Erratum

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The following errors were introduced during the typesetting process. Image panels (g), (h), and (i) of the original figure 4 were mistakenly interchanged. The corrected figure is displayed below.
Figure 4. Visual results. (a) Filtered backprojection. (b) CG, iteration 9. (c) S-CG-2, iteration 50. (d) S-CG, iteration 51. (e) S-CG-CD, iteration 43. (f) S-PCG, iteration 20. (g) S-PCG-2, iteration 13. (h) FISTA, iteration 61. (i) Phantom.
Total variation superiorized conjugate gradient method for image reconstruction

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Abstract
The conjugate gradient (CG) method is commonly used for the relatively-rapid solution of least squares problems. In image reconstruction, the problem can be ill-posed and also contaminated by noise; due to this, approaches such as regularization should be utilized. Total variation (TV) is a useful regularization penalty, frequently utilized in image reconstruction for generating images with sharp edges. When a non-quadratic norm is selected for regularization, as is the case for TV, then it is no longer possible to use CG. Non-linear CG is an alternative, but it does not share the efficiency that CG shows with least squares and methods such as fast iterative shrinkage-thresholding algorithms (FISTA) are preferred for problems with TV norm. A different approach to including prior information is superiorization. In this paper it is shown that the conjugate gradient method can be superiorized. Five different CG variants are proposed, including preconditioned CG. The CG methods superiorized by the total variation norm are presented and their performance in image reconstruction is demonstrated. It is illustrated that some of the proposed variants of the superiorized CG method can produce reconstructions of superior quality to those produced by FISTA and in less computational time, due to the speed of the original CG for least squares problems. In the Appendix we examine the behavior of one of the superiorized CG methods (we call it S-CG); one of its input parameters is a positive number ε. It is proved that, for any given ε that is greater than the half-squared-residual for the least squares solution, S-CG terminates in a finite number of steps with an output for which the half-squared-residual is less than or equal to ε. Importantly, it is also the case that

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the output will have a lower value of TV than what would be provided by unsuperiorized CG for the same value $\varepsilon$ of the half-squared residual.

Keywords: image reconstruction, superiorization, total variation, conjugate gradient

(Some figures may appear in colour only in the online journal)

1. Introduction

Solving least squares problems with linear models has a long history in image reconstruction. The least squares (LS) problem for image reconstruction is stated as: find

$$x_{\text{LS}} = \arg \min_x \frac{1}{2} \| y - Ax \|_2^2,$$

(1)

where $y$ is an $L$-dimensional vector containing the captured data, usually the sinogram in computed tomography (CT), $x$ is a $J$-dimensional vector containing the image to be reconstructed, and $A$ is an $L \times J$ system matrix, used for discrete approximation of the line integrals or the Radon transform in CT.

The LS problem is convex and its solution satisfies the linear system

$$A^T Ax_{\text{LS}} = A^T y.$$

(2)

This is a widely understood approach to the LS problem, with many tools available from linear algebra to solve it or analyze it [1, 2]. LS is also strongly connected to maximum likelihood (ML) estimation for Gaussian noise models [3], which is a well-understood topic from statistics.

Due to the large dimensionality of the problems in image reconstruction, direct solving of (2) is not practical and iterative methods are usually preferred. The conjugate gradient (CG) method [4] is a good choice since it converges very rapidly (just a few iterations often provide acceptable results) and frequently it can use fast computational operators instead of numerical matrices. When the system is ill-conditioned, it is still possible to use preconditioning, getting even faster convergence.

In image reconstruction problems (where $A^T A$ is singular or ill-conditioned and data are noisy) regularization should be utilized. This can be done by adding a penalty to the right hand side of (1) (commonly used penalties are total variation (TV) norm and sparsity promoting norms, such as the $\ell_1$-norm of a transform of $x$; see, for example, [5, 6]). This results in changing (1) to

$$x_{\text{RLS}} = \arg \min_x \left( \frac{1}{2} \| y - Ax \|_2^2 + \lambda R(x) \right),$$

(3)

whose solution satisfies

$$A^T A x_{\text{RLS}} + \lambda \nabla R(x_{\text{RLS}}) = A^T y.$$

(4)

which is a nonlinear system of equations.

One method for solving (4) is nonlinear CG (NLCG), which is a direct generalization of CG for solving nonlinear systems [7, 8]. However, if $R(x)$ is an $\ell_1$-norm or the TV norm, then NLCG may face some issues, such as non-differentiability and the lack of a specific fast line search.
A way of dealing with non-differentiability is to use subgradients [9, chapter 8], but this may put the optimization process into trouble, since the negative of a subgradient is not necessarily a descent direction. This difficulty can be overcome by using a strictly convex approximation that replaces the non-differentiable norm with a differentiable one, such as the Hyperbola function or the Huber norm [10]. For example, if \( R(x) = \|Rx\|_1 \), where \( R \) is an \( n \times J \) matrix and \( \|Rx\|_1 \) is the \( \ell_1 \)-norm of \( Rx \), then \( \nabla R(x) \approx R^TWRx \) for

\[
W = \text{diag} \left( \frac{1}{\sqrt{w_1^2 + \kappa^2}}, \ldots, \frac{1}{\sqrt{w_n^2 + \kappa^2}} \right)
\]

where \( w = (w_1, \ldots, w_n)^T = Rx \) and \( \kappa \) a small positive number. For the lack of a specific line search in NLCG, we note that some alternatives exist when \( \ell_1 \)-norm is used [11], but for other cases general line searches, such as back tracking (which may be costly), has to be used [4]. Such considerations indicate that NLCG is not as good a choice for solving (3) as CG is for solving the least squares problem (1).

For such reasons, other approaches are preferred. One of these is forward-backward splitting [12], which is utilized by the iterative shrinkage-thresholding algorithm (ISTA) [13], TWIST [14] and fast ISTA (FISTA) [15] that are based on proximal operators and Nesterov acceleration. In these approaches, the gradient of only the quadratic part of (3) is utilized and is combined with the proximal operator for the non-differentiable part \( R(x) \). In ISTA, we can write the iterations as

\[
x_{k+1} = \text{prox}_{\lambda c^2} R(x) \left( x_k + \frac{1}{c^2} A^T (y - Ax_k) \right),
\]

where the proximal operator is defined as

\[
\text{prox}_{\mu R(x)}(b) = \arg \min_x \left( \frac{1}{2} \|b - x\|_2^2 + \mu R(x) \right).
\]

The proximal operator has been demonstrated to deal well with the non-differentiability of the \( \ell_1 \)-norm and TV. Proximal operators look like denoising [16], but they are connected with the subdifferential and are known to satisfy (4) at convergence if \( \nabla R(x) \) is a subgradient of \( R(x) \). Proximal operators for some \( R(x) \) are quite simple to implement in practice; for example, the proximal operator of the \( \ell_1 \)-norm can be found by soft-thresholding or shrinkage-thresholding. Other cases, including total variation, are not so easy. For TV, some recent approaches using a dual formulation [17, 18] allow us to use iterative algorithms, such as the gradient projection (GP) and the fast gradient projection (FGP) [19] algorithms as an iterative solution for the proximal operator.

Even though regularization is very commonly used, it is not the only way of including prior information into the solution; a more-recently introduced approach is superiorization [20, 21]. With a similar purpose to Tikhonov regularization [4, 22], superiorization makes use of extra information about the desired image to improve the reconstructed result. However, instead of adding a side penalty to the original optimization problem, superiorization preserves the original iterative algorithm and includes perturbation steps between iterations. These steps shift the solutions obtained along the iterations to a better path of solutions; ones that are superior according to a secondary criterion, while preserving performance according to the original optimization criterion. Published proofs of such behavior assume that the iterative algorithm that is being superiorized has the property of being ‘(strong) perturbation resilient’; see, for example, [20, 21].
Regularization changes an originally ill-posed problem into a different well-posed problem, that may require a new optimization algorithm for solving it. (This was the case when regularizing least squares with sparsity priors.) On the other hand, superiorization is an algorithm-preserving approach, which perturbs the original algorithm towards a better path of intermediate solutions. Considering a general algorithmic step $x_{k+1} = P(x_k)$, superiorization changes it to

$$x_{k+1} = P(x_k + \gamma_k v_k),$$

(8) where $v_k$ is a nonascending direction for $R(x)$ (which might be obtained using gradient, proximal operator or something else) and $\gamma_k$ is a step size that ensures that the next point is superiorized according to the cost provided by the secondary criterion, i.e. $R(x_k + \gamma_k v_k) \leq R(x_k)$. Therefore we do not need an essentially new algorithm, but rather just the inclusion of superiorization steps, which shift the solution of the original algorithm to a better solution at each iteration. When appropriate conditions are satisfied, both regularization and superiorization provide good reconstructed images.

Superiorization has been proven successful in many applications [20, 21, 23–26]. In this paper, superiorization is applied to the conjugate gradient algorithm to solve least squares problems, using the proximity function\(^5\) $f$ that is defined by the half-squared-residual $f(x) = \frac{1}{2} \|y - Ax\|^2_2$ as the primary criterion and total variation as the secondary criterion (see, for example, [21]). Our aim was to keep the good speed of CG, in spite of it being perturbed for superiorization.

It is demonstrated in this paper that there are a number of ways to achieve our aim; we propose five different versions and some of which are very effective. Experimental results illustrate superiorized CG producing reconstructed images of similar quality to those produced by FISTA, but faster.

The paper is organized as follows. Section 2 presents the CG method and an introduction to superiorization. In section 3 the proposed superiorized CG methods are presented. In section 4 the results of some experiments comparing various methods are shown. The conclusions and a discussion are in section 5. A convergence proof of one of the proposed superiorized CG methods is presented in the appendix.

2. Review of methods

The conjugate gradient algorithm (CG) is an effective way of solving (2); its details are provided in algorithms 1 and 2. Several versions of conjugate gradient algorithms for solving (2) have been published since the original version by Hetenes and Stiefel in 1952, some of which are preferred to the original for stability reasons, see [1, 27]. However, our focus is superiorization, which can be illustrated on any variant of the algorithm. In the parameter list of the algorithm CG($A, y, x_0, \epsilon, x$), the input parameters are the matrix $A$ and the vector $y$ (as specified immediately after (1)), the initial guess $x_0$ at the solution (a $J$-dimensional vector), the error $\epsilon$ that we are willing to tolerate according to the primary criterion and the output parameter is $x$, which is an approximation to the desired $x_{LS}$ of (1).

Using $k$ as the iteration counter, CG terminates as soon as $f(x_k) \leq \epsilon$ (recall that $f(x) = \frac{1}{2} \|y - Ax\|^2_2$ is the primary criterion), where $\epsilon$ is a user-specified input parameter.

\(^5\) As defined in the superiorization literature, the proximity function $f$ is a measure of how badly the constraints are violated; it is not to be confused with the proximal operator as defined in (7).
Given the user-specified initial guess \( x_0 \) at the solution, the initial vectors \( g_0 \) and \( p_0 \) in CG are specified as
\[
g_0 = A^T(Ax_0 - y), \quad (9)
\]
\[
p_0 = -g_0. \quad (10)
\]
In each iteration the tentative solution is updated by
\[
x_{k+1} = x_k + \alpha_k p_k, \quad (11)
\]
where \( p_k \) is a search direction with step-size \( \alpha_k \) (defined as \( \alpha \) in Step 2 of algorithm 2). Part of the efficiency of CG is due to the facts that each new search direction is conjugated with all previous directions and the step-size \( \alpha_k \) minimizes the primary criterion with respect to \( \alpha \):
\[
\alpha_k = \arg \min_\alpha f(x_k + \alpha p_k). \quad (12)
\]

The directions are created according to
\[
p_{k+1} = -g_{k+1} + \beta_k p_k \quad (13)
\]
(with \( \beta_k \) defined as \( \beta \) in Step 6 of algorithm 2), where the new gradient is given by
\[
g_{k+1} = A^T(Ax_{k+1} - y), \quad (14)
\]
considering the new point \( x_{k+1} \), or recursively, which is computationally more efficient, by
\[
g_{k+1} = g_k + \alpha_k A^T A p_k. \quad (15)
\]

The computation of the new direction removes part of the previous direction from the gradient; the specified \( \beta_k \) results in
\[
p_{k+1}^T A^T A p_k = (-g_{k+1} + \beta_k p_k)^T A^T A p_k = 0, \quad (16)
\]
which shows that the directions are conjugated.

---

**Algorithm 1.** Standard linear conjugate gradient CG\((A, y, x_0, \varepsilon, x)\).

1: set \( k = 0 \)
2: set \( g_0 = A^T(Ax_0 - y) \)
3: set \( p_0 = -g_0 \)
4: set \( \delta_0 = \|g_0\|^2_2 \)
5: while \( f(x_k) > \varepsilon \)
6: call CG-STEP\((A, x, p, g, \delta, x_{k+1}, p_{k+1}, g_{k+1}, \delta_{k+1})\)
7: set \( k = k + 1 \)
8: set \( x = x_k \)

**Algorithm 2.** CG-STEP\((A, x, p, g, \delta, x', p', g', \delta')\)

1: set \( h = A^T A p \)
2: set \( \alpha = \delta / p^T h \)
3: set \( x' = x + \alpha p \)
4: set \( g' = g + \alpha h \)
5: set \( \delta' = \|g'\|^2_2 \)
6: set \( \beta = \delta'/\delta \)
7: set \( p' = -g' + \beta p \)
In each iteration Step 6 of CG calls CG-STEP(\(A_k, x_k, p_k, g_k, \delta_k, x_{k+1}, p_{k+1}, g_{k+1}, \delta_{k+1}\)), which means that it requires several items from the previous iteration. Thus writing the algorithmic step of CG as \(x_{k+1} = P(x_k)\) is an oversimplification; the vectors \(x_k, g_k, p_k\) depend on all three of \(x_k, g_k, p_k\). This matters when we try to superiorize CG, for the following essential reason: the proof of convergence of the sequence \((x_k)_{k=0}^\infty\) produced by CG to \(x_{LS}\) involves the maintenance, as iterations proceed, of certain mathematical relations involving \(x_k, g_k, p_k\). It is therefore not advisable (for convergence according to the primary criterion) to superiorize by updating \(x_k\) according to (8), without taking care of the matching updates of \(g_k\) and \(p_k\) so that the mathematical relations used in the proof of convergence of the sequence \((x_k)_{k=0}^\infty\) are maintained.

The conjugate gradient method is generally-speaking fast, however its convergence speed can be affected by the conditioning of the matrix \(A^T A\), being slower as the condition number increases [4]. In computed tomography problems, this may mean more iterations and a very long reconstruction time. In order to achieve a good speed of convergence, preconditioned conjugate gradient (PCG) can be a good alternative. In this work we utilize a preconditioning matrix \(M\) constructed from the filtering part of filtered backprojection reconstruction method [28, chapter 8]. Each PCG iteration acts very similarly, but not exactly, to a filtered backprojection reconstruction. In algorithm 3, we describe the standard PCG, which at each iteration calls PCG-STEP(\(A_k, x_k, p_k, g_k, \delta_k, x_{k+1}, p_{k+1}, g_{k+1}, \delta_{k+1}, M\)), as described in algorithm 4.6.

The computation of the new direction in PCG removes part of the previous direction from the gradient.

\[
p_{k+1}^T A^T A p_k = (z_{k+1} + \delta_k p_k)^T A^T A p_k = 0.
\]

In the next section we present five superiorized CG-like algorithms. In the appendix we discuss a proof of convergence for one such algorithm. In section 4 we report on experimental results for all five algorithms and compare such results with what can be obtained by pure CG and also with FISTA, which is one of most efficacious previously-published alternatives to superiorization for solving (4). We devote the rest of this section to a discussion relevant to FISTA.

As indicated in the Introduction, the NLCG approach for solving (4) is based on making use of the gradient \(g_k = A^T (Ax_k - y) + \lambda \nabla R(x_k)\), relying on different options, as seen in [4, 8, 29, 30]. However, for non-differentiable \(R(x_k)\), such as TV or the \(\ell_1\)-norm, the concept of subdifferential needs to be considered [9, chapter 8]. If we substitute any subgradient in the subdifferential for \(\nabla R(x_k)\) in the previous formula for \(g_k\), then \(-g_k\) is not necessarily a descent direction and NLCG may fail to converge.

---

**Algorithm 3.** Standard preconditioned conjugate gradient PCG(\(A, y, x_0, \varepsilon, x, M\)).

1: set \(k = 0\)
2: set \(g_0 = A^T (Ax_0 - y)\)
3: set \(z_0 = M g_0\)
4: set \(p_0 = -z_0\)
5: set \(\delta_0 = g_0^T z_0\)
6: while \(f(x_k) > \varepsilon\)
   7: call PCG-STEP(\(A, x_k, p_k, g_k, \delta_k, x_{k+1}, p_{k+1}, g_{k+1}, \delta_{k+1}, M\))
8: set \(k = k + 1\)
9: set \(x = x_k\)

---

It is not desirable for algorithm 4 to act exactly like an inverse (as does filtered backprojection) because this would result in getting from the initial point to one satisfying \(f(x_k) < \varepsilon\) too quickly, not letting the superiorization to do its task of improving the solution according to the secondary criterion.
Algorithm 4. PCG-STEP(A, x, p, g, δ, x', p', g', δ', M).

1: set \( h = A^T A p \)
2: set \( \alpha = \delta / p^T h \)
3: set \( x' = x + \alpha p \)
4: set \( g' = g + \alpha h \)
5: set \( z' = M g' \)
6: set \( \delta' = g'^T z' \)
7: set \( \beta = \delta' / \delta \)
8: set \( p' = -z' + \beta p \)

For this reason, proximal operators such as the ones used in (6) do a better job. The FISTA algorithm [15] is specified by

\[
\begin{align*}
\text{x}_k &= \text{prox}_{\lambda c_2 R(\cdot)} \left( \text{u}_k + \frac{1}{\ell^2} A^T (y - A \text{x}_k) \right), \\
\text{u}_{k+1} &= \text{x}_k + \frac{t_k - 1}{t_{k+1}} (\text{x}_k - \text{x}_{k-1})
\end{align*}
\]

where \( t_{k+1} = \left( 1 + \sqrt{1 + 4 t_k^2} \right) / 2 \), with \( t_1 = 1 \) and \( \text{u}_1 = \text{x}_0 \). This generates a momentum that accelerates the ISTA algorithm specified by (6), giving to FISTA a convergence rate of order \( 1/k^2 \), as compared to \( 1/k \) that is the order of the convergence rate of ISTA.

### 3. Superiorizing the conjugate gradient method

In this section we introduce five superiorized CG-like algorithms. We start with a discussion of notation. Roughly speaking, if a not-superiorized iterative algorithm produces a sequence \( (\text{x}_k)_{k=0}^{\infty} \) that converges to \( \text{x}_{LS} \) by using algorithmic steps of the kind \( \text{x}_{k+1} = \text{P}(\text{x}_k) \), then its superiorized version works according to a formula such as (8), in which \( \text{v}_k \) is a nonascending direction for \( R(\cdot) \) and \( \gamma_k \) is a step size that ensures that the next point is superior according to the cost provided by the secondary criterion; see, for example, [21]. It has been shown that, under reasonable assumptions, if the sequence of the \( \gamma_k \) is summable, then the superiorized sequence of the \( \text{x}_k \) will retain the desirable property of the original algorithm of producing a good approximation to \( \text{x}_{LS} \). In practice, the \( \gamma_k \) are typically chosen to be a subsequence of

\[
\gamma_k = \gamma_0 a^k,
\]

where both \( \gamma_0 \) and \( a \) are positive real numbers, with \( a \) strictly less than 1.

We now introduce an important clarifying notation for perturbations of vectors in a superiorized version of an iterative algorithm. As an example, if the perturbation is done as indicated in (8), then we use \( \text{x}_{k+1} \) to denote \( \text{x}_k + \gamma_k \text{v}_k \), which means that (8) can be replaced by \( \text{x}_{k+1} = \text{P}(\text{x}_{k+1}) \).

Similar notation will be adopted for other intermediate vectors in the description of superiorized algorithms. Furthermore, for \( k \geq 1 \), we will use the notation \( \text{x}_{k-1} \) to denote \( \text{x}_{(k-1)+\frac{1}{2}} \).

In the superiorized algorithms described below we use the general notation \( \text{perturbed}(\text{x}) \) to denote the perturbed version of the vector \( \text{x} \). For example, if the superiorization is done according to the discussion in the paragraph that contains (8), then

\[
\text{perturbed}(\text{x}_k) = \text{x}_k + \gamma_k \text{v}_k.
\]
This, combined with the notation introduced in the previous paragraph, implies that \( x_{k+1} \) = perturbed \((x_k)^7\).

### 3.1. CG-K and its superiorization S-CG-K

In our first approach to superiorizing CG, we introduce the idea of the algorithm CG-K (where K is a fixed positive integer), whose one iterative step is defined as K iterative steps of CG. Details of a step CG-K\((A, y, x_0, x)\) of this algorithm are provided in algorithm 6. The parameters in the list for this algorithm CG-K\((A, y, x_0, x)\) are to be interpreted in the same way as for CG\((A, y, x_0, \varepsilon, x)\). The only difference between CG-K and CG is in Step 5, which specifies the termination condition.

In each iterative step of the superiorized version of CG-K, we restart CG using the perturbed output of the previous K iterations of CG as the input for the next K iterations. Details of this superiorized version are provided in algorithm 5. The parameter list of the superiorized algorithm S-CG-K\((A, y, x_0, \varepsilon, x)\) is to be interpreted in the same way as for CG\((A, y, x_0, \varepsilon, x)\). The integer K is not considered a parameter; we think of S-CG-1, S-CG-2, etc as different algorithms that call CG-1, CG-2, etc, respectively.

In order to see how S-CG-K\((A, y, x_0, \varepsilon, x)\) overcomes the previously mentioned difficulty with directly superiorizing CG, observe that in order to obtain \( x_{k+1} \) from \( x_k \) (Steps 4 and 5 of algorithm 5), we do not need to to worry about the maintenance of mathematical relations with other vectors. Since CG converges to an LS solution for any initial vector (in particular, for \( x_{k+1} \)), \( x_{k+1} \) will be a good approximation to the LS solution if K is large enough. We found that, in practice, K can be as low as 2 or 3 for computed tomography problems.

The S-CG-K algorithm calls the algorithm CG-K, which in turn calls the algorithm CG-STEP that is also called in algorithm 1 for CG. This implies that for S-CG-K one can make use of any code or implementation for standard CG that is available for many computer architectures [31, 32].

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#### Algorithm 5. S-CG-K\((A, y, x_0, \varepsilon, x)\).

1: set \( k = 0 \)
2: set \( x_{-1} = x_0 \)
3: while \( f(x_{-1}) > \varepsilon \)
4: set \( x_{-1} = \) perturbed\((x_k)\)
5: call CG-K\((A, y, x_{k+1}, x_{k+1})\)
6: set \( k = k + 1 \)
7: set \( x = x_{k+1} \)

#### Algorithm 6. CG-K\((A, y, x_0, x)\).

1: set \( k = 0 \)
2: set \( g_0 = A^T(Ax_0 - y) \)
3: set \( p_0 = -g_0 \)
4: set \( \delta_0 = \|g_0\|_2^2 \)
5: while \( k \leq K \)
6: call CG-STEP\((A, x_k, p_k, \varepsilon_k, \delta_k, x_{k+1}, p_{k+1}, \varepsilon_{k+1}, \delta_{k+1})\)
7: set \( k = k + 1 \)
8: set \( x = x_k \)

---

7 We note that, as is shown in [26], the proximal operator from (7) may be utilized to provide an alternative definition of the perturbed vector (21).
3.2. Perturbation resilient CG for superiorization

Note that just repeated applications of the CG-K step (that is, using algorithm 5 without perturbations, meaning that $x_{k+\frac{1}{2}} = x_k$) does not reproduce the original CG. In order to have an algorithm that performs exactly as CG, but is resilient to perturbations, we need to design some alternative algorithmic steps. For this purpose we utilized some steps proposed for NLCG [4, 33]. Here, we present two variants of such steps described in algorithms 8 and 10, respectively; the only important difference between them is the definition of $\beta$. When combining these with perturbed superiorization steps, we obtain the superiorized versions of two variants of CG; they are presented as S-CG and S-CG-CD in algorithms 7 and 9, respectively.

An individual step of the proposed variant of the CG algorithm, as specified in algorithm 8 (the PR is short for ‘perturbation resilient’), is not as efficient computationally as algorithm 2. This is because the trick of replacing (14) by the computationally more efficient (15) is mathematically incorrect when using CG-PR-STEP and so Step 1 of algorithm 8, which is similar to (14), needs to be explicitly (rather than recursively) computed. However, repeated applications of the CG-PR-STEP (that is, using algorithm 7 without perturbations, meaning that Step 9 is replaced by $x_{k+\frac{1}{2}} = x_k$) results in a perturbation resilient iterative algorithm for solving the LS problem. Thus its superiorized version (S-CG) should return an output that is superior according to a secondary criterion (in our case TV), while preserving performance according to the original LS-minimization criterion.

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**Algorithm 7.** S-CG($A, y, x_0, \varepsilon, x$).

1: set $x_\frac{1}{2} = x_0$
2: set $g_0 = A^T(Ax_0 - y)$
3: set $p_0 = -g_0$
4: set $h_0 = A^TAp_0$
5: set $\alpha = -g_0^Tg_0/p_0^Tg_0$
6: set $x_1 = x_0 + \alpha p_0$
7: set $k = 1$
8: while $f(x_{k-\frac{1}{2}}) > \varepsilon$
9:    set $x_{k+\frac{1}{2}} = \text{perturbed}(x_k)$
10:   call CG-PR-STEP($A, y, x_{k+\frac{1}{2}}, p_{k-1}, h_{k-1}, x_{k+1}, p_k, h_k$)
11:   set $k = k + 1$
12: set $x = x_{k-\frac{1}{2}}$

**Algorithm 8.** CG-PR-STEP($A, y, x, p, h, x', p', h'$).

1: set $g' = A^T(Ax - y)$
2: set $\beta = g'^T h / p'^T h$
3: set $p' = -g' + \beta p$
4: set $h' = A^TAp'$
5: set $\alpha = -g'^T p' / p'^T h'$
6: set $x' = x + \alpha p'$

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Algorithm 9. S-CG-CD(A, y, x₀, ε, x).

1: set \( x_1 = x_0 \)
2: set \( g_0 = A^T(Ax_0 - y) \)
3: set \( p_0 = -g_0 \)
4: set \( h_0 = A^TAp_0 \)
5: set \( x_1 = x_0 + \alpha p_0 \)
6: set \( k = 1 \)
7: while \( f(x_{k-1}) > \varepsilon \)
8: set \( x_{k+1} = \text{perturbed}(x_k) \)
9: call CG-CD-STEP(A, y, x, p, g, x′, p′, g′)
10: set \( k = k + 1 \)
11: set \( x = x_{k-1} \)

Algorithm 10. CG-CD-STEP(A, y, x, p, g, x′, p′, g′).

1: set \( g′ = A^T(Ax - y) \)
2: set \( \beta = -\|g′\|^2 / g′p \)
3: set \( p′ = -g′ + \beta p \)
4: set \( h′ = A^TAp′ \)
5: set \( \alpha = -g′^Tp′ / p′h′ \)
6: set \( x′ = x + \alpha p′ \)

Furthermore, different definitions of \( \beta \) can be utilized \[8, 29\]. One of these, namely \( \beta = -\|g′\|^2 / g′p \), is very effective; we use it in Step 2 of algorithm 10. (It has been referred to in the literature as the ‘conjugate descent’ rule, hence the ‘CD’ in the name of the algorithm.) This choice of \( \beta \) provides a smooth behavior of the superiorized CG algorithm and it resulted in the best reconstruction quality among all our experimentally-tested algorithms.

3.3. PCG-K and its superiorization S-PCG-K

As is the case with standard CG, the PCG algorithm cannot be directly superiorized. However, the same modifications that we proposed for CG can be done also to PCG. The first of these is superiorized PCG-K (S-PCG-K). The operator for each iteration of S-PCG-K (algorithm 11) is specified by PCG-K (algorithm 12), with K being the number of iterations of preconditioned CG, similarly to what was defined for CG-K. In practice, a small number K is sufficient for S-PCG-K to achieve good results. (In fact, a large value of K may be undesirable. This is because, the output of such PCG-K would be very close to the minimum of the least squares, defined in (1), resulting in early violation of the condition in Step 3 of algorithm 11. This would prevent the execution of the number of perturbations by Step 4 of algorithm 11 that is needed to get to a noticeably superior output according to the secondary criterion.) The not-superiorized version of S-PCG-K (that is, using algorithm 11 without perturbations, meaning that Step 4 is replaced by \( x_{k+1} = x_k \)) is a nonexpansive algorithm and, consequently, it is strongly perturbation resilient [21].

8 Different \( \beta \)s for NLCG \[8, 29\] produce the same result for the LS problem (the gradient and conjugate directions are unique). This fails for non-quadratic criteria or for superiorized algorithms.
3.4. Perturbation resilient PCG for superiorization

Since repeated application of PCG-K does not mimic the PCG steps exactly, a second variant of preconditioned CG was proposed for superiorization; this new superiorized algorithm is provided as algorithm 13. As was done for CG, the standard version of preconditioned CG was modified so that it becomes perturbation resilient. This way the algorithm will eventually converge to the LS solution, considering that bounded and summable perturbations are applied [21]. This algorithm is named S-PCG.

Algorithm 11. S-PCG-K(A, y, x₀, ε, x, M).

1: set \( k = 0 \)
2: set \( x_{-\frac{1}{2}} = x_0 \)
3: while \( f(x_{-\frac{1}{2}}) > \varepsilon \)
4: set \( x_{\frac{1}{2}} = \text{perturbed}(x_k) \)
5: call PCG-K(A, y, x_{\frac{1}{2}}, x_{k+1}, M)
6: set \( k = k + 1 \)
7: set \( x = x_{\frac{1}{2}} \)

Algorithm 12. PCG-K(A, y, x₀, x, M).

1: set \( k = 0 \)
2: set \( g_0 = A^T(Ax_0 - y) \)
3: set \( z_0 = Mg_0 \)
4: set \( p_0 = -z_0 \)
5: set \( \delta_0 = g_0^Tz_0 \)
6: while \( k \leq K \)
7: call PCG-STEP(A, x_k, p_k, \delta_k, x_{k+1}, p_{k+1}, \delta_{k+1}, M)
8: set \( k = k + 1 \)
9: set \( x = x_k \)

Algorithm 13. S-PCG(A, y, x₀, ε, x, M).

1: set \( x_{\frac{1}{2}} = x_0 \)
2: set \( g_0 = A^T(Ax_0 - y) \)
3: set \( z_0 = Mg_0 \)
4: set \( p_0 = -z_0 \)
5: set \( h_0 = A^TAp_0 \)
6: set \( \alpha = -g_0^Tp_0/p_0^Th_0 \)
7: set \( x_1 = x_0 + \alpha p_0 \)
8: set \( k = 1 \)
9: while \( f(x_{-\frac{1}{2}}) > \varepsilon \)
10: set \( x_{\frac{1}{2}} = \text{perturbed}(x_k) \)
11: call PCG-PR-STEP(A, y, x_{\frac{1}{2}}, x_{k-\frac{1}{2}}, p_{k-\frac{1}{2}}, h_{k-\frac{1}{2}}, x_{k+1}, p_k, h_k, M)
12: set \( k = k + 1 \)
13: set \( x = x_{\frac{1}{2}} \)
Algorithm 14. PCG-PR-STEP(A, y, x, p, h, x’, p’, h’, M).

1: set \( g' = A^T(Ax - y) \)
1: set \( x' = Mg' \)
1: set \( \beta = z'^T h / p'^T h \)
1: set \( p' = -z' + \beta p \)
1: set \( h' = A^TAp' \)
1: set \( \alpha = -g'^T p' / p'^T h' \)
1: set \( x' = x + \alpha p' \)

3.5. Filters for preconditioning

In order to specify more precisely the details of S-PCG and S-PCG-K, we complete this section with a discussion of the preconditioning filter \( M \) used in Step 3 of algorithm 12, Step 3 of algorithm 13 and Step 2 of algorithm 14. It is a filter applied in the frequency domain, in the same way as many filtering operations utilized in the filtered back projection method [28, chapter 8]. It can be defined as

\[
z = A^T F^T C F (Ax - y),
\]

where \( F \) represents a set of 1D Fourier transforms applied to each projection and \( C \) is a diagonal matrix with the filter factors in the frequency domain for each projection information (in Fourier domain). The filter factors can be written as

\[
c(\omega) = (|\omega| + \mu) \times (0.54 + 0.46 \cos(\omega)),
\]

where \( \omega \) is the frequency, \( \mu \) is a small number to avoid any singularity in the preconditioning matrix, and \((0.54 + 0.46 \cos(\omega))\) is the Hamming window, to reduce the gain in high frequencies that may amplify noise too much. The Hamming window is commonly used to ‘regularize’ the filter factors in filtered backprojection [28].

4. Experimental results

In these experiments we utilized a parallel ray tomographic simulation with 256 angles, uniformly spaced between 0 and 180 degrees, and 512 rays/angle. Gaussian noise with zero mean and \( \sigma^2 \) variance was added to the synthetically generated data, where \( \sigma^2 \) was computed to provide 5% of noise, or SNR of approximately 26dB. We reconstruct the images with \( 512 \times 512 \) pixels, using the following methods:

- CG: algorithm 1, the conjugate gradient method for solving problem (1);
- S-CG-2: algorithm 5 with \( K = 2 \), the superiorized CG algorithm using the operator CG-2 of algorithm 6;
- S-CG: algorithm 7, the superiorized CG algorithm using the perturbation resilient CG operator of algorithm 8;
- S-CG-CD: algorithm 9, variant of S-CG using the CG-CD operator of algorithm 10;
- S-PCG-2: algorithm 11 with \( K = 2 \), the superiorized preconditioned CG algorithm using the operator PCG-2 of algorithm 12;
- S-PCG: algorithm 13; the superiorized preconditioned CG algorithm using the operator PCG-PR-STEP of algorithm 14;
- FISTA: a reference method for the TV-regularized LS problem, specified by (18).
For all the algorithms, we selected the initial guess at the solution, \( x_0 \), to be the \( J \)-dimensional vector all of whose components are zero. The \( \varepsilon \) value for the stopping criterion (as in Step 5 of algorithm 1 and Step 3 of algorithm 5, etc) is defined as 
\[
\varepsilon = \frac{1}{2} N \sigma^2
\]
where \( \sigma^2 \) is the noise variance and \( N = 256 \times 512 \) is the number of elements of the data vector. For all superiorized algorithms, the constant \( a \), in (20), was set to .975 and \( \gamma_0 \) was manually selected to achieve the best performance (it is different for each method). Algorithms for all these methods (except for FISTA) are specified in the previous two sections and, in each case, the output \( x \) of the algorithm is provided by its last step. The following paragraphs explain the correct interpretation of the results reported in figures 1–3.

In figure 1 we compare algorithm performance in terms of quality and reconstruction speed, as judged by reconstruction error versus time. Each open circle on the curves corresponds to an iteration. The red boxes indicate the iteration when the stopping criterion is first satisfied, the number of open circles on the curve up to the red box is the number iterations \( k \) needed.
to reach the stopping point (for example, this is 9 for CG). The output images are shown in figure 4, in which the $k$ used to get the output is also indicated. For illustration purposes, we show error values even beyond the stopping criterion. We see in figure 1 that the algorithm S-CG-CD has the lowest error among all reported algorithms and that S-PCG-2 is the superiorized algorithm that satisfied the stopping criterion in the least amount of time.

Figure 2 reports on the half-squared-residual $f$ of the reconstructed images over time. Again we report beyond the iteration provided by the stopping criterion, with the purpose to demonstrate the behavior of superiorization algorithms, which converge to the (not regularized) least squares solution. On the other hand, regularized algorithms, such as FISTA, stay nearly at the same value of $f$ as the iterations go beyond the stopping criterion.

In figure 3, we show how the smoothness, as measured by the TV norm of the reconstructed images, behaves over time. Starting with a zero-valued image $x_0$ (whose TV norm is 0), we see that the reconstructed images rapidly reach having a TV norm very close to the TV norm of the phantom. After a while the TV norm of the superiorization algorithms grows again, due to the reduction of the $\gamma_k$ values in the perturbations (21); but this is not relevant as far as the output is concerned, since it happens after the stopping criterion is satisfied.

**Figure 3.** TV norm versus time.

**Table 1.** Robustness/sensitivity for measurement errors of five of the algorithms. For each algorithm and each noise level we report the mean ± standard deviation over the ten randomly generated projection data sets of the reconstruction error $\text{Err}$ at the time of termination, which is the $\text{Err}(x_{k-1})$ of figure 1. The reported $k$ is the median of the terminating iteration number of the ten reconstructions.

| Noise Level | 2.5%         | 5%         | 10%        |
|-------------|--------------|------------|------------|
|             | $k$ | $\text{Err}$ | $k$ | $\text{Err}$ | $k$ | $\text{Err}$ |
| S-CG-2      | 62  | 0.1340 ± 0.0035 | 49  | 0.2247 ± 0.0048 | 38  | 0.3571 ± 0.0066 |
| S-CG        | 75  | 0.1308 ± 0.0042 | 51  | 0.3135 ± 0.0033 | 44  | 0.6033 ± 0.0086 |
| S-CG-CD     | 57  | 0.0731 ± 0.0017 | 43  | 0.1664 ± 0.0041 | 36  | 0.3300 ± 0.0062 |
| S-PCG       | 27  | 0.1019 ± 0.0038 | 20  | 0.2312 ± 0.0042 | 12  | 0.3921 ± 0.0067 |
| S-PCG-2     | 22  | 0.1296 ± 0.0036 | 13  | 0.2524 ± 0.0034 | 6   | 0.4491 ± 0.0100 |
Figure 4 presents the output reconstructions produced by the tested methods, indicating the number of iterations required to reach those results. As a reference, a reconstruction produced by a filtered backprojection method [28, chapter 8] is also shown. These results can be used for subjective visual evaluation.

Figures 1–4 give an anecdotal illustration of the behavior of our algorithms. We now report on an experimental study of robustness/sensitivity for measurement errors for the five algorithms that we consider (based on figure 1) most deserving further investigation, namely S-CG-2, S-CG, S-CG-CD, S-PCG and S-PCG-2. For the anecdotal study described above, Gaussian noise with zero mean and $\sigma^2$ variance was added to the synthetically generated data,
where $\sigma^2$ was computed to provide 5% of noise. For the robustness/sensitivity for measurement errors we carried out experiments in which $\sigma^2$ was computed to provide 2.5%, 5% and 10% of noise. Everything else stayed the same as specified at the beginning of this section; in particular, we use $\varepsilon = \frac{1}{2} N \sigma^2$ for the stopping criterion. For each noise level we generated ten (random) projection data sets and reconstructed from each data set by each of the five algorithms. In table 1 we report on the results of these experiments. We can conclude from these results the following. S-CG-CD reached the lowest reconstruction error among the tested reconstruction methods for all three levels of noise and this conclusion is robust, since the differences in means are many times the associated standard deviations. This method of choice (S-CG-CD) is sensitive to noise in the data; in fact, for the range that we tried the reconstruction error seems to depend approximately linearly on the noise level. Just as shown in figure 1, which reports on the anecdotal experiment, S-PCG and SPCG-2 require less computer time, but the results produced by them have significantly higher reconstruction error than the results produced by S-CG-CD.

5. Discussion and conclusions

In this paper we have applied the superiorization approach to the conjugate gradient method, as well as to its preconditioned version. The total variation norm, commonly utilized as a regularizing penalty, was utilized as the secondary criterion for superiorization. In the Appendix we prove for one of the superiorized versions of the conjugate gradient method (namely, S-CG) that it behaves in the manner that is expected for a superiorized algorithm (roughly meaning that it gets as good results as the unsuperiorized version according to the primary criterion, but with improvements according to the secondary criterion; see, for example, [21] for a more precise discussion). The experimental results have illustrated that the proposed algorithms are fast, achieving as good results as algorithms such as FISTA, but in less time; see the plots for S-CG-CD, S-PCG and S-PCG-2 in figure 1.

An item that is missing from this paper is a thorough mathematical analysis of the convergence properties of all the presented algorithms. Termination is proved only for S-CG. Since that proof takes up quite a lot of space (see the Appendix), we did not consider it appropriate to take up additional space for other termination proofs. This is so especially since our termination proofs tend to consist of first proving that the iterative algorithm that is being superiorized has the property of being ‘strongly perturbation resilient’ and then appealing to general theorems that the termination of the superiorized algorithm follows; see, for example, [20, 21]. However, look at [34], which states the following.

- We are not able to establish that pSART is a strongly perturbation resilient algorithm, as the conditions under which the algorithm converges are not well understood. In our numerical experiments, however, the superiorized pSART algorithm is successful in every instance. It produces solutions that are as constraints compatible as those produced by pSART, with TV or ATV values that are typically 30–60% lower. As the authors note in [21], strong perturbation resilience is a sufficient condition for the success of superiorization, but not a necessary one. Thus, the inability to prove whether or not an algorithm is strongly perturbation resilient does not preclude the use of superiorization to obtain solutions that are improved with respect to the chosen secondary criterion.

We share the attitude expressed in the above paragraph, which implies that it is reasonable in practice to superiorize an iterative algorithm, even if there is no mathematical theorem at hand to validate the superiorization of that particular algorithm.
More specifically, our paper does not contain an analysis of the convergence rate of our algorithms. We consider such results marginal to our main interest, since we intend to use superiorized algorithms in such a way that they terminate in a finite number of steps. However, other researchers have a different attitude. For example, [35] states:

- Once an algorithm is proved to be bounded perturbation resilient, superiorization can be used, and this allows flexibility in choosing the bounded perturbations in order to obtain a superior solution. We show that the perturbed algorithms converge at the rate of \( O\left(\frac{1}{t}\right) \).

In conclusion, in this paper we have proposed a method that provides a practical solution for the image reconstruction problem when good reconstruction quality and low reconstruction time are both important requirements for the desired reconstruction algorithm.

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Appendix. Proof that superiorized CG (algorithm 7) terminates

The specifications of the parameters of algorithm 7 are:

- \( J \) is a positive integer (the dimensionality of the output vector of the algorithm).
- \( L \) is a positive integer (the number of data elements in the sinogram).
- \( A \) is an \( L \times J \) (system) matrix.
- \( y \) is an \( L \)-dimensional (measurement) vector.
- \( \varepsilon \) is a positive number (used for algorithm termination).
- \( x_0 \) is a \( J \)-dimensional (input) vector (the initial guess vector).
- \( x \) is a \( J \)-dimensional (output) vector.

The quadratic objective function for the data fidelity constraints (the primary criterion) is the half-squared-residual

\[
 f(x) = \frac{1}{2} \| y - Ax \|_2^2 .
\]  

(A.1)

We define

\[
 \varepsilon_0 = \min_x \frac{1}{2} \| y - Ax \|_2^2 .
\]  

(A.2)

This implies that \( \varepsilon_0 = f(x_{LS}) \); see (1). We note that termination of algorithm 7 can happen only if the condition in Step 8 of the algorithm is violated. That means that \( f\left(x_{k-\frac{1}{2}}\right) \leq \varepsilon \) and also that the output \( x \) of the algorithm satisfies \( f(x) \leq \varepsilon \).

**Theorem A.1.** Given any positive number \( \varepsilon \) such that \( \varepsilon > \varepsilon_0 \), algorithm 7 terminates.

We prove this theorem through a sequence of intermediate results. We note the fact that if Step 10 of algorithm 7 is executed, it has to be the case that at that time \( k \geq 1 \). Also, we consider what happens during the execution of Step 10 of algorithm 7, which is a call to algorithm 8: After executing Step 1, all occurrences of \( g' \) in algorithm 8 may be also denoted as \( g_{k+\frac{1}{2}} \), where
\( g_{k+\frac{1}{2}} = A^T \left( Ax_{k+\frac{1}{2}} - y \right) \),
\[(A.3)\]

which is consistent with (14) and is notation that we use from now on.

**Proposition A.2.** Upon the execution of Step 10 of algorithm 7, it is the case that, for all integers \( n \) such that \( 0 \leq n \leq k \),
\[ \langle g_{n+1}, p_n \rangle = 0, \]
\[(A.4)\]

where, \( g_{n+1} \) is defined by (14) with the \( k \) there replaced by \( n \).

**Proof.** We first prove that (A.4) holds for \( n = 0 \). It follows from (14) and Steps 5 and 6 of algorithm 7 that
\[ g_1 = g_0 + \alpha A^T A p_0. \]

Combining this with Steps 4 and 5 of algorithm 7, we have that
\[ \langle g_1, p_0 \rangle = \langle g_0, p_0 \rangle + \alpha \langle A^T A p_0, p_0 \rangle \]

\[ = \langle g_0, p_0 \rangle - \langle A p_0, A p_0 \rangle \]
\[ = 0. \]
\[(A.5)\]

Note that (A.5) always holds after Step 6 of algorithm 7 since \( g_1 \) and \( p_0 \) do not get changed after their initial assignments.

Next we prove that, for \( k \geq 1 \), upon the execution of Step 10 of algorithm 7,
\[ \langle g_{k+1}, p_k \rangle = 0. \]
\[(A.6)\]

It follows from (14), (A.3) and Step 6 of algorithm 8 that, upon the execution of Step 10 of algorithm 7,
\[ g_{k+1} = g_{k+\frac{1}{2}} + \alpha A^T A p_k. \]
\[(A.7)\]

Combining this with Steps 4 and 5 of algorithm 8, we have that
\[ \langle g_{k+1}, p_k \rangle = \langle g_{k+\frac{1}{2}}, p_k \rangle + \alpha \langle A^T A p_k, p_k \rangle \]

\[ = \langle g_{k+\frac{1}{2}}, p_k \rangle - \langle g_{k+\frac{1}{2}}, p_k \rangle \langle A p_k, A p_k \rangle \]
\[ = 0. \]
\[(A.8)\]

We note that, for \( k \geq 1 \), \( x_{k+1} \) and \( p_k \) do not get changed once they are obtained by an execution of Step 10 of algorithm 7. Combing this fact and (14), we know that, for \( k \geq 1 \), \( g_{k+1} \) does not get changed once it is obtained. From these facts and (A.5), (A.8), it follows that, upon the execution of Step 10 of algorithm 7, it is the case that, for all integers \( n \) such that \( 0 \leq n \leq k \), (A.4) holds.

**Proposition A.3.** Just before an execution of Step 10 of algorithm 7, it holds that
\[ h_{k-1} = A^T A p_{k-1}. \]
\[(A.9)\]
Proof. From Step 4 of algorithm 7, we know that, for \( k = 1 \), (A.9) holds just before the execution of Step 10 of algorithm 7. By Step 4 of algorithm 8, we see that upon an execution of Step 10 of algorithm 7, it holds that
\[
h_k = A^T A p_k. \tag{A.10}
\]
These facts and the repeated executions of the while loop of algorithm 7 imply that, for \( k \geq 1 \), (A.9) holds just before the execution of Step 10 of algorithm 7. □

Proposition A.4. Upon the execution of Step 10 of algorithm 7, it is the case that
\[
\langle A p_k, A p_{k-1} \rangle = 0. \tag{A.11}
\]

Proof. By proposition A.3, we know that (A.9) holds just before the execution of Step 10 of algorithm 7. Consider now the execution of Step 10 of algorithm 7, which is a call to algorithm 8. It is easily shown that, upon the execution of Step 2 of algorithm 8,
\[
\beta = \frac{\langle g_{k+1}, A^T A p_{k-1} \rangle}{\langle A p_{k-1}, A p_{k-1} \rangle}. \tag{A.12}
\]
Combining this with Step 3 of algorithm 8, we have that
\[
\langle A p_k, A p_{k-1} \rangle = \langle p_k, A^T A p_{k-1} \rangle
= -\langle g_{k+1}, A^T A p_{k-1} \rangle
+ \frac{\langle g_{k+1}, A^T A p_{k-1} \rangle}{\langle A p_{k-1}, A p_{k-1} \rangle} \langle p_{k-1}, A^T A p_{k-1} \rangle
= 0. \tag{A.13}
\]
The remaining two steps of algorithm 8 do not change the validity of (A.13). □

In Step 9 of algorithm 7 the procedure \( x_{k+\frac{1}{2}} = \text{perturbed}(x_k) \) is called to add a perturbation to the vector \( x_k \) and thus produce a new vector \( x_{k+\frac{1}{2}} \) that is generally better than \( x_k \) according to a secondary criterion. Using (21), this \( x_{k+\frac{1}{2}} \) is expressed as
\[
x_{k+\frac{1}{2}} = x_k + u_k, \tag{A.14}
\]
where \( u_k = \gamma_k v_k \) is the overall perturbation at the superiorization stage. In the superiorization methodology, the sequence of the perturbations \( (u_k)_{k=0}^\infty \) for all \( k \geq 0 \) in (A.14) are bounded and the norm of the sequence is summable, that is
\[
\sum_{k=0}^\infty \| u_k \| < \infty. \tag{A.15}
\]
In what follows we use \( c \) be the Euclidean norm \( \| A \|_2 \) of the matrix \( A \); that is
\[
c = \sup_{\| x \|_2 \neq 0} \frac{\| A x \|_2}{\| x \|_2}. \tag{A.16}
\]
We note that
\[ c^2 = \|A^T A\|_2, \]  
(A.17)

and that \( c \) is the largest singular value of \( A \). Another notation that we use in the rest of this paper is \( \eta_1 = \frac{1}{4c^2} \).

**Proposition A.5.** Suppose that the \( x_{k+\frac{1}{2}} \) produced by the execution of Step 9 of algorithm 7 is expressed as (A.14) in which the \( u_k \) satisfies
\[ \|u_k\|_2 = \eta_0 \|g_k\|_2, \]  
(A.18)

with \( 0 < \eta_0 \leq \eta_1 \) and
\[ g_k = A^T (Ax_k - y). \]  
(A.19)

Then, upon the execution of Step 10 of algorithm 7, it is the case that
\[ 2f(x_{k+\frac{1}{2}}) - 2f(x_{k+1}) \geq \frac{1}{16c^2} \|g_k\|_2^2. \]  
(A.20)

**Proof.** We look at the details of what happens during the execution of Step 10 of algorithm 7, which is a call to algorithm 8. It follows from (A.1) that
\[ 2f(x_{k+\frac{1}{2}}) - 2f(x_{k+1}) = \left\langle Ax_{k+\frac{1}{2}} - y, Ax_{k+\frac{1}{2}} - y \right\rangle - \left\langle Ax_{k+1} - y, Ax_{k+1} - y \right\rangle. \]  
(A.21)

From Step 6 of algorithm 8, we see that,
\[ x_{k+1} = x_{k+\frac{1}{2}} + \alpha p_k. \]  
(A.22)

Combining this with (A.21) we have that
\[
2f(x_{k+\frac{1}{2}}) - 2f(x_{k+1}) \\
= \left\langle Ax_{k+\frac{1}{2}} - y, Ax_{k+\frac{1}{2}} - y \right\rangle \\
- \left\langle (Ax_{k+\frac{1}{2}} - y) + \alpha Ap_k, (Ax_{k+\frac{1}{2}} - y) + \alpha Ap_k \right\rangle \\
= -2\alpha \left\langle Ax_{k+\frac{1}{2}} - y, Ap_k \right\rangle - \alpha^2 \|Ap_k\|^2_2 \\
= -2\alpha \left\langle g_{k+\frac{1}{2}}, p_k \right\rangle - \alpha^2 \|Ap_k\|^2_2. 
\]  
(A.23)

From Steps 4 and 5 of algorithm 8, it follows that
\[ \alpha = -\frac{\left\langle g_{k+\frac{1}{2}}, p_k \right\rangle}{\|Ap_k\|^2_2}. \]  
(A.24)

Combining this with (A.23), we know that
\[
2f(x_{k+\frac{1}{2}}) - 2f(x_{k+1}) \\
= 2 \frac{\left\langle g_{k+\frac{1}{2}}, p_k \right\rangle^2}{\|Ap_k\|^2_2} - \frac{\left\langle g_{k+\frac{1}{2}}, p_k \right\rangle^2}{\|Ap_k\|^2_2} \\
= \frac{\left\langle g_{k+\frac{1}{2}}, p_k \right\rangle^2}{\|Ap_k\|^2_2}. 
\]  
(A.25)
Now we calculate $\langle g_{k+\frac{1}{2}}, p_k \rangle$. By Step 3 of algorithm 8, we have that
\[ p_k = -g_{k+\frac{1}{2}} + \beta p_{k-1}. \tag{A.26} \]

It follows that
\[ \langle g_{k+\frac{1}{2}}, p_k \rangle = -\left\| g_{k+\frac{1}{2}} \right\|_2^2 + \left\langle g_{k+\frac{1}{2}}, \beta p_{k-1} \right\rangle. \tag{A.27} \]

By (A.19) and (A.14) we have that
\[ g_{k+\frac{1}{2}} = g_k + A^T A u_k. \tag{A.28} \]

From (A.4) of proposition A.2 with $n = k - 1$, we have that
\[ \langle g_k, \beta p_{k-1} \rangle = 0. \tag{A.29} \]

Combining these two facts, we have that
\[ \langle g_{k+\frac{1}{2}}, \beta p_{k-1} \rangle = \langle A u_k, \beta A p_{k-1} \rangle \leq \|A u_k\|_2 \cdot \|\beta A p_{k-1}\|_2. \tag{A.30} \]

It follows from Step 3 of algorithm 8 that
\[ A p_k = -A g_{k+\frac{1}{2}} + \beta A p_{k-1}. \tag{A.31} \]

Combining this with the orthogonality expressed in (A.11) of proposition A.4, we have that
\[ \left\| A g_{k+\frac{1}{2}} \right\|_2^2 = \|A p_k\|_2^2 + \|\beta A p_{k-1}\|_2^2. \tag{A.32} \]

Consequently,
\[ \|A p_k\|_2 \leq \left\| A g_{k+\frac{1}{2}} \right\|_2, \tag{A.33} \]

and
\[ \|\beta A p_{k-1}\|_2 \leq \left\| A g_{k+\frac{1}{2}} \right\|_2. \tag{A.34} \]

From this and (A.30), we know that
\[ \langle g_{k+\frac{1}{2}}, \beta p_{k-1} \rangle \leq \|A u_k\|_2 \cdot \left\| A g_{k+\frac{1}{2}} \right\|_2 \leq c^2 \|u_k\|_2 \cdot \|g_{k+\frac{1}{2}}\|_2 \]
\[ = c^2 \eta_0 \|g_k\|_2 \cdot \left\| g_{k+\frac{1}{2}} \right\|_2. \tag{A.35} \]

The second inequality of (A.35) comes from (A.16) and the equality comes from (A.18).
By (A.28), (A.17) and (A.18), we have that
\[
\|g_{k+\frac{1}{2}}\|_2 \geq \|g_k\|_2 - \|A^T A u_k\|_2 \\
\geq \|g_k\|_2 - c^2 \eta_0 \|g_k\|_2 \\
= (1 - c^2 \eta_0) \|g_k\|_2.
\] (A.36)

From this and the assumption that \(0 < \eta_0 \leq \frac{1}{4c^2}\), it follows that
\[
\|g_{k+\frac{1}{2}}\|_2 \geq \frac{3}{4} \|g_k\|_2 \geq \frac{\|g_k\|_2}{2}.
\] (A.37)

From this and (A.35), it follows that
\[
\langle g_{k+\frac{1}{2}}, p_{k-1} \rangle \leq 2c^2 \eta_0 \|g_{k+\frac{1}{2}}\|_2^2.
\] (A.38)

From this and (A.27), it follows that
\[
\langle g_{k+\frac{1}{2}}, p_k \rangle \leq -(1 - 2c^2 \eta_0) \|g_{k+\frac{1}{2}}\|_2^2.
\] (A.39)

Combining this with the assumption that \(0 < \eta_0 \leq \frac{1}{4c^2}\), we have that
\[
\langle g_{k+\frac{1}{2}}, p_k \rangle^2 \geq \frac{1}{4} \|g_{k+\frac{1}{2}}\|_2^4.
\] (A.40)

From this and (A.25) and (A.33), it follows that
\[
2f(x_{k+\frac{1}{2}}) - 2f(x_{k+1}) = \frac{\langle g_{k+\frac{1}{2}}, p_k \rangle^2}{\|A p_k\|_2^2} \\
\geq \frac{\|g_{k+\frac{1}{2}}\|_2^4}{4 \|A p_{k+\frac{1}{2}}\|_2^2} \\
\geq \frac{\|g_{k+\frac{1}{2}}\|_2^2}{4c^2}.
\] (A.41)

From this and (A.37) and (A.20) follows.

Lemma A.6. Let \(\eta_2\) be the positive solution to the quadratic equation on the variable \(\eta\):
\[
(2 + c^2 \eta) \eta = \frac{1}{32c^2}.
\] (A.42)

During the execution of algorithm 7, suppose that, for some integer \(k\), immediately after the execution of Step 9 of algorithm 7, the returned \(x_{k+\frac{1}{2}}\) is expressed as (A.14) in which the \(u_k\) satisfies (A.18) with \(0 < \eta_0 \leq \eta_1 = \min \{\eta_1, \eta_2\}\) and \(g_k\) defined in (A.19). Then, upon the execution of Step 10 of algorithm 7, it is the case that
2f(x_k) - 2f(x_{k+1}) \geq \frac{1}{32c^2} \| \mathbf{g}_k \|_2^2. \quad (A.43)

**Proof.** By (A.1) and (A.14), we have that immediately after the execution of Step 9 of algorithm 7

\[
2f(x_k) - 2f(x_{k+\frac{1}{2}}) = \langle Ax_k - y, Ax_k - y \rangle - \langle Ax_{k+\frac{1}{2}} - y, Ax_{k+\frac{1}{2}} - y \rangle
\]

\[
= -2 \langle Ax_k - y, Au_k \rangle - \| Au_k \|_2^2. \quad (A.44)
\]

Combining this with (A.19), we know that

\[
2f(x_k) - 2f(x_{k+\frac{1}{2}}) = -2 \langle \mathbf{g}_k, u_k \rangle - \| Au_k \|_2^2. \quad (A.45)
\]

It follows that

\[
\left\| 2f(x_k) - 2f(x_{k+\frac{1}{2}}) \right\| \leq 2 \| \mathbf{g}_k \|_2 \| u_k \|_2 + c^2 \| u_k \|_2^2
\]

\[
= (2 + c^2 \eta_0) \eta_0 \| \mathbf{g}_k \|_2^2. \quad (A.46)
\]

The second inequality of (A.46) comes from (A.16) and the equality comes from (A.18).

Let

\[
\varphi(\eta) = \left( 2 + c^2 \eta \right) \eta. \quad (A.47)
\]

By the definition of \( \eta_2 \), we know that \( \varphi(\eta_2) = \frac{1}{32c^2} \). Since \( \varphi(\eta) \) is a monotone increasing function of \( \eta \) for \( \eta > 0 \), and \( \varphi(0) = 0 \), \( \eta_0 \leq \eta_2 \), we have that

\[
0 < \varphi(\eta_0) \leq \varphi(\eta_2) = \frac{1}{32c^2}. \quad (A.48)
\]

Combining this with (A.46), it follows that

\[
\left\| 2f(x_{k+\frac{1}{2}}) - 2f(x_k) \right\| \leq \frac{1}{32c^2} \| \mathbf{g}_k \|_2^2. \quad (A.49)
\]

From this and (A.20) obtained by proposition A.5, it follows that, upon the execution of Step 10 of algorithm 7,

\[
2f(x_k) - 2f(x_{k+1}) \geq -\frac{1}{32c^2} \left\| \mathbf{R}_k \right\|_2^2 + \frac{1}{16c^2} \left\| \mathbf{R}_k \right\|_2^2 \quad (A.50)
\]
Now we are ready to complete the proof of theorem A.1.

**Proof.** Since $x_{LS}$ is a minimizer of $f(x)$ if and only if
\[ g(x_{LS}) = A^T (Ax_{LS} - y) = 0, \]
we know that for any $x$ such that $f(x) > \epsilon_0, \|g(x)\|_2 > 0$.

Given a positive $\epsilon$ such that $\epsilon > \epsilon_0$, define
\[ \theta = \inf_x \{ \|g(x)\|_2 \mid f(x) > \epsilon \}. \]
Then $\theta > 0$.

Let $c$ be as specified in (A.16), $\eta_1 = \frac{1}{\sqrt{2}}$, and $\eta_2$ be the positive solution to the quadratic equation (A.42) of $\eta, \eta = \min \{\eta_1, \eta_2\}$. During the execution of algorithm 7, the sequence of the perturbations $(u_k)_{k=1}^{\infty}$ for all $k \geq 1$ in (A.14) generated by execution of Step 9 of algorithm 7, satisfies (A.15). Hence, there exists an integer $K$ such that $\|u_k\|_2 \leq \eta \theta$ for all $k \geq K$. Let $S = \{2f(x_k) \mid k \geq K\}$ be the sequence of $2f(x_k)$ of which the $x_k$ for $k \geq K$ is generated by an execution of Step 10 of algorithm 7. By lemma A.6, we know that $0 < 2f(x_{k+1}) < 2f(x_k)$, hence the sequence in $S$ is strictly decreasing and bounded.

We prove this theorem with the method of proof by contradiction. Suppose that the algorithm 7 never terminates. Then for any $k \geq K$, it holds that
\[ f(x_k) > \epsilon. \]
Let
\[ \xi = \inf \{ 2f(x_k) \mid k \geq K \}. \]
Now we prove that if the algorithm 7 never terminates, then there exists a $k \geq K$ such that
\[ 2f(x_k) < \xi, \]
which contradicts the definition of $\xi$.

Let $\delta = \frac{\theta^2}{32c^2}$. By the definition of $\xi$, we know that there exists an integer $k \geq K$ such that
\[ 2f(x_k) \leq \xi + \frac{\delta}{2}. \]
From the facts that $\|u_k\|_2 \leq \eta \theta$ and $\|g_k\|_2 \geq \theta$ for $k \geq K$ with $g_k$ defined in (A.19), we know that the precondition of lemma A.6 is satisfied for $k \geq K$. It follows from lemma A.6 that
\[
2f(x_{k+1}) \leq 2f(x_k) - \frac{1}{32c^2} \|g_k\|_2^2 \\
\leq 2f(x_k) - \delta \\
\leq \xi - \frac{\delta}{2}.
\]
The second inequality of (A.57) comes from the facts that $\|g_k\|_2 \geq \theta$ and $\delta = \frac{\theta^2}{32c^2}$. The third inequality of (A.57) comes from (A.56). Then we know that (A.55) holds for $k + 1$, which contradicts the definition of $\xi$. Hence algorithm 7 terminates. \(\square\)
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References

[1] Björck A 1996 Numerical Methods for Least Squares Problems (Philadelphia, PA: SIAM)
[2] Barrett H H and Myers K J 2004 Foundations of Image Science (Hoboken, NJ: Wiley)
[3] Kim K and Shevlyakov G 2008 Why Gaussianity? IEEE Signal Process. Mag. 25 102–13
[4] Vogel C R 2002 Computational Methods for Inverse Problems (Philadelphia, PA: SIAM)
[5] Bovik A C 2000 Handbook of Image and Video Processing 1st edn (San Diego, CA: Academic)
[6] Romberg J K 2008 Imaging via compressive sampling IEEE Signal Process. Mag. 25 14–20
[7] Dai Y, Han J, Liu G, Sun D, Yin H and Yuan Y 2000 Convergence properties of nonlinear conjugate gradient methods SIAM J. Optim. 10 345–58
[8] Hager W and Zhang H 2006 A survey of nonlinear conjugate gradient methods Pac. J. Optim. 2 35–58
[9] Rockafellar R T and Wets R J B 1998 Variational Analysis (Berlin: Springer)
[10] Beck A and Teboulle M 2009 Fast iterative shrinkage-thresholding algorithm for linear inverse problems SIAM J. Imaging Sci. 2 183–202
[11] Parikh N and Boyd S 2014 Proximal algorithms Found. Trends Optim. 1 127–239
[12] Censor Y, Garduño E, Davidi R and Herman G T 2010 Perturbation resilience and superiorization of iterative algorithms Inverse Problems 26 065008
[13] Hansen P C 1998 Rank-Deficient and Discrete Ill-Posed Problems: Numerical Aspects of Linear Inversion (Philadelphia, PA: SIAM)
[14] Censor Y, Davidi R, Herman G T, Schulte R W and Tetroshvili L 2014 Projected subgradient minimization versus superiorization J. Optim. Theory Appl. 160 730–47
[15] Garduño E and Herman G T 2014 Superiorization of the ML-EM algorithm IEEE Trans. Nucl. Sci. 61 162–72
[16] Schrapp M J and Herman G T 2014 Data fusion in x-ray computed tomography using a superiorization approach Rev. Sci. Instrum. 85 053701
[17] Helou E S, Zibetti M V W and Miqueles E X 2017 Superiorization of incremental optimization algorithms for statistical tomographic image reconstruction Inverse Problems 33 044010
[18] Björck A, Elfving T and Strakos Z 1998 Stability of conjugate gradient and Lanczos methods for linear least squares problems SIAM J. Matrix Anal. Appl. 19 720–36
[19] Herman G T 2009 Fundamentals of Computerized Tomography: Image Reconstruction from Projections 2nd edn (London: Springer)
[29] Dai Y-H and Kou C-X 2013 A nonlinear conjugate gradient algorithm with an optimal property and an improved Wolfe line search SIAM J. Optim. 23 296–320
[30] Luenberger D G and Ye Y 2008 Linear and Nonlinear Programming 3rd edn (New York: Springer)
[31] Frayssé V and Giraud L 2000 A set of conjugate gradient routines for real and complex arithmetics Technical Report TR/PA/00/47 CERFACS Toulouse, France
[32] Bolz J, Farmer I, Grinspun E and Schröder P 2003 Sparse matrix solvers on the GPU: conjugate gradients and multigrid ACM Trans. Graph. 22 917–24
[33] Shewchuk J R 1994 An introduction to the conjugate gradient method without the agonizing pain Technical Report Carnegie Mellon University Pittsburgh, PA
[34] Humphries T, Winn J and Faridani A 2017 Superiorized algorithm for reconstruction of CT images from sparse-view and limited-angle polyenergetic data Phys. Med. Biol. 62 6762–83
[35] Dong Q, Gibali A, Jiang D and Tang Y 2017 Bounded perturbation resilience of extragradient-type methods and their applications J. Inequalities Appl. 280