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Comparison of A-posteriori parameter choice rules for linear discrete ill-posed problems

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ABSTRACT

Tikhonov regularization is one of the most popular methods for computing approximate solutions of linear discrete ill-posed problems with error-contaminated data. A regularization parameter, $\mu > 0$, balances the influence of a fidelity term, which measures how well the data is approximated, and of a regularization term, which dampens the propagation of the data error into the computed approximate solution. The quality of the computed solution is affected by the value of the regularization parameter μ. The discrepancy principle is a popular a-posteriori rule for determining a suitable value of μ. It performs quite well when a fairly accurate estimate of the norm of the error in the data is known. A modification of the discrepancy principle, proposed independently by Gfrerer and Raus, also can be used to determine μ. Analysis of this modification in an infinite-dimensional Hilbert space setting suggests that it will determine a value of μ that yields an approximate solution of higher quality than the approximate solution obtained when using the (standard) discrepancy principle to compute μ. This paper compares these a-posteriori rules for determining μ when applied to the solution of many linear discrete ill-posed problems with different amounts of error in the data. Our comparison shows that in a discrete setting, the discrepancy principle generally gives a value of μ that yields a computed solution of higher quality than the value of μ furnished by the modified discrepancy principle.

1. Introduction

We are concerned with the solution of minimization problems of the form

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \|A\boldsymbol{x} - \boldsymbol{b}\|, \tag{1}$$

where $\|\cdot\|$ denotes the Euclidean vector norm, $A \in \mathbb{R}^{m\times n}$ is an ill-conditioned matrix whose singular values "cluster" at the origin, and the data vector $\boldsymbol{b} \in \mathbb{R}^m$ is contaminated by an unknown error $\boldsymbol{e} \in \mathbb{R}^m$. The error may, for instance, be caused by measurement inaccuracies. Least-squares problems of this kind arise in many areas of science and engineering. They usually stem from the discretization of a linear ill-posed problem, such as a Fredholm integral equation of the first kind, and are commonly referred to as linear discrete ill-posed problems.

Let $\boldsymbol{b}_{\text{true}}$ denote the unavailable error-free vector associated with $\boldsymbol{b}$. Thus,

$$\boldsymbol{b} = \boldsymbol{b}_{\text{true}} + \boldsymbol{e}. \tag{2}$$

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We would like to determine the solution $\boldsymbol{x}_{\text{true}}$ of minimal Euclidean norm of the unavailable linear system of equations

$$A\boldsymbol{x} = \boldsymbol{b}_{\text{true}},$$

which we assume to be consistent. We determine an approximation of $\boldsymbol{x}_{\text{true}}$ by computing a suitable approximate solution of (1). Note that the least-squares solution of minimal norm of (1) typically is a poor approximation of $\boldsymbol{x}_{\text{true}}$ due to the error $\boldsymbol{e}$ in $\boldsymbol{b}$ and the presence of tiny positive singular values of A.

Tikhonov regularization is a commonly used technique for determining a useful approximation of $\boldsymbol{x}_{\text{true}}$. It is based on replacing the problem (1) by the penalized least-squares problem

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \left\{ \|A\boldsymbol{x} - \boldsymbol{b}\|^2 + \mu\|\boldsymbol{x}\|^2 \right\}. \tag{3}$$

The parameter $\mu > 0$ is a regularization parameter that balances the influence of the first term (the fidelity term) and the second term (the regularization term). The solution of (3) can be expressed as

$$\boldsymbol{x}_\mu := (A^TA + \mu I)^{-1}A^T\boldsymbol{b}, \tag{4}$$

where the superscript ^{T} denotes transposition. This solution exists for all $\mu > 0$.

The quality of the solution $\boldsymbol{x}_\mu$ of (3) is affected by the value of μ: A too large value of μ gives an over-smoothed solution that lacks details that the desired solution $\boldsymbol{x}_{\text{true}}$ may have, while a too small value of $\mu > 0$ yields a vector $\boldsymbol{x}_\mu$ that is unnecessarily, and possibly severely, contaminated by propagated error that stems from the error $\boldsymbol{e}$ in $\boldsymbol{b}$.

Assume that the norm

$$\epsilon = \|\boldsymbol{e}\| > 0, \tag{5}$$

or an accurate approximation thereof, is known. The *discrepancy principle* prescribes that $\mu > 0$ be determined so that the solution $\boldsymbol{x}_\mu$ of (3) satisfies

$$\|A\boldsymbol{x}_\mu - \boldsymbol{b}\| = \eta\epsilon, \tag{6}$$

where $\eta > 1$ is a user-specified constant independent of ϵ. This is a non-linear equation for μ as a function of $\epsilon > 0$. It has a unique solution $\mu = \mu(\epsilon)$ for most reasonable values of ϵ. A proof in an infinite-dimensional Hilbert space setting that $\boldsymbol{x}_{\mu(\epsilon)} \to \boldsymbol{x}_{\text{true}}$ as $\epsilon \searrow 0$ can be found, e.g., in [1].

The quality of the computed solution $\boldsymbol{x}_{\mu(\epsilon)}$ is sensitive to the accuracy of ϵ defined by (5): when $\epsilon \gg \|\boldsymbol{e}\|$, the regularization parameter μ determined by (6) is unnecessarily large, and $\epsilon \ll \|\boldsymbol{e}\|$ results in a too small value of μ. The sensitivity of μ and $\boldsymbol{x}_\mu$ to inaccuracies in an available estimate of $\|\boldsymbol{e}\|$ has been investigated by Hämarik et al. [2], who proposed alternatives to the discrepancy principle when only a poor estimate of $\|\boldsymbol{e}\|$ is known. In the present paper, we will assume that a fairly accurate estimate of $\|\boldsymbol{e}\|$ is available. Such an estimate may be known for the problem at hand or can be determined by a denoising method; see, e.g., [3–5] and references therein for a variety of such methods. The norm of the difference between the given vector $\boldsymbol{b}$ and a denoised version can be used as an estimate of the norm of the noise in $\boldsymbol{b}$. This is illustrated in [6].

Introduce the function

$$\phi_2(\mu) := \mu^2\boldsymbol{b}^T(AA^T + \mu I)^{-2}\boldsymbol{b}. \tag{7}$$

Eq. (6) for μ can be expressed as

$$\phi_2(\mu) = \eta^2\epsilon^2; \tag{8}$$

see, e.g., [7,8] for details. The function ϕ_2 is monotonically increasing with μ. It may be beneficial to replace μ by $\nu = 1/\mu$ before solving Eq. (8) by Newton's method; see [7,8] for discussions. We will denote the solution of (8) by μ_2 and the associated approximation of $\boldsymbol{x}_{\text{true}}$ determined by Tikhonov regularization by $\boldsymbol{x}_{\mu_2}$.

In the following variation of the discrepancy principle, which is referred to as the *modified discrepancy principle* by Hämarik et al. [2], the function (7) is replaced by

$$\phi_3(\mu) := \mu^3\boldsymbol{b}^T(AA^T + \mu I)^{-3}\boldsymbol{b}, \tag{9}$$

and Eq. (8) is replaced by

$$\phi_3(\mu) = \eta^2\epsilon^2. \tag{10}$$

We denote the solution by μ_3. This approach to determine the regularization parameter was first proposed by Gfrerer [9] and Raus [10]. Analysis in an infinite-dimensional Hilbert space setting by Gfrerer [9] suggests that the solution $\boldsymbol{x}_{\mu_3}$ should be a more accurate approximation of $\boldsymbol{x}_{\text{true}}$ than $\boldsymbol{x}_{\mu_2}$. The modified discrepancy principle is discussed by, e.g., Engl et al. [1, Section 5.1], Hanke and Hansen [8], Hansen [11, Section 7.3], and Neubauer [12].

The function ϕ_3 is monotonically increasing with μ. Therefore (10) has a unique solution for reasonable values of ϵ. We may compute it, e.g., by Newton's method.

Proposition 1. *Let μ_j be the unique solution of $\phi_j(\mu) = \eta^2\epsilon^2$ for $j \in \{2, 3\}$. Then $\mu_3 \le \mu_2$. Generally, the inequality is strict.*

The proposition shows that the modified discrepancy principle typically regularizes more than the (standard) discrepancy principle. We present a proof at the end of the following section after having introduced the singular value decomposition of the matrix A.

It is the purpose of the present paper to compare the quality of the solutions $\boldsymbol{x}_{\mu_2}$ and $\boldsymbol{x}_{\mu_3}$ when solving linear discrete ill-posed problems by Tikhonov regularization.

This paper is organized as follows. Section 2 defines the singular value decomposition (SVD) of A. Substituting this decomposition into (8) and (10) makes the evaluation of these functions easy and fast for each value of μ. However, the computation of the SVD of a large matrix is expensive. We therefore discuss in Section 3 how to, instead of using the SVD of A, use a small matrix that is computed by carrying out a few steps of Golub–Kahan bidiagonalization applied to A. Section 4 contains computed examples. Concluding remarks can be found in Section 5.

2. The singular value decomposition

Introduce the SVD of the matrix $A \in \mathbb{R}^{m\times n}$. For notational simplicity, we assume that $m \geq n$, but this restriction easily can be removed. Thus,

$$A = U\Sigma V^T, \tag{11}$$

where the matrices

$$U = [\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_m] \in \mathbb{R}^{m\times m} \text{ and } V = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_n] \in \mathbb{R}^{n\times n}$$

have orthonormal columns $\boldsymbol{u}_j$ and $\boldsymbol{v}_j$, respectively, and

$$\Sigma = \operatorname{diag}[\sigma_1, \sigma_2, \ldots, \sigma_n] \in \mathbb{R}^{m\times n}.$$

The σ_j are referred to as singular values and satisfy $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$. We refer to [13] for details and properties of the SVD.

Let

$$\widetilde{\boldsymbol{b}} = [\widetilde{b}_1, \widetilde{b}_2, \ldots, \widetilde{b}_m]^T := U^T\boldsymbol{b}.$$

Substituting the SVD (11) into (7) and (9) gives, for $\mu > 0$,

$$\phi_p(\mu) = \mu^p\widetilde{\boldsymbol{b}}^T(\Sigma\Sigma^T + \mu I)^{-p}\widetilde{\boldsymbol{b}} = \sum_{j=1}^{n}\frac{\widetilde{b}_j^2}{(\sigma_j^2/\mu + 1)^p} + \sum_{j=n+1}^{m}\widetilde{b}_j^2 \tag{12}$$

for $p \in \{2, 3\}$. The right-hand side of (12) can easily and inexpensively be evaluated for many different values of $\mu > 0$. This makes fast solution of (8) or (10) possible.

Having solved (8) or (10) for $\mu = \mu_2$ or $\mu = \mu_3$, respectively, we compute the associated solutions $\boldsymbol{x}_{\mu_2}$ or $\boldsymbol{x}_{\mu_3}$ of (3) by substituting (11) into (4) and letting $\mu = \mu_2$ or $\mu = \mu_3$ in

$$\boldsymbol{x}_\mu = \sum_{j=1}^{n}\frac{\sigma_j\widetilde{b}_j}{\sigma_j^2 + \mu}\boldsymbol{v}_j$$

Proof of Proposition 1. The function

$$p \to \frac{\widetilde{b}_j^2}{(\sigma_j^2/\mu + 1)^p}$$

is decreasing. Therefore, for fixed $\mu > 0$, $\phi_3(\mu) \leq \phi_2(\mu)$. The inequality is strict if $\widetilde{b}_j\sigma_j \neq 0$. The function

$$\mu \to \frac{\widetilde{b}_j^2}{(\sigma_j^2/\mu + 1)^p}$$

also is decreasing. In order for $\phi_2(\mu_2) = \phi_3(\mu_3)$, we must have $\mu_3 \leq \mu_2$. The inequality is strict if $\widetilde{b}_j\sigma_j \neq 0$ for at least one index $1 \leq j \leq n$. □

3. Bidiagonalization and quadrature

This section outlines an approach to solve large-scale Tikhonov regularization problem (3). Details of this approach are described in [7]. It uses the connection between partial Golub–Kahan bidiagonalization of the matrix A and certain Gauss-type quadrature rules that can be used to bound quantities of interest when determining the regularization parameter μ.

3.1. Bidiagonalization

It is unattractive to compute the SVD of a large matrix $A \in \mathbb{R}^{m\times n}$ due to the high computational cost; see [13, p. 493]. A Tikhonov regularization problem (3) with a large matrix A can be reduced to a fairly small Tikhonov regularization problem by the application of a variety of Krylov subspace methods; see, e.g., Gazzola et al. [14] for a recent survey. One of the most popular reduction methods is Golub–Kahan bidiagonalization; see [7,8,13]. Application of $\ell \leq \min\{m, n\}$ steps of Golub–Kahan bidiagonalization to A with initial vector $\boldsymbol{b}$ yields the decompositions

$$AV_\ell = U_{\ell+1}C_{\ell+1,\ell}, \qquad A^T U_\ell = V_\ell C_{\ell,\ell}^T, \tag{13}$$

where the matrices $U_{\ell+1} = [\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_{\ell+1}] \in \mathbb{R}^{m\times(\ell+1)}$ and $V_\ell = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_\ell] \in \mathbb{R}^{n\times\ell}$ have orthonormal columns with $\boldsymbol{u}_1 = \boldsymbol{b}/\|\boldsymbol{b}\|$. The matrix U_ℓ is made up of the first ℓ columns of $U_{\ell+1}$ and $C_{\ell+1,\ell}$ is lower bidiagonal with positive diagonal and subdiagonal entries,

$$C_{\ell+1,\ell} = \begin{bmatrix} \gamma_1 & & & & 0 \\ \delta_2 & \gamma_2 & & & \\ & \ddots & \ddots & & \\ & & \delta_{\ell-1} & \gamma_{\ell-1} & \\ & & & \delta_\ell & \gamma_\ell \\ 0 & & & & \delta_{\ell+1} \end{bmatrix} \in \mathbb{R}^{(\ell+1)\times\ell}. \tag{14}$$

It has leading principal submatrix $C_{\ell,\ell} \in \mathbb{R}^{\ell\times\ell}$; see, e.g., [13] for details. In this section, we may have $m \geq n$ or $m < n$. We assume that ℓ is chosen small enough so that the decompositions (13) with the stated properties exist. This is the generic situation. The value of ℓ used in the application of this paper, generally, is quite small; in particular, it is much smaller than $\min\{m, n\}$. Each step of Golub–Kahan bidiagonalization requires the evaluation of one matrix–vector product with A and the evaluation of one matrix–vector product with A^T. When A is large, these matrix–vector product evaluations constitute the dominating cost of the bidiagonalization process.

The range of V_ℓ is the Krylov subspace

$$\mathcal{K}_\ell(A^TA, A^T\boldsymbol{b}) = \operatorname{span}\{A^T\boldsymbol{b}, (A^TA)A^T\boldsymbol{b}, \ldots, (A^TA)^{(\ell-1)}A^T\boldsymbol{b}\}. \tag{15}$$

We seek to compute an approximate solution $\boldsymbol{x}_{\mu,\ell} = V_\ell \boldsymbol{y}_{\mu,\ell}$ of (3) in this subspace. Applying a Galerkin method to the normal equations associated with (3) yields

$$V_\ell^T(A^TA + \mu I)V_\ell \boldsymbol{y}_{\mu,\ell} = V_\ell^T A^T \boldsymbol{b},$$

which, by using the decompositions (13), can be expressed as

$$(C_{\ell+1,\ell}^T C_{\ell+1,\ell} + \mu I)\boldsymbol{y}_{\mu,\ell} = C_{\ell+1,\ell}^T \boldsymbol{e}_1 \|\boldsymbol{b}\|, \tag{16}$$

where $\boldsymbol{e}_1 = [1, 0, \ldots, 0]^T$ denotes the first axis vector. The solution of (16), by rewriting the equations as an equivalent least-squares problem, is described in [7].

It remains to determine how many bidiagonalization steps, ℓ, to carry out. The computed solution $\boldsymbol{x}_{\mu,\ell}$ cannot satisfy the discrepancy or modified discrepancy principles when ℓ is too small, while letting ℓ be large may make the application of Golub–Kahan bidiagonalization unnecessarily expensive. We will determine upper and lower bounds for the functions (7) and (9) with the aid of quadrature rules that can be evaluated by using the connection between Gauss-type quadrature and the decompositions (13). This approach for computing upper and lower bounds for the function (7) has previously been described in [7].

3.2. Quadrature rules

We review the technique used in [7] for computing bounds for the function (7). This method also can be applied to bound the function (9). We refer to [7] for details. Extensions and many references can be found in [15,16].

Consider the spectral factorization

$$AA^T = W\Lambda W^T,$$

where $\Lambda = \operatorname{diag}[\lambda_1, \lambda_2, \ldots, \lambda_m] \in \mathbb{R}^{m\times m}$ and the matrix $W \in \mathbb{R}^{m\times m}$ is orthogonal. Substitution into (7) or (9) yields

$$\begin{aligned} \phi_p(\mu) &= \boldsymbol{b}^T W(\mu^{-1}\Lambda + I)^{-p} W^T \boldsymbol{b} \\ &= \sum_{j=1}^m \frac{\widehat{\beta}_j^2}{(\mu^{-1}\lambda_j + 1)^p}, \end{aligned} \tag{17}$$

where $\widehat{\boldsymbol{b}} = [\widehat{\beta}_1, \widehat{\beta}_2, \ldots, \widehat{\beta}_m]^T := W^T \boldsymbol{b}$. The sum in (17) can be expressed as a Stieltjes integral

$$\phi_p(\mu) = \int_0^\infty \frac{1}{(\mu^{-1}\lambda + 1)^p} d\omega(\lambda) \tag{18}$$

with a piece-wise constant distribution function ω with jump discontinuities of height $\widehat{\beta}_j^2$ at the eigenvalues λ_j; $d\omega$ is the associated measure.

We will approximate the integral (18) by Gauss-type quadrature rules. One can show that

$$G_{\ell,p}(\mu) := \|\boldsymbol{b}\|^2 \boldsymbol{e}_1^T (\mu^{-1} C_{\ell,\ell} C_{\ell,\ell}^T + I_\ell)^{-p} \boldsymbol{e}_1.$$

is an ℓ-node Gauss quadrature rule for approximating the integral (18) and

$$R_{\ell+1,p}(\mu) := \|\boldsymbol{b}\|^2 \boldsymbol{e}_1^T (\mu^{-1} C_{\ell+1,\ell} C_{\ell+1,\ell}^T + I_{\ell+1})^{-p} \boldsymbol{e}_1.$$

is an $(\ell+1)$-node Gauss–Radau quadrature rule with a fixed nodes at the origin for approximating the same integral; see, e.g., [7,15,16] for details.

Since the derivatives of the integrand in (18) (as a function of λ) of even order are negative on the interval of integration and the derivatives of odd order are positive, the remainder formulas for the error in Gauss and Gauss–Radau quadrature show that, generically,

$$G_{\ell,p}(\mu) < \phi_p(\mu) < R_{\ell+1,p}(\mu), \qquad \mu > 0, \qquad p \in \{2, 3\}. \tag{19}$$

The quadrature errors of the rules $G_{\ell,p}(\mu)$ and $R_{\ell+1,p}(\mu)$ decrease as ℓ increases; see [17]. Thus, we can compute upper and lower bounds for the integral (18) of desired accuracy by using the decompositions (13) with ℓ chosen sufficiently large. Following [7], we increase ℓ until we can determine a value of μ, denoted by μ_ℓ, that satisfies

$$\epsilon^2 \le G_{\ell,p}(\mu_\ell) \text{ and } R_{\ell+1,p}(\mu_\ell) \le \epsilon^2 \alpha^2 \tag{20}$$

for some constant $\alpha > 1$ independent of μ and ℓ. This is done by solving

$$\phi_{\ell,p}(\mu) = \epsilon^2 \tag{21}$$

by Newton's method, where $\phi_{\ell,p}(\mu) := G_{\ell,p}(\mu)$. Details for $p = 2$ are provided in [7]; the computations when $p = 3$ are carried out in the same manner.

It follows from (19) that

$$\epsilon^2 < \phi_p(\mu_\ell) < \epsilon^2 \alpha^2.$$

For many linear discrete ill-posed problems, the required number of bidiagonalization steps, ℓ, is quite small. This is illustrated in the following section. Having determined μ_ℓ as described, we compute the corresponding approximate solution $\boldsymbol{x}_{\mu_\ell,\ell}$ in the Krylov subspace (15) as outlined in Section 3.1. Here we only note that the dominating computational expense for determining $\boldsymbol{x}_{\mu_\ell,\ell}$ is the evaluation of the decompositions (13). Note that it is not necessary to compute the SVD of any matrix in the method of this section.

4. Computed examples

This section presents computed examples with several of the linear discrete ill-posed problems that are available in the MATLAB package Regularization Tools by Hansen [18]. All problems are discrete ill-posed problems; many are discretizations of Fredholm integral equations of the first kind. The problems are described in [18]. Further discussions on some of the problems can be found in [19–22].

The discretized problems have matrices $A \in \mathbb{R}^{2000\times 2000}$. The codes in the Regularization Tools provide the "exact solution" $\boldsymbol{x}_{\text{true}}$, which is used to compute the "exact right-hand side" $\boldsymbol{b}_{\text{true}} := A\boldsymbol{x}_{\text{exact}}$. The error $\boldsymbol{e}$ in $\boldsymbol{b}$ (cf. (2)) is Gaussian with zero mean and the variance is chosen to correspond to a specified noise level $\|\boldsymbol{e}\|/\|\boldsymbol{b}_{\text{true}}\| \in \{10^{-1}, 10^{-2}, 10^{-3}\}$. For each problem and each noise level, we generate 10 random noise vectors $\boldsymbol{e}$. The tables report averages of the relative error

$$\text{RE} := \frac{\|\boldsymbol{x}_{\text{computed}} - \boldsymbol{x}_{\text{true}}\|}{\|\boldsymbol{x}_{\text{true}}\|} \tag{22}$$

achieved for the 10 noise vectors of specified noise level, as well as standard deviations (SD), when using the discrepancy principle and the modified discrepancy principle to determine the regularization parameter.

The iterations with Newton's method applied to the solution of (8) or (10) use the initial iterate $\mu^{(0)} = 0$. Both $\phi_p(0)$ and the derivative $\phi_p'(0)$ can be evaluated by taking limits of $\phi_p(\mu)$ and $\phi_p'(\mu)$ as $\mu \searrow 0$; see [7] for details when $p = 2$. Formulas for $p = 3$ can be evaluated similarly. Newton's method determines iterates $\mu^{(k)}$, $k = 1, 2, \ldots$. The iterations with Newton's method are terminated as soon as an iterate $\mu^{(k)}$ satisfies

$$|\phi_p(\mu^{(k)})| \le 2 \cdot 10^{-3} \|\boldsymbol{e}\|. \tag{23}$$

Table 1
Modified Discrepancy Principle (MD) vs. Discrepancy Principle (D) using the SVD to determine the regularization parameter μ. The table shows the average relative error (avg. RE) and its standard deviation (SD).

Noise level	Problem	Avg. RE		SD	
		MD	D	MD	D
10^{-3}	baart	1.1×10^{-1}	1.1×10^{-1}	4.5×10^{-3}	5.3×10^{-3}
	foxgood	1.0×10^{-2}	7.5×10^{-3}	2.5×10^{-3}	2.6×10^{-3}
	shaw	4.9×10^{-2}	4.6×10^{-2}	1.2×10^{-3}	1.9×10^{-3}
	gravity	1.3×10^{-2}	1.0×10^{-2}	2.2×10^{-3}	2.0×10^{-3}
	deriv2	3.7×10^{-1}	1.4×10^{-1}	2.3×10^{-1}	5.6×10^{-3}
	heat	3.0×10^{-2}	2.3×10^{-2}	2.2×10^{-3}	1.3×10^{-3}
	phillips	9.0×10^{-3}	6.3×10^{-3}	9.3×10^{-4}	1.0×10^{-3}
10^{-2}	baart	1.6×10^{-1}	1.5×10^{-1}	1.1×10^{-2}	1.4×10^{-2}
	foxgood	2.9×10^{-2}	1.6×10^{-2}	8.8×10^{-3}	7.6×10^{-3}
	shaw	7.7×10^{-2}	6.3×10^{-2}	1.7×10^{-2}	1.5×10^{-2}
	gravity	2.9×10^{-2}	2.1×10^{-2}	4.9×10^{-3}	5.8×10^{-3}
	deriv2	3.4×10^{-1}	2.0×10^{-1}	1.9×10^{-1}	1.3×10^{-2}
	heat	8.4×10^{-2}	6.4×10^{-2}	7.9×10^{-3}	6.8×10^{-3}
	phillips	2.3×10^{-2}	1.7×10^{-2}	1.7×10^{-3}	3.7×10^{-3}
10^{-1}	baart	2.7×10^{-1}	2.3×10^{-1}	6.2×10^{-2}	4.7×10^{-2}
	foxgood	5.5×10^{-2}	3.2×10^{-2}	2.1×10^{-2}	1.5×10^{-2}
	shaw	1.8×10^{-1}	1.3×10^{-1}	8.8×10^{-2}	3.3×10^{-2}
	gravity	7.1×10^{-2}	5.0×10^{-2}	1.3×10^{-2}	1.4×10^{-2}
	deriv2	4.1×10^{-1}	3.1×10^{-1}	1.5×10^{-1}	2.7×10^{-2}
	heat	7.1×10^{-1}	1.7×10^{-1}	7.9×10^{-1}	1.7×10^{-2}
	phillips	5.9×10^{-2}	4.1×10^{-2}	8.5×10^{-3}	8.2×10^{-3}

The solution of (21) is carried out similarly with an analogous stopping criterion, i.e., $\phi_p(\mu^{(k)})$ is replaced by $\phi_{\ell,p}(\mu^{(k)})$ in (23).

Table 1 shows results for the situation described in Section 2 when the SVD of A is computed, while Table 2 displays the corresponding results when the solution is computed by first carrying out a few bidiagonalization steps as described in Section 3. The parameters η and α in (6) and (20), respectively, are set to 1.01.

Table 1 shows the average relative error to be smaller when the parameter μ is determined by the discrepancy principle than when it is determined by the modified discrepancy principle for all problems and all noise levels. The better performance of the discrepancy principle depends on that the regularization parameter determined by the discrepancy principle generally is strictly larger than the regularization parameter obtained by the modified discrepancy principle; see Proposition 1. The standard deviation of the relative error is for some problems slightly larger for the discrepancy principle than for the modified discrepancy principle. The computations are carried out by using the SVD of A as described in Section 2. Results similar to those of Table 1 are obtained for smaller and larger matrices A. The table indicates that there is no reason to use the modified discrepancy principle when an accurate estimate of the norm of the error $\boldsymbol{e}$ is available.

Table 2 is analogous to Table 1 and shows results for the situation when the regularization parameter μ is computed by the method of Section 3. The table shows the average relative error to be smaller when the parameter μ is determined by the discrepancy principle than when it is determined by the modified discrepancy principle for all problems and all noise levels. For some problems, the standard deviation of the relative error is somewhat larger when the discrepancy principle is used. The solution method reduces the matrix A in the large Tikhonov regularization problem (3) to a small bidiagonal matrix $C_{\ell+1,\ell}$; see (13) and (14). Table 2 reports for each problem the average value of ℓ for each noise realization. We remark that the computation of an approximation of $\boldsymbol{x}_{\text{true}}$ in a Krylov subspace of dimension ℓ entails regularization in addition to the regularization furnished by choosing a regularization parameter $\mu > 0$. The table shows the discrepancy principle to yield a smaller average relative error (22) than the modified discrepancy principle. Analogous results are obtained for Tikhonov regularization problem (3) with a matrix A of different size.

5. Conclusion

The average relative errors reported for the discrepancy principle are smaller than those achieved with the modified discrepancy principle for a variety of linear discrete ill-posed problems solved by Tikhonov regularization. This holds both when the solution is computed by a method that is well suited for small to moderately sized problems based on first evaluating the SVD of the matrix of the problem, and when the solution is determined by a method that is well suited for large-scale problems based on reducing the given problem to a smaller one by carrying out a few steps of Golub–Kahan bidiagonalization. We conclude that when a fairly accurate estimate of the noise level in the data $\boldsymbol{b}$ is available, the discrepancy principle performs better than the modified discrepancy principle. When no such estimate is available, then it may be beneficial to use other methods for determining the regularization parameter such as methods described in [2] or so-called heuristic parameter choice rules; see, e.g., [23–25] for discussions of the latter.

Table 2
Modified Discrepancy Principle (MD) vs. Discrepancy Principle (D) using bidiagonalization to determine the regularization parameter μ. The table shows the average number of bidiagonalization steps (avg. ℓ), the average relative error (avg. RE), and its standard deviation (SD).

Noise	Problem	Avg. ℓ		Avg. RE		SD	
level		MD	D	MD	D	MD	D
10^{-3}	baart	4.9	5.0	1.2×10^{-1}	1.0×10^{-1}	8.8×10^{-3}	3.4×10^{-2}
	foxgood	4	4	1.1×10^{-2}	8.0×10^{-3}	2.6×10^{-3}	2.3×10^{-3}
	shaw	8	8	4.9×10^{-2}	4.2×10^{-2}	1.1×10^{-3}	1.4×10^{-3}
	gravity	9	9.1	1.6×10^{-2}	1.3×10^{-2}	1.1×10^{-3}	1.6×10^{-3}
	deriv2	14.8	15.2	1.5×10^{-1}	1.4×10^{-1}	4.5×10^{-3}	4.4×10^{-3}
	heat	21	22	3.3×10^{-2}	2.3×10^{-2}	1.6×10^{-3}	1.5×10^{-3}
	phillips	9.8	10.6	1.1×10^{-2}	6.8×10^{-3}	9.8×10^{-4}	1.5×10^{-3}
10^{-2}	baart	4	4	1.6×10^{-1}	1.5×10^{-1}	3.4×10^{-3}	7.1×10^{-3}
	foxgood	3	3	2.9×10^{-2}	1.9×10^{-2}	5.2×10^{-3}	7.1×10^{-3}
	shaw	6	6	1.0×10^{-1}	9.3×10^{-2}	8.7×10^{-3}	1.0×10^{-2}
	gravity	7	7	3.5×10^{-2}	2.7×10^{-2}	1.9×10^{-3}	2.4×10^{-3}
	deriv2	8	8.1	2.4×10^{-1}	2.2×10^{-1}	5.8×10^{-3}	9.2×10^{-3}
	heat	14	15	9.9×10^{-2}	7.2×10^{-2}	3.4×10^{-3}	4.4×10^{-3}
	phillips	7.2	7.5	2.8×10^{-2}	2.2×10^{-2}	2.4×10^{-3}	2.3×10^{-3}
10^{-1}	baart	3	3	3.0×10^{-1}	2.7×10^{-1}	2.0×10^{-2}	2.3×10^{-2}
	foxgood	3	3	7.9×10^{-2}	3.9×10^{-2}	1.2×10^{-2}	1.3×10^{-2}
	shaw	5	5	1.6×10^{-1}	1.4×10^{-1}	1.1×10^{-2}	2.1×10^{-2}
	gravity	5	5	8.3×10^{-2}	6.0×10^{-2}	7.7×10^{-3}	7.0×10^{-3}
	deriv2	4	4	3.7×10^{-1}	3.5×10^{-1}	7.8×10^{-3}	8.2×10^{-3}
	heat	9	9	2.5×10^{-1}	2.1×10^{-1}	1.1×10^{-2}	1.1×10^{-2}
	phillips	4.9	6.4	9.0×10^{-2}	4.3×10^{-2}	1.0×10^{-2}	6.9×10^{-3}

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