A semi-smooth Newton method for general projection equations applied to the nearest correlation matrix problem

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Abstract

In this paper, we extend and investigate the properties of the semi-smooth Newton method when applied to a general projection equation in finite dimensional spaces. We first present results concerning Clarke's generalized Jacobian of the projection onto a closed convex cone. We then describe the iterative process for the general cone case and establish two global convergence theorems combined with a local quadratic convergence result. We apply these results to the constrained quadratic conic programming problem, emphasizing its connection to the projection equation. To illustrate the performance of our method, we conduct numerical experiments focusing on semidefinite least squares, in particular the nearest correlation matrix problem. In this scenario, we benchmark our outcomes against previous literature, presenting performance profiles and tabulated results for clarity and comparison.

Keywords: Conic programming, nearest correlation matrix, quadratic programming, semi-smooth Newton method.

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1 Introduction

We begin by considering the following special nonlinear system:

$$\Pi_{\mathcal{K}}(x) + Tx = b, \tag{1}$$

where $\mathcal{K} \subseteq \mathbb{X}$ is a nonempty closed convex cone of a finite dimensional vector space $\mathbb{X}$ equipped with the inner product $\langle \cdot, \cdot \rangle$, $\Pi_{\mathcal{K}}(x)$ denotes the projection of $x \in \mathbb{X}$ onto $\mathcal{K}$, $b \in \mathbb{X}$, and $T \colon \mathbb{X} \to \mathbb{X}$ is a linear operator. Several particular cases of equation (1equation.1) have been studied, for instance, in [1, 3–6, 8, 12, 15, 22, 29]. Among these problems, particular attention has been given to the cases in which $\mathcal{K}$ is the n-dimensional nonnegative orthant or the second order cone. For these cases, novel iterative methods have been proposed; see, for instance, [1, 3, 6].

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Equation (1equation.1) is closely related to the quadratic cone-constrained programming:

$$\begin{pmatrix} \min & \frac{1}{2}\langle x, Qx\rangle + \langle q, x\rangle, \\ \text{s.t.} & x \in \mathcal{K}, \end{pmatrix} \tag{2}$$

for a linear operator $Q\colon \mathbb{X} \to \mathbb{X}$ and a vector $q \in \mathbb{X}$. The particularly relevant case arises when $\mathbb{X} = \mathbb{R}^n$ and $\mathcal{K}$ is either the nonnegative orthant or the second order cone. The connection between equation (1equation.1) and problem (2equation.2) is established by setting $T = (Q - \mathrm{Id})^{-1}$ (where Id is the $n \times n$ identity matrix) and $b = -Tq$. Moreover, the projection onto $\mathcal{K}$ of a solution of equation (1equation.1) satisfies the first order necessary optimality conditions for problem (2equation.2). Here, we also prove that this property holds in the general case, that is, for any closed convex cone $\mathcal{K}$ in a finite dimensional vector space $\mathbb{X}$ and considering any linear operator $Q\colon \mathbb{X} \to \mathbb{X}$. Additional linear equality constraints are also considered in problem (2equation.2).

In this work, we generalize and focus our attention on the *semi-smooth Newton method* for solving equation (1equation.1). This method finds a zero of the mapping $F\colon \mathbb{X} \to \mathbb{X}$,

$$F(x) = \Pi_{\mathcal{K}}(x) + Tx - b, \qquad x \in \mathbb{X}. \tag{3}$$

Starting from a point $x^0 \in \mathbb{X}$, the classical semi-smooth Newton method iterates as follows:

$$x^{k+1} = x^k - \left[F'(x^k)\right]^{-1} F(x^k), \qquad k \in \mathbb{N}, \tag{4}$$

where $F'(x^k)$ is a generalized Jacobian of F at x^k. When applied to (3equation.3), this iteration takes the following simple form:

$$\left(V(x^k) + T\right) x^{k+1} = b, \qquad k \in \mathbb{N}, \tag{5}$$

where $V(x^k) \in \partial_C \Pi_{\mathcal{K}}(x^k)$ is a Clarke's generalized Jacobian of the projection $\Pi_{\mathcal{K}}$ at x^k. This is a consequence of the relation $V(x^k)x^k = \Pi_{\mathcal{K}}(x^k)$ which we will prove later.

Our approach enables us to address the relevant case where $\mathcal{K} = \mathbb{S}^n_+$, the cone of $n \times n$ positive semidefinite matrices. In this scenario, a subdifferential $V(x^k)$ can be computed through the spectral decomposition of the symmetric matrix x^k. Specifically, we consider the quadratic cone-constrained problem (2equation.2). We also incorporate additional linear constraints to the problem in the form $\mathcal{A}x = f$, with $\mathcal{A}\colon \mathbb{X} \to \mathbb{Y}$ being a linear mapping between finite dimensional inner product vector spaces and $f \in \mathbb{Y}$, adapting our results accordingly; see problem (14equation.14) below. This optimization problem is well-known and has numerous applications. Our main contribution is the further study of the properties of the semi-smooth Newton method (5equation.5), proving its Q-linear global convergence under standard conditions on the linear operator T for a general cone $\mathcal{K}$ and establishing a local quadratic convergence theorem. This yields a simple and effective algorithm for this general problem, allowing a more detailed study in the particular case of the cone of positive semidefinite matrices, especially the nearest correlation matrix problem. Previous studies of the semi-smooth Newton method for the projection equation have considered only the cases where the cone is the nonnegative orthant or the second order cone.

The paper is organized as follows: We start by introducing our notation and presenting some preliminary results needed for our analysis. In Section 2section.2, we present general results about the projection operator onto cones and its differentiability. In Section 3section.3, we present the semi-smooth Newton method and prove the previously mentioned global convergence theorems. Section 4section.4 is devoted to exploring the relationship between equation (1equation.1) and

the quadratic conic programming problem (2equation.2), with special emphasis on the case where $\mathcal{K} = \mathbb{S}^n_+$, including additional linear constraints. In Section 6section.6, we present some numerical experiments for the positive semidefinite cone $\mathbb{S}^n_+$, focusing particularly on semidefinite least squares problems. Specifically, we include a comparison with the algorithms from [27, 28] in the context of the nearest correlation matrix and the nearest Euclidean distance matrix problem, which has been well-studied in finance, econometrics, and risk management; see for instance, [16]. We finally illustrate the performance of the proposed iteration for the nearest Euclidean distance matrix problem, which also arises in the multidimensional scaling and molecular conformation from nuclear magnetic resonance data in computational chemistry; see for instance, [25].

1.1 Notations and preliminaries

In this section, we present some relevant results and definitions that are used throughout this paper. We denote the nonnegative integers by $\mathbb{N}$ and by Id the identity operator. The bracket notation $\langle \cdot, \cdot \rangle$ denotes the inner product in any finite dimensional space $\mathbb{X}$. Given a linear operator $T\colon \mathbb{X} \to \mathbb{X}$, we use the notation $\|T\|$ for the operator norm of T, that is, $\|T\| := \max\{\|Tx\| \mid x \in \mathbb{X}, \|x\| = 1\}$, where $\|x\| := \sqrt{\langle x, x \rangle}$ is the norm associated with the inner product. We also denote by T^* its adjoint linear operator $T^*\colon \mathbb{X} \to \mathbb{X}$, that is, $\langle Tx, y \rangle = \langle x, T^* y \rangle$, for all $x, y \in \mathbb{X}$. When T is self-adjoint, that is, $T = T^*$, we say that T is positive semidefinite (definite) if $\langle Tx, x \rangle \geq 0$ (> 0, respectively), for all $x \in \mathbb{X}, x \neq 0$ and we denote by $\lambda_{\min}(T)$ and $\lambda_{\max}(T)$ the smallest and largest eigenvalues of T, respectively. For a cone $\mathcal{K} \subseteq \mathbb{X}$, the dual of $\mathcal{K}$ is denoted by $\mathcal{K}^* = \{y \in \mathbb{X} \mid \langle y, x \rangle \geq 0, \forall x \in \mathcal{K}\}$. When $\mathbb{X} = \mathbb{S}^n$ is the set of symmetric $n \times n$ real matrices with the inner product $\langle A, B \rangle = \operatorname{trace}(AB), A, B \in \mathbb{S}^n$, we consider the self-dual cone $\mathcal{K} = \mathbb{S}^n_+$ of positive semidefinite matrices.

The projection of a point x onto a closed convex cone $\mathcal{K} \neq \emptyset$ is denoted by $\Pi_{\mathcal{K}}(x)$ where $\Pi_{\mathcal{K}}(x) = \operatorname{argmin}\{\|y - x\| \mid y \in \mathcal{K}\}$. For a given mapping $F\colon \mathbb{X} \to \mathbb{X}$, we denote the set where it is differentiable by D_F and the Jacobian at a point $x \in D_F$ by $F'(x)$. The set of Clarke's generalized Jacobians at a point $x \in \mathbb{X}$ is denoted by $\partial_C F(x)$ and it is defined by

$$\partial_C F(x) := \operatorname{conv}\left\{ \lim_{k \to \infty} F'(x_k) \mid x_k \to x, x_k \in D_F \right\},$$

that is, the convex hull of all limits of Jacobians of F in a neighborhood of x. Throughout this paper, any Clarke's generalized Jacobian of the projection $\Pi_{\mathcal{K}}$ at x will be denoted by $V(x)$, so we may omit any explicit reference to a particular mapping F whenever the context is clear.

We will use the well-known results below, which we state in the context of a general finite dimensional inner product space $\mathbb{X}$ as follows.

Theorem 1.1 (Mean Value Theorem [9], Proposition 2.6.5, Page 79)**.** *Let $F\colon \mathbb{X} \to \mathbb{X}$ be a Lipschitz mapping. Then, we have*

$$F(y) - F(x) \in \operatorname{conv}\left(\partial_C F([x, y])\right)(y - x),$$

that is, $F(y) - F(x) = U(z)(y - x)$ for some $U(z) \in \partial_C F(z)$ and z is a convex combination of x and y.

Lemma 1.1 (Banach's Lemma [18], Page 351)**.** *Let $E\colon \mathbb{X} \to \mathbb{X}$ be a mapping onto $\mathbb{X}$. If $\|E\| < 1$, then $E - \mathrm{Id}$ is invertible and*

$$\|(E - \mathrm{Id})^{-1}\| \leq \frac{1}{1 - \|E\|}.$$

Lemma 1.2 (Weyl's inequality [18], Theorem 4.3.1, Page 239)**.** *Let $A, B\colon \mathbb{X} \to \mathbb{X}$ be self-adjoint linear operators. Then, it holds*

$$\lambda_{\min}(A) + \lambda_{\min}(B) \leq \lambda_{\min}(A+B) \leq \lambda_{\max}(A+B) \leq \lambda_{\max}(A) + \lambda_{\max}(B).$$

Finally, an important result that guarantees the existence and uniqueness of solutions of equation (1equation.1) is the contraction mapping principle.

Theorem 1.2 (Contraction mapping principle [26], Thm. 8.2.2, page 153)**.** *Let $\Phi\colon \mathbb{X} \to \mathbb{X}$ and suppose that there exists $\lambda \in [0,1)$ such that $\|\Phi(y) - \Phi(x)\| \leq \lambda \|y - x\|$, for all $x, y \in \mathbb{X}$. Then, there exists a unique $\overline{x} \in \mathbb{X}$ such that $\Phi(\overline{x}) = \overline{x}$.*

2 On the projection mapping onto a closed convex cone

In this section, we study some useful results that will be important in the well-definiteness and global convergence of the semi-smooth Newton method for equation (1equation.1). We begin by presenting the following result on the properties of generalized Jacobians.

Theorem 2.1. *The projection operator $\Pi_{\mathcal{K}}\colon \mathbb{X} \to \mathcal{K}$ is differentiable almost everywhere. The Jacobian $\Pi'_{\mathcal{K}}(x)$ (when it exists) and any generalized Jacobian $V(x) \in \partial_C \Pi_{\mathcal{K}}(x)$ for all $x \in \mathbb{X}$, are self-adjoint and positive semidefinite operators. Moreover, the following properties hold:*

(i) $\|V(x)\| \leq 1$, $\forall V(x) \in \partial_C \Pi_{\mathcal{K}}(x)$ *with* $x \in \mathbb{X}$.

(ii) $\Pi'_{\mathcal{K}}(x)x = \Pi_{\mathcal{K}}(x), \forall x \in D_{\Pi_{\mathcal{K}}}$.

(iii) $V(x)x = \Pi_{\mathcal{K}}(x), \forall V(x) \in \partial_C \Pi_{\mathcal{K}}(x)$ *with* $x \in \mathbb{X}$.

(iv) *For all $x \in \mathbb{X}$,*

$$0 \leq \lambda_{min}(V(x)) \leq \lambda_{max}(V(x)) \leq 1, \forall V(x) \in \partial_C \Pi_{\mathcal{K}}(x).$$

Proof. The fact that the projection is differentiable almost everywhere is well-known due to its non-expansiveness (that is, the projection is 1-Lipschitz). When $\Pi'_{\mathcal{K}}(x)$ exists, it is self-adjoint and positive semidefinite due to [13, Proposition 2.2]. Now, let $x \in \mathbb{X}$ and $V(x) \in \partial_C \Pi_{\mathcal{K}}(x)$. By definition, there exist $V_1(x), \ldots, V_m(x)$ and sequences $\{x_k^j\} \subset D_{\Pi_{\mathcal{K}}}$ such that $\lim_{k\to\infty} x_k^j = x$, $\Pi'_{\mathcal{K}}(x_k^j) \to V_j(x)$, $\forall j = 1, \ldots, m$, and $V(x) = \sum_{j=1}^m \alpha_j V_j(x)$, with $\sum_{j=1}^m \alpha_j = 1$ and $\alpha_j \in [0,1]$ for all j. By the continuity of the inner product, we can deduce that each $V_j(x)$ is also self-adjoint and positive semidefinite, and therefore, by linearity, the same holds true for $V(x)$. The positive semidefiniteness and self-adjointness of $V(x)$ were also proved in [24, Proposition 1].

To prove item (i), note that $\|\Pi'_{\mathcal{K}}(x_k^j)\| \leq 1$ for all j and k due to non-expansiveness. Hence

$$\begin{aligned}\|V(x)\| &= \left\| \sum_{j=1}^m \alpha_j V_j(x) \right\| \leq \sum_{j=1}^m \alpha_j \|V_j(x)\| \\ &= \sum_{j=1}^m \alpha_j \lim_{k\to\infty} \|\Pi'_{\mathcal{K}}(x_k^j)\| \leq 1.\end{aligned}$$

For item (ii), note that since $\mathcal{K}$ is a cone, $\Pi_{\mathcal{K}}(\cdot)$ is positive homogeneous, that is, $\Pi_{\mathcal{K}}(tx) = t\Pi_{\mathcal{K}}(x), \forall t \geq 0$ for any $x \in \mathbb{X}$. Let $x \in D_{\Pi_{\mathcal{K}}}$. If $x = 0$, the equality is evident. Assume that $x \neq 0$. By the definition of $\Pi'_{\mathcal{K}}(x)$, we have that

$$0 = \lim_{t \to 0} \frac{\|\Pi_{\mathcal{K}}(x + tx) - \Pi_{\mathcal{K}}(x) - t\Pi'_{\mathcal{K}}(x)x\|}{\|tx\|} = \frac{\|\Pi_{\mathcal{K}}(x) - \Pi'_{\mathcal{K}}(x)x\|}{\|x\|}.$$

Hence, $\Pi'_{\mathcal{K}}(x)x = \Pi_{\mathcal{K}}(x)$ proving item (ii).

In order to prove item (iii), by noting that $V(x)x - \Pi_{\mathcal{K}}(x) = \sum_{j=1}^{m} \alpha_j (V_j(x)x - \Pi_{\mathcal{K}}(x))$, it is enough to show that for all $j = 1, \ldots, m$, $V_j(x)x = \Pi_{\mathcal{K}}(x)$. Recalling that $\Pi'_{\mathcal{K}}(x_k^j) \to V_j(x)$, we have that

$$\begin{aligned} \|V_j(x)x - \Pi'_{\mathcal{K}}(x_k^j)x_k^j\| &\leq \|V_j(x)x - V_j(x)x_k^j\| + \|V_j(x)x_k^j - \Pi'_{\mathcal{K}}(x_k^j)x_k^j\| \\ &\leq \|V_j(x)\|\|x - x_k^j\| + \|V_j(x) - \Pi'_{\mathcal{K}}(x_k^j)\|\|x_k^j\| \\ &\to 0. \end{aligned}$$

Using item (ii) and the continuity of $\Pi_{\mathcal{K}}(\cdot)$ we conclude that

$$\begin{aligned} \|V_j(x)x - \Pi_{\mathcal{K}}(x)\| &\leq \|V_j(x)x - \Pi_{\mathcal{K}}(x_k^j)\| + \|\Pi_{\mathcal{K}}(x_k^j) - \Pi_{\mathcal{K}}(x)\| \\ &= \|V_j(x)x - \Pi'_{\mathcal{K}}(x_k^j)x_k^j\| + \|\Pi_{\mathcal{K}}(x_k^j) - \Pi_{\mathcal{K}}(x)\| \to 0. \end{aligned}$$

Finally, for item (iv), it is enough to note that $0 \leq \lambda_{\min}(V_j(x)) \leq \lambda_{\max}(V_j(x)) \leq 1$ for all $j = 1, \ldots, m$ due to the fact that $V_j(x)$ is self-adjoint and positive semidefinite with $\|V_j(x)\| \leq 1$. The result now follows easily from Lemma 1.2lemma.1.2. □

We conclude the section with the following useful result.

Lemma 2.1. *Let $x, y \in \mathbb{X}$ and $V(x) \in \partial_C \Pi_{\mathcal{K}}(x)$. Then $\|\Pi_{\mathcal{K}}(y) - \Pi_{\mathcal{K}}(x) - V(x)(y - x)\| \leq \|y - x\|$.*

Proof. By Theorem 1.1theorem.1.1 we have that

$$\Pi_{\mathcal{K}}(y) - \Pi_{\mathcal{K}}(x) - V(x)(y - x) = (V(z) - V(x))(y - x),$$

where z is a convex combination of x and y and $V(z) \in \partial_C \Pi_{\mathcal{K}}(z)$. The result follows from the fact that $\|V(z) - V(x)\| \leq 1$ due to Lemma 1.2lemma.1.2 and Theorem 2.1theorem.2.1 item (iv). □

Item (ii) from Theorem 2.1theorem.2.1 provides a foundation for introducing the semi-smooth Newton method for solving equation (1equation.1). Specifically, since the projection can be expressed as:

$$\Pi_{\mathcal{K}}(x) = V(x)x,$$

where $V(x) \in \partial_C \Pi_{\mathcal{K}}(x)$, we have that $F(x)$ as defined in (3equation.3) can be written as:

$$F(x) = (V(x) + T)x - b,$$

with $V(x) + T \in \partial_C F(x)$. Then, iteration (4equation.4) can be expressed as:

$$x^{k+1} = x^k - (V(x^k) + T)^{-1}[(V(x^k) + T)x^k - b] = (V(x^k) + T)^{-1}b.$$

In the next section, we explore the convergence properties of this iteration.

3 A semi-smooth Newton method for general projection equations

In this section, we define a semi-smooth Newton method for solving equation (1equation.1) and study the convergence along with the sufficient conditions required to achieve it. Our goal is to extend the application of the semi-smooth Newton method, previously studied in [3, 6], for the cases where $\mathcal{K} \subseteq \mathbb{R}^n$ is either the nonnegative orthant or the second order cone. This extension considers any closed convex cone $\mathcal{K} \subseteq \mathbb{X}$. We first establish a sufficient condition for the existence and uniqueness of the solution to equation (1equation.1).

Theorem 3.1 (Sufficient condition for existence and uniqueness of a solution)**.** *If T is invertible and $\|T^{-1}\| < 1$, then equation* (1equation.1) *has a unique solution for any $b \in \mathbb{X}$.*

Proof. Equation (1equation.1) has a unique solution if and only if the mapping $\Phi(x) = -T^{-1}\Pi_{\mathcal{K}}(x) + T^{-1}b$ has a unique fixed point. Hence, it is sufficient to prove that Φ is a contraction and use Theorem 1.2theorem.1.2 to guarantee the existence and uniqueness of a fixed point. From the definition of Φ, we have

$$\Phi(x) - \Phi(y) = -T^{-1}(\Pi_{\mathcal{K}}(x) - \Pi_{\mathcal{K}}(y)).$$

Since $\|\Pi_{\mathcal{K}}(x) - \Pi_{\mathcal{K}}(y)\| \leq \|x - y\|$ we deduce that $\|\Phi(x) - \Phi(y)\| \leq \|T^{-1}\|\|x - y\|$ concluding that Φ is a contraction since $\|T^{-1}\| < 1$. □

We define the semi-smooth Newton method for the mapping $F(x) = \Pi_{\mathcal{K}}(x) + Tx - b$ starting on an initial point $x^0 \in \mathbb{X}$ as the iteration

$$(V(x^k) + T)x^{k+1} = b,\ k \in \mathbb{N} \tag{6}$$

with $V(x) \in \partial_C \Pi_{\mathcal{K}}(x)$.

Notice that if $x^k \to \overline{x}$, then $\overline{x}$ is a solution of equation (1equation.1). To see this, we subtract $(V(x^k) + T)x^k$ from both sides of (6equation.6). Using that $\Pi_{\mathcal{K}}(x^k) = V(x^k)x^k$, we arrive at $(V(x^k) + T)(x^{k+1} - x^k) = b - \Pi_{\mathcal{K}}(x^k) - Tx^k$. Since $V(x^k) + T$ is bounded, the left-hand side converges to zero, while from the continuity of the projection the right-hand side converges to $b - \Pi_{\mathcal{K}}(\overline{x}) - T\overline{x}$. Therefore, $\overline{x}$ is a solution of (1equation.1).

We start by showing a sufficient condition for stopping the method (6equation.6) at a solution.

Proposition 3.1 (Stopping criterion)**.** *If $V(x^{k+1}) = V(x^k)$, then x^{k+1} is a solution of equation* (1equation.1)*.*

Proof. From Theorem 2.1theorem.2.1 item (iii) and (6equation.6), we have that

$$\Pi_{\mathcal{K}}(x^{k+1}) + Tx^{k+1} = (V(x^{k+1}) + T)x^{k+1} = (V(x^k) + T)x^{k+1} = b.$$

Hence, x^{k+1} is a solution of equation (1equation.1). □

Now, we show a sufficient condition for the global convergence of iteration (6equation.6). Provided certain conditions regarding the norm of the inverse of T are met, we can guarantee the existence and uniqueness of the solution of equation (1equation.1). In addition to that, by imposing an additional norm condition, we obtain global linear convergence.

Theorem 3.2 (Sufficient condition for global Q-linear convergence)**.** *Let $b \in \mathbb{X}$ and $T\colon \mathbb{X} \to \mathbb{X}$ be an invertible linear operator. Assume that $\|T^{-1}\| < 1$. Then, equation* (1equation.1) *has a unique solution $\overline{x}$ and for any initial point x^0, the semi-smooth Newton sequence generated by equation* (6equation.6) *is well-defined. Additionally, if $\|T^{-1}\| < \frac{1}{2}$ then the sequence $\{x^k\}$ converges Q-linearly to $\overline{x}$ and satisfies*

$$\|x^{k+1} - \overline{x}\| \leq \frac{\|T^{-1}\|}{1 - \|T^{-1}\|}\|x^k - \overline{x}\|,\ k \in \mathbb{N}.$$

Proof. First we know from Theorem 2.1theorem.2.1 that $\|V(x)\| \leq 1$ for any $x \in \mathbb{X}$. Since $\|T^{-1}\| < 1$ we deduce that $\|T^{-1}V(x)\| < 1$ for every $x \in \mathbb{X}$. Lemma 1.1lemma.1.1 implies that $-T^{-1}V(x) - \mathrm{Id}$ is invertible and therefore $V(x)+T$ is also invertible. In particular the semi-smooth Newton method (6equation.6) is well-defined. Let $\overline{x}$ be the only solution of problem (1equation.1) (which exists and is unique due to Theorem 3.1theorem.3.1). So, this point satisfies the relation $(V(\overline{x})+T)\overline{x} - b = 0$. Combining with (6equation.6) we deduce that

$$(V(x^k) + T)(x^{k+1} - \overline{x}) = (V(\overline{x}) - V(x^k))\overline{x} = V(\overline{x})\overline{x} - V(x^k)x^k - V(x^k)(\overline{x} - x^k).$$

Since $V(\overline{x})\overline{x} = \Pi_{\mathcal{K}}(\overline{x})$ and $V(x^k)x^k = \Pi_{\mathcal{K}}(x^k)$, using Lemma 2.1lemma.2.1, we obtain

$$\|x^{k+1} - \overline{x}\| \leq \|(V(x^k) + T)^{-1}\|\|(\Pi_{\mathcal{K}}(\overline{x}) - \Pi_{\mathcal{K}}(x^k) - V(x^k)(\overline{x} - x^k))\| \leq \|(V(x^k) + T)^{-1}\|\|\overline{x} - x^k\|.$$

But $\|(V(x^k) + T)^{-1}\| = \|(T(T^{-1}V(x^k) + \mathrm{Id}))^{-1}\| \leq \|(-T^{-1}V(x^k) - \mathrm{Id})^{-1}\|\|T^{-1}\|$. Lemma 1.1lemma.1.1 for $E = -T^{-1}V(x^k)$ along with the fact that $\|E\| = \|T^{-1}V(x^k)\| < 1$ implies that

$$\|(T^{-1}V(x^k) + \mathrm{Id})^{-1}\| \leq \frac{1}{1 - \|T^{-1}V(x^k)\|} \leq \frac{1}{1 - \|T^{-1}\|}.$$

Thus, we have that $\|x^{k+1} - \overline{x}\| \leq \frac{\|T^{-1}\|}{1-\|T^{-1}\|}\|x^k - \overline{x}\|$ with $\frac{\|T^{-1}\|}{1-\|T^{-1}\|} < 1$ due to the assumption that $\|T^{-1}\| < \frac{1}{2}$. Hence, x^k converges Q-linearly to the unique solution $\overline{x}$. □

Theorem 3.2theorem.3.2 states that with only a norm condition on the operator T^{-1}, namely $\|T^{-1}\| < \frac{1}{2}$, we can achieve Q-linear convergence of the method. We now prove that for the case where T is a positive definite linear mapping, the weaker norm condition $\|T^{-1}\| < 1$ is sufficient to ensure Q-linear convergence of iteration (6equation.6) to the unique solution of problem (1equation.1).

Theorem 3.3. *Let $b \in \mathbb{X}$ and $T\colon \mathbb{X} \to \mathbb{X}$ be a positive definite linear operator. Then, equation* (1equation.1) *has a unique solution $\overline{x} \in \mathbb{X}$ and for any initial point $x^0 \in \mathbb{X}$, the semi-smooth Newton sequence generated by* (6equation.6) *is well-defined. Additionally, if $\|T^{-1}\| < 1$ then the sequence $\{x^k\}$converges Q-linearly to $\overline{x}$ and satisfies*

$$\|x^{k+1} - \overline{x}\| \leq \|T^{-1}\|\|x^k - \overline{x}\|,\ k \in \mathbb{N}.$$

Proof. First notice that from Lemma 1.2lemma.1.2 and the positive definiteness of T, it follows that $\mathrm{Id}+T$ is invertible with $\|(\mathrm{Id}+T)^{-1}\| < 1$. Using Moreau's decomposition [17, Theorem 3.2.5], we can write any $x \in \mathbb{X}$ as $x = \Pi_{\mathcal{K}}(x) - \Pi_{\mathcal{K}^*}(-x)$. Now, it follows directly that x is a solution of equation (1equation.1) if and only if x is a fixed point of $\Phi(x) = (\mathrm{Id} + T)^{-1}(b - \Pi_{\mathcal{K}^*}(-x))$. Since

$$\Phi(x) - \Phi(y) = (\mathrm{Id} + T)^{-1}(-\Pi_{\mathcal{K}^*}(-x) + \Pi_{\mathcal{K}^*}(-y)), \quad x, y \in \mathbb{X},$$

we deduce that Φ is a contraction due to the non-expansiveness of the projection. This gives existence and uniqueness of a solution of problem (1equation.1).

By Theorem 2.1theorem.2.1 item (iv) and Lemma 1.2lemma.1.2, it follows that $V(x) + T$ is positive definite with $\|(V(x) + T)^{-1}\| \leq \|T^{-1}\|$ for all $x \in \mathbb{X}$. Hence, iteration (6equation.6) is well-defined for every starting point $x^0 \in \mathbb{X}$. The Q-linear convergence when $\|T^{-1}\| < 1$ now follows from the relation $\|x^{k+1} - \overline{x}\| \leq \|(V(x^k) + T)^{-1}\|\|x^k - \overline{x}\|$ deduced in the proof of Theorem 3.2theorem.3.2. □

Note that although the assumption of positive definiteness is sufficient for existence and uniqueness of the solution without imposing a condition on the norm of T^{-1}, it alone does not guarantee the convergence of Newton's method; see [1, Example 1].

In the following section, we present relevant applications of our results to quadratic conic programming.

4 Application to quadratic conic programming

In this section, we connect equation (1equation.1) with the important quadratic conic programming problem:

$$\begin{pmatrix} \min & \frac{1}{2}\langle x, Qx\rangle + \langle q, x\rangle, \\ \text{s.t.} & x \in \mathcal{K}. \end{pmatrix} \tag{7}$$

This problem has been widely studied and has multiple applications such as semidefinite least squares and, in particular, the nearest correlation matrix problem which we will present next.

The Lagrangian of the problem is given by:

$$L(x, \mu) := \frac{1}{2}\langle x, Qx\rangle + \langle q, x\rangle - \langle \mu, x\rangle,$$

where $\mu \in \mathcal{K}^*$. Then, the well-known complementary KKT conditions (see [7, page 267]) for problem (7equation.7) are given by

$$\begin{aligned} Q\overline{x} + q - \overline{\mu} &= 0, \\ \langle \overline{\mu}, \overline{x}\rangle &= 0, \\ \overline{x} &\in \mathcal{K}, \\ \overline{\mu} &\in \mathcal{K}^*. \end{aligned}$$

Or equivalently,

$$\langle Q\overline{x} + q, \overline{x}\rangle = 0, \quad Q\overline{x} + q \in \mathcal{K}^*, \quad \overline{x} \in \mathcal{K}. \tag{8}$$

In order to find a solution to the KKT system (8equation.8), we use the following modified projection equation:

$$(Q - \mathrm{Id})\Pi_{\mathcal{K}}(x) + x = -q. \tag{9}$$

With this in mind, we have the following connection between the solutions of equation (9equation.9) and the ones of the KKT conditions (8equation.8) above. The following theorem is a generalization of Proposition 4 of [6].

Theorem 4.1 (KKT points and solutions of a generalized projection equation)**.** *If x is solution of equation* (9equation.9)*, then $\overline{x} = \Pi_{\mathcal{K}}(x)$ is a solution of the KKT system* (8equation.8)*. On the other hand, if $\overline{x}$ is a solution of system* (8equation.8)*, then $x = \overline{x} - (Q\overline{x} + q)$ is a solution of equation* (9equation.9)*.*

Proof. For the first part, let x be a solution of equation (9equation.9). Using Moreau's decomposition [17, Theorem 3.2.5] for x, we have

$$x = \Pi_{\mathcal{K}}(x) - \Pi_{\mathcal{K}^*}(-x), \tag{10}$$

and

$$\langle \Pi_{\mathcal{K}}(x), \Pi_{\mathcal{K}^*}(-x) \rangle = 0. \tag{11}$$

By hypothesis we get that

$$Q\Pi_{\mathcal{K}}(x) + q = \Pi_{\mathcal{K}}(x) - x = \Pi_{\mathcal{K}^*}(-x) \in \mathcal{K}^*,$$

where we used (10equation.10) in the last equality. Now using the previous equation and (11equation.11), we have

$$\langle Q\Pi_{\mathcal{K}}(x) + q, \Pi_{\mathcal{K}}(x) \rangle = \langle \Pi_{\mathcal{K}^*}(-x), \Pi_{\mathcal{K}}(x) \rangle = 0,$$

implying that $\overline{x} = \Pi_{\mathcal{K}}(x) \in \mathcal{K}$ solves (8equation.8).

For the second part, let $\overline{x}$ be a solution of (8equation.8) and $x := \overline{x} - (Q\overline{x} + q)$. Since $\overline{x} \in \mathcal{K}$, $Q\overline{x} + q \in \mathcal{K}^*$ with $\langle Q\overline{x} + q, \overline{x} \rangle = 0$, it follows by Moreau's decomposition that $\overline{x} = \Pi_{\mathcal{K}}(x)$. Thus, replacing $\Pi_{\mathcal{K}}(x)$ by $\overline{x}$ and x by $\overline{x} - (Q\overline{x} + q)$ in (9equation.9), we obtain:

$$(Q - \mathrm{Id})\Pi_{\mathcal{K}}(x) + x = (Q - \mathrm{Id})\overline{x} + \overline{x} - (Q\overline{x} + q) = -q.$$

Therefore, x is a solution of equation (9equation.9), which concludes the proof. □

Theorem 4.1theorem.4.1 establishes a significant connection between the KKT system (8equation.8) and equation (9equation.9). In particular, it asserts that if (9equation.9) does not have a solution, then the quadratic conic programming problem (7equation.7) admits no point that satisfies the complementary optimality conditions.

We now extend our previous results to the case of equation (9equation.9). The proofs of the next three results use Theorem 3.1theorem.3.1 and closely follow the ideas presented in [6], hence we omit some details for brevity. We begin by presenting two propositions regarding the existence and uniqueness of solutions as follows:

Proposition 4.1. *If $\|Q - \mathrm{Id}\| < 1$, then equation* (9equation.9) *has a unique solution for any $q \in \mathbb{X}$.*

Proof. Similar to the proof of Theorem 3.1theorem.3.1 but replacing T by $(Q - \mathrm{Id})^{-1}$. □

Proposition 4.2. *If Q is invertible and $\|Q^{-1} - \mathrm{Id}\| < 1$, then equation* (9equation.9) *has a unique solution for any $q \in \mathbb{X}$.*

Proof. Similar to the proof of Theorem 3.1theorem.3.1 but defining $\Phi(x) = (Q^{-1} - \mathrm{Id})\Pi_{\mathcal{K}^*}(-x) - Q^{-1}q$ and using that $x = \Pi_{\mathcal{K}}(x) - \Pi_{\mathcal{K}^*}(-x)$ and the fact that the projection $\Pi_{\mathcal{K}^*}(\cdot)$ is non-expansive. □

The Newton iteration (6equation.6) for the case of equation (9equation.9), that is, when $T = (Q - \mathrm{Id})^{-1}$ and $b = -(Q - \mathrm{Id})^{-1}q$ can be written after multiplying by $Q - \mathrm{Id}$ as:

$$((Q - \mathrm{Id})V(x^k) + \mathrm{Id})x^{k+1} = -q,\ k \in \mathbb{N} \tag{12}$$

with $V(x^k) \in \partial_C \Pi_{\mathcal{K}}(x^k)$. Let us now specialize our Q-linear convergence results to this case.

Theorem 4.2. *Let $q \in \mathbb{X}$ and $Q\colon \mathbb{X} \to \mathbb{X}$ be a linear operator. Assume that $Q - \mathrm{Id}$ is invertible and $\|Q - \mathrm{Id}\| < 1$. Then, equation* (9equation.9) *has a unique solution $\overline{x}$, and for any initial point x^0 the semi-smooth Newton sequence generated by* (12equation.12) *is well-defined. Additionally, if $\|Q - \mathrm{Id}\| < \frac{1}{2}$ then the sequence $\{x^k\}$ converges Q-linearly to $\overline{x}$ and satisfies*

$$\|x^{k+1} - \overline{x}\| \leq \frac{\|Q - \mathrm{Id}\|}{1 - \|Q - \mathrm{Id}\|}\|x^k - \overline{x}\|,\ k \in \mathbb{N}.$$

Proof. Similar to the proof of Theorem 3.2theorem.3.2. □

Before stating a result analogous to Theorem 3.3theorem.3.3, we need the following lemma.

Lemma 4.1. *Let $x \in \mathbb{X}$ and $V(x) \in \partial_C \Pi_{\mathcal{K}}(x)$. If Q is a positive definite linear mapping, then $(Q - \mathrm{Id})V(x) + \mathrm{Id}$ is invertible.*

Proof. By contradiction let us suppose that there exists $u \neq 0$ with $((Q - \mathrm{Id})V(x) + \mathrm{Id})u = 0$, or equivalently that

$$QV(x)u = (V(x) - \mathrm{Id})u. \tag{13}$$

Since Q is positive definite and $V(x)$ is self-adjoint, we have that

$$0 \leq \langle QV(x)u, V(x)u\rangle = \langle V(x)^* QV(x)u, u\rangle = \langle V(x)QV(x)u, u\rangle = \langle (V(x)^2 - V(x))u, u\rangle \leq 0,$$

where the last inequality is due to Theorem 2.1theorem.2.1, item (iv). Then, $\langle QV(x)u, V(x)u\rangle = 0$, which implies that $V(x)u = 0$. But by (13equation.13), we conclude that $u = 0$, which is a contradiction. Hence, the operator $(Q - \mathrm{Id})V(x) + \mathrm{Id}$ is invertible. □

Finally, we present a sufficient condition for the convergence of the semi-smooth Newton method which is analogous to Theorem 3.3theorem.3.3 applied to the quadratic conic programming problem when Q is positive definite.

Theorem 4.3. *Let $q \in \mathbb{X}$ and $Q\colon \mathbb{X} \to \mathbb{X}$ be a positive definite linear operator. Then, for any initial point $x^0 \in \mathbb{X}$, the semi-smooth Newton sequence generated by* (6equation.6) *is well-defined. Additionally, if $Q - \mathrm{Id}$ is invertible, then equation* (9equation.9) *has a unique solution $\overline{x} \in \mathbb{X}$ and, if $\|Q - \mathrm{Id}\| < 1$ then $\{x^k\}$ generated by* (12equation.12) *converges Q-linearly to $\overline{x}$ satisfying*

$$\|x^{k+1} - \overline{x}\| \leq \|Q - \mathrm{Id}\|\|x^k - \overline{x}\|, \quad k \in \mathbb{N}.$$

Proof. Using Lemma 4.1lemma.4.1, the proof follows the lines of the proof of Theorem 3.3theorem.3.3. □

We next consider an extension of the quadratic conic programming problem (7equation.7) by including additional linear constraints. That is, given a linear mapping $\mathcal{A}\colon \mathbb{X} \to \mathbb{Y}$, where $\mathbb{Y}$ is also a finite dimensional inner product vector space, and given $f \in \mathbb{Y}$, we consider the problem

$$\begin{pmatrix} \min & \frac{1}{2}\langle x, Qx\rangle + \langle q, x\rangle, \\ \text{s.t.} & \mathcal{A}x = f, \\ & x \in \mathcal{K}. \end{pmatrix} \tag{14}$$

The Lagrangian function associated with (14equation.14) is given by:

$$L(x, \lambda, \mu) = \frac{1}{2}\langle x, Qx\rangle + \langle q, x\rangle + \langle \lambda, \mathcal{A}x - f\rangle - \langle \mu, x\rangle, \tag{15}$$

where $\lambda \in \mathbb{Y}$ and $\mu \in \mathbb{X}$. The complementary KKT conditions for problem (14equation.14) are given by:

$$\begin{aligned} Q\overline{x} + q + \mathcal{A}^*\overline{\lambda} - \overline{\mu} &= 0, \\ \mathcal{A}\overline{x} &= f, \\ \langle \overline{\mu}, \overline{x}\rangle &= 0, \\ \overline{x} &\in \mathcal{K}, \\ \overline{\mu} &\in \mathcal{K}^*, \end{aligned}$$

where the Lagrange multipliers are $\overline{\mu} \in \mathcal{K}^*$ and $\overline{\lambda} \in \mathbb{Y}$. This system can be rewritten as the following complementary system:

$$\left\langle \begin{pmatrix} Q\overline{x} + \mathcal{A}^*\overline{\lambda} + q \\ \mathcal{A}\overline{x} - f \end{pmatrix}, \begin{pmatrix} \overline{x} \\ \overline{\lambda} \end{pmatrix} \right\rangle = 0, \quad \begin{pmatrix} Q\overline{x} + \mathcal{A}^*\overline{\lambda} + q \\ \mathcal{A}\overline{x} - f \end{pmatrix} \in K^*, \quad (\overline{x}, \overline{\lambda}) \in K, \tag{16}$$

where $K = \mathcal{K} \times \mathbb{Y}$ and its dual is given by $K^* = \mathcal{K}^* \times \{0\}$. Thus, by Theorem 4.1theorem.4.1, this system may be solved by means of the following projection equation

$$\left(\begin{pmatrix} Q & \mathcal{A}^* \\ \mathcal{A} & 0 \end{pmatrix} - \mathrm{Id} \right) \Pi_K(x, \lambda) + \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} -q \\ f \end{pmatrix}, \tag{17}$$

where a solution $(\overline{x}, \overline{\lambda})$ of (17equation.17) is such that $\Pi_K(\overline{x}, \overline{\lambda}) = (\Pi_{\mathcal{K}}(\overline{x}), \overline{\lambda})$ solves the complementary system (16equation.16). Notice that equation (17equation.17) can be rewritten as:

$$\begin{pmatrix} (Q - \mathrm{Id})\Pi_{\mathcal{K}}(x) + \mathcal{A}^*\lambda + x \\ \mathcal{A}\Pi_{\mathcal{K}}(x) \end{pmatrix} = \begin{pmatrix} -q \\ f \end{pmatrix}. \tag{18}$$

Finally, for any starting point $x^0 \in \mathbb{X}$, the semi-smooth Newton method applied to (18equation.18), noticing that (17equation.17) and (9equation.9) have the same structure, and after simplifications, results in:

$$\begin{pmatrix} (Q - \mathrm{Id})V(x^k)x^{k+1} + x^{k+1} + \mathcal{A}^*\lambda^{k+1} \\ \mathcal{A}V(x^k)x^{k+1} \end{pmatrix} = \begin{pmatrix} -q \\ f \end{pmatrix}, \tag{19}$$

for $k \in \mathbb{N}$. The convergence of the sequence $\{(x^k, \lambda^k)\}$ generated by iteration (19equation.19) is guaranteed by applying Theorems 4.2theorem.4.2 and 4.3theorem.4.3 with respect to equation (17equation.17).

5 The nearest correlation matrix problem

In this section, we describe the application of the semi-smooth Newton method to the nearest correlation matrix problem. This specific problem represents a special case of the broader positive semidefinite least squares problem (referenced as (20equation.20) below), a well-studied area notable for its significant applications and established algorithms; see [16, 21].

Let $\mathbb{X} = \mathbb{S}^n$ be denoted the set of symmetric $n \times n$ matrices with real entries and $\mathcal{K} = \mathbb{S}^n_+ \subset \mathbb{S}^n$ be denoted the cone of positive semidefinite matrices. Given any finite dimensional inner product space $\mathbb{Y}$ and a linear mapping $\mathcal{A}\colon \mathbb{S}^n \to \mathbb{Y}$, we consider the problem:

$$\begin{pmatrix} \min & \frac{1}{2}\|X - G\|_F^2, \\ \text{s.t.} & \mathcal{A}(X) = f, \\ & X \in \mathbb{S}^n_+, \end{pmatrix} \tag{20}$$

where $G \in \mathbb{S}^n$ and $f \in \mathbb{Y}$ are given and the Frobenius norm is defined as $\|A\|_F := \sqrt{\langle A, A\rangle}$, where $\langle A, B\rangle := \operatorname{trace}(AB)$ for $A, B \in \mathbb{S}^n$.

Since $\frac{1}{2}\|X - G\|_F^2 = \frac{1}{2}\langle X, X\rangle - \langle X, G\rangle + \frac{1}{2}\langle G, G\rangle$, problem (20equation.20) is an instance of (14equation.14) with $Q = \mathrm{Id}$ and $q = -G$. Thus, substituting in (19equation.19) we arrive at the following iteration for the semi-smooth Newton method for finding a solution $(X, \Lambda) \in \mathbb{S}^n \times \mathbb{Y}$ of (17equation.17):

$$\begin{pmatrix} X^{k+1} + \mathcal{A}^*(\Lambda^{k+1}) \\ \mathcal{A}V(X^k)X^{k+1} \end{pmatrix} = \begin{pmatrix} G \\ f \end{pmatrix}. \tag{21}$$

The nearest correlation matrix problem is the particular case where $\mathbb{Y} = \mathbb{R}^n$ and $\mathcal{A} = \operatorname{diag}\colon \mathbb{S}^n \to \mathbb{R}^n$ which maps a symmetric matrix to its diagonal vector. Its adjoint $\mathcal{A}^* = \operatorname{Diag}\colon \mathbb{R}^n \to \mathbb{S}^n$ maps a vector to a diagonal matrix with the given vector in its diagonal. The right-hand side vector $f \in \mathbb{R}^n$ will be fixed at the vector $e \in \mathbb{R}^n$ of all ones. Namely, let us consider problem:

$$\begin{pmatrix} \min & \frac{1}{2}\|X - G\|_F^2, \\ \text{s.t.} & \operatorname{diag}(X) = e, \\ & X \in \mathbb{S}^n_+. \end{pmatrix} \tag{22}$$

Thus, substituting in (18equation.18) we aim at solving the following projection equation for $(\overline{X}, \overline{\lambda}) \in \mathbb{S}^n \times \mathbb{R}^n$:

$$\overline{X} + \operatorname{Diag}(\overline{\lambda}) = G, \tag{23}$$

$$\operatorname{diag}(\Pi_{\mathbb{S}^n_+}(\overline{X})) = e, \tag{24}$$

by means of the semi-smooth Newton iteration

$$X^{k+1} + \operatorname{Diag}(\lambda^{k+1}) = G, \tag{25}$$

$$\operatorname{diag}(V(X^k)X^{k+1}) = e, \tag{26}$$

which is obtained from (21equation.21).

From (23equation.23) and (25equation.25) we deduce that the off-diagonal entries of $\overline{X}$ and X^{k+1} are equal to the corresponding off-diagonal entries of G. Thus, by defining the linear operator

$M(X) = \text{Diag}(\text{diag}(X))$, we have that $D^{k+1} = M(X^{k+1})$. We also define $\hat{G} = G - M(G)$. Hence, we obtain

$$X^{k+1} = D^{k+1} + \hat{G}, \tag{27}$$

$$\lambda^{k+1} = \text{diag}(G) - \text{diag}(D^{k+1}). \tag{28}$$

Now, a simple calculation substituting (27equation.27) in (26equation.26) and noticing that $\text{diag}(V(X^k)D^{k+1}) = M(V(X^k))\,\text{diag}(D^{k+1})$ since D^{k+1} is diagonal, gives

$$\begin{aligned} e = \text{diag}(V(X^k)X^{k+1}) &= \text{diag}(V(X^k)(D^{k+1} + \hat{G})), \\ &= \text{diag}(V(X^k)D^{k+1}) + \text{diag}(V(X^k)\hat{G}), \\ &= M(V(X^k))\,\text{diag}(D^{k+1}) + \text{diag}(V(X^k)\hat{G}). \end{aligned}$$

Then, solving the linear system for D^{k+1}, we arrive at the following expression for the semi-smooth Newton method:

$$\text{diag}(D^{k+1}) = (M(V(X^k)))^{-1}[e - \text{diag}(V(X^k)\hat{G})]. \tag{29}$$

Above expression gives us a fully computable iteration for our Newton method applied to the nearest correlation matrix problem. In particular, we compute the generalized Jacobian as $V(X) = UDU^T$ from the spectral decomposition $X = U\Lambda U^T$, where D is a diagonal matrix with $D_{ii} = 1$ if $\Lambda_{ii} > 0$ and $D_{ii} = 0$ if $\Lambda_{ii} \leq 0$. This choice is such that $V(X)H = U\left(D_e^+ \circ (U^THU)\right)U^T$, for any $H \in \mathbb{S}^n$, where D_e^+ is the matrix formed by the lines $\text{sgn}(\Lambda_{ii}^+)e^T$ and $\circ$ denotes the Hadamard product, so we are considering a particular case of the generalized Jacobian structure of the projection given in [23, Theorem 4.3]. This gives a convenient choice in order to achieve a simple and easy-to-evaluate iteration. When iteration (29equation.29) is not defined, we use in our implementation the pseudoinverse, corresponding to the least squares solution of the underlying system, although this situation never arose in our tests. The particular choice of $V(X)$ also allows us to apply it in more general structures, such as block diagonal problems, computing the projection and the generalized Jacobian of each block with a similar expressions, which we do not exploit in this paper. We prove next that the iteration is well-defined when $\text{diag}(X^k) > 0$:

Proposition 5.1. *Let $X \in \mathbb{S}^n$. If $\text{diag}(X) > 0$, then $\text{diag}(V(X)) > 0$.*

Proof. Let $X = U\Lambda U^T$ and $i \in \{1, \ldots, n\}$. Denote by u_j the j-th row of $U, j = 1, \ldots, n$. We have

$$X_{ii} = \sum_{j=1}^{n} \Lambda_{jj}(u_j)_i^2 > 0.$$

Then there exists k such that $\Lambda_{kk}(u_k)_i^2 > 0$. In particular, $\Lambda_{kk} > 0$ and $(u_k)_i^2 > 0$. Then, $V(X) = UDU^T$ with $D_{kk} = 1$. Therefore,

$$V(X)_{ii} = \sum_{j=1}^{n} D_{jj}(u_j)_i^2 = D_{kk}(u_k)_i^2 + \sum_{j \neq k} D_{jj}(u_j)_i^2 \geq (u_k)_i^2 > 0,$$

proving the result. □

Finally, we present a result ensuring that the method (29equation.29), near the solution, is not only well-defined but also has local quadratic convergence.

Theorem 5.1. *The semi-smooth Newton method defined by* (29equation.29) *is well-defined and converges quadratically to a solution* $(\overline{X}, \overline{\lambda})$ *of* (23equation.23)-(24equation.24) *when* (X_0, λ_0) *is sufficiently close to* $(\overline{X}, \overline{\lambda})$.

Proof. The result was proved in [27, Corollary 3.7], but it relies on the non-singularity of the iteration matrix (29equation.29), so we only need to prove this. Since $\operatorname{diag}(\Pi_{\mathbb{S}^n_+}(\overline{X})) = e > 0$, using Proposition 5.1proposition.5.1 we have that $V(\Pi_{\mathbb{S}^n_+}(\overline{X})) > 0$. By the definition of the generalized Jacobian we use, and using the fact that the nonnegative eigenvalues of both $\overline{X}$ and $\Pi_{\mathbb{S}^n_+}(\overline{X})$ are the same, we have $V(\Pi_{\mathbb{S}^n_+}(\overline{X})) = V(\overline{X})$, implying $\operatorname{diag}(V(\overline{X})) > 0$. Since the mappings diag and $\Pi_{\mathbb{S}^n_+}$ are continuous and strongly semi-smooth, we obtain a neighborhood $\mathcal{Y}$ of $\overline{X}$ where $\operatorname{diag}(V(X)) > 0$ for all $X \in \mathcal{Y}$. Hence, the method is locally well-defined and quadratic convergence is established. □

It turns out that in [27], a method closely resembling ours was proposed for the nearest correlation matrix problem (30equation.30). In their approach, a semi-smooth Newton method is applied to the following function:

$$\tilde{F}(y) := \mathcal{A}\Pi_{\mathbb{S}^n_+}(G + \mathcal{A}^* y) - e,$$

where $\mathcal{A} = \operatorname{diag}$. A significant contribution of their work is providing a formula for computing the matrix-vector operation $h \mapsto V_y h$, where V_y belongs to the (B-)subdifferential of $\tilde{F}$ at y, without needing to compute V_y explicitly. The drawback of this approach is that they must then resort to an iterative procedure for computing each Newton step, without exploiting the diagonal structure of the operator $\mathcal{A}$. In our approach, we explicitly compute the subdifferential, which allows us to explicitly solve the diagonal Newtonian linear system. We note that both methods require computing the full spectral decomposition of an $n \times n$ matrix at each iteration. The algorithm in [27] also adds a linesearch procedure in order to ensure global convergence. Their global strategy is easily adaptable to our case, but the impact in the experiments was minimal since no reduction of a stepsize was necessary. For a fair comparison, in our study, we chose not to use a linesearch procedure in either method.

6 Numerical experiments

6.1 Nearest correlation matrix problem

In order to observe the behavior of the method, we conducted four experiments from [27] (Experiments 5.5 to 5.8). In these four experiments the nearest correlation matrix problem was solved using randomly generated data. We remind the definition of the problem:

$$\begin{pmatrix} \min & \frac{1}{2}\|X - G\|_F^2, \\ \text{s.t.} & \operatorname{diag}(X) = e, \\ & X \in \mathbb{S}^n_+. \end{pmatrix} \tag{30}$$

Experiment 1 involves generating the matrix G as $G := C + \alpha R$, where C is a random correlation matrix generated by the `randcorr` Matlab command, $R_{ij} \in [-1, 1]$ is random, and $\alpha \geq 0$ is chosen. In Experiment 2, G is defined as a matrix of random numbers $G_{ij} \in [-1, 1]$ with $G_{ii} = 1$ for $i = 1, \ldots, n$. Experiment 3 is analogous to Experiment 2, but in this case $G_{ij} \in [0, 2]$. Finally,

Experiment 4 defines G as

$$G := \begin{pmatrix} \frac{\ell}{1-\ell}(E_\ell - \mathrm{Id}_\ell) & 0 \\ 0 & 0 \end{pmatrix} + D + \alpha R,$$

where $1 \leq \ell \leq n$, $\alpha \geq 0$, Id_ℓ is the identity matrix of dimension ℓ, E_ℓ is a matrix of 1's of dimension ℓ, D is a random diagonal matrix with $D_{ii} \in [-20000, 20000]$, and R is a random matrix such that $R_{ij} \in [-1, 1]$. The comparison is made using performance profiles [10]. We built 10 random problems for each choice of parameters. For Experiment 1, we fixed $n = 3000$ and tested all values of $\alpha \in \{0.01, 0.1, 1, 10\}$. Experiments 2 and 3 used $n \in \{1000, 2000, 3000\}$, while Experiment 4 used $n \in \{5000, 8000, 10000\}$ with $\alpha = 0.001$ and $\ell = n/2$.

The experiments were ran in a 2.30 GHz Intel(R) Core(TM) i5-8300H processor, 16 GB of RAM and operating system Windows 10 using Matlab 9.5.0.944444 (R2018b). We stopped the execution of the methods when the Euclidean residual error is smaller than 10^{-5} and we report the CPU time required by both methods.

In Experiment 1, our method was in general slower than that of Qi and Sun [27]. For $\alpha = 0.01$, our method took on average 65% more CPU time. This percentage was 137% and 499% for $\alpha = 1$ and 10, respectively. Conversely, for $\alpha = 0.1$, their method took on average 13% more CPU time than ours. In Figure 1figure.1, we present a performance profile for Experiment 1 with $\alpha = 0.1$.

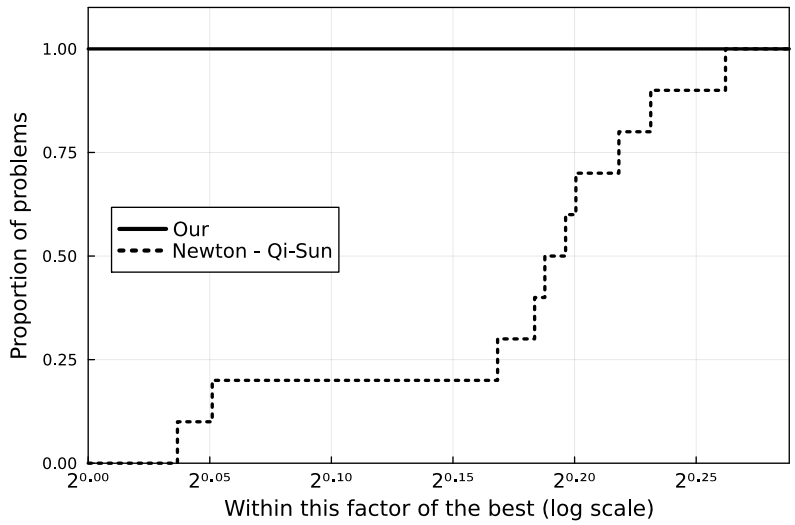
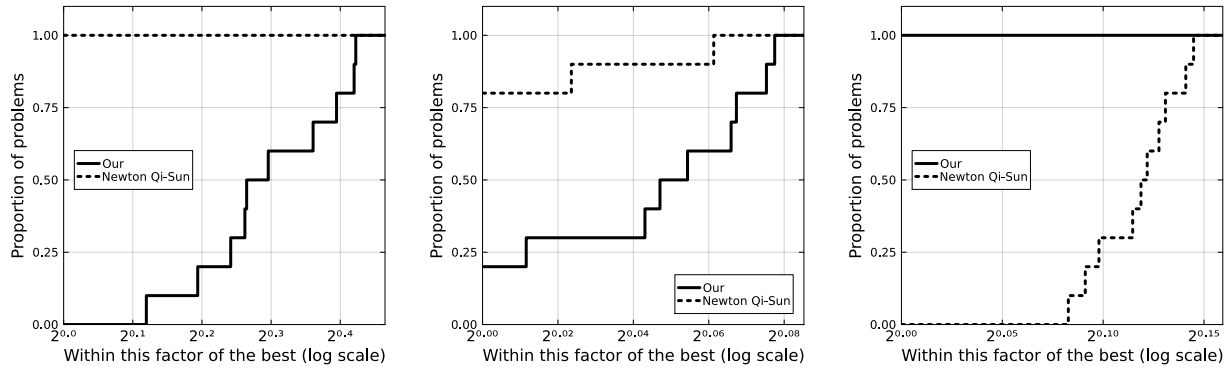


Figure 1: Performance profile for Experiment 1 with $\alpha = 0.1$.

In Experiments 2 and 3, we observed that our method was slower compared to [27]. For Experiment 2 our method took on average 1.6 times the CPU time required by the method from [27] for $n = 1000$, 2 times for $n = 2000$ and 2.5 times for $n = 3000$. The situation was worse regarding Experiment 3 where we observe that our method took around 4 times the total CPU time required by the method from [27] for $n = 1000$. It was 7 times slower for $n = 2000$ and 9 times slower for $n = 3000$. The situation is much more favorable in Experiment 4. In Figures 2asubfigure.2.1, 2bsubfigure.2.2, and 2csubfigure.2.3, we present the performance profiles concerning $n = 5000$, $n = 8000$, and $n = 10000$, respectively. In Table 1table.1 we show the average total CPU time and the average number of iterations for both methods and all dimensions tested.

For Experiment 4, we observed that the method of Qi and Sun was faster in all problems with dimension 5000 and in about 75% of the problems with dimension 8000, while our method was

faster in all problems of dimension 10000. In Table 1table.1 we can see that our method in general requires more iterations to converge, yet the computation of the iteration is cheaper. This pattern was consistent across other experiments we conducted. Despite this, the difference in the number of iterations was not significant enough in order for the better iteration cost to yield a better overall performance. In Experiment 4, we noted that as the dimension increases, our method becomes more efficient compared to the method of Qi and Sun as the number of iterations becomes similar. We could not, however, replicate this behavior for other values of α. This suggests that although we can exploit the diagonal structure of the linear system in order to compute Newton's direction, while Qi and Sun's method resorts to a conjugate gradient method, the subgradient they compute is somewhat more efficient towards solving the problem than the one we obtain in our approach. Specifically, in Experiments 2 and 3 where the matrix G is far from being positive semidefinite, the better subgradient of Qi and Sun pays off considerably. Nonetheless, our method shows potential superiority for the low noise level regime ($\alpha \approx 0$) and high values of n in Experiments 1 and 4.



(a) $n = 5000$ (b) $n = 8000$ (c) $n = 10000$

Figure 2: Performance profiles for Experiment 4.

	$n = 5000$		$n = 8000$		$n = 10000$	
Method	time (s)	it	time (s)	it	time (s)	it
Our	972.99	13	3677.27	10	6880.66	10
Qi-Sun	791.12	8	3588.47	8	7463.56	9

Table 1: Average total CPU time and number of iterations for $n = 5000$, $n = 8000$, and $n = 10000$ in Experiment 4.

Notice that the sufficient conditions of Theorems 4.2theorem.4.2 and 4.3theorem.4.3 do not hold for this problem. Despite this, we did not observe any convergence failures in any of the experiments we ran.

The method of Qi and Sun is tailored to the nearest correlation matrix problem, while our method applies to the general minimization of a quadratic function subject to conic linear constraints. Therefore, it is natural to compare our results with such a general method. Hence, to complete our numerical experiments, we ran ten instances of each of the four experiments using the two-phase augmented Lagrangian method proposed in [20] for convex quadratic minimization with linear semidefinite constraints. Experiment 1 was run with $\alpha = 0.1$, Experiments 2 and 3 with $n = 3000$, and Experiment 4 was run with $n = 5000$. While our algorithm stops with a tolerance for the KKT

residual, their algorithm uses a relaxed stopping criterion (with tolerance 10^{-6}), where the residual is scaled by the norm of the matrix G, which can be very large for high dimensions. In the sequel, for each experiment, we report the ratio of the average of CPU time taken by each algorithm to stop together with the average of the unscaled residual found. In Experiment 1 their method took 75% more CPU time than our method to stop and their residual was of order 10^{-5} compared to 10^{-14} from our method. In Experiment 2, our method found a solution with KKT residual of order 10^{-13} while, using roughly the same amount of time, their method found a solution with residual of order 10^{-1}. In Experiment 3 their algorithm stopped at a solution with KKT residual of order 10^{-3} while our method found a solution with KKT residual of order 10^{-13} (taking 125% of the time). In Experiment 4, the situation was similar but our method was run in half the CPU time needed by their method and their residual was of order 10^{-2} while ours was of order 10^{-12}. In summary, our method was able to significantly reduce the KKT residual quickly, while their method struggled to find accurate solutions. The general conclusion of our numerical experiments for the nearest correlation matrix problem is that although our method is a general one, it is more efficient than other general algorithm while being still competitive with a tailored algorithm, at least in the low noise regime ($\alpha \approx 0$) and for large n.

6.2 Nearest Euclidean distance matrix problem

In order to emphasize the generality of our approach, we consider a related matrix problem but defined on a different cone. Let $\mathbb{X} = \mathbb{S}^n$. We are interested in the so-called hollow subspace $\{X \in \mathbb{S}^n : \operatorname{diag}(X) = 0\}$. In this subspace, a matrix D is called a *Euclidean distance matrix* if there exists a dimension $r \leq n-1$ and points $p_1, \ldots, p_n$ in $\mathbb{R}^r$ such that $D_{ij} = \|p_i - p_j\|^2, i, j = 1, \ldots, n$. The smallest such r is the embedding dimension of D. It is well-known (see [28] and the references therein) that a matrix D in the hollow subspace of $\mathbb{S}^n$ is a Euclidean distance matrix if and only if $-D \in \mathcal{K}_+^n := \{X \in \mathbb{S}^n \colon z^T X z \geq 0, \forall z \in e^\perp\}$. The embedding dimension of D is $r = \operatorname{rank}(JDJ)$, where $J := \operatorname{Id} - \frac{1}{n} e e^T$.

Given a data matrix $D \in \mathbb{S}^n$, we are interested in computing the nearest Euclidean distance matrix to D. This problem can be written as an instance of (14equation.14) as follows:

$$\begin{pmatrix} \min & \frac{1}{2}\|X - G\|_F^2, \\ \text{s.t.} & \operatorname{diag}(X) = 0, \\ & X \in \mathcal{K}_+^n, \end{pmatrix} \tag{31}$$

where $G = -D$ and $-X$ is the Euclidean distance matrix sought.

The system of projection equations for this problem, analogous to (23equation.23)-(24equation.24), is

$$X + \operatorname{Diag}(\lambda) = G, \tag{32}$$

$$\operatorname{diag}(X) + \operatorname{diag}(\Pi_{\mathbb{S}_+^n}(-JXJ)) = 0, \tag{33}$$

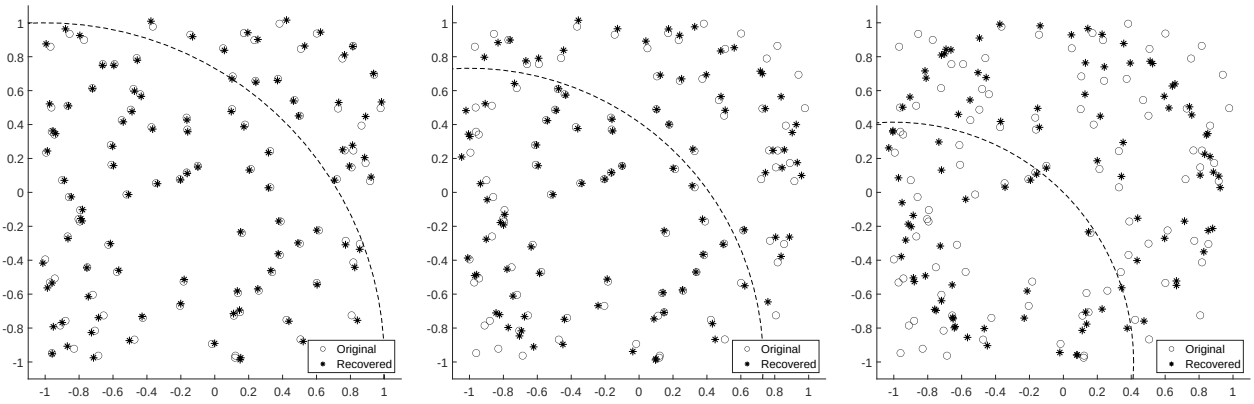
where we used that the projection $\Pi_{\mathcal{K}_+^n}(X)$ is equal to $X + \Pi_{\mathbb{S}_+^n}(-JXJ)$; see (29) in [14].

Using a similar computation conducted for the nearest correlation matrix problem, we deduce that the semi-smooth Newton method's iteration for this problem can be stated as:

$$\left[\operatorname{Id} - M(V(-JX^kJ)J) + \frac{1}{n} V(-JX^kJ)J\right] \operatorname{diag}(D^{k+1}) + g^k = 0, \tag{34}$$

with $g^k := \operatorname{diag}(\hat{G}) + \operatorname{diag}(V(-JX^kJ)[-J\hat{G}J])$, $V(-JX^kJ) \in \partial_C \Pi_{\mathbb{S}^n_+}(-JX^kJ)$, $M(X) := \operatorname{Diag}(\operatorname{diag}(X))$, $\hat{G} := G - M(G)$, and $X^{k+1} := D^{k+1} + \hat{G}$.

To illustrate the algorithm, we randomly generated $n = 100$ points $p_1, \ldots, p_n$ in $\mathbb{R}^2$ in the square $[-1, 1] \times [-1, 1]$ and we computed the Euclidean distance matrix D^{true} associated, where $D^{\text{true}}_{ij} := \|p_i - p_j\|^2, i, j = 1, \ldots, n$. To define the matrix $G = -D$ used in (31equation.31), we simulate the situation where only distances to nearby points are known. That is, given a maximum range $R > 0$, we define $D_{ij} := D^{\text{true}}_{ij}$ when $\|p_i - p_j\| \leq \sqrt{R}$ and $D_{ij} := R^*$ otherwise, where $R^* \geq 0$ is some fixed estimate for large distances. We then solve the problem using iteration (34equation.34) until a precision of 10^{-6} on the unscaled Euclidean KKT residual is reached. We recover the points from the Euclidean distance matrix found using Matlab's classical multidimensional scaling function `cmdscale` and the procrustes analysis function `procrustes`. Figure 3figure.3 shows the results for $R = 4$, $R = 3$, and $R = 2$, where we chose an appropriate estimate R^* for squared distances larger than R. We compared our results with the Newton method proposed by Qi in [28], where they considered the computation of an efficient subgradient for the function $F(y) := \operatorname{diag}(\Pi_{\mathcal{K}^n_+}(G + \operatorname{Diag}(y)))$, solving the linear system by a preconditioned conjugate gradient method similarly to [27].



(a) $R = 4, R^* = 5.5$ (b) $R = 3, R^* = 4.0$ (c) $R = 2, R^* = 3.5$

Figure 3: After computing the matrix of squared distances of the original points, for each point, squared distances larger than R are replaced by R^* in the matrix. The nearest Euclidean distance matrix is computed and the points are recovered. A circular sector of radius $\sqrt{R}$ centered at $(-1, -1)$ is shown in the picture in order to roughly depict which distances were replaced by R^*. One can see that the algorithm is able to recover the overall structure of the original configuration and that the solution quality degrades as the amount of missing information increases.

In this experiment, for all three values of R, our method required between 0.01 and 0.02 seconds to reach the desired accuracy, whereas Qi's method took between 0.03 and 0.05 seconds. In terms of iteration count, our method converged in 18 to 20 iterations, while Qi's method consistently converged in 6 iterations.

We also carried out a more complete comparison of our method and the one from [28], namely, Examples 5.2, 5.3, 5.4 and 5.5 from [28]. The results were consistent with those in the above experiment and with what we have reported for the nearest correlation matrix problem. That is, although the algorithm by Qi in general performs less iterations due to a more efficient subgradient used, our iteration is significantly cheaper. Therefore, the overall performance in terms of CPU time depends heavily on problem structure and dimension. In all problems we ran, we start both

methods at $X = G$.

In Figure 3figure.3, we were able to somewhat recover the original points for $R = 4$ and $R = 3$, however, when $R = 2$, the solution obtained is not accurate. In particular, due to the lack of data in D, the nearest Euclidean distance $-X$ to D, where X is a solution to (31equation.31), may be far from D^{true}. That is, there are too many distances fixed at R^* which the algorithm commits to, while replacing the true distances given in D. This explains the circular pattern present in Figure 3csubfigure.3.3. The solution obtained also varies considerably with R^*, even for the successful cases of $R = 4$ and $R = 3$.

In order to recover the original points when $R = 2$, we describe a more accurate representation of the problem, termed *Euclidean distance matrix completion problem* [19]. Given a set of known distances $D_{ij} = D_{ij}^{\text{true}}$, one is interested in *completing* the matrix D in order to obtain a Euclidean distance matrix. Formally, for $G = -D$, we consider the problem

$$\begin{pmatrix} \min & \frac{1}{2}\|H \circ (X - G)\|_F^2, \\ \text{s.t.} & \operatorname{diag}(X) = 0, \\ & X \in \mathcal{K}_+^n, \end{pmatrix} \tag{35}$$

where H_{ij} is set as 1 if D_{ij} is known, that is, if $D_{ij} = D_{ij}^{\text{true}}$ and H_{ij} is set as 0 otherwise. Operator $\circ$ denotes the Hadamard product, hence, the objective function effectively removes from the objective function the unknown entries of $G = -D$. Note that this formulation does not require an approximation R^* for unknown distances. This is known as the H-weighted least squares formulation, see [28]. Problem (35equation.35) is an instance of our general quadratic problem (14equation.14) where the linear operator Q corresponds to $X \mapsto (H \circ H) \circ X$ and $q = -(H \circ H) \circ G$. For our choice of H, we have $H \circ H = H$. Notice that, following [2], the graph of prescribed distances D_{ij} may not be chordal, that is, a cycle of known distances D_{12}, D_{23}, D_{34}, and D_{41} may be known without any intermediate distances D_{13} or D_{24} being prescribed. This happens, for instance, if in the original configuration four points correspond to the vertices of a square of radius $\sqrt{R}$. Hence, the sufficient condition for existence of solution may not be met [2]. However, problem (35equation.35) has a global minimizer $-D^{\text{true}}$ by construction, such that the objective function vanishes (ignoring possible truncation errors in D^{true}). Hence, unless multiple global minimizers exist, we expect to recover the original configuration with our method at least when multiple starting points are considered to avoid local minimizers. Figure 4figure.4 shows the points recovered from $-X$, where X is the solution found for problem (35equation.35) in 639 iterations of the algorithm (in 5.1 seconds) applied to completing the matrix D computed previously with $R = 2$ and an unspecified R^*. This corresponds to a single run with initial point equal to G and tolerance 10^{-6} of the KKT residual as previously. We also recovered exactly the original points for $R = 4$ and $R = 3$ in 28 and 78 iterations, corresponding to computation times of 0.3 and 0.7 seconds, respectively, with the same starting point and tolerance as previously. The number of iterations may be reduced by considering a more refined starting point and linesearch procedures. See, for instance, [11].

7 Concluding remarks

In this paper, we investigated the global and local convergence properties of the semi-smooth Newton method when applied to a general projection equation within finite dimensional spaces. We also highlighted the intrinsic connection between the solutions of this projection equation and the constrained quadratic conic programming problem. Comparative experiments on semidefinite least squares problems, in particular, the nearest correlation matrix problem and the nearest Eu-

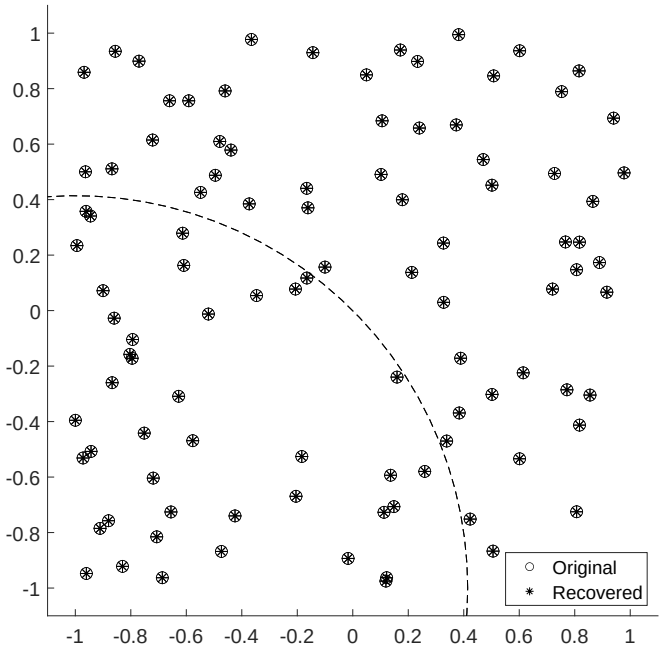


Figure 4: Recovered points for $R = 2$ using the formulation of problem (35equation.35).

clidean distance matrix problem, benchmark the proposed method against existing literature and underscore its efficacy. The method demonstrated remarkable adaptability in quadratic conic programming, yielding good results on both a symmetric and a nonsymmetric cone, namely $\mathbb{S}^n_+$ and $\mathcal{K}^n_+$, respectively. Moreover, an important variation – the H-weighted nearest Euclidean distance matrix problem – was successfully solved. The methodology introduced herein paves the way for future research into the versatility and performance of the semi-smooth Newton method in addressing a broader class of conic-constrained problems via generalized projection equations.

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