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Error estimates for Arnoldi–Tikhonov regularization for ill-posed operator equations

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Abstract

Most of the literature on the solution of linear ill-posed operator equations, or their discretization, focuses only on the infinite-dimensional setting or only on the solution of the algebraic linear system of equations obtained by discretization. This paper discusses the influence of the discretization error on the computed solution. We consider the situation when the discretization used yields an algebraic linear system of equations with a large matrix. An approximate solution of this system is computed by first determining a reduced system of fairly small size by carrying out a few steps of the Arnoldi process. Tikhonov regularization is applied to the reduced problem and the regularization parameter is determined by the discrepancy principle. Errors incurred in each step of the solution process are discussed. Computed examples illustrate the error bounds derived.

Keywords: inverse problems, regularization methods, Arnoldi decomposition, convergence analysis

1. Introduction

Let $A : \mathcal{X} \to \mathcal{Y}$ be an injective linear operator between the Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$, and assume that A is not continuously invertible. We are concerned with the solution of operator equations of the form

$$Ax = y, \qquad x \in \mathcal{X}, \quad y \in \mathcal{Y}. \tag{1.1}$$

Let $\|\cdot\|_{\mathcal{X}}$ and $\|\cdot\|_{\mathcal{Y}}$ denote the norms of the spaces $\mathcal{X}$ and $\mathcal{Y}$, respectively. We will assume that equation (1.1) is consistent and are interested in determining the solution of minimal norm. We denote this solution by $\widehat{x}$. The solution $\widehat{x}$ might not depend continuously on y. Therefore its computation is an ill-posed problem.

The right-hand side y of (1.1) is assumed not to be available; only an error-contaminated approximation $y^\delta \in \mathcal{Y}$ of y is known. We assume that y^δ satisfies

$$\|y - y^\delta\|_{\mathcal{Y}} \leqslant \delta, \tag{1.2}$$

with a known bound $\delta > 0$. The solution of the equation

$$Ax = y^\delta, \qquad x \in \mathcal{X}, \quad y^\delta \in \mathcal{Y}, \tag{1.3}$$

obtained by replacing y by y^δ in (1.1), if it exists, generally, is not a meaningful approximation of the desired solution $\widehat{x}$ since A is not continuously invertible. In fact, equation (1.3) might not have a solution even when equation (1.1) does. A regularization method, which replaces the operator A by a nearby operator, such that the solution of the modified equation so obtained exists and is less sensitive to the error in y^δ, has to be used to obtain a meaningful approximation of $\widehat{x}$.

The numerical solution of (1.3) requires discretization at a certain stage of the process. In general, this can be done in two ways:

(i) *Regularize then discretize:* In this approach, the infinite-dimensional ill-posed problem is transformed into a well-posed problem, e.g. by means of *Tikhonov regularization*. Then the well-known error estimates for the regularized solution, see, e.g. [7] for regularization in Hilbert spaces, can be applied. In a second step the now well-posed regularized equation is discretized, and available error estimators for well posed-problems, e.g. from the theory of finite elements, can be used. This approach has been followed in, e.g. [4, 10, 16, 20].

(ii) *Discretize then regularize:* The discretization of the ill-posed operator equation (1.3) yields a linear system of algebraic equations

$$A_n x_n = y_n^\delta \tag{1.4}$$

with an ill-conditioned, possibly singular, matrix $A_n \in \mathbb{R}^{n,n}$, and vectors $x_n, y_n^\delta \in \mathbb{R}^n$. Well-known methods from linear algebra are used for its solution; see, e.g. [3, 11, 13]. The difficulty with this approach is to obtain convergence and convergence rate results for the distance between the solution of the infinite-dimensional problem (1.1) and its discretized counterpart x_n fulfilling (1.4), see, e.g. [5, 18].

As mentioned above, the approach (i) works particularly well for different variants of Tikhonov regularization. Iterative methods, however, require frequent application of the operator, and maybe of its adjoint, which is only possible in a discretized form. Iterative methods therefore belong to category (ii). An analysis of approach (ii) has been carried out for an adaptive version of Landweber iteration [24], but to the best of our knowledge this approach has not been investigated for Krylov subspace methods. Additionally, methods that work exceptionally well in finite dimensions but have no infinite-dimensional counterpart, or for which an error analysis is missing in infinite dimensions, belong to category (ii). The latter holds for the method discussed in the present paper.

In this paper, we start with two continuous linear operator equations (1.1) and (1.3), and discretize the latter to obtain the linear system of algebraic equation (1.4). We are concerned with the situation when the matrix A_n is large and, in particular, when A_n is too large to make the computation of its singular value decomposition attractive. Then we apply the Arnoldi process to compute an approximation of fairly low rank of the matrix A_n in (1.4). We replace A_n in (1.4) by this low-rank approximation, and compute an approximate solution of the linear system of equations with the aid of Tikhonov regularization. The replacement of A_n by a low-rank approximation reduces the computational effort required for Tikhonov regularization when the matrix A_n is large, which is the situation of interest to us. Our approach allows us to solve problems with a matrix A_n that is too large to make the use of direct solution methods, which require factorization of a large matrix, e.g. of A_n or a related matrix, too expensive to be attractive or feasible. We will discuss the effect on the computed solution of discretization errors that stem from replacing the operator A by the matrix A_n, as well as the effect of the error in the right-hand side y^δ. Moreover, we are concerned with the influence on the computed solution of the replacement of the matrix A_n in the linear system (1.4) by a low-rank matrix determined by the Arnoldi process. We remark that Tikhonov regularization based on partial Arnoldi decomposition, and some variations thereof, have been described in [3, 6, 8, 14, 15] and in references therein. The contribution of this paper is to provide an error analysis.

This paper is organized as follows. Section 2 discusses results by Natterer [18] on the discretization of integral operators. Discretization yields the linear system of algebraic equation (1.4). We assume that the matrix A_n determined by discretization is so large that factorization is unattractive or unfeasible. Section 3 reviews the Arnoldi process for computing an approximation of fairly low rank of the matrix A_n in (1.4). We use this low-rank approximation in Tikhonov regularization and obtain a quite efficient solution method. To analyze the performance of this solution approach, we have to take into account the discretization error as well as the error incurred by approximating the matrix A_n by the low-rank approximation furnished by the Arnoldi process. Section 4 applies bounds due to Neubauer [20] to the computed solution obtained by the Tikhonov regularized problem that uses the approximation of the matrix A_n in (1.4) computed with the Arnoldi process. We remark that while the bounds provided by Natterer [18] shed light on the influence of the discretization error on the computed solution, they are not useful for assessing the effect of approximating the matrix A_n by a low-rank approximation determined by the Arnoldi process. We will comment further on this issue in remark 4.10 of section 4. A few computed examples that illustrate the theory are presented in section 5, and concluding remarks can be found in section 6.

2. Discretization of the operator equation

To be able to numerically compute an approximate solution of equation (1.3) in the infinite-dimensional Hilbert space $\mathcal{X}$, the equation first has to be discretized. This results in the finite-dimensional equation (1.4). We introduce a discretization and define a finite-dimensional least-squares problem similarly as Natterer [18], who investigated regularization properties of projection methods.

Introduce the finite-dimensional subspaces

$$\mathcal{X}_n \subset \mathcal{X}, \qquad \dim(\mathcal{X}_n) = n,$$
$$\mathcal{Y}_n = A\mathcal{X}_n,$$

and define projectors $P_n : \mathcal{X} \to \mathcal{X}_n$ and $Q_n : \mathcal{Y} \to \mathcal{Y}_n$. The space $\mathcal{X}_n$ is chosen for its convenience to use in applications and for the approximation properties of its elements. For instance, $\mathcal{X}_n$ may be a space of piece-wise polynomials or finite elements.

Consider the linear system of equations

$$Q_n A P_n x = Q_n y^\delta. \tag{2.1}$$

We identify the matrix A_n and vector y_n^δ in (1.4) with the finite-dimensional operator $Q_n A P_n$ and the right-hand side $Q_n y^\delta$ in (2.1), respectively. The unique least-squares solution of minimal norm of equation (2.1) is given by $x_n := A_n^\dagger y_n^\delta$, where $A_n^\dagger$ denotes the Moore–Penrose pseudoinverse of the matrix A_n. We identify this solution of (2.1) with the solution in $\mathbb{R}^n$ of (1.4).

Let $\{e_j\}_{j=1}^n$ form a convenient basis for $\mathcal{X}_n$, such as a basis of piece-wise polynomials or finite elements with local support. Consider the representation

$$x_n = \sum_{j=1}^n x_j^{(n)} e_j \tag{2.2}$$

of an element $x_n \in \mathcal{X}_n$. We identify the function x_n with the vector

$$\vec{x}_n = [x_1^{(n)}, x_2^{(n)}, \ldots, x_n^{(n)}]^T \in \mathbb{R}^n.$$

To shed light on how $\|x_n\|_{\mathcal{X}}$ relates to $\|\vec{x}_n\|_2$, we introduce an orthonormal basis $\{\widehat{e}_j\}_{j=1}^n$ for $\mathcal{X}_n$. There is a nonsingular matrix $M_n = [m_{ij}] \in \mathbb{R}^{n\times n}$ such that

$$[e_1, e_2, \ldots, e_n] = [\widehat{e}_1, \widehat{e}_2, \ldots, \widehat{e}_n] M_n,$$

i.e. $e_j = \sum_{i=1}^n m_{i,j} \widehat{e}_i$ for $j = 1, 2, \ldots, n$. For instance, when the basis $\{\widehat{e}_j\}_{j=1}^n$ is determined from $\{e_j\}_{j=1}^n$ by the Gram–Schmidt process, the matrix M_n is upper triangular.

We obtain from (2.2) that

$$x_n = [e_1, e_2, \ldots, e_n]\vec{x}_n = [\widehat{e}_1, \widehat{e}_2, \ldots, \widehat{e}_n] M_n \vec{x}_n.$$

It follows that

$$\|x_n\|_{\mathcal{X}} = \|M_n \vec{x}_n\|_2 \leqslant \|M_n\|_2 \|\vec{x}_n\|_2 = \sigma_{\max}(M_n)\|\vec{x}_n\|_2, \tag{2.3}$$

where $\sigma_{\max}(M_n)$ denotes the largest singular value of the matrix M_n. Let $\sigma_{\min}(M_n)$ stand for the smallest singular value of M_n. Then we obtain analogously to (2.3) that

$$\|x_n\|_{\mathcal{X}} \geqslant \sigma_{\min}(M_n)\|\vec{x}_n\|_2.$$

We will assume that there are constants $c_{\min}$ and $c_{\max}$ (independent of n) such that

$$0 < c_{\min} \leqslant \sigma_{\min}(M_n), \qquad \sigma_{\max}(M_n) \leqslant c_{\max} < \infty \qquad \forall n.$$

Then

$$c_{\min}\|\vec{x}_n\|_2 \leqslant \|x_n\|_{\mathcal{X}} \leqslant c_{\max}\|\vec{x}_n\|_2. \tag{2.4}$$

Thus, the norms $\|\cdot\|_{\mathcal{X}}$ and $\|\cdot\|_2$ are equivalent. We will therefore simply write $\vec{x}_n$ as x_n.

Another way of obtaining an estimate (2.4) is by using the decomposition (2.2) directly: let $\langle\cdot,\cdot\rangle$ denote the inner product in $\mathcal{X}$ and define the norm $\|x\|_{\mathcal{X}} = \langle x, x\rangle^{1/2}$. Since the functions $e_1, e_2, \ldots, e_n$ are linearly independent, the Gram matrix $D_n = (\langle e_j, e_i\rangle)_{i,j=1,\ldots n}$ is positive definite. Moreover,

$$\begin{aligned}\|x_n\|_{\mathcal{X}}^2 &= \langle \sum_{j=1}^n x_j^{(n)} e_j, \sum_{j=1}^n x_j^{(n)} e_j\rangle \\ &= \sum_{j=1}^n \sum_{i=1}^n x_j^{(n)} x_j^{(n)} \langle e_j, e_i\rangle = \vec{x}_n^T D_n \vec{x}_n.\end{aligned}$$

The constants $c_{\min}$ and $c_{\max}$ in (2.4) can be chosen as the square root of the minimal and maximal eigenvalues of D_n, respectively. For instance, if the set $\{e_j\}_{j=1}^n$ forms an orthonormal basis for $\mathcal{X}_n$, then $D_n = I$ and (2.4) holds with $c_{\min} = c_{\max} = 1$. This is the situation when an orthonormal wavelet basis is used for the discretization. Another simple example is the use of linear B-spline fuctions (hat functions). Let $\{t_1, t_2, \ldots, t_n\}$ be an equidistant partition of the interval $[0, 1]$, and let $e_1, e_2, \ldots, e_n$ denote normalized hat functions associated with this partition. Define the subspace $\mathcal{X}_n = \text{span}\{e_1, e_2 \ldots, e_n\}$. A simple calculation shows that

$$D_n = \begin{bmatrix} 1 & \frac{1}{2\sqrt{2}} & 0 & 0 & 0 & \cdots & 0 \\ \frac{1}{2\sqrt{2}} & 1 & \frac{1}{4} & 0 & 0 & \ddots & 0 \\ 0 & \frac{1}{4} & 1 & \frac{1}{4} & 0 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & 0 & \frac{1}{4} & 1 & \frac{1}{4} & 0 \\ 0 & \ddots & \ddots & 0 & \frac{1}{4} & 1 & \frac{1}{2\sqrt{2}} \\ 0 & \cdots & \ddots & 0 & 0 & \frac{1}{2\sqrt{2}} & 1 \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

This tridiagonal matrix is diagonally dominant. The upper and lower bounds $1 \pm \frac{1}{4}(1 + \sqrt{2})$ for the eigenvalues of D_n can be determined by using Gershgorin disks; see, e.g. [27]. These bounds are independent of the dimension n. It follows that we may choose $\sigma_{\min} = \frac{1}{2}(3 - \sqrt{2})^{1/2}$ and $\sigma_{\max} = \frac{1}{2}(5 + \sqrt{2})^{1/2}$ independently of n. Hence, (2.4) also holds in the present situation. The bounds (2.4) will be explicitly used in section 4.

The solution $x_n \in \mathcal{X}_n$ of (2.1) might not be a useful approximation of the desired solution $\widehat{x}$ of (1.1) due to a large propagated error stemming from the error in the available data y_n^δ. We therefore would like to determine a bound for $\|\widehat{x} - x_n\|_{\mathcal{X}}$. This is generally not possible without some additional assumptions on the solution $\widehat{x}$ of (1.1); in particular, it is not sufficient that A and A_n be close.

Let $\Omega \subseteq \mathbb{R}^N$, $\mathcal{X} = L_2(\Omega)$, and define the Sobolev spaces $\mathcal{H}^l = \mathcal{H}^l(\Omega)$ for $l \in \mathbb{R}$. Assume that

$$\|Ax\|_{\mathcal{Y}} \sim \|x\|_{\mathcal{H}^{-l}} \tag{2.5}$$

holds for all $x \in \mathcal{H}^{-l}$ and some $0 < l < \infty$, i.e. the operator $A : \mathcal{H}^{-l} \to \mathcal{Y}$ is continuously invertible. The theory developed by Natterer [18] requires that (2.5) holds for a finite value of l.

Example 2.1. Let $\Omega \subset \mathbb{R}^2$, $Z = \{(\omega, t) \in \mathbb{R}^3 : \omega \in \mathbb{R}^2,\ \|\omega\| = 1,\ t \in \mathbb{R}\}$. Let $\omega^\perp$ be a unit vector perpendicular to ω, and define the Radon transform

$$A : L_2(\Omega) \to L_2(Z),$$
$$(Ax)(\omega, s) := \int_{\mathbb{R}} x(s\omega + t\omega^\perp)\, \mathrm{d}t.$$

Then (2.5) holds with $l = 1/2$; see [19]. □

Example 2.2. Let

$$A : L_2(\mathbb{R}^d) \to L_2(\mathbb{R}^d),$$
$$(Ax)(\omega, s) := (k * x)(s) = \int_{\mathbb{R}^d} k(s-t)x(t)\,\mathrm{d}t,\ s \in \mathbb{R}^d,$$

for some kernel function $k \in L_2(\mathbb{R}^d)$. If the Fourier transform $\hat{k}$ of k satisfies

$$|\hat{k}(\xi)| \sim (1 + |\xi|^2)^{-\beta/2},$$

then (2.5) holds with $l = \beta$, see, e.g. [9]. □

Assume that the minimal norm solution $\widehat{x}$ of (1.1) lives in $\mathcal{H}^k$. Natterer [18] shows that if the operator A is injective and the subspaces $\mathcal{X}_n$, $n = 1, 2, \ldots$, are chosen so that an inverse estimate is fulfilled (see [18, equation (4.1)–(4.5)] for details on the latter), then one obtains the bound

$$\|\widehat{x} - x_n\|_{\mathcal{X}} \leqslant C\left(h(n)^k \|\widehat{x}\|_{\mathcal{H}^k} + h(n)^{-l}\delta\right) \tag{2.6}$$

for some constant C that can be chosen independently of $h(n)$, $\widehat{x}$, and δ. Here, $h = h(n) > 0$ is a discretization parameter that depends on the approximation property of the subspaces $\mathcal{X}_n$, $n = 1, 2, \ldots$, i.e. on how well $\widehat{x}$ can be approximated by an element in $\mathcal{X}_n$; in particular, $h \searrow 0$ as $n \to \infty$. The parameter $\delta > 0$ in (2.6) is the bound (1.2); see [18]. An optimal dimension of the discretized problem is given by

$$n \sim h^{-1}\left(\left(\frac{\delta}{\|\widehat{x}\|_{\mathcal{H}^k}}\right)^{1/(k+l)}\right) \tag{2.7}$$

and yields the bound

$$\|\widehat{x} - x_n\|_{\mathcal{X}} \leqslant C' \|\widehat{x}\|_{\mathcal{H}^k}^{l/(k+l)} \delta^{k/(k+l)} \tag{2.8}$$

for some constant $C' > 0$; see Natterer [18] for details. For instance, spline and finite element approximation spaces $\mathcal{X}_n$ allow for bounds of the type (2.6) and (2.8). Natterer [18] proposes that the dimension n of the solution subspace of the discretized problem (1.4) be chosen according to (2.7). This choice provides regularization of the operator equation (1.3) and no further regularization is necessary.

We note that the use of wavelet-based projection methods also has been investigated for the solution of ill-posed problems. Regularization properties of wavelet methods have been shown by Dicken and Maaß [5].

Convergence rates analogous to (2.8), when h is chosen according to (2.7), also can be established in a different setting; see Mathé and Pereverzev [17]. They assume that the operator A is continuously invertible in Hilbert scales (which resembles the condition (2.5)), and show convergence rates in a stochastic noise setting with respect to norms of the relevant Hilbert scales; see [17, theorem 6.3].

We conclude this section with a comment on condition (1.2). Let $y_n = Q_n y$ and $y_n^\delta = Q_n y^\delta$. We will assume that $\|y - y^\delta\|_{\mathcal{Y}} \approx \|y_n - y_n^\delta\|_{\mathcal{Y}}$. Then (1.2) translates to

$$\|y_n - y_n^\delta\|_{\mathcal{Y}} \lessapprox \delta. \tag{2.9}$$

It is convenient to replace the norm in (2.9) by the Euclidean norm. This can be achieved analogously as in the beginning of this section: let $\{f_j\}_{j=1}^n$ form a convenient basis for $\mathcal{Y}_n$, such as $f_j = Ae_j$, where $\{e_j\}_{j=1}^n$ is a basis for $\mathcal{X}_n$. Represent the element $y_n \in \mathcal{Y}_n$ as

$$y_n = \sum_{j=1}^{n} y_j^{(n)} f_j,$$

and define the vector $\vec{y}_n = (y_1^{(n)}, y_2^{(n)}, \ldots, y_n^{(n)})^T \in \mathbb{R}^n$. We would like to bound $\|y_n\|_{\mathcal{Y}}$ in terms of $\|\vec{y}_n\|_2$. Introduce an orthonormal basis $\{\widehat{f}_j\}_{j=1}^n$ for $\mathcal{Y}_n$. There is a nonsingular matrix $N_n \in \mathbb{R}^{n\times n}$ such that

$$[f_1, f_2, \ldots, f_n] = [\widehat{f}_1, \widehat{f}_2, \ldots, \widehat{f}_n] N_n.$$

It follows similarly as (2.3) that

$$\|y_n\|_{\mathcal{Y}} \leqslant \sigma_{\max}(N_n)\|\vec{y}_n\|_2,$$

where $\sigma_{\max}(N_n)$ denotes the largest singular value of N_n. We will assume that there is an upper bound $d_{\max}$, independent of n, such that

$$\sigma_{\max}(N_n) \leqslant d_{\max} < \infty.$$

In computations, we will apply the discrepancy principle based on the inequality

$$\|y_n - y_n^\delta\|_2 \leqslant \delta, \tag{2.10}$$

which implies that

$$\|y_n - y_n^\delta\|_{\mathcal{Y}} \lessapprox d_{\max}\delta.$$

3. Arnoldi decomposition of a matrix

Let A_n and y_n^δ be as in (1.4), and assume that n is large. The Arnoldi process is a popular approach to reduce a large matrix to a small one by evaluating matrix-vector products with the large matrix and applying Gram–Schmidt orthogonalization. The small matrix, denoted by $H_{\ell+1,\ell}$ below, is an orthogonal projection of A_n. Application of $1 \leqslant \ell \ll n$ steps of the Arnoldi process to the matrix A_n with initial vector y_n^δ gives the decomposition

$$A_n V_{n,\ell} = V_{n,\ell+1} H_{\ell+1,\ell}, \tag{3.1}$$

where the columns of the matrix $V_{n,\ell+1} \in \mathbb{R}^{n,\ell+1}$ form an orthonormal basis for the Krylov subspace

$$\mathcal{K}_{\ell+1}(A_n, y_n^\delta) := \operatorname{span}\{y_n^\delta, A_n y_n^\delta, \ldots, A_n^\ell y_n^\delta\}$$

with respect to the inner product

$$\langle u, w\rangle := \frac{1}{n}\sum_{j=1}^{n} u_j w_j, \quad u = (u_1, \ldots, u_n)^T,\ w = (w_1, \ldots, w_n)^T \in \mathbb{R}^n \tag{3.2}$$

and associated norm

$$\|u\|_2 := \sqrt{\langle u, u\rangle};$$

see, e.g. [26]. We also will denote the spectral norm of a matrix by $\|\cdot\|_2$. The matrix $V_{n,\ell}$ in (3.1) is made up of the first ℓ columns of $V_{n,\ell+1}$, and $H_{\ell+1,\ell} \in \mathbb{R}^{\ell+1,\ell}$ is an upper Hessenberg matrix, i.e. all entries below the subdiagonal vanish. We assume the generic situation that the subspace $\mathcal{K}_{\ell+1}(A_n, y_n)$ is of dimension $\ell + 1$ for all $\ell \geqslant 0$, otherwise the computations simplify; see below.

Algorithm 1. The Arnoldi process.

1: **Input:** $A_n \in \mathbb{R}^{n,n}$, $y_n^\delta \in \mathbb{R}^n \backslash \{0\}$, number of steps ℓ.
2: $v_1 := y_n^\delta / \|y_n^\delta\|_2$
3: **for:** $j = 1$ **to** ℓ
4: $\quad w := A_n v_j$
5: $\quad$ **for** $k = 1$ **to** j
6: $\quad\quad h_{k,j} := \langle v_j, w \rangle$
7: $\quad\quad w := w - v_j h_{k,j}$
8: $\quad$ **end for**
9: $\quad h_{j+1,j} := \|w\|_2$; $v_{j+1} := w / h_{j+1,j}$
10: **end for**
11: **Output:** Upper Hessenberg matrix $H_{\ell+1,\ell} = [h_{k,j}] \in \mathbb{R}^{\ell+1,\ell}$, matrix
12: $\quad\quad V_{n,\ell+1} = [v_1, v_2, \ldots, v_{\ell+1}] \in \mathbb{R}^{n,\ell+1}$ with orthonormal columns

Algorithm 1 describes the Arnoldi process for computing the decomposition (3.1). The algorithm is said to break down in iteration j if $h_{k+1,k} > 0$ for $1 \leqslant k < j$, and $h_{j+1,j} = 0$ in line 9. Then the decomposition (3.1) simplifies to

$$A_n V_{n,j} = V_{n,j} H_{j,j}$$

and the solution of (1.4) lives in the Krylov subspace $\mathcal{K}_j(A_n, y_n^\delta)$ if the matrix $H_{j,j}$ is nonsingular. This is secured, e.g. if the matrix A_n is nonsingular. A discussion on how to continue the Arnoldi process in case of breakdown when $H_{j,j}$ is singular is provided in [25].

We remark that the Arnoldi process simplifies to the Lanczos process when the matrix A_n is symmetric; see [26, chapter 6].

4. The Arnoldi–Tikhonov method

The results of section 2 suggest that the discretized system can be solved without further regularization if the discretization is carried out on a suitably (but not too) fine grid. However, numerical realization of regularization by discretization only often leads to difficulties, because an appropriate value of the dimension n of the solution subspace generally is not known before the computations are begun. For instance, when $\mathcal{X}_n$ is a finite element space, it may be necessary to determine several discretizations and associated solutions (for different values of n) to find a suitable n-value. We therefore prefer to first discretize the spaces $\mathcal{X}$ and $\mathcal{Y}$ to obtain n-dimensional subspaces $\mathcal{X}_n$ and $\mathcal{Y}_n$, respectively, that allow approximation of elements of $\mathcal{X}$ and $\mathcal{Y}$ with sufficient accuracy, and then regularize (1.4) by Tikhonov's method. In the remainder of this section, we identify the spaces $\mathcal{X}_n$ and $\mathcal{Y}_n$ with $\mathbb{R}^n$ and the finite-dimensional operator $Q_n A P_n$ in (2.1) with the matrix $A_n \in \mathbb{R}^{n,n}$ in (1.4).

The solution method considered consists of three steps:

1. **Discretization of the (infinite-dimensional) operator equation.** This requires an estimate of the distance between the solution of the infinite-dimensional system and the solution of its finite-dimensional approximation.

Table 1. Example 5.1: the Phillips test problem. The noise level (5.3) is 1%.

n	ℓ	h_ℓ	α	$\|x^\delta_{\alpha,n,\ell} - x_n\|_2/\|x_n\|_2$	$\|x^\delta_{\alpha,n,\ell} - x^\delta_{\alpha,n}\|_2/\|x_n\|_2$
1000	20	$1.14 \cdot 10^{-1}$	4.90	$2.28 \cdot 10^{-1}$	$3.64 \cdot 10^{-4}$
1000	30	$1.13 \cdot 10^{-1}$	4.96	$2.28 \cdot 10^{-1}$	$3.60 \cdot 10^{-4}$
1000	40	$1.12 \cdot 10^{-1}$	4.90	$2.26 \cdot 10^{-1}$	$3.60 \cdot 10^{-4}$
2000	20	$8.15 \cdot 10^{-2}$	3.82	$1.95 \cdot 10^{-1}$	$3.73 \cdot 10^{-4}$
2000	30	$8.13 \cdot 10^{-2}$	3.81	$1.94 \cdot 10^{-1}$	$3.69 \cdot 10^{-4}$
2000	40	$8.06 \cdot 10^{-2}$	3.79	$1.94 \cdot 10^{-1}$	$3.67 \cdot 10^{-4}$
4000	20	$5.78 \cdot 10^{-2}$	2.97	$1.68 \cdot 10^{-1}$	$3.25 \cdot 10^{-4}$
4000	30	$5.77 \cdot 10^{-2}$	2.97	$1.67 \cdot 10^{-1}$	$3.24 \cdot 10^{-4}$
4000	40	$5.75 \cdot 10^{-2}$	2.96	$1.67 \cdot 10^{-1}$	$3.23 \cdot 10^{-4}$

2. **Definition of a regularized finite-dimensional system.** Estimate the distance between the solution of the finite-dimensional system and its regularized version.
3. **Compute an approximate solution of the regularized solution.** Estimate the distance between the solution of the regularized finite-dimensional system and its computed approximation.

The error of the computed solution is bounded by the sum of the norms of these three errors. We will discuss each one of these errors separately.

Let the Arnoldi decomposition (3.1) be available, and introduce the approximation

$$A_n^{(\ell)} := V_{n,\ell+1} H_{\ell+1,\ell} V_{n,\ell}^* \tag{4.1}$$

of the matrix A_n. In what follows, we need to compute an estimate for the distance between A_n and $A_n^{(\ell)}$. To this end we may compute the operator norm $\|A_n - A_n^{(\ell)}\|_2$, which can be evaluated as the largest singular value of the matrix $A_n - A_n^{(\ell)}$. It has recently been shown that a few of the largest singular values of a large matrix that stems from the discretization of a linear ill-posed problem can be computed quite inexpensively; see [22] for discussions and illustrations. Alternatively, we may use the easily computable Frobenius norm,

$$\|A_n\|_F := \sqrt{\sum_{i,j=1}^{n} |a_{ij}|^2},$$

where $A_n = [a_{ij}]_{i,j=1}^n$, and apply the bound

$$\|A_n - A_n^{(\ell)}\|_2 \leqslant \|A_n - A_n^{(\ell)}\|_F.$$

Assume that

$$\|A_n - A_n^{(\ell)}\|_2 \leqslant h_\ell \tag{4.2}$$

for some scalar $h_\ell > 0$ and define the Tikhonov functional

$$J_{\alpha,n,\ell}(x_n) := \|A_n^{(\ell)} x_n - y_n^\delta\|_2^2 + \alpha \|x_n\|_2^2, \tag{4.3}$$

where $\alpha > 0$ is a regularization parameter. We will solve the minimization problem

$$x^\delta_{\alpha,n,\ell} := \arg\min_{x_n \in \mathbb{R}^n} \{J_{\alpha,n,\ell}(x_n)\}. \tag{4.4}$$

For comparison, we also define the Tikhonov functional $J_{\alpha,n}$ obtained by replacing $A_n^{(\ell)}$ in (4.3) by A_n, i.e.

$$J_{\alpha,n}(x_n) := \|A_n x_n - y_n^\delta\|_2^2 + \alpha\|x_n\|_2^2$$

and solve the minimization problem

$$x_{\alpha,n}^\delta := \arg\min_{x_n\in\mathbb{R}^n} \{J_{\alpha,n}(x_n)\}. \tag{4.5}$$

Let us fix n. We would like to choose the parameter pair $\{\ell,\alpha\}$ so that $x_{\alpha,n,\ell}^\delta$ is an accurate approximation of the solution $\widehat{x}$ of minimal norm of the operator equation (1.1).

The proper choice of the parameter pair $\{\ell,\alpha\}$ has been studied by Neubauer [20], who considers the computation of an approximate solution of an operator equation

$$Tx = y^\delta, \qquad T : \widetilde{\mathcal{X}} \to \widetilde{\mathcal{Y}},$$

where $\widetilde{\mathcal{X}}$ and $\widetilde{\mathcal{Y}}$ are Hilbert spaces, by first discretizing and then solving the discretized equation using Tikhonov regularization,

$$x_{\alpha,\ell}^{h,\delta} := \left(T_{h,\ell}^* T_{h,\ell} + \alpha I\right)^{-1} T_{h,\ell}^* y_n^\delta.$$

Here $T_{h,\ell}$ denotes a discretization and modification of T (see below), and $T_{h,\ell}^*$ is the adjoint of $T_{h,\ell}$. Neubauer [20] requires the operator $T_{h,\ell}$ to satisfy

$$\begin{aligned} \|T - T_{h,\ell}\|_2 &\leqslant h_\ell, \\ T_{h,\ell} &:= R_\ell T_h, \\ R_\ell &\to I \text{point-wise as } \ell \text{ increases,} \end{aligned}$$

where R_ℓ is an orthogonal projector onto an ℓ-dimensional subspace $\mathcal{W}_\ell \subset \widetilde{\mathcal{Y}}$ to be specified below. The dimension ℓ is finite and typically quite small. Moreover, T_h is a discretization of T and $T_{h,\ell}$ is a modification of T_h determined by R_ℓ.

In our application of the results of Neubauer [20], we let $T := A_n$ and $\widetilde{\mathcal{X}} := \widetilde{\mathcal{Y}} := \mathbb{R}^n$. Thus, we set

$$\begin{aligned} T &:= A_n, \\ T_{h,\ell} &:= A_n^{(\ell)}, \qquad \|A_n - A_n^{(\ell)}\|_2 \leqslant h_\ell, \\ \mathcal{W}_\ell &:= \overline{\mathcal{R}(A_n^{(\ell)})}, \\ R_\ell &:= P_{\overline{\mathcal{R}(A_n^{(\ell)})}}, \end{aligned} \tag{4.6}$$

where $P_{\overline{\mathcal{R}(A_n^{(\ell)})}}$ denotes the orthogonal projector onto the (closure of the) range of $A_n^{(\ell)}$. The operator T_h is not important to us; we only use $T_{h,\ell}$. We are in a position to show the following results.

Proposition 4.1. *Assume that the Arnoldi process does not break down. With the operators defined as above, we have*

$$\mathcal{W}_\ell \subset \overline{\mathcal{R}(A_n)}, \tag{4.7}$$

$$\mathcal{R}(R_\ell A_n^{(\ell)}) = \mathcal{W}_\ell, \tag{4.8}$$

$$\|R_\ell(A_n - A_n^{(\ell)})\|_2 \leqslant h_\ell,$$

$$\|R_\ell(y - y_n^\delta)\|_2 \leqslant \delta, \tag{4.9}$$

$$R_\ell \to I \text{ point-wise onto } \mathcal{R}(A_n), \tag{4.10}$$

where the bound (4.9) is inspired by (2.10).

Proof. First note that the ranges of the operators (matrices) A_n and $A_n^{(\ell)}$ are closed as they are maps between finite-dimensional spaces. It follows from (3.1) and (4.1) that

$$A_n^{(\ell)} = A_n V_{n,\ell} V_{n,\ell}^* \tag{4.11}$$

and, therefore,

$$\mathcal{W}_\ell = \mathcal{R}(A_n^{(\ell)}) \subset \mathcal{R}(A_n),$$

i.e. property (4.7) holds. Furthermore,

$$\mathcal{R}(R_\ell A_n^{(\ell)}) = \mathcal{R}(P_{\mathcal{R}(A_n^{(\ell)})} A_n^{(\ell)}) = \mathcal{R}(A_n^{(\ell)}) = \mathcal{W}_\ell.$$

This establishes (4.8). Finally, we have

$$\begin{aligned} \|R_\ell(A_n - A_n^{(\ell)})\|_2 &\leqslant \|R_\ell\|_2 \|A_n - A_n^{(\ell)}\|_2 \overset{(4.6)}{\leqslant} h_\ell, \\ \|R_\ell(y - y_n^\delta)\|_2 &\leqslant \|R_\ell\|_2 \|y - y_n^\delta\|_2 \leqslant \delta. \end{aligned}$$

It remains to show (4.10). According to (4.7), we have $\mathcal{R}(A_n^{(\ell)}) \subset \mathcal{R}(A_n)$. We will show that for every $y_n \in \mathcal{R}(A_n)$, there exists an $\ell \geqslant 1$ such that $y_n \in \mathcal{R}(A_n^{(\ell)})$. Let $x_n \in \mathbb{R}^n$ and define $y_n = A_n x_n$. Note that $V_{n,\ell} V_{n,\ell}^*$ is an orthogonal projector onto the space $\mathcal{R}(V_{n,\ell})$. Assuming that the Arnoldi process does not break down, there is an $\ell \geqslant 1$ (in the worst case, $\ell = n$) such that $x_n \in \mathcal{R}(V_{n,\ell})$ and, therefore, $V_{n,\ell} V_{n,\ell}^* x_n = x_n$. It follows from (4.11) that

$$y_n = A_n x_n = A_n V_{n,\ell} V_{n,\ell}^* x_n = A_n^{(\ell)} x_n,$$

i.e. $y_n \in \mathcal{R}(A_n^{(\ell)})$ and, consequently, $R_\ell y_n = y_n$. This shows the point-wise convergence of the projector R_ℓ to I as ℓ increases. □

Thus, the requirements of Neubauer [20, assumption 2.3] are fulfilled, and we get the following result from [20, proposition 2.6 and theorem 3.1]:

Proposition 4.2. *Let x_n be an approximate solution of (2.1) such that*

$$x_n = (A_n^* A_n)^\nu v_n, \quad v_n \in \mathcal{N}(A_n)^\perp, \ \nu \in [0,1], \tag{4.12}$$

$$\|v_n\| \leqslant \rho \qquad \forall n \in \mathbb{N}, \tag{4.13}$$

for some constant $\rho \geqslant 0$ independent of n, and assume that $\|y_n - Q_n y^\delta\|_2 \leqslant \delta$. Let the regularization parameter $\alpha > 0$ satisfy

$$\alpha^3 \left\langle \left(A_n^{(\ell)} \left(A_n^{(\ell)} \right)^* + \alpha I \right)^{-3} R_\ell y_n^\delta, R_\ell y_n^\delta \right\rangle = (E h_\ell + C\delta)^2, \tag{4.14}$$

where the inner product $\langle \cdot, \cdot \rangle$ is defined by (3.2) and the constants $C > 1$ and $E > 3\|x_n\|_2$ are chosen such that

$$0 \leqslant E h_\ell + C\delta \leqslant \|R_\ell y_n^\delta\|_2. \tag{4.15}$$

Then the associated solution of (4.4) satisfies

$$\|x^{\delta}_{\alpha,n,\ell} - x_n\|_2 = O\left((\delta + h_\ell)^{2\nu/(2\nu+1)}\right) + p(l,\nu) \tag{4.16}$$

with

$$p(l,\nu) = \begin{cases} 0 & \text{if } \nu = 0, \\ \gamma_l \|(I - R_\ell)z\| & \text{if } \nu = \frac{1}{2},\ A_n^* z_n = (A_n^* A_n)^{1/2} v_n, \\ \gamma_l^2 \|v_n\|_2 & \text{if } \nu = 1, \\ (4/\pi)\gamma_l^{2\nu}\|v_n\| & \text{otherwise,} \end{cases}$$

$$\gamma_l = \|(I - R_\ell)A_n\|_2^2 \, \|v_n\|_2.$$

Additionally, o has to be replaced by $\mathcal{O}$ for $\nu = 1$.

Remark 4.3. The smoothness condition (4.12) is for infinite-dimensional problems a fairly strong restriction. In finite dimension, we observe that (4.12) implies that $x_n \in \mathcal{N}(A_n)^{\perp}$. Therefore, there is a unique $v_n \in \mathcal{N}(A_n)^{\perp}$ such that $x_n = (A_n^* A_n)^{\nu} v_n$. However, the uniform boundedness of $\|v_n\|$, see inequality (4.13), generally remains an open problem; see proposition 4.5 below.

Remark 4.4. The quantities in (4.16) may depend on n. Generally, h_ℓ does not vary much as ℓ is kept fixed and n is increased; see section 5 for illustrations. When n is fixed and ℓ increases, h_ℓ decreases. We are interested in choosing ℓ large enough so that both terms in the right-hand side of (4.16) are sufficiently small; see corollary 4.6 below. Moreover, condition (4.15) requires ℓ to be large enough.

Let us now give an example where the uniform boundedness of the source elements v_n, required in proposition 4.2, can be guaranteed:

Proposition 4.5. *Let the conditions of proposition 4.2 except for condition (4.13) hold. Assume that A is self-adjoint, fulfilling (2.5), $A_n = P_n A P_n$, and the solution $x \in \mathcal{H}^k$ of the equation $Ax = y$ fulfills a source condition with $\nu = 1/2$ and source element $v \in \mathcal{H}^{\tilde{k}}$. If A_n is injective, then also the solutions of the equations $A_n x_n = y_n$, $n = 1, 2, \ldots$, fulfill a source condition with $\nu = 1/2$, and the associated source elements v_n are uniformly bounded.*

Proof. For $\nu = 1/2$ and a self-adjoint operator A, the source condition transfers to

$$x = (A^* A)^{1/2} v = Av. \tag{4.17}$$

As A_n is also self-adjoint, finite-dimensional, and injective, x_n also fulfills a source condition; see remark 4.3,

$$x_n = (A_n^* A_n)^{1/2} v_n = A_n v_n$$

with a unique v_n. As A fulfills (2.5), the distance between x and x_n can be bounded by

$$\|x - x_n\|_{\mathcal{X}} \leqslant C' \|x\|_{\mathcal{H}^k}^{l/(k+l)} \delta_n^{k/(k+l)},$$

see (2.8), and $\delta_n = \|y - y_n\| \searrow 0 \text{as} n \to \infty$. Using again (2.8) for solving (4.17) with $\tilde{\delta}_n = \|x - x_n\|$, we obtain with $v \in \mathcal{H}^{\tilde{k}}$,

$$\|v - v_n\|_{\mathcal{X}} \leqslant C' \|v\|_{\mathcal{H}^{\tilde{k}}}^{l/(\tilde{k}+l)} \delta_n^{\tilde{k}/(\tilde{k}+l)},$$

i.e. $v_n \to v$ and consequently $\|v_n\|$ is uniformly bounded as $n \to \infty$. □

The best convergence rates can be achieved for $\nu = 1$:

Corollary 4.6. *Assume that the conditions of proposition 4.2 hold, let $\nu = 1$, and let $\hat{\alpha}$ solve (4.14). Then for ℓ such that*

$$\max\{h_\ell, \|(I - R_\ell)A_n^{(\ell)}\|_2\} \sim \delta,$$

we have

$$\|x_{\hat{\alpha},n,\ell}^{\delta} - x_n\|_2 = \mathcal{O}\left(\delta^{2/3}\right) \text{ as } \delta \searrow 0.$$

Proof. The first term on the right-hand side of (4.16) behaves like $\mathcal{O}(\delta^{2/3})$ if $h_\ell \sim \delta$. For the second term, we have

$$\begin{aligned}\|(I - R_\ell)A_n\|_2 &\leqslant \|(I - R_\ell)A_n^{(\ell)}\|_2 + \|(I - R_\ell)(A_n - A_n^{(\ell)})\|_2 \\ &\leqslant \|(I - R_\ell)A_n^{(\ell)}\|_2 + h_\ell.\end{aligned}$$

Since $R_\ell \to I$ as $\ell \to n$, we can choose ℓ large enough such that $\|(I - R_\ell)A_n^{(\ell)}\|_2 \leqslant \delta$ and obtain

$$\|x_{\hat{\alpha},n,\ell}^{\delta} - x_n\|_2 = \mathcal{O}\left(\delta^{2/3}\right) + 2\delta^2\|v\|_2 = \mathcal{O}\left(\delta^{2/3}\right)$$

as $\delta \searrow 0$. □

With the same argument we achieve optimal convergence rates for each $\nu \in (0, 1)$ if $p(l, \nu) = o(\delta^{2\nu/(2\nu+1)})$, which holds for l small enough.

Now let us further specify the orthogonal projector R_ℓ.

Proposition 4.7. *Let $A_n^{(\ell)} = V_{n,\ell+1}H_{\ell+1,\ell}V_{n,\ell}^*$ be defined by (4.1) and let $H_{\ell+1,\ell} = U_{\ell+1}\Sigma_{\ell+1,\ell}W_\ell^*$ denote a singular value decomposition, i.e. $U_{\ell+1} \in \mathbb{R}^{\ell+1,\ell+1}$ and $W_\ell^* \in \mathbb{R}^{\ell,\ell}$ are orthogonal matrices, whereas $\Sigma_{\ell+1,\ell} \in \mathbb{R}^{\ell+1,\ell}$ is a diagonal matrix with non-negative diagonal entries arranged in nonincreasing order. In particular, all entries of the last row of $\Sigma_{\ell+1,\ell}$ vanish. Then the projector $R_\ell : \mathbb{R}^n \to P_{\overline{\mathcal{R}(A_n^{(\ell)})}}$ is given by*

$$R_\ell = V_{n,\ell+1}U_{\ell+1}I_{q,\ell+1}U_{\ell+1}^*V_{n,\ell+1}^*, \tag{4.18}$$

where $I_{q,\ell+1} \in \mathbb{R}^{\ell+1,\ell+1}$ is defined in (4.21) below and $q \geqslant 0$ denotes the rank of the matrix $H_{\ell+1,\ell}$.

Proof. It is well known that

$$P_{\overline{\mathcal{R}(A_n^{(\ell)})}} = A_n^{(\ell)}\left(A_n^{(\ell)}\right)^{\dagger}.$$

Moreover,

$$\left(A_n^{(\ell)}\right)^\dagger = \left(V_{n,\ell+1} H_{\ell+1,\ell} V_{n,\ell}^*\right)^\dagger = V_{n,\ell} H_{\ell+1,\ell}^\dagger V_{n,\ell+1}^*. \tag{4.19}$$

The singular value decomposition of $H_{\ell+1,\ell}$ yields

$$H_{\ell+1,\ell}^\dagger = W_\ell \Sigma_{\ell+1,\ell}^\dagger U_{\ell+1}^*. \tag{4.20}$$

Now using (4.19) and (4.20), we obtain

$$A_n^{(\ell)} \left(A_n^{(\ell)}\right)^\dagger = V_{n,\ell+1} U_{\ell+1} \Sigma_{\ell+1,\ell} \Sigma_{\ell+1,\ell}^\dagger U_\ell^* V_{n,\ell+1}^*.$$

Finally, when $H_{\ell+1,\ell}$ is of rank $q \leqslant \ell$, we have

$$I_{q,\ell+1} := \Sigma_{\ell+1,\ell} \Sigma_{\ell+1,\ell}^\dagger = \begin{pmatrix} I_q & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{R}^{\ell+1,\ell+1} \tag{4.21}$$

with I_q being the $q \times q$ identity matrix. □

The use of the discrepancy principle requires the solution of equation (4.14). The following result is concerned with the evaluation of the left-hand side of this equation.

Proposition 4.8. *Under the assumptions of proposition 4.7, and with the same notation, it holds*

$$\left\langle \left(A_n^{(\ell)} \left(A_n^{(\ell)}\right)^* + \alpha I\right)^{-3} R_\ell y_n^\delta,\ R_\ell y_n^\delta \right\rangle$$

$$= \left(R_\ell y_n^\delta\right)^* V_{n,\ell+1} U_{\ell+1} \left(\Lambda_{\ell+1} + \alpha I_{\ell+1}\right)^{-3} U_{\ell+1}^* V_{n,\ell+1}^* R_\ell y_n^\delta \tag{4.22}$$

$$= \left(y_n^\delta\right)^* V_{n,\ell+1} U_{\ell+1} I_{q,\ell+1} \left(\Lambda_{\ell+1} + \alpha I_{\ell+1}\right)^{-3} I_{q,\ell+1} U_{\ell+1}^* V_{n,\ell+1}^* y_n^\delta, \tag{4.23}$$

where $\Lambda_{\ell+1} \in \mathbb{R}^{\ell+1,\ell+1}$ is a diagonal matrix made up by the squares of the singular values of the Hessenberg matrix $H_{\ell+1,\ell} \in \mathbb{R}^{\ell+1,\ell}$ and with the last diagonal entry zero.

Proof. We first show (4.22). Using the notation of proposition 4.7, we obtain

$$\left(A_n^{(\ell)}\right)^* = V_{n,\ell} H_{\ell+1,\ell}^* V_{n,\ell+1}^* = V_{n,\ell} W_\ell \Sigma_{\ell+1,\ell}^* U_{\ell+1}^* V_{n,\ell+1}^*,$$

and taking into account that the matrices U_ℓ and W_ℓ are orthogonal, and that the matrices $V_{n,\ell}$ and $V_{n,\ell+1}$ have orthonormal columns, yields

$$\begin{aligned} A_n^{(\ell)} \left(A_n^{(\ell)}\right)^* &= (V_{n,\ell+1} U_{\ell+1} \Sigma_{\ell+1,\ell} W_\ell^* V_{n,\ell}^*)(V_{n,\ell} W_\ell \Sigma_{\ell+1,\ell}^* U_{\ell+1}^* V_{n,\ell+1}^*) \\ &= V_{n,\ell+1} U_{\ell+1} \Sigma_{\ell+1,\ell} \Sigma_{\ell+1,\ell}^* U_{\ell+1}^* V_{n,\ell+1}^* \\ &= V_{n,\ell+1} U_{\ell+1} \Lambda_{\ell+1} U_{\ell+1}^* V_{n,\ell+1}^*, \end{aligned}$$

where

$$\Lambda_{\ell+1} := \operatorname{diag}\left(\sigma_1^2, \sigma_2^2, \ldots, \sigma_\ell^2, 0\right) \in \mathbb{R}^{\ell+1,\ell+1}$$

and $\sigma_1 \geqslant \sigma_2 \geqslant \ldots \geqslant \sigma_\ell \geqslant 0$ are the singular values of the matrix $H_{\ell+1,\ell}$. We obtain

$$A_n^{(\ell)}\left(A_n^{(\ell)}\right)^* + \alpha I = V_{n,\ell+1}U_{\ell+1}\left(\Lambda_{\ell+1} + \alpha I_{\ell+1}\right)U_{\ell+1}^* V_{n,\ell+1}^* + \alpha(I - V_{n,\ell+1}V_{n,\ell+1}^*).$$

Since $V_{n,\ell+1}V_{n,\ell+1}^*$ and $I - V_{n,\ell+1}V_{n,\ell+1}^*$ are complementary orthogonal projectors, it follows that

$$\left(A_n^{(\ell)}\left(A_n^{(\ell)}\right)^* + \alpha I\right)^3 = V_{n,\ell+1}U_{\ell+1}\left(\Lambda_{\ell+1} + \alpha I_{\ell+1}\right)^3 U_{\ell+1}^* V_{n,\ell+1}^* + \alpha^3(I - V_{n,\ell+1}V_{n,\ell+1}^*).$$

Introduce the vector

$$z_n^\delta := V_{n,\ell+1}U_{\ell+1}\left(\Lambda_{\ell+1} + \alpha I_{\ell+1}\right)^{-3} U_{\ell+1}^* V_{n,\ell+1}^* R_\ell y_n^\delta.$$

Then

$$\left(A_n^{(\ell)}\left(A_n^{(\ell)}\right)^* + \alpha I\right)^3 z_n^\delta = R_\ell y_n^\delta$$

and, therefore,

$$\left(A_n^{(\ell)}\left(A_n^{(\ell)}\right)^* + \alpha I\right)^{-3} R_\ell y_n^\delta = z_n^\delta.$$

This shows (4.22). Equation (4.23) now follows by substituting (4.18) into (4.22). □

In actual computations, the matrix $H_{\ell+1,\ell}$ typically is small; see section 4 for illustrations. The singular value decomposition of $H_{\ell+1,\ell}$ therefore is quite inexpensive to compute and the left-hand side of (4.22) easily can be evaluated.

Corollary 4.9. *Let the conditions in section 2 hold and choose n according to (2.7). Assume that $1 \leqslant \ell \leqslant n$ is large enough so that (4.14) has a solution, which we denote by $\hat{\alpha}$. Consider the regularized solution $x_{\hat{\alpha},n,\ell}^\delta$, defined by (4.4) with $\alpha = \hat{\alpha}$, an element in $\mathcal{X}_n$. Assume that the conditions of corollary 4.6 hold. Then*

$$\|\widehat{x} - x_{\hat{\alpha},n,\ell}^\delta\|_{\mathcal{X}} \leqslant C'\|\widehat{x}\|_{\mathcal{H}^k}^{l/(k+l)}\delta^{k/(k+l)} + \mathcal{O}(\delta^{2/3}) \text{ as } \delta \searrow 0 \tag{4.24}$$

for a suitable constant $C' > 0$ with the parameter l the same as in (2.5).

Proof. Let $x_n \in \mathcal{X}_n$ be the minimal-norm solution (2.2) of (2.1) with n chosen according to (2.7). Then we obtain by the triangle inequality and (2.8) that

$$\begin{aligned}\|\widehat{x} - x_{\hat{\alpha},n,\ell}^\delta\|_{\mathcal{X}} &\leqslant \|\widehat{x} - x_n\|_{\mathcal{X}} + \|x_n - x_{\hat{\alpha},n,\ell}^\delta\|_{\mathcal{X}} \\ &\leqslant C'\|\widehat{x}\|_{\mathcal{H}^k}^{l/(k+l)}\delta^{k/(k+l)} + \|x_n - x_{\hat{\alpha},n,\ell}^\delta\|_{\mathcal{X}}.\end{aligned}$$

Now considering x_n and $x_{\hat{\alpha},n,\ell}^\delta$ elements in $\mathbb{R}^n$, we obtain from (2.4) that

$$c_{\min}\|\widehat{x} - x_{\hat{\alpha},n,\ell}^\delta\|_2 \leqslant \|\widehat{x} - x_{\hat{\alpha},n,\ell}^\delta\|_{\mathcal{X}} \leqslant c_{\max}\|\widehat{x} - x_{\hat{\alpha},n,\ell}^\delta\|_2.$$

The inequality (4.24) now follows from corollary 4.6. □

Remark 4.10. We conclude this section with a comment on why our analysis requires results by both Natterer [18] and Neubauer [20], because it may appear more natural to choose $T_{h,\ell} = A_n^{(\ell)}$ and apply Neubauer's result, only, without invoking those of Natterer. Our reason for using the bounds provided by Natterer is that in order to be able to use the results of Neubauer, without applying those of Natterer, we need a bound for

$$\|A - A_n^{(\ell)}\|,$$

where we consider $A_n^{(\ell)}$ an operator from $\mathcal{X}$ to $\mathcal{Y}$ and $\|\cdot\|$ denotes the appropriate operator norm. For many standard discretizations with suitable basis functions such a bound can be determined. However, this is not the case for the Arnoldi approximation $A_n^{(\ell)}$, as the Arnoldi process depends on the starting vector. Therefore, we need a discrete approximation A_n of A so that we are able to evaluate

$$\|A_n - A_n^{(\ell)}\|_2$$

numerically. Here $A_n^{(\ell)}$ is considered a matrix. The application of the Arnoldi process to A_n gives an approximation of the solution of the *discretized equation*. Natterer's bounds are required to bound the distance to the solution of the infinite-dimensional problem.

5. Computed examples

We apply the Arnoldi–Tikhonov method to a few ill-posed operator equations and illustrate the influence of different discretizations. All computations were carried out using MATLAB with about 15 significant decimal digits.

Example 5.1. Consider the Fredholm integral equation of the first kind discussed by Phillips [23],

$$\int_{-6}^{6} \kappa(s,t)x(t)\mathrm{d}t = g(t), \qquad -6 \leqslant s \leqslant 6, \tag{5.1}$$

where the solution $x(t)$, kernel $\kappa(s,t)$, and right-hand side $y(s)$ are given by

$$\begin{aligned} x(t) &= \begin{cases} 1 + \cos\left(\frac{\pi t}{3}\right), & |t| < 3, \\ 0, & |t| \geqslant 3, \end{cases} \\ \kappa(s,t) &= x(s-t), \\ y(s) &= (6 - |s|)\left(1 + \frac{1}{2}\cos\left(\frac{\pi s}{3}\right)\right) + \frac{9}{2\pi}\sin\left(\frac{\pi|s|}{3}\right). \end{aligned} \tag{5.2}$$

We discretize this integral equation by a Nyström method based on the composite trapezoidal rule with n nodes. This yields a nonsymmetric matrix $A_n \in \mathbb{R}^{n,n}$. The vector $x_n \in \mathbb{R}^n$ is a discretization of the exact solution (5.2). We define the associated right-hand side $y_n = A_n x_n$, which is assumed to be unknown. An associated contaminated right-hand side, $y_n^\delta \in \mathbb{R}^n$, which is assumed to be known, is obtained by adding a vector $e_n \in \mathbb{R}^n$, with normally distributed random entries with mean zero, that models 'noise', to y_n. The noise vector e_n is scaled to cor-

respond to a prescribed noise level

$$\nu = \frac{\|e_n\|_2}{\|y_n\|_2}. \tag{5.3}$$

We will use $\delta = \nu\|y_n\|_2$ when determining the regularization parameter α by solving (4.14).

Application of ℓ steps of the Arnoldi process to the matrix A_n with initial vector $v_1 = y^\delta/\|y^\delta\|_2$ yields the decomposition (3.1), as well as the low-rank approximation $A_n^{(\ell)}$ of A_n defined by (4.1). Table 1 displays the approximation error

$$h_\ell = \|A_n - A_n^{(\ell)}\|_2; \tag{5.4}$$

see (4.2).

We determine the regularization parameter α by solving (4.14) with $E = 3\|x_n\|_2$ and $C = 1$, as suggested by proposition 4.2, and then solve the regularized problem (4.4) with the low-rank matrix $A_n^{(\ell)}$ for $x_{\alpha,n,\ell}^\delta$. The inequality (4.15) holds for all examples in this section. Table 1 shows the relative error $\|x_{\alpha,n,\ell}^\delta - x_n\|_2/\|x_n\|_2$. This error depends both on the error in y_n^δ and on the approximation error (5.4). For fixed n, the approximation error (5.4) is seen to decrease as ℓ increases in table 1.

Let $x_{\alpha,n}^\delta$ denote the solution of the regularized problem (4.5) with the matrix A_n. We are interested in how much the replacement of A_n by the low-rank approximation $A_n^{(\ell)}$ affects the quality of the computed solution. Therefore, we tabulate the normalized difference $\|x_{\alpha,n,\ell}^\delta - x_{\alpha,n}^\delta\|_2/\|x_n\|_2$. Table 1 shows this difference to be much smaller than $\|x_{\alpha,n,\ell}^\delta - x_n\|_2/\|x_n\|_2$. Hence, the use of $A_n^{(\ell)}$ instead of A_n, with a fixed value of α, does not affect the quality of the computed solution significantly.

Table 1 shows results for different problem sizes, $n \in \{1000, 2000, 4000\}$, and noise level 1%. The quality of the computed solution $x_{\alpha,n,\ell}^\delta$ is seen not to be very sensitive to the problem size n or to the number of steps ℓ carried out with the Arnoldi process. For n fixed, table 1 shows h_ℓ to decrease as ℓ increases. Also the relative error $\|x_{\alpha,n,\ell}^\delta - x_n\|_2/\|x_n\|_2$ can be seen to decrease slowly as ℓ increases. Moreover, the error decreases when n increases and ℓ is kept fixed.

The quality of the computed solution is, of course, sensitive to the noise level. This is illustrated by table 2, which shows results for noise level 0.1%. The α-values of table 2 are smaller than of table 1, as can be expected. Moreover, the relative errors $\|x_{\alpha,n,\ell}^\delta - x_n\|_2/\|x_n\|$ reported in table 2 are smaller than the corresponding errors of table 1.

We would like the ℓth singular value of $A_n^{(\ell)}$, i.e. of $H_{\ell+1,\ell}$, to be much smaller than the first one (the largest singular value). Then $A_n^{(\ell)}$ captures all essential properties of A_n. To illustrate that this is the case, we display in table 3 the largest and smallest singular values, $\sigma_1^{(\ell)}$ and $\sigma_\ell^{(\ell)}$, respectively, of the matrix $H_{\ell+1,\ell}$ in the definition (4.1) of $A_n^{(\ell)}$. The table shows singular values for the matrices $H_{\ell+1,\ell}$ determined for table 1. The size of the largest singular value is seen to be independent of ℓ, while the smallest singular value decreases slowly as ℓ and n increase.

In the computations reported in tables 1–3, we assumed that the noise level δ is known exactly. In the next couple of tables, we illustrate the situation when only an upper bound for the noise level is known. To investigate the sensitivity of the computed solution to the error in δ, we repeat some of the computations of tables 1 and 2 with the value of δ increased by 50% and 100% in equation (4.14), but without changing the noise vector e_n.

Table 2. Example 5.1: the Phillips test problem. The noise level (5.3) is 0.1%.

n	ℓ	h_ℓ	α	$\|x^\delta_{\alpha,n,\ell} - x_n\|_2/\|x_n\|_2$	$\|x^\delta_{\alpha,n,\ell} - x^\delta_{\alpha,n}\|_2/\|x_n\|_2$
1000	20	$1.14 \cdot 10^{-1}$	4.44	$2.13 \cdot 10^{-1}$	$4.20 \cdot 10^{-4}$
1000	30	$1.13 \cdot 10^{-1}$	4.42	$2.12 \cdot 10^{-1}$	$4.16 \cdot 10^{-4}$
1000	40	$1.12 \cdot 10^{-1}$	4.36	$2.11 \cdot 10^{-1}$	$4.14 \cdot 10^{-4}$
2000	20	$8.15 \cdot 10^{-2}$	3.27	$1.77 \cdot 10^{-1}$	$4.28 \cdot 10^{-4}$
2000	30	$8.13 \cdot 10^{-2}$	3.26	$1.77 \cdot 10^{-1}$	$4.22 \cdot 10^{-4}$
2000	40	$8.06 \cdot 10^{-2}$	3.24	$1.76 \cdot 10^{-1}$	$4.20 \cdot 10^{-4}$
4000	20	$5.78 \cdot 10^{-2}$	2.42	$1.48 \cdot 10^{-1}$	$3.69 \cdot 10^{-4}$
4000	30	$5.77 \cdot 10^{-2}$	2.41	$1.47 \cdot 10^{-1}$	$3.67 \cdot 10^{-4}$
4000	40	$5.75 \cdot 10^{-2}$	2.41	$1.47 \cdot 10^{-1}$	$3.66 \cdot 10^{-4}$

Table 3. Example 5.1: the Phillips test problem. Largest and smallest singular values $\sigma_1^{(\ell)} \geqslant \ldots \geqslant \sigma_\ell^{(\ell)}$ of the matrices $H_{\ell+1,\ell}$ in the definition (4.1) of the approximations $A_n^{(\ell)}$ of A_n used in table 1.

n	ℓ	$\sigma_1^{(\ell)}$	$\sigma_\ell^{(\ell)}$
1000	20	5.80	$2.44 \cdot 10^{-4}$
1000	30	5.80	$9.36 \cdot 10^{-5}$
1000	40	5.80	$3.37 \cdot 10^{-5}$
2000	20	5.80	$2.26 \cdot 10^{-4}$
2000	30	5.80	$6.44 \cdot 10^{-5}$
2000	40	5.80	$2.11 \cdot 10^{-5}$
4000	20	5.80	$1.99 \cdot 10^{-4}$
4000	30	5.80	$3.38 \cdot 10^{-5}$
4000	40	5.80	$1.54 \cdot 10^{-5}$

Table 4 is analogous to table 1 and displays relative errors for the situation when the computations are carried out with the same data as for table 1, but the noise level is assumed to be 50% larger. As can be expected, the errors $\|x^\delta_{\alpha,n,\ell} - x_n\|_2/\|x_n\|_2$ are larger than the corresponding errors in table 1. However, they are still small enough so that the computed solutions $x^\delta_{\alpha,n,\ell}$ furnish meaningful approximations of x_n. The relative differences $\|x^\delta_{\alpha,n,\ell} - x^\delta_{\alpha,n}\|_2/\|x_n\|_2$ are somewhat smaller than the corresponding differences in table 1, which shows that the error introduced by using the Arnoldi process is negigible also when the noise level is overestimated. Table 5 differs from table 4 only in that the true noise level is 0.1%. Since the noise level is smaller in table 2 than in table 1, a 50% overestimation of the noise level only has a small effect on the errors $\|x^\delta_{\alpha,n,\ell} - x_n\|_2/\|x_n\|_2$ reported in table 5.

Tables 6 and 7 are analogous to (parts of) tables 4 and 5, respectively, and display the error $\|x^\delta_{\alpha,n,\ell} - x_n\|_2/\|x_n\|_2$ for the situation when the noise level has been overestimated by 100%. As expected, the errors reported in the tables 6 and 7 are larger than those reported in tables 4 and 5, respectively, but not by much. We conclude that the solution method gives useful computed solutions also in the situation when the noise level in the data y_n^δ is significantly overestimated. □

Table 4. Example 5.1: this table is analogous to table 1 with the noise level (5.3) overestimated by 50%.

n	ℓ	$\|x^{\delta}_{\alpha,n,\ell} - x_n\|_2/\|x_n\|_2$	$\|x^{\delta}_{\alpha,n,\ell} - x^{\delta}_{\alpha,n}\|_2/\|x_n\|_2$
1000	20	$2.36 \cdot 10^{-1}$	$3.26 \cdot 10^{-4}$
1000	30	$2.36 \cdot 10^{-1}$	$3.23 \cdot 10^{-4}$
1000	40	$2.34 \cdot 10^{-1}$	$3.23 \cdot 10^{-4}$
4000	20	$1.78 \cdot 10^{-1}$	$3.01 \cdot 10^{-4}$
4000	30	$1.78 \cdot 10^{-1}$	$3.00 \cdot 10^{-4}$
4000	40	$1.77 \cdot 10^{-1}$	$2.99 \cdot 10^{-4}$

Table 5. Example 5.1: this table is analogous to table 2 with the noise level (5.3) overestimated by 50%.

n	ℓ	$\|x^{\delta}_{\alpha,n,\ell} - x_n\|_2/\|x_n\|_2$	$\|x^{\delta}_{\alpha,n,\ell} - x^{\delta}_{\alpha,n}\|_2/\|x_n\|_2$
1000	20	$2.14 \cdot 10^{-1}$	$4.16 \cdot 10^{-4}$
1000	30	$2.13 \cdot 10^{-1}$	$4.12 \cdot 10^{-4}$
1000	40	$2.12 \cdot 10^{-1}$	$4.10 \cdot 10^{-4}$
4000	20	$1.49 \cdot 10^{-1}$	$3.66 \cdot 10^{-4}$
4000	30	$1.49 \cdot 10^{-1}$	$3.65 \cdot 10^{-4}$
4000	40	$1.48 \cdot 10^{-1}$	$3.64 \cdot 10^{-4}$

Table 6. Example 5.1: this table is analogous to table 1 with the noise level (5.3) overestimated by 100%.

n	ℓ	$\|x^{\delta}_{\alpha,n,\ell} - x_n\|_2/\|x_n\|_2$	$\|x^{\delta}_{\alpha,n,\ell} - x^{\delta}_{\alpha,n}\|_2/\|x_n\|_2$
1000	20	$2.45 \cdot 10^{-1}$	$2.91 \cdot 10^{-4}$
1000	30	$2.44 \cdot 10^{-1}$	$2.88 \cdot 10^{-4}$
1000	40	$2.42 \cdot 10^{-1}$	$2.88 \cdot 10^{-4}$

Example 5.2. This example also considers the integral equation (5.1), but uses a different discretization. The discretization is computed with the MATLAB function phillips from Regularization Tools by Hansen [12]. This function uses a Galerkin method with n orthonormal box functions as test and trial functions and yields a symmetric indefinite matrix $A_n \in \mathbb{R}^{n\times n}$. The vector $x_n \in \mathbb{R}^n$ is a scaled discretization of the exact solution (5.2). Since the matrix A_n is symmetric, the Arnoldi process (Algorithm 1) simplifies to the Lanczos process. Table 8 is analogous to table 1 and shows results for the noise level (5.3) 1%. Results for noise level 0.1% are displayed in table 9, which is analogous to table 2. Due to the different scaling of matrices and right-hand sides in this and the previous examples, the quantities h_ℓ and α will differ. However, the relative errors tabulated in the last two columns are comparable, and it is clear that the Galerkin method of the present example furnishes more accurate approximations of x_n than the Nyström discretization of Example 5.1. The exact solution x_n and the computed approximation $x^{\delta}_{\alpha,n,\ell}$ for $n = 2000$, $\ell = 30$, and $\nu = 1 \cdot 10^{-2}$, are shown in figure 1. □

Table 7. Example 5.1: this table is analogous to table 2 with the noise level (5.3) overestimated by 100%.

n	ℓ	$\|x^{\delta}_{\alpha,n,\ell} - x_n\|_2/\|x_n\|_2$	$\|x^{\delta}_{\alpha,n,\ell} - x^{\delta}_{\alpha,n}\|_2/\|x_n\|_2$
4000	20	$1.50 \cdot 10^{-1}$	$3.64 \cdot 10^{-4}$
4000	30	$1.50 \cdot 10^{-1}$	$3.63 \cdot 10^{-4}$
4000	40	$1.49 \cdot 10^{-1}$	$3.62 \cdot 10^{-4}$

Table 8. Example 5.2: the Phillips test problem. The noise level (5.3) is 1%.

n	ℓ	h_ℓ	α	$\frac{\|x^{\delta}_{\alpha,n,\ell} - x_n\|_2}{\|x_n\|_2}$	$\frac{\|x^{\delta}_{\alpha,n,\ell} - x^{\delta}_{\alpha,n}\|_2}{\|x_n\|_2}$
1000	20	$1.76 \cdot 10^{-2}$	$1.48 \cdot 10^{0}$	$1.10 \cdot 10^{-1}$	$1.39 \cdot 10^{-14}$
1000	30	$5.40 \cdot 10^{-3}$	$9.92 \cdot 10^{-1}$	$8.65 \cdot 10^{-2}$	$1.87 \cdot 10^{-14}$
1000	40	$2.38 \cdot 10^{-3}$	$7.94 \cdot 10^{-1}$	$8.58 \cdot 10^{-2}$	$2.29 \cdot 10^{-14}$
2000	20	$1.76 \cdot 10^{-2}$	$1.49 \cdot 10^{0}$	$1.10 \cdot 10^{-1}$	$1.76 \cdot 10^{-14}$
2000	30	$5.39 \cdot 10^{-3}$	$9.98 \cdot 10^{-1}$	$8.70 \cdot 10^{-2}$	$2.50 \cdot 10^{-14}$
2000	40	$2.21 \cdot 10^{-3}$	$8.63 \cdot 10^{-1}$	$7.99 \cdot 10^{-2}$	$2.81 \cdot 10^{-14}$
4000	20	$1.80 \cdot 10^{-2}$	$1.50 \cdot 10^{0}$	$1.11 \cdot 10^{-1}$	$2.60 \cdot 10^{-14}$
4000	30	$5.80 \cdot 10^{-3}$	$1.02 \cdot 10^{0}$	$8.83 \cdot 10^{-2}$	$3.73 \cdot 10^{-14}$
4000	40	$2.57 \cdot 10^{-3}$	$8.83 \cdot 10^{-1}$	$8.11 \cdot 10^{-2}$	$4.38 \cdot 10^{-14}$

Table 9. Example 5.2: the Phillips test problem. The noise level (5.3) is 0.1%.

n	ℓ	h_ℓ	α	$\frac{\|x^{\delta}_{\alpha,n,\ell} - x_n\|_2}{\|x_n\|_2}$	$\frac{\|x^{\delta}_{\alpha,n,\ell} - x^{\delta}_{\alpha,n}\|_2}{\|x_n\|_2}$
1000	20	$1.76 \cdot 10^{-2}$	$8.73 \cdot 10^{-1}$	$8.02 \cdot 10^{-2}$	$2.16 \cdot 10^{-14}$
1000	30	$5.40 \cdot 10^{-3}$	$3.55 \cdot 10^{-1}$	$4.73 \cdot 10^{-2}$	$5.05 \cdot 10^{-14}$
1000	40	$2.40 \cdot 10^{-3}$	$2.21 \cdot 10^{-1}$	$3.66 \cdot 10^{-2}$	$8.52 \cdot 10^{-14}$
2000	20	$1.75 \cdot 10^{-2}$	$8.71 \cdot 10^{-1}$	$8.01 \cdot 10^{-2}$	$2.91 \cdot 10^{-14}$
2000	30	$5.39 \cdot 10^{-3}$	$3.55 \cdot 10^{-1}$	$4.73 \cdot 10^{-2}$	$6.63 \cdot 10^{-14}$
2000	40	$2.22 \cdot 10^{-3}$	$2.14 \cdot 10^{-1}$	$3.60 \cdot 10^{-2}$	$1.09 \cdot 10^{-13}$
4000	20	$1.76 \cdot 10^{-2}$	$8.73 \cdot 10^{-1}$	$8.03 \cdot 10^{-2}$	$4.45 \cdot 10^{-14}$
4000	30	$5.78 \cdot 10^{-3}$	$3.73 \cdot 10^{-1}$	$4.86 \cdot 10^{-2}$	$9.99 \cdot 10^{-14}$
4000	40	$2.57 \cdot 10^{-3}$	$2.31 \cdot 10^{-1}$	$3.74 \cdot 10^{-2}$	$1.63 \cdot 10^{-13}$

Example 5.3. We turn to the Fredholm integral equation of the first kind discussed by Baart [1],

$$\int_0^{\pi} \kappa(s,t)x(t)\mathrm{d}t = g(s), \qquad 0 \leqslant s \leqslant \frac{\pi}{2},$$

where $\kappa(s,t) = \exp(s\cos(t))$ and $g(s) = 2\sinh(s)/s$. The solution is given by $x(t) = \sin(t)$. We discretize this integral equation by a Galerkin method using n orthonormal box functions as test and trial functions. The discretization is computed with the MATLAB function baart from [12] and gives a nonsymmetric matrix $A_n \in \mathbb{R}^{n,n}$ and a vector $x_n \in \mathbb{R}^n$ that is a scaled discretization of the exact solution. Similarly as in example 5.1, we define the 'unknown' exact right-hand side by $y_n = A_n x_n$, and obtain the associated contaminated right-hand side

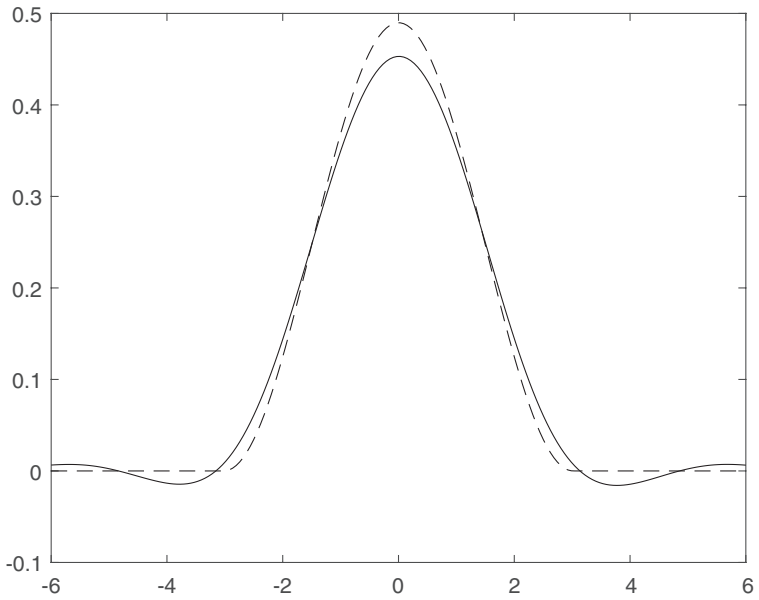

Figure 1. Example 5.2: exact solution x_n (dashed curve) and computed solution $x^{\delta}_{\alpha,n,\ell}$ (continuous curve) for $n = 2000$, $\ell = 30$, and noise level $\nu = 1\%$.

Table 10. Example 5.3: the Baart test problem for $\ell = 10$, three sizes n, and two noise levels ν.

n	h_ℓ	ν	α	$\frac{\|x^{\delta}_{\alpha,n,\ell} - x_n\|_2}{\|x_n\|_2}$	$\frac{\|x^{\delta}_{\alpha,n,\ell} - x^{\delta}_{\alpha,n}\|_2}{\|x_n\|_2}$
1000	$3.01 \cdot 10^{-4}$	$1 \cdot 10^{-2}$	$5.25 \cdot 10^{-3}$	$3.30 \cdot 10^{-1}$	$9.73 \cdot 10^{-5}$
2000	$4.70 \cdot 10^{-4}$	$1 \cdot 10^{-2}$	$5.28 \cdot 10^{-3}$	$3.30 \cdot 10^{-1}$	$1.55 \cdot 10^{-4}$
4000	$3.16 \cdot 10^{-4}$	$1 \cdot 10^{-2}$	$5.17 \cdot 10^{-3}$	$3.29 \cdot 10^{-1}$	$1.28 \cdot 10^{-4}$
1000	$3.01 \cdot 10^{-4}$	$1 \cdot 10^{-3}$	$1.98 \cdot 10^{-3}$	$1.86 \cdot 10^{-1}$	$3.23 \cdot 10^{-4}$
2000	$4.70 \cdot 10^{-4}$	$1 \cdot 10^{-3}$	$2.27 \cdot 10^{-3}$	$1.90 \cdot 10^{-1}$	$4.49 \cdot 10^{-4}$
4000	$3.16 \cdot 10^{-4}$	$1 \cdot 10^{-3}$	$2.00 \cdot 10^{-3}$	$1.86 \cdot 10^{-1}$	$4.36 \cdot 10^{-4}$

$y^{\delta}_n \in \mathbb{R}^n$, which is assumed to be known, by adding a vector $e_n \in \mathbb{R}^n$ with normally distributed entries with zero mean to y_n. The vector e_n is scaled to correspond to a prescribed noise level. A few computed results are displayed in table 10. The table shows the relative error $\|x^{\delta}_{\alpha,n,\ell} - x_n\|_2 / \|x_n\|_2$ to be independent of n for n large, and to decrease as the noise level (5.3) decreases.

The singular values of the matrices A_n, when ordered in decreasing order, decrease rapidly with increasing index. It therefore is not meaningful to choose ℓ larger than 10. The largest singular value of all the matrices $H_{11,10}$ generated for table 10 is 3.23 and the smallest one for all matrices is about $1 \cdot 10^{-13}$.

We remark that since the singular values of A decrease exponentially with their index number, the condition (2.5) is not valid for any finite l. Nevertheless, this example illustrates that the approximation method described in this paper also can be applied in this situation. □

6. Conclusion and extensions

The paper presents an analysis of the influence of discretization and truncation errors on the computed approximate solution. These errors are caused by replacing an operator A first by a large matrix A_n, which in turn is approximated by a matrix $A_n^{(\ell)}$ of rank at most $\ell \ll n$. The choice of the regularization parameter in Tikhonov regularization is discussed. Computed examples illustrate the theory.

The matrix $A_n^{(\ell)}$ is determined by the application of ℓ steps of the Arnoldi process to the large matrix A_n. Other approaches to determine low-rank approximations are available, such as methods based on Golub–Kahan bidiagonalization or block Golub–Kahan bidiagonalization; see, e.g. Bentbib *et al* [2] and Gazzola *et al* [8]. The analyses for these methods differ from the one of this paper and are presently being pursued.

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References

[1] Baart M L 1982 The use of auto-correlation for pseudo-rank determination in noisy ill-conditioned linear least-squares problems *IMA J. Numer. Anal.* **2** 241–7
[2] Bentbib A H, El Guide M, Jbilou K, Onunwor E and Reichel L 2018 Solution methods for linear discrete ill-posed problems for color image restoration *BIT Numer. Math.* **58** 555–78
[3] Calvetti D, Morigi S, Reichel L and Sgallari F 2000 Tikhonov regularization and the *L*-curve for large, discrete ill-posed problems *J. Comput. Appl. Math.* **123** 423–46
[4] Clason C, Kaltenbacher B and Wachsmuth D 2016 Functional error estimators for the adaptive discretization of inverse problems *Inverse Problems* **32** 104004
[5] Dicken V and Maaß P 1997 Wavelet–Galerkin methods for ill-posed problems *J. Inverse Ill-Posed Probl.* **4** 507–19
[6] Donatelli M and Reichel L 2014 Square smoothing regularization matrices with accurate boundary conditions *J. Comput. Appl. Math.* **272** 334–49
[7] Engl H W, Hanke M and Neubauer A 1996 *Regularization of Inverse Problems* (Dordrecht: Kluwer)
[8] Gazzola S, Novati P and Russo M R 2015 On Krylov projection methods and Tikhonov regularization *Electron. Trans. Numer. Anal.* **44** 83–123
[9] Gerth D and Ramlau R 2014 A stochastic convergence analysis for Tikhonov regularization with sparsity constraints *Inverse Problems* **30** 055009
[10] Haber E, Heldmann S and Ascher U 2007 Adaptive finite volume method for distributed nonsmooth parameter identification *Inverse Problems* **23** 1659–76
[11] Hanke M and Hansen P C 1993 Regularization methods for large-scale problems *Surv. Math. Ind.* **3** 253–315
[12] Hansen P C 2007 Regularization tools version 4.0 for Matlab 7.3 *Numer. Algorithms* **46** 189–94
[13] Hansen P C 1998 *Rank-Deficient and Discrete Ill-Posed Problems* (Philadelphia, PA: SIAM)
[14] Hochstenbach M E, McNinch N and Reichel L 2012 Discrete ill-posed least-squares problems with a solution norm constraint *Linear Algebr. Appl.* **436** 3801–18
[15] Lewis B and Reichel L 2009 Arnoldi–Tikhonov regularization methods *J. Comput. Appl. Math.* **226** 92–102

[16] Maaß P, Pereverzev S V, Ramlau R and Solodky S G 2001 An adaptive discretization scheme for Tikhonov-regularization with *a posteriori* parameter selection *Numer. Math.* **87** 485–502
[17] Mathé P and Pereverzev S 2001 Optimal discretization of inverse problems in Hilbert scales. Regularization and self-regularization of projection methods *SIAM J. Numer. Anal.* **38** 1999–2012
[18] Natterer F 1977 Regularization of ill-posed problems by projection methods *Numer. Math.* **28** 329–41
[19] Natterer F 2001 *The Mathematics of Computerized Tomography* (Philadelphia, PA: SIAM)
[20] Neubauer A 1986 An *a posteriori* parameter choice for Tikhonov regularization in the presence of modeling error *Appl. Numer. Math.* **4** 203–22
[21] Neuman A, Reichel L and Sadok H 2012 Algorithms for range restricted iterative methods for linear discrete ill-posed problems *Numer. Algorithms* **59** 325–31
[22] Onunwor E and Reichel L 2017 On the computation of a truncated SVD of a large linear discrete ill-posed problem *Numer. Algorithms* **75** 359–80
[23] Phillips D L 1962 A technique for the numerical solution of certain integral equations of the first kind *J. ACM* **9** 84–97
[24] Ramlau R 1999 A modified Landweber method for inverse problems *Numer. Funct. Anal. Optim.* **20** 79–98
[25] Reichel L and Ye Q 2005 Breakdown-free GMRES for singular systems *SIAM J. Matrix Anal. Appl.* **26** 1001–21
[26] Saad Y 2003 *Iterative Methods for Sparse Linear Systems* 2nd edn (Philadelphia, PA: SIAM)
[27] Varga R S 2004 *Geršgorin and His Circles* (Berlin: Springer)