Generalized Conjugate Gradient Methods for ℓ_1 Regularized Convex Quadratic Programming with Finite Convergence

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Abstract

The conjugate gradient (CG) method is an efficient iterative method for solving large-scale strongly convex quadratic programming (QP). In this paper we propose some generalized CG (GCG) methods for solving the ℓ_1-regularized (possibly not strongly) convex QP that terminate at an optimal solution in a finite number of iterations. At each iteration, our methods first identify a face of an orthant and then either perform an exact line search along the direction of the negative projected minimum-norm subgradient of the objective function or execute a CG subroutine that conducts a sequence of CG iterations until a CG iterate crosses the boundary of this face or an approximate minimizer of over this face or a subface is found. We determine which type of step should be taken by comparing the magnitude of some components of the minimum-norm subgradient of the objective function to that of its rest components. Our analysis on finite convergence of these methods makes use of an error bound result and some key properties of the aforementioned exact line search and the CG subroutine. We also show that the proposed methods are capable of finding an approximate solution of the problem by allowing some inexactness on the execution of the CG subroutine. The overall arithmetic operation cost of our GCG methods for finding an ϵ-optimal solution depends on ϵ in $O(\log(1/\epsilon))$, which is superior to the accelerated proximal gradient method [2, 23] that depends on ϵ in $O(1/\sqrt{\epsilon})$. In addition, our GCG methods can be extended straightforwardly to solve box-constrained convex QP with finite convergence. Numerical results demonstrate that our methods are very favorable for solving ill-conditioned problems.

Keywords: conjugate gradient method, convex quadratic programming, ℓ_1-regularization, sparse optimization, finite convergence

AMS subject classifications: 65C60, 65K05, 65Y20, 90C06, 90C20, 90C25

1 Introduction

The conjugate gradient (CG) method is an efficient numerical method for solving *strongly* convex quadratic programming (QP) in the form of

$$\min_{x \in \Re^n} \frac{1}{2} x^T B x - c^T x, \tag{1.1}$$

or equivalently, the linear system $Bx = c$, where $B \in \Re^{n \times n}$ is a symmetric *positive definite* matrix and $c \in \Re^n$. It terminates at the unique optimal solution of (1.1) in a finite number of iterations. Moreover, it is suitable for solving large-scale problems since it only requires matrix-vector multiplications per iteration (e.g., see [24] for details). The CG method has also been generalized to minimize a convex quadratic function over a box or a ball (e.g., see [11, 12, 25, 26, 27]).

In this paper we are interested in generalizing the CG method to solve the ℓ_1 regularized convex QP:

$$F^* = \min_{x \in \Re^n} F(x) := \frac{1}{2} x^T A x - b^T x + \tau \|x\|_1, \tag{1.2}$$

where $A \in \Re^{n \times n}$ is a symmetric *positive semidefinite* matrix, $b \in \Re^n$ and $\tau \geq 0$ is a regularized parameter. Throughout this paper we make the following assumption for problem (1.2).

Assumption 1 *The set of optimal solutions of problem* (1.2), *denoted by $\mathcal{S}^*$, is nonempty.* [1]

Over the last decade, a great deal of attention has been focused on problem (1.2) due to numerous applications in image sciences, machine learning, signal processing and statistics (e.g., see [8, 16, 5, 14, 30, 29] and the references therein). Considerable effort has been devoted to developing efficient algorithms for solving (1.2) (e.g., see [2, 23, 30, 33, 15, 32, 31, 22]). These methods are iterative methods and capable of producing an approximate solution to (1.2). Nevertheless, they generally cannot terminate at an optimal solution of (1.2). Recently, Byrd et al. [6] proposed a method called iiCG to solve (1.2) that combines the iterative soft-thresholding algorithm (ISTA) [2, 10, 30] with the CG method. Under the assumption that A is symmetric positive definite, it was shown in [6] that the sequence generated by iiCG converges to the unique optimal solution of (1.2), and if additionally this solution satisfies strict complementarity, iiCG terminates in a finite number of iterations. Its convergence is, however, unknown when A is positive semidefinite (but not definite), which is typical for many instances of (1.2) arising in applications.

In this paper we propose some generalized CG (GCG) methods for solving (1.2) that terminate at an optimal solution of (1.2) in a finite number of iterations with no additional assumption. At each iteration, our methods first identify a certain face of some orthant and then either perform an exact line search along the direction of the negative projected minimum-norm subgradient of F or execute a CG subroutine that conducts a sequence of CG iterations until a CG iteration crosses the boundary of this face or an approximate minimizer of F over this face or a subface is found. The purpose of the exact line search step is to release some zero components of the current iterate so that the value of F is sufficiently reduced. The aim of executing a CG routine is to update the nonzero components of the current iterate, which also results in a reduction on F. We determine which type of step should be taken by comparing the magnitude of some components of the minimum-norm subgradient of F to that of its rest components. Our methods are substantially different from the iiCG method [6]. In fact, at each iteration, iiCG either performs a *proximal gradient* step or executes a *single* CG iteration. It determines which type of step should be conducted by comparing the magnitude of some components of a *proximal gradient* of F to that of its rest components.

In order to analyze the convergence of our GCG methods, we establish some error bound results for problem (1.2). We also conduct some exclusive analysis on the aforementioned exact line search and the CG subroutine. Using these results, we show that the GCG methods terminate at an optimal solution of (1.2) in a finite number of iterations. To the best of our knowledge, the GCG methods are the first methods for solving (1.2) with finite convergence. We also show that our methods are capable of finding an approximate solution of (1.2) by allowing some inexactness on the execution of the CG subroutine. The overall arithmetic operation cost of our GCG methods for finding an ϵ-optimal solution depends on ϵ in $O(\log(1/\epsilon))$, which is superior to the accelerated

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[1]Since the objective function of (1.2) is a convex piecewise quadratic function, problem (1.2) has at least an optimal solution if and only if its objective function is bounded below.

proximal gradient method [2, 23] that depends on ϵ in $O(1/\sqrt{\epsilon})$. In addition, it shall be mentioned that these methods can be extended to solve the following box-constrained convex QP with finite convergence:

$$\min_{l \leq x \leq u} \frac{1}{2} x^T A x - b^T x, \tag{1.3}$$

where $A \in \Re^{n \times n}$ is symmetric positive semidefinite, $b \in \Re^n$, $l, u \in \bar{\Re}^n$ with $\bar{\Re} = [-\infty, \infty]$. As for finite convergence, the existing CG type methods [11, 12] for (1.3), however, require that A be symmetric positive definite. The extension of our methods to problem (1.3) is not included in this paper due to the length limitation.

The rest of the paper is organized as follows. In Section 2, we establish some results on error bound for problem (1.2). In Section 3, we propose several GCG methods for solving problem (1.2) and establish their finite convergence. In Section 4, we discuss the application of our GCG methods to solve the ℓ_1 regularized least-squares problems and develop a practical termination criterion for them. We conduct numerical experiments in Section 5 to compare the performance of our GCG methods with some state-of-the-art algorithms for solving problem (1.2). In Section 6 we present some concluding remarks. Finally, in the appendix we study some convergence properties of the standard CG method for solving (possibly not strongly) convex QP.

1.1   Notation and terminology

For a nonzero symmetric positive semidefinite matrix A, we define a generalized condition number of A as

$$\kappa(A) = \|A\|\|A^+\| = \frac{\lambda_{\max}(A)}{\lambda_{\min}^+(A)}, \tag{1.4}$$

where A^+ is the Moore-Penrose pseudoinverse of A, $\lambda_{\max}(A)$ is the largest eigenvalue of A and $\lambda_{\min}^+(A)$ is the smallest *positive* eigenvalue of A. Clearly, it reduces to the standard condition number when A is symmetric positive definite. In addition, for any index set $J \in \{1, \ldots, n\}$, $|J|$ is the cardinality of J and A_{JJ} is the submatrix of A formed by its rows and columns indexed by J. Analogously, b_J is the subvector of $b \in \Re^n$ formed by its components indexed by J. In addition, the range space and rank of a matrix B are denoted by $\text{Range}(B)$ and $\text{rank}(B)$, respectively.

Let $\text{sgn} : \Re^n \to \{-1, 0, 1\}^n$ be the standard sign operator, which is conventionally defined as follows

$$[\text{sgn}(x)]_i = \begin{cases} 1 & \text{if } x_i > 0; \\ 0 & \text{if } x_i = 0; \\ -1 & \text{if } x_i < 0, \end{cases} \quad i = 1, \ldots .n.$$

Let F be defined in (1.2) and

$$f(x) = \frac{1}{2} x^T A x - b^T x. \tag{1.5}$$

Let $v(x)$ be the *minimum-norm subgradient* of F at x, which is the projection of the zero vector onto the subdifferential of F at x. It follows that

$$v_i(x) = \begin{cases} \nabla_i f(x) + \tau \, \text{sgn}(x_i) & \text{if } x_i \neq 0; \\ \min\left(\nabla_i f(x) + \tau, \max(0, \nabla_i f(x) - \tau)\right) & \text{if } x_i = 0, \end{cases} \quad i = 1, \ldots, n, \tag{1.6}$$

where $\nabla_i f(x)$ denotes the ith partial derivative of f at x. It is known that x is an optimal solution of problem (1.2) if and only if $0 \in \partial F(x)$, where ∂F denotes the subdifferential of F. Since $0 \in \partial F(x)$ is equivalent to $v(x) = 0$, x is an optimal solution of (1.2) if and only if $v(x) = 0$.

For any $x \in \Re^n$, we define

$$\begin{aligned} I_-(x) &= \{i : x_i < 0\}, \quad I_+(x) = \{i : x_i > 0\}, \\ I_0(x) &= \{i : x_i = 0\}, \quad I_0^c(x) = \{i : x_i \neq 0\}, \end{aligned} \tag{1.7}$$

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and also define
$$\mathcal{H}(x) = \{y \in \Re^n : y_i = 0, \ i \in I_0(x)\}, \qquad F_x^* = \min\{F(y) : y \in \mathcal{H}(x)\}. \tag{1.8}$$

In addition, given any closed set $S \subseteq \Re^n$, $\mathrm{dist}(x, S)$ denotes the distance from x to S, and $\mathcal{P}_S(x)$ denotes the projection of x to S. Finally, we define

$$\mathcal{I}^* = \{J \subseteq I_0(x^*) : x^* \in \mathcal{S}^*\}, \qquad \mathcal{L}(n) = \max\{\ell : \mathcal{C}_i \notin \mathcal{I}^*, \ i = 1, \ldots, \ell, \text{ are distinct subsets in } \{1, \ldots, n\}\} + 1. \tag{1.9}$$

2   Error bound results

In this section we develop some error bound results for problem (1.2). To proceed, let $\mathcal{S}(\delta) := \{x : F(x) - F^* \le \delta\}$ for any $\delta \ge 0$, where F and F^* are defined in (1.2). We first bound the gap between $F(x)$ and F^* by $\|v(x)\|$ for all $x \in \mathcal{S}(\delta)$.

Theorem 2.1 *Let F, F^* and v be defined in (1.2) and (1.6), respectively. Then for any $\delta \ge 0$, there exists some $\eta > 0$ (depending on δ) such that*

$$F(x) - F^* \le \eta\|v(x)\|^2, \qquad \forall x \in \mathcal{S}(\delta).$$

Proof. Let X^* denote the set of optimal solutions of (1.2). Notice that F is a convex piecewise quadratic function. By [21, Theorem 2.7], there exists some $\eta > 0$ such that

$$\mathrm{dist}(x, X^*) \le \sqrt{\eta}\sqrt{F(x) - F^*}, \qquad \forall x \in \mathcal{S}(\delta). \tag{2.1}$$

Let $x^* \in X^*$ be such that $\|x - x^*\| = \mathrm{dist}(x, X^*)$. By $v(x) \in \partial F(x)$ and the convexity of F, one has

$$F(x) - F^* = F(x) - F(x^*) \le \langle v(x), x - x^* \rangle \le \|v(x)\|\|x - x^*\| = \|v(x)\|\mathrm{dist}(x, X^*),$$

which together with (2.1) implies that the conclusion holds. ∎

We next bound the gap between $F(x)$ and F_x^* by the magnitude of some components of $v(x)$ for all $x \in \mathcal{S}(\delta)$.

Theorem 2.2 *Let F and F_x^* be defined in (1.2) and (1.8), respectively. Then for any $\delta \ge 0$, there exists some $\hat{\eta} > 0$ (depending on δ) such that*

$$F(x) - F_x^* \le \hat{\eta}\|[v(x)]_J\|^2, \qquad \forall x \in \mathcal{S}(\delta),$$

where $J = I_0^c(x)$.

Proof. Let $x \in \mathcal{S}(\delta)$ be arbitrarily chosen, $I = I_0(x)$ and $J = I_0^c(x)$. If $J = \emptyset$, it is clear that $x = 0$ and hence $F_x^* = F(x)$. Also, by convention $\|[v(x)]_J\| = 0$. These imply the conclusion holds. We now assume $J \ne \emptyset$. Consider the problem

$$\hat{F}_J^* = \min_{z \in \Re^{|J|}} \hat{F}_J(z) := \frac{1}{2}z^T A_{JJ} z - b_J^T z + \tau\|z\|_1. \tag{2.2}$$

In view of the definitions of F_x^*, $\hat{F}_J$, $\hat{F}_J^*$, F, F^* and J, one can observe that

$$\hat{F}_J(x_J) = F(x), \qquad \hat{F}_J^* = F_x^* \ge F^*.$$

This together with $x \in \mathcal{S}(\delta)$ implies that $\hat{F}_J(x_J) - \hat{F}_J^* \le F(x) - F^* \le \delta$. By (1.6), (2.2) and the definition of J, we also observe that $[v(x)]_J$ is the minimum-norm subgradient of $\hat{F}_J$ at x_J. In addition, notice that problem

(2.2) is in the same form as (1.2). By these facts and applying Theorem 2.3 to problem (2.2), there exists some $\eta_J > 0$ (depending on δ and J) such that

$$F(x) - F_x^* = \hat{F}_J(x_J) - \hat{F}_J^* \leq \eta_J \|[v(x)]_J\|. \tag{2.3}$$

Let $\hat{\eta} = \max\{\eta_J : J = I_0^c(x),\ x \in \mathcal{S}(\delta)\}$, which is finite due to the fact that all possible choices of J are finite. The conclusion immediately follows from this and (2.3). ∎

The error bound presented in Theorem 2.2 is a local error bound as it depends on δ. In addition, Theorem 2.2 only ensures the existence of some parameter η for the error bound, but its actual value is generally unknown. We next derive a global error bound with a known η for problem (1.2) when A is symmetric positive definite. To proceed, we first establish a lemma as follows.

Lemma 2.1 *Suppose $A \neq 0$ and $b \in \text{Range}(A)$. Let $f(x)$ be defined in (1.5) and $f^* = \min_{x \in \Re^n} f(x)$. Then there holds:*

$$\frac{1}{2\|A\|}\|\nabla f(x)\|^2 \leq f(x) - f^* \leq \frac{\|A^+\|}{2}\|\nabla f(x)\|^2, \qquad \forall x \in \Re^n.$$

Proof. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$ be all eigenvalues of A and $\{u_i\}_{i=1}^n$ the corresponding orthonormal eigenvectors. In addition, let x^* be an optimal solution of the problem $\min_{x \in \Re^n} f(x)$. Clearly, $Ax^* = b$. Moreover, for any $x \in \Re^n$, we have $x - x^* = \sum_{i=1}^n \alpha_i u_i$ for some $\{\alpha_i\}_{i=1}^n$. These imply

$$\nabla f(x) = Ax - b = A(x - x^*) = \sum_{i=1}^n \lambda_i \alpha_i u_i. \tag{2.4}$$

Let $\ell = \text{rank}(A)$. It follows that $\lambda_i = 0$ for all $i > \ell$. In view of this and (2.4), we have

$$\|\nabla f(x)\|^2 = \sum_{i=1}^n \lambda_i^2 \alpha_i^2 = \sum_{i=1}^\ell \lambda_i^2 \alpha_i^2.$$

This together with the fact $\lambda_1 \geq \cdots \geq \lambda_\ell > 0$ yields

$$\frac{1}{\lambda_1}\|\nabla f(x)\|^2 = \frac{1}{\lambda_1}\sum_{i=1}^\ell \lambda_i^2 \alpha_i^2 \ \leq\ \sum_{i=1}^\ell \lambda_i \alpha_i^2 \ \leq\ \frac{1}{\lambda_\ell}\sum_{i=1}^\ell \lambda_i^2 \alpha_i^2 = \frac{1}{\lambda_\ell}\|\nabla f(x)\|^2.$$

Using the definitions of f and x^*, (2.4), $x - x^* = \sum_{i=1}^n \alpha_i u_i$ and $\lambda_i = 0$ for all $i > \ell$, one can observe that

$$f(x) - f^* = \frac{1}{2}(x - x^*)^T A(x - x^*) = \frac{1}{2}\sum_{i=1}^n \lambda_i \alpha_i^2 = \frac{1}{2}\sum_{i=1}^\ell \lambda_i \alpha_i^2.$$

The conclusion then immediately follows from the last two relations and the fact that $\lambda_1 = \|A\|$ and $\lambda_\ell = 1/\|A^+\|$. ∎

Theorem 2.3 *Let F and F_x^* be defined in (1.2) and (1.8), respectively. Suppose that A is symmetric positive definite. Then there holds:*

$$F(x) - F_x^* \leq \frac{\|A^{-1}\|}{2}\|[v(x)]_J\|^2, \qquad \forall x \in \Re^n,$$

where $J = I_0^c(x)$.

Proof. Let $x \in \Re^n$ be arbitrarily chosen and let $J = I_0^c(x)$. If $J = \emptyset$, it is clear that $x = 0$ and hence $F_x^* = F(x)$. Also, by convention $\|[v(x)]_J\| = 0$. These imply the conclusion holds. We now assume $J \neq \emptyset$. Consider the problem

$$\tilde{F}_J^* = \min_{z \in \Re^{|J|}} \tilde{F}_J(z) := \frac{1}{2} z^T A_{JJ} z + (-b_J + \text{sgn}(x_J))^T z.$$

Since A is positive definite, so is A_{JJ}. It then follows that $\text{sgn}(x_J) - b_J \in \text{Range}(A_{JJ})$. By applying Lemma 2.1 to this problem, we obtain that

$$\tilde{F}_J(x_J) - \tilde{F}_J^* \leq \frac{\|(A_{JJ})^{-1}\|}{2} \|\nabla \tilde{F}_J(x_J)\|^2. \tag{2.5}$$

In addition, by the definitions of F, $\tilde{F}_J$ and J, one can observe that $\tilde{F}_J(y_J) \leq F(y)$ for all $y \in \mathcal{H}(x)$, where $\mathcal{H}(x)$ is defined in (1.8). This together with the definitions of $\tilde{F}_J^*$ and F_x^* implies $\tilde{F}_J^* \leq F_x^*$. Also, we observe that $\tilde{F}_J(x_J) = F(x)$ and $[v(x)]_J = \nabla \tilde{F}_J(x_J)$. Using these relations and (2.5), we have

$$F(x) - F_x^* \leq \tilde{F}_J(x_J) - \tilde{F}_J^* \leq \frac{\|(A_{JJ})^{-1}\|}{2} \|\nabla \tilde{F}_J(x_J)\|^2 \leq \frac{\|A^{-1}\|}{2} \|[v(x)]_J\|^2,$$

and hence the conclusion holds. $\blacksquare$

3 Generalized conjugate gradient methods for (1.2)

In this section we propose several GCG methods for solving problem (1.2), which terminate at an optimal solution in a finite number iterations. A key ingredient of these methods is to apply a truncated projected CG (TPCG) method to a sequence of convex QP over certain faces of some orthants in $\Re^n$.

3.1 Truncated projected conjugate gradient methods

In this subsection we present two TPCG methods for finding an (perhaps very roughly) approximate solution to a convex QP on a face of some orthant in $\Re^n$ in the form of

$$
\begin{aligned}
\min_{x} \quad & q(x) := f(x) + c^T x \\
\text{s.t.} \quad & x_j = 0, \quad j \in J_0, \\
& x_j \leq 0, \quad j \in J_-, \\
& x_j \geq 0, \quad j \in J_+,
\end{aligned}
\tag{3.1}
$$

where f is defined in (1.5), $c \in \Re^n$, and $J_-, J_0, J_+ \subseteq \{1, \dots, n\}$ form a partition of $\{1, \dots, n\}$. For convenience of presentation, we denote by Ω the feasible region of (3.1).

For the first TPCG method, each iterate is obtained by applying the standard projected CG (PCG) method [2] to the problem

$$\min_{x}\{q(x) : x_j = 0, \ j \in J_0\} \tag{3.2}$$

until an approximate solution of (3.2) is found or a PCG iterate crosses the boundary of Ω. In the former case, the method outputs the resulting approximate solution. But in the latter case, it outputs the intersection point between the boundary of Ω and the line segment joining the last two PCG iterates. Let x^0 be an arbitrary feasible point of problem (3.1) and $\epsilon \geq 0$ be given. We now present the first TPCG method for problem (3.1).

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[2]The PCG method applied to problem (3.2) is equivalent to the CG method applied to the problem $\min q(x_{J_0^c}, 0)$, where J_0^c is the complement of J_0 in $\{1, \dots, n\}$.

Subroutine 1: $y = \text{TPCG1}(A, b, c, J_0, J_-, J_+, x^0, \epsilon)$

Input: A, b, c, J_0, J_-, J_+, x^0, ϵ.

Set $r^0 = Ax^0 - b + c$, $\mathcal{H} = \{x \in \Re^n : x_j = 0, \ j \in J_0\}$, $p^0 = \mathcal{P}_{\mathcal{H}}(r^0)$, $d^0 = -p^0$, $k = 0$.

Repeat

1) $\alpha_k = \min\{\alpha_k^{\text{cg}}, \alpha_k^{\text{tc}}\}$, where

$$\alpha_k^{\text{cg}} = \frac{\|p^k\|^2}{(d^k)^T A d^k}, ^3 \quad \alpha_k^{\text{tc}} = \max\{\alpha : x^k + \alpha d^k \in \Omega\}.$$

2) $x^{k+1} = x^k + \alpha_k d^k$.

3) If $\alpha_k^{\text{cg}} > \alpha_k$, return $y = x^{k+1}$ and terminate.

4) $r^{k+1} = r^k + \alpha_k A d^k$.

5) $p^{k+1} = \mathcal{P}_{\mathcal{H}}(r^{k+1})$. If $\|p^{k+1}\|_\infty \leq \epsilon$, return $y = x^{k+1}$ and terminate.

6) $d^{k+1} = -p^{k+1} + \frac{\|p^{k+1}\|^2}{\|p^k\|^2} d^k$.

7) $k \leftarrow k + 1$.

Output: y.

Remark 1: The iterations of the above TPCG method are almost identical to those of PCG applied to problem (3.2) except that the step length α_k is chosen to be an intermediate one when an iterate of PCG crosses the boundary of Ω. In addition, if $\alpha_k^{\text{cg}} > \alpha_k$ holds at some k, the output y is on the boundary of Ω. If $\|p^{k+1}\|_\infty \leq \epsilon$ holds at some k, the output y is an approximate optimal solution of problem (3.1).

We next show that under a mild assumption the above method terminates in a finite number of iterations.

Theorem 3.1 *Assume that problem* (3.1) *has at least an optimal solution. Suppose that x^0 is a feasible point of problem* (3.1) *and $\epsilon \geq 0$. Let $B = A_{J_0^c J_0^c}$, where J_0^c is the complement of J_0 in $\{1, \ldots, n\}$. The following statements hold:*

(i) *If problem* (3.2) *is bounded below, Subroutine 1 terminates in at most $\min(M, \text{rank}(B))$ [4] iterations, where*

$$M = \left\lceil \frac{\log \epsilon - \log(2\sqrt{\kappa(B)}\|p^0\|)}{\log(\kappa(B) - 1) - \log(\kappa(B) + 1)} \right\rceil.$$

(ii) *If problem* (3.2) *is unbounded below, Subroutine 1 terminates in at most $\text{rank}(B) + 1$ iterations.*

Proof. (i) Assume that problem (3.2) is bounded. Suppose for contradiction that Subroutine 1 does not terminate in $\min(M, \text{rank}(B))$ iterations. Then the iterates x^k, $k = 1, \ldots, \min(M, \text{rank}(B))$ of Subroutine 1 are

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[3] If $\|p^k\| \neq 0$ and $(d^k)^T A d^k = 0$, we set $\alpha_k^{\text{cg}} = \infty$.

[4] By convention, we define $\log 0 = -\infty$. It follows that $M = -\infty$ and hence $\min(M, \text{rank}(B)) = \text{rank}(B)$ when $\epsilon = 0$.

identical to those generated by the PCG method applied to problem (3.2). Let q^* denote the optimal value of (3.2). It follows from Theorem A.3 (iii) that for $k = 1, \ldots, \min(M, \mathrm{rank}(B))$,

$$q(x^k) - q^* \leq 4 \left(\frac{\sqrt{\kappa(B)} - 1}{\sqrt{\kappa(B)} + 1} \right)^{2k} \left(q(x^0) - q^* \right).$$

By the definition of p^k and Lemma 2.1, we have

$$\|p^k\|^2 \leq 2\|B\|(q(x^k) - q^*), \qquad q(x^0) - q^* \leq \|B^+\|\|p^0\|^2/2.$$

Using these relations, we obtain that

$$\|p^k\|^2 \leq 4\kappa(B) \left(\frac{\sqrt{\kappa(B)} - 1}{\sqrt{\kappa(B)} + 1} \right)^{2k} \|p^0\|^2.$$

In view of this and Theorem A.2 (i), one can easily conclude that the PCG method must terminate at x^k satisfying $\|p^k\|_\infty \leq \epsilon$ for some $0 \leq k \leq \min(M, \mathrm{rank}(B))$. This contradict the above supposition.

(ii) Assume that problem (3.2) is unbounded. Suppose for contradiction that Subroutine 1 does not terminate in $\mathrm{rank}(B) + 1$ iterations. Then the iterates x^k, $k = 1, \ldots, \mathrm{rank}(B) + 1$, of Subroutine 1 are identical to those generated by the PCG method applied to problem (3.2). By Theorem A.2 (ii), there must exist some $0 \leq i \leq \mathrm{rank}(B) + 1$ such that $q(x^i + \alpha d^i) \to -\infty$ as $\alpha \to \infty$. Recall that x^l is in Ω and problem (3.1) has at least an optimal solution. Thus there exists a least $\alpha \geq 0$ such that $x^{i+1} = x^i + \alpha d^i$ lies on the boundary of Ω and Subroutine 1 thus terminates at iteration i, which is a contradiction to the above supposition. ∎

Remark 2: It follows from Theorem 3.1 that when $\epsilon = 0$, TPCG1 executes at most (but possibly much less than) $n + 1$ PCG iterations. On the other hand, when $\epsilon > 0$, the number of PCG iterations executed in TPCG1 depends on ϵ in $O(\log(1/\epsilon))$.

As seen from step 3) of Subroutine 1, it immediately terminates once an iterate crosses the boundary of Ω. In this case, the output y may be a rather poor approximate solution to problem (3.1). In order to improve the quality of y, we resort an active set approach by iteratively applying Subroutine 1 to minimize q over a decremental subset of Ω, which is formed by incorporating the active constraints of the iterate obtained from the immediately preceding execution of Subroutine 1. Let x^0 be an arbitrary feasible point of problem (3.1) and $\epsilon \geq 0$ be given. We now present this improved TPCG method for problem (3.1) as follows.

Subroutine 2: $y = \mathrm{TPCG2}(A, b, c, J_0, J_-, J_+, x^0, \epsilon)$

Input: A, b, c, J_0, J_-, J_+, x^0, ϵ.

Set $\mathcal{H}_0 = \{x \in \Re^n : x_j = 0, \ j \in J_0\}$, $J_0^0 = J_0$, $J_-^0 = J_-$, $J_+^0 = J_+$, $k = 0$.

Repeat

    1) If $\|\mathcal{P}_{\mathcal{H}_k}(Ax^k - b + c)\|_\infty \leq \epsilon$, return $y = x^k$ and terminate.

    2) $x^{k+1} = \mathrm{TPCG1}(A, b, c, J_0^k, J_-^k, J_+^k, x^k, \epsilon)$.

    3) $J_0^{k+1} = I_0(x^{k+1})$, $J_-^{k+1} = I_-(x^{k+1})$, $J_+^{k+1} = I_+(x^{k+1})$, $\mathcal{H}_{k+1} = \mathcal{H}(x^{k+1})$.

    4) $k \leftarrow k + 1$.

Output: y.

We next show that under some suitable assumptions, Subroutine 2 terminates in a finite number of iterations.

Theorem 3.2 *Assume that problem (3.1) has at least an optimal solution. Let $\mathcal{H}_0 = \{x \in \Re^n : x_j = 0, \ j \in J_0\}$ and Ω be the feasible region of problem (3.1). Suppose that x^0 is a feasible point (3.1) and $\epsilon \geq 0$. Then the following statements hold:*

(i) Subroutine 2 is well defined.

(ii) Subroutine 2 terminates in at most $n + 1 - |J_0|$ iterations. Moreover, its output y satisfies $y \in \Omega$ and $\|\mathcal{P}_{\mathcal{H}(y)}(Ay - b + c)\|_\infty \leq \epsilon$, where $\mathcal{H}(\cdot)$ is defined in (1.8).

(iii) Suppose additionally that $\|\mathcal{P}_{\mathcal{H}_0}(Ax^0 - b + c)\|_\infty > \epsilon$ and $x^0 - \alpha \mathcal{P}_{\mathcal{H}_0}(Ax^0 - b + c) \in \Omega$ for sufficiently small $\alpha > 0$. Then $q(y) < q(x^0)$, where q is defined in (3.1).

Proof. (i) Observe that in step 2) of Subroutine 2, Subroutine 1 (namely, TPCG1) is applied to the problem

$$
\begin{aligned}
\min_x \quad & q(x) \\
\text{s.t.} \quad & x_j = 0, \quad j \in J_0^k, \\
& x_j \leq 0, \quad j \in J_-^k, \\
& x_j \geq 0, \quad j \in J_+^k,
\end{aligned}
\tag{3.3}
$$

where q is defined in (3.1). Let Ω_k denote the feasible region of (3.3). In view of the updating scheme of Subroutine 2 and the definitions of J_0^k, J_-^k and J_+^k, it is not hard to observe that $\emptyset \neq \Omega_k \subseteq \Omega$. By the assumption that (3.1) has at least an optimal solution, so does (3.3). It then follows from Theorem 3.1 that x^{k+1} shall be successfully generated by Subroutine 1. Using this observation and an inductive argument, we can conclude that Subroutine 2 is well defined.

(ii) Suppose for contradiction that Subroutine 2 does not terminate in $K = n + 1 - |J_0|$ iterations. Then $\|\mathcal{P}_{\mathcal{H}_{k+1}}(Ax^{k+1} - b + c)\|_\infty > \epsilon$ for all $0 \leq k \leq K$. Since $\{x^k\}_{k=0}^K$ are generated by Subroutine 1, one can observe that $I_0(x^k) \subseteq I_0(x^{k+1})$ and hence $\mathcal{H}_k \supseteq \mathcal{H}_{k+1}$ for every $0 \leq k \leq K$. It then follows from these and the definition of $\mathcal{H}(\cdot)$ that for all $0 \leq k \leq K$,

$$\|\mathcal{P}_{\mathcal{H}_k}(Ax^{k+1} - b + c)\|_\infty \geq \|\mathcal{P}_{\mathcal{H}_{k+1}}(Ax^{k+1} - b + c)\|_\infty > \epsilon.$$

This implies that when Subroutine 1 is applied to (3.3), it terminates at a boundary point x^{k+1} of the feasible region of (3.3). It then follows that

$$I_0(x^0) \subsetneq I_0(x^1) \subsetneq \cdots \subsetneq I_0(x^K).$$

Thus $\{|I_0(x^k)|\}_{k=0}^K$ is strictly increasing, which along with $K = n + 1 - |J_0|$ and $|I_0(x^0)| \geq |J_0|$ leads to $|I_0(x^K)| \geq n + 1$. This contradicts the trivial fact $|I_0(x^K)| \leq n$. Therefore, Subroutine 2 must terminate at some y in at most $n + 1 - |J_0|$ iterations. Clearly, $y \in \Omega$. We now prove $\|\mathcal{P}_{\mathcal{H}(y)}(Ay - b + c)\|_\infty \leq \epsilon$ by considering two separate cases as follows.

Case 1): $\|\mathcal{P}_{\mathcal{H}_0}(Ax^0 - b + c)\|_\infty \leq \epsilon$. In this case, Subroutine 2 terminates at $k = 0$ and outputs $y = x^0$. By $x^0 \in \Omega$ and the definition of $\mathcal{H}(\cdot)$, one can see that $\mathcal{H}(x^0) \subseteq \mathcal{H}_0$ and hence

$$\|\mathcal{P}_{\mathcal{H}(x^0)}(Ax^0 - b + c)\|_\infty \leq \|\mathcal{P}_{\mathcal{H}_0}(Ax^0 - b + c)\|_\infty \leq \epsilon,$$

which together with $y = x^0$ implies $\|\mathcal{P}_{\mathcal{H}(y)}(Ay - b + c)\|_\infty \leq \epsilon$.

Case 2): $\|\mathcal{P}_{\mathcal{H}_0}(Ax^0 - b + c)\|_\infty > \epsilon$. In this case, Subroutine 2 must terminate at some iteration $k \geq 1$. It then follows that $\|\mathcal{P}_{\mathcal{H}_k}(Ax^k - b + c)\|_\infty \leq \epsilon$ and $y = x^k$. In addition, we observe from the definitions of $\mathcal{H}(\cdot)$ and $\mathcal{H}_k$ that $\mathcal{H}(x^k) = \mathcal{H}_k$ for $k \geq 1$. It then immediately follows that $\|\mathcal{P}_{\mathcal{H}(y)}(Ay - b + c)\|_\infty \leq \epsilon$.

(iii) We now prove statement (iii). Since $\|\mathcal{P}_{\mathcal{H}_0}(Ax^0 - b + c)\|_\infty > \epsilon$, x^1 must be generated by calling the subroutine $\text{TPCG1}(A, b, c, J_0, x^0, \epsilon)$, whose first iteration performs a projected gradient step to find a point $x(\alpha^*)$, where

$$\alpha^* = \arg\min_{\alpha \geq 0}\{q(x(\alpha)) : x(\alpha) \in \Omega\},$$

and $x(\alpha) = x^0 - \alpha \mathcal{P}_{\mathcal{H}_0}(\nabla q(x^0)) = x^0 - \alpha \mathcal{P}_{\mathcal{H}_0}(Ax^0 - b + c)$. By the assumption that $x^0 - \alpha \mathcal{P}_{\mathcal{H}_0}(Ax^0 - b + c) \in \Omega$ for sufficiently small $\alpha > 0$, one can see that $\alpha^* > 0$ and $q(x(\alpha^*)) < q(x^0)$. We also observe that the value of q is non-increasing along the subsequent iterates of the subroutine $\text{TPCG1}(A, b, c, J_0, x^0, \epsilon)$. These observations and the definition of x^1 imply that $q(x^1) < q(x^0)$. In addition, q is non-increasing along the iterates generated in Subroutine 1. Hence, $q(x^{k+1}) \leq q(x^k)$ for all $k \geq 1$. It then follows $q(x^k) < q(x^0)$ for all $k \geq 1$. Notice that $y = x^k$ for some $k \geq 1$. Hence, $q(y) < q(x^0)$. ∎

Remark 3: As seen from Theorem 3.2, the subroutine TPCG1 is executed in TPCG2 at most (but possibly much less than) $n + 1$ times. In view of this and Remark 2, one can see that when $\epsilon = 0$, the number of PCG iterations executed in TPCG2 is at most $(n+1)^2$. On the other hand, when $\epsilon > 0$, its number of PCG iterations depends on ϵ in $O(\log(1/\epsilon))$.

3.2   The first generalized conjugate gradient method for (1.2)

In this subsection we propose a GCG method for solving problem (1.2). We show that this method terminates at an optimal solution of (1.2) in a finite number of iterations. Before proceeding, we introduce some notations that will be used through the next several subsections.

Given any $x \in \Re^n$, we define

$$
\begin{aligned}
I_0^0(x) &= \{i \in I_0(x) : 0 \in [\nabla_i f(x) - \tau, \nabla_i f(x) + \tau]\}, \\
I_0^+(x) &= \{i \in I_0(x) : \nabla_i f(x) + \tau < 0\}, \\
I_0^-(x) &= \{i \in I_0(x) : \nabla_i f(x) - \tau > 0\},
\end{aligned}
\tag{3.4}
$$

where $I_0(\cdot)$ is given in (1.7). Also, we define $c(\cdot; \tau) : \Re^n \to \{-\tau, 0, \tau\}^n$ as follows:

$$
c_i(x; \tau) = \begin{cases}
\tau & \text{if } i \in I_+(x) \cup I_0^+(x); \\
0 & \text{if } i \in I_0^0(x); \\
-\tau & \text{if } i \in I_-(x) \cup I_0^-(x),
\end{cases}
\quad i = 1, \ldots, n,
\tag{3.5}
$$

where $I_-(\cdot)$ and $I_+(\cdot)$ are defined in (1.7). It then follows from (1.6) and (3.5) that

$$v_i(x) = \nabla_i f(x) + c_i(x; \tau), \quad \forall i \notin I_0^0(x). \tag{3.6}$$

In addition, given any $y \in \Re^n$, we define

$$Q(x; y) = f(x) + c(y; \tau)^T x.$$

The main idea of our GCG method is as follows. Given a current iterate x^k, we check to see whether $v(x^k) = 0$ or not. If yes, then x^k is an optimal solution of (1.2). Otherwise, we find next iterate x^{k+1} by applying Subroutine 2 with initial point x^k and $\epsilon = 0$ to the problem

$$
\begin{aligned}
\min_x \quad & Q(x; x^k) \\
\text{s.t.} \quad & x_j = 0, \quad j \in J_0^k, \\
& x_j \leq 0, \quad j \in J_-^k, \\
& x_j \geq 0, \quad j \in J_+^k,
\end{aligned}
\tag{3.7}
$$

where $J_0^k = I_0^0(x^k)$, $J_-^k = I_-(x^k) \cup I_0^-(x^k)$ and $J_+^k = I_+(x^k) \cup I_0^+(x^k)$. That is, x^{k+1} is obtained by executing the subroutine $\text{TPCG2}(A, b, c^k, J_0^k, J_-^k, J_+^k, x^k, 0)$. As later shown, such x^{k+1} satisfies the following properties:

$$F(x^{k+1}) < F(x^k), \tag{3.8}$$

$$x^{k+1} \in \text{Arg}\min\{F(x) : x_i = 0, \ i \in I_0(x^{k+1})\}.^5 \tag{3.9}$$

By these relations, one can observe that there is no repetition among $\{I_0(x^k) : k \geq 1\}$. Notice that $\{I_0(x) : x \in \Re^n\}$ is a finite set. Thus the method must terminate in a finite number of iterations. Moreover, we will show that it terminates at an optimal solution of (1.2). We now present our GCG method as follows.

GCG method 1 for problem (1.2): $y = \text{GCG1}(A, b, \tau, x^0, \epsilon)$

Input: A, b, τ, x^0, ϵ.

Set $k = 0$.

Repeat

    1) If $\|v(x^k)\|_\infty \leq \epsilon$, return $y = x^k$ and terminate.

    2) $J_0^k = I_0^0(x^k)$, $J_-^k = I_-(x^k) \cup I_0^-(x^k)$, $J_+^k = I_+(x^k) \cup I_0^+(x^k)$, $c^k = c(x^k; \tau)$.

    3) $x^{k+1} = \text{TPCG2}(A, b, c^k, J_0^k, J_-^k, J_+^k, x^k, 0)$.

    4) $k \leftarrow k + 1$.

Output: y.

We next show that the above GCG method terminates in a finite number of iterations, and moreover it finds an optimal solution of problem (1.2) when $\epsilon = 0$.

Theorem 3.3 *Under Assumption 1, the following statements hold:*

    (i) GCG *method 1 terminates in at most $\mathcal{L}(n)$ iterations, where $\mathcal{L}(n)$ is defined in (1.9).*

    (ii) Let y be the output of GCG *method 1. Then $s \in \partial F(y)$ for some s with $\|s\|_\infty \leq \epsilon$, and moreover, y is an optimal solution of problem (1.2) when $\epsilon = 0$.*

Proof. (i) We first show that (3.8) and (3.9) hold at iteration k at which GCG method 1 has not yet terminated, that is, $\|v(x^k)\|_\infty > \epsilon$. Let Ω_k denote the feasible region of problem (3.7). By (3.5) and the definitions of J_0^k, J_-^k and J_+^k, one can observe that $c_i(x^k; \tau)x_i = \tau|x_i|$ for all $x \in \Omega_k$. This along with the definitions of $Q(\cdot; \cdot)$, f and F yields

$$F(x) = Q(x; x^k), \qquad \forall x \in \Omega_k. \tag{3.10}$$

It then follows from Assumption 1 that problem (3.7) is bounded below and hence has at least an optimal solution. By this and Theorem 3.2, x^{k+1} shall be successfully generated in step 3) by the subroutine TPCG2. We next show that x^{k+1} satisfies (3.8) and (3.9). To this end, let

$$\bar{\mathcal{H}} = \{x \in \Re^n : x_i = 0, \ i \in I_0^0(x^k)\}. \tag{3.11}$$

---

    [5]By convention, the symbol Arg stands for the set of the solutions of the associated optimization problem. When this set is known to be a singleton, we use the symbol arg to stand for it instead.

By (3.6), (3.11) and the definition of c^k, we have

$$\mathcal{P}_{\bar{\mathcal{H}}}(Ax^k - b + c^k) = \mathcal{P}_{\bar{\mathcal{H}}}(\nabla f(x^k) + c(x^k; \tau)) = \mathcal{P}_{\bar{\mathcal{H}}}(v(x^k)). \qquad (3.12)$$

Observe from (1.6) and (3.4) that $v_i(x^k) < 0$ if $i \in I_0^+(x^k)$; and $v_i(x^k) > 0$ if $i \in I_0^-(x^k)$. By (3.11), one can see that $[\mathcal{P}_{\bar{\mathcal{H}}}(v(x^k))]_i = 0$ if $i \in I_0^0(x^k)$ and $[\mathcal{P}_{\bar{\mathcal{H}}}(v(x^k))]_i = v_i(x^k)$ otherwise. These imply that $[\mathcal{P}_{\bar{\mathcal{H}}}(v(x^k))]_i = 0$ if $i \in I_0^0(x^k)$; $[\mathcal{P}_{\bar{\mathcal{H}}}(v(x^k))]_i < 0$ if $i \in I_0^+(x^k)$; and $[\mathcal{P}_{\bar{\mathcal{H}}}(v(x^k))]_i > 0$ if $i \in I_0^-(x^k)$. In view of these relations, (3.12) and the definition of Ω_k, one can observe that when $\alpha > 0$ is sufficiently small,

$$x^k - \alpha \mathcal{P}_{\bar{\mathcal{H}}}(Ax^k - b + c^k) = x^k - \alpha \mathcal{P}_{\bar{\mathcal{H}}}(v(x^k)) \in \Omega_k.$$

In addition, we observe that $\|\mathcal{P}_{\bar{\mathcal{H}}}(v(x^k))\|_\infty = \|v(x^k)\|_\infty$, which along with (3.12) and $\|v(x^k)\|_\infty > \epsilon$ yields $\|\mathcal{P}_{\bar{\mathcal{H}}}(Ax^k - b + c^k)\|_\infty > \epsilon$. Recall that x^{k+1} is resulted from the subroutine TPCG2 when applied to problem (3.7) starting at x^k. It then follows from Theorem 3.2 that $x^{k+1} \in \Omega_k$, $\mathcal{P}_{\hat{\mathcal{H}}}(Ax^{k+1} - b + c^k) = 0$ and $Q(x^{k+1}; x^k) < Q(x^k; x^k)$, where

$$\hat{\mathcal{H}} = \{x \in \Re^n : x_i = 0, \ i \in I_0(x^{k+1})\}.$$

In view of (3.10), $Q(x^{k+1}; x^k) < Q(x^k; x^k)$ and $x^k, x^{k+1} \in \Omega_k$, we see that (3.8) holds. In addition, since $x^{k+1} \in \Omega_k$, the nonzero components of x^{k+1} share the same sign as the corresponding ones of x^k. Using this fact, (3.5) and the definition of c^k, one can observe that $c^k = c(x^k; \tau) \in \tau \partial \|x^{k+1}\|_1$, which along with the definition of F implies that $Ax^{k+1} - b + c^k \in \partial F(x^{k+1})$. It then follows from this, $\mathcal{P}_{\hat{\mathcal{H}}}(Ax^{k+1} - b + c^k) = 0$ and $x^{k+1} \in \hat{\mathcal{H}}$ that

$$x^{k+1} \in \text{Arg} \min\{F(x) : x \in \hat{\mathcal{H}}\}.$$

This relation and the definition of $\hat{\mathcal{H}}$ immediately imply that (3.9) holds.

We are now ready to prove that GCG method 1 terminates in at most $\mathcal{L}(n)$ iterations, where $\mathcal{L}(n)$ is defined in (1.9). Suppose for contradiction that it does not terminate in $\mathcal{L}(n)$ iterations. Then this method generates x^{k+1} satisfying (3.8) and (3.9) for $k = 0, \ldots, \mathcal{L}(n)$. It then follows that for $k = 1, \ldots, \mathcal{L}(n)$,

$$\min\{F(x) : x_i = 0, \ i \in I_0(x^{k+1})\} \ < \ \min\{F(x) : x_i = 0, \ i \in I_0(x^k)\}.$$

This implies $I_0(x^i) \notin \mathcal{I}^*$ and $I_0(x^i) \not\subseteq I_0(x^j)$ for all $i, j = 1, \ldots, \mathcal{L}(n)$ and $j > i$, where $\mathcal{I}^*$ is defined in (1.9). This contradicts the definition of $\mathcal{L}(n)$. Thus the method must terminate in at most $\mathcal{L}(n)$ iterations.

(ii) Since y is the output of GCG method 1, one has $\|v(y)\|_\infty \leq \epsilon$. We also know that $v(y) \in \partial F(y)$. Hence, statement (ii) holds with $s = v(y)$. Clearly, when $\epsilon = 0$, we have $0 \in \partial F(y)$ and thus y is an optimal solution of (1.2). ∎

Remark 4: In view of Theorem 3.3 and Remark 3, one can observe that the number of PCG iterations executed within GCG method 1 is at most $\mathcal{L}(n)(n+1)^2$.

3.3   The second generalized conjugate gradient method for (1.2)

The first GCG method proposed in Subsection 3.2 enjoys a nice theoretical property, that is, it terminates at an optimal solution of problem (1.2) in a finite number of iterations when its input parameter ϵ is set to 0. Nevertheless, as observed from step 3) of that method, PCG is required to solve some associated optimization problems exactly. This is not an issue from a theoretical perspective due to the finite convergence of PCG. It is, however, generally hard to achieve that due to numerical errors. In this subsection we propose a GCG method for (1.2) in which the involved PCG is only required to find an approximate solution of the associated optimization problems, which makes the method more practical. To proceed, we introduce some notations and state several facts as follows.

Let $v(\cdot)$ and $I_0(\cdot)$ be defined in (1.6) and (1.7), respectively. We define the projected minimum-norm subgradient $v^{\mathrm{p}} : \Re^n \to \Re^n$ as follows:

$$(v^{\mathrm{p}}(x))_i = \begin{cases} v_i(x) & \text{if } i \in I_0(x), \\ 0 & \text{otherwise,} \end{cases} \qquad \forall x \in \Re^n, \tag{3.13}$$

which is the projection of $v(x)$ onto the subspace $\{y \in \Re^n : y_i = 0, \; i \notin I_0(x)\}$. As later shown, the direction $-v^{\mathrm{p}}(x)$ is a descent direction for F at x when $v^{\mathrm{p}}(x) \neq 0$. We now assume $v^{\mathrm{p}}(x) \neq 0$. The exact line search starting at x along $-v^{\mathrm{p}}(x)$ can be performed by computing

$$\alpha^* = \arg\min_{\alpha \geq 0} F\left(x - \alpha v^{\mathrm{p}}(x)\right) \tag{3.14}$$

and setting $x^+ = x - \alpha^* v^{\mathrm{p}}(x)$. We can show that α^* has a closed-form expression. Indeed, by virtue of (1.6), (3.4) and (3.13), one can observe that for all $\alpha \geq 0$,

$$x_i - \alpha(v^{\mathrm{p}}(x))_i = \begin{cases} \geq 0 & \text{if } i \in I_0^+(x), \\ \leq 0 & \text{if } i \in I_0^-(x), \\ = x_i & \text{otherwise.} \end{cases}$$

This together with (3.5) implies that

$$\tau \|x - \alpha v^{\mathrm{p}}(x)\|_1 = c(x;\tau)^T (x - \alpha v^{\mathrm{p}}(x)), \qquad \forall \alpha \geq 0.$$

It follows from this and the definitions of F and f that

$$F\left(x - \alpha v^{\mathrm{p}}(x)\right) = f\left(x - \alpha v^{\mathrm{p}}(x)\right) + c(x;\tau)^T (x - \alpha v^{\mathrm{p}}(x)), \qquad \forall \alpha \geq 0. \tag{3.15}$$

Using this relation and (3.14), we obtain that

$$(v^{\mathrm{p}}(x))^T [\nabla f(x - \alpha^* v^{\mathrm{p}}(x)) + c(x;\tau)] = 0. \tag{3.16}$$

Observe from (1.6) and (3.13) that $[v^{\mathrm{p}}(x)]_i = 0$ for every $i \in I_0^0(x)$. This together with (3.6), (3.13), (3.16) and the definition of f implies that

$$\begin{aligned} 0 &= (v^{\mathrm{p}}(x))^T [\nabla f(x) - \alpha^* A v^{\mathrm{p}}(x) + c(x;\tau)] \\ &= (v^{\mathrm{p}}(x))^T [v(x) - \alpha^* A v^{\mathrm{p}}(x)] = \|v^{\mathrm{p}}(x)\|^2 - \alpha^* (v^{\mathrm{p}}(x))^T A v^{\mathrm{p}}(x). \end{aligned}$$

It follows from this and the assumption $v^{\mathrm{p}}(x) \neq 0$ that $(v^{\mathrm{p}}(x))^T A v^{\mathrm{p}}(x) \neq 0$ and hence

$$\alpha^* = \frac{\|v^{\mathrm{p}}(x)\|^2}{(v^{\mathrm{p}}(x))^T A v^{\mathrm{p}}(x)} \geq 0. \tag{3.17}$$

Given $x^0 \in \Re^n$, one knows from Theorem 2.2 that there exists some $\eta > 0$ that may depend on x^0 such that

$$F(x) - F_x^* \leq \frac{\eta}{2\|A\|} \|[v(x)]_{I_0^c(x)}\|^2 \text{ for all } x \text{ with } F(x) \leq F(x^0), \tag{3.18}$$

where F_x^* is defined in (1.8). Especially, when A is symmetric positive definite, one can see from Theorem 2.3 that the above η can be chosen as $\kappa(A)$, where $\kappa(A)$ is defined in (1.4). In general, the actual value of the above η may be unknown. In what follows, we first assume that the η associated with (3.18) is known. For the case where the η is unknown, we can estimate it by executing a try-and-test strategy that will be discussed afterwards.

We next propose the second GCG method for problem (1.2). Unlike the first GCG method that always performs TPCG2 (namely Subroutine 2), each iteration of the method presented below either executes the subroutine TPCG2 or performs the exact line search along the negative projected minimum-norm subgradient of F. Following a similar strategy proposed by Dostal and Schöberl [12] for solving a box-constrained convex QP, we determine which type of step should be taken by comparing the magnitude of some components of the minimum-norm subgradient of F to that of its rest components. In particular, given a current iterate x^k, if

$$\left\|[v(x^k)]_{I_0(x^k)}\right\| > \sqrt{\eta}\left\|[v(x^k)]_{I_0^c(x^k)}\right\|, \tag{3.19}$$

where η is given in (3.18), it indicates that the zero components of x^k are more far from being optimal compared to its nonzero components. It is thus plausible to release some of zero components of x^k by minimizing F along the direction $-v^{\mathrm{p}}(x^k)$ to obtain a new iterate x^{k+1}, that is,

$$x^{k+1} = x^k - \alpha_k v^{\mathrm{p}}(x^k),$$

where α_k is computed by (3.17) with x replaced by x^k. Analogously, if (3.19) is violated at x^k, it is more beneficial to improve the nonzero components of x^k, which can be made by the subroutine TPCG2 to result in x^{k+1}.

Let η be given in (3.18) and $\epsilon \geq 0$. The second GCG method for problem (1.2) is presented in detail as follows.

GCG method 2 for problem (1.2): $y = \mathrm{GCG2}(A, b, \tau, x^0, \eta, \epsilon)$

Input: A, b, τ, x^0, η, ϵ.

Set $k = 0$.

Repeat

  1) If $\|v(x^k)\|_\infty \leq \epsilon$, return $y = x^k$ and terminate.

  2) $J_0^k = I_0^0(x^k)$, $J_-^k = I_-(x^k) \cup I_0^-(x^k)$, $J_+^k = I_+(x^k) \cup I_0^+(x^k)$, $c^k = c(x^k; \tau)$.

  3) If (3.19) holds, do

$$x^{k+1} = x^k - \alpha_k v^{\mathrm{p}}(x^k), \quad \alpha_k = \frac{\|v^{\mathrm{p}}(x^k)\|^2}{(v^{\mathrm{p}}(x^k))^T A v^{\mathrm{p}}(x^k)}; \tag{3.20}$$

  else

$$x^{k+1} = \mathrm{TPCG2}\left(A, b, c^k, J_0^k, J_-^k, J_+^k, x^k, \frac{\epsilon}{\max(\sqrt{n\eta}, 1)}\right). \tag{3.21}$$

  4) $k \leftarrow k + 1$.

Output: y.

Before establishing convergence of GCG method 2, we study two sufficient descent properties of F at x along the direction of $-v^{\mathrm{p}}(x)$.

Lemma 3.1 *Suppose that $x \in \Re^n$ satisfies $v^{\mathrm{p}}(x) \neq 0$. Let $x^+ = x - \alpha^* v^{\mathrm{p}}(x)$, where α^* be defined in (3.17). Then there holds:*

$$F(x^+) = F(x) - \frac{\|v^{\mathrm{p}}(x)\|^4}{2(v^{\mathrm{p}}(x))^T A v^{\mathrm{p}}(x)} \leq F(x) - \frac{\|v^{\mathrm{p}}(x)\|^2}{2\|A\|}. \tag{3.22}$$

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Proof. In view of (3.5), one has $c(x;\tau)^T x = \tau \|x\|_1$ and hence

$$F(x) = f(x) + c(x;\tau)^T x.$$

Using this, (3.14)-(3.16) and the definition of f, we have

$$
\begin{aligned}
F(x) &= f(x) + c(x;\tau)^T x = f(x - \alpha^* v^{\mathrm{p}}(x)) + c(x;\tau)^T(x - \alpha^* v^{\mathrm{p}}(x)) \\
&\quad + \alpha^* (v^{\mathrm{p}}(x))^T [\nabla f(x - \alpha^* v^{\mathrm{p}}(x)) + c(x;\tau)] + \tfrac{1}{2}(\alpha^*)^2 (v^{\mathrm{p}}(x))^T A v^{\mathrm{p}}(x) \\
&= F(x - \alpha^* v^{\mathrm{p}}(x)) + \tfrac{1}{2}(\alpha^*)^2 (v^{\mathrm{p}}(x))^T A v^{\mathrm{p}}(x) \\
&= F(x^+) + \frac{\|v^{\mathrm{p}}(x)\|^4}{2(v^{\mathrm{p}}(x))^T A v^{\mathrm{p}}(x)} \geq F(x^+) + \frac{\|v^{\mathrm{p}}(x)\|^2}{2\|A\|},
\end{aligned}
$$

where the last inequality follows from $z^T A z \leq \|A\| \|z\|^2$ for all $z \in \Re^n$. ∎

Lemma 3.2 *Let η be given in (3.18). Suppose that $x \in \Re^n$ satisfies $F(x) \leq F(x^0)$ and*

$$\left\| [v(x)]_{I_0(x)} \right\| > \sqrt{\eta} \left\| [v(x)]_{I_0^c(x)} \right\|. \tag{3.23}$$

Let F_x^* be defined in (1.8) and $x^+ = x - \alpha^* v^{\mathrm{p}}(x)$, where α^* is defined in (3.17). Then $F(x^+) < F_x^*$.

Proof. Let $J = I_0^c(x)$. It follows from (3.22) and (3.18) that

$$
\begin{aligned}
F(x^+) &\leq F(x) - \frac{\|v^{\mathrm{p}}(x)\|^2}{2\|A\|} \leq F_x^* + \frac{\eta}{2\|A\|} \|(v(x))_J\|^2 - \frac{\|v^{\mathrm{p}}(x)\|^2}{2\|A\|}, \\
&= F_x^* + \frac{\|v^{\mathrm{p}}(x)\|^2}{2\|A\|} \left(\frac{\eta \|(v(x))_J\|^2}{\|v^{\mathrm{p}}(x)\|^2} - 1 \right).
\end{aligned}
$$

The conclusion follows from this inequality, $\|v^{\mathrm{p}}(x)\| = \|[v(x)]_{I_0(x)}\|$ and (3.23). ∎

We next show that GCG method 2 terminates in a finite number of iterations, and moreover it terminates at an optimal solution of problem (1.2) when $\epsilon = 0$.

Theorem 3.4 *Under Assumption 1, the following statements hold:*

(i) GCG *method 2 terminates in at most $2\mathcal{L}(n)$ iterations, where $\mathcal{L}(n)$ is defined in (1.9).*

(ii) *Let y be the output of* GCG *method 2. Then $s \in \partial F(y)$ for some s with $\|s\|_\infty \leq \epsilon$, and moreover, y is an optimal solution of problem (1.2) if $\epsilon = 0$.*

Proof. (i) We first claim that $F(x^{k+1}) \leq F(x^k)$ for all $k \geq 0$. Indeed, x^{k+1} is generated by (3.20) or (3.21). If it is generated by (3.20), it follows from (3.22) that $F(x^{k+1}) \leq F(x^k)$. On the other hand , if x^{k+1} is generated by (3.21), one can observe from the subroutine TPCG2 that $F(x^{k+1}) \leq F(x^k)$.

Secondly, we claim that the number of executions of (3.20) is at most $\mathcal{L}(n)$. Indeed, let

$$\mathcal{K} = \{k : x^{k+1} \text{ is generated by (3.20)}\}.$$

By the updating scheme of GCG method 2, it can be observed that (3.19) holds at x^k for all $k \in \mathcal{K}$. In addition, by the monotonicity of $\{F(x^k)\}$, it is clear that $F(x^k) \leq F(x^0)$ for every $k \in \mathcal{K}$. It then follows from Lemma 3.2 that $F(x^{k+1}) < F_{x^k}^*$ for all $k \in \mathcal{K}$. By (1.8), we know that $F(x^{k+1}) \geq F_{x^{k+1}}^*$. In view of these relations and the monotonicity of $\{F(x^k)\}$, one has $F_{x^{j+1}}^* \leq F(x^j) \leq F(x^{i+1}) < F_{x^{i+1}}^*$ for all $i, j \in \mathcal{K}$ and $j > i$. It follows

from this relation and (1.8) that $I_0(x^{i+1}) \notin \mathcal{I}^*$ and $I_0(x^{i+1}) \not\subseteq I_0(x^{j+1})$ for all $i, j \in \mathcal{K}$ and $j > i$, where $\mathcal{I}^*$ is defined in (1.9). By this and (1.9), we see that $|\mathcal{K}| \leq \mathcal{L}(n)$ and thus this claim holds.

Thirdly, we claim that (3.21) cannot be executed at any two consecutive iterations. Suppose for contradiction that (3.21) is executed at iterations k and $k + 1$ for some $k \geq 0$. By the updating scheme of GCG method 2, we then know that (3.19) does not hold at x^k and x^{k+1}. It follows from (3.21) and Theorem 3.2 that

$$\|\mathcal{P}_{\mathcal{H}(x^{k+1})}(Ax^{k+1} - b + c^k)\|_\infty \leq \frac{\epsilon}{\max(\sqrt{n}\eta, 1)}, \tag{3.24}$$

where $\mathcal{H}(\cdot)$ is defined in (1.8). Observe that all nonzero components of x^{k+1} share the same sign as the corresponding ones of x^k. This together with (3.5) implies that $c_i(x^{k+1}; \tau) = c_i(x^k; \tau) = c_i^k$ for all $i \in I_0^c(x^{k+1})$. Using this fact, (3.6) and the definition of $\mathcal{H}(\cdot)$, we have

$$\|\mathcal{P}_{\mathcal{H}(x^{k+1})}(Ax^{k+1} - b + c^k)\|_\infty = \|\mathcal{P}_{\mathcal{H}(x^{k+1})}(Ax^{k+1} - b + c^{k+1})\|_\infty = \|\mathcal{P}_{\mathcal{H}(x^{k+1})}(v(x^{k+1}))\|_\infty.$$

It follows from this, (3.24) and the definition of $\mathcal{H}(\cdot)$ that

$$\left\| [v(x^{k+1})]_{I_0^c(x^{k+1})} \right\|_\infty \leq \frac{\epsilon}{\max(\sqrt{n}\eta, 1)} \leq \epsilon. \tag{3.25}$$

In view of this and the fact that (3.19) does not hold at $k + 1$, one has

$$\begin{aligned}
\left\| [v(x^{k+1})]_{I_0(x^{k+1})} \right\|_\infty &\leq \left\| [v(x^{k+1})]_{I_0(x^{k+1})} \right\| \leq \sqrt{\eta} \left\| [v(x^{k+1})]_{(I_0(x^{k+1}))^c} \right\|, \\
&\leq \sqrt{n}\eta \left\| [v(x^{k+1})]_{I_0^c(x^{k+1})} \right\|_\infty \leq \frac{\epsilon\sqrt{n}\eta}{\max(\sqrt{n}\eta, 1)} \leq \epsilon.
\end{aligned}$$

This together with (3.25) yields $\|v(x^{K+1})\|_\infty \leq \epsilon$. Hence, GCG method 2 terminates at x^{k+1} and thus (3.21) will not be executed at iteration $k + 1$, which contradicts the above supposition. Therefore, this claim holds.

From the last claim above, one can see that (3.21) is executed at most once between every two adjacent executions of (3.20). In view of this fact, the second claim above and the updating scheme of GCG method 2, we can conclude that it must terminate in at most $2\mathcal{L}(n)$ iterations.

(ii) The proof of the second statement is similar to that of Theorem 3.3. ∎

Remark 5: From the proof of Theorem 3.4, we know that the subroutine TPCG2 is called in GCG2 at most $\mathcal{L}(n)$ times. In view of this and Remark 3, one can observe that when $\epsilon = 0$, the number of PCG iterations executed within GCG method 2 is at most $\mathcal{L}(n)(n + 1)^2$. On the other hand, when $\epsilon > 0$, its number of PCG iterations depends on ϵ in $O(\log(1/\epsilon))$.

The above GCG method is suitable for the case where the η associated with (3.18) is known. From the proof of Theorem 3.4, it can be observed that the error bound (3.18) with a known η ensures that $I_0(x^i)$ is not a subset of $I_0(x^j)$ for all $I^0(x^i), I^0(x^j) \in \mathcal{C}_\eta$ with $j > i$, where

$$\mathcal{C}_\eta = \left\{ I_0(x^k) : x^k \text{ satisfies (3.19) with the given } \eta. \right\}. \tag{3.26}$$

When such η is unknown, we can start with a guess of η, denoted by $\hat{\eta}$. Then we run the subroutine GCG2 with η replaced by $\hat{\eta}$ until some x^k is found with the property: (a) $\|v(x^k)\|_\infty \leq \epsilon$ or (b) x^k satisfies (3.19) with η replaced by $\hat{\eta}$ and $I_0(x^k)$ is a supset of some member in $\mathcal{C}_{\hat{\eta}}$ that was previously generated, where $\mathcal{C}_{\hat{\eta}}$ is defined according to (3.26) by replacing η by $\hat{\eta}$. If (a) occurs, x^k is a desired approximate solution of problem (1.2). On the other hand , if (b) occurs, it follows from the above observation that $\hat{\eta}$ is clearly a wrong guess of η, and we need to increase $\hat{\eta}$ and repeat the above process starting with x^k. These observations lead to the following variant of GCG method 2.

A variant of GCG **method 2 for problem** (1.2): $y = \mathrm{GCG2_v}(A, b, \tau, x^0, \eta_0, \rho, \epsilon)$

Input: A, b, τ, x^0, η_0, $\rho > 1$, ϵ.

Set $k = 0$, $\hat{\eta} = \eta_0$, $\mathcal{C} = \emptyset$.

Repeat

1) If $\|v(x^k)\|_\infty \leq \epsilon$, return $y = x^k$ and terminate.

2) $J_0^k = I_0^0(x^k)$, $J_-^k = I_-(x^k) \cup I_0^-(x^k)$, $J_+^k = I_+(x^k) \cup I_0^+(x^k)$, $c^k = c(x^k; \tau)$.

3) If (3.19) holds with $\eta = \hat{\eta}$, do

   if $\mathcal{C} \neq \emptyset$ and some member in $\mathcal{C}$ is a subset of $I_0(x^k)$, set

$$\hat{\eta} \leftarrow \rho\hat{\eta}, \ \mathcal{C} \leftarrow \emptyset, \ x^{k+1} = x^k; \tag{3.27}$$

   else

$$\mathcal{C} \leftarrow \mathcal{C} \cup \{I_0(x^k)\},$$
$$x^{k+1} = x^k - \alpha_k v^{\mathrm{p}}(x^k), \quad \alpha_k = \frac{\|v^{\mathrm{p}}(x^k)\|^2}{(v^{\mathrm{p}}(x^k))^T A v^{\mathrm{p}}(x^k)}; \tag{3.28}$$

   else

$$x^{k+1} = \mathrm{TPCG2}\left(A, b, c^k, J_0^k, J_-^k, J_+^k, x^k, \frac{\epsilon}{\max(\sqrt{n}\hat{\eta}, 1)}\right). \tag{3.29}$$

4) $k \leftarrow k + 1$.

Output: y.

We now briefly discuss how to choose η_0 for the above method. When the η associated with (3.18) is known, we simply choose $\eta_0 = \eta$. It can be observed from the proof below that the variant of GCG method 2 with such a choice of η_0 is identical to GCG method 2. In addition, when A is symmetric positive definite, we see from Theorem 2.3 that $\eta = \kappa(A)$ satisfies the error bound (3.18). Thus, it is reasonable to choose $\eta_0 = \kappa(A)$ when the η associated with (3.18) is unknown.

We next show that the variant of GCG method 2 terminates in a finite number of iterations, and moreover it terminates at an optimal solution of problem (1.2) when $\epsilon = 0$.

Theorem 3.5 *Under Assumption 1, the following statements hold:*

(i) *The variant of* GCG *method 2 terminates in at most*

$$N = \max\left(\left\lceil \frac{\log \eta^* - \log \eta_0}{\log \rho} \right\rceil + 1, 1\right)(2^{n+1} - 1) \tag{3.30}$$

iterations, where η^* is the smallest η satisfying (3.18).

(ii) *Let y be the output of the variant of* GCG *method 2. Then $s \in \partial F(y)$ for some s with $\|s\|_\infty \leq \epsilon$, and moreover, y is an optimal solution of problem (1.2) if $\epsilon = 0$.*

Proof. (i) Let η^* be the smallest η satisfying (3.18). By the monotonicity of $\{F(x^k)\}$ and a similar argument as in the proof of Theorem 3.4, one can show that if $\hat{\eta} \geq \eta^*$ at some iteration K, then $I_0(x^i) \nsubseteq I_0(x^k)$ for all $I_0(x^i) \in \mathcal{C}$ with $i < k$ and every $k \geq K$ such that (3.19) holds at x^k with $\eta = \hat{\eta}$. Thus $\hat{\eta}$ will no longer be updated for all $k \geq K$. By this fact and the updating scheme of the variant of GCG method 2, it is not hard to show that $\hat{\eta}$ can be updated by (3.27) in at most $\max(\lceil (\log \eta^* - \log \eta_0)/\log \rho \rceil, 0)$ times. Hence, the number of distinct $\hat{\eta}$ arising in this method is at most $\max(\lceil (\log \eta^* - \log \eta_0)/\log \rho \rceil, 0) + 1$. Observe that if (3.19) holds at some x^k, then $I_0(x^k) \neq \emptyset$. In view of this and the updating scheme of $\mathcal{C}$, one can see that if $\mathcal{C} \neq \emptyset$, then all members of $\mathcal{C}$ are distinct nonempty subsets of $\{1, \ldots, n\}$. It follows that for each $\hat{\eta}$, the number of members of $\mathcal{C}$ is at most $2^n - 1$ and hence the number of executions of (3.28) is at most $2^n - 1$. By this fact and a similar argument as in the proof of Theorem 3.4, one can show that for each $\hat{\eta}$, the number of executions of (3.29) is also at most $2^n - 1$. Thus for each $\hat{\eta}$, the total number of executions of (3.27), (3.28) and (3.29) is at most $1 + 2(2^n - 1) = 2^{n+1} - 1$. The conclusion of the first statement immediately follows from these facts.

(ii) The proof of the second statement is similar to that of Theorem 3.3. ∎

Remark 6: From the proof of Theorem 3.5, we know that the subroutine TPCG2 is called in $\mathrm{GCG2}_v$ at most $\max(\lceil (\log \eta^* - \log \eta_0)/\log \rho \rceil + 1, 1)(2^n - 1)$ times. In view of this and Remark 3, one can observe that when $\epsilon = 0$, the number of PCG iterations executed in $\mathrm{GCG2}_v$ is at most $\max(\lceil (\log \eta^* - \log \eta_0)/\log \rho \rceil + 1, 1)(2^n - 1)(n+1)^2$. On the other hand, when $\epsilon > 0$, the number of PCG iterations executed in this method depends on ϵ in $O(\log(1/\epsilon))$.

3.4   The third generalized conjugate gradient method for (1.2)

Notice that the subroutine TPCG2 is used in the variant of GCG method 2. Given that TPCG2 is generally more expensive than the subroutine TPCG1, a natural question is whether one could replace TPCG2 by TPCG1 there. In what follows, we propose a third GCG method by performing such a replacement and also modifying the associated J_0^k, J_-^k and J_+^k accordingly.

GCG method 3 for problem (1.2): $y = \mathrm{GCG3}(A, b, \tau, x^0, \eta_0, \rho, \epsilon)$

Input: A, b, τ, x^0, η_0, $\rho > 1$, ϵ.

Set $k = 0$, $\hat{\eta} = \eta_0$, $\mathcal{C} = \emptyset$.

Repeat

1) If $\|v(x^k)\|_\infty \leq \epsilon$, return $y = x^k$ and terminate.

2) $J_0^k = I_0(x^k)$, $J_-^k = I_-(x^k)$, $J_+^k = I_+(x^k)$, $c^k = c(x^k; \tau)$.

3) If (3.19) holds with $\eta = \hat{\eta}$, do

   if $\mathcal{C} \neq \emptyset$ and some member in $\mathcal{C}$ is a subset of $I_0(x^k)$, set

$$\hat{\eta} \leftarrow \rho\hat{\eta}, \ \mathcal{C} \leftarrow \emptyset, \ x^{k+1} = x^k; \tag{3.31}$$

   else

$$\mathcal{C} \leftarrow \mathcal{C} \cup \{I_0(x^k)\},$$
$$x^{k+1} = x^k - \alpha_k v^{\mathrm{p}}(x^k), \quad \alpha_k = \frac{\|v^{\mathrm{p}}(x^k)\|^2}{(v^{\mathrm{p}}(x^k))^T A v^{\mathrm{p}}(x^k)}; \tag{3.32}$$

   else

$$x^{k+1} = \mathrm{TPCG1}\left(A, b, c^k, J_0^k, J_-^k, J_+^k, x^k, \frac{\epsilon}{\max(\sqrt{n}\hat{\eta}, 1)}\right). \tag{3.33}$$

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4) $k \leftarrow k + 1$.

Output: y.

Remark 7: The parameter η_0 for this method can be chosen similarly as for the variant of GCG method 2. In particular, when the η associated with (3.18) is known, we choose $\eta_0 = \eta$. Otherwise, we can choose $\eta_0 = \kappa(A)$.

We next show that GCG method 3 terminates in a finite number of iterations, and moreover it terminates at an optimal solution of problem (1.2) when $\epsilon = 0$.

Theorem 3.6 *Under Assumption 1, the following statements hold:*

(i) GCG *method 3 terminates in at most*

$$\max\left(\left\lceil \frac{\log \eta^* - \log \eta_0}{\log \rho} \right\rceil + 1, 1\right)(1 + (n+2)(2^n - 1))$$

iterations, where η^* is the smallest η satisfying (3.18).

(ii) *Let y be the output of* GCG *method 3. Then $s \in \partial F(y)$ for some s with $\|s\|_\infty \leq \epsilon$, and moreover, y is an optimal solution of problem (1.2) if $\epsilon = 0$.*

Proof. (i) We first claim that $F(x^{k+1}) \leq F(x^k)$ for all $k \geq 0$. Indeed, if x^{k+1} is generated by (3.31), $F(x^{k+1}) = F(x^k)$. In addition, if x^{k+1} is updated by (3.32), it follows from Lemma 3.1 that $F(x^{k+1}) \leq F(x^k)$. On the other hand , if x^{k+1} is generated by (3.33), one can observe from the subroutine TPCG1 that $F(x^{k+1}) \leq F(x^k)$.

Secondly, we claim that (3.33) cannot be executed at any $n + 2$ consecutive iterations. Suppose for contradiction that (3.33) is executed at iterations $i, i + 1, \ldots, i + n + 1$ iterations for some $i \geq 0$. This along with the updating scheme of GCG method 3 implies that (3.19) with $\eta = \hat{\eta}$ does not hold at these $n + 2$ iterations. We now show that the subroutine TPCG1 executed in (3.33) must terminate at a boundary point x^{k+1} of the feasible region of problem (3.1) with $c = c^k$, $J_0 = J_0^k$, $J_- = J_-^k$ and $J_+ = J_+^k$ for all $i \leq k \leq i+n$. Suppose not. By the termination criteria of TPCG1, there exists some $i \leq k \leq i + n$ such that

$$\|\mathcal{P}_{\mathcal{H}}(Ax^{k+1} - b + c^k)\|_\infty \leq \frac{\epsilon}{\max(\sqrt{n\hat{\eta}}, 1)}, \tag{3.34}$$

where

$$\mathcal{H} = \{x \in \Re^n : x_j = 0, \ j \in J_0^k\}.$$

Observe from the subroutine TPCG1 that for such k, $J_0^k = I_0(x^k) \subseteq I_0(x^{k+1})$ and moreover the nonzero components of x^{k+1} share the same sign as the corresponding ones of x^k, which implies

$$c_i(x^{k+1}; \tau) = c_i(x^k; \tau) = c_i^k, \quad \forall i \notin I_0(x^{k+1}).$$

Using these relations and (3.34), one can have

$$\|\mathcal{P}_{\hat{\mathcal{H}}}(Ax^{k+1} - b + c(x^{k+1}; \tau))\|_\infty \leq \frac{\epsilon}{\max(\sqrt{n\hat{\eta}}, 1)},$$

where

$$\hat{\mathcal{H}} = \{x \in \Re^n : x_i = 0, \ i \in I_0(x^{k+1})\}.$$

It follows from this and (1.6) that

$$\left\| [v(x^{k+1})]_{I_0^c(x^{k+1})} \right\|_\infty \leq \frac{\epsilon}{\max(\sqrt{n}\hat\eta, 1)} \leq \epsilon.$$

In view of this, the fact that (3.19) with $\eta = \hat\eta$ does not hold at x^{k+1}, and a similar argument as in the proof of Theorem 3.4, one can show that $\|[v(x^{k+1})]_{I_0(x^{k+1})}\|_\infty \leq \epsilon$. It then follows that $\|v(x^{k+1})\|_\infty \leq \epsilon$, which implies that GCG method 3 terminates at x^{k+1} and thus (3.33) will no longer be executed at iteration $k + 1$. This contradicts the second supposition above. Therefore, TPCG1 must terminate at a boundary point x^{k+1} of the feasible region of problem (3.1) with $c = c^k$, $J_0 = J_0^k$, $J_- = J_-^k$ and $J_+ = J_+^k$ for all $i \leq k \leq i + n$. This together with the definition of J_0^k, J_-^k and J_+^k implies that $I_0(x^k) \subsetneq I_0(x^{k+1})$ and hence $|I_0(x^k)| < |I_0(x^{k+1})|$ for all $i \leq k \leq i + n$, which leads to $|I_0(x^{i+n+1})| \geq n + 1$ and contradicts the trivial fact $|I_0(x^{i+n+1})| \leq n$. Thus the above claim holds.

From the second claim above, we can see that for each $\hat\eta$, (3.33) is executed at most $n + 1$ times between every two adjacent executions of (3.32). In addition, by the monotonicity of $\{F(x^k)\}$ and a similar argument as in the proof of Theorem 3.4, one can show that for each $\hat\eta$, the number of executions of (3.32) is at most $2^n - 1$. Therefore, for each $\hat\eta$ the number of executions of (3.33) is at most $(n + 1)(2^n - 1)$. It follows that for each $\hat\eta$, the total number of executions of (3.31), (3.32) and (3.33) is at most $1 + (n + 2)(2^n - 1)$. Also, by a similar argument as in the proof of Theorem 3.5, we know that the number of distinct $\hat\eta$ arising in this method is at most $\max(\lceil(\log\eta^* - \log\eta_0)/\log\rho\rceil, 0) + 1$. The conclusion of the first statement immediately follows from these facts.

(ii) The proof of the second statement is similar to that of Theorem 3.3. ∎

Remark 8: From the proof of Theorem 3.6, one knows that the subroutine TPCG1 is called in GCG3 at most $(n + 1)\max(\lceil(\log\eta^* - \log\eta_0)/\log\rho\rceil + 1, 1)(2^n - 1)$ times. In view of this and Remark 2, we can observe that when $\epsilon = 0$, the number of PCG iterations executed in GCG3 is at most $\max(\lceil(\log\eta^* - \log\eta_0)/\log\rho\rceil + 1, 1)(2^n - 1)(n + 1)^2$. On the other hand, when $\epsilon > 0$, its number of PCG iterations depends on ϵ in $O(\log(1/\epsilon))$.

3.5   The fourth generalized conjugate gradient method for (1.2)

In this subsection we propose the fourth GCG method for problem (1.2), which enhances GCG method 3 by incorporating a proximal gradient scheme. In particular, we perform a proximal gradient step over a subspace immediately after executing the subroutine TPCG1, which makes the iterates cross orthants more rapidly and also shrinks some nonzero components of the iterates to zero. This strategy is similar to the one proposed by Dostal and Schöberl [12] for solving a box-constrained convex QP.

GCG **method 4 for problem** (1.2): $y = \mathrm{GCG4}(A, b, \tau, x^0, t, \eta_0, \rho, \xi, \epsilon)$

Input: A, b, τ, x^0, $t \in (0, 2/\|A\|)$, η_0, $\rho > 1$, $0 < \xi < 1$, ϵ.

Set $k = 0$, $\hat\eta = \eta_0$, $\hat\epsilon = \epsilon$, $\mathcal{C} = \emptyset$.

Repeat

1) If $\|v(x^k)\|_\infty \leq \epsilon$, return $y = x^k$ and terminate.

2) $J_0^k = I_0(x^k)$, $J_-^k = I_-(x^k)$, $J_+^k = I_+(x^k)$, $c^k = c(x^k; \tau)$.

3) If (3.19) holds with $\eta = \hat\eta$, do

   set $\hat\epsilon \leftarrow \epsilon$;

if $\mathcal{C} \neq \emptyset$ and some member in $\mathcal{C}$ is a subset of $I_0(x^k)$, set

$$\hat{\eta} \leftarrow \rho\hat{\eta}, \ \mathcal{C} \leftarrow \emptyset, \ x^{k+1} = x^k; \tag{3.35}$$

else

$$\mathcal{C} \leftarrow \mathcal{C} \cup \{I_0(x^k)\}, \tag{3.36}$$

$$x^{k+1} = x^k - \alpha_k v^{\mathrm{P}}(x^k), \quad \alpha_k = \frac{\|v^{\mathrm{P}}(x^k)\|^2}{(v^{\mathrm{P}}(x^k))^T A v^{\mathrm{P}}(x^k)}; \tag{3.37}$$

else

$$y^{k+1} = \mathrm{TPCG1}\left(A, b, c^k, J_0^k, J_-^k, J_+^k, x^k, \frac{\sqrt{(2t^{-1} - \|A\|)\|A\|}}{(t^{-1} + \|A\|)\sqrt{n\hat{\eta}}} \hat{\epsilon}\right), \tag{3.38}$$

$$x^{k+1} = \arg\min\left\{\frac{1}{2}\|x - (y^{k+1} - t(Ay^{k+1} - b))\|^2 + t\tau\|x\|_1 : x \in \mathcal{H}(y^{k+1})\right\}, \tag{3.39}$$

$$\hat{\epsilon} \leftarrow \xi\hat{\epsilon}.$$

4) $k \leftarrow k + 1$.

Output: y.

Remark: (a) When the η associated with (3.18) is known, one can choose $\eta_0 = \eta$. Otherwise, one can choose $\eta_0 = \kappa(A)$.

(b) It is not hard to see that subproblem (3.39) has a closed-form solution, which is given as follows:

$$x_i^{k+1} = \begin{cases} \mathrm{sgn}(a_i)\max(|a_i| - t\tau, 0) & \text{if } i \notin I_0(y^{k+1}), \\ 0 & \text{otherwise,} \end{cases} \quad i = 1, \ldots, n,$$

where $a_i = y_i^{k+1} - t((Ay^{k+1})_i - b_i)$ for $i = 1, \ldots, n$.

We next show that GCG method 4 terminates in a finite number of iterations, and moreover it terminates at an optimal solution of problem (1.2) when $\epsilon = 0$.

Theorem 3.7 *Under Assumption 1, the following statements hold:*

(i) GCG *method 4 terminates in at most*

$$\max\left(\left\lceil \frac{\log \eta^* - \log \eta_0}{\log \rho} \right\rceil + 1, 1\right)(1 + (M + 1)(2^n - 1)),$$

iterations, where η^* is the smallest η satisfying (3.18) *and*

$$M = \max\left(\left\lceil \frac{\max(\log \eta_0 - \log \eta^*, -\log \eta^*)}{2\log \xi} \right\rceil + n + 1, n + 1\right). \tag{3.40}$$

(ii) Let y be the output of GCG *method 4. Then $s \in \partial F(y)$ for some s with $\|s\|_\infty \leq \epsilon$, and moreover, y is an optimal solution of problem* (1.2) *if $\epsilon = 0$.*

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Proof. (i) We first claim that $F(x^{k+1}) \leq F(x^k)$ for all $k \geq 0$. By the same argument as in the proof of Theorem 3.6, one can see that this claim holds if x^{k+1} is generated by (3.35) or (3.36). We now show that it also holds if x^{k+1} is obtained by (3.39). Indeed, by the definition of f, it is not hard to observe that

$$f(x^{k+1}) \leq f(y^{k+1}) + \langle \nabla f(y^{k+1}), x^{k+1} - y^{k+1} \rangle + \frac{\|A\|}{2} \|x^{k+1} - y^{k+1}\|^2. \tag{3.41}$$

In addition, notice that the objective of (3.39) is strongly convex. Then one can see from (3.39) that for all $x \in \mathcal{H}(y^{k+1})$,

$$\frac{1}{2}\|x - (y^{k+1} - t(Ay^{k+1} - b))\|^2 + t\tau\|x\|_1 \geq \frac{1}{2}\|x^{k+1} - (y^{k+1} - t(Ay^{k+1} - b))\|^2$$
$$+ t\tau\|x^{k+1}\|_1 + \frac{1}{2}\|x - x^{k+1}\|^2. \tag{3.42}$$

Substituting $x = y^{k+1}$ into (3.42), using $\nabla f(y^{k+1}) = Ay^{k+1} - b$, and upon some manipulation, one has

$$\langle \nabla f(y^{k+1}), x^{k+1} - y^{k+1} \rangle \leq \tau\|y^{k+1}\|_1 - \tau\|x^{k+1}\|_1 - t^{-1}\|x^{k+1} - y^{k+1}\|^2.$$

Combining this inequality with (3.41) and using the definition of F, we obtain that

$$F(y^{k+1}) \geq F(x^{k+1}) + \frac{1}{2}\left(\frac{2}{t} - \|A\|\right)\|x^{k+1} - y^{k+1}\|^2. \tag{3.43}$$

This together with $t \in (0, 2/\|A\|)$ implies $F(x^{k+1}) \leq F(y^{k+1})$. In addition, one can observe from (3.38) that $F(y^{k+1}) \leq F(x^k)$. It thus follows that $F(x^{k+1}) \leq F(x^k)$.

Secondly, we claim that (3.38) cannot be executed at any $M+1$ consecutive iterations, where M is defined in (3.40). Suppose for contradiction that (3.38) is executed at iterations $i, i+1, \ldots, i+M$ iterations for some $i \geq 0$. This along with the updating scheme of GCG method 4 implies that (3.19) with $\eta = \hat{\eta}$ does not hold at these $M+1$ iterations and thus $\hat{\epsilon}$ is updated at them. By the updating scheme on $\hat{\epsilon}$, it is not hard to verify that $\hat{\epsilon} \leq \min(\sqrt{\eta_0}, 1)\epsilon/\sqrt{\eta^*}$ at the iterations $i + M_1, \ldots, i + M$, where $M_1 = M - (n+1)$. We now show that the subroutine TPCG1 executed in (3.38) must terminate at a boundary point x^{k+1} of the feasible region of problem (3.1) with $c = c^k$, $J_0 = J_0^k$, $J_- = J_-^k$ and $J_+ = J_+^k$ for all $i + M_1 \leq k \leq i + M - 1$. Suppose not. By the termination criteria of TPCG1, there exists some $i + M_1 \leq k \leq i + M - 1$ such that

$$\|\mathcal{P}_{\mathcal{H}}(Ay^{k+1} - b + c^k)\|_\infty \leq \frac{\sqrt{(2t^{-1} - \|A\|)\|A\|}\ \hat{\epsilon}}{(t^{-1} + \|A\|)\sqrt{n\hat{\eta}}}, \tag{3.44}$$

where

$$\mathcal{H} = \{x \in \Re^n : x_j = 0,\ j \in J_0^k\}.$$

Observe from (3.38) that $J_0^k = I_0(x^k) \subseteq I_0(y^{k+1})$ and moreover the nonzero components of y^{k+1} share the same sign as the corresponding ones of x^k, which implies

$$c_i(y^{k+1}; \tau) = c_i(x^k; \tau) = c_i^k, \quad \forall i \notin I_0(y^{k+1}).$$

Using these relations, (3.44) and (1.6), we have

$$\left\|[v(y^{k+1})]_{I_0^c(y^{k+1})}\right\|_\infty = \|\mathcal{P}_{\hat{\mathcal{H}}}(Ay^{k+1} - b + c(y^{k+1}; \tau))\|_\infty \leq \frac{\sqrt{(2t^{-1} - \|A\|)\|A\|}\ \hat{\epsilon}}{(t^{-1} + \|A\|)\sqrt{n\hat{\eta}}}, \tag{3.45}$$

where

$$\hat{\mathcal{H}} = \{x \in \Re^n : x_i = 0,\ i \in I_0(y^{k+1})\}. \tag{3.46}$$

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By the monotonicity of $\{F(x^l)\}$, we know that $F(x^k) \leq F(x^0)$, which along with $F(y^{k+1}) \leq F(x^k)$ implies $F(y^{k+1}) \leq F(x^0)$. Using this relation, (3.18) with $\eta = \eta^*$ and (3.45), we obtain that

$$
\begin{aligned}
F(y^{k+1}) - F^*_{y^{k+1}} & \leq \frac{\eta^*}{2\|A\|} \|[v(x)]_{I_0^c(y^{k+1})}\|^2 \leq \frac{n\eta^*}{2\|A\|} \|[v(x)]_{I_0^c(y^{k+1})}\|_\infty^2 \\
& \leq \frac{\eta^*(2t^{-1} - \|A\|)\hat{\epsilon}^2}{2\hat{\eta}(t^{-1} + \|A\|)^2},
\end{aligned}
\tag{3.47}
$$

where η^* is the smallest η satisfying (3.18). Notice that $I_0(y^{k+1}) \subseteq I_0(x^{k+1})$, which along with (1.8) implies that $F(x^{k+1}) \geq F^*_{y^{k+1}}$. In view of this, (3.43) and (3.47), one has

$$
\frac{1}{2}\left(\frac{2}{t} - \|A\|\right) \|x^{k+1} - y^{k+1}\|^2 \leq F(y^{k+1}) - F(x^{k+1}) \leq F(y^{k+1}) - F^*_{y^{k+1}} \leq \frac{\eta^*(2t^{-1} - \|A\|)\hat{\epsilon}^2}{2\hat{\eta}(t^{-1} + \|A\|)^2}.
$$

It then follows that

$$
\|x^{k+1} - y^{k+1}\| \leq \frac{\hat{\epsilon}\sqrt{\eta^*}}{\sqrt{\hat{\eta}}(t^{-1} + \|A\|)}.
$$

By the first-order optimality condition of (3.39), one has

$$
0 \in \mathcal{P}_{\hat{\mathcal{H}}}(t^{-1}(x^{k+1} - y^{k+1}) + \nabla f(y^{k+1}) + \tau \partial \|x^{k+1}\|_1),
$$

where $\hat{\mathcal{H}}$ is defined in (3.46). It then follows from the last two relations that

$$
\begin{aligned}
\mathrm{dist}(0, \mathcal{P}_{\hat{\mathcal{H}}}(\nabla f(x^{k+1}) + \tau \partial \|x^{k+1}\|_1)) & \leq \|t^{-1}(x^{k+1} - y^{k+1}) + \nabla f(y^{k+1}) - \nabla f(x^{k+1})\| \\
& \leq (t^{-1} + \|A\|)\|x^{k+1} - y^{k+1}\| \leq \hat{\epsilon}\sqrt{\eta^*/\hat{\eta}}.
\end{aligned}
$$

This along with (1.6), (3.46) and $I_0(y^{k+1}) \subseteq I_0(x^{k+1})$ implies that

$$
\left\|[v(x^{k+1})]_{I_0^c(x^{k+1})}\right\| \leq \hat{\epsilon}\sqrt{\eta^*/\hat{\eta}}.
\tag{3.48}
$$

By the above supposition, we know that (3.38) is executed at iteration $k+1$ and hence (3.19) with $\eta = \hat{\eta}$ does not hold at x^{k+1}. In view of this fact and (3.48), we further have

$$
\left\|[v(x^{k+1})]_{I_0(x^{k+1})}\right\| \leq \sqrt{\hat{\eta}}\left\|[v(x^{k+1})]_{I_0^c(x^{k+1})}\right\| \leq \hat{\epsilon}\sqrt{\eta^*}.
\tag{3.49}
$$

As shown above, $\hat{\epsilon} \leq \epsilon \min(\sqrt{\eta_0}, 1)/\sqrt{\eta^*}$ at iteration $k+1$. In view of this, $\hat{\eta} \geq \eta_0$, (3.48) and (3.49), we have $\|v(x^{k+1})\|_\infty \leq \epsilon$, which implies that GCG method 4 terminates at x^{k+1} and thus (3.38) will no longer be executed at iteration $k+1$. This contradicts the second supposition above. Therefore, TPCG1 must terminate at a boundary point x^{k+1} of the feasible region of problem (3.1) with $c = c^k$, $J_0 = J_0^k$, $J_- = J_-^k$ and $J_+ = J_+^k$ for all $i + M_1 \leq k \leq i + M - 1$. This together with the definitions of J_0^k, J_-^k and J_+^k implies that $I_0(x^k) \subsetneq I_0(x^{k+1})$ and hence $|I_0(x^k)| < |I_0(x^{k+1})|$ for all $i + M_1 \leq k \leq i + M - 1$, which leads to $|I_0(x^{i+M})| \geq M - M_1 = n + 1$ and contradicts the trivial fact $|I_0(x^{i+M})| \leq n$. Thus the above claim holds.

From the second claim above, we can see that for each $\hat{\eta}$, (3.38) is executed at most M times between every two adjacent executions of (3.37). By a similar argument as in the proof of Theorem 3.6, we know that for each $\hat{\eta}$, the number of executions of (3.37) is at most $2^n - 1$. Thus, for each $\hat{\eta}$ the number of executions of (3.38) is at most $M(2^n - 1)$. It then follows that for each $\hat{\eta}$, the total number of executions of (3.35), (3.37) and (3.38) is at most $1 + (M + 1)(2^n - 1)$. In addition, by a similar argument as in the proof of Theorem 3.5, we know that the number of distinct $\hat{\eta}$ arising in this method is at most $\max(\lceil(\log \eta^* - \log \eta_0)/\log \rho\rceil, 0) + 1$. The conclusion of the first statement immediately follows from these facts.

(ii) The proof the second statement is similar to that of Theorem 3.3. ∎

Remark 9: From the proof of Theorem 3.7, we know that the subroutine TPCG1 is called in GCG4 at most $M \max(\lceil (\log \eta^* - \log \eta_0)/\log \rho \rceil + 1, 1)(2^n - 1)$ times, where M is defined (3.40). In view of this and Remark 2, one can observe that when $\epsilon = 0$, the number of PCG iterations executed within GCG4 is at most $M \max(\lceil (\log \eta^* - \log \eta_0)/\log \rho \rceil + 1, 1)(2^n - 1)(n + 1)$. On the other hand, when $\epsilon > 0$, its number of PCG iterations depends on ϵ in $O(\log(1/\epsilon))$.

4 The l_1 regularized least squares problem

In this section we consider a special class of problem (1.2) in the form of

$$\bar{F}^* = \min_{x \in \Re^n} \bar{F}(x) := \frac{1}{2}\|\bar{A}x - \bar{b}\|^2 + \tau \|x\|_1, \tag{4.1}$$

which has important applications in compressed sensing and sparse regression. The GCG methods proposed in Section 3 can be suitably applied to solve problem (4.1). As shown in Section 3, these methods are able to find an exact optimal solution of (4.1) within a finite number of iterations when the associated accuracy parameter ϵ is set to 0, assuming no numerical errors. Despite this nice property, in practice it may be more interesting to find an approximate solution for two mains reasons. One is that only a subset of real numbers can be represented precisely in computer and thus the truncation errors generally cannot be avoided. Another reason is that even if an exact optimal solution can be found, it may take many iterations to do that, which can be too expensive for large-scale problems. An approximate solution usually suffices for practical purpose.

Given a tolerance parameter $\delta > 0$, we are interested in applying the GCG methods to find a δ-optimal solution for problem (4.1), that is, a point x_δ such that $\bar{F}(x_\delta) - \bar{F}^* \leq \delta$. Notice that $\bar{F}^*$ is typically unknown. To terminate these methods properly, we need a suitable lower bound on $\bar{F}^*$. In what follows, we derive some lower bounds for $\bar{F}^*$. Before proceeding, we first establish a technical lemma.

Lemma 4.1 *Let x^* be an arbitrary optimal solution of problem (4.1). Then for any $x \in \Re^n$, the following inequalities hold:*

$$\left| \|\bar{A}x - \bar{b}\|^2 - \|\bar{A}x^* - \bar{b}\|^2 \right| \leq 2\left(\sqrt{\bar{F}(x)} + \sqrt{\bar{F}^*} \right) \sqrt{\bar{F}(x) - \bar{F}^*},$$

$$\left| \|x\|_1 - \|x^*\|_1 \right| \leq \frac{1}{\tau}\left[\bar{F}(x) - \bar{F}^* + \left(\sqrt{\bar{F}(x)} + \sqrt{\bar{F}^*} \right) \sqrt{\bar{F}(x) - \bar{F}^*} \right]. \tag{4.2}$$

Proof. One can observe that

$$\bar{F}^* = \min_{x \in \Re^n} \frac{1}{2}\|\bar{A}x - \bar{b}\|^2 + \tau \|x\|_1] = \min_{u \in \mathrm{Range}(\bar{A})} \underbrace{\frac{1}{2}\|u - \bar{b}\|^2 + \tau \min_{\bar{A}x = u} \|x\|_1}_{\phi(u)}. \tag{4.3}$$

Notice that ϕ is strongly convex in u. Hence, the latter problem in (4.3) has a unique optimal solution, denoted by u^*. By the definition of ϕ, one has

$$\bar{F}^* \leq \phi(\bar{A}x^*) = \frac{1}{2}\|\bar{A}x^* - \bar{b}\|^2 + \tau \min_{\bar{A}x = \bar{A}x^*} \|x\|_1 \leq \frac{1}{2}\|\bar{A}x^* - \bar{b}\|^2 + \tau \|x^*\|_1 = \bar{F}^*,$$

which implies $\phi(\bar{A}x^*) = \bar{F}^*$ and hence $u^* = \bar{A}x^*$. In addition, by the strong convexity of ϕ and the first-order optimality condition of (4.3), we obtain that

$$\phi(u) - \bar{F}^* \geq \frac{1}{2}\|u - u^*\|^2, \qquad \forall u \in \mathrm{Range}(\bar{A}).$$

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In view of this relation, the definition of ϕ, and $u^* = \bar{A}x^*$, one has

$$\bar{F}(x) - \bar{F}^* \ \geq \ \phi(\bar{A}x) - \bar{F}^* \ \geq \ \frac{1}{2}\|\bar{A}(x - x^*)\|^2, \qquad \forall x \in \Re^n,$$

which yields

$$\|\bar{A}(x - x^*)\| \leq \sqrt{2(\bar{F}(x) - \bar{F}^*)}. \tag{4.4}$$

Notice from the definition of $\bar{F}$ that

$$\|\bar{A}x^* - \bar{b}\| \ \leq \ \sqrt{2\bar{F}^*}, \quad \|\bar{A}x - \bar{b}\| \ \leq \ \sqrt{2\bar{F}(x)}, \quad \forall x \in \Re^n.$$

Using these relations, (4.4) and the definition of $\bar{F}$, we have

$$
\begin{aligned}
\left|\|\bar{A}x - \bar{b}\|^2 - \|\bar{A}x^* - \bar{b}\|^2\right| \ &\leq \ (\|\bar{A}x - \bar{b}\| + \|\bar{A}x^* - \bar{b}\|)\|\bar{A}(x - x^*)\| \\
&\leq \ 2\left(\sqrt{\bar{F}(x)} + \sqrt{\bar{F}^*}\right)\sqrt{\bar{F}(x) - \bar{F}^*}, \\
\left|\|x\|_1 - \|x^*\|_1\right| \ &= \ \tfrac{1}{\tau}\left|(\bar{F}(x) - \tfrac{1}{2}\|\bar{A}x - \bar{b}\|^2) - (\bar{F}^* - \tfrac{1}{2}\|\bar{A}x^* - \bar{b}\|^2)\right|, \\
&\leq \ \tfrac{1}{\tau}\left[\bar{F}(x) - \bar{F}^* + \tfrac{1}{2}\left|\|\bar{A}x - \bar{b}\|^2 - \|\bar{A}x^* - \bar{b}\|^2\right|\right], \\
&\leq \ \tfrac{1}{\tau}\left[\bar{F}(x) - \bar{F}^* + \left(\sqrt{\bar{F}(x)} + \sqrt{\bar{F}^*}\right)\sqrt{\bar{F}(x) - \bar{F}^*}\right].
\end{aligned}
$$

∎

In the following propositions we derive two computable lower bounds for $\bar{F}^*$.

Proposition 4.1 *Let $\{x^k\}$ be a sequence of approximate solutions to problem (4.1), and let*

$$\bar{F}_{\mathrm{low}_1}(x^k) := \bar{F}(x^k) - \langle\bar{A}^T(\bar{A}x^k - \bar{b}), x^k\rangle - \tau\|x^k\|_1 + \min\left(1 - \frac{\|\bar{A}^T(\bar{A}x^k - \bar{b})\|_\infty}{\tau}, 0\right)\bar{F}(x^k), \tag{4.5}$$

where $\langle\cdot,\cdot\rangle$ denotes the inner product of two associated vectors. Then the following statements hold:

(i) $\bar{F}^* \geq \bar{F}_{\mathrm{low}_1}(x^k)$ for all k;

(ii) If $\bar{F}(x^k) \to \bar{F}^*$, then $\bar{F}_{\mathrm{low}_1}(x^k) \to \bar{F}^*$.

Proof. Let x^* be an arbitrary optimal solution of (4.1).
(i) Using the definition of $\bar{F}$, we have

$$\tau\|x^*\|_1 \leq \bar{F}(x^*) \leq \bar{F}(x^k),$$

which implies

$$\|x^*\|_1 \leq \tau^{-1}\bar{F}(x^k), \qquad \forall k. \tag{4.6}$$

It then follows that $x^* \in \Delta_k := \{x \in \Re^n : \|x\|_1 \leq \tau^{-1}\bar{F}(x^k)\}$. By the convexity of $\|\bar{A}\cdot -\bar{b}\|^2/2$, one has

$$\bar{F}(x) = \frac{1}{2}\|\bar{A}x - \bar{b}\|^2 + \tau\|x\|_1 \ \geq \ \frac{1}{2}\|\bar{A}x^k - \bar{b}\|^2 + \langle\bar{A}^T(\bar{A}x^k - \bar{b}), x - x^k\rangle + \tau\|x\|_1,$$

Using this and the fact $x^* \in \Delta_k$, we have

$$
\begin{aligned}
\bar{F}^* &= \min_{x \in \Delta_k} \bar{F}(x) \geq \min_{x \in \Delta_k} \left\{ \tfrac{1}{2} \|\bar{A}x^k - \bar{b}\|^2 + \langle \bar{A}^T(\bar{A}x^k - \bar{b}), x - x^k \rangle + \tau \|x\|_1 \right\}, \\
&= \tfrac{1}{2} \|\bar{A}x^k - \bar{b}\|^2 - \langle \bar{A}^T(\bar{A}x^k - \bar{b}), x^k \rangle + \min_{x \in \Delta_k} \left\{ \langle \bar{A}^T(\bar{A}x^k - \bar{b}), x \rangle + \tau \|x\|_1 \right\}, \\
&= \bar{F}(x^k) - \langle \bar{A}^T(\bar{A}x^k - \bar{b}), x^k \rangle - \tau \|x^k\|_1 + \min_{x \in \Delta_k} \left\{ \langle \bar{A}^T(\bar{A}x^k - \bar{b}), x \rangle + \tau \|x\|_1 \right\}, \\
&= \bar{F}(x^k) - \langle \bar{A}^T(\bar{A}x^k - \bar{b}), x^k \rangle - \tau \|x^k\|_1 + \min\left(1 - \tfrac{\|\bar{A}^T(\bar{A}x^k - \bar{b})\|_\infty}{\tau}, 0\right) \bar{F}(x^k),
\end{aligned}
$$

which together with (4.5) implies that statement (i) holds.

(ii) Suppose $\bar{F}(x^k) \to \bar{F}^*$. Recall that x^* is an optimal solution of (4.1). By the first optimality condition of (4.1) at x^*, one has

$$
0 \in \bar{A}^T(\bar{A}x^* - \bar{b}) + \tau \partial \|x^*\|_1 \tag{4.7}
$$

and hence $\|\bar{A}^T(\bar{A}x^* - \bar{b})\|_\infty \leq \tau$. In view of (4.4) and the assumption $\bar{F}(x^k) \to \bar{F}^*$, we have $\|\bar{A}(x^k - x^*)\| \to 0$ and hence $\bar{A}x^k \to \bar{A}x^*$, which implies

$$
\langle \bar{A}^T(\bar{A}x^k - \bar{b}), x^k \rangle = \langle \bar{A}x^k - \bar{b}, \bar{A}x^k \rangle \to \langle \bar{A}x^* - \bar{b}, \bar{A}x^* \rangle = \langle \bar{A}^T(\bar{A}x^* - \bar{b}), x^* \rangle, \tag{4.8}
$$

$$
\min\left(1 - \frac{\|\bar{A}^T(\bar{A}x^k - \bar{b})\|_\infty}{\tau}, 0\right) \to \min\left(1 - \frac{\|\bar{A}^T(\bar{A}x^* - \bar{b})\|_\infty}{\tau}, 0\right) = 0, \tag{4.9}
$$

where the last equality is due to $\|\bar{A}^T(\bar{A}x^* - \bar{b})\|_\infty \leq \tau$. In addition, by the the assumption $\bar{F}(x^k) \to \bar{F}^*$ and (4.2), we have $\|x^k\|_1 \to \|x^*\|_1$. Also, by (4.7), one can observe that x^* is an optimal solution to the problem

$$
\min_x \langle \bar{A}^T(\bar{A}x^* - \bar{b}), x \rangle + \tau \|x\|_1.
$$

Notice that the objective of this problem is positive homogeneous. Hence, its optimal value is 0. It then follows that

$$
\langle \bar{A}^T(\bar{A}x^* - \bar{b}), x^* \rangle + \tau \|x^*\|_1 = 0.
$$

Using this relation, $\bar{F}(x^k) \to \bar{F}^*$, $\|x^k\|_1 \to \|x^*\|_1$, (4.8), (4.9) and taking limits on both sides of (4.5), we have $\bar{F}_{\text{low}_1}(x^k) \to \bar{F}^*$. $\blacksquare$

As seen from Proposition 4.1, $\bar{F}_{\text{low}_1}(x^k)$ is a suitable lower bound for $\bar{F}^*$. We next derive another lower bound.

Proposition 4.2 *(i) Let $\{x^k\}$ be a sequence of approximate solutions to problem (4.1), v be defined in (1.6) with $f(x) = \|\bar{A}x - \bar{b}\|^2/2$, and let*

$$
\bar{F}_{\text{low}_2}(x^k) := \bar{F}(x^k)(1 - \tau^{-1}\|v(x^k)\|_\infty) - \langle v(x^k), x^k \rangle. \tag{4.10}
$$

The following statements hold:

(i) $\bar{F}^* \geq \bar{F}_{\text{low}_2}(x^k)$ for all k.

(ii) If $\{x^k\}$ is bounded and $v(x^k) \to 0$, then $\bar{F}_{\text{low}_2}(x^k) \to \bar{F}^*$.

Proof. (i) Let x^* be an arbitrary optimal solution of (4.1). In view of (1.6), one knows that $v(x^k) \in \partial \bar{F}(x^k)$. Using this relation and (4.6), we obtain that

$$
\begin{aligned}
\bar{F}^* &= \bar{F}(x^*) \geq \bar{F}(x^k) + \langle v(x^k), x^* - x^k \rangle = \bar{F}(x^k) - \langle v(x^k), x^k \rangle + \langle v(x^k), x^* \rangle \\
&\geq \bar{F}(x^k) - \langle v(x^k), x^k \rangle - \|v(x^k)\|_\infty \|x^*\| \geq \bar{F}(x^k)(1 - \tau^{-1}\|v(x^k)\|_\infty) - \langle v(x^k), x^k \rangle,
\end{aligned}
$$

and hence statement (i) holds.

(ii) Assume that $\{x^k\}$ is bounded and $v(x^k) \to 0$. Then $\{\bar{F}(x^k)\}$ is bounded. It follows from this and Lemma 2.3 with $F = \bar{F}$ and $F^* = \bar{F}^*$ that there exists some $\eta > 0$ such that $\bar{F}(x^k) - \bar{F}^* \leq \eta \|v(x^k)\|$ for all k. This along with $v(x^k) \to 0$ and the definition of $\bar{F}^*$ implies $\bar{F}(x^k) \to \bar{F}^*$. The conclusion of this statement immediately follows from this relation, (4.10), $v(x^k) \to 0$ and the boundedness of $\{x^k\}$. ∎

We next propose a practical termination criterion for the GCG methods by using the above two lower bounds on $\bar{F}^*$. This criterion may also be useful for any other methods for solving problem (4.1).

Theorem 4.1 *Let x^0 be an arbitrary initial point for the* GCG *methods. Given any $\delta \geq 0$, let*

$$
\epsilon = \tau \delta / (2 \bar{F}(x^0)). \tag{4.11}
$$

Let $\{x^k\}$ be the sequence generated by the GCG *methods applied to problem (4.1) starting at x^0 with the above ϵ as the input accuracy parameter. Suppose that these methods are terminated once $\|v(x^k)\|_\infty \leq \epsilon$ or*

$$
\bar{F}(x^k) - \max(\bar{F}_{\mathrm{low}_1}(x^k), \bar{F}_{\mathrm{low}_2}(x^k)) \leq \delta \tag{4.12}
$$

holds. Then the GCG *methods terminate within a finite number of iterations at a δ-optimal solution x^k of (4.1), that is, $\bar{F}(x^k) - \bar{F}^* \leq \delta$.*

Proof. In view of Theorems 3.3-3.7, one can see that at least one of the above termination criteria must be satisfied at some iteration k. Also, one can observe that $\bar{F}(x^k) \leq \bar{F}(x^0)$. We next show that $\bar{F}(x^k) - \bar{F}^* \leq \delta$ holds by considering two cases.

Case 1): $\|v(x^k)\|_\infty \leq \epsilon$ holds. By the definition of $\bar{F}$, one has $\tau \|x^k\|_1 \leq \bar{F}(x^k)$, which yields $\|x^k\|_1 \leq \tau^{-1} \bar{F}(x^k)$. Using this relation and (4.10), we obtain that

$$
\bar{F}_{\mathrm{low}_2}(x^k) \geq \bar{F}(x^k)(1 - \tau^{-1}\|v(x^k)\|_\infty) - \|v(x^k)\|_\infty \|x^k\|_1 \geq \bar{F}(x^k)(1 - 2\tau^{-1}\|v(x^k)\|_\infty).
$$

It follows from this, $\bar{F}^* \geq \bar{F}_{\mathrm{low}_2}(x^k)$, $\|v(x^k)\|_\infty \leq \epsilon$, $\bar{F}(x^k) \leq \bar{F}(x^0)$ and (4.11) that

$$
\bar{F}(x^k) - \bar{F}^* \leq 2\tau^{-1}\bar{F}(x^k)\|v(x^k)\|_\infty \leq 2\tau^{-1}\bar{F}(x^0)\|v(x^k)\|_\infty \leq 2\tau^{-1}\bar{F}(x^0)\epsilon = \delta.
$$

Case 2): (4.12) holds. It follows from Propositions 4.1 and 4.2 that

$$
\max(\bar{F}_{\mathrm{low}_1}(x^k), \bar{F}_{\mathrm{low}_2}(x^k)) \geq \bar{F}^*,
$$

which together with (4.12) implies $\bar{F}(x^k) - \bar{F}^* \leq \delta$. ∎

5   Numerical results

In this section we conduct numerical experiments to test the performance of the GCG methods proposed in Section 3 and compare them with some closely related methods, which are the fast iterative shrinkage-thresholding algorithm (FISTA) [2] with a constant stepsize $1/L$, the interleaved ISTA-CG method (iiCG) [6],

and the nonmonotone proximal gradient method (NPG) [30] without continuation. It shall be mentioned that four iiCG algorithms were proposed in [6] that differ in the choice of stepsize (fixed or variable) and proximal step (ISTA or reduced ISTA). As observed in our experiment, the iiCG algorithm with the ISTA step and the variable stepsize determined by the subroutine ISTA-BB-LS described in [6] outperforms the others. Therefore, we only include this one in our numerical comparison. In addition, extensive numerical experiments conducted in [6] demonstrate that the iiCG methods are competitive with the other state-of-the-art codes including PSSgb [28], N83 [3], pdNCG [13], SALSA [1], TWIST [4], FPC_AS [15], l1_ls [20] and YALL1 [9]. Therefore, we will not compare our methods with them in this paper.

We choose $x^0 = 0$ as the initial point for all methods and terminate them once the termination criterion (4.12) with some δ is met. It then follows from Theorem 4.1 that the approximate solution obtained by them is a δ-optimal solution of (4.1). For the GCG methods, we set $t = 2/(\|\bar{A}\|^2 + 10^{-4})$, $\eta_0 = \kappa^2(\bar{A})$, $\rho = 10$, $\xi = 0.5$ and $\epsilon = \tau\delta/(2\bar{F}(x^0))$, where τ and $\bar{F}$ are given in (4.1). For FISTA, iiCG and NPG, we choose the same parameters as mentioned in [2, 6, 30] except M. In particular, we set $L = \|\bar{A}\|^2$ (i.e., the Lipschitz constant of the gradient of $\|\bar{A}x - \bar{b}\|^2/2$) for FISTA, $c = 10^{-4}$ and $\xi = 0.005$ for iiCG, and $\sigma = 10^{-2}$, $\alpha_{\max} = 1/\alpha_{\min} = 10^{30}$ and $\eta = 2$ for NPG. For the purpose of comparison of these methods, we do not include the time for evaluating these parameters in the CPU time reported below. The codes of all methods are written in Matlab. All computations are performed by Matlab R2015b running on a Dell Optiplex 9020 personal computer with a 3.40-GHz Intel Core i7-4770 processor and 32 GB of RAM.

In the first experiment we test the performance of the GCG methods, particularly, GCG2$_v$, GCG3 and GCG4 and also compare them with FISTA, iiCG and NPG for solving problem (4.1) in which $\bar{A}$ is well-conditioned, namely, with a small $\kappa(\bar{A})$. We randomly generate $\bar{A} \in \Re^{m \times n}$ and $\bar{b} \in \Re^m$ in the same manner as described in l_1-magic [7]. In particular, given $\sigma > 0$ and positive integers m, n, s with $m < n$ and $s < n$, we first generate a matrix $W \in \Re^{n \times m}$ with entries randomly chosen from a standard normal distribution. We then compute an orthonormal basis, denoted by B, for the range space of W, and set $\bar{A} = B^T$. In addition, we randomly generate a vector $\tilde{x} \in \Re^n$ with only s nonzero components that are ± 1, and generate a vector $v \in \Re^m$ with entries randomly chosen from a standard normal distribution. Finally, we set $\bar{b} = \bar{A}\tilde{x} + \sigma v$. In particular, we choose $\sigma = 10^{-5}$ for all instances. In addition, we set $\tau = 0.1$ for problem (4.1), and $M = 5$ for iiCG and NPG that is the same as in [6, 30].

In Table 1 we present the computational results obtained by those methods based on the termination criterion (4.12) with $\delta = 10^{-2}$. The parameters m, n and s of each instance are listed in the first three columns, respectively. We observe from the experiment that the approximate solutions found by these methods have almost same cardinality and nearly equal objective value. We only report in the rest of columns of Table 1 the average cardinality of their approximate solutions and also the CPU times (in seconds) of each method. From Table 1, one can see that GCG4 consistently outperforms GCG2$_v$ and GCG3 in terms of CPU time. Though GCG4 is slower than FISTA, it is competitive with iiCG and NPG.

We next compare the performance of the aforementioned methods for solving problem (4.1) in which $\bar{A}$ is ill-conditioned, namely, with a large $\kappa(\bar{A})$. The data $\bar{A}$ and $\bar{b}$ are similarly generated as above except that $\bar{A}$ is set to $B^T D$ rather than B^T, where D is an $n \times n$ diagonal matrix whose ith diagonal entry is $\min(i^2, 10^6)$ for all i. In addition, we set $\tau = 1$ for (4.1), and $M = 15$ for iiCG and NPG that generally gives better performance than the other choices of M in this experiment. We present in Table 2 the computational results obtained by those methods based on the termination criterion with $\delta = 10^{-2}$. As in the first experiment, the approximate solutions found by those methods have almost same cardinality and nearly equal objective value. We thus only report the average cardinality of these approximate solutions and also the CPU times (in seconds) of each method. One can see from Table 2 that GCG2$_v$ consistently outperforms the other methods in terms of CPU time and appears to be more favorable for solving problem (4.1) with ill-conditioned $\bar{A}$.

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Table 1: Comparison on the methods for (4.1) with well-conditioned $\bar{A}$

Problem			Cardinality	CPU Time					
m	n	s		GCG2$_\mathrm{v}$	GCG3	GCG4	FISTA	IICG	NPG
120	512	20	24	0.01	0.01	0.01	0.00	0.01	0.01
240	1024	40	56	0.06	0.05	0.03	0.00	0.03	0.02
360	1536	60	77	0.13	0.18	0.07	0.01	0.07	0.07
480	2048	80	113	0.28	0.50	0.17	0.02	0.14	0.14
600	2560	100	137	0.52	1.23	0.26	0.05	0.26	0.24
720	3072	120	155	0.82	2.41	0.46	0.08	0.42	0.34
840	3584	140	188	1.58	3.47	0.57	0.14	0.54	0.47
960	4096	160	212	1.67	5.19	0.73	0.18	0.79	0.65
1080	4608	180	247	2.93	7.17	1.10	0.25	1.03	0.88
1200	5120	200	269	3.10	9.90	1.34	0.32	1.34	1.19

Table 2: Comparison on the methods for (4.1) with ill-conditioned $\bar{A}$

Problem			Cardinality	CPU Time					
m	n	s		GCG2$_\mathrm{v}$	GCG3	GCG4	FISTA	IICG	NPG
120	512	20	36	0.17	0.39	0.23	0.36	0.60	6.23
240	1024	40	57	0.85	2.02	1.22	1.06	2.94	16.88
360	1536	60	77	2.48	6.81	3.35	2.72	3.37	7.02
480	2048	80	114	6.19	22.27	9.66	8.26	11.40	50.74
600	2560	100	140	16.72	45.82	20.63	29.17	32.00	251.68
720	3072	120	154	27.67	89.63	39.82	55.43	86.16	171.91
840	3584	140	186	49.55	148.23	67.83	98.76	201.14	84.37
960	4096	160	212	96.08	233.86	110.54	153.72	298.99	635.62
1080	4608	180	261	159.04	351.05	174.62	230.58	406.29	463.51
1200	5120	200	285	227.87	468.09	272.06	320.31	720.73	6198.07

6   Concluding remarks

In this paper we proposed generalized CG (GCG) methods for solving ℓ_1 regularized convex QP. When the tolerance parameter ϵ is set to 0, our GCG methods terminate at an optimal solution in a finite number of iterations, assuming no numerical errors. We also show that our methods are capable of finding an approximate solution of the problem by allowing some inexactness on the execution of the CG subroutine. Numerical results demonstrate that our methods are very favorable for solving ill-conditioned problems.

It can be observed that the main computation of our GCG methods lies in executing PCG iterations over a sequence of subspaces. Given any $\epsilon > 0$, one can see from Remarks 4-9 that the number of PCG iterations of these methods for finding an approximate solution x satisfying $\|v(x)\| \leq \sqrt{\epsilon}$ depends on ϵ in $O(\log(1/\epsilon))$. It follows from this and Theorem 2.3 that the number of PCG iterations for finding an ϵ-optimal solution by these methods depends on ϵ in $O(\log(1/\epsilon))$. Therefore, the overall operation cost of the GCG methods for finding an ϵ-optimal solution depends on ϵ in $O(\log(1/\epsilon))$, which is superior to the accelerated proximal gradient (APG) method [2, 23] whose operation cost depends on ϵ in $O(1/\sqrt{\epsilon})$. In addition, at each iteration the main computation of APG is on full-dimensional matrix-vector products while that of PCG is on lower-dimensional matrix-vector products.

Our GCG methods can be extended to solve the box-constrained convex QP (1.3) by properly modifying

the definitions of $v(\cdot)$, $v^{\mathrm{p}}(\cdot)$, $I_0(\cdot)$, $I_+(\cdot)$, $I_-(\cdot)$, $I_0^0(\cdot)$, $I_0^+(\cdot)$, $I_0^-(\cdot)$ and also the subroutines TPCG1 and TPCG2. The similar convergence results as in this paper can also be established. Due to the length limitation, such an extension is left in a separate paper.

A   Appendix: The CG method for convex QP

In this appendix we study CG method for solving (possibly not strongly) convex quadratic programming:

$$f^* = \inf_{x \in \Re^n} f(x) := \frac{1}{2} x^T A x - b^T x, \tag{A.1}$$

where $A \in \Re^{n \times n}$ is symmetric positive semidefinite, $b \in \Re^n$ and $f^* \in [-\infty, \infty)$. It is well-known that (A.1) has at least an optimal solution and f^* is finite if $b \in \mathrm{Range}(A)$, and $f^* = -\infty$ otherwise. The standard CG method (e.g., see [24, Chapter 5]) is proposed mainly for the case where A is symmetric positive definite. In order to make the CG method applicable to the general convex QP (A.1), one has to modify the termination criterion of the standard CG method, which is usually in terms of the gradient of the objective of (A.1). The resulting CG method is presented as follows.

CG method for (A.1)**:**

Input: A, b, x^0.

Set $r^0 = Ax^0 - b$, $p^0 = -r^0$, $k = 0$.

while $Ap^k \neq 0$

$$\alpha_k = \frac{\|r^k\|^2}{(p^k)^T A p^k}; \tag{A.2}$$

$$x^{k+1} = x^k + \alpha_k p^k; \tag{A.3}$$
$$r^{k+1} = r^k + \alpha_k A p^k; \tag{A.4}$$

$$\beta_{k+1} = \frac{\|r^{k+1}\|^2}{\|r^k\|^2}; \tag{A.5}$$

$$p^{k+1} = -r^{k+1} + \beta_{k+1} p^k; \tag{A.6}$$
$$k \leftarrow k + 1.$$

end (while)

The convergence of the CG method for (A.1) has been well studied when A is symmetric positive definite (e.g., see [24] and the references therein). Nevertheless, for the case where A is symmetric positive semidefinite, it has only been partially studied in the literature (e.g., see [19, 18, 17]). As a self-contained reference, we next provide a more comprehensive study on the convergence of the CG method for problem (A.1) with A being symmetric positive *semidefinite*.

Theorem A.1 *The following statements hold for the above CG method:*

(i) *The CG method is well defined.*

(ii) *Suppose that the CG method has not yet terminated at the kth iterate, that is, $Ap^k \neq 0$ for some $k \geq 0$. Then the following properties hold:*

$$(r^i)^T r^j = 0, \qquad \text{for } i \neq j, \ i, j = 0, 1, \ldots, k,$$
$$\text{span}\{r^0, r^1, \ldots, r^k\} = \text{span}\{r^0, Ar^0, \ldots, A^k r^0\},$$
$$\text{span}\{p^0, p^1, \ldots, p^k\} = \text{span}\{r^0, Ar^0, \ldots, A^k r^0\}, \tag{A.7}$$
$$(p^i)^T A p^j = 0, \qquad \text{for } i \neq j, \ i, j = 0, 1, \ldots, k, \tag{A.8}$$

where span *denotes the subspace spanned by the associated vectors.*

Proof. (i) We first claim that

$$\text{if } Ap^k \neq 0 \text{ for some } k \geq 0, \text{ then } r^k \neq 0. \tag{A.9}$$

Indeed, since $p^0 = -r^0$, it is clear that $Ap^0 \neq 0$ yields $r^0 \neq 0$. Suppose for contradiction that $Ap^k \neq 0$ for some $k > 0$ but $r^k = 0$. It then follows from (A.5) that $\beta_k = \|r^k\|^2 / \|r^{k-1}\|^2 = 0$. This together with (A.6) and $r^k = 0$ gives $p^k = -r^k + \beta_k p^{k-1} = 0$, which contradicts the assumption $Ap^k \neq 0$ and thus (A.9) holds. In addition, since A is symmetric positive semidefinite, one can see that $(p^k)^T A p^k \neq 0$ if and only if $Ap^k \neq 0$. By this fact, (A.9) and an inductive argument, it is not hard to see that the CG method is well defined.

(ii) The proof of statement (ii) is identical to that of [24, Theorem 5.3]. ∎

The following result shows that the CG method terminates in a finite number of iterations and produces either an optimal solution of (A.1) or a direction along which f is unbounded below.

Theorem A.2 *Let $\ell = \text{rank}(A)$. The following properties hold for the CG method:*

(i) If $b \in \text{Range}(A)$, the CG method terminates at some iteration $0 \leq k \leq \ell$ and x^k is an optimal solution of (A.1);

(ii) If $b \notin \text{Range}(A)$, the CG method terminates at some iteration $0 \leq k \leq \ell + 1$ and $f(x^k + \alpha p^k) \to -\infty$ as $\alpha \to \infty$.

Proof. (i) Assume that $b \in \text{Range}(A)$. Suppose for contradiction that the CG method does not terminate for all $0 \leq k \leq \ell$. It then follows that $Ap^k \neq 0$ and hence $p^k \neq 0$ for every $0 \leq k \leq \ell$. From (A.8) we also know that $\{p^i\}_{i=0}^{\ell}$ are conjugate with respect to A. Thus $\{p^i\}_{i=0}^{\ell}$ are linearly independent. In view of this and (A.7), one can see that the dimension of $\text{span}\{r^0, Ar^0, \ldots, A^\ell r^0\}$ is $\ell + 1$. On the other hand, by the assumption $b \in \text{Range}(A)$, we observe that $r^0 = Ax^0 - b \in \text{Range}(A)$. It yields $\text{span}\{r^0, Ar^0, \ldots, A^\ell r^0\} \subseteq \text{Range}(A)$, which along with $\ell = \text{rank}(A)$ implies that the dimension of $\text{span}\{r^0, Ar^0, \ldots, A^\ell r^0\}$ is at most ℓ. This leads to a contradiction. Thus the CG method terminates at some $0 \leq k \leq \ell$ with $Ap^k = 0$. We next show that x^k is an optimal solution of (A.1). Since (A.1) is a convex problem, it suffices to show $\nabla f(x^k) = 0$. Notice that $r^k = Ax^k - b$, which along with the assumption $b \in \text{Range}(A)$ implies that $r^k = A\xi$ for some vector ξ. By this and $Ap^k = 0$, we have $(r^k)^T p^k = \xi^T A p^k = 0$. Since the exact line search is performed at each iteration of CG, one has $(r^k)^T p^{k-1} = 0$. In addition, it follows from (A.6) that $r^k = -p^k + \beta_k p^{k-1}$. Using these relations, we have $\|r^k\|^2 = (r^k)^T (-p^k + \beta_k p^{k-1}) = 0$. Hence, $\nabla f(x^k) = r^k = 0$ as desired.

(ii) Assume that $b \notin \text{Range}(A)$. Suppose for contradiction that the CG method does not terminate for all $0 \leq k \leq \ell + 1$. By a similar argument as in statement (i), one knows that $\{p^i\}_{i=0}^{\ell+1}$ are linearly independent. Using this and (A.7), we see that the dimension of $\text{span}\{r^0, Ar^0, \ldots, A^{\ell+1} r^0\}$ is $\ell + 2$. In addition, notice that $\text{span}\{r^0, Ar^0, \ldots, A^{\ell+1} r^0\} \subseteq \text{span}\{r^0 \cup \text{Range}(A)\}$. This and $\ell = \text{rank}(A)$ imply that the dimension of $\text{span}\{r^0, Ar^0, \ldots, A^{\ell+1} r^0\}$ is at most $\ell + 1$, which leads to a contradiction. Thus the CG method terminates

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at some $0 \leq k \leq \ell + 1$ with $Ap^k = 0$. It remains to show that $f(x^k + \alpha p^k) \to -\infty$ as $\alpha \to \infty$. By the same argument as above, one has $(r^k)^T p^{k-1} = 0$. Also, by the assumption $b \notin \text{Range}(A)$, we know that $r^k \neq 0$. In addition, notice from (A.6) that $p^k = -r^k + \beta_k p^{k-1}$. It follows from these relations that $(r^k)^T p^k = -\|r^k\|^2 < 0$. In view of this and $Ap^k = 0$, we have

$$f(x^k + \alpha p^k) = f(x^k) + \alpha(r^k)^T p^k + \frac{1}{2}\alpha^2 (p^k)^T Ap^k = f(x^k) + \alpha(r^k)^T p^k \ \to -\infty \text{ as } \alpha \to \infty.$$

■

We next study some further convergence properties of the CG method under the following assumption.

Assumption 2 $b \in \text{Range}(A)$.

This Assumption implies that problem (A.1) has at least an optimal solution and f^* is finite. As shown above, the CG method terminates at an optimal solution of (A.1) in a finite number of iterations. We next show that the convergence of CG may depend on the eigenvalue distribution and a certain condition number of A. To this end, let $\ell = \text{rank}(A)$ and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_\ell > 0$ be all nonzero eigenvalues of A. In addition, let $W \in \Re^{n \times \ell}$ and $V \in \Re^{n \times (n-\ell)}$ such that

$$A = [W \ V]\begin{bmatrix} \hat{A} & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} W^T \\ V^T \end{bmatrix}, \quad [W \ V]^T[W \ V] = I, \quad \hat{A} = \text{diag}(\lambda_1, \ldots, \lambda_\ell),$$

which is a standard eigenvalue decomposition of A. Clearly, $A = W\hat{A}W^T$ and $\hat{A} = W^T AW$. Moreover, it is not hard to observe that

$$A = AWW^T, \qquad WW^T x = x \quad \forall x \in \text{Range}(A). \tag{A.10}$$

Let $\{r^k\}$, $\{p^k\}$ and $\{x^k\}$ be generated by the above CG method. Define

$$\hat{b} = W^T b, \quad \hat{r}^k = W^T r^k, \quad \hat{p}^k = W^T p^k, \quad \hat{x}^k = W^T x^k. \tag{A.11}$$

Lemma A.1 Let $\hat{A}$, $\{\alpha_k\}$, $\{\beta_k\}$, $\{r^k\}$, $\{\hat{r}^k\}$, $\{\hat{x}^k\}$ and $\{\hat{p}^k\}$ be defined above. Under Assumption 2, the following relations hold for any $k \geq 0$ such that $r^k \neq 0$:

(i) $\alpha_k = \frac{\|\hat{r}^k\|^2}{(\hat{p}^k)^T \hat{A} \hat{p}^k}$;

(ii) $\hat{x}^{k+1} = \hat{x}^k + \alpha_k \hat{p}^k$;

(iii) $\hat{r}^{k+1} = \hat{r}^k + \alpha_k \hat{A} \hat{p}^k$;

(iv) $\beta_{k+1} = \frac{\|\hat{r}^{k+1}\|^2}{\|\hat{r}^k\|^2}$;

(v) $\hat{p}^{k+1} = -\hat{r}^{k+1} + \beta_{k+1}\hat{p}^k$.

Proof. We observe from (A.9) and Theorem A.2 (i) that under Assumption 2, $Ap^k \neq 0$ if and only if $r^k \neq 0$. It follows that if $r^k \neq 0$ for some $k \geq 0$, the CG method does not terminate at iteration k and $(\alpha_k, x^{k+1}, r^{k+1}, \beta_{k+1}, p^{k+1})$ must be generated. Thus $\hat{x}^{k+1}$, $\hat{r}^{k+1}$ and $\hat{p}^{k+1}$ are well defined. It is known for the CG method that $r^k = Ax^k - b$, which along with Assumption 2 implies that $r^k \in \text{Range}(A)$. It then follows from (A.10) that $WW^T r^k = r^k$. Using this relation, $A = W\hat{A}W^T$ and (A.11), we have

$$\|\hat{r}^k\|^2 = (W^T r^k)^T (W^T r^k) = (r^k)^T (WW^T r^k) = (r^k)^T r^k = \|r^k\|^2, \tag{A.12}$$

$$(\hat{p}^k)^T \hat{A} \hat{p}^k = (W^T p^k)^T \hat{A}(W^T p^k) = (p^k)^T (W\hat{A}W^T)p^k = (p^k)^T Ap^k,$$

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which together with (A.2) yields statement (i). Pre-multiplying (A.3) by W^T and using (A.11), one can see that statement (ii) holds. In addition, pre-multiplying (A.4) by W^T and using (A.10), (A.11) and $\hat{A} = W^T A W$, we have

$$\hat{r}^{k+1} = W^T r^{k+1} = W^T r^k + \alpha_k W^T A p^k = \hat{r}^k + \alpha_k (W^T A W)(W^T p^k) = \hat{r}^k + \alpha_k \hat{A} \hat{p}^k$$

and thus statement (iii) holds. Statement (iv) follows from (A.5) and (A.12). Finally, statement (v) follows from (A.11) and the pre-multiplication of (A.6) by W^T. ∎

We are now ready to establish some further convergence properties for the CG method for solving problem (A.1).

Theorem A.3 *Let $\{x^k\}$ be generated by the CG method applied to problem (A.1) and $\ell = \mathrm{rank}(A)$. Under Assumption 2, the following properties hold:*

(i) *If A has $\hat{\ell}$ distinct nonzero eigenvalues, the CG method terminates at an optimal solution of problem (A.1) in at most $\hat{\ell}$ iterations;*

(ii) $f(x^k) - f^* \leq \left(\frac{\lambda_k - \lambda_\ell}{\lambda_k + \lambda_\ell} \right)^2 \left(f(x^0) - f^* \right)$ *for all $1 \leq k \leq \ell$;*

(iii) $f(x^k) - f^* \leq 4 \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^{2k} \left(f(x^0) - f^* \right)$ *for all $k \geq 0$, where $\kappa(A)$ is defined in (1.4).*

Proof. Let W, $\hat{A}$, $\hat{b}$, $\{\alpha_k\}$, $\{\hat{x}^k\}$, $\{\hat{r}^k\}$, $\{\beta_k\}$ and $\{\hat{p}^k\}$ be defined above. Recall that for the CG method, $A p^k \neq 0$ if and only if $r^k \neq 0$. This along with (A.12) implies that $A p^k \neq 0$ if and only if $\hat{r}^k \neq 0$. In view of (A.10), (A.11), $\hat{A} = W^T A W$ and $r^0 = A x^0 - b$, one has

$$\hat{r}^0 = W^T r^0 = W^T(A x^0 - b) = W^T(A W W^T x^0 - b) = (W^T A W)W^T x^0 - W^T b = \hat{A}\hat{x}^0 - \hat{b}.$$

Using these and statements (i)-(v) of Lemma A.1, we observe that $\{\alpha_k\}$, $\{\hat{x}^k\}$, $\{\hat{r}^k\}$, $\{\beta_k\}$ and $\{\hat{p}^k\}$ can be viewed as the sequences generated by the CG method applied to the problem

$$\hat{f}^* = \min_{\hat{x} \in \mathcal{R}^\ell} \hat{f}(\hat{x}) := \frac{1}{2}\hat{x}^T \hat{A}\hat{x} - \hat{b}^T \hat{x}. \tag{A.13}$$

Claim that the following relations hold for problems (A.1) and (A.13).

(a) $f(x) = \hat{f}(W^T x)$ for all $x \in \mathcal{R}^n$;

(b) $f(W\hat{x}) = \hat{f}(\hat{x})$ for all $\hat{x} \in \mathcal{R}^\ell$;

(c) $f^* = \hat{f}^*$.

Indeed, since $b \in \mathrm{Range}(A)$, it follows from (A.10) that $W W^T b = b$. Using this, $A = W\hat{A}W^T$ and (A.11), we see that for any $x \in \mathcal{R}^n$,

$$(W^T x)^T \hat{A}(W^T x) = x^T A x, \qquad \hat{b}^T(W^T x) = (b^T W W^T)x = b^T x,$$

which along with the definitions of f and $\hat{f}$ imply that property (a) holds. In addition, by (A.11), $\hat{A} = W^T A W$ and the definitions of f and $\hat{f}$, one has for any $\hat{x} \in \mathcal{R}^\ell$,

$$f(W\hat{x}) = \frac{1}{2}\hat{x}^T(W^T A W)\hat{x} + (W^T b)^T\hat{x} = \frac{1}{2}\hat{x}^T \hat{A}\hat{x} + \hat{b}^T\hat{x} = \hat{f}(\hat{x})$$

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and hence property (b) holds. Combining properties (a) and (b), it is not hard to see that property (c) holds.

Notice that $\hat{A}$ is symmetric positive definite. Thus $\{\hat{x}^k\}$ is the sequence generated by the CG method for solving the strongly convex quadratic program (A.13) with $\hat{x}^0 = W^T x^0$. It follows that the convergence results of the CG method for strongly convex QP, which are presented in [24, Theorems 5.4 and 5.5 and equation (5.36)], hold for $\{\hat{x}^k\}$. Let $\hat{x}^*$ be the unique optimal solution of (A.13). We are now ready to prove statements (i)-(iii) by using this observation and the above properties (a)-(c).

(i) Notice that [24, Theorem 5.4] holds for $\{\hat{x}^k\}$. Then there exists some $0 \leq k \leq \hat{\ell}$ such that $\hat{r}^k = 0$, which along with (A.12) implies $r^k = 0$. It follows that $Ap^k = 0$ and x^k is an optimal solution of (A.1). Hence, the CG method terminates at an optimal solution of (A.1) in at most $\hat{\ell}$ iterations.

(ii) Applying [24, Theorem 5.5] to problem (A.13), one has

$$\|\hat{x}^k - \hat{x}^*\|_{\hat{A}}^2 \leq \left(\frac{\lambda_k - \lambda_\ell}{\lambda_k + \lambda_\ell}\right)^2 \|\hat{x}^0 - \hat{x}^*\|_{\hat{A}}^2, \quad \forall 1 \leq k \leq \ell,$$

where $\|\hat{x}\|_{\hat{A}} = \sqrt{\hat{x}^T \hat{A} \hat{x}}$ for any $\hat{x} \in \Re^\ell$. Observe that $\hat{f}(\hat{x}) - \hat{f}^* = \|\hat{x} - \hat{x}^*\|_{\hat{A}}^2 / 2$ for all $\hat{x}$. It thus follows that

$$\hat{f}(\hat{x}^k) - \hat{f}^* \leq \left(\frac{\lambda_k - \lambda_\ell}{\lambda_k + \lambda_\ell}\right)^2 (\hat{f}(\hat{x}^0) - \hat{f}^*), \quad \forall\, 1 \leq k \leq \ell.$$

The conclusion of this statement follows from this relation, $\hat{x}^k = W^T x^k$ and the above properties (a) and (c).

(iii) Applying [24, equation (5.36)] to problem (A.13), we have

$$\|\hat{x}^k - \hat{x}^*\|_{\hat{A}}^2 \leq 4 \left(\frac{\sqrt{\kappa(\hat{A})} - 1}{\sqrt{\kappa(\hat{A})} + 1}\right)^{2k} \|\hat{x}^0 - \hat{x}^*\|_{\hat{A}}^2, \quad \forall k \geq 0.$$

Notice that A shares the same nonzero eigenvalues with $\hat{A}$. It follows from (1.4) that $\kappa(A) = \kappa(\hat{A})$. The conclusion of this statement then follows from these relations and a similar argument as for statement (ii). ∎

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