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THE MINIMAL-NORM GAUSS-NEWTON METHOD AND SOME OF ITS REGULARIZED VARIANTS*

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Abstract. Nonlinear least-squares problems appear in many real-world applications. When a nonlinear model is used to reproduce the behavior of a physical system, the unknown parameters of the model can be estimated by fitting experimental observations by a least-squares approach. It is common to solve such problems by Newton's method or one of its variants such as the Gauss-Newton algorithm. In this paper, we study the computation of the minimal-norm solution to a nonlinear least-squares problem, as well as the case where the solution minimizes a suitable semi-norm. Since many important applications lead to severely ill-conditioned least-squares problems, we also consider some regularization techniques for their solution. Numerical experiments, both artificial and derived from an application in applied geophysics, illustrate the performance of the different approaches.

Key words. nonlinear least-squares, nonlinear inverse problem, regularization, Gauss-Newton method

AMS subject classifications. 65F22, 65H10, 65F20

1. Introduction.

Let us assume that $F(\mathbf{x}) = [F_1(\mathbf{x}), \dots, F_m(\mathbf{x})]^T$ is a nonlinear twice continuously Frechét-differentiable function with values in $\mathbb{R}^m$ for any $\mathbf{x} \in \mathbb{R}^n$. For a given $\mathbf{b} \in \mathbb{R}^m$, we consider the nonlinear least-squares data fitting problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \|\mathbf{r}(\mathbf{x})\|^2, \qquad \mathbf{r}(\mathbf{x}) = F(\mathbf{x}) - \mathbf{b}, \tag{1.1}$$

where $\|\cdot\|$ denotes the Euclidean norm and $\mathbf{r}(\mathbf{x}) = [r_1(\mathbf{x}), \dots, r_m(\mathbf{x})]^T$ is the residual vector function between the model expectation $F(\mathbf{x})$ and the vector $\mathbf{b}$ of measured data. The solution to the nonlinear least-squares problem gives the best model fit to the data in the sense of the minimum sum of squared errors. Classical approaches to the numerical solution of a nonlinear least-squares problem consist of applying Newton's method and its variants such as the Gauss-Newton method [4, 25, 34].

Linear least-squares problems have been widely studied; an exhaustive review can be found in [4]. There also exists a vast literature concerning regularization methods for discrete linear inverse problems; see [14, 21]. The same references discuss numerical methods for the solution of nonlinear least-squares problems, as well as suitable regularization techniques.

The Gauss-Newton method and its variants have been investigated in many papers; see, e.g., [7, 19, 29, 32, 40]. The application of the Levenberg-Marquardt method to ill-posed problems was studied in [8, 26], and in [18] it was applied to an inverse problem in groundwater hydrology. In [36], an iterative algorithm based on the minimization of the Tikhonov functional by the gradient method was developed. The application of Tikhonov regularization to nonlinear inverse problems has been further investigated in [31, 37]. The case where the regularizing term is substituted by a penalty term which promotes the selection of a sparse solution was analyzed in [38].

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At the kth step of the Gauss-Newton method, the current approximation is computed by solving, in the least-squares sense, a linearization of the original nonlinear problem. When the Jacobian of the residual function does not have full column rank, the solution is not unique, and the usual approach is to select the one having minimal norm. This ensures that each update of the solution of the nonlinear least-squares problem has minimal norm, but this property does not apply to the solution itself. The same is true when a regularization technique is introduced.

The idea of constructing an iterative method for the computation of the minimal norm solution of a nonlinear least-squares problem was first studied by Eriksson et al. In [15, 16, 17], the case where the Jacobian is rank-deficient or ill-conditioned was analyzed, and solution techniques based on the Gauss-Newton method and on Tikhonov regularization in standard form were proposed.

In this paper, we review the results obtained by Eriksson et al. and extend them by introducing the minimization of the semi-norm $\|L\mathbf{x}\|$, where L is a regularization matrix; see equation (4.1). In case of lack of a unique solution, the employment of such a semi-norm is often essential to select an effective reconstruction when suitable a priori information is available. We further analyze the computation of the regularized minimal-L-norm solution in two standard procedures for approximating the solution of ill-conditioned nonlinear least-squares problems, namely, the truncated generalized singular value decomposition (TGSVD) applied to the Gauss-Newton method and Tikhonov regularization in general form, whose solutions are given by (5.5) and (5.14), respectively. Though the two regularized solutions are different, they both converge to the minimal-L-norm solution when the regularization level decreases. The new algorithms are finally applied to a small-scale test problem and to the inversion of a medium-size nonlinear model typical in applied geophysics. The numerical results are compared to those produced by the classical approaches.

The paper is organized as follows: Section 2 recalls Newton and Gauss-Newton methods as well as some basic computational tools. In Sections 3 we review the results from Eriksson et al. on the computation of the minimal-norm solution to a nonlinear least-squares problem, and in Section 4 we extend them to the minimal-L-norm solution. Two regularization techniques for ill-conditioned problems are introduced in Section 5. We discuss in Section 6 some details of our implementation and report the results of numerical experiments in Section 7. Section 8 contains concluding remarks.

2. Mathematical preliminaries. We will rewrite the minimization problem (1.1) as

$$\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x}), \qquad \text{where } f(\mathbf{x}) = \frac{1}{2}\|\mathbf{r}(\mathbf{x})\|^2 = \frac{1}{2}\sum_{i=1}^{m} r_i(\mathbf{x})^2.$$

Let the Jacobian of the residual vector function $\mathbf{r}(\mathbf{x})$ be $J(\mathbf{x}) \in \mathbb{R}^{m\times n}$, defined by

$$[J(\mathbf{x})]_{ij} = \frac{\partial r_i(\mathbf{x})}{\partial x_j}, \qquad i = 1,\dots,m,\ j = 1,\dots,n,$$

and the Hessian matrix of $r_i(\mathbf{x})$ be $G_i(\mathbf{x}) = \nabla^2 r_i(\mathbf{x}) \in \mathbb{R}^{n\times n}$, $i = 1,\dots,m$, with entries given by

$$[G_i(\mathbf{x})]_{jk} = \frac{\partial^2 r_i(\mathbf{x})}{\partial x_j \partial x_k}, \qquad j,k = 1,\dots,n.$$

Then, the gradient and the Hessian of $f(\mathbf{x})$, written in matrix form, are given by

$$\nabla f(\mathbf{x}) = \frac{\partial f}{\partial \mathbf{x}} = J(\mathbf{x})^T \mathbf{r}(\mathbf{x}), \tag{2.1}$$

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and

$$\nabla^2 f(\mathbf{x}) = J(\mathbf{x})^T J(\mathbf{x}) + Q(\mathbf{x}), \qquad \text{where } Q(\mathbf{x}) = \sum_{i=1}^{m} r_i(\mathbf{x}) G_i(\mathbf{x}). \tag{2.2}$$

If the point $\mathbf{x}^*$ is a local minimum for a twice continuously differentiable function $f(\mathbf{x})$, then $\mathbf{x}^*$ is a stationary point, i.e., the gradient (2.1) of f at $\mathbf{x}^*$ is zero. Conversely, a sufficient condition for a stationary point to be a local minimum is that the Hessian $\nabla^2 f(\mathbf{x}^*)$ is positive definite.

Newton's method for optimization [4] is based on the minimization of the second-order Taylor approximation of the function $f(\mathbf{x})$,

$$\tilde{f}(\mathbf{x}+\mathbf{s}) = f(\mathbf{x}) + \nabla f(\mathbf{x})^T \mathbf{s} + \frac{1}{2}\mathbf{s}^T \nabla^2 f(\mathbf{x}) \mathbf{s}.$$

The minimizer is obtained by equating to zero the derivative with respect to $\mathbf{s}$,

$$\frac{\partial \tilde{f}(\mathbf{x}+\mathbf{s})}{\partial \mathbf{s}} = \nabla f(\mathbf{x}) + \nabla^2 f(\mathbf{x}) \mathbf{s} = 0.$$

Starting from an initial guess $\mathbf{x}^{(0)}$, assuming that the Hessian of $f(\mathbf{x})$ is invertible in $\mathbf{x}^{(k)}$, and substituting (2.1) and (2.2), the iteration of Newton's method is obtained:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \left(J(\mathbf{x}^{(k)})^T J(\mathbf{x}^{(k)}) + Q(\mathbf{x}^{(k)}) \right)^{-1} J(\mathbf{x}^{(k)})^T \mathbf{r}(\mathbf{x}^{(k)}). \tag{2.3}$$

Newton's method is rarely used for nonlinear least-squares problem because computing the mn^2 derivatives appearing in $Q(\mathbf{x})$ is often computationally too expensive. Initially, we assume that the problem is *overdetermined*, i.e., $m \geq n$. An alternative to Newton's method is to neglect the term $Q(\mathbf{x}^{(k)})$ in (2.3), obtaining the Gauss-Newton method. If $m \geq n$ and $J_k = J(\mathbf{x}^{(k)})$ is full-rank, then the matrix $J_k^T J_k$ is nonsingular, and we can write

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \left(J_k^T J_k \right)^{-1} J_k^T \mathbf{r}(\mathbf{x}^{(k)}), \qquad k = 0, 1, 2, \ldots$$

In this case, the matrix $J_k^\dagger = \left(J_k^T J_k \right)^{-1} J_k^T$ is the Moore-Penrose pseudoinverse of J_k. If $m = n$, then the iteration simplifies to $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - J_k^{-1} \mathbf{r}(\mathbf{x}^{(k)})$.

For *underdetermined* full-rank problems ($m < n$), the iteration of the Gauss-Newton method becomes

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - J_k^T \left(J_k J_k^T \right)^{-1} \mathbf{r}(\mathbf{x}^{(k)}).$$

The behavior of the Gauss-Newton method can be expected to be similar to that of Newton's method when the term $Q(\mathbf{x})$ is negligible, i.e., when the quantities $|r_i(\mathbf{x})| \|G_i(\mathbf{x})\|$, $i = 1, \ldots, m$, are small compared to $J^T J$, where $J = J(\mathbf{x})$. This happens if the functions $r_i(\mathbf{x})$ are mildly nonlinear in a neighborhood of the solution or if the problem is consistent.

We can give a different characterization of the Gauss-Newton method. It replaces the nonlinear problem by a sequence of linear approximations of $\mathbf{r}(\mathbf{x})$, obtained through a first-order Taylor series expansion. The residual at the new iterate is approximated by

$$\mathbf{r}(\mathbf{x}^{(k+1)}) \simeq \mathbf{r}(\mathbf{x}^{(k)}) + J_k \mathbf{s}.$$

Chosen an initial point $\mathbf{x}^{(0)}$, if $\mathbf{x}^{(k)}$ denotes the current approximation, the new approximation is

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{s}^{(k)}, \qquad k = 0, 1, 2, \ldots, \tag{2.4}$$

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where the step $\mathbf{s}^{(k)}$ is computed as a solution to the linear least-squares problem

$$\min_{\mathbf{s}\in\mathbb{R}^n} \|\mathbf{r}(\mathbf{x}^{(k)}) + J_k\mathbf{s}\|^2. \tag{2.5}$$

As already noted, the Gauss-Newton method for solving nonlinear least-squares problems is attractive, compared to Newton's method, because the computation of the second-order term $Q(\mathbf{x})$ is often unfeasible for large scale problems.

In order to ensure convergence, (2.4) is replaced by the damped Gauss-Newton method

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k\mathbf{s}^{(k)}, \tag{2.6}$$

where the scalar α_k is a step length. To determine it, the *Armijo-Goldstein principle* selects α_k as the largest number in the sequence 2^{-i}, $i = 0, 1, \ldots$, for which a substantial reduction in the residual occurs, that is,

$$\|\mathbf{r}(\mathbf{x}^{(k)})\|^2 - \|\mathbf{r}(\mathbf{x}^{(k)} + \alpha_k\mathbf{s}^{(k)})\|^2 \geq \frac{1}{2}\alpha_k\|J_k\mathbf{s}^{(k)}\|^2. \tag{2.7}$$

The step length α_k may also be determined by solving the minimization problem

$$\min_{\alpha} \|\mathbf{r}(\mathbf{x}^{(k)} + \alpha\mathbf{s}^{(k)})\|^2.$$

In [40], this approach is denoted as *Gauss-Newton algorithm with line search*.

The solution to (2.5) may not be unique: this situation happens when the matrix J_k does not have full column rank. To make the solution unique, the new iterate $\mathbf{x}^{(k+1)}$ can be obtained by solving the following minimal-norm linear least-squares problem

$$\begin{cases} \min\limits_{\mathbf{s}\in\mathbb{R}^n} \|\mathbf{s}\|^2 \\ \text{s. t. } \min\limits_{\mathbf{s}\in\mathbb{R}^n} \|J_k\mathbf{s} + \mathbf{r}(\mathbf{x}^{(k)})\|^2, \end{cases} \tag{2.8}$$

which has the solution

$$\mathbf{s}^{(k)} = -J_k^{\dagger}\mathbf{r}(\mathbf{x}^{(k)}).$$

Such *minimal-norm solution* is orthogonal to the null space $\mathcal{N}(J_k)$ of J_k. This is generally assumed to be a good choice among the infinite many solutions to the problem unless other constraints for the solution are available.

In order to select different solutions, the term $\|\mathbf{s}\|^2$ in (2.8) is often substituted by $\|L\mathbf{s}\|^2$, where $L \in \mathbb{R}^{p\times n}$ $(p \leq n)$ is a matrix which incorporates available a priori information on the solution. When $p < n$ or whenever the null space of L is nontrivial, $\|L\mathbf{x}\|$ is a seminorm, i.e., there exist vectors $\mathbf{x} \neq 0$ such that $\|L\mathbf{x}\| = 0$. The constraint $p \leq n$ is not restrictive. Indeed (see, e.g., [21]), if $p > n$, it is possible to perform the compact QR factorization $L = QR$ with $Q \in \mathbb{R}^{p\times p_1}$, $R \in \mathbb{R}^{p_1\times n}$, and $p_1 = \operatorname{rank}(L) \leq n$. In this case the matrix L can be substituted by R, as $\|L\mathbf{x}\| = \|R\mathbf{x}\|$ for any vector $\mathbf{x}$.

The matrix L is typically a diagonal weighting matrix or a $p \times n$ discrete approximation of a derivative operator, in which case L is a banded matrix with full row rank. For example, the matrices

$$D_1 = \begin{bmatrix} 1 & -1 & & \\ & \ddots & \ddots & \\ & & 1 & -1 \end{bmatrix} \quad \text{and} \quad D_2 = \begin{bmatrix} 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \end{bmatrix} \tag{2.9}$$

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of size $(n-1)\times n$ and $(n-2)\times n$, respectively, are approximations to the first and second derivative operators. Regularization operators of this form are often referred to as smoothing operators. An effective choice of L is such that the solution $\mathbf{s}$ is (at least approximately) in the null space of L. If $L = D_1$, then $\mathcal{N}(L)$ contains constant vectors, while $\mathcal{N}(D_2)$ includes constant and linearly varying vectors. Other regularization matrices might be used. For instance, the regularization matrix

$$L = \begin{bmatrix} I_n \otimes D_1 \\ D_1 \otimes I_n \end{bmatrix},$$

where I_n denotes the identity matrix of order n and $\otimes$ stands for the Kronecker product, is commonly used in image restoration [6, 30].

When a regularization matrix is introduced, formulation (2.8) becomes

$$\begin{cases} \min\limits_{\mathbf{s}\in\mathbb{R}^n} \|L\mathbf{s}\|^2 \\ \text{s. t. } \min\limits_{\mathbf{s}\in\mathbb{R}^n} \|J_k\mathbf{s} + \mathbf{r}(\mathbf{x}^{(k)})\|^2. \end{cases} \tag{2.10}$$

It is important to remark that both (2.8) and (2.10) impose some kind of regularity on the update vector $\mathbf{s}$ for the solution $\mathbf{x}^{(k)}$ and not on the solution itself. We will explore in this paper what the consequence is of imposing a regularity constraint directly on the solution $\mathbf{x}$ of problem (1.1). Approaches of this kind were studied by Eriksson and Wedin [15, 16, 17]: they proposed a minimal-norm Gauss-Newton method and a Tikhonov regularization method in standard form. We extend, in Theorem 4.2, the minimal-norm Gauss-Newton method by introducing a regularization matrix L. Moreover, in Section 5 we investigate Tikhonov regularization in general form and the use of truncated SVD/GSVD in the minimal-norm Gauss-Newton method.

In Section 5.2 we will see that, in the limit, the minimal-norm Gauss-Newton iteration and the iteration obtained through Tikhonov regularization in standard form are closely related; the same happens for the minimal-L-norm Gauss-Newton iteration and Tikhonov regularization in general form.

We conclude this section by recalling the *singular value decomposition* (SVD) of a matrix J and the *generalized singular value decomposition* (GSVD) of a matrix pair (J, L), which will be useful in the rest of the paper.

The SVD is a matrix decomposition of the form

$$J = U\Sigma V^T, \tag{2.11}$$

where $U = [\mathbf{u}_1, \ldots, \mathbf{u}_m] \in \mathbb{R}^{m\times m}$ and $V = [\mathbf{v}_1, \ldots, \mathbf{v}_n] \in \mathbb{R}^{n\times n}$ are matrices with orthonormal columns. The non-zero diagonal elements of the diagonal matrix $\Sigma \in \mathbb{R}^{m\times n}$ are the *singular values* $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$ with $r = \operatorname{rank}(J) \leq \min(m, n)$.

Let $J \in \mathbb{R}^{m\times n}$ and $L \in \mathbb{R}^{p\times n}$ be matrices with $\operatorname{rank}(J) = r$ and $\operatorname{rank}(L) = p$. Assume that $m + p \geq n$ and

$$\operatorname{rank}\left(\begin{bmatrix} J \\ L \end{bmatrix}\right) = n,$$

which corresponds to requiring that $\mathcal{N}(J) \cap \mathcal{N}(L) = \{0\}$. The GSVD is a matrix decomposition of the form

$$J = U\Sigma_J W^{-1}, \qquad L = V\Sigma_L W^{-1}, \tag{2.12}$$

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where $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{p\times p}$ are matrices with orthonormal columns $\mathbf{u}_i$ and $\mathbf{v}_i$, respectively, and $W \in \mathbb{R}^{n\times n}$ is nonsingular. If $m \geq n \geq r$, then the matrices $\Sigma_J \in \mathbb{R}^{m\times n}$ and $\Sigma_L \in \mathbb{R}^{p\times n}$ have the form

$$\Sigma_J = \left[\begin{array}{c} O_{n-r} \\ \hline C \\ \hline & I_d \\ \hline O_{(m-n)\times n} \end{array}\right], \qquad \Sigma_L = \left[\begin{array}{c|c} I_{p-r+d} & \\ \hline & S \end{array} \begin{array}{c} \\ \hline O_{p\times d} \end{array}\right], \tag{2.13}$$

where $d = n - p$,

$$\begin{aligned} C &= \operatorname{diag}(c_1, \ldots, c_{r-d}), & 0 < c_1 \leq c_2 \leq \cdots \leq c_{r-d} < 1, \\ S &= \operatorname{diag}(s_1, \ldots, s_{r-d}), & 1 > s_1 \geq s_2 \geq \cdots \geq s_{r-d} > 0, \end{aligned}$$

with $c_i^2 + s_i^2 = 1$, for $i = 1, \ldots, r-d$. The identity matrix of size k is denoted by I_k, while O_k and $O_{k\times\ell}$ are zero matrices of size k and $k \times \ell$, respectively; a matrix block has to be omitted when one of its dimensions is zero. The scalars $\gamma_i = \frac{c_i}{s_i}$ are called *generalized singular values*, and they appear in nondecreasing order.

If $r \leq m < n$, then the matrices $\Sigma_J \in \mathbb{R}^{m\times n}$ and $\Sigma_L \in \mathbb{R}^{p\times n}$ take the form

$$\Sigma_J = \left[\begin{array}{c|c} O_{m\times(n-m)} & \begin{array}{ccc} O_{m-r} & & \\ & C & \\ & & I_d \end{array} \end{array}\right], \qquad \Sigma_L = \left[\begin{array}{c|c} I_{p-r+d} & \\ \hline & S \end{array} \begin{array}{c} \\ \hline O_{p\times d} \end{array}\right], \tag{2.14}$$

where the blocks are defined as above.

3. Nonlinear minimal-norm solution. Let us discuss the computation of the minimal-norm solution to the nonlinear problem (1.1),

$$\begin{cases} \min\limits_{\mathbf{x}\in\mathbb{R}^n} \|\mathbf{x}\|^2 \\ \text{s. t.} \ \min\limits_{\mathbf{x}\in\mathbb{R}^n} \|F(\mathbf{x}) - \mathbf{b}\|^2. \end{cases} \tag{3.1}$$

We consider the following iterative method of type (2.4), based on a first-order linearization of the problem:

$$\begin{cases} \min\limits_{\mathbf{s}\in\mathbb{R}^n} \|\mathbf{x}^{(k)} + \mathbf{s}\|^2 \\ \text{s. t.} \ \min\limits_{\mathbf{s}\in\mathbb{R}^n} \|J_k\mathbf{s} + \mathbf{r}(\mathbf{x}^{(k)})\|^2, \end{cases} \tag{3.2}$$

where $J_k = J(\mathbf{x}^{(k)})$ is the Jacobian of F in $\mathbf{x}^{(k)}$. We will denote this as the *minimal-norm Gauss-Newton* (MNGN) method.

A theorem similar to the following one is presented, in a slightly general form, in [15, 16, 17]. We provide here a statement and a proof in terms of the SVD, which is useful from a computational point of view.

THEOREM 3.1. *Let $\mathbf{x}^{(k)} \in \mathbb{R}^n$, and let $\widetilde{\mathbf{x}}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{s}^{(k)}$ be the Gauss-Newton iteration for (1.1), where the step $\mathbf{s}^{(k)}$ is determined by solving (2.8). Then, the iteration $\mathbf{x}^{(k+1)}$ for (3.2), starting from the same point $\mathbf{x}^{(k)}$, is given by*

$$\mathbf{x}^{(k+1)} = \widetilde{\mathbf{x}}^{(k+1)} - V_2 V_2^T \mathbf{x}^{(k)},$$

where $\operatorname{rank}(J_k) = r$ and the columns of the matrix $V_2 = [\mathbf{v}_{r+1}, \ldots, \mathbf{v}_n]$ are orthonormal vectors in $\mathbb{R}^n$ spanning the null space of J_k.

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Proof. Let $U\Sigma V^T$ be the singular value decomposition of the matrix J_k. The norm of the solution $\mathbf{x}^{(k+1)}$ of (3.2) may be expressed as

$$\|\mathbf{x}^{(k+1)}\|^2 = \|V^T(\mathbf{x}^{(k)} + \mathbf{s})\|^2 = \|\mathbf{y} + \mathbf{z}^{(k)}\|^2,$$

with $\mathbf{y} = V^T\mathbf{s}$ and $\mathbf{z}^{(k)} = V^T\mathbf{x}^{(k)}$. Replacing J_k by its SVD and setting $\mathbf{b}^{(k)} = U^T\mathbf{r}(\mathbf{x}^{(k)})$, we can rewrite (3.2) as the following diagonally constrained least-squares problem

$$\begin{cases} \min\limits_{\mathbf{y}\in\mathbb{R}^n} \|\mathbf{y} + \mathbf{z}^{(k)}\|^2 \\ \text{s. t.} \ \min\limits_{\mathbf{y}\in\mathbb{R}^n} \|\Sigma\mathbf{y} + \mathbf{b}^{(k)}\|^2. \end{cases}$$

Solving the second minimization problem uniquely determines the components $y_i = -\sigma_i^{-1}b_i^{(k)}$, $i = 1, \ldots, r$, while the entries y_i, $i = r+1, \ldots, n$, are undetermined. In order to minimize the norm of the solution

$$\|\mathbf{y} + \mathbf{z}^{(k)}\|^2 = \sum_{i=1}^{r}\left(-\frac{b_i^{(k)}}{\sigma_i} + z_i^{(k)}\right)^2 + \sum_{i=r+1}^{n}\left(y_i + z_i^{(k)}\right)^2,$$

we set $y_i = -z_i^{(k)} = -\mathbf{v}_i^T\mathbf{x}^{(k)}$, $i = r+1, \ldots, n$. The solution to (3.2), that is, the next approximation to the solution of (3.1), is then

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=1}^{r}\frac{b_i^{(k)}}{\sigma_i}\mathbf{v}_i - \sum_{i=r+1}^{n}(\mathbf{v}_i^T\mathbf{x}^{(k)})\mathbf{v}_i, \tag{3.3}$$

where the last summation can be written in matrix form as $V_2V_2^T\mathbf{x}^{(k)}$.

Similarly, we rewrite (2.8) as the following diagonal least-squares problem

$$\begin{cases} \min\limits_{\mathbf{y}\in\mathbb{R}^n} \|\mathbf{y}\|^2 \\ \text{s. t.} \ \min\limits_{\mathbf{y}\in\mathbb{R}^n} \|\Sigma\mathbf{y} + \mathbf{b}^{(k)}\|^2, \end{cases}$$

with $\mathbf{y} = V^T\mathbf{s}$, obtaining

$$\widetilde{\mathbf{x}}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{s}^{(k)} = \mathbf{x}^{(k)} - \sum_{i=1}^{r}\frac{b_i^{(k)}}{\sigma_i}\mathbf{v}_i.$$

Then,

$$\mathbf{x}^{(k+1)} = \widetilde{\mathbf{x}}^{(k+1)} - V_2V_2^T\mathbf{x}^{(k)},$$

where the columns of $V_2 = [\mathbf{v}_{r+1}, \ldots, \mathbf{v}_n]$ are a basis for $\mathcal{N}(J_k)$. This completes the proof. ∎

REMARK 3.2. Let $\mathcal{P}_{\mathcal{N}(J_k)}$ represent the orthogonal projector onto $\mathcal{N}(J_k)$. Since $\mathcal{P}_{\mathcal{N}(J_k)} = V_2V_2^T$, the above theorem shows that, unlike the Gauss-Newton method, the $(k+1)$th iterate of the MNGN method is orthogonal to the null space of J_k. Then, equation (3.3) may be expressed in the more general form [15, 16, 17]

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \begin{bmatrix} J_k^\dagger & \mathcal{P}_{\mathcal{N}(J_k)} \end{bmatrix}\begin{bmatrix} \mathbf{r}(\mathbf{x}^{(k)}) \\ \mathbf{x}^{(k)} \end{bmatrix}.$$

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REMARK 3.3. It is useful to remember that $V_2V_2^T = I_n - V_1V_1^T$ with the matrix $V_1 = [\mathbf{v}_1, \ldots, \mathbf{v}_r]$. So, the updated solution can be obtained without necessarily computing the singular vectors $\mathbf{v}_i$, $i = r+1, \ldots, n$, i.e., when a compact SVD is available

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{s}^{(k)} - V_2V_2^T\mathbf{x}^{(k)} = \mathbf{s}^{(k)} + V_1V_1^T\mathbf{x}^{(k)}.$$

REMARK 3.4. In the first numerical example of Section 7, the approach of projecting the iterates orthogonally to the null space of J_k will also be applied to Newton's method. This approach is only heuristic in this case. It will be shown that the solution at convergence coincides with the one produced by the MNGN method but that the speed of convergence of Newton's method degrades.

4. Nonlinear minimal-L-norm solution. Let us introduce a regularization matrix $L \in \mathbb{R}^{p\times n}$, $p \leq n$. We seek to compute the minimal-L-norm solution to the nonlinear problem (1.1), that is, the vector $\mathbf{x}$ which solves the constrained problem

$$\begin{cases} \min\limits_{\mathbf{x}\in\mathbb{R}^n} \|L\mathbf{x}\|^2 \\ \text{s. t. } \min\limits_{\mathbf{x}\in\mathbb{R}^n} \|F(\mathbf{x}) - \mathbf{b}\|^2. \end{cases} \tag{4.1}$$

Similarly to the previous section, we consider an iterative method of type (2.4), where the step $\mathbf{s}^{(k)}$ is the solution of the linearized problem

$$\begin{cases} \min\limits_{\mathbf{s}\in\mathbb{R}^n} \|L(\mathbf{x}^{(k)} + \mathbf{s})\|^2 \\ \text{s. t. } \min\limits_{\mathbf{s}\in\mathbb{R}^n} \|J_k\mathbf{s} + \mathbf{r}(\mathbf{x}^{(k)})\|^2. \end{cases} \tag{4.2}$$

We will denote this as the *minimal-L-norm Gauss-Newton* (MLNGN) method.

Let $J_k = U\Sigma_J W^{-1}$, $L = V\Sigma_L W^{-1}$ be the GSVD of the matrix pair (J_k,L). We indicate by $\mathbf{w}_i$ the column vectors of the matrix W and by $\widehat{\mathbf{w}}^j$ the rows of W^{-1}, that is,

$$W = [\mathbf{w}_1, \ldots, \mathbf{w}_n], \qquad W^{-1} = \begin{bmatrix} \widehat{\mathbf{w}}^1 \\ \vdots \\ \widehat{\mathbf{w}}^n \end{bmatrix}.$$

The columns of W and the rows of W^{-1} form a pair of biorthogonal bases, i.e., $\widehat{\mathbf{w}}^i\mathbf{w}_j = \delta_{ij}$.

LEMMA 4.1. *If* $r = \operatorname{rank}(J_k)$, *then*

$$\mathcal{N}(J_k) = \operatorname{span}(\mathbf{w}_1, \ldots, \mathbf{w}_{n-r}).$$

Proof. Any vector $\mathbf{x}$ in $\mathbb{R}^n$ can be represented in the basis $\{\mathbf{w}_i\}_{i=1}^n$ by writing

$$\mathbf{x} = W(W^{-1}\mathbf{x}) = \sum_{j=1}^{n} (\widehat{\mathbf{w}}^j\mathbf{x})\mathbf{w}_j. \tag{4.3}$$

From the GSVD of (J_k, L), we obtain

$$J_k\mathbf{x} = \sum_{i=1}^{m} \delta_i\mathbf{u}_i,$$

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where $\boldsymbol{\delta} = (\delta_1, \ldots, \delta_n)^T = \Sigma_J W^{-1}\mathbf{x}$. When $m \geq n$, (2.13) leads to

$$\delta_i = \begin{cases} 0, & i = 1, \ldots, n-r, \\ c_{i-n+r}(\widehat{\mathbf{w}}^i\mathbf{x}), & i = n-r+1, \ldots, p, \\ \widehat{\mathbf{w}}^i\mathbf{x}, & i = p+1, \ldots, n, \\ 0, & i = n+1, \ldots, m, \end{cases}$$

so that $J_k\mathbf{x} = 0$ if and only if $\widehat{\mathbf{w}}^i\mathbf{x} = 0$, for $i = n-r+1, \ldots, n$. By (4.3), this means that

$$\mathbf{x} \in \operatorname{span}(\mathbf{w}_1, \ldots, \mathbf{w}_{n-r}).$$

When $m < n$, from (2.14) we obtain

$$\delta_i = \begin{cases} 0, & i = 1, \ldots, m-r, \\ c_{i-m+r}(\widehat{\mathbf{w}}^{i-m+n}\mathbf{x}), & i = m-r+1, \ldots, m+p-n, \\ \widehat{\mathbf{w}}^{i-m+n}\mathbf{x}, & i = m+p-n+1, \ldots, m, \end{cases}$$

so the same conclusion holds true: $\mathbf{x} \in \mathcal{N}(J_k)$ if and only if $\mathbf{x} \in \operatorname{span}(\mathbf{w}_1, \ldots, \mathbf{w}_{n-r})$. ∎

THEOREM 4.2. *Let $\mathbf{x}^{(k)} \in \mathbb{R}^n$, and let $\widetilde{\mathbf{x}}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{s}^{(k)}$ be the Gauss-Newton iteration for (1.1), where the step $\mathbf{s}^{(k)}$ has been determined by solving (2.10). Then, the iteration $\mathbf{x}^{(k+1)}$ for (4.2), starting from the same point $\mathbf{x}^{(k)}$, is given by*

$$\mathbf{x}^{(k+1)} = \widetilde{\mathbf{x}}^{(k+1)} - W_1\widehat{W}_1\mathbf{x}^{(k)}, \tag{4.4}$$

where $\widehat{W}_1 \in \mathbb{R}^{(n-r)\times n}$ contains the first $n-r$ rows of W^{-1} and $W_1 \in \mathbb{R}^{n\times(n-r)}$ is composed by the first $n-r$ columns of W.

Proof. Replacing J_k and L with their GSVD and setting $\mathbf{y} = W^{-1}\mathbf{s}$, $\mathbf{z}^{(k)} = W^{-1}\mathbf{x}^{(k)}$, and $\mathbf{b}^{(k)} = U^T\mathbf{r}(\mathbf{x}^{(k)})$, (4.2) can be rewritten as the following diagonal least-squares problem

$$\begin{cases} \min\limits_{\mathbf{y}\in\mathbb{R}^n} \|\Sigma_L(\mathbf{y} + \mathbf{z}^{(k)})\|^2 \\ \text{s. t. } \min\limits_{\mathbf{y}\in\mathbb{R}^n} \|\Sigma_J\mathbf{y} + \mathbf{b}^{(k)}\|^2. \end{cases} \tag{4.5}$$

When $m \geq n$, the diagonal linear system in the constraint is solved by a vector $\mathbf{y}$ with entries

$$y_i = \begin{cases} -\dfrac{b_i^{(k)}}{c_{i-n+r}}, & i = n-r+1, \ldots, p, \\ -b_i^{(k)}, & i = p+1, \ldots, n, \end{cases}$$

while the components y_i, for $i = 1, \ldots, n-r$, can be determined by minimizing the norm

$$\|\Sigma_L(\mathbf{y} + \mathbf{z}^{(k)})\|^2 = \sum_{i=1}^{n-r}\left(y_i + z_i^{(k)}\right)^2 + \sum_{i=n-r+1}^{p}\left(-\frac{b_i^{(k)}}{\gamma_{i-n+r}} + s_{i-n+r}z_i^{(k)}\right)^2, \tag{4.6}$$

where $\gamma_i = \frac{c_i}{s_i}$ are the generalized singular values of the matrix pair (J_k, L). The minimum of (4.6) is reached for

$$y_i = -z_i^{(k)} = -\widehat{\mathbf{w}}^i\mathbf{x}^{(k)}, \qquad i = 1, \ldots, n-r,$$

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and the solution to (4.2), that is, the next approximation for the solution of (4.1), is

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=1}^{n-r} z_i^{(k)} \mathbf{w}_i - \sum_{i=n-r+1}^{p} \frac{b_i^{(k)}}{c_{i-n+r}} \mathbf{w}_i - \sum_{i=p+1}^{n} b_i^{(k)} \mathbf{w}_i, \tag{4.7}$$

where the first summation at the right-hand side can be rewritten in the form $W_1 \widehat{W}_1 \mathbf{x}^{(k)}$. Applying the same procedure to (2.10), we obtain

$$\widetilde{\mathbf{x}}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=n-r+1}^{p} \frac{b_i^{(k)}}{c_{i-n+r}} \mathbf{w}_i - \sum_{i=p+1}^{n} b_i^{(k)} \mathbf{w}_i, \tag{4.8}$$

from which (4.4) follows. We note that the last summation in (4.7) and (4.8) is the component of the update vector $\mathbf{s}$ in the null space of L.

When $m < n$, (2.14) yields the following solution for the diagonal system in (4.5),

$$y_i = \begin{cases} -\dfrac{b_{i-n+m}^{(k)}}{c_{i-n+r}}, & i = n-r+1, \ldots, p, \\ -b_{i-n+m}^{(k)}, & i = p+1, \ldots, n, \end{cases}$$

from which, after minimizing the weighted norm like in (4.6), we obtain

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=1}^{n-r} z_i^{(k)} \mathbf{w}_i - \sum_{i=n-r+1}^{p} \frac{b_{i-n+m}^{(k)}}{c_{i-n+r}} \mathbf{w}_i - \sum_{i=p+1}^{n} b_{i-n+m}^{(k)} \mathbf{w}_i. \tag{4.9}$$

Since solving (2.10) when $m < n$ leads to a formula similar to (4.8) with $b_{i-n+m}^{(k)}$ in place of $b_i^{(k)}$, the validity of (4.4) is confirmed. □

5. Regularization. The nonlinear function $F(\mathbf{x})$ is considered ill-conditioned in a domain $\mathcal{D} \subset \mathbb{R}^n$ when the condition number $\kappa(J)$ of the Jacobian $J = J(\mathbf{x})$ is very large for any $\mathbf{x} \in \mathcal{D}$. In this situation, it is common to apply a regularization procedure to each step of the Gauss-Newton method.

The truncated singular value decomposition (TSVD) solves (2.8) after substituting J_k by its best rank-ℓ approximation, that is,

$$J_k^{(\ell)} = \operatorname*{argmin}_{\operatorname{rank}(M)=\ell} \|J_k - M\|_2 = \sum_{i=1}^{\ell} \sigma_i \mathbf{u}_i \mathbf{v}_i^T, \tag{5.1}$$

where $(\sigma_i, \mathbf{u}_i, \mathbf{v}_i)$ is the ith singular triplet for J_k; see (2.11). Here, ℓ plays the role of a regularization parameter, which has to be carefully chosen. Its role is to approximate the initial least-squares problem by a better-conditioned problem. Choosing its value amounts to finding a compromise between fidelity to the original model and numerical stability.

Another classical approach is Tikhonov regularization, in which the minimization problem (2.5) is replaced by

$$\min_{\mathbf{s} \in \mathbb{R}^n} \left\{ \|J_k \mathbf{s} + \mathbf{r}(\mathbf{x}^{(k)})\|^2 + \lambda^2 \|\mathbf{s}\|^2 \right\}, \tag{5.2}$$

for a fixed value of the parameter $\lambda > 0$. The regularization parameter λ controls the balance between the two terms of the functional, i.e., the weights attributed to the residual term and to the regularization term.

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If a regularization matrix $L \in \mathbb{R}^{p\times n}$ is introduced, then (2.8) becomes (2.10), and the regularized solution is computed by the truncated generalized singular value decomposition (TGSVD). If the Tikhonov approach is followed, then the standard form functional (5.2) is expressed in general form

$$\min_{\mathbf{s}\in\mathbb{R}^n} \left\{ \|J_k\mathbf{s} + \mathbf{r}(\mathbf{x}^{(k)})\|^2 + \lambda^2\|L\mathbf{s}\|^2 \right\}. \tag{5.3}$$

We stress that both (5.2) and TSVD applied to (2.8) impose a regularity constraint on the update vector $\mathbf{s}$ for the solution $\mathbf{x}^{(k)}$ and not on the solution itself in the same matter as (5.3) and TGSVD applied to (2.10) do.

5.1. Truncated minimal-norm solution. When the function F is ill-conditioned, we propose a *truncated minimal-norm Gauss-Newton* (TMNGN) method to solve (3.2). We choose a value for the truncation parameter $1 \le \ell \le r$, an initial solution $\mathbf{x}_\ell^{(0)}$, and compute

$$\mathbf{x}_\ell^{(k+1)} = \mathbf{x}_\ell^{(k)} - \sum_{i=1}^{\ell} \frac{b_i^{(\ell,k)}}{\sigma_i}\mathbf{v}_i - V_{2,\ell}V_{2,\ell}^T\mathbf{x}_\ell^{(k)}, \qquad k = 0, 1, 2, \ldots, \tag{5.4}$$

where $V_{2,\ell} = [\mathbf{v}_{\ell+1}, \ldots, \mathbf{v}_n]$, until convergence. In the above formula, $\mathbf{b}^{(\ell,k)} = U^T\mathbf{r}(\mathbf{x}_\ell^{(k)})$ as in the proof of Theorem 3.1. Notice that the columns of $V_{2,\ell}$ form a basis for the null space of the rank-ℓ approximation (5.1) of the Jacobian.

In case a partial SVD is computed, say, up to the truncation index ℓ, the last term may be expressed as $(I - V_{1,\ell}V_{1,\ell}^T)\mathbf{x}_\ell^{(k)}$, where $V_{1,\ell} = [\mathbf{v}_1, \ldots, \mathbf{v}_\ell]$. There are several methods for computing a partial SVD for large scale problems [1, 2, 3, 27, 41].

To solve (4.2), we employ a *truncated minimal-L-norm Gauss-Newton* (TMLNGN) method. This consists of choosing an integer $0 \le \ell \le p - n + r = r - d$ (see (4.7) and (4.9)) and computing, for $k = 0, 1, 2, \ldots$ until convergence, the iterates

$$\mathbf{x}_\ell^{(k+1)} = \mathbf{x}_\ell^{(k)} - \sum_{i=p-\ell+1}^{p} \frac{b_{i-N}^{(\ell,k)}}{c_{i-n+r}}\mathbf{w}_i - \sum_{i=p+1}^{n} b_{i-N}^{(\ell,k)}\mathbf{w}_i - W_{1,\ell}\widehat{W}_{1,\ell}\mathbf{x}_\ell^{(k)}, \tag{5.5}$$

where $N = \max(n - m, 0)$. The matrix $W_{1,\ell} \in \mathbb{R}^{n\times(p-\ell)}$ contains the first $p - \ell$ columns of W, and $\widehat{W}_{1,\ell} \in \mathbb{R}^{(p-\ell)\times n}$ the first $p - \ell$ rows of W^{-1}. Again, the columns of $W_{1,\ell}$ span the null space of $J_k^{(\ell)}$.

In formulas (5.4) and (5.5), the solution at convergence will be denoted by $\mathbf{x}_\ell$. Under the assumption that the exact data vector $\widehat{\mathbf{b}}$ is perturbed by noise

$$\mathbf{b} = \widehat{\mathbf{b}} + \mathbf{e}, \tag{5.6}$$

the classical discrepancy principle introduced by Morozov [33] will be used to estimate the optimal value of the regularization parameter, namely, selecting the smallest truncation parameter ℓ such that

$$\|F(\mathbf{x}_\ell) - \mathbf{b}\| \le \tau\|\mathbf{e}\|, \tag{5.7}$$

where $\tau > 1$ is a constant independent of the noise level $\|\mathbf{e}\|$. When the noise level is unknown, heuristic methods are commonly used, such as the L-curve criterion [20, 23, 24]. For an analysis of other heuristic methods; see [22, 28, 35, 39].

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5.2. Minimal-norm Tikhonov solution. We assume here that a regularizing term is added to the least-squares problem (1.1), transforming it into the minimization of the nonlinear Tikhonov functional

$$\min_{\mathbf{x}\in\mathbb{R}^n} \left\{ \|F(\mathbf{x}) - \mathbf{b}\|^2 + \lambda^2 \|L\mathbf{x}\|^2 \right\}, \tag{5.8}$$

where $\lambda > 0$ is a continuous regularization parameter and $L \in \mathbb{R}^{p\times n}$ is a regularization matrix. We will apply the Gauss-Newton method to the solution of (5.8) and compare the iterates to those derived from the application of the same method to (1.1) followed by the Tikhonov regularization of each step as in (5.3).

Linearizing (5.8), we obtain

$$\min_{\mathbf{s}\in\mathbb{R}^n} \left\{ \|J_k\mathbf{s} + \mathbf{r}(\mathbf{x}^{(k)})\|^2 + \lambda^2 \|L(\mathbf{x}^{(k)} + \mathbf{s})\|^2 \right\}. \tag{5.9}$$

We first analyze the case $L = I_n$.

THEOREM 5.1. *Let* $\operatorname{rank}(J_k) = r$. *The iteration for* (5.9) *is given by*

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=1}^{r} \frac{\sigma_i b_i^{(k)} + \lambda^2 z_i^{(k)}}{\sigma_i^2 + \lambda^2} \mathbf{v}_i - V_2 V_2^T \mathbf{x}^{(k)}, \tag{5.10}$$

where $\mathbf{b}^{(k)} = U^T \mathbf{r}(\mathbf{x}^{(k)})$, $\mathbf{z}^{(k)} = V^T \mathbf{x}^{(k)}$, *and* $V_2 = [\mathbf{v}_{r+1}, \ldots, \mathbf{v}_n]$ *is defined as in Theorem 3.1.*

Proof. Computing the gradient of the function (5.9) with $L = I_n$ yields the normal equations associated to the penalized least-squares problem

$$(J_k^T J_k + \lambda^2 I_n)\mathbf{s} = -J_k^T \mathbf{r}(\mathbf{x}^{(k)}) - \lambda^2 \mathbf{x}^{(k)}. \tag{5.11}$$

By employing the singular value decomposition $J_k = U\Sigma V^T$, the normal equations (5.11) become

$$(\Sigma^T\Sigma + \lambda^2 I_n)\mathbf{y} = -\Sigma^T \mathbf{b}^{(k)} - \lambda^2 \mathbf{z}^{(k)}, \tag{5.12}$$

with $\mathbf{y} = V^T\mathbf{s}$, $\mathbf{b}^{(k)} = U^T\mathbf{r}(\mathbf{x}^{(k)})$, and $\mathbf{z}^{(k)} = V^T\mathbf{x}^{(k)}$. The solution to the diagonal normal equations (5.12),

$$y_i = \begin{cases} -\dfrac{\sigma_i b_i^{(k)} + \lambda^2 z_i^{(k)}}{\sigma_i^2 + \lambda^2}, & i = 1, \ldots, r, \\ -z_i^{(k)}, & i = r+1, \ldots, n, \end{cases}$$

leads to the Tikhonov-Gauss-Newton (TikGN) iterate, which solves (5.9):

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=1}^{r} \frac{\sigma_i b_i^{(k)} + \lambda^2 z_i^{(k)}}{\sigma_i^2 + \lambda^2} \mathbf{v}_i - \sum_{i=r+1}^{n} z_i^{(k)} \mathbf{v}_i.$$

The last summation can be rewritten in matrix form as $V_2 V_2^T \mathbf{x}^{(k)}$, where $V_2 = [\mathbf{v}_{r+1}, \ldots, \mathbf{v}_n]$. This completes the proof. ∎

The normal equations associated to (5.2) are

$$(J_k^T J_k + \lambda^2 I_n)\mathbf{s} = -J_k^T \mathbf{r}(\mathbf{x}^{(k)}),$$

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which become after substituting the SVD of J_k,

$$(\Sigma^T\Sigma + \lambda^2 I_n)\mathbf{y} = -\Sigma^T \mathbf{b}^{(k)}.$$

The solution to this diagonal system

$$y_i = \begin{cases} -\dfrac{\sigma_i b_i^{(k)}}{\sigma_i^2 + \lambda^2}, & i = 1, \dots, r, \\ 0, & i = r+1, \dots, n, \end{cases}$$

produces the iterate

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=1}^{r} \frac{\sigma_i b_i^{(k)}}{\sigma_i^2 + \lambda^2} \mathbf{v}_i. \tag{5.13}$$

Comparing equation (5.13), where the approximate solution is obtained by imposing the regularity constraint on the update vector $\mathbf{s}$, to the iteration (5.10), where the regularity constraint is imposed on the approximate solution $\mathbf{x}^{(k+1)}$, we see that the TikGN method implements a different filtering technique with respect to the standard application of Tikhonov regularization to the Gauss-Newton iteration and produces approximate solutions which are orthogonal to the null space of the Jacobian matrix J_k.

REMARK 5.2. Since $V_2 V_2^T = I_n - V_1 V_1^T$, the updated solution (5.10) can be expressed without the explicit use of the singular vectors $\mathbf{v}_i$, $i = r+1, \dots, n$, in the form

$$\mathbf{x}^{(k+1)} = V_1 V_1^T \mathbf{x}^{(k)} - \sum_{i=1}^{r} \frac{\sigma_i b_i^{(k)} + \lambda^2 z_i^{(k)}}{\sigma_i^2 + \lambda^2} \mathbf{v}_i.$$

This is useful when a compact SVD is available.

Formula (5.10) immediately yields the following result.

COROLLARY 5.3. *When the regularization parameter λ approaches zero, the TikGN iterate computed by* (5.10) *converges to the MNGN solution* (3.3)*, that is,*

$$\mathbf{x}_{MNGN}^{(k+1)} = \lim_{\lambda \to 0^+} \mathbf{x}_{TikGN}^{(k+1)}.$$

We now turn to the case $L \neq I_n$. We will denote the resulting method by TikLGN.

THEOREM 5.4. *Let* $\operatorname{rank}(J_k) = r$. *The iteration for the TikLGN approach* (5.9) *is*

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=n-r+1}^{p} \xi_i \mathbf{w}_i - \sum_{i=p+1}^{n} b_{i-N}^{(k)} \mathbf{w}_i - W_1 \widehat{W}_1 \mathbf{x}^{(k)}, \tag{5.14}$$

with

$$\xi_i = \frac{c_{i-n+r} b_{i-N}^{(k)} + \lambda^2 s_{i-n+r}^2 z_i^{(k)}}{c_{i-n+r}^2 + \lambda^2 s_{i-n+r}^2}, \qquad i = n-r+1, \dots, p,$$

where $N = \max(n-m, 0)$ *and* W_1 *and* $\widehat{W}_1$ *are defined as in Theorem* 4.2.

Proof. Let us consider the generalized singular value decomposition (GSVD) (2.12) of the matrix pair (J_k, L). We initially assume that $m \geq n \geq r = \operatorname{rank}(J_k)$ and that L has full rank, i.e., $\operatorname{rank}(L) = p$. We have $J_k = U \Sigma_J W^{-1}$ and $L = V \Sigma_L W^{-1}$, with Σ_J and Σ_L given by (2.13).

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Substituting the GSVD in the normal equations associated to (5.9) ,

$$(J_k^T J_k + \lambda^2 L^T L)\mathbf{s} = -J_k^T \mathbf{r}(\mathbf{x}^{(k)}) - \lambda^2 L^T L \mathbf{x}^{(k)},$$

leads to

$$(D + \lambda^2 H)\mathbf{y} = -\Sigma_J^T \mathbf{b}^{(k)} - \lambda^2 H \mathbf{z}^{(k)}, \tag{5.15}$$

where

$$D = \begin{bmatrix} O_{n-r} & & \\ & C^2 & \\ & & I_{n-p} \end{bmatrix}, \qquad H = \begin{bmatrix} I_{n-r} & & \\ & S^2 & \\ & & O_{n-p} \end{bmatrix},$$

$\mathbf{y} = W^{-1}\mathbf{s}$, $\mathbf{b}^{(k)} = U^T \mathbf{r}(\mathbf{x}^{(k)})$, and $\mathbf{z}^{(k)} = W^{-1}\mathbf{x}^{(k)}$. The diagonal system (5.15) yields the iterate

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=n-r+1}^{p} \xi_i \mathbf{w}_i - \sum_{i=p+1}^{n} b_i^{(k)} \mathbf{w}_i - W_1 \widehat{W}_1 \mathbf{x}^{(k)}, \tag{5.16}$$

where

$$\xi_i = \frac{c_{i-n+r} b_i^{(k)} + \lambda^2 s_{i-n+r}^2 z_i^{(k)}}{c_{i-n+r}^2 + \lambda^2 s_{i-n+r}^2}, \qquad i = n-r+1, \ldots, p.$$

Similarly, when $r \leq m < n$, the TikLGN approach leads to the iterate

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=n-r+1}^{p} \xi_i' \mathbf{w}_i - \sum_{i=p+1}^{n} b_{i-n+m}^{(k)} \mathbf{w}_i - W_1 \widehat{W}_1 \mathbf{x}^{(k)}, \tag{5.17}$$

with

$$\xi_i' = \frac{c_{i-n+r} b_{i-n+m}^{(k)} + \lambda^2 s_{i-n+r}^2 z_i^{(k)}}{c_{i-n+r}^2 + \lambda^2 s_{i-n+r}^2}, \qquad i = n-r+1, \ldots, p.$$

Introducing $N = n - m$ if $m < n$ and zero otherwise, the overdetermined (5.16) and the underdetermined (5.17) cases may be condensed into the single expression (5.14), and this completes the proof. □

The normal equations associated to (5.3), if $m \geq n \geq r$, are

$$(J_k^T J_k + \lambda^2 L^T L)\mathbf{s} = -J_k^T \mathbf{r}(\mathbf{x}^{(k)}),$$

that is,

$$(D + \lambda^2 H)\mathbf{y} = -\Sigma_J^T \mathbf{b}^{(k)},$$

where D, H, and $\mathbf{b}^{(k)}$ are defined as above. This diagonal system yields

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=n-r+1}^{p} \frac{c_{i-n+r} b_i^{(k)}}{c_{i-n+r}^2 + \lambda^2 s_{i-n+r}^2} \mathbf{w}_i - \sum_{i=p+1}^{n} b_i^{(k)} \mathbf{w}_i. \tag{5.18}$$

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When $r \leq m < n$, the iteration induced by (5.3) is

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=n-r+1}^{p} \frac{c_{i-n+r} b_{i-n+m}^{(k)}}{c_{i-n+r}^2 + \lambda^2 s_{i-n+r}^2} \mathbf{w}_i - \sum_{i=p+1}^{n} b_{i-n+m}^{(k)} \mathbf{w}_i. \tag{5.19}$$

We can condense the overdetermined (5.18) and the underdetermined (5.19) cases into a single expression, introducing N defined as in the Theorem 5.4:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \sum_{i=n-r+1}^{p} \frac{c_{i-n+r} b_{i-N}^{(k)}}{c_{i-n+r}^2 + \lambda^2 s_{i-n+r}^2} \mathbf{w}_i - \sum_{i=p+1}^{n} b_{i-N}^{(k)} \mathbf{w}_i.$$

Comparing (5.14) to this formula shows, as in the case $L = I_n$, that the minimal-L-norm approach and the traditional Tikhonov method produce different reconstructions. Also, when the regularization parameter λ approaches zero, the TikLGN solution converges to the MLNGN solution.

COROLLARY 5.5. *For the iterations computed by the MLNGN method* (4.7) *and by the TikLGN method* (5.16)*, it holds that*

$$\mathbf{x}_{MLNGN}^{(k+1)} = \lim_{\lambda \to 0^+} \mathbf{x}_{TikLGN}^{(k+1)}.$$

In formulas (5.10) and (5.14), the solution at convergence will be denoted by $\mathbf{x}_\lambda$, and also in this case we will consider the right-hand side $\mathbf{b}$ to be affected by noise as in (5.6). The regularization parameter λ will be estimated by the discrepancy principle [33], substituting $F(\mathbf{x}_\ell)$ by $F(\mathbf{x}_\lambda)$ in (5.7).

6. Implementation details. In some situations, the `gsvd` routine provided by Matlab produces unexpected results. We observed that when the norm of the Jacobian matrix J_k is very small, the GSVD of (J_k, L) may produce an inaccurate factor W, which prevents the Gauss-Newton method (4.2) to converge. To overcome such numerical issues, when $\|J_k\|_\infty < \rho$ (in the experiments we set $\rho = 10^{-6}$), we rescale the least-squares problem (4.2) to obtain

$$\begin{cases} \min\limits_{\mathbf{s} \in \mathbb{R}^n} \|L(\mathbf{x}^{(k)} + \mathbf{s})\|^2 \\ \text{s. t. } \min\limits_{\mathbf{s} \in \mathbb{R}^n} \|\widetilde{J}_k \mathbf{s} + \widetilde{\mathbf{r}}_k\|^2, \end{cases}$$

with $\widetilde{J}_k = \rho^{-1} J_k$ and $\widetilde{\mathbf{r}}_k = \rho^{-1} \mathbf{r}(\mathbf{x}^{(k)})$, before applying the algorithms described in the preceding sections. The Armijo-Goldstein principle (2.7) is modified accordingly. Similarly, the Tikhonov approach (5.9) is rescaled.

We adopt the following stopping rule for all the iterative methods. We iterate until either the difference between two successive approximations is small enough

$$\|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\| < \delta \|\mathbf{x}^{(k)}\|$$

or until a chosen maximum number of iterations $K_{\max}$ is reached. In our tests, we set $\delta = 10^{-8}$ and $K_{\max} = 60$.

In the case of ill-conditioned problems, it is useful to consider an additional stopping criterion in order to detect the unboundedness of the solution for a particular value of the regularization parameter. The iteration is interrupted when one of the preceding conditions is reached or when the ratio between the norms of the kth approximate solution and the initial point is larger than 10^8.

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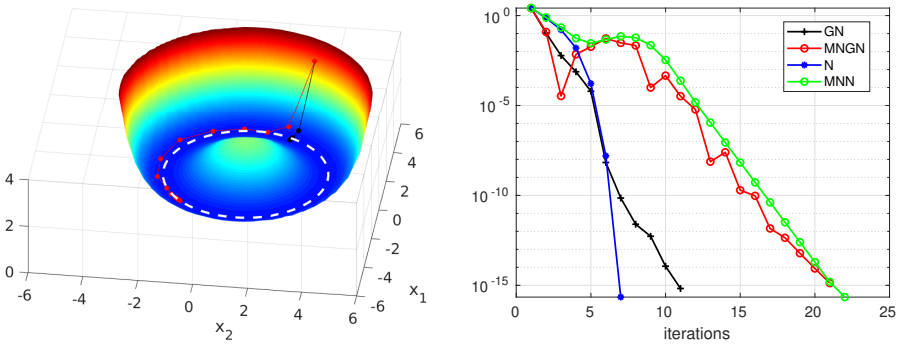

FIG. 7.1. *Convergence of problem (7.1) with* $\alpha = \beta = \frac{1}{9}$ *and* $\mathbf{x}^{(0)} = (5, 3)^T$. *In the 3D graph on the left, the white dashed line represents the locus of the solutions, the red dots are the iterations of the MNGN method, and the black ones correspond to the GN method. The graph on the right reports the residuals for each method.*

7. Numerical examples. In this section, we present two classes of numerical examples. In the first one, we apply the minimal-norm Gauss-Newton (MNGN) method of Section 3 to a well-conditioned problem of small dimension in order to visualize its convergence and compare it to the standard Gauss-Newton iteration. In the second numerical example, we apply the regularization techniques of Sections 5.1 and 5.2, that is, the truncated minimal-L-norm Gauss-Newton (TMLNGN) method and the minimal-L-norm Tikhonov-Gauss-Newton (TikLGN) method, to an ill-conditioned nonlinear problem of larger size. In each experiment, we solve problem (1.1) for a particular function $F(\mathbf{x})$ with values in $\mathbb{R}^m$ for $\mathbf{x} \in \mathbb{R}^n$.

The numerical experiments were performed on an Intel Xeon computer (12 cores, 24 threads) with 32 GB RAM, running the Debian GNU/Linux operating system. The computational code, implemented in Matlab R2019a, is available upon request.

7.1. A well-conditioned example. In this example, we let $m = 1$ and $\mathbf{x} = (x_1, x_2)^T$ in $\mathbb{R}^2$. The residual $r : \mathbb{R}^2 \to \mathbb{R}$ is the nonlinear function defined by

$$r(\mathbf{x}) = F(\mathbf{x}) - b = \left[\alpha(x_1 - 1)^2 + \beta(x_2 - 1)^2 - 1\right]^2 + 1,$$

depending upon the parameters $\alpha, \beta \in \mathbb{R}$. We minimize the objective function

$$f(\mathbf{x}) = \frac{1}{2} r(\mathbf{x})^2 = \frac{1}{2} \left\{ \left[\alpha(x_1 - 1)^2 + \beta(x_2 - 1)^2 - 1\right]^2 + 1 \right\}^2, \tag{7.1}$$

which can be graphically represented by a surface.

In this case, the least-squares problem (1.1) is underdetermined, so it has infinitely many solutions. We solve it by Newton's method (2.3), the Gauss-Newton method (2.6), the minimal-norm Gauss-Newton method (3.3), and the "projected" Newton method discussed in Remark 3.4.

First we consider $\alpha = \beta = \frac{1}{9}$. Figure 7.1 illustrates the progress of the iterations: the graph on the left displays the iterates produced by the MNGN and the GN methods in a 3D representation of $f(\mathbf{x})$. The one on the right reports the residuals corresponding to the above methods, to Newton's method (N), and to the "projected" Newton method (MNN). The last two methods converge to the same solutions as the GN and MNGN methods, respectively, so they are not represented in the 3D plot.

All the methods reach convergence as the residuals converge to zero. We see that MNGN takes longer to converge as it must "travel" across the solutions locus to reach the minimal-norm solution, which is the one nearby the origin. On the contrary, GN converges to the

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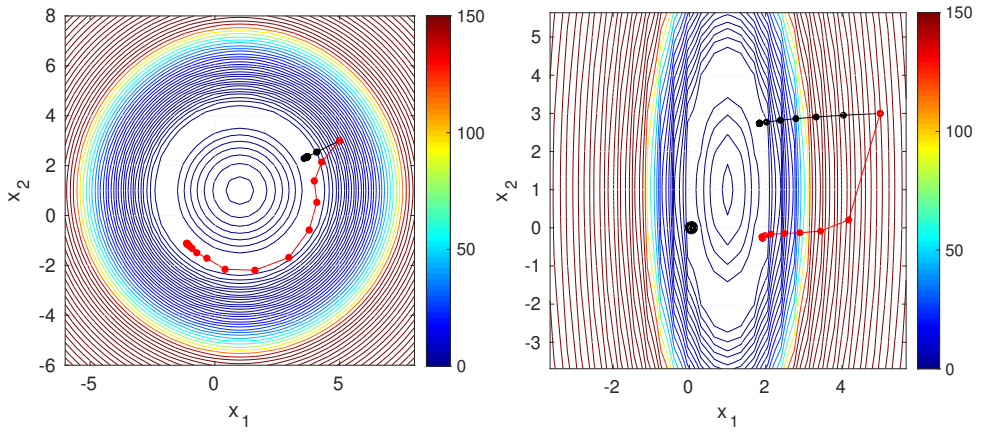

FIG. 7.2. *Contour plots for problem (7.1): on the left* $\alpha = \beta = \frac{1}{9}$, *on the right* $\alpha = 1$ *and* $\beta = \frac{1}{10}$. *The red dots are the iterates of the MNGN method and the black ones the approximations produced by the GN method. The thick black dot in the graph on the right is the minimal-norm solution.*

solution closer to the initial point. This fact is even clearer in the contour plot on the left of Figure 7.2.

Observing the residuals, we see that Newton's method has the highest convergence rate. Anyway, if we trivially project its iterates orthogonally to the null space of the Jacobian (see Remark 3.4), then it converges to the minimal-norm solution, but its speed of convergence degrades and equals the MNGN method. So, no computational gain is derived from its higher complexity.

It is also interesting to observe that the residuals of the MNGN method are not monotonically decreasing. The method, in some measure, is able to step away from the local attraction basin in order to chase the minimal-norm solution. Anyway, the dependence upon the initial point $\mathbf{x}^{(0)}$ is obviously maintained. This is shown in the contour plot on the right of Figure 7.2, which illustrates the convergence of the GN and MNGN methods when $\alpha = 1$ and $\beta = \frac{1}{10}$, starting from the same initial point. The MNGN method converges, in this case, to a solution with a smaller norm (i.e., with a smaller distance from the origin) than the one computed by the GN method but not to the minimal-norm solution identified by a thick black dot in the graph.

7.2. An ill-conditioned example. Electromagnetic induction (EMI) techniques are used to investigate soil properties in a non-destructive way. A nonlinear forward model for predicting the EM response of the subsoil was described in [42]. A regularized inversion algorithm was studied in [10, 12] and recently extended to process complex-valued data sets [11]. The algorithm, as well as the forward model, were coded in Matlab and included in a publicly available software package [9], which has already been employed in real-world applications [5, 11, 13].

In the model, the soil is assumed to have a layered structure with n layers. As it is usual in many applications, we let the magnetic permeability take the constant value $\mu_0 = 4\pi 10^{-7}\mathrm{H/m}$ (Henry/meter), that is, the value in the empty space. Let σ_i denote the electrical conductivity in the ith layer.

A measuring device generates an electromagnetic (primary) field and senses the induced (secondary) electromagnetic field. According to the instrument configuration (orientation of the coils, height above the ground, inter-coil distance, alternating current frequency) multiple measurements are available; see [10]. We will denote them by b_i, $i = 1, \ldots, m$, and the model

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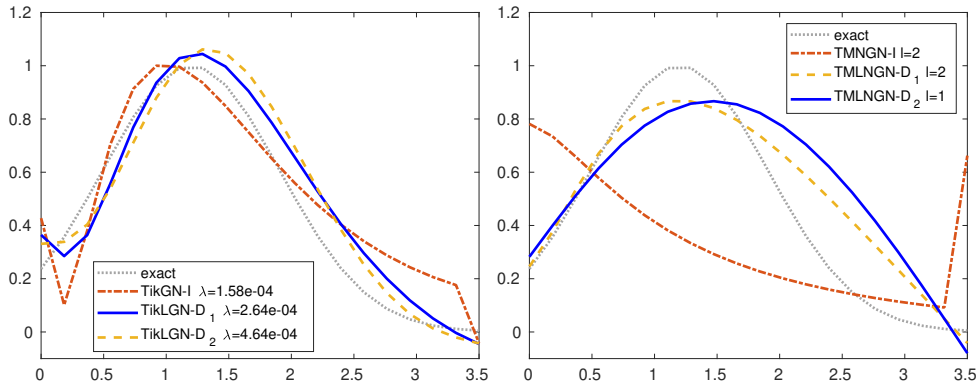

FIG. 7.3. *Electromagnetic data inversion: $m = n = 20$, noise level $\varepsilon = 10^{-2}$, comparison of the solution corresponding to the regularization matrices $L = I$, D_1, and D_2. The initial point is $\boldsymbol{\sigma}^{(0)} = 50\mathbf{e}$. The exact solution is compared to the solutions computed by TikGN/TikLGN on the left and by TMNGN/TMLNGN on the right. The parameters λ and ℓ are the best possible.*

prediction by $F(\boldsymbol{\sigma})$, where $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_n)^T$. Then, the problem of data inversion consists of computing the conductivity vector $\boldsymbol{\sigma}$ which determines the best fit to the data vector $\mathbf{b}$, that is, the one which solves the problem

$$\min_{\boldsymbol{\sigma} \in \mathbb{R}^n} \|\mathbf{r}(\boldsymbol{\sigma})\|^2, \qquad \text{with } \mathbf{r}(\boldsymbol{\sigma}) = F(\boldsymbol{\sigma}) - \mathbf{b}. \tag{7.2}$$

In our numerical simulation, we fix the following test model for the electrical conductivity as a function of depth,

$$\sigma(z) = \mathrm{e}^{-(z-1.2)^2}. \tag{7.3}$$

We discretize the soil by $n = 20$ uniformly spaced layers up to the depth of $3.5\mathrm{m}$ (meters), and we assign to each layer the conductivity $\sigma_i = \sigma(z_i)$, $i = 1, \ldots, n$, with $z_1 = 0\mathrm{m}$ and $z_n = 3.5\mathrm{m}$. We choose the configuration of an existing device (the Geophex GEM-2), using a single pair of coils at $1.66\mathrm{m}$ distance and 5 different current frequencies. This means that it can acquire 5 measurements for each sampling. The forward model generates a noise-free data vector $\mathbf{b}$ of m synthetic measurements, corresponding to placing the instrument at two different heights above the ground ($0.75\mathrm{m}$ and $1.5\mathrm{m}$) with the coils either in vertical orientation ($m = 10$) or in vertical and horizontal orientations ($m = 20$). To simulate experimental errors, the noise-free data vector $\widehat{\mathbf{b}}$ is perturbed by

$$\mathbf{b} = \widehat{\mathbf{b}} + \frac{\varepsilon \|\widehat{\mathbf{b}}\|}{\sqrt{m}} \mathbf{w},$$

where $\mathbf{w}$ is a normally distributed random vector with zero mean and unitary variance and ε represents the noise level.

We solve problem (7.2) by the damped Gauss-Newton method with the damping parameter determined by the Armijo-Goldstein principle. Each step of the iterative method is regularized by one of the methods described in this paper. In the standard case, when $L = I$, we display the solutions computed by the TMNGN (5.4) and TikGN (5.10) methods; when a regularization matrix is present, that is, when $L = D_1$ or D_2 (see (2.9)), we apply the TMLNGN (5.5) and TikLGN (5.14) methods.

The regularization parameters λ and ℓ are chosen both by minimizing the 2-norm error with respect to the exact solution in order to ascertain the best possible performance of the

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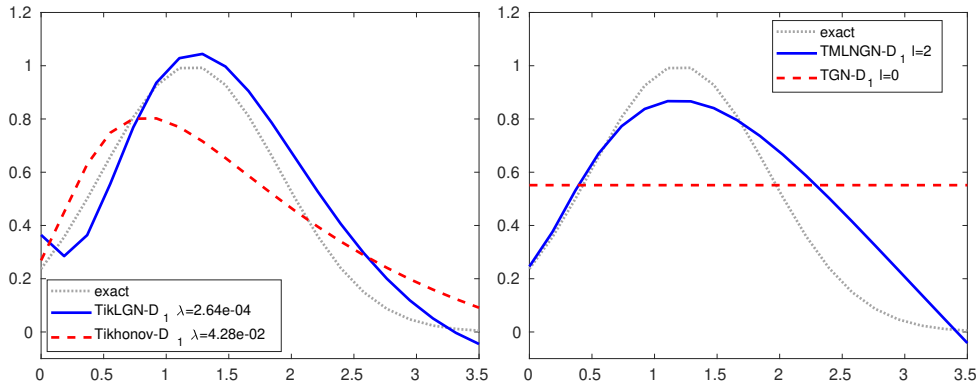

FIG. 7.4. *Electromagnetic data inversion:* $m = n = 20$, *noise level* $\varepsilon = 10^{-2}$, *regularization matrix* $L = D_1$, *initial point* $\boldsymbol{\sigma}^{(0)} = 50\mathbf{e}$. *The exact solution is compared to the solutions computed by TikLGN and the standard Tikhonov method (on the left) and by TMLNGN and by the Gauss-Newton method regularized by TGSVD, labelled as TGN (on the right). The parameters* λ *and* ℓ *are the best possible.*

methods and by the discrepancy principle (see Section 5) to test the algorithms in a realistic situation.

We start by discussing the importance of the regularization matrix L for the accuracy of the solution. The data set is composed by $m = 20$ measurements, the noise level is $\varepsilon = 10^{-2}$, a value consistent with experimental data sets, and the initial vector is $\boldsymbol{\sigma}^{(0)} = 50\mathbf{e}$ with $\mathbf{e} = (1, \ldots, 1)^T \in \mathbb{R}^{20}$.

The model function (7.3) is smooth, favoring a regularizing term based on the approximation of the first or second derivatives. The graphs in Figure 7.3 compare the solutions obtained by the regularization matrices $L = I$, D_1, and D_2. The computation is performed by using a Tikhonov approach (graph on the left) and by truncating the SVD/GSVD in the minimal-norm Gauss-Newton iteration (on the right). In the first case the solution corresponding to $L = I$ is evidently less accurate than the others. In the second one, the minimal-norm method TMNGN converges to a solution which is totally different from the model function, while the other two reconstructions are close to it. We also observe that in this case, as it happened in other experiments, Tikhonov regularization can reach a higher accuracy than the truncated SVD/TSVD approach. This is probably due to the fact that the regularization parameter λ can be varied continuously, while the parameter ℓ can only take integer values. In this example and in the following one, both parameters are chosen by minimizing the 2-norm error.

In many cases, especially when the initial vector used to initialize the iteration is close enough to the solution of the problem, the minimal-norm and the standard approaches produce similar approximations. Anyway, when the initial vector is rather far away from the solution, there are cases in which the minimal-norm methods are significantly more accurate and less sensible to the presence of local minima than the traditional approaches.

Figure 7.4 shows one of these cases. Here the minimal-norm algorithms are compared to the traditional approaches, namely, Tikhonov regularization (5.3) and the Gauss-Newton method regularized by TGSVD, labeled as TGN. The regularization matrix is the discretization of the first derivative operator; the other parameters are the same as in the previous example. We observe from the graph at the left of Figure 7.4 that the TikLGN method (5.9) reproduces very closely the exact solution, while the Tikhonov approach (5.3) is far less accurate. The graph at the right shows that, with the same data set, the reconstruction obtained by TGN is completely wrong, while the one produced by TMLNGN is acceptable.

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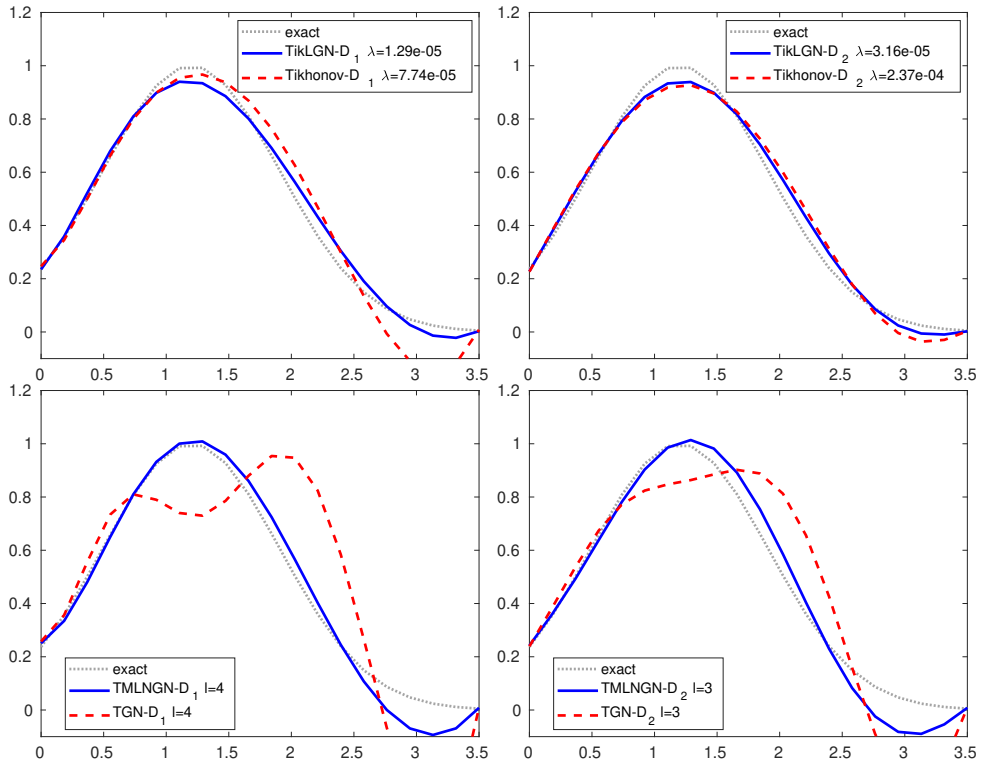

FIG. 7.5. *Electromagnetic data inversion:* $m = 10$, $n = 20$, *noise level* $\varepsilon = 10^{-4}$, *regularization matrix* $L = D_1$ *(left column) and* $L = D_2$ *(right column). The initial point is* $\boldsymbol{\sigma}^{(0)} = 1.5\mathbf{e}$. *The exact solution is compared to the solutions computed by TikLGN and the standard Tikhonov method (top row) and by TMLNGN/TGN (bottom row). The parameters* λ *and* ℓ *have been chosen by the discrepancy principle.*

In Figure 7.5 we illustrate the performance of the discrepancy principle in estimating the regularization parameters λ and ℓ. In this example, we consider $m = 10$ data values, the initial solution $\boldsymbol{\sigma}^{(0)} = 1.5\mathbf{e}$, and the noise level $\varepsilon = 10^{-4}$. The regularization matrix is the discretization of the first derivative for the graphs in the left column and of the second derivative for the right column. The graphs in the top row concern the reconstructions obtained by the TikLGN and Tikhonov methods with λ determined by the discrepancy principle. All solutions are acceptable, but the minimal-L-norm ones are slightly more accurate. At the bottom row we report the results obtained by the TMLNGN method and the Gauss-Newton method regularized by TGSVD (TGN). In this case, the TGN solutions, with ℓ estimated by (5.7), are strongly underregularized compared to the minimal-norm reconstructions.

8. Conclusions. This paper explores the solution of a nonlinear least-squares problem in the case its solution lacks unicity. The usual approach is to compute the minimal-norm solution of a linearization of the problem, generating an iterative method which does not guarantee that the converged solution itself has a minimal norm or minimizes a suitable semi-norm. Here, we develop various techniques to impose such constraint on the solution. In the case of ill-conditioned problems, we also propose two regularization algorithms, namely the truncated minimal-L-norm Gauss-Newton method and the minimal-L-norm Tikhonov-Gauss-Newton method. In the numerical experiments, we compare the newly proposed methods to the classical approaches. The results show that the two classes of methods produce, in general,

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different results. The new methods are in some cases less sensitive to the initial guess without a significant increase in the computational load.

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