Projected Newton Method for noise constrained Tikhonov regularization

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October 2019

Abstract. Tikhonov regularization is a popular approach to obtain a meaningful solution for ill-conditioned linear least squares problems. A relatively simple way of choosing a good regularization parameter is given by Morozov’s discrepancy principle. However, most approaches require the solution of the Tikhonov problem for many different values of the regularization parameter, which is computationally demanding for large scale problems. We propose a new and efficient algorithm which simultaneously solves the Tikhonov problem and finds the corresponding regularization parameter such that the discrepancy principle is satisfied. We achieve this by formulating the problem as a nonlinear system of equations and solving this system using a line search method. We obtain a good search direction by projecting the problem onto a low dimensional Krylov subspace and computing the Newton direction for the projected problem. This projected Newton direction, which is significantly less computationally expensive to calculate than the true Newton direction, is then combined with a backtracking line search to obtain a globally convergent algorithm, which we refer to as the Projected Newton method. We prove convergence of the algorithm and illustrate the improved performance over current state-of-the-art solvers with some numerical experiments.

Keywords: Newton method, Krylov subspace, Tikhonov regularization, discrepancy principle, bidiagonalization

1. Introduction

Large scale ill-posed linear inverse problems of the form $Ax = b$ with $A \in \mathbb{R}^{m \times n}, x \in \mathbb{R}^n$ and $b \in \mathbb{R}^m$ where $m \geq n$ arise in countless scientific and industrial applications. The singular values of such a matrix typically decay to zero, which means the condition number $\kappa(A)$ is very large. This in turn means that small perturbations in the right-hand side $b$ can cause huge changes in the solution $x$. The right-hand side $b$ is generally the perturbed version of the unknown exact measurements or observations $b_{ex} = b + e$. Thus we know that for ill-posed problems some form of regularization has to be used.
Projected Newton Method

in order to deal with the noise $e$ in the data $b$ and to find a good approximation for the true solution $x_{ex}$ of $Ax = b_{ex}$. One of the most widely used methods to do so is Tikhonov regularization [1]. In its standard form, the Tikhonov solution to the inverse problem is given by

$$x_{\alpha} = \arg \min_{x \in \mathbb{R}^n} \frac{1}{2}||Ax - b||^2 + \frac{\alpha}{2}||x||^2$$  \hspace{1cm} (1)

where $\alpha > 0$ is the regularization parameter and $|| \cdot ||$ is the standard Euclidean norm. By taking the gradient of the objective function of (1) and equating it to zero, it follows that the Tikhonov solution can alternatively be characterized as the solution of the linear system of normal equations

$$(A^TA + \alpha I)x_{\alpha} = A^Tb$$  \hspace{1cm} (2)

where $I$ is the $n \times n$ identity matrix [2]. The choice of the regularization parameter is very important since its value has a significant impact on the quality of the reconstruction. If, on the one hand, $\alpha$ is chosen too large, focus lies on minimizing the regularization term $||x||^2$ in (1). The corresponding reconstruction $x_{\alpha}$ will therefore no longer be a good solution for the linear system $Ax = b$, will typically have lost many details and be what is referred to as “oversmoothed”. If, on the other hand, $\alpha$ is chosen too small, focus lies on minimizing the residual $||Ax - b||^2$. This, however, means that the measurement errors $e$ are not suppressed and that the reconstruction $x_{\alpha}$ will be “overfitted” to the measurements.

One way of choosing the regularization parameter is the L-curve method. If $x_{\alpha}$ is the solution of the Tikhonov problem (1), then the curve $(||Ax_{\alpha} - b||, ||x_{\alpha}||)$ typically has a rough “L” shape, see figure 1. Heuristically, the value for the regularization parameter corresponding to the corner of this “L” has been proposed as a good regularization parameter because it balances model fidelity (minimizing the residual) and regularizing the solution (minimizing the regularization term) [3, 4, 5, 2]. The problem with this method is that in order to find this value, the linear system (2) has to be solved for many different values of $\alpha$, which can be computationally expensive and inefficient for large scale problems.

Another way of choosing the regularization parameter is Morozov’s discrepancy principle [6]. Here, the regularization parameter is chosen such that

$$||Ax_{\alpha} - b|| = \eta \epsilon$$  \hspace{1cm} (3)

with $\epsilon = ||e||$ the size of the measurement error and $1 \leq \eta$ a tolerance value. The idea behind this choice is that finding a solution $x_{\alpha}$ with a lower residual can only lead to overfitting. Similarly to the L-curve, we can look at the curve $(\alpha, ||Ax_{\alpha} - b||)$, which is often referred to as the discrepancy curve or D-curve, see figure 1. Note that in practice we never have the exact value $\epsilon$, so this approach assumes we have a good estimate for the “noise-level” of the inverse problem. We could use a root-finding method like the secant or regula falsi method [7, 8] to find the regularization parameter $\alpha$ which satisfies (3), but this would again require us to solve the linear system (2) multiple times.
In this paper we develop a new and efficient algorithm, which we call the **Projected Newton method**, that simultaneously updates the solution \( x \) and the regularization parameter \( \alpha \) such that the Tikhonov equation (2) and Morozov’s discrepancy principle (3) are both satisfied. We start by considering an equivalent formulation as a constrained optimization problem, which we refer to as the noise constrained Tikhonov problem. By taking the gradient of the Lagrangian of the optimization problem, this formulation naturally leads to a nonlinear system of equations that can be solved using a Newton type method, which is precisely the approach taken in [9]. For large scale problems, however, computing the Newton direction is computationally demanding. We therefore propose the project the noise constrained Tikhonov problem onto a low dimensional Krylov subspace. In each iteration of the Projected Newton method we first expand the Krylov subspace with one dimension and then compute the Newton direction for the projected problem, which is much cheaper to compute than the actual Newton direction. This **projected Newton direction** is then combined with a backtracking line search to obtain a robust and globally convergent algorithm.

The rest of the paper is organized as follows. Section 2 introduces the noise constrained Tikhonov problem and reviews some basic properties of Newton’s method and the approach taken in [9]. The main novel contribution of this work is presented in section 3 where we derive the Projected Newton method. In section 4 a convergence result is formulated and proven for the new algorithm. Experimental results, as well as a reference method, can be found in section 5. Lastly, this work is concluded and possible future research directions are proposed in section 6.

2. Newton’s method for noise constrained Tikhonov regularization

Let us consider the following equality constrained optimization problem:

\[
\min_{x \in \mathbb{R}^n} \frac{1}{2}||x||^2 \quad \text{subject to} \quad \frac{1}{2}||Ax||^2 = \frac{\sigma^2}{2}
\]
where we denote $\sigma = \eta \varepsilon$ for the value used in the discrepancy principle, see (3). The Lagrangian of (4) is given by
\[
L(x, \lambda) = \frac{1}{2}||x||^2 + \lambda \left( \frac{1}{2}||Ax - b||^2 - \sigma^2 \right)
\] (5)
where $\lambda \in \mathbb{R}$ is the Lagrange multiplier. It follows from classical constrained optimization theory that if $x^*$ is a solution of (4) then there exists a Lagrange multiplier $\lambda^*$ such that $F(x^*, \lambda^*) = 0$ with
\[
F(x, \lambda) = \begin{pmatrix}
\lambda A^T (Ax - b) + x \\
\frac{1}{2}||Ax - b||^2 - \sigma^2
\end{pmatrix}.
\] (6)
The first component of this nonlinear function is the gradient of the Lagrangian with respect to $x$, i.e. $\nabla_x L(x, \lambda)$, while the second component is simply the constraint. These are in fact the first order optimality conditions, also known as Karush-Kuhn-Tucker or KKT conditions \[10\]. Note that any point $(x, \lambda)$ with $\lambda > 0$ that is a root of the first component of (6) is a Tikhonov solution (2) with $\alpha = 1/\lambda$:
\[
\lambda A^T (Ax - b) + x = 0 \iff A^T (Ax - b) + \frac{1}{\lambda} x = 0 \\
\iff A^T (Ax - b) + \alpha x = 0 \\
\iff (A^T A + \alpha I) x = A^T b.
\]
In \[9\] it is shown that (4) has a unique solution $x^*$ and that the corresponding Lagrange multiplier $\lambda^*$ is strictly positive. Now if we write $\alpha^* = 1/\lambda^*$ it follows from the discussion above that $(x^*, \alpha^*)$ satisfies the Tikhonov equations (2) as well as the discrepancy principle (3). This means that if we solve (4), we have simultaneously found the regularization parameter and corresponding Tikhonov solution that satisfies the discrepancy principle. Henceforth we refer to (4) as the noise constrained Tikhonov problem.

A modification of Newton’s method to solve the nonlinear system of equations $F(x, \lambda) = 0$ is presented in \[9\], which the author refers to as the Lagrange Method since it is based on the Lagrangian (5). The Newton direction for this particular problem starting from a point $(x, \lambda)$ is defined as the solution of the linear system
\[
J(x, \lambda) \begin{pmatrix}
\Delta x \\
\Delta \lambda
\end{pmatrix} = -F(x, \lambda)
\] (7)
where $J(x, \lambda) \in \mathbb{R}^{n \times (n+1)}$ is the Jacobian matrix of $F(x, \lambda)$ and is given by
\[
J(x, \lambda) = \begin{pmatrix}
\lambda A^T A + I & A^T (Ax - b) \\
(Ax - b)^T A & 0
\end{pmatrix}.
\]
We can express the determinant of this matrix as
\[
\det J(x, \lambda) = -(Ax - b)^T A (\lambda A^T A + I)^{-1} A^T (Ax - b) \det(\lambda A^T A + I).
\]
due to the $2 \times 2$ block structure of the matrix $[11]$. Thus we know that $J(x, \lambda)$ is nonsingular when $\lambda \geq 0$ and $A^T(Ax - b) \neq 0$. Indeed, this follows from the fact that both $\lambda A^T + I$ and $(\lambda A^T + I)^{-1}$ are positive definite and hence $\text{det} \ J(x, \lambda) < 0$.

It is well known that the Newton direction is a descent direction for the merit function $f(x, \lambda) = \frac{1}{2}||F(x, \lambda)||^2$, which can be seen from the following calculation

$$
\nabla f(x, \lambda)^T \left( \begin{array}{c} \Delta x \\ \Delta \lambda \end{array} \right) = \left( J(x, \lambda)^T F(x, \lambda) \right)^T \left( -J(x, \lambda)^{-1} F(x, \lambda) \right)
$$

$$
= -||F(x, \lambda)||^2 \leq 0.
$$

Now it follows from Taylor’s theorem [10] that starting from the point $(x, \lambda)$, we can either find a step-length $\gamma > 0$ such that $f(x + \gamma \Delta x, \lambda + \gamma \Delta \lambda) < f(x, \lambda)$ or we have found the solution to $F(x, \lambda) = 0$. In [9] a different merit function is chosen, namely

$$
m(x, \lambda) = \frac{1}{2}||A^T(Ax - b) + x||^2 + \frac{w}{2} \left( \frac{1}{2}||Ax - b||^2 - \frac{\sigma^2}{2} \right)^2
$$

with $w \in \mathbb{R}$ a fixed weight. Note that for $w = 1$ this merit function coincides with the usual merit function $f(x, \lambda)$. The Lagrange method calculates in each iteration an approximate solution $\tilde{\Delta}$ to (7) using the Krylov subspace method MINRES [12] and then chooses the step-length $\gamma$ such that there is a sufficient decrease of the merit function $m(x, \lambda)$, i.e.

$$
m(x + \gamma \Delta x, \lambda + \gamma \Delta \lambda) < m(x, \lambda) + c\gamma \nabla m(x, \lambda)^T \tilde{\Delta}
$$

with $c \in (0, 1)$ and such that $\lambda > 0$ and $A^T(Ax - b) \neq 0$ by means of a backtracking line search. Furthermore it is shown that by choosing a specific tolerance $\xi$ for the relative residual $||J(x, \lambda)\tilde{\Delta} + F(x, \lambda)|| \leq \xi ||F(x, \lambda)||$ such a step-length $\gamma$ can always be found and that the algorithm converges to the unique solution of the noise constrained Tikhonov problem (4). Even when solving (7) to a certain tolerance with a Krylov subspace method, calculating the Newton direction is computationally expensive for large scale problems since each MINRES iteration requires a matrix-vector product with $A$ and $A^T$.

**Remark 2.1.** The Lagrange method is able to solve the more general equality constrained optimization problem

$$
\min_{x \in \mathbb{R}^n} \phi(x) \quad \text{subject to} \quad \frac{1}{2}||Ax - b||^2 = \frac{\sigma^2}{2}
$$

where $\phi(x)$ is a general regularization functional. However, since we are concerned with the Tikhonov solution, we only consider the functional $\phi(x) = ||x||^2/2$.

3. Projected Newton method

In this section we derive the Projected Newton method by projecting the noise constrained Tikhonov problem (4) onto a $k$ dimensional Krylov subspace $K_k(A^T A, A^T b)$,
where $k$ is the iteration index of the new algorithm. In each iteration we expand the basis $V_k$ for the Krylov subspace by the bidiagonalization algorithm proposed by Paige and Saunders [13, 14] and calculate an approximate solution in the Krylov subspace using a single Newton iteration on the projected system. We show that by calculating the Newton direction in the projected space, which can be done very efficiently for small values of $k$, we get a descent direction for the merit function $m(x, \lambda)$. We start our discussion by a brief review of the bidiagonal decomposition [15].

3.1. Bidiagonalization

**Theorem 3.1** (Bidiagonal decomposition). If $A \in \mathbb{R}^{m \times n}$ with $m \geq n$, then there exists orthonormal matrices

$$U = (u_0, u_1, \ldots, u_{m-1}) \in \mathbb{R}^{m \times m} \quad \text{and} \quad V = (v_0, v_1, \ldots, v_{n-1}) \in \mathbb{R}^{n \times n}$$

and a lower bidiagonal matrix

$$B = \begin{pmatrix}
\mu_0 & 
\nu_1 &
\mu_1 & 
\nu_2 &
\ddots &
\nu_{k-1} &
\mu_{k-1} & 
\nu_{n-1} &
\nu_n \\
0 & 
0 &
0 & \ddots &
0 &
0 & \ddots &
0 &
0 & 
\mu_n
\end{pmatrix} \in \mathbb{R}^{(n+1) \times n},$$

such that

$$A = U \begin{pmatrix} B \\ 0 \end{pmatrix} V^T.$$

**Proof.** See [15].

Starting from a given unit vector $u_0 \in \mathbb{R}^m$ it is possible to generate the columns of $U$, $V$ and $B$ recursively using the Bidiag1 procedure proposed by Paige and Saunders [13, 14], see algorithm [2]. Reorthogonalization can be added for numerical stability. Note that this bidiagonal decomposition is the basis for the LSQR algorithm and that after $k$ steps of Bidiag1 starting with the initial vector $u_0 = b/\|b\|$ we have matrices $V_k = [v_0, v_1, \ldots, v_{k-1}] \in \mathbb{R}^{n \times k}$ and $U_{k+1} = [u_0, u_1, \ldots, u_k] \in \mathbb{R}^{m \times (k+1)}$ with orthonormal columns and a lower bidiagonal matrix $B_{k+1,k} \in \mathbb{R}^{(k+1) \times k}$ that satisfy

$$AV_k = U_{k+1}B_{k+1,k} \quad (10)$$
$$A^T U_{k+1} = V_k B_{k+1,k}^T + \mu_k v_k e_{k+1}^T \quad (11)$$

with $e_{k+1} = (0, 0, \ldots, 0, 1)^T \in \mathbb{R}^{k+1}$. Here, the matrix $B_{k+1,k}$ consists of the first $k + 1$ rows and $k$ columns of $B$.

The columns of $V_k$ and $U_k$ both span a Krylov subspace of dimension $k$, more specifically we have

$$\begin{cases}
\text{span } V_k = K_k(A^T A, A^T b) \\
\text{span } U_k = K_k(A A^T, b)
\end{cases}$$
where for a general square matrix \( M \) and vector \( z \) the Krylov subspace of dimension \( k \) is defined as

\[
K_k(M, z) = [z, Mz, M^2z, \ldots, M^{k-1}z].
\]

**Algorithm 1 Bidiag**

1. Choose initial unit vector \( u_0 \) (typically \( b / \| b \| \)).
2. Set \( v_0v_{-1} = 0 \)
3. for \( k = 0, 1, \ldots, n - 1 \) do
4. \( r_k = A^T u_k - v_k v_{k-1} \)
5. Reorthogonalize \( r_k \) w.r.t. \( V_k \) if necessary.
6. \( \mu_k = \| r_k \| \) and \( v_k = r_k / \mu_k \).
7. \( p_k = A v_k - \mu_k u_k \)
8. Reorthogonalize \( p_k \) w.r.t. \( U_{k+1} \) if necessary.
9. \( v_{k+1} = \| p_k \| \) and \( u_{k+1} = p_k / v_{k+1} \).
10. end for

3.2. **The projected Newton direction**

In order to solve the noise constrained Tikhonov problem \( 4 \) we calculate a series of approximate solutions in the Krylov subspace spanned by the columns of the orthonormal basis \( V_k \):

\[
x_k \in \text{span} \ V_k = K_k(A^T A, A^T b) = [A^T b, (A^T A) A^T b, \ldots, (A^T A)^{k-1} A^T b].
\]

This means that \( x_k = V_k y_k \) for some \( y_k \in \mathbb{R}^k \) with \( k \geq 1 \) and \( x_0 = 0 \). Using \( 10 \) and the fact that \( V_k \) and \( U_{k+1} \) are orthonormal matrices we have \( \| x_k \| = \| V_k y_k \| = \| y_k \| \) and

\[
\| A x_k - b \| = \| A V_k y_k - b \| = \| U_{k+1} B_{k+1, k} y_k - U_{k+1} c_{k+1} \| = \| B_{k+1, k} y_k - c_{k+1} \| \quad (12)
\]

where \( c_{k+1} = (\| b \|, 0, \ldots, 0)^T \in \mathbb{R}^{k+1} \). So now we can see that the projected minimization problem of dimension \( k \):

\[
\min_{x_k \in \text{span} \ V_k} \frac{1}{2} \| x_k \|^2 \quad \text{subject to} \quad \frac{1}{2} \| A x_k - b \|^2 = \frac{\sigma^2}{2} \quad (13)
\]

can alternatively be written using the bidiagonal decomposition as

\[
\min_{y_k \in \mathbb{R}^k} \frac{1}{2} \| y_k \|^2 \quad \text{subject to} \quad \frac{1}{2} \| B_{k+1, k} y_k - c_{k+1} \|^2 = \frac{\sigma^2}{2}. \quad (14)
\]

Similarly as explained in section \( 2 \) the solution \( y_k^* \) of \( 14 \) with corresponding Langrange multiplier \( \lambda_k^* \) satisfies \( F^{(k)}(y_k^*, \lambda_k^*) = 0 \) where the equation is now given by

\[
F^{(k)}(y, \lambda) = \left( \lambda B_{k+1, k}^T (B_{k+1, k} y - c_{k+1}) + y \right) + \frac{1}{2} \| B_{k+1, k} y - c_{k+1} \|^2 - \frac{\sigma^2}{2}.
\]  \quad (15)
The function \( F^{(k)}(y, \lambda) \) can be seen as a projected version of the function \( F(x, \lambda) \) given by (6). The Jacobian \( J^{(k)}(y, \lambda) \in \mathbb{R}^{(k+1) \times (k+1)} \) of \( F^{(k)}(y, \lambda) \) is given by

\[
J^{(k)}(y, \lambda) = \begin{pmatrix}
\lambda B_{k+1,k}^T B_{k+1,k} + I_k & B_{k+1,k}^T (B_{k+1,k} y - c_{k+1}) \\
(B_{k+1,k} y - c_{k+1})^T B_{k+1,k} & 0
\end{pmatrix}
\]

where \( I_k \) is the \( k \times k \) identity matrix. If \( \lambda \geq 0 \) then \( \lambda B_{k+1,k}^T B_{k+1,k} + I_k \) is a positive definite matrix and we again have that \( J^{(k)}(y, \lambda) \) is nonsingular if and only if

\[
B_{k+1,k}^T (B_{k+1,k} y - c_{k+1}) \neq 0.
\]

Let us denote \( \tilde{y}_{k-1} = (y_{k-1}^T, 0)^T \in \mathbb{R}^k \) for \( k \geq 1 \) where \( y_{k-1} \) is an approximation of the solution of the projected minimization problem of dimension \( k-1 \) and \( y_0 = (\ ) \) an empty vector. Note that \( \tilde{y}_{k-1} \) can be seen as a good initial guess for the projected minimization problem of dimension \( k \), see (14). If \( J^{(k)}(\tilde{y}_{k-1}, \lambda_{k-1}) \) is nonsingular – a condition we will enforce by step-length selection – we can calculate the Newton direction for the projected function \( F^{(k)}(y, \lambda) \) starting from the point \( (\tilde{y}_{k-1}, \lambda_{k-1}) \), i.e.:

\[
\begin{pmatrix}
\Delta y_k \\
\Delta \lambda_k
\end{pmatrix} = -J^{(k)}(\tilde{y}_{k-1}, \lambda_{k-1})^{-1} F^{(k)}(\tilde{y}_{k-1}, \lambda_{k-1})
\]

We can then update \( \tilde{y}_{k-1} \) and \( \lambda_{k-1} \) by

\[
\begin{cases}
y_k = \tilde{y}_{k-1} + \gamma \Delta y_k \\
\lambda_k = \lambda_{k-1} + \gamma \Delta \lambda_k
\end{cases}
\]

with a suitably chosen step-length \( \gamma \). This gives us a corresponding update for \( x_{k-1} \):

\[
x_k = V_k y_k = V_k \tilde{y}_{k-1} + \gamma V_k \Delta y_k \\
= V_{k-1} y_{k-1} + \gamma V_k \Delta y_k \\
= x_{k-1} + \gamma \underbrace{V_k \Delta y_k}_{:= \Delta x_k}.
\]

By multiplying the Newton step \( \Delta y_k \) for the projected variable \( \tilde{y}_{k-1} \) by \( V_k \) we obtain a step \( \Delta x_k \) for \( x_{k-1} \). Note that this step is different from the Newton step that would be obtained by solving (7) for \( (x_{k-1}, \lambda_{k-1}) \). However, we will show that the step \( (\Delta x_k^T, \Delta \lambda_k)^T \) is a descent direction for \( m(x_{k-1}, \lambda_{k-1}) \), see (8), which is the main result of the current section. For ease of notation we prove the result for \( w = 1 \), which means \( m(x, \lambda) = f(x, \lambda) = \frac{1}{2} ||F(x, \lambda)||^2 \), however the proof easily generalizes for all \( w \in \mathbb{R} \). We start by proving the following lemma:

**Lemma 3.2.** Let \( F(x, \lambda) \) be defined as (4) and \( F^{(k)}(y, \lambda) \) as (15). Furthermore let \( \tilde{y}_{k-1} = (y_{k-1}^T, 0)^T \in \mathbb{R}^k \) and \( x_{k-1} \in \mathbb{R}^n \) be such that \( x_{k-1} = V_k \tilde{y}_{k-1} \) for the orthonormal basis \( V_k \) generated by Bidiag1. Then we have following equality:

\[
||F(x_{k-1}, \lambda_{k-1})|| = ||F^{(k)}(\tilde{y}_{k-1}, \lambda_{k-1})||.
\]

\( (18) \)
Proof. First note that we can write
\[ \|F(x_{k-1}, \lambda_{k-1})\|^2 = \|\lambda_{k-1}A^T(Ax_{k-1} - b) + x_{k-1}\|^2 + \left( \frac{1}{2} \|Ax_{k-1} - b\|^2 - \frac{\sigma^2}{2} \right)^2. \]
Similarly as shown in (12) we have that \(\|Ax_{k-1} - b\| = \|B_{k+1,k}\|\). Now let us take a closer look at the first term:
\[
\|\lambda_{k-1}A^T(Ax_{k-1} - b) + x_{k-1}\|
\]
\[= \|\lambda_{k-1}A^T(AV_ky_{k-1} - b) + V_ky_{k-1}\| \]
\[= \|\lambda_{k-1}A^TU_{k+1}(B_{k+1,k}y_{k-1} - c_{k+1}) + V_ky_{k-1}\| \]
\[= \|\lambda_{k-1}V_kB_{k+1,k}^T(B_{k+1,k}y_{k-1} - c_{k+1}) + V_ky_{k-1}\| \]
\[= \|\lambda_{k-1}B_{k+1,k}^T(B_{k+1,k}y_{k-1} - c_{k+1}) + y_{k-1}\|. \]
The second to last equality follows from the fact that the last element of \((B_{k+1,k}y_{k-1} - c_{k+1})\) is zero and that the matrices \(V_kB_{k+1,k}^T \) and \(V_kB_{k+1,k}^T + \mu_kv_k\) only differ in the last column. Now the proof follows from the fact that we have
\[ \|F^{(k)}(\bar{y}_{k-1}, \lambda_{k-1})\|^2 = \|\lambda_{k-1}B_{k+1,k}^T(B_{k+1,k}y_{k-1} - c_{k+1}) + y_{k-1}\|^2 \]
\[+ \left( \frac{1}{2} \|B_{k+1,k}y_{k-1} - c_{k+1}\|^2 - \frac{\sigma^2}{2} \right)^2. \]
\[\]
Lemma 3.3. Let \(F(x, \lambda)\) be defined as (6) and \(F^{(k)}(y, \lambda)\) as (15). Furthermore let \(\bar{y}_{k-1} = (y_{k-1}^T, 0)^T \in \mathbb{R}^k\) and \(x_{k-1} \in \mathbb{R}^n\) be such that \(x_{k-1} = V_k\bar{y}_{k-1}\) for the orthonormal basis \(V_k\) generated by Bidiag1. Then we have following equality:
\[
\begin{pmatrix}
V_k^T \\
0 \\
1
\end{pmatrix} J(x_{k-1}, \lambda_{k-1}) F(x_{k-1}, \lambda_{k-1}) = J^{(k)}(\bar{y}_{k-1}, \lambda_{k-1}) F^{(k)}(\bar{y}_{k-1}, \lambda_{k-1}). \tag{19}
\]
Proof. Let us first introduce notations \(t_{k+1} = B_{k+1,k}\) and
\[ \zeta_k = \frac{1}{2} \left( \|Ax_{k-1} - b\|^2 - \sigma^2 \right) = \frac{1}{2} \left( \|t_{k+1}\|^2 - \sigma^2 \right). \]
The left-hand side of equality (19) can be rewritten as
\[
\begin{pmatrix}
V_k^T \\
0 \\
1
\end{pmatrix} J(x_{k-1}, \lambda_{k-1}) F(x_{k-1}, \lambda_{k-1})
\]
\[= \begin{pmatrix}
V_k^T \\
0 \\
1
\end{pmatrix} \begin{pmatrix}
\lambda_{k-1}A^TA + I \\
(Ax_{k-1} - b)^T A
\end{pmatrix} \begin{pmatrix}
\lambda_{k-1}A^T(Ax_{k-1} - b) + x_{k-1} \\
0
\end{pmatrix} \frac{\zeta_k}{\zeta_k}
\]
\[= \begin{pmatrix}
\lambda_{k-1}V_k^TA + V_k^T \\
V_k^T \\
(Ax_{k-1} - b)^TA
\end{pmatrix} \begin{pmatrix}
\lambda_{k-1}A^T(Ax_{k-1} - b) + x_{k-1} \\
0
\end{pmatrix} \frac{\zeta_k}{\zeta_k}
\]
\[= \begin{pmatrix}
\lambda_{k-1}V_k^TA + V_k^T \lambda_{k-1}A^T(Ax_{k-1} - b) + x_{k-1} + \zeta_k V_k^TA^T(Ax_{k-1} - b) \\
\lambda_{k-1}(Ax_{k-1} - b)^TA^T(Ax_{k-1} - b) + (Ax_{k-1} - b)^TAx_{k-1}
\end{pmatrix} \frac{\zeta_k}{\zeta_k}. \]
Similarly we can rewrite the right-hand side of equality (19) as

\[
J^{(k)}(\bar{y}_{k-1}, \lambda_{k-1})F^{(k)}(\bar{y}_{k-1}, \lambda_{k-1}) = \begin{pmatrix}
\lambda_{k-1} B^T_{k+1,k} B_{k+1,k} + I_k & B^T_{k+1,k} t_{k+1} \\
t^T_{k+1} B_{k+1,k} & 0
\end{pmatrix} \begin{pmatrix}
\lambda_{k-1} B^T_{k+1,k} t_{k+1} + \bar{y}_{k-1} \\
\zeta_k
\end{pmatrix} = \begin{pmatrix}
(\lambda_{k-1} B^T_{k+1,k} B_{k+1,k} + I_k)(\lambda_{k-1} B^T_{k+1,k} t_{k+1} + \bar{y}_{k-1}) + \zeta_k B^T_{k+1,k} t_{k+1} \\
\lambda_{k-1} t^T_{k+1} B_{k+1,k} B_{k+1,k} t_{k+1} + t^T_{k+1} B_{k+1,k} \bar{y}_{k-1}
\end{pmatrix}.
\]

We can now compare all individual terms and check if they are indeed equal. Let us work out the last component as an example:

\[
\lambda_{k-1}(Ax_{k-1} - b)^T A A^T (Ax_{k-1} - b) + (Ax_{k-1} - b)^T A x_{k-1} = \lambda_{k-1}(AV_k \bar{y}_{k-1} - b)^T A A^T (AV_k \bar{y}_{k-1} - b) + (AV_k \bar{y}_{k-1} - b)^T A V_k \bar{y}_{k-1} = \lambda_{k-1} t^T_{k+1} U_{k+1} A A^T U_{k+1} t_{k+1} + t^T_{k+1} U_{k+1} A V_k \bar{y}_{k-1} = \lambda_{k-1} t^T_{k+1} B_{k+1,k} B_{k+1,k} t_{k+1} + t^T_{k+1} B_{k+1,k} \bar{y}_{k-1} = \lambda_{k-1} t^T_{k+1} B_{k+1,k} B_{k+1,k} t_{k+1} + t^T_{k+1} B_{k+1,k} \bar{y}_{k-1}.
\]

The last equality follows from the fact that \(U_{k+1} A A^T U_{k+1}\) and \(B_{k+1,k} B_{k+1,k}\) only differ in the last column and that the last element of \(t_{k+1}\) is equal to zero. Indeed, using (11) we have

\[
U_{k+1} A A^T U_{k+1} = (V_k B^T_{k+1,k} + \mu_k v_k e^T_{k+1})^T (V_k B^T_{k+1,k} + \mu_k v_k e^T_{k+1}) = B_{k+1,k} V_k V_k^T B^T_{k+1,k} + 2 \mu_k e_{k+1} v^T_k V_k B^T_{k+1,k} + \mu^2_k e^T_{k+1} e^T_{k+1} = B_{k+1,k} B^T_{k+1,k} + \mu^2_k e^T_{k+1} e^T_{k+1}
\]

which shows that these matrices only differ in the last element. Equality of the first component can be proven similarly.

\[\square\]

Lemmas 3.2 and 3.3 allow us to prove the main result of the current section:

**Theorem 3.4.** Let \(\frac{\Delta y_k}{\Delta \lambda_k}\) be defined as in (17) and let \(\Delta x_k = V_k \Delta \lambda_k\), where \(V_k\) is the orthonormal matrix generated by Bidiag1. Then we have

\[
\begin{pmatrix}
\Delta x_k \\
\Delta \lambda_k
\end{pmatrix}^T \nabla f(x_{k-1}, \lambda_{k-1}) = -||F(x_{k-1}, \lambda_{k-1})||^2 \leq 0
\]

which means that \(\frac{\Delta x_k}{\Delta \lambda_k}\) is a descent direction for \(f(x_{k-1}, \lambda_{k-1})\).
Proof. The result now follows from an easy calculation:

\[
\begin{pmatrix}
\Delta x_k \\
\Delta \lambda_k
\end{pmatrix}^T \nabla f(x_{k-1}, \lambda_{k-1}) = \begin{pmatrix}
V_k \Delta y_k \\
\Delta \lambda_k
\end{pmatrix}^T J(x_{k-1}, \lambda_{k-1}) F(x_{k-1}, \lambda_{k-1}) = \begin{pmatrix}
\Delta y_k \\
\Delta \lambda_k
\end{pmatrix}^T \begin{pmatrix}
V_k^T & 0 \\
0 & 1
\end{pmatrix} J(x_{k-1}, \lambda_{k-1}) F(x_{k-1}, \lambda_{k-1})
\]

\[
\begin{aligned}
\sum_{i=1}^{k+1} \left( \frac{\partial F^T}{\partial y_{k-1}(\bar{y}_{k-1}, \bar{\lambda}_{k-1})} \frac{y_{k-1}}{V_k} \right)^2 & < 0
\end{aligned}
\]

Theorem 3.4 implies that we can compute the Newton direction for the projected function \(F^{(k)}(\bar{y}_{k-1}, \bar{\lambda}_{k-1})\), which we refer to as a projected Newton direction, and obtain a descent direction for \(f(x_{k-1}, \lambda_{k-1})\) by multiplying the step \(\Delta y_k\) with the Krylov subspace basis \(V_k\). Alternatively, this can be seen as performing a single Newton iteration on the projected minimization problem of dimension \(k\) with initial guess \((y_{k-1}^T, 0)^T\), where \(y_{k-1}\) is the approximate solution of the \(k-1\) dimensional projected optimization problem and then multiplying the result \(y_k\) with \(V_k\) to obtain an approximate solution \(x_k = V_k y_k\) of the noise constrained Tikhonov problem \([1]\). Subsequently, the Krylov subspace basis is expanded and the procedure is repeated until a sufficiently accurate solution is found.

When \(k \ll n\) calculating the projected Newton step is much cheaper than calculating the actual Newton direction for \(F(x_{k-1}, \lambda_{k-1})\), since the former requires us to solve a \((k+1) \times (k+1)\) linear system, while the latter is found by solving an \((n+1) \times (n+1)\) linear system. Moreover, theorem 3.4 guarantees the existence of a step-length \(\gamma > 0\) such that

\[
\frac{1}{2} ||F(x_k, \lambda_k)||^2 < \left( \frac{1}{2} - c\gamma \right) ||F(x_{k-1}, \lambda_{k-1})||^2
\]

(21)

with \(c \in (0, 1)\). Equation (21) is often referred to in literature as a sufficient decrease condition. A step-length \(\gamma\) for which the sufficient decrease condition holds is in practice often found using a so-called backtracking line search. We start by setting \(\gamma = 1\) (which corresponds to taking a full Newton step) and check if (21) holds. If not, we decrease \(\gamma\) by a factor \(\tau \in (0, 1)\), say \(\tau = 0.9\), and check if \(\gamma := \tau \gamma\) satisfies the condition. This procedure is then repeated until a suitable step-length is found.
Remark 3.5. The sufficient decrease condition \( (21) \) can be efficiently computed in the Krylov subspace. First of all, from lemma 3.2 we know how to compute the previous residual norm using \( F(k)(y,\lambda) \). So what we need to know is how the compute \( ||F(x_k,y_k)|| \). Let us denote \( B_{k,k} \in \mathbb{R}^{k \times k} \) for \( k \geq 1 \) the square matrix containing the first \( k \) columns of \( B_{k+1,k} \). We can then show similarly as in the proof of lemma 3.2 that \( ||F(x_k,y_k)|| = ||\bar{F}(k)(\bar{y}_k,\lambda_k)|| \) with

\[
\bar{F}(k)(y,\lambda) = \left( \lambda B_{k+1,k+1}^T(B_{k+1,k+1} y - c_{k+1}) + y \right)
\]

Note that the only difference between \( \bar{F}(k) \) and \( F(k) \) is the multiplication with the matrix \( B_{k+1,k+1} \) instead of \( B_{k+1,k} \). This norm can thus be computed if we have the basis \( V_{k+1}, U_{k+1} \) and matrix \( B_{k+1,k+1} \) in iteration \( k \).

Following the discussion above, we can now formulate the Projected Newton method, see algorithm 2.

Remark 3.6. For notational convenience we choose to present algorithm 2 with merit function \( f(x,\lambda) \), however the algorithm can easily be reformulated to allow the more general merit function \( m(x,\lambda) \) as defined in \((8)\). Note that the results presented in the current section as well as the convergence results presented in the following section, section 4, can also be proven for this choice of merit function.

Remark 3.7. Algorithm 2 can be adapted to allow for general form Tikhonov regularization. In its general form, the Tikhonov problem is written as

\[
x_\alpha = \arg\min_{x \in \mathbb{R}^n} \frac{1}{2} \|Ax - b\|^2 + \frac{\alpha}{2} \|L(x - x_0)\|^2,
\]

with \( x_0 \in \mathbb{R}^n \) an initial estimate and \( L \in \mathbb{R}^{p \times n} \) a regularization matrix, both chosen to incorporate prior knowledge or to place specific constraints on the solution \([16, 2]\). If \( L \) is a square invertible matrix, then the problem can be written in the standard form

\[
z_\alpha = \arg\min_{z \in \mathbb{R}^n} \frac{1}{2} \|\bar{A}z - r_0\|^2 + \frac{\alpha}{2} \|z\|^2,
\]

by using the transformation

\[
z = L(x - x_0), \quad \bar{A} = AL^{-1}, \quad r_0 = b - Ax_0.
\]

When \( L \) is not square invertible, some form of pseudoinverse has to be used, but the reformulation of the problem remains the same \([2]\).

After solving \((23)\), the solution of \((22)\) can be found as

\[
x = x_0 + L^{-1}z.
\]

For this reason, we focus our attention on the standard form Tikhonov problem \([4]\).
that \( \phi \) projected minimization problem (13) to the more convenient form (14) we use the fact in literature as Basis Pursuit denoising \([20, 21, 22]\). Hence, we would like to be \( \ell \)

TV is important to preserve edges in a reconstructed image, the total variation functional \( \phi \) regularization functional \( \phi \) Tikhonov regularization. However, in many applications a different

Remark 3.8. In its current form, the Projected Newton method can only be used for (general form) Tikhonov regularization. However, in many applications a different regularization functional \( \phi(x) \) produces better reconstructions. For instance, when it is important to preserve edges in a reconstructed image, the total variation functional \( \text{TV}(x) \) is a good candidate \([17, 18, 19]\) . Another popular regularization functional is the \( \ell_1 \)-norm \( || \cdot ||_1 \), which is known to produce a sparse solution and is often referred to in literature as Basis Pursuit denoising \([20, 21, 22]\). Hence, we would like to be able to solve the more general regularization problem \([7]\). However, to reformulate the projected minimization problem (13) to the more convenient form (14) we use the fact that \( \phi(x_k) = \phi(V_k y_k) = \phi(y_k) \) for the Tikhonov functional \( \phi(x) = ||x||^2/2 \), which is not true in general. Hence, at the current time, it is unclear how the projection step can be

\begin{algorithm}
\textbf{Algorithm 2} Projected Newton method
\begin{algorithmic}[1]
\State \( \bar{y}_0 = 0; x_0 = 0; \tau = 0.9; \alpha = 10^{-4}; \psi = 10^{-16}; k = 1; \) \# Initialization
\State \( u_0 = b/||b||; r_0 = A^T u_0; \mu_0 = ||r_0||; v_0 = r_0/\mu_0; \) \# Calculate \( B_{1,1}, V_1 \) and \( U_1 \)
\While {\( ||F^{(k)}(\bar{y}_{k-1}, \lambda_{k-1})|| > \text{tol} \)} \# Check for convergence
\State \( p_{k-1} = Av_{k-1} - \mu_{k-1}u_{k-1}; \) \# Calculate \( B_{k+1,1} \) and \( U_{k+1} \)
\State \( v_k = ||p_{k-1}||; u_k = p_{k-1}/v_k; \)
\State \( r_k = A^T u_k - \nu_kv_{k-1}; \) \# Calculate \( B_{k+1,k} \) and \( V_{k+1} \)
\State \( \nu_k = ||p_{k-1}||; r_k = p_{k-1}/v_k; \)
\State \( \mu_k = ||r_k||; v_k = r_k/\mu_k; \)
\EndWhile
\State \( y_k = y_{k-1} + \gamma_k\Delta y_k; \gamma_k = \tau(\lambda_{k-1}/\Delta \lambda_k); \lambda_k = \lambda_{k-1} + \gamma_k\Delta \lambda_k; \) \# Ensure positivity \( \lambda_k \)
\EndIf
\State \( \gamma_k = \tau(\lambda_{k-1}/\Delta \lambda_k); \lambda_k = \lambda_{k-1} + \gamma_k\Delta \lambda_k; \)
\EndIf
\EndWhile
\State \( y_k = y_{k-1} + \gamma_k\Delta y_k; \) \# Check for convergence
\EndWhile
\State \( x_k = V_k y_k; \) \# Update the solution
\State \( k = k + 1; \) \# Increase iteration index
\EndWhile
\State \( \text{return } x_k, \lambda_k \)
\end{algorithmic}
\end{algorithm}

Remark 3.8. In its current form, the Projected Newton method can only be used for (general form) Tikhonov regularization. However, in many applications a different regularization functional \( \phi(x) \) produces better reconstructions. For instance, when it is important to preserve edges in a reconstructed image, the total variation functional \( \text{TV}(x) \) is a good candidate \([17, 18, 19]\) . Another popular regularization functional is the \( \ell_1 \)-norm \( || \cdot ||_1 \), which is known to produce a sparse solution and is often referred to in literature as Basis Pursuit denoising \([20, 21, 22]\). Hence, we would like to be able to solve the more general regularization problem \([7]\). However, to reformulate the projected minimization problem (13) to the more convenient form (14) we use the fact that \( \phi(x_k) = \phi(V_k y_k) = \phi(y_k) \) for the Tikhonov functional \( \phi(x) = ||x||^2/2 \), which is not true in general. Hence, at the current time, it is unclear how the projection step can be
generalized for other regularization terms.

One idea is to solve a series of Tikhonov problems using the Projected Newton method, where we approximate the regularization term \( \phi(x) \) with a regularization term of the form \( ||Lx||_2^2 \) and then improve the approximation based on the obtained solution. Every subsequent Tikhonov problem would then be a better approximation of the general regularization problem (9). Similar approaches have been taken in [16, 23, 24].

4. Proof of convergence

In this section we show that, under the assumption that the iterates \( \{(x_k, \lambda_k)\}_{k \in \mathbb{N}} \) remain bounded, algorithm 2 converges to the solution of the noise constrained Tikhonov problem (4), i.e the limit point \( (x^*, \lambda^*) \) solves the nonlinear system of equations \( F(x, \lambda) = 0 \). The analysis in this section closely resembles the convergence analysis presented in [9].

First of all, we know by condition (16) that the projected Jacobian matrix \( J^{(k+1)}(\bar{y}_k, \lambda_k) \) is never singular since we enforce positivity of \( \lambda_k \) and require that \( B^T_{k+1, k}(B_{k+1, k} \bar{y}_k - c_{k+1}) \neq 0 \). Indeed, the first \( k \) elements of \( B^T_{k+2, k+1}(B_{k+2, k+1} \bar{y}_k - c_{k+2}) \) are equal to \( B^T_{k+1, k}(B_{k+1, k} \bar{y}_k - c_{k+1}) \) and is thus not equal to zero. Moreover, it is easy to see that a suitable step-length always exists which satisfies all the required inequalities.

We will use the following lemma to prove global convergence:

**Lemma 4.1.** Let \( f : Z \subset \mathbb{R}^{n+1} \rightarrow \mathbb{R} \) be a continuous function. Suppose there exists a sequence \( \{z_k\}_{k \in \mathbb{N}} \) such that:

\[
\begin{align*}
\bullet & \quad f(z_{k+1}) \leq f(z_k) \quad \forall k \in \mathbb{N} \\
\bullet & \quad z_k \rightarrow z^* \quad \forall k \in S \subset \mathbb{N}
\end{align*}
\]

Then

\[
\lim_{k \rightarrow \infty} f(z_k) = \lim_{k \in S} f(z_k) = f(z^*)
\]

**Proof.** See Lemma 4.1, page 89 of [25].

The following theorem is a fundamental result in calculus:

**Theorem 4.2 (Bolzano-Weierstrass Theorem).** Every bounded sequence in the Euclidean space \( \mathbb{R}^{n+1} \) has a convergent subsequence.

**Proof.** See Theorem 11.17, page 299 of [26].

We can now prove global convergence of algorithm 2 to the solution of the noise constrained Tikhonov problem:

**Theorem 4.3.** Suppose \( \{(x_k, \lambda_k)\}_{k \in \mathbb{N}} \) generated by algorithm 2 is a bounded sequence, then it converges to the solution of \( F(x, \lambda) = 0 \).
Proof. This proof closely resembles the proof of Theorem 4.1 in [9]. By the Bolzano-Weierstrass Theorem the sequence \( \{(x_k, \lambda_k)\}_{k \in \mathbb{N}} \) has a convergent subsequence. Hence we have an index set \( S \) such that

\[
(x_k, \lambda_k) \rightarrow (x^*, \lambda^*) \quad \forall k \in S \subset \mathbb{N}.
\]

Moreover, due the backtracking line search we know that \( f(x_k, \lambda_k) \) is a decreasing sequence. Hence, from the lemma 4.1 we now have that

\[
f(x_k, \lambda_k) \rightarrow f(x^*, \lambda^*) \quad \forall k \in \mathbb{N}.
\]

From the backtracking line search it also follows that

\[
f(x_{k+1}, \lambda_{k+1}) - f(x_k, \lambda_k) < -2c\gamma_{k+1}f(x_k, \lambda_k) < 0
\]

and as a consequence we have

\[
-2c \lim_{k \to \infty} \gamma_{k+1}f(x_k, \lambda_k) = 0.
\]

Since \( (1/\gamma_{k+1}) \geq 1 > 0 \) for all \( k \), we know

\[
\lim_{k \to \infty} f(x_k, \lambda_k) = f(x^*, \lambda^*) = 0
\]

We thus have \( \frac{1}{2}||F(x^*, \lambda^*)|| = f(x^*, \lambda^*) = 0.\)

What remains to show is convergence of the entire sequence \( \{(x_k, \lambda_k)\}_{k \in \mathbb{N}} \) to \( (x^*, \lambda^*) \). Assume that \( \{(x_k, \lambda_k)\}_{k \in \mathbb{N}} \) does not converge to \( (x^*, \lambda^*) \). Then there exists another index set \( \tilde{S} \neq S \) such that

\[
(x_k, \lambda_k) \rightarrow (\tilde{x}, \tilde{\lambda}) \quad \forall k \in \tilde{S} \subset \mathbb{N}
\]

and \( (\tilde{x}, \tilde{\lambda}) \neq (x^*, \lambda^*) \). But we can then show that \( (\tilde{x}, \tilde{\lambda}) \) is also a solution of our equations. However, we know that the solution is unique so we have a contraction, i.e. the entire sequence has to converge. \( \square \)

5. Numerical experiments

In this section we report the results of some numerical experiments with test problems from image deblurring and computed tomography. Moreover, to thoroughly test the robustness of the Projected Newton method, we apply the algorithm to 164 matrices from the Suite Sparse matrix collection [27]. We start this section by explaining another Krylov subspace method for automatic regularization based on the discrepancy principle, namely Generalized bidiagonal-Tikhonov, which we use to compare our newly developed method.
5.1. Reference method: Generalized bidiagonal-Tikhonov

In [16, 28, 29] a generalized Arnoldi-Tikhonov method (GAT) was introduced that iteratively solves the Tikhonov problem \([11]\) using a Krylov subspace method based on the Arnoldi decomposition of the matrix \(A\). Simultaneously, after each Krylov iteration, the regularization parameter is updated in order to approximate the value for which the discrepancy is equal to \(\eta \epsilon\). This is done using one step of the secant method to find the intersection of the discrepancy curve with the tolerance for the discrepancy principle, see figure \([1]\) but in the current Krylov subspace. Because the method is based on the Arnoldi decomposition, it only works for square matrices. However, by replacing the Arnoldi decomposition with the bidiagonal decomposition we used in section \([3]\) the method can be adapted to non-square matrices.

The update for the regularization parameter is done based on the regularized and the non-regularized residual. Let, in the \(k\)th iteration, \(z_k\) be the solution without regularization, i.e. \(\alpha = 0\), and \(y_k\) the solution with the current best regularization parameter, i.e. \(\alpha = \alpha_{k-1}\). We can then update the regularization parameter using

\[
\alpha_k = \frac{\eta \epsilon - r(z_k)}{r(y_k) - r(z_k)} \alpha_{k-1},
\]

(24)

where \(r(z_k) = ||B_{k+1,k}z_k - c_{k+1}||\) and \(r(y_k) = ||B_{k+1,k}y_k - c_{k+1}||\) are the residuals. A brief sketch of this method is given in algorithm \([3]\) but for more information we refer to [16, 28, 29]. Note that in the original GAT method, the non-regularized iterates \(z_k\) are equivalent to the GMRES \([30]\) iterations for the solution of \(Ax = b\). Now, because the Arnoldi decomposition is replaced with the bidiagonal decomposition, they are equivalent to the LSQR iterations for the solution of \(Ax = b\).

Remark 5.1. We use the same stopping criterion in algorithm \([3]\) as in algorithm \([2]\) for a fair comparison between both methods. Note however that since GBiT is based on the standard formulation of the Tikhonov problem \([1]\), we have to invert the parameter \(\alpha\). Moreover, evaluating this norm would require two additional matrix vector products in each iteration, which is a computationally expensive addition to the algorithm. In an actual implementation GBiT would use a different stopping criterion.

Remark 5.2. Note the difference between GBiT (and by extension GAT) and Projected Newton. While both methods solve the inverse problem in increasingly larger Krylov subspaces, the value that is minimized in each Krylov subspace and the way the regularization parameter is updated are different. GBiT solves the projected Tikhonov normal equations \([2]\) in each Krylov subspace using a fixed regularization parameter and only afterwards updates the regularization parameter for the next Krylov iteration. The Projected Newton method performs a single iteration of Newton to simultaneously update the solution and regularization parameter and then expands the Krylov subspace basis.
Projected Newton Method

Algorithm 3 Generalized bidiagonal-Tikhonov (GBiT) \[ \text{Input: } A, b, \alpha_0, \sigma, \text{tol} \]

1. \( x_0 = 0; \quad k = 1; \)
2. \( \textbf{while} \left\| F \left( x_{k-1}, \frac{1}{\alpha_{k-1}} \right) \right\| < \text{tol} \textbf{do} \)
3. \( \text{Calculate } U_{k+1}, B_{k+1,k} \text{ and } V_k \text{ using Bidiag1} \)
4. \( \text{Solve } B^T_{k+1,k}B_{k+1,k}z_k = B^T_{k+1,k}c_{k+1} \text{ for } z_k. \)
5. \( \text{Solve } (B^T_{k+1,k}B_{k+1,k} + \alpha_{k-1}I_k)y_k = B^T_{k+1,k}c_{k+1} \text{ for } y_k. \)
6. \( \text{Calculate } \alpha_k \text{ using } (24). \)
7. \( x_k = V_ky_k; \quad k = k + 1; \)
8. \( \textbf{end while} \)

Figure 2. The images “hst” and “satellite”, which represent the exact solution \( x_{ex} \), together with the distorted images, which represent the exact (i.e. noise-free) right-hand side \( b_{ex} \), generated by the different blurring functions from the IR tools package [31].

5.2. Image deblurring

Image deblurring is a rich source of linear inverse problems. For example in astronomy, when a ground-based telescope takes a picture of an object in space, the image is typically blurred due to the rapidly changing index of refraction of the atmosphere. Extraterrestrial photographs taken of earth are typically degraded by motion blur due to the slow camera shutter speed relative to the fast spacecraft motion [32]. A post-processing phase is then necessary to improve the quality of the picture. Other examples include microscopy, crowd surveillance, positron emmision tomography and many more, see for instance [33, 34, 35].

We use the matlab package IR tools [31] for generating test problems. This package
contains several functions that generate a matrix $A$, which models the blurring operator in different scenarios, and a corresponding right-hand side $b_{ex}$, which is a distorted version of the exact image. The function PRblurrotation, for example, generates data for an image deblurring problem where the blur simulates rotational motion blur. We consider the functions PRblurgauss, PRblurmotion and PRblurspeckle applied to the exact image “hst” and the functions PRblurdefocus, PRblurshake and PRblurrotation applied to the image “satellite”, see figure 2. These figures are also part of the IR tools package. For more information we refer the reader to [31].

We solve the deblurring test problems described above using GBiT, the Lagrange method and the Projected Newton method with tolerance $10^{-8}$. We apply reorthogonalization to the bidiagonalization procedure in both GBiT and Projected Newton. We set weight $w = 1$ for the merit function (8), $\alpha_0 = \lambda_0 = 1$ as initial regularization parameter and set the maximum number of iterations to 500. We take test images of size $256 \times 256$ and add 10% Gaussian noise to the right-hand side $b_{ex}$. For simplicity, we solve the Newton system (7) for the Lagrange method with a fixed precision of $10^{-6}$ using the Krylov subspace method MINRES and put the maximum number of iterations of MINRES equal to 100. The results of the experiment can be found in the top half of table 1. While the number of Newton iterations for the Lagrange method is quite small, the total number of matrix vector product is large since each Krylov iteration requires a matrix vector product with $A$ and $A^T$. Moreover, the backtracking line search also requires two matrix vector products each time the step-length is reduced. It can also be observed the the number of iterations for GBiT and Projected Newton seem to be similar. Note that both methods require two matrix vector products in each iteration and one matrix vector product for initialization. This assumes that we also use the projected function to check for convergence in GBiT, otherwise we get an additional two matrix vector products each iteration. See figure 3 for an example of the convergence history of all three methods in function of the number of matrix vector products.

5.3. Computed tomography

As a second class of test problems we consider x-ray computed tomography [38]. Here, the goal is to reconstruct the attenuation factor of an object based on the loss of intensity in the x-rays after they passed through the object. Classically, the reconstruction is done using analytical methods based on the Fourier and Radon transformations [39]. In the last decades interest has grown in algebraic reconstruction methods due to their flexibility when it comes to incorporating prior knowledge and handling limited data. Here, the problem is written as a linear system $Ax = b$, where $x$ represents the attenuation of the object in each pixel, the right-hand side $b$ is related to the intensity measurements of the x-rays and $A$ is a projection matrix. The precise structure of $A$ depends on the experimental set-up, but it is typically very sparse. For more information we refer to [40, 2, 41].
Table 1. Results of the numerical experiments as explained in section 5.2 (top) and section 5.3 (bottom). For the Lagrange method the column \#N denotes the number of Newton iterations, while \#\bar{K} denotes the average number of Krylov iterations per Newton iteration. For GBiT and the Projected Newton method (PN) \#K denotes the number of Krylov subspace iterations. The column MV gives the total number of matrix vector products for each of the methods. This includes the matrix vector products necessary for the backtracking line search in the Lagrange method.

Figure 3. Convergence history of PRblurgauss for the Lagrange method, Projected Newton and GBiT in function of the number of matrix vector products. For the Lagrange method, the circles denote the Newton iterations.
Projected Newton Method

Figure 4. The modified Shepp–Logan phantom (top) and grains image (bottom) of size $256 \times 256$ as exact solution $x_{ex}$ [36, 37] and corresponding sinogram $b_{ex}$ with 360 projection angles in $[0, \pi]$.

For our computed tomography experiments we consider a parallel beam geometry and use the ASTRA toolbox [42, 43] in order to generate the projection matrix $A$. To generate the test images we use the AIR tools package [36, 37]. As a first test problem we take the modified Shepp–Logan phantom of size $128 \times 128$ and take 180 projection angles in $[0, \pi]$, which corresponds to a matrix $A$ of size $23,040 \times 16,384$. We consider the same experimental set-up but with the Shepp–Logan phantom of size $256 \times 256$ and with 360 projection angles in $[0, \pi]$. We denote these two test problems as shepp128 and shepp256 respectively. For a third and fourth test problem we take the image grains as exact solution and again consider problem sizes $128 \times 128$ and $256 \times 256$ with 180 and 360 projection angles respectively. We denote these problems as grains128 and grains256. The exact solution $x_{ex}$ and the exact (noise-free) right-hand side $b_{ex}$, typically called a sinogram in computed tomography, for the problems shepp256 and grains256 are shown in figure 4. We again solve these test problems with the Lagrange method, Projected Newton and GBiT and use the same parameters as in section 5.2. The results of the experiment are shown in the bottom half of table 1. We can observe that the Lagrange method is not competitive compared to the other two algorithms in terms of matrix vector products. For the problems with the Shepp–Logan phantom we have the same number of Krylov iterations for GBiT and Projected Newton. However, for the grains test problems, the latter algorithm slightly outperforms the former. We investigate the number of Krylov iterations for these methods in a bit more detail in section 5.4.
It is well known that the Krylov subspace bases $V_k$ and $U_{k+1}$ are not guaranteed to be perfectly orthogonal (i.e. up to machine precision) if we apply the Bidiag1 algorithm in finite precision arithmetic without reorthogonalization [44, 45, 46]. However, our derivation of the Projected Newton method and proof of convergence heavily rely on the fact that they are. Hence, we are interested in the effect loss of orthogonality of the computed basis vectors has on convergence. To study this effect we solve test problem shepp128 using GBiT and Projected Newton with and without reorthogonalization. We use the same parameters as before but set the tolerance well below machine precision to check the attainable accuracy and set the maximum number of iterations to 100. The result is shown in figure 5.

In the first few iterations the effect of not reorthogonalizing in unnoticeable since at that point the basis vectors are still relatively orthogonal. However, from iteration 28 onward we can clearly see the difference. The effect is quite similar for GBiT and Projected Newton: while the left plot shows a decreasing series $||F(x_k, \lambda_k)||$, this value increases in some of the iterations on the right plot. Note that with our choice of merit function $f(x, \lambda)$, this behavior for Projected Newton in the right plot is not possible in exact arithmetic. Indeed, the backtracking line search in the Projected Newton method, see line 16 in algorithm 2, ensures that (21) holds, which means $||F(x_k, \lambda_k)|| < ||F(x_{k-1}, y_{k-1})||$ for all $k$. However, while this irregular behavior causes a small delay in convergence, it has hardly any effect on the attainable accuracy for this particular experiment. GBiT and Projected Newton with reorthogonalization both reach a tolerance of $10^{-10}$ in 59 iterations, while it takes them both 66 iterations when no reorthogonalization is applied. The effect might be more pronounced for other linear inverse problems, but a more thorough analysis of the loss of orthogonality is left as future work.
Projected Newton Method

Figure 6. Number of iterations (y-axis) needed for GBiT and Projected Newton to converge to the solution of the inverse problem with matrix (x-axis) from the SuiteSparse Matrix Collection and exact solution $x_{ex,i} = \sin(ih)$ for $h = 2\pi/(n + 1)$. Tolerance for convergence is set to $10^{-8}$ and 10% Gaussian noise is added. For both methods the initial regularization parameter is set to 1 and the maximum number of iterations is 500. Black circles indicate when the method did not converge to the desired tolerance within the maximum number of iterations.

Remark 5.3. When the number of Krylov iterations is small the computational overhead of reorthogonalizing the basis vectors is rather limited. However, if we need to perform a lot of Krylov iterations to converge, the additional cost is non-negligible. To reorthogonalize the bases $V_{k+1}$ and $U_{k+1}$ in iteration $k$ we need to calculate $2k$ dot-products, $2k$ multiplications of a vector with a scalar and $2k$ vector additions with vectors of length $n$. This amount to an additional $O(8kn)$ floating point operations. We could use more sophisticated techniques like partial reorthogonalization to reduce the computation overhead. We refer the reader to [46] for more information.

5.4. SuiteSparse Matrix Collection

As a final experiment we compare the number of Krylov subspace iterations needed for GBiT and Projected Newton to converge. We leave out the Langrange method in this experiment since it is clearly not competitive with the Krylov subspace based approaches, see table 1. We selected all real valued rectangular matrices from the SuiteSparse Matrix Collection [27] with number of rows and columns less than 10,000, resulting in a total of 164 matrices $A \in \mathbb{R}^{m \times n}$. When $m < n$ we take the transpose of the matrix. Next, we normalize the matrix such that the problem is well-scaled and then we generate a solution vector $x_{ex} \in \mathbb{R}^n$ with entries $x_{ex,i} = \sin(ih)$ for $h = 2\pi/(n + 1)$ and $1 \leq i \leq n$, calculate the right-hand side $b_{ex} = Ax_{ex} \in \mathbb{R}^m$ and add 10% Gaussian noise. We compare the total number of iterations that GBiT and Projected Newton need to converge to the solution with tolerance $\text{tol} = 10^{-8}$. We again use $\lambda_0 = \alpha_0 = 1$ for all problems and set weight $w = 10^{10}$ for the merit function (8) and put the maximum
Figure 7. Convergence history of GBiT and Projected Newton method applied to four selected matrices from the SuiteSparse Matrix Collection, see section 5.4. Left: two examples where Projected Newton significantly outperforms GBiT, due to the quadratic (local) convergence rate of Newton’s method. Right: two examples where convergence of GBiT and Projected Newton is very similar, since the convergence rate is determined by the dimension of the Krylov subspace.

The results of the experiment are given by figure 6. We have ordered the 164 matrices by the number of iterations needed for Projected Newton to converge. First note that the Projected Newton method converges for each of the 164 matrices within the maximum number of iteration, while GBiT does not converge to the desired tolerance for three of the matrices. Moreover, the number of iterations for Projected Newton to converge for these particular problems is less than or equal to the number of iterations of GBiT. Note however that for 90 of the 164 matrices, which is approximately 55%, the number of iterations for both methods is exactly the same. An intuitive explanation for this observation is the following: the rate of convergence of both methods is either limited by the dimension of the Krylov subspace, in which case both methods behave quite similarly, or convergence is determined by the rate of convergence of the root-finder. In the latter case, Projected Newton outperforms GBiT, since Newton’s method
has a quadratic (local) convergence while the secant method has only a linear rate of convergence. We illustrate this hypothesis with a few representative examples, see figure 7.

6. Conclusions & outlook

In this work we develop a new algorithm which simultaneously calculates the regularization parameter and corresponding Tikhonov regularized solution of an ill-posed least squares problem such that the discrepancy principle is satisfied. In section 2 we describe how this problem can be characterized as a constrained optimization problem. By projecting the problem onto a low dimensional Krylov subspace using the bidiagonalization procedure, we obtain a projected optimization problem, for which a Newton direction can be calculated very efficiently. We then show that this projected Newton direction produces a descent direction for the original problem. This result allows us to formulate the Projected Newton algorithm for which we prove a global convergence result. We consider some test problems from image deblurring and computed tomography to show the validity of the approach and compare Projected Newton with two other algorithms, namely the Lagrange method from [9] and the Generalized bidiagonal-Tikhonov method (GBiT), which uses the same bidiagonalization procedure. A first observation we make is that the Lagrange method is not competitive compared to the Krylov subspace based approaches in terms of the number of matrix vector products with $A$ and $A^T$. Next, we compare the number of Krylov subspace iterations needed for GBiT and Projected Newton to converge to a solution with the same tolerance. While in the majority of the experiments reported both methods roughly perform the same number of iterations, the Projected Newton method significantly outperforms GBiT for a large portion of the inverse problems. We hypothesize that this is due to the fact that, when convergence is not determined by the dimension of the Krylov subspace, the quadratic convergence rate of Newton’s method beats the linear rate of convergence of the secant method, which is used in GBiT.

A first possible future research direction is explained in remark 3.8. Since the Projected Newton method in its current form is only able to solve the general form Tikhonov problem, we are interested in how similar ideas can be used to solve the more general regularization problem (9). Although this work presents a solid theoretical foundation for the algorithm, some interesting research questions remain unanswered. A more formal discussion of the rate of convergence of the Projected Newton method is desirable. Furthermore, finite precision behavior of the algorithm is also something that would benefit from further investigation. More specifically, we are interested in the importance of the reorthogonalization step in the bidiagonalization algorithm, since the proofs we present rely heavily on the fact that we have an orthonormal basis. It is well known that a loss of orthogonality can be observed if we apply the bidiagonalization procedure without reorthogonalization. A small numerical experiment investigating loss or orthogonality is shown in section 5.3 but a formal analysis deserves to be treated as
Acknowledgments

We would like to acknowledge the Department of Mathematics and Computer Science, University of Antwerp, for financial support. This work was funded in part by the IOF-SBO project entitled “High performance iterative reconstruction methods for Talbot Lau grating interferometry based phase contrast tomography”.

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