A semi-smooth Newton method for a special piecewise linear system with application to positively constrained convex quadratic programming

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Abstract

In this paper a special piecewise linear system is studied. It is shown that, under a mild assumption, the semi-smooth Newton method applied to this system is well defined and the method generates a sequence that converges linearly to a solution. Besides, we also show that the generated sequence is bounded, for any starting point, and a formula for any accumulation point of this sequence is presented. As an application, we study the convex quadratic programming problem under a positive constraint. The numerical results suggest that this method achieves accurate solutions to large scale problems in few iterations.

Keywords: Piecewise linear system, quadratic programming, convex set, convex cone, semi-smooth Newton method.

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1 Introduction

In this paper we consider the following special piecewise linear system:

$$x^+ + Tx = b, \tag{1}$$

where the data consists of b a real matrix of size $n \times 1$ and T a nonsingular real matrix of size $n \times n$, the variable x is a real matrix of size $n \times 1$ and x^+ is the matrix with i-th component equal to $(x_i)^+ = \max\{x_i, 0\}$. In [7] was proposed a semi-smmooth Newton's method for solving (1). Under suitable assumption was showed the finite convergence to a solution of (1). Some works dealing with (1) and its generalizations include [8, 9, 12, 20, 38]. It is worth mentioning that a similar equation has been studied in [27].

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The purpose of the present paper is to discuss the semi-smmooth Newton's method introduced in [7], to solve (1), under new assumptions. As an application, we use the obtained results to study the remarkable instance of (1),

$$[Q - \mathrm{Id}]\, x^{+} + x = -\tilde{b}, \tag{2}$$

where the data consists of Q a symmetric positive definite real matrix of size $n \times n$ and $\tilde{b}$ a real matrix of size $n \times 1$. Moreover, we present some computational experiments designed to investigate its practical viability. It is worth pointing out that the semi-smmooth Newton's method for solving (2) was studied in [17] and some computational tests were presented in [3]. The results obtained in this paper improve the ones of [17].

As we will show, the system (2) arises from the optimality condition of the convex quadratic programming problem under a positive constraint,

$$\begin{aligned} &\text{Minimize } \ \frac{1}{2} x^{\top} Q x + x^{\top} \tilde{b} + c \\ &\text{subject to } \ x \in \mathbb{R}^n_+. \end{aligned} \tag{3}$$

where c is a real number and $\mathbb{R}^n_+$ is the nonnegative orthant. Positively constrained convex quadratic programming is equivalent to the problem of projecting the point onto a simplicial cone. The interest in the subject of projection arises in several situations, having a wide range of applications in pure and applied mathematics such as Convex Analysis (see e.g. [21]), Optimization (see e.g. [4, 10, 11, 36]), Numerical Linear Algebra (see e.g. [37]), Statistics (see e.g. [6, 15, 22]), Computer Graphics (see e.g. [18]) and Ordered Vector Spaces (see e.g. [1, 23, 24, 32, 33]). The projection onto a general simplicial cone is difficult and computationally expensive, this problem has been studied e.g. in [2, 16, 19, 30, 31]. It is a special convex quadratic program and its KKT optimality conditions consists in a linear complementarity problem (LCP) associated with it, see e.g [29, 30]. Therefore, the problem of projecting onto simplicial cones can be solved by active set methods [5, 25, 26, 29] or any algorithms for solving LCPs, see e.g [5, 29] and special methods based on its geometry, see e.g [30, 29]. Other fashionable ways to solve this problem are based on the classical von Neumann algorithm (see e.g. the Dykstra algorithm [14, 15, 40]). Nevertheless, these methods are also quite expensive (see the numerical results in [28] and the remark preceding section 6.3 in [39]).

Following the ideas of [27], we show that the approach using semi-smooth Newton's method, for solving (3), has potential advantages over existing methods. The main advantage appears to be the global, linear convergence and to achieve accurate solutions of large scale problems in few iterations. Our numerical results suggest, for a given class of problem, that the number of required iterations is almost unchanged. The numerical results also indicate a remarkable robustness with respect to the starting point.

The organization of the paper is as follows. In Section 1.1, some notations and and preliminaries used in the paper are presented. In Section 2 we study the convergence properties of the semi-smooth Newton's method for solving (1). In Section 3 the results of Section 2 are applied to find a solution of (3). In Section 4 we present some computational tests. Some final remarks are made in Section 5.

1.1 Notations and preliminaries

In this subsection we present the notations and some auxiliary results used throughout the paper. Let $\mathbb{R}^n$ be the n-dimensional Euclidean space with the canonical inner product $\langle \cdot, \cdot \rangle$ and induced norm $\| \cdot \|$. The i-th component of a vector $x \in \mathbb{R}^n$ is denoted by x_i . We use the partial ordering for vectors, defined by $x \leq y$ meaning $x_i \leq y_i$, for all $i = 1, \ldots, n$. For $x \in \mathbb{R}^n$, $\mathrm{sgn}(x)$ will denote a vector with components equal to 1, 0 or -1 depending on whether the corresponding component of the vector x is positive, zero or negative. If $a \in \mathbb{R}$ and $x \in \mathbb{R}^n$, then denote $a^+ := \max\{a, 0\}$, $a^- := \max\{-a, 0\}$ and x^+ and x^- the vectors with i-th component equal to $(x_i)^+$ and $(x_i)^-$, respectively. From the definitions of x^+ and x^- we have $x = x^+ - x^-$, $\langle x^+, x^- \rangle = 0$ and $x^+, x^- \in \mathbb{R}^n_+$.

Lemma 1. *Let $x, y \in \mathbb{R}^n$. Then $\|y^+ - x^+ - \mathrm{diag}(\mathrm{sgn}(x^+))(y - x)\| \leq \|y - x\|$.*

Proof. For each $i \in \{1, \ldots, n\}$, we have two possibilities:

(a) $x_i < 0$. In this case, $\mathrm{sgn}(x_i^+) = 0$. Thus, $|y_i^+ - x_i^+ - \mathrm{sgn}(x_i^+)(y_i - x_i)| = |y_i^+| \leq |y_i - x_i|$.

(b) $x_i \geq 0$. In this case, $\mathrm{sgn}(x_i^+) = 1$. Hence, $|y_i^+ - x_i^+ - \mathrm{sgn}(x_i^+)(y_i - x_i)| = |y_i^+ - y_i| \leq |y_i - x_i|$.

Combining (a) and (b) we have $(y_i^+ - x_i^+ - \mathrm{sgn}(x_i^+)(y_i - x_i))^2 \leq (y_i - x_i)^2$, for all $i = 1, \ldots, n$, which implies the desired inequality. □

The set of all $m \times n$ matrices with real entries is denoted by $\mathbb{R}^{m \times n}$ and $\mathbb{R}^n \equiv \mathbb{R}^{n \times 1}$. The matrix Id denotes the $n \times n$ identity matrix. If $x \in \mathbb{R}^n$ then $\mathrm{diag}(x)$ will denote an $n \times n$ diagonal matrix with (i, i)-th entry equal to x_i, $i = 1, \ldots, n$. Denote $\|M\| := \max\{\|Mx\| \ : \ x \in \mathbb{R}^n, \ \|x\| = 1\}$ for any $M \in \mathbb{R}^{n \times n}$. The next useful result was proved in 2.1.1, page 32 of [34].

Lemma 2. *Let $E \in \mathbb{R}^{n \times n}$. If $\|E\| < 1$, then $E - \mathrm{Id}$ is invertible and $\|(E - \mathrm{Id})^{-1}\| \leq 1/\left(1 - \|E\|\right)$.*

We end this section with the contraction mapping principle (see 8.2.2, page 153 of [34]).

Theorem 1 (contraction mapping principle)**.** *Let $\phi : \mathbb{R}^n \to \mathbb{R}^n$. Suppose that there exists $\lambda \in [0, 1)$ such that $\|\phi(y) - \phi(x)\| \leq \lambda \|y - x\|$, for all $x, y \in \mathbb{R}^n$. Then there exists a unique $\bar{x} \in \mathbb{R}^n$ such that $\phi(\bar{x}) = \bar{x}$.*

2 A semi-smooth Newton method for a piecewise linear systems

In this section we present and analyze the semi-smooth Newton's method for solving (1). We begin with an existence result of solution to the equation (1).

Proposition 1. *Let $\lambda \in \mathbb{R}$. If $\left\|T^{-1}\right\| \leq \lambda < 1$ then (1) has unique solution for any $b \in \mathbb{R}^n$.*

Proof. The equation (1) has a solution if only if $\phi(x) = -T^{-1}x^+ + T^{-1}b$ has a fixed point. It follows from definition of ϕ that

$$\phi(y) - \phi(x) = -T^{-1}(y^+ - x^+), \qquad x, y \in \mathbb{R}^n.$$

Since $\left\|T^{-1}\right\| < \lambda < 1$, the last equality implies that $\|\phi(y) - \phi(x)\| \leq \lambda \|y - x\|$, for all $x, y \in \mathbb{R}^n$. Hence ϕ is a contraction. Therefore applying Theorem 1 we conclude that ϕ has precisely a unique fixed point and consequently (1) has a unique solution. □

The assumption $\left\|T^{-1}\right\| < 1$ in Proposition 1 is sufficient to the uniqueness of solution of (1). The next example shows that it is also necessary.

Example 1. *Consider the function $F : \mathbb{R}^2 \to \mathbb{R}^2$ defined by $F(x) = x^+ + Tx - b$, where*

$$T = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad b = \begin{bmatrix} 0 \\ 2 \end{bmatrix}.$$

Note that $\|T^{-1}\| = 1$ and there holds $F(x^*) = F(x^{**}) = 0$, where $x^* = [1, 1]^T$ and $x^{**} = [0, 1]^T$.

The *semi-smooth Newton method* introduced in [35] for finding the zero of the function

$$F(x) := x^+ + Tx - b, \qquad x \in \mathbb{R}^n. \tag{4}$$

with starting point $x^0 \in \mathbb{R}^n$, it is formally defined by

$$F(x^k) + V^k\left(x^{k+1} - x^k\right) = 0, \qquad V^k \in \partial F(x^k), \qquad k = 0, 1, \ldots, \tag{5}$$

where V^k is any subgradient in $\partial F(x^k)$ the Clarke generalized Jacobian of F at x^k (see Definition 2.6.1 on page 70 of [13]). Letting

$$P(x) := \operatorname{diag}(\operatorname{sgn}(x^+)), \qquad x \in \mathbb{R}^n, \tag{6}$$

it easy to see that

$$P(x) + T \in \partial F(x), \qquad x \in \mathbb{R}^n.$$

Since $P(x)x = x^+$ for all $x \in \mathbb{R}^n$, taking $V^k = P(x^k) + T$, equation (5) becomes

$$\left[P(x^k) + T\right] x^{k+1} = b, \qquad k = 0, 1, \ldots, \tag{7}$$

which define formally the *semi-smooth Newton sequence* $\{x^k\}$ for solving (1) (see, [7]). We devote the rest of this section to studying the convergence properties of this sequence.

Proposition 2. *Assume that the matrix $P(x) + T$ is nonsingular for all $x \in \mathbb{R}^n$. Then, $\{x^k\}$ is well defined and bounded from any starting point. Moreover, for each accumulation point $\bar{x}$ of $\{x^k\}$ there exists an $\hat{x} \in \mathbb{R}^n$ such that*

$$\left[P(\hat{x}^+) + T\right] \bar{x} = b. \tag{8}$$

In particular, if $sgn(\bar{x}^+) = sgn(\hat{x}^+)$, then $\bar{x}$ is a solution of (1).

Proof. To prove this result we follow similar arguments of Proposition 3 of [27]. □

Next proposition gives a condition for the Newton iteration (7) to finish in a finite number of steps.

Proposition 3. *If in* (7) *it happens that $sgn((x^{k+1})^+) = sgn((x^k)^+)$, then x^{k+1} is a solution of* (1).

Proof. Since $\operatorname{sgn}((x^{k+1})^+) = \operatorname{sgn}((x^k)^+)$ we have $P(x^{k+1}) = P(x^k)$. Thus, (7) gives

$$\left[P(x^{k+1}) + T\right] x^{k+1} = b.$$

Because $P(x^{k+1})x^{k+1} = (x^{k+1})^+$, the last equality yields $(x^{k+1})^+ + Tx^{k+1} = b$, which implies that x^{k+1} is a solution of (1). □

Theorem 2. *Let $b \in \mathbb{R}^n$ and $T \in \mathbb{R}^{n\times n}$ be a nonsingular matrix. Assume that $\left\|T^{-1}\right\| < 1$. Then, for any starting point $x^0 \in \mathbb{R}^n$, $\{x^k\}$ is well-defined. Additionally, if*

$$\left\|T^{-1}\right\| < 1/2, \tag{9}$$

then $\{x^k\}$ converges Q-linearly to $x^* \in \mathbb{R}^n$, the unique solution of (1)*, as follows*

$$\|x^* - x^{k+1}\| \le \frac{\|T^{-1}\|}{1 - \|T^{-1}\|}\|x^* - x^k\|, \qquad k = 0, 1, \ldots. \tag{10}$$

Proof. Let $x \in \mathbb{R}^n$. Since $\left\|T^{-1}\right\| < 1$, the definition of $P(x)$ implies $\|T^{-1}P(x)\| \leq \|T^{-1}\| < 1$. Thus, Lemma 2 implies that $-T^{-1}P(x) - \mathrm{Id}$ is nonsingular. Because T is nonsingular and

$$P(x) + T = -T\left[-T^{-1}P(x) - \mathrm{Id}\right], \qquad x \in \mathbb{R}^n,$$

we conclude that $P(x) + T$ is also nonsingular. Hence, for any starting point $x^0 \in \mathbb{R}^n$, (7) implies that $\{x^k\}$ is well-defined .

Using Proposition 1, we conclude that (1) has unique solution $x^* \in \mathbb{R}^n$. Since $x^* \in \mathbb{R}^n$ is the solution of (1), we have $[P(x^*) + T]x^* - b = 0$, which together with definition of $\{x^k\}$ in (7) and (6) imples

$$x^* - x^{k+1} = -[P(x^k)+T]^{-1}\left[[P(x^*)+T]x^* - b - [P(x^k)+T]x^k + b - [P(x^k)+T](x^* - x^k)\right], \quad k = 0, 1, \ldots.$$

On the other hand, since $P(x)x = x^+$ for all $x \in \mathbb{R}^n$, after simple algebraic manipulations we obtain

$$[P(x^*) + T]x^* - b - [P(x^k) + T]x^k + b - [P(x^k) + T](x^* - x^k) = (x^*)^+ - (x^k)^+ - P(x^k)(x^* - x^k),$$

for $k = 0, 1, \ldots$. Combining two above equalities and using properties of the norm we have

$$\|x^* - x^{k+1}\| \leq \left\|P(x^k) + T]^{-1}\right\| \left\|(x^*)^+ - (x^k)^+ - P(x^k)(x^* - x^k)\right\|, \qquad k = 0, 1, \ldots.$$

It follows from Lemma 1 that $\left\|(x^*)^+ - (x^k)^+ - P(x^k)(x^* - x^k)\right\| \leq \|x^* - x^k\|$, for $k = 0, 1, \ldots$, and last inequality becomes

$$\|x^* - x^{k+1}\| \leq \left\|[P(x^k) + T]^{-1}\right\| \|x^* - x^k\|, \qquad k = 0, 1, \ldots. \tag{11}$$

On the other hand, after some algebra and using properties of the norm, we have

$$\left\|[P(x^k) + T]^{-1}\right\| = \left\|[-T^{-1}P(x^k) - \mathrm{Id}]^{-1}\left[-T^{-1}\right]\right\| \leq \left\|[T^{-1}P(x^k) + \mathrm{Id}]^{-1}\right\| \|T^{-1}\|, \quad k = 0, 1, \ldots.$$

which combined with Lemma 2 and considering that $\|T^{-1}P(x^k)\| \leq \|T^{-1}\| < 1$, implies

$$\left\|[P(x^k) + T]^{-1}\right\| \leq \frac{\|T^{-1}\|}{1 - \|T^{-1}\|}, \qquad k = 0, 1, \ldots.$$

Thus, last inequality together with (11) gives (10). Assumption (9) implies $\|T^{-1}\|/(1 - \|T^{-1}\|) < 1$. Therefore, (10) implies that $\{x^k\}$ converges Q-linearly, from any starting point x^0, to the solution x^* of (1). Hence the theorem is proven. □

Theorem 3. *Assume that* (1) *has solutions. If* $[P(x)+T]^{-1}$ *exists with its lines either non-negative or non-positive for all* $x \in \mathbb{R}^n$, *then* $\{x^k\}$ *generated by* (7) *converges after finite steps for the unique solution of the* (1).

Proof. First of all note that the sequence generated by (7) satisfies

$$F(x^k) + [P(x^k) + T](x^{k+1} - x^k) = 0, \qquad k = 0, 1, \ldots. \tag{12}$$

where the function F is defined in (4). By direct computation, we have

$$F(y) - F(x) - [P(x) + T](y - x) = P(y)y - P(x)y \geq 0, \qquad x, y \in \mathbb{R}^n. \tag{13}$$

For arbitrary $x^0 \in \mathbb{R}^n$, the above inequality and (12) imply that

$$F(x^1) \geq F(x^0) + [P(x^0) + T](x^1 - x^0) = 0.$$

Thus, applying an induction argument we conclude that

$$F(x^k) = [P(x^k) + T]x^k - b \geq 0, \qquad k = 1, 2, \ldots. \tag{14}$$

Let x^* be a solution of (1). Letting $y = x^*$ and $x = x^k$ in (13), we obtain

$$0 = F(x^*) \geq F(x^k) + [P(x^k) + T](x^* - x^k). \tag{15}$$

Since $s_i = (s_{i1}, \ldots, s_{in})^T$, the $i-$th line of $[T + P(x)]^{-1} =: (s_{ij})$, has all elements either non-negative or non-positive, we have only two options: $\text{sgn}(s_i^T)$ has its components equal to -1 or 0, or $\text{sgn}(s_i^T)$ has its components equal 0 or 1. Multiplying both sides of (15) by $[T + P(x^k)]^{-1}$ and using (14), we have

$$x_i^* \leq x_i^k - s_i F(x^k) \leq x_i^k, \qquad i \in I_+ := \left\{1 \leq i \leq n : \text{sgn}(s_i^T) \in \{0, 1\}\right\}, \tag{16}$$

for all $k \geq 1$, and similarly

$$x_i^* \geq x_i^k - s_i F(x^k) \geq x_i^k, \qquad i \in I_- := \left\{1 \leq i \leq n : \text{sgn}(s_i^T) \in \{-1, 0\}\right\}. \tag{17}$$

Note that as $[T + P(x^k)]^{-1}$ exists, then there are no indexes i and j such that $s_i = s_j$, thus $I_+ \cap I_- = \emptyset$ and $I_+ \cup I_- = \{1, 2 \ldots, n\}$. It follows from (5), (7) and $V^k = P(x^k) + T$ that

$$x^{k+1} = [T + P(x^k)]^{-1} b = x^k - [P(x^k) + T]^{-1} F(x^k), \qquad k = 0, 1, \ldots.$$

Therefore, using (14) and the definition of I_+, we obtain

$$x_i^* \leq x_i^{k+1} \leq x_i^k, \qquad i \in I_+, \tag{18}$$

where the first inequality above follows from (16), and analogously using (17), we have

$$x_i^* \geq x_i^{k+1} \geq x_i^k, \qquad i \in I_-. \tag{19}$$

Hence, $\{x^k\}$ converges, because $\{x_i^k\}$ is monotone and bounded by x_i^* for $i = 1, \ldots, n$. Thus, $\{x_i^k\}$ has a limit u_i. Therefore, $\{x^k\}$ converges to the vector u with components u_i. By using again (12), we have

$$\|F(u)\| = \lim_{k \to \infty} \|F(x^k)\| = \lim_{k \to \infty} \|[P(x^k) + T](x^{k+1} - x^k)\| \leq (1 + \|T\|) \lim_{k \to \infty} \|x^{k+1} - x^k\| = 0.$$

Therefore, u is a solution. Furthermore, for any two solutions x^* and y^*, (13) implies

$$0 = F(x^*) - F(y^*) \geq [T + P(y^*)](x^* - y^*). \tag{20}$$

Then, multiplying by $[T + P(y^*)]^{-1}$ we obtain

$$y_i^* \geq x_i^* \quad i \in I_+ \quad \text{and} \quad y_i^* \leq x_i^* \quad i \in I_-.$$

The result follows by reversing the roles of x^* and y^* in (20). Thus, the problem has a unique solution equal to the limit of the sequence $\{x^k\}$ generated by (7).

Finally we establish the finite termination of the sequence $\{x^k\}$ at the unique solution of problem (1). Let x^* be the solution of (1). Since $P(x)$ has only 2^n different choices, for all $x \in \mathbb{R}^n$, then there exist j and $\ell \geq 1$ such that $P(x^j) = P(x^{j+\ell})$. This statement implies that

$$x^{j+1} = [T + P(x^j)]^{-1}b = [T + P(x^{j+\ell})]^{-1}b = x^{j+\ell+1}.$$

Applying inductively this argument,

$$x^{j+1} = x^{j+\ell+1}, \;\; x^{j+2} = x^{j+\ell+2}, \;\; \ldots, \; x^{j+\ell} = x^{j+2\ell}, \;\; x^{j+\ell+1} = x^{j+2\ell+1} = x^{j+1}.$$

Now using (18) and (19), we obtain

$$x_i^{j+1} \geq x_i^{j+2} \geq \cdots \geq x_i^{j+\ell+1} = x_i^{j+1}, \qquad i \in I_+,$$

and

$$x_i^{j+1} \leq x_i^{j+2} \leq \cdots \leq x_i^{j+\ell+1} = x_i^{j+1}, \qquad i \in I_-.$$

Hence, $x^{j+1} = x^{j+2}$ and in view Proposition 3 we conclude that $x^{j+2} = x^*$. □

The invertibility of $P(x) + T$, for all $x \in \mathbb{R}^n$, is sufficient to the well-definedness of the semi-smooth Newton method. However, the next example show that, for the convergence of these methods, an additional condition on T must be assumed, for instance, (9) or $[P(x) + T]^{-1}$ exists with its lines either non-positive or non-negative for all $x \in \mathbb{R}^n$.

Example 2. *Consider the function $F : \mathbb{R}^2 \to \mathbb{R}^2$ defined by $F(x) = x^+ + Tx - b$, where*

$$T = \begin{bmatrix} -2 & 3 \\ -1 & 1 \end{bmatrix}, \qquad b = \begin{bmatrix} -5 \\ -3 \end{bmatrix}.$$

Note that $\|T^{-1}\| = 3,86...$ and the matrix $P(x) + T$ is invertible, for all $x \in \mathbb{R}^2$. Moreover, F has $x^* = [2, -1]^T$ as the unique zero. Applying semi-smooth Newton method starting with $x^0 = [-3, 3]^T$, for finding the zero of F, the generated sequence oscillates between the points

$$x^1 = \begin{bmatrix} 4 \\ 1 \end{bmatrix}, \qquad x^2 = \begin{bmatrix} -1 \\ -2 \end{bmatrix}.$$

3 Application to quadratic programming

In this section, we apply the results of Section 2 to solve (2), in order to find a solution of (3). We begin showing that, from each solution of (2), we obtain a solution of (3).

Proposition 4. *If the vector x^* is a solution of* (2)*, then $(x^*)^+$ is a solution of* (3)*.*

Proof. The optimality conditions of the problem in (3) are given by

$$x \in \mathbb{R}^n_+, \qquad Qx + \tilde{b} \in \mathbb{R}^n_+, \qquad \left\langle Qx + \tilde{b}, x \right\rangle = 0. \tag{21}$$

We claim that $(x^*)^+$ is a solution of (21). We know that $(x^*)^+ - x^* = (x^*)^-$. Thus, if $x^* \in \mathbb{R}^n$ is a solution of (2), then

$$Q(x^*)^+ + \tilde{b} = (x^*)^-.$$

Hence, by using $(x^*)^- \in \mathbb{R}^n_+$ and $\langle (x^*)^-, (x^*)^+ \rangle = 0$, the last equality easily implies that

$$Q(x^*)^+ + \tilde{b} \in \mathbb{R}^n_+, \qquad \langle Q(x^*)^+ + \tilde{b}, (x^*)^+ \rangle = 0.$$

Combining this with $(x^*)^+ \in \mathbb{R}^n_+$, we conclude that $(x^*)^+$ is a solution of (21) as claimed, which completes the proof. □

The *semi-smooth Newton method* for solving (2), with starting point $x^0 \in \mathbb{R}^n$, is given by

$$x^{k+1} = -\Big([Q - \mathrm{Id}]\, P(x^k) + \mathrm{Id}\Big)^{-1} \tilde{b}, \qquad k = 0, 1, \ldots. \tag{22}$$

Remark 1. *If $Q - \mathrm{Id}$ is a nonsingular matrix, $T = [Q - \mathrm{Id}]^{-1}$ and $b = -T\tilde{b}$, then (2) and (1) are equivalent. Moreover, (22) becomes*

$$x^{k+1} = \Big[T^{-1}P(x^k) + \mathrm{Id}\Big]^{-1} T^{-1}b = \Big[P(x^k) + T\Big]^{-1} b, \qquad k = 0, 1, \ldots,$$

which is the semi-smooth Newton method defined in (7).

Proposition 5. *Let $\lambda \in \mathbb{R}$. If $\|Q - \mathrm{Id}\| \leq \lambda < 1$ then (2) has a unique solution.*

Proof. The proof follows by combining Remark 1 with Proposition 1. □

The next result shows that the semismooth Newton defined in (22) is always well defined.

Lemma 3. *Let $x \in \mathbb{R}^n$. The following matrix is nonsingular*

$$[Q - \mathrm{Id}]\, P(x) + \mathrm{Id}. \tag{23}$$

As a consequence, the semi-smooth Newton sequence $\{x^k\}$ is well-defined, for any starting point $x^0 \in \mathbb{R}^n$.

Proof. The proof of the first part of the lemma, follows similar argument to the proof of Lemma 5 of [17]. To prove the second part of the lemma, combine the definition of $\{x^k\}$ in (22) and the first part of the lemma. □

Proposition 6. *If in (22) it happens that $sgn((x^{k+1})^+) = sgn((x^k)^+)$, then x^{k+1} is a solution of (2).*

Proof. The proof follows combining Remark 1 and Proposition 3. □

Proposition 7. *The sequence $\{x^k\}$, defined in (22), is bounded from any starting point. Moreover, for each accumulation point $\bar{x}$ of $\{x^k\}$, there exists an $\hat{x} \in \mathbb{R}^n$ such that*

$$([Q - \mathrm{Id}]\, P(\hat{x}) + \mathrm{Id})\, \bar{x} = -A^\top b. \tag{24}$$

In particular, if $sgn(\bar{x}^+) = sgn(\hat{x}^+)$ then $\bar{x}$ is a solution of (2).

Proof. Using Remark 1 and Proposition 2 the result follows. □

Theorem 4. *The sequences $\{x^k\}$ generated by the semi-smooth Newton Method (22) for solving (2), is well defined for any starting point $x^0 \in \mathbb{R}^n$. Moreover, if*

$$\|Q - \mathrm{Id}\| < 1/2, \tag{25}$$

then the sequence $\{x^k\}$ converges Q-linearly to $u \in \mathbb{R}^n$, the unique solution of (2), as follows

$$\|x^* - x^{k+1}\| \leq \frac{\|Q - \mathrm{Id}\|}{1 - \|Q - \mathrm{Id}\|} \|x^* - x^k\|, \qquad k = 0, 1, \ldots, \tag{26}$$

and u^+ is a solution of (3).

Proof. The well-definedness, for any starting point $x^0 \in \mathbb{R}^n$, follows from Lemma 3. For concluding the proof combine, Proposition 4, Remark 1 and Theorem 2. □

Let us present an important equivalent form of problem (3).

Example 3. *Given $A \in \mathbb{R}^{n\times n}$ a nonsingular matrix, $A\mathbb{R}^n_+ := \{Ax \ : \ x \in \mathbb{R}^n_+\}$ and $z \in \mathbb{R}^n$. The projection $P_{A\mathbb{R}^n_+}(z)$ of the point z onto the cone $A\mathbb{R}^n_+$ is defined by*

$$P_{A\mathbb{R}^n_+}(z) := argmin\left\{\frac{1}{2}\|z-y\|^2 \ : \ y \in A\mathbb{R}^n_+\right\}.$$

From the definition of the simplical cone associated with the matrix A, the problem of projecting the point $z \in \mathbb{R}^n$ onto a simplicial cone $A\mathbb{R}^n_+$ may be stated as the following positively constrained quadratic programming problem

$$\begin{aligned} &\text{Minimize } \ \frac{1}{2}\|z-Ax\|^2, \\ &\text{subject to } \ x \in \mathbb{R}^n_+. \end{aligned}$$

Hence, if $v \in \mathbb{R}^n$ is the unique solution of this problem then we have $P_{A\mathbb{R}^n_+}(z) = Av$. The above problem is equivalent to the following nonegatively constrained quadratic programming problem

$$\begin{aligned} &\text{Minimize } \ \frac{1}{2}x^\top \tilde{Q}x + x^\top \tilde{b} + \tilde{c} \\ &\text{subject to } \ x \in \mathbb{R}^n_+, \end{aligned} \tag{27}$$

by taking $\tilde{Q} = A^\top A$, $\tilde{b} = -A^\top z$ and $\tilde{c} = z^\top z/2$. The optimality condition for problem (27) *implies that its solution can be obtained by solving the following linear complementarity problem*

$$y - \tilde{Q}x = \tilde{b}, \qquad x \geq 0, \qquad y \geq 0, \qquad \langle x, y\rangle = 0. \tag{28}$$

Remark 2. *It is easy to establish that corresponding to each nonnegative quadratic problems* (27) *and each linear complementarity problems* (28) *associated to symmetric positive definite matrices, there are equivalent problems of projection onto simplicial cones. Therefore, the problem of projecting onto simplicial cones can be solved by active set methods [5, 25, 26, 29] or any algorithms for solving LCPs, see e.g [5, 29] and special methods based on its geometry, see e.g [30, 29]. Other fashionable ways to solve this problem are based on the classical von Neumann algorithm (see e.g. the Dykstra algorithm [14, 15, 40]). Nevertheless, these methods are also quite expensive (see the numerical results in [28] and the remark preceding section 6.3 in [39])*

4 Computational results

In this section we test our semi-smooth Newton method (22) to find solutions on generated random instances of (2). We present two types of experiments. In one of them, we guarantee that for each test problem the hypotheses given in Theorem 4 are satisfied and in the other they are not.

All programs were implemented in MATLAB Version 7.11 64-bit and run on a 3.40GHz Intel Core $i5-4670$ with 8.0GB of RAM. All MATLAB codes and generated data of this paper are available in `http://orizon.mat.ufg.br/pages/34449-publications`.

All experiments are based on the following general considerations:

- In order to accurately measure the method's runtime for a problem, each one of the test problems was solved 10 times and the runtime data collected. Then, we defined the corresponding *method's runtime for a problem* as the median of these measurements.

- Let $\operatorname{Tol} X \in \mathbb{R}_+$ be a relative bound, we consider that the method converged to the solution and stopped the execution when, for some k, the condition

$$\|u - x^k\| < \operatorname{Tol} X(1 + \|u\|),$$

  is satisfied. If the previous stopping criteria are not met within 100 iterations, we declare that the method did not converge.

4.1 When the hypotheses of Theorem 4 are satisfied

In this experiment, we studied the behavior of the method on sets of 100 randomly generated test problems of dimension $n = 2000, 3000, 4000, 5000$, respectively. Furthermore, we analyzed the influence of the initial point in the convergence of the method on 1000 randomly generated test problems of dimension $n = 100$. For each test problem in this experiment the hypotheses given in the Theorem 4 are satisfied, generating each of them as follows:

1. To construct the matrix $Q \in \mathbb{R}^{n \times n}$ satisfying the assumption (25) in Theorem 4, we first chose a random number β from the standard uniform distribution on the open interval $(0, 1/2)$. Secondly, we compute the matrices S, V and D, respectively, from the singular value decomposition of a generated $n \times n$ real nonsingular matrix containing random values drawn from the uniform distribution on the interval $[-10^6, 10^6]$. Finally, we compute the matrix Q from

$$Q = S \operatorname{sqrt}\left(I + \frac{\beta}{\sigma} V\right) D,$$

   were σ is the largest singular value of V and $\operatorname{sqrt}(I + \frac{\beta}{\sigma} V)$ is the square root of the diagonal matrix $I + \frac{\beta}{\sigma} V$.

2. We have chosen the solution $u \in \mathbb{R}^n$ containing random values drawn from the uniform distribution on the interval $[-10^6, 10^6]$ and then we have computed $\tilde{b} \in \mathbb{R}^n$ from equation (2).

3. Finally we have chosen a starting point $x^0 \in \mathbb{R}^n$ containing random values drawn from the uniform distribution on the interval $[-10^6, 10^6]$.

In accordance with the theoretical convergence of the method, ensured by Theorem 4, the computational convergence is obtained in all cases.

The computational results to analyze the behavior of the method on sets of 100 generated random test problems of different dimensions, are reported in Table 1. From these, it can be noted that for the same dimension, to achieve higher accuracy, the method does not experience a significant increase in the number of iterations or in runtime. On the other hand, the increase in the dimension of the problems does not necessarily involve an increase in the number of iterations to achieve the same accuracy, however, a larger runtime is consumed. A larger runtime consumption is associated with the fact that the semi-smooth Newton method (22) requieres the solution of a linear system in each iteration, whose computational effort increases with the dimension of the problem. Another important aspect that can be checked in Table 1 is the ability of the method to converge in about three iterations on average.

n	Total Iterations			Total Time		
2000	278	291	293	137.17	143.37	144.29
3000	285	293	296	451.75	463.81	468.33
4000	289	302	304	1049.23	1094.25	1100.82
5000	284	300	305	1964.60	2074.63	2109.27
Tol X	10^{-6}	10^{-8}	10^{-10}	10^{-6}	10^{-8}	10^{-10}

Table 1: Total overall iterations and total time in seconds, performed and consumed, respectively by the semi-smooth Newton method (22) to solve the 100 test problems of each dimension for different accuracies.

In order to study the influence of the initial point in the convergence of the method, we have generated 1000 test problems of dimension $n = 100$ and we have associated to each of them 1000 generated initial points. We have solved each problem with each of the 1000 corresponding initial points. Then, we have computed the standard deviation (STD) $\overline{d}_i$ and the mean value (MEAN) $\overline{m}_i$ of the number of iterations performed by the method to solve the problem i taking each one of the 1000 initial points. Finally we have computed the mean of all $\overline{d}_i$ and the mean of all $\overline{m}_i$, $\;i = 1, ..., 1000$. All cases converged, indicating robustness of the method with respect to the starting point. The results are shown in Table 2. The standard deviation of the number of iterations performed by the method to solve the problem i with the 1000 initial points gives us an idea of the influence of the initial point in the number of iterations performed by the method in each problem. The reported means of these standard deviation values give us an idea of the influence of the initial point in the number of iterations performed by the method in all the problems in general. The results in the table show that on average the number of iterations performed by our method to find the solution for a problem varies only very slightly with the chosen starting point. Again we see that the average number of iterations performed is less than three.

Tol X	MEAN $\left(\{\overline{d}_i\}_{i=1,...,1000}\right)$	MEAN $\left(\{\overline{m}_i\}_{i=1,...,1000}\right)$
10^{-6}	0.2501	2.3410
10^{-8}	0.2560	2.3470
10^{-10}	0.2564	2.3478

Table 2: Influence of the initial point in the convergence of the semi-smooth Newton method (22) on a total of 1000 test problems of dimension $n = 100$ each of them with 1000 generated initial points for different accuracies.

4.2 When the hypotheses of Theorem 4 are not satisfied

In this experiment, we studied the behavior of the method on 1000 test problems of dimension $n = 1000$, where the hypotheses given in the Theorem 4 are not all satisfied.

In this case, the test problems were built almost as in the previous experiment. The only difference was in the construction of the matrix $Q \in \mathbb{R}^{n\times n}$ not satisfying the assumption (25) of Theorem 4. Namely, we chose the random number β from the standard uniform distribution on the interval $[lb, ub)$, where $\frac{1}{2} \leq lb < ub$. Then, $\|Q - I\| = \beta$.

According to the obtained numerical results, we can conjecture that our method converges to a much broader class of problems, not satisfying the hypotheses of Theorem 4. However we detected that convergence with high accuracy to the solution largely depends on the magnitude of the value of the norm in condition (25). This idea can be observed inspecting Table 3. As the magnitude of the value of the norm in (25) increases sufficiently, the number of problems for which the method converges to the solution with greater accuracy decreases. This phenomenon, of course, is not associated to the convergence of the method for a specific problem, but, rather, there is an optimum accuracy achievable due to the accumulated errors. Small tolerances do not ensure obtaining accurate results. It can be the case that convergence is overlooked and unnecessary iterations are performed. It is important to note in the table that, even when the hypothesis is unfulfilled, the method converges for these problems, however it can be noted that the number of iterations performed by the method increases with respect of the previous experiments in which the hypotheses were fulfilled.

$\beta \in [lb, ub)$	Solved Problems			Iterations		
$[0.5, 10^3)$	1000	1000	1000	6.3960	6.3980	6.3980
$[10^3, 10^4)$	1000	1000	1000	7.6030	7.6080	7.6080
$[10^4, 10^5)$	1000	1000	1000	8.0140	8.0170	8.0170
$[10^5, 10^6)$	1000	1000	678	8.2490	8.2520	8.2316
$[10^6, 10^7)$	1000	1000	0	8.3170	8.3180	-
$[10^7, 10^8)$	1000	686	0	8.3190	8.3397	-
Tol X	10^{-6}	10^{-8}	10^{-10}	10^{-6}	10^{-8}	10^{-10}

Table 3: Number of problems solved by the semi-smooth Newton method (22) on a total of 1000 test problems of dimension $n = 1000$ of each condition ($lb \leq \|Q - I\| < ub$) for different accuracies, and the mean number of iterations performed by the semi-smooth Newton method (22) to solve one problem in each case.

5 Conclusions

In this paper we studied a special class of convex quadratic programming under positive constraint, which, via its optimality conditions, is reduced to finding the unique solution of a nonsmooth system of equations. Our main result shows that, under a mild assumption on the simplicial cone, we can apply a semi-smooth Newton method for finding a unique solution of the obtained associated nonsmooth system of equations and that the generated sequence converges linearly to the solution for any starting point. It would be interesting to see whether the used technique can be applied for solving more general convex programs.

Since the optimality condition of a positive constrained convex quadratic programming problem is equivalent to a linear complementarity problem, which is equivalent to the problem of finding the unique solution of a nonsmooth system of equations, another interesting problem to address is to compare our semi-smooth Newton method with active set methods [5, 25, 26, 29].

This paper is a continuation of [17], where we studied the problem of projection onto a simplicial cone by using a semi-smooth Newton method. We expect that the results of this paper become a further step towards solving general convex optimization problems. We foresee further progress in this topic in the near future.

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