ yields

$$\left(f^{[1]}(\lambda^k)\right)_{ij} = \begin{cases} 1, & i,j \in \alpha^*, \\ 0, & i,j, \in \gamma^*, \\ \dfrac{\lambda_i^k - (\lambda_j^k)_+}{\lambda_i^k - \lambda_j^k}, & i \in \alpha^*, j \in \beta^*, \\ \dfrac{\lambda_i^k}{\lambda_i^k - \lambda_j^k}, & i \in \alpha^*, j \in \gamma^*, \end{cases}$$

and $(f^{[1]}(\lambda^k))_{ij} = (f^{[1]}(\lambda^k))_{ji}$ (i.e., it is symmetric). Because $0 \le (f^{[1]}(\lambda^k))_{ij} \le 1$ for all i, j, there exists a sequence (still denoted by $\{y^k\}$ without loss of generality) such that $f^{[1]}(\lambda^k)$ converges to a matrix, say M^*. It is easy to see that $M^* \in \mathcal{M}$. The boundedness of $\{P^k\}$ also implies that there exists a sequence (also denoted by $\{y^k\}$) such that $P^k \to P^*$. Then we have

$$C(y^*) = \lim_{k\to\infty} C(y^k) = \lim_{k\to\infty} P^k\text{Diag}[\lambda^k](P^k)^T = P^*\text{Diag}[\lambda](P^*)^T.$$

Hence, $P^* \in \mathcal{O}_{C(y^*)}$, and consequently we have by (15) that

$$Vh = \lim_{k\to\infty} F'(y^k)h \in \{\mathcal{A}WH : \ W \in \mathcal{W}\} \qquad \forall h \in \mathbb{R}^n.$$

Since $V \in \partial_B F(y^*)$ is arbitrary, we establish our result. □

Now we are ready to prove our main result in this section.

PROPOSITION 3.6. *Each element $V \in \partial_B F(y^*)$ is positive definite. Consequently, each element $V \in \partial F(y^*)$ is also positive definite.*

Proof. Let $V \in \partial_B F(y^*)$ be arbitrarily chosen. We want to show that for any $0 \neq h \in \mathbb{R}^n$

$$h^T V h > 0.$$

We note that it follows from Lemma 3.5 that there exist $M \in \mathcal{M}$ and $P \in \mathcal{O}_{C(y^*)}$ such that

$$Vh = \mathcal{A}\left(P(M \circ (P^T H P)\right) P^T.$$

Then

$$\begin{aligned}\langle h, Vh\rangle &= \langle \mathcal{A}^* h, P(M \circ (P^T H P))P^T\rangle \\ &= \langle P^T H P, M \circ (P^T H P)\rangle.\end{aligned}$$

Let $\tilde{H} := P^T H P$. Then we have

$$\begin{aligned}\langle h, Vh\rangle &= \langle \tilde{H}, M \circ \tilde{H}\rangle \\ &\geq \sum_{i\in\alpha^*}\left(\sum_{j\in\alpha^*\cup\beta^*} \tilde{H}_{ij}^2 + \sum_{j\in\gamma^*} \tau_{ij}\tilde{H}_{ij}^2\right) \\ &\geq \tau \sum_{i\in\alpha^*}\sum_{j=1}^{n} \tilde{H}_{ij}^2,\end{aligned}$$

where $\tau = \min_{i\in\alpha^*, j\in\gamma^*} \tau_{ij} > 0$. Because V is positive semidefinite, we see that $\langle h, Vh\rangle = 0$ only if

$$\tilde{H}_{ij} = 0 \qquad \forall i \in \alpha^* \text{ and } j \in \{1, \ldots, n\}.$$

The above condition is equivalent to

$$(\tilde{H}_{i1}, \tilde{H}_{i2}, \ldots, \tilde{H}_{in}) = (0, 0, \ldots, 0) \qquad \forall i \in \alpha^*.$$

By recalling that $\tilde{H} = P^T H P$ and $H = \mathrm{Diag}[h]$, we have

$$(\tilde{H}_{i1}, \tilde{H}_{i2}, \ldots, \tilde{H}_{in}) = (h_1 P_{1i}, h_2 P_{2i}, \ldots, h_n P_{ni})P = (0, 0, \ldots, 0)$$

if and only if

$$(h_1 P_{1i}^2, h_2 P_{2i}^2, \ldots, h_n P_{ni}^2) = (0, 0, \ldots, 0) \ \text{ (because } P \text{ is nonsingular).}$$

Summarizing over $i \in \alpha^*$ in the above relation yields

$$\left(h_1 \sum_{i\in\alpha^*} P_{1i}^2, h_2 \sum_{i\in\alpha^*} P_{2i}^2, \ldots, h_n \sum_{i\in\alpha^*} P_{ni}^2\right) = (0, 0, \ldots, 0).$$

According to Lemma 3.3, the above condition holds if and only if

$$(h_1, h_2, \ldots, h_n) = (0, 0, \ldots, 0),$$

i.e., $h = 0$. This establishes the positive definiteness of V.

Since $\partial_B F(y^*)$ is compact and its every element is positive definite, any convex combination of its elements is also positive definite. That is, every element of $\partial F(y^*)$ is positive definite. □

The first of two important consequences of the above regularity result is on the convergence of Newton's method (11). It is just a direct application of Theorem 2.1, given that we have already known that F is strongly semismooth and every element in $\partial F(y^*)$ is positive definite.

COROLLARY 3.7. *Newton's method* (11) *is quadratically convergent, provided that* y^0 *is sufficiently close to* y^*.

The second corollary is on the uniqueness of the solution to (10) and its strong semismoothness.

COROLLARY 3.8. *For any given* $G \in \mathcal{S}^n$ *and* $0 < b \in \mathbb{R}^n$, *there is a unique solution* y^* *to* (10). *If* y^* *is viewed as a function of* G *and* b, *denoted* $y^*(G, b)$, *then* y^* *is strongly semismooth with respect to* $(G, b) \in \mathcal{S}^n \times \mathbb{R}^n_{++}$. *Consequently,* X^* *as a function of* G *and* b *is also strongly semismooth with respect to* $(G, b) \in \mathcal{S}^n \times \mathbb{R}^n_{++}$.

Proof. The proof of Proposition 3.6 is independent of the choice of G and b as long as it belongs to $\mathcal{S}^n \times \mathbb{R}^n_{++}$. Hence, the Clarke inverse theorem says that there is a unique solution $y^*(G, b)$ for any $(G, b) \in \mathcal{S}^n \times \mathbb{R}^n_{++}$. We note that the existence of a solution is guaranteed because $0 < b \in \mathbb{R}^n_{++}$ and $b \in \mathrm{int}\mathcal{A}(\mathcal{S}^n_+)$. The strong semismoothness of y^* follows from a result of Sun [45] on an implicit theorem of strongly semismooth functions. Since X^* is composed of strongly semismooth functions, it is also strongly semismooth with respect to $(G, b) \in \mathcal{S}^n \times \mathbb{R}^n_{++}$. □

4. Extensions.

4.1. The *W*-weighted version. In practice, the W-weighted version of (1) is very useful [25]:

$$\begin{array}{ll} \min & \frac{1}{2}\|G - X\|_W^2 \\ \text{s.t.} & X_{ii} = 1, \quad i = 1, \ldots, n, \\ & X \succeq 0, \end{array} \tag{16}$$

where $W \in \mathcal{S}^n$ is positive definite and for any $Y \in \mathcal{S}^n$,

$$\|Y\|_W = \|W^{1/2} Y W^{1/2}\|.$$

Let

$$\bar{G} = W^{1/2} G W^{1/2} \quad \text{and} \quad \bar{X} = W^{1/2} X W^{1/2}.$$

Then problem (16) becomes standard in the form of (1):

$$\begin{array}{ll} \min & \frac{1}{2}\|\bar{G} - \bar{X}\|^2 \\ \text{s.t.} & (W^{-1/2} \bar{X} W^{-1/2})_{ii} = 1, \quad i = 1, \ldots, n, \\ & \bar{X} \succeq 0. \end{array}$$

In fact, the constraint $\bar{X} \succeq 0$ should be $W^{-1/2} \bar{X} W^{-1/2} \succeq 0$. It is easy to see that they are equivalent. For simplicity, we drop the bars in the above formulation and

have

$$\begin{array}{ll} \min & \frac{1}{2}\|G-X\|^2 \\ \text{s.t.} & \left(W^{-1/2}XW^{-1/2}\right)_{ii}=1, \quad i=1,\ldots,n, \\ & X \succeq 0. \end{array} \tag{17}$$

Define the linear operator $\mathcal{A}: \mathcal{S}^n \mapsto \mathbb{R}^n$ by

$$(\mathcal{A}X)_i = \left(W^{-1/2}XW^{-1/2}\right)_{ii}, \quad i=1,\ldots,n. \tag{18}$$

The adjoint operator $\mathcal{A}^*: \mathbb{R}^n \mapsto \mathcal{S}^n$ is given by

$$\begin{aligned} \langle \mathcal{A}^* y, X\rangle &= \langle y, \mathcal{A}X\rangle \\ &= \langle y, \mathrm{diag}[W^{-1/2}XW^{-1/2}]\rangle \\ &= \langle \mathrm{Diag}[y], W^{-1/2}XW^{-1/2}\rangle \\ &= \langle W^{-1/2}\mathrm{Diag}[y]W^{-1/2}, X\rangle. \end{aligned}$$

Hence

$$\mathcal{A}^* y = W^{-1/2}\mathrm{Diag}[y]W^{-1/2}. \tag{19}$$

It is easy to see that $e \in \mathrm{int}\mathcal{A}\mathcal{S}^n_+$. With this fact, we once again get (10) with $\mathcal{A}$ and $\mathcal{A}^*$ defined by (18) and (19), respectively. With no difficulty, we can develop parallel results as in Lemmas 3.3–3.5 and in Proposition 3.6. For example, Lemma 3.3 now becomes the following result.

LEMMA 4.1. *Suppose that $b > 0$ in* (10) *and that $\mathcal{A}$ and $\mathcal{A}^*$ are defined by* (18) *and* (19)*, respectively. Then $\alpha^* \neq \emptyset$. Moreover, for any $P \in \mathcal{O}_{C(y^*)}$ we have*

$$\sum_{\ell \in \alpha^*} \hat{P}^2_{i\ell} > 0 \qquad \forall i = 1,\ldots,n\,,$$

where $\hat{P} = W^{-1/2}P$.

The proof follows just that of Lemma 3.3 and makes use of (18). Lemmas 3.4 and 3.5 remain true with $H = \mathcal{A}^*h = W^{-1/2}\mathrm{Diag}[h]W^{-1/2}$ for $h \in \mathbb{R}^n$. The proof for Proposition 3.6 is also true now with $\tilde{H} = P^T H P$ and H as just defined. Starting from

$$(\tilde{H}_{i1}, \tilde{H}_{i2}, \ldots, \tilde{H}_{in}) = (0, 0, \ldots, 0) \qquad \forall i \in \alpha^*$$

in the proof of Proposition 3.6, we have

$$\left(h_1 \sum_{i\in\alpha^*} \hat{P}^2_{1i}, h_2 \sum_{i\in\alpha^*} \hat{P}^2_{2i}, \ldots, h_n \sum_{i\in\alpha^*} \hat{P}^2_{ni}\right) = (0, 0, \ldots, 0)$$

by noticing

$$\tilde{H} = P^T W^{-1/2}\mathrm{Diag}[h]W^{-1/2}P = \hat{P}\mathrm{Diag}[h]\hat{P}.$$

According to Lemma 4.1, the above condition holds if and only if

$$(h_1, h_2, \ldots, h_n) = (0, 0, \ldots, 0).$$

This proves Proposition 3.6 with $\mathcal{A}$ and $\mathcal{A}^*$ defined by (18) and (19), respectively. Therefore, for the W-weighted version, Newton's method is quadratically convergent.

4.2. The case of lower bounds. The nearest correlation matrix is often rank-deficient [25]. To avoid the ill-conditionedness and to increase the stability, one often requires the matrix to be not less than a positive diagonal matrix. This gives the so-called calibration of correlation matrices, i.e.,

$$\begin{array}{ll} \min & \frac{1}{2}\|G - X\|^2 \\ \text{s.t.} & X \succeq \alpha I, \\ & \mathcal{A}X = e\,, \end{array} \tag{20}$$

where $\alpha \in (0,1)$ and $\mathcal{A}X = \mathrm{diag}[X]$. We will see that it is quite straightforward to apply the generalized Newton method to this case.

First, we note that the following condition is automatically valid:

$$\left\{\mathcal{A}^*y :\ (1-\alpha)y^Te \geq 0,\ y \in \mathbb{R}^n\right\} \cap (-\mathcal{S}^n_+) = \{0\}.$$

This condition corresponds to the condition [37, (2.17)], so that [37, Thm. 2.2] (this theorem considers only the case which corresponds to $G = 0$ in (20); however, it also holds for $G \neq 0$) implies that the unique solution of (20) has the following representation:

$$X^* = (G - \alpha I + \mathcal{A}^*y^*)_+ + \alpha I,$$

where y^* is a solution of the following equation:

$$\mathcal{A}(G - \alpha I + \mathcal{A}^*y)_+ + \alpha\mathcal{A}I = e,$$

which is obviously equivalent to

$$\mathcal{A}(G - \alpha I + \mathcal{A}^*y)_+ = (1-\alpha)e. \tag{21}$$

We now note that this equation actually defines a new problem similar to (1):

$$\begin{array}{ll} \min & \frac{1}{2}\|(G - \alpha I) - X\|^2 \\ \text{s.t.} & \mathcal{A}e = (1-\alpha)e, \\ & X \in \mathcal{S}^n_+. \end{array} \tag{22}$$

Hence, by following the discussion in section 1 and noting that $(1-\alpha)e > 0$, we know that the unique solution of problem (22) has the form

$$X^* = (G - \alpha I + \mathcal{A}^*y^*)_+,$$

where y^* is the unique solution of (21). We note that the uniqueness of y^* follows from Corollary 3.8 applied to (22). Therefore, Newton's method also applies to (21) and is quadratically convergent by Corollary 3.7, and hence solves (20).

A more complicated problem of the *calibration of covariance matrix* was also discussed by Malick [35] and is defined by

$$\begin{array}{ll} \min & \frac{1}{2}\|X - \tilde{Q}\|^2 \\ \text{s.t.} & X \succeq \alpha I, \\ & \langle I, X\rangle = \mathrm{tr}(\tilde{Q}), \\ & \langle G_i, X\rangle = \sigma_i^2, \quad i = 1, \ldots, m, \end{array} \tag{23}$$

where $\alpha > 0$, $\tilde{Q}$ is a first estimate of the true covariance matrix Q used in portfolio risk analysis, and σ_i^2 represent "ex-post" volatilities of well-chosen portfolios; $G_i \in \mathcal{S}^n$. We now demonstrate how Newton's method can be applied to this problem.

The feasibility of problem (23) requires

$$\mathrm{tr}(\tilde{Q}) \geq n\alpha.$$

To facilitate our analysis, let

$$b_0 := \mathrm{tr}(\tilde{Q}),\ b_i := \sigma_i^2,\ i = 1, \ldots, m, \quad \text{and} \quad b := (b_0, b_1, \ldots, b_m)^T \in \mathbb{R}^{m+1},$$

$$G_0 := I,\ \mathcal{A} := (G_0, G_1, \ldots, G_m)$$

with

$$\mathcal{A}X := (\langle G_0, X\rangle, \langle G_1, X\rangle, \ldots, \langle G_m, X\rangle)^T \in \mathbb{R}^{m+1}.$$

Suppose that G_i's are positive semidefinite nonzero matrices. Then $\mathrm{tr}(G_i) > 0$ for each i. Let α be chosen such that

$$0 < \alpha < \min\{b_i/\mathrm{tr}(G_i) \mid i = 0, 1, \ldots, m\}. \tag{24}$$

We also assume that for any $y \in \mathbb{R}^{m+1}$ with $y_\ell > 0$ for some $\ell \in \{0, 1, \ldots, m\}$, we have

$$\mathcal{A}^* y := \sum_{i=1}^{m} G_i y_i \not\preceq 0. \tag{25}$$

Conditions (24) and (25) indicate how α and G_i are chosen in problem (23). Under these two conditions, we see that condition (2.17) in [37] is valid for problem (23), i.e.,

$$\{\mathcal{A}^* y :\ y^T(b - \alpha z^0) \geq 0\} \cap (-\mathcal{S}_+^n) = \{0\},$$

where $z^0 := \mathcal{A}I = (\mathrm{tr}(G_0), \mathrm{tr}(G_1), \ldots, \mathrm{tr}(G_m))^T \in \mathbb{R}^{m+1}$. Hence, once again [37, Thm. 2.2] implies that the unique solution of (23) has the representation

$$X^* = (\tilde{Q} - \alpha I + \mathcal{A}^* y^*)_+ + \alpha I\,,$$

where y^* is a solution to the following equation:

$$\mathcal{A}(\tilde{Q} - \alpha I + \mathcal{A}^* y)_+ = b - \alpha z^0. \tag{26}$$

Now the generalized Newton method can be applied to this equation. If we further assume that the matrices $G_i, i = 1, \ldots, m$, are mutually diagonalizable, Newton's method is also quadratically convergent following our results in the last section. To see this, let $P \in \mathcal{O}$ be a matrix such that G_i are simultaneously diagonalizable by P, i.e.,

$$G_i = P\Gamma^i P^T,\ \ i = 1, \ldots, m,$$

where each Γ^i is a nonnegative diagonal matrix. Let $\Gamma^0 = I$ and define

$$\mathcal{L} := (\Gamma^0, \Gamma^1, \ldots, \Gamma^m)$$

so that

$$\mathcal{L}X = (\langle \Gamma^0, X\rangle, \langle \Gamma^1, X\rangle, \ldots, \langle \Gamma^m, X\rangle)^T$$

and

$$\mathcal{L}^* y = \sum_{i=0}^{m} \Gamma^i y_i.$$

Then (26) becomes

$$\mathcal{L}(P^T(\tilde{Q} - \alpha I)P + \mathcal{L}^* y)_+ = \tilde{b}\,, \tag{27}$$

where $\tilde{b} := \mathrm{diag}[P^T(b - \alpha z^0)P]$. Since $b - \alpha z^0 > 0$ by the assumed conditions, we see that $\tilde{b} > 0$. Now we note that (27) defines a new problem given by

$$\begin{array}{ll} \min & \dfrac{1}{2}\|P^T(\tilde{Q} - \alpha I)P - X\|^2 \\ \text{s.t.} & \langle \Gamma^i, X\rangle = \tilde{b}_i, \quad i = 0, \ldots, m, \\ & X \in \mathcal{S}^n_+. \end{array}$$

It is easy to repeat the arguments for problem (1) to verify that Newton's method for the above problem is quadratically convergent.

Finally, we note that all the assumptions made so far for problem (23) are automatically satisfied if each $G_i = E_i$, where E_i is the diagonal matrix whose only nonzero element is its ith diagonal element and equals 1.

4.3. The nonsymmetric case. In some applications [31], X may be only required to be positive semidefinite but not necessarily symmetric. Then we have the following matrix nearness problem:

$$\begin{array}{ll} \min & \dfrac{1}{2}\| X - G \|^2 \\ \text{s.t.} & \mathcal{A}X = b, \\ & X \in \mathcal{K}^n\,, \end{array} \tag{28}$$

where $\mathcal{K}^n$ is the cone of $n \times n$ positive semidefinite matrices (not necessarily symmetric)

$$\mathcal{K}^n = \{X \in \mathbb{R}^{n\times n} \,|\, X \text{ is positive semidefinite}\}\,.$$

By assuming the strong CHIP on $\{\mathcal{K}^n, \mathcal{A}^{-1}(b)\}$, we know from section 1 that the unique solution X^* to problem (28) has the representation

$$X^* = \Pi_{\mathcal{K}^n}(G + \mathcal{A}^* y^*) \tag{29}$$

and y^* is a solution of the equation

$$F(y) := \mathcal{A}\Pi_{\mathcal{K}^n}(G + \mathcal{A}^* y) = b, \quad y \in \mathbb{R}^n\,. \tag{30}$$

Next, we derive an explicit formula for computing $\Pi_{\mathcal{K}^n}(X)$ for a given $X \in \mathbb{R}^{n\times n}$. It is easy to see that $\Pi_{\mathcal{K}^n}(X)$ is the unique solution to

$$\begin{array}{ll} \min & \dfrac{1}{2}\| Y - X \|^2 \\ \text{s.t.} & \dfrac{1}{2}(Y + Y^T) \in \mathcal{S}^n_+\,. \end{array} \tag{31}$$

Since the Slater condition for problem (31) holds automatically, $\Pi_{\mathcal{K}^n}(X)$, together with the Lagrange multiplier $\Lambda \in \mathcal{S}^n_+$, satisfies the KKT conditions [34, Chap. 8]

$$\begin{cases} Y - X - \Lambda = 0, \\ \dfrac{1}{2}(Y + Y^T) \in \mathcal{S}^n_+, \quad \Lambda \in \mathcal{S}^n_+, \quad \dfrac{1}{2}(Y + Y^T)\Lambda = 0\,. \end{cases}$$

These conditions can be equivalently written as

$$\begin{cases} Y - X - \Lambda = 0, \\ \Lambda - \Pi_{\mathcal{S}^n_+}[\Lambda - \frac{1}{2}(Y + Y^T)] = 0\,, \end{cases}$$

which imply

$$\Lambda - \frac{1}{2}(Y + Y^T) = -\frac{1}{2}(X + X^T)$$

and

$$\Lambda = \frac{1}{2}\Pi_{\mathcal{S}^n_+}[-(X + X^T)]\,.$$

Hence

$$\Pi_{\mathcal{K}^n}(X) = X + \frac{1}{2}\Pi_{\mathcal{S}^n_+}[-(X + X^T)] = \frac{1}{2}(X - X^T) + \frac{1}{2}\Pi_{\mathcal{S}^n_+}(X + X^T)\,.$$

Therefore, by [46, Thm 4.13], we get the following result.

PROPOSITION 4.2. *The metric projection operator* $\Pi_{\mathcal{K}^n}(\cdot)$ *is strongly semismooth at any* $X \in \mathbb{R}^{n\times n}$.

Proposition 4.2 implies that the function F defined in (30) is strongly semismooth everywhere on $\mathbb{R}^n$. Then, in a similar way as for the symmetric case, we may use our Newton's method to find a solution of $F(y) = b$.

To establish the quadratic convergence of Newton's method, we restrict ourselves to the case that the linear operator $\mathcal{A} : \mathbb{R}^{n\times n} \mapsto \mathbb{R}^n$ is defined by $\mathcal{A}X = \mathrm{diag}[X]$. In this case, the adjoint of $\mathcal{A}$ is $\mathcal{A}^* y = \mathrm{Diag}[y]$ (note that the inner product in $\mathbb{R}^{n\times n}$ is $\langle X, Y\rangle = \mathrm{tr}(X^T Y)$.) Noticing that

$$\mathcal{A}(X - X^T) = 0,$$

we see that the nonsmooth equation (30) becomes

$$F(y) = \frac{1}{2}\mathcal{A}\Pi_{\mathcal{S}^n_+}(C(y) + C^T(y)) = b,$$

where as before we denote $C(y) = G + \mathcal{A}^* y$. In a more explicit form we have

$$F(y) = \mathcal{A}\Pi_{\mathcal{S}^n_+}\left(\frac{1}{2}(G + G^T) + \mathcal{A}^* y\right) = b. \tag{32}$$

This is the nonsmooth equation derived from the following standard problem in the form of (1):

$$\begin{array}{ll} \min & \dfrac{1}{2}\|(G + G^T)/2 - X\|^2 \\ \text{s.t.} & X_{ii} = b_i, \quad i = 1, \ldots, n, \\ & X \in \mathcal{S}^n_+\,. \end{array} \tag{33}$$

Under the condition that $b > 0$, we see from our previous results for the symmetric case similar to (33) that Proposition 3.6 holds for (32). Hence, Newton's method is quadratically convergent for the special case.

5. Numerical results. In numerical experiments, we used the following globalized version of Newton's method for solving the dual problem (8). Recall that for any $y \in \mathbb{R}^n$, $\nabla\theta(y) = F(y) - b$ and $b = e$.

ALGORITHM 5.1. NEWTON'S METHOD.

Step 0. *Given* $y^0 \in \mathbb{R}^n$, $\eta \in (0,1)$, $\rho, \sigma \in (0, 1/2)$. $k := 0$.

Step 1. *Select an element* $V_k \in \partial F(y^k)$ *and apply the conjugate gradient (CG) method of Hestenes and Stiefel* [23] *to find an approximate solution* d^k *to*

$$\nabla\theta(y^k) + V_k d = 0 \tag{34}$$

such that

$$\|\nabla\theta(y^k) + V_k d^k\| \le \eta_k \|\nabla\theta(y^k)\|, \tag{35}$$

where $\eta_k := \min\{\eta, \|\nabla\theta(y^k)\|\}$. *If* (35) *is not achievable or if the condition*

$$\nabla\theta(y^k)^T d^k \le -\eta_k \|d^k\|^2 \tag{36}$$

is not satisfied, let $d^k := -B_k^{-1}\nabla\theta(y^k)$, *where* B_k *is any symmetric positive definite matrix in* $\mathcal{S}^n$.

Step 2. *Let* m_k *be the smallest nonnegative integer* m *such that*

$$\theta(y^k + \rho^m d^k) - \theta(y^k) \le \sigma\rho^m \nabla\theta(y^k)^T d^k.$$

Set $t_k := \rho^{m_k}$ *and* $y^{k+1} := y^k + t_k d^k$.

Step 3. *Replace* k *by* $k+1$ *and go to Step* 1.

An alternative to calculating the Newton direction is to apply the CG method to the following perturbed Newton equation:

$$\nabla\theta(y^k) + (V_k + \varepsilon_k I)\, d = 0 \quad \text{with} \quad \varepsilon_k > 0.$$

The classical choice of ε_k is the norm of the residue, i.e., $\varepsilon_k = \|F(y^k) - b\|$. Since V_k is always positive semidefinite, the matrix $(V_k + \varepsilon_k I)$ is always positive definite for any $\varepsilon^k > 0$.

We provide a proof for the sake of completeness.

The global convergence analysis of Algorithm 5.1 is quite standard. Since the CG method is used to calculate the Newton direction, it is actually an inexact Newton direction that was used in our implementation. Hence, our local convergence analysis is a bit different from the standard ones. We provide a proof for the sake of completeness.

First, we need the following result due to Facchinei [21, Thm. 3.3 and Remark 3.4]. A similar result was also obtained by Pang and Qi [41].

LEMMA 5.2. *Suppose that, for every* k,

$$\nabla\theta(y^k)^T d^k \le -\hat{\rho}\|d^k\|^2$$

for some $\hat{\rho} > 0$. *Then, for any* $\mu \in (0, 1/2)$, *there exists a* $\bar{k}$ *such that for all* $k \ge \bar{k}$,

$$\theta(y^k + d^k) \le \theta(y^k) + \mu\nabla\theta(y^k)^T d^k\,.$$

THEOREM 5.3. *Suppose that in Algorithm* 5.1 *both* $\{\|B_k\|\}$ *and* $\{\|B_k^{-1}\|\}$ *are uniformly bounded. Then the iteration sequence* $\{y^k\}$ *generated by Algorithm* 5.1 *converges to the unique solution* y^* *of* $F(y) = b$ *quadratically.*

Proof. Since for any $k \geq 0$, d^k is always a descent direction of $\theta(\cdot)$ at y^k, Algorithm 5.1 is well defined. Moreover, from the coercive property of θ we know that $\{y^k\}$ is bounded. Then, by employing standard convergence analysis (cf. [12, Thm 6.3.3]), we can conclude that

$$\lim_{k\to\infty} \nabla\theta(y^k) = 0\,,$$

which, together with the convexity of $\theta(\cdot)$ and the boundedness of $\{y^k\}$, implies that $y^k \to y^*$.

Since, by Proposition 3.6, any element $V \in \partial F(y^*)$ is positive definite, it holds that for all k sufficiently large, V_k is positive definite and $\{\|V_k^{-1}\|\}$ is uniformly bounded. Hence, for all k sufficiently large, the CG method can find d^k such that both (35) and (36) are satisfied. This, together with the facts that $\nabla\theta(y^*) = 0$ and $\nabla\theta(\cdot)$ is strongly semismooth at y^*, further implies that for all k sufficiently large,

(37)
$$\begin{aligned}
\|y^k + d^k - y^*\| &= \|y^k + V_k^{-1}[(\nabla\theta(y^k) + V_k d^k) - \nabla\theta(y^k)] - y^*\| \\
&\leq \|y^k - y^* - V_k^{-1}\nabla\theta(y^k)\| + \|V_k^{-1}(\nabla\theta(y^k) + V_k d^k)\| \\
&\leq \|V_k^{-1}\|\|\nabla\theta(y^k) - \nabla\theta(y^*) - V_k(y^k - y^*)\| + \eta_k\|V_k^{-1}\|\|\nabla\theta(y^k)\| \\
&\leq O(\|y^k - y^*\|^2) + \|V_k^{-1}\|\|\nabla\theta(y^k)\|^2 \\
&\leq O(\|y^k - y^*\|^2) + O(\|\nabla\theta(y^k) - \nabla\theta(y^*)\|)^2, \\
&= O(\|y^k - y^*\|^2),
\end{aligned}$$

where in the last equality we used the Lipschitz continuity of $\nabla\theta(\cdot)$. From (37) and the fact that $y^k \to y^*$, we have for all k sufficiently large that

$$y^k - y^* = -d^k + O(\|d^k\|^2) \qquad \text{and} \qquad \|d^k\| \to 0. \tag{38}$$

For each $k \geq 0$, let $r^k := \nabla\theta(y^k) + V_k d^k$. Then for all k sufficiently large,

$$\begin{aligned}
-\nabla\theta(y^k)^T d^k &= \langle d^k, V_k d^k\rangle - \langle d^k, r^k\rangle \\
&\geq \langle d^k, V_k d^k\rangle - \|d^k\|\|r^k\| \\
&\geq \langle d^k, V_k d^k\rangle - \eta_k\|d^k\|\|\nabla\theta(y^k)\| \\
&= \langle d^k, V_k d^k\rangle - \|d^k\|\|\nabla\theta(y^k)\|^2 \\
&\geq \langle d^k, V_k d^k\rangle - \|d^k\|\|y^k - y^*\|^2, \qquad (39)
\end{aligned}$$

which, together with (38) and the uniform positive definiteness of V_k, implies that there exists $\hat\rho > 0$ such that for all k sufficiently large,

$$-\nabla\theta(y^k)^T d^k \geq \hat\rho\|d^k\|^2.$$

It then follows from Lemma 5.2 that for all k sufficiently large, $t_k = 1$ and

$$y^{k+1} = y^k + d^k\,.$$

The proof is completed by observing (37). ∎

Next, we discuss several issues regarding the implementation of Algorithm 5.1.

(a) *Forming the Newton matrix.* In Algorithm 5.1, we need to find a $V \in \partial F(y)$ to form (34). For a given $y \in \mathbb{R}^n$, let $C(y)$ have the following spectral decomposition:

$$C(y) = P\mathrm{Diag}[\lambda(y)]P^T, \quad P \in \mathcal{O}_{C(y)}.$$

Let

$$M_y := \begin{pmatrix} E_{\alpha\alpha} & E_{\alpha\beta} & (\tau_{ij}(y))_{\substack{i\in\alpha\\ j\in\gamma}} \\ E_{\beta\alpha} & 0 & 0 \\ (\tau_{ji}(y))_{\substack{i\in\alpha\\ j\in\gamma}} & 0 & 0 \end{pmatrix}, \qquad \tau_{ij}(y) := \frac{\lambda_i(y)}{\lambda_i(y) - \lambda_j(y)}, \quad i \in \alpha, j \in \gamma.$$

Define the matrix $V_y \in \mathbb{R}^{n\times n}$ by

$$V_y h = \mathcal{A}P\left(M_y \circ (P^T H P)\right) P^T, \quad h \in \mathbb{R}^n, \tag{40}$$

where $H := \mathrm{Diag}[h]$.

PROPOSITION 5.4. *Let the matrix V_y be defined by* (40). *Then*

$$V_y \in \partial_B F(y) \subseteq \partial F(y).$$

Proof. Recall that the scalar-valued function $f(t) = \max(0, t), t \in \mathbb{R}$. For each $k > 0$, let $t_k := -1/k$. We now consider the sequence $\{z^k\}$ with z^k given by $z^k := y - t_k e = y + (1/k)e$. Then $\lambda(y) - t_k e$ is the spectrum of $C(z^k)$, i.e.,

$$C(z^k) = C(y) - t_k C(e) = P\mathrm{Diag}[\lambda(y) - t_k e]P^T = P\mathrm{Diag}[\lambda(y) + (1/k)e]P^T.$$

Let $\bar{k} > 0$ be sufficiently large such that $1/\bar{k} < \min\{|\lambda_i(y)| \,|\, i \in \alpha \cup \gamma\}$ (recall the definitions of α and γ). Then, for each $k \geq \bar{k}$, the matrix-valued function $f : \mathcal{S}^n \to \mathcal{S}^n$ is differentiable at $C(z^k)$ because $C(z^k)$ is nonsingular and in this case, by Lemma 3.1, f is differentiable at $C(z^k)$ and for any $Z \in \mathcal{S}^n$,

$$f'(C(z^k))Z = P\left(f^{[1]}(\lambda(y) + (1/k)e) \circ (P^T Z P)\right) P^T.$$

Therefore, from Lemma 3.4 we know that for each $k \geq \bar{k}$, F is differentiable at z^k and for any $h \in \mathbb{R}^n$,

$$F'(z^k)h = \mathcal{A}f'(C(z^k))H,$$

where $H := \mathrm{Diag}[h]$. After direct computations we can see that

$$M_y = \lim_{k\to\infty} f^{[1]}(\lambda(y) + (1/k)e).$$

Hence, for each $h \in \mathbb{R}^n$,

$$\lim_{k\to\infty} F'(z^k)h = \mathcal{A}P\left(M_y \circ (P^T H P)\right) P^T,$$

which, together with (40), implies that

$$V_y = \lim_{k\to\infty} F'(z^k).$$

Thus, by the definition of $\partial_B F(y)$, $V_y \in \partial_B F(y)$. The proof is completed by observing that $\partial F(y) = \mathrm{co}\,\partial_B F(y)$. ∎

We see from Proposition 5.4 that we can obtain an element $V_y \in \partial F(y)$ by the spectral decomposition of $C(y)$. Since we use the CG method to solve (34), we do not need to form V_y explicitly.

(b) *Testing examples.* We tested the following four classes of problems.

Example 5.5. C is a randomly generated $n \times n$ correlation matrix by `gallery ('randcorr',n)` of MATLAB 7.0.1. R is a random $n \times n$ symmetric matrix with $R_{ij} \in [-1, 1]$, $i, j = 1, 2, \ldots, n$. Then we set

$$G = C + \alpha R\,,$$

where $\alpha = 0.01, 0.1, 1.0, 10.0$. We fix $n = 1000$ in our numerical reports. This problem was tested by Higham [25].

Example 5.6. G is a randomly generated symmetric matrix as in the first example of Malick [35] with $G_{ij} \in [-1, 1]$ and $G_{ii} = 1.0$, $i, j = 1, 2, \ldots, n$, and $n = 500, 1000, 1500, 2000$.

Example 5.7. G is a randomly generated symmetric matrix with $G_{ij} \in [0, 2]$ and $G_{ii} = 1.0$, $i, j = 1, 2, \ldots, n$, and $n = 500, 1000, 1500, 2000$.

Example 5.8. G is a randomly generated symmetric matrix as in the second example of Malick [35] with

$$G_{ii} \in [-2.0 \times 10^4, 2.0 \times 10^4],\ i = 1, 2, \ldots, n.$$

We add to G a perturbed $n \times n$ random symmetric matrix with entries in $[-\alpha, \alpha]$, where $\alpha = 0.0, 0.01, 0.1, 1.0$. We report our numerical results for $n = 1000$.

(c) *Initial parameters.* In our numerical experiments, two initial points were used: (i) $b - \mathrm{diag}(G)$; and (ii) $b - \mathrm{diag}(G) + e$. Other initial points may be used. For example, we may start from a positive point, i.e., $y^0 > 0$, such that $C(y^0)$ is positive definite. The performance of Newton's method is similar, as we reported below. We set other parameters as $\eta = 10^{-5}$, $\rho = 0.5$, and $\sigma = 2.0 \times 10^{-4}$. For simplicity, we fix $B_k \equiv I$ for all $k \geq 0$.

(d) *Comparison and observations.* For the purpose of comparison, we tested the performance of the BFGS method with the Wolfe line search used by Malick [35] and the alternating projection method employed by Higham [25]. The details of the implementation of the BFGS method can be found in [39, Chap. 8]. As observed by Malick [35, Thm. 5.1], Higham's method is the following standard gradient optimization algorithm applied to (8):

$$y^{k+1} := y^k - \nabla\theta(y^k)\,, \quad k = 0, 1, \ldots,$$

and is therefore called the gradient method. We also tested a hybrid method that combines the BFGS method and Newton's method. The hybrid method, which is called BFGS-N here, starts with the BFGS method and switches to Newton's method when $\|\nabla\theta(y^k)\| \leq 1.0$.

All tests were carried out in MATLAB 7.0.1 running on a PC Pentium IV. In our experiments, our stopping criterion is

$$\|\nabla\theta(y^k)\| \leq 10^{-5}\,.$$

The reason that we chose 10^{-5} instead of 10^{-6} or higher accuracy is because the BFGS method and the gradient method ran into difficulty for a higher accuracy in a few cases. Our numerical results are reported in Tables 1–4, where Init., Iter., Func.,

TABLE 1
Numerical results of Example 5.5.

Init.	Algorithm	α	cputime	Iter.	Func.	Res.
(i)	Newton	0.01	2 m 13 s	1	2	2.6×10^{-7}
		0.1	2 m 58 s	3	4	2.0×10^{-8}
		1.0	3 m 38 s	5	6	2.7×10^{-8}
		10.0	4 m 13 s	7	8	9.9×10^{-8}
	BFGS	0.01	2 m 19 s	2	3	2.3×10^{-7}
		0.1	3 m 03 s	5	6	8.0×10^{-7}
		1.0	6 m 27 s	18	19	9.7×10^{-6}
		10.0	15 m 10 s	53	54	6.4×10^{-6}
	BFGS-N	0.01	2 m 16 s	1	2	7.2×10^{-8}
		0.1	3 m 10 s	4	5	4.9×10^{-11}
		1.0	3 m 50 s	7	8	4.0×10^{-6}
		10.0	6 m 00 s	15	16	2.6×10^{-10}
	Gradient	0.01	2 m 20s	2	3	6.0×10^{-6}
		0.1	4 m 56 s	13	14	6.6×10^{-6}
		1.0	24 m 38 s	107	108	9.3×10^{-6}
		10.0	1 h 57 m 54 s	500	501	8.2×10^{-3}
(ii)	Newton	0.01	0.22 s	2	3	1.4×10^{-6}
		0.1	3 m 12 s	4	5	1.1×10^{-10}
		1.0	3 m 41 s	5	6	4.5×10^{-7}
		10.0	4 m 39 s	7	8	1.2×10^{-7}
	BFGS	0.01	2 m 50 s	3	4	6.9×10^{-8}
		0.1	3 m 25 s	6	7	6.9×10^{-6}
		1.0	8 m 09 s	19	20	6.3×10^{-6}
		10.0	15 m 11 s	53	54	7.9×10^{-6}
	BFGS-N	0.01	2 m 39 s	2	3	4.6×10^{-6}
		0.1	3 m 08 s	4	5	6.3×10^{-7}
		1.0	4 m 16 s	7	8	4.0×10^{-6}
		10.0	6 m 37 s	15	16	2.3×10^{-9}
	Gradient	0.01	02 m 48s	3	4	5.1×10^{-6}
		0.1	5 m 24 s	14	15	6.0×10^{-6}
		1.0	24m 06 s	106	107	9.2×10^{-6}
		10.0	1 h 59 m 53 s	500	501	8.4×10^{-3}

and Res. stand for, respectively, the initial point used, the number of iterations, the number of function evaluations of θ, and the residual $\|\nabla\theta(y^k)\|$ at the final iterate of an algorithm (we set a maximum of 500 iterations). LS failed means that the line search failed (the steplength is too small to proceed) during the computation.

An outstanding observation is that Newton's method took less than 10 iterations for all the problems to reach the reported accuracy and the quadratic convergence was observed. The BFGS method performed quite well for Examples 5.5, 5.6, and 5.8, while there are four line search failures in Example 5.7. Sometimes it took much longer to reach the required accuracy. Numerical results for BFGS-N clearly showed that Newton's method can be used to save a lot of computing time required by the BFGS method. The gradient method is generally outperformed by the BFGS method. Compared to the numerical results reported in [49] on the inexact primal-dual path following interior point methods for the similar tested examples, our proposed Newton method is much faster (4 to 5 times) in terms of the cputime. The main reason is that the proposed Newton method needs fewer iterations and at each iteration it needs only one eigenvalue decomposition instead of two as in the inexact primal-dual path following interior point methods [49].

More specific observations are included in the following remarks.

TABLE 2
Numerical results of Example 5.6.

Init.	Algorithm	n	cputime	Iter.	Func.	Res.
(i)	Newton	500	16.6 s	5	6	1.0×10^{-9}
		1,000	1 m 49 s	5	6	3.3×10^{-8}
		1,500	5 m 44 s	5	6	2.7×10^{-7}
		2,000	12 m 34 s	5	6	1.5×10^{-6}
	BFGS	500	32.1 s	16	17	5.5×10^{-6}
		1,000	4 m 03 s	19	20	5.7×10^{-6}
		1,500	13 m 26 s	20	21	9.1×10^{-6}
		2,000	33 m 10 s	22	23	3.9×10^{-6}
	BFGS-N	500	15.1 s	6	7	4.0×10^{-6}
		1,000	2 m 00 s	7	8	3.6×10^{-6}
		1,500	7 m 44 s	7	8	7.4×10^{-6}
		2,000	17 m 06 s	8	9	1.9×10^{-11}
	Gradient	500	2 m 43 s	76	77	9.2×10^{-6}
		1,000	25 m 26 s	106	107	9.0×10^{-6}
		1,500	1 h 24 m 44 s	126	127	9.5×10^{-6}
		2,000	3 h 41 m 16 s	144	145	1.0×10^{-5}
(ii)	Newton	500	16.4 s	5	6	4.3×10^{-9}
		1,000	1 m 50 s	5	6	9.4×10^{-8}
		1,500	6 m 10 s	5	6	7.0×10^{-7}
		2,000	13 m 38 s	5	6	2.2×10^{-6}
	BFGS	500	32.2 s	17	18	8.1×10^{-6}
		1,000	4 m 14 s	19	20	7.0×10^{-6}
		1,500	15 m 23 s	21	22	4.9×10^{-6}
		2,000	35 m 04 s	22	23	3.9×10^{-6}
	BFGS-N	500	14.8 s	6	7	6.7×10^{-6}
		1,000	2 m 02 s	7	8	3.3×10^{-6}
		1,500	5 m 57 s	7	8	9.5×10^{-6}
		2,000	18 m 35 s	8	9	8.3×10^{-11}
	Gradient	500	2 m 25 s	78	79	9.4×10^{-6}
		1,000	21 m 31 s	105	106	9.0×10^{-6}
		1,500	1 h 46 m 40 s	127	128	9.7×10^{-6}
		2,000	3 h 34 m 59 s	144	145	9.4×10^{-6}

Remark 5.9. Newton's method takes less cputime and fewer iterations. For all the tested examples, it is observed that the Newton method always took the unit steplength and achieved the quadratic convergence at the last several iterations. Typically, Newton's method was terminated in two or three steps after the residue of the gradient was below 10^{-1} or 10^{-2}.

Remark 5.10. The major cost in Newton's method includes two parts: (1) the spectral decomposition and (2) the CG method for solving the linear system. In order to form the linear system, we need the computation of the full eigensystem. So it seems that the computing time involved in part (1) is inevitable. The computing time in part (2) may be reduced by making use of the special structure of $\partial_B F(y)$, $y \in \mathbb{R}^n$. We did not explore the latter in our implementation, as we are quite satisfied with the performance of Newton's method.

Remark 5.11. The major cost in the BFGS method and the gradient is the spectral decomposition. By doing a partial spectral decomposition as outlined in [25], we may be able to save some cputime. We did not exploit this, as we do not know the distributions of the eigenvalues of the optimal correlation matrix.

Remark 5.12. It can be seen clearly from the numerical results for BFGS-N that Newton's steps reduced the cputime committed by the BFGS method substantially.

TABLE 3
Numerical results of Example 5.7.

Init.	Algorithm	n	cputime	Iter.	Func.	Res.
(i)	Newton	500	34.3 s	8	9	3.7×10^{-9}
		1,000	4 m 55 s	9	10	3.1×10^{-9}
		1,500	14 m 04 s	9	10	4.5×10^{-7}
		2,000	33 m 52 s	9	10	2.6×10^{-6}
	BFGS	500	2 m 46 s	88	89	9.4×10^{-6}
		1,000	LS failed	110	119	2.3×10^{-5}
		1,500	LS failed	111	123	4.7×10^{-5}
		2,000	LS failed	112	129	8.1×10^{-5}
	BFGS-N	500	43.1 s	12	13	1.4×10^{-7}
		1,000	6 m 09 s	15	17	9.8×10^{-10}
		1,500	19 m 03 s	15	17	3.6×10^{-10}
		2,000	1 h 08 m 36 s	20	28	1.1×10^{-7}
	Gradient	500	15 m 53 s	500	501	3.7×10^{-2}
		1,000	2 h 01 m 01 s	500	501	1.3×10^{-1}
		1,500	5 h 25 m 42 s	500	501	2.0×10^{-1}
		2,000	–	–	–	–
(ii)	Newton	500	35.6 s	8	9	1.7×10^{-7}
		1,000	4 m 34 s	9	10	6.1×10^{-8}
		1,500	15 m 37 s	9	10	6.2×10^{-7}
		2,000	40 m 06 s	9	10	3.8×10^{-6}
	BFGS	500	2 m 51 s	89	90	9.3×10^{-6}
		1,000	26 m 01 s	116	118	9.6×10^{-6}
		1,500	LS failed	122	126	2.6×10^{-5}
		2,000	3 h 43 m 33 s	139	140	1.0×10^{-5}
	BFGS-N	500	45.2 s	12	15	2.4×10^{-6}
		1,000	6 m 16 s	15	17	2.6×10^{-9}
		1,500	18 m 55 s	15	17	8.3×10^{-8}
		2,000	50 m 56 s	14	18	7.0×10^{-7}
	Gradient	500	15 m 13 s	500	501	3.7×10^{-2}
		1,000	1 h 54 m 18 s	500	501	1.2×10^{-1}
		1,500	5 h 22 m 08 s	500	501	1.9×10^{-1}
		2,000	–	–	–	–

If one can calculate $F(y)$ much less costly than via the computation of the full eigensystem, then it may be a good choice to start with a method such as the BFGS, which costs less than Newton's method at each step, and then switch to Newton's method when the iterates are close to the solution. In this case, BFGS-N may be an ideal choice.

6. Conclusion. In this paper, a close look at the nearest correlation matrix problem as the best approximation from a convex set in a Hilbert space led us to consider Newton's method. Theoretically, we proved that Newton's method is well defined and is quadratically convergent. Our theoretical results were then extended to such problems as the W-weighted nearest correlation problem, the case with lower bounds, and the nonsymmetric case. Numerically, Newton's method is shown to be extremely efficient, taking less than 10 iterations to solve all the test problems. This research opens the possibility of developing Newton's method for other least-square semidefinite problems. We shall pursue this possibility in our future research.

Acknowledgments. The authors are grateful to Professor N. J. Higham for suggesting the present title and to the referees for their helpful comments.

TABLE 4
Numerical results of Example 5.8.

Init.	Algorithm	α	cputime	Iter.	Func.	Res.
(i)	Newton	0.0	9.4 s	1	2	2.3×10^{-13}
		0.01	1 m 52 s	5	6	1.4×10^{-6}
		0.1	2 m 33 s	6	7	3.9×10^{-7}
		1.0	4 m 19 s	8	9	1.6×10^{-8}
	BFGS	0.0	28.0 s	2	9	4.6×10^{-13}
		0.01	5 m 00 s	23	27	1.4×10^{-6}
		0.1	5 m 23 s	27	29	8.9×10^{-6}
		1.0	9 m 24 s	50	52	9.1×10^{-6}
	BFGS-N	0.0	8.7 s	1	2	1.6×10^{-13}
		0.01	2 m 03 s	5	6	1.4×10^{-6}
		0.1	2 m 25 s	11	12	4.1×10^{-9}
		1.0	6 m 11 s	20	25	2.0×10^{-9}
	Gradient	0.0	27 m 29 s	500	501	1.6×10^{-2}
		0.01	1 h 36 m 35 s	500	501	5.6×10^{-2}
		0.1	1 h 26 m 35 s	500	501	4.0×10^{-1}
		1.0	1 h 51 m 23 s	500	501	4.0×10^{0}
(ii)	Newton	0.0	14.3 s	2	3	1.4×10^{-13}
		0.01	2 m 19 s	6	7	1.3×10^{-6}
		0.1	3 m 08 s	7	8	2.1×10^{-7}
		1.0	4 m 11 s	8	9	1.7×10^{-7}
	BFGS	0.0	32.6 s	3	10	7.2×10^{-11}
		0.01	3 m 47 s	17	20	4.6×10^{-6}
		0.1	5 m 50 s	25	28	6.9×10^{-7}
		1.0	LS failed	60	74	1.1×10^{-5}
	BFGS-N	0.0	12.7 s	2	3	2.7×10^{-13}
		0.01	2 m 06 s	6	7	1.3×10^{-6}
		0.1	2 m 33 s	9	10	2.5×10^{-9}
		1.0	6 m 36 s	21	25	3.4×10^{-7}
	Gradient	0.0	27 m 35 s	500	501	1.6×10^{-2}
		0.01	1 h 25 m 10 s	500	501	5.6×10^{-2}
		0.1	1 h 28 m 51 s	500	501	4.0×10^{-1}
		1.0	1 h 23 m 17 s	500	501	4.0×10^{0}

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