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ERROR ESTIMATES FOR ARNOLDI–TIKHONOV REGULARIZATION FOR ILL-POSED OPERATOR EQUATIONS

RONNY RAMLAU* AND LOTHAR REICHEL†

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.

Key words. ill-posed problem, Arnoldi's method, Tikhonov regularization

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

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

Denote the solution, if it exists, by $\widehat{x}$. The determination of this solution is an ill-posed problem since $\widehat{x}$ might not depend continuously on y.

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

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

with a known bound $\delta > 0$, where $\| \cdot \|_{\mathcal{Y}}$ denotes the norm in $\mathcal{Y}$. 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 $\widehat{x}$.

Numerical solution of (1.3) requires discretization of the equation. The discretization, to be specified below, 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 $x_n, y_n^\delta \in \mathbb{R}^n$. We are concerned with the situation when the matrix A_n is large, and in particular too large to make the computation of its singular value decomposition attractive.

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Most of the existing literature on the solution of linear ill-posed operator equations (1.3) or their discretization (1.4) consider either the infinite-dimensional setting (1.3) only and, thus, neglect the necessary discretization, or focus on the solution of the linear system of algebraic equations (1.4) with an ill-conditioned or singular matrix, and neglect the fact that these equations stem from an underlying continuous formulation. Only a few papers, most prominently by Natterer [11] and Neubauer [13], consider both continuous and discrete aspects, but then do not discuss fast solution methods for the discretized systems.

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 equations (1.4). We then 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 equation 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. We also 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 [2, 4, 5, 8, 9] 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 [11] on the discretization of integral operators. Discretization yields the linear system of algebraic equations (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 the low-rank approximation in Tikhonov regularization and obtain a quite efficient solution method. To analyze the performance 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 [13] to the computed solution furnished 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 [11] 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 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 [11], 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 the 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 right-hand side $Q_n y^{\delta}$ in (2.1). A unique solution of the linear system of equations (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

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

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

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

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

$$0 < c_{\min} \leq \sigma_{\min}(M_n), \qquad \sigma_{\max}(M_n) \leq c_{\max} < \infty \qquad \forall n. \tag{2.4}$$

Then

$$c_{\min}\|\vec{x}_n\|_2 \le \|x_n\|_{\mathcal{X}} \le c_{\max}\|\vec{x}_n\|_2. \tag{2.5}$$

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

$$\|Ax\|_{\mathcal{Y}} \sim \|x\|_{\mathcal{H}^{-l}} \tag{2.6}$$

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 [11] requires a finite value of l such that (2.6) holds to exist.

Example 2.1. Consider the mildly ill-posed Volterra integral equation of the first kind

$$[Ax](s) = \int_0^s x(t)dt, \qquad 0 \le s \le 1.$$

Then (2.6) holds with $l = 1$. $\quad\square$

Example 2.2. Let

$$[Ax](s) = \int_{-6}^6 k(s-t)x(t)dt, \qquad -6 \le s \le 6,$$

with

$$k(t) = \begin{cases} 1 + \cos\left(\frac{\pi}{3}t\right), & -3 \le t \le 3, \\ 0, & \text{otherwise.} \end{cases}$$

This integral operator is discussed by Phillips [16]. The kernel k has jump discontinuities in the second derivative at $t = \pm 3$. It follows that $l = 2$. $\quad\square$

Example 2.3 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

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

Then (2.6) holds with $l = 1/2$; see [12]. $\quad\square$

Example 2.4. Let

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

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 (2.6) holds with $l = \beta$, see, e.g., [6]. We remark that square integrability of the kernel is not required. $\square$

Natterer [11] shows that if the operator A is injective and the subspaces $\mathcal{X}_n$, $n = 1, 2, \dots$, are chosen so that an inverse estimate is fulfilled (see [11, eq. (4.1)-(4.5)] for details on the latter), then one obtains for $\widehat{x} \in \mathcal{H}^k$ the bound

$$\|\widehat{x} - x_n\|_{\mathcal{X}} \leq C \left(h(n)^k \|\widehat{x}\|_{\mathcal{H}^k} + h(n)^{-l}\delta \right) \tag{2.7}$$

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 $\mathcal{X}_n$, $n = 1, 2, \dots$, 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 (2.7) is the bound (1.2); see [11]. An optimal dimension of the discretized problem is given by

$$n \approx h^{-1} \left(\left(\frac{\delta}{\|\widehat{x}\|_{\mathcal{H}^k}} \right)^{1/(k+l)} \right) \tag{2.8}$$

and yields the bound

$$\|\widehat{x} - x_n\|_{\mathcal{X}} \leq C' \|\widehat{x}\|_{\mathcal{H}^k}^{l/(k+l)} \delta^{k/(k+l)} \tag{2.9}$$

for some constant $C' > 0$; see Natterer [11] for details. For instance, spline and finite element approximation spaces $\mathcal{X}_n$ allow for bounds of the type (2.7) and (2.9). Natterer [11] proposes that the dimension n of the solution subspace of the discretized problem (1.4) be chosen according to (2.8). 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 [3].

Convergence rates analogous to (2.9), when h is chosen according to (2.8), also can be established in a different setting; see Mathé and Pereverzev [10]. They assume that the operator A is continuously invertible in Hilbert scales (which resembles the condition (2.6)), and show convergence rates in a stochastic noise setting with respect to norms of the relevant Hilbert scales; see [10, 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

$$\|y_n - y_n^\delta\|_{\mathcal{Y}} \lesssim \delta. \tag{2.10}$$

It is convenient to replace the norm in (2.10) by the Euclidean norm. This can be achieved analogously as in the begining 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

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

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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

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

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

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

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

$$\|y_n - y_n^\delta\|_2 \le \delta, \tag{2.11}$$

which implies that

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

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. Application of $1 \le \ell \ll n$ 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

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

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., [18]. 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 $\ell \ge 0$, otherwise the computations simplify; see below.

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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:     $w := A_n v_j$

5:     **for** $k = 1$ **to** j

6:         $h_{k,j} := \langle v_j, w \rangle$

7:         $w := w - v_j h_{k,j}$

8:     **end for**

9:     $h_{j+1,j} := \|w\|_2$; $v_{j+1} := w/h_{j+1,j}$

10: **end for**

11: **Output:** Upper Hessenberg matrix $H_{\ell+1,\ell} = [h_{k,j}] \in \mathbb{R}^{\ell+1,\ell}$, matrix

12:         $V_{n,\ell+1} = [v_1, v_2, \ldots, v_{\ell+1}] \in \mathbb{R}^{n,\ell+1}$ with orthonormal columns

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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 $1 \leq k < j$, 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 [17].

We remark that the Arnoldi process simplifies to the Lanczos process when the matrix A_n is symmetric; see [18, 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 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 proposed solution method 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.

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 [15] 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

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

Assume that

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

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

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

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 the operator equation (1.1). If the latter equation does not have a solution, then we let $\widehat{x}$ denote the least-squares solution of minimal norm. We assume this least-squares solution to exist.

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The proper choice of the parameter pair $\{\ell, \alpha\}$ has been studied by Neubauer [13], 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 [13] requires the operator $T_{h,\ell}$ to satisfy

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

where R_ℓ is an orthogonal projector onto a finite-dimensional subspace $\mathcal{W}_\ell \subset \widetilde{\mathcal{Y}}$ to be specified below. Here, 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 [13], we let $T := A_n$ and $\widetilde{\mathcal{X}} := \widetilde{\mathcal{Y}} := \mathbb{R}^n$. Thus, we set

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

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*

$$\mathcal{W}_\ell \subset \overline{\mathcal{R}(A_n)}, \tag{4.7}$$
$$\mathcal{R}(R_\ell A_n^{(\ell)}) = \mathcal{W}_\ell, \tag{4.8}$$
$$\|R_\ell(A_n - A_n^{(\ell)})\|_2 \le h_\ell,$$
$$\|R_\ell(y - y_n^\delta)\|_2 \le \delta, \tag{4.9}$$
$$R_\ell \to I \; \text{point-wise onto } \mathcal{R}(A_n), \tag{4.10}$$

where the bound (4.9) *is inspired by* (2.11).

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,

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

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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

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

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 $\ell \geq 1$ 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 $\ell \geq 1$ (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. $\square$

Thus, the requirements of Neubauer [13, Assumption 2.3] are fulfilled, and we get the following result from [13, Proposition 2.6 and Theorem 3.1]:

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

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

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

for some constant $\rho \geq 0$ independent of n, and assume that $\|y_n - Q_n y^\delta\|_2 \leq \delta$. 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

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

Then the associated solution of (4.4) satisfies

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

with

$$
p(l,\nu) = \begin{cases}
0 & \text{if } \nu = 0 \\
\gamma_l \|(I - R_\ell)z\| & \text{if } \nu = \frac{1}{2}, \ A_n^* z_n = (A_n^* A_n)^{1/2} v_n, \\
\gamma_l^2 \|v_n\|_2 & \text{if } \nu = 1, \\
(4/\pi)\gamma_l^{2\nu} \|v_n\| & \text{otherwise,}
\end{cases} \tag{4.17}
$$

$$\gamma_l = \|(I - R_\ell)A_n\|_2^2 \|v_n\|_2 \tag{4.18}$$

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 relatively strong restriction. In finite dimension it is enough for (4.12) to hold for all x_n that A_n is injective. However, the uniform boundedness of $\|v_n\|$ (inequality (4.13)) generally remains an open problem (see Proposition 4.5).*

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 the following corollary. Also, the condition (4.15) requires ℓ has 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 hold. Assume A is self adjoint, fulfilling (2.6), $A_n = P_n A P_n$, 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 $A_n x_n = y_n$ fulfill a source condition with $\nu = 1/2$, and the associated source elements v_n are uniformly bounded.*

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

$$x = (A^* A)^{1/2} v = Av. \tag{4.19}$$

As A_n is also self adjoint, finite dimensional and injective, x_n also fulfills a source condition (see Remark 4.3)

$$x_n = (A_n^* A_n)^{1/2} v_n = A_n v_n \tag{4.20}$$

with a unique v_n. As A fulfills (2.6), the distance between x and x_n can be estimated by

$$\|x - x_n\|_{\mathcal{X}} \le C' \|x\|_{\mathcal{H}^k}^{l/(k+l)} \delta_n^{k/(k+l)} \tag{4.21}$$

see (2.9), and $\delta_n = \|y - y_n\| \searrow 0$ as $n \to \infty$. Using again (2.9) for solving (4.19) with $\tilde{\delta}_n = \|x - x_n\|$, we obtain with $v \in \mathcal{H}^{\tilde{k}}$

$$\|v - v_n\|_{\mathcal{X}} \le C' \|v\|_{\mathcal{H}^{\tilde{k}}}^{l/(\tilde{k}+l)} \delta_n^{\tilde{k}/(\tilde{k}+l)} , \tag{4.22}$$

i.e., $v_n \to v$ and consequently $\|v_n\|$ is uniformly bounded. $\square$

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

COROLLARY 4.6. *Assume that the conditions of Proposition 4.2 hold, $\nu = 1$ 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

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

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

$$\|(I - R_\ell)A_n\|_2 \leq \|(I - R_\ell)A_n^{(\ell)}\|_2 + \|(I - R_\ell)(A_n - A_n^{(\ell)})\|_2$$
$$\leq \|(I - R_\ell)A_n^{(\ell)}\|_2 + h_\ell.$$

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

$$R_\ell = V_{n,\ell+1}U_{\ell+1}I_{q,\ell+1}U_{\ell+1}^*V_{n,\ell+1}^*, \tag{4.23}$$

where $I_{q,\ell+1} \in \mathbb{R}^{\ell+1,\ell+1}$ is defined in (4.26) below and $q \geq 0$ 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,

$$\left(A_n^{(\ell)}\right)^\dagger = \left(V_{n,\ell+1}H_{\ell+1,\ell}V_{n,\ell}^*\right)^\dagger = V_{n,\ell}H_{\ell+1,\ell}^\dagger V_{n,\ell+1}^*. \tag{4.24}$$

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

$$H_{\ell+1,\ell}^\dagger = W_\ell \Sigma_{\ell+1,\ell}^\dagger U_{\ell+1}^*. \tag{4.25}$$

Now using (4.24) and (4.25), 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 $q \leq \ell$, we have

$$I_{q,\ell+1} := \Sigma_{\ell+1,\ell}\Sigma_{\ell+1,\ell}^\dagger = \begin{pmatrix} I_q & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{R}^{\ell+1,\ell+1} \tag{4.26}$$

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*

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

$$= \left(R_\ell y_n^\delta \right)^* V_{n,\ell+1} U_{\ell+1} \left(\Lambda_{\ell+1} + \alpha I_{\ell+1} \right)^{-3} U_{\ell+1}^* V_{n,\ell+1}^* R_\ell y_n^\delta \tag{4.27}$$

$$= \left(y_n^\delta \right)^* V_{n,\ell+1} U_{\ell+1} I_{q,\ell+1} \left(\Lambda_{\ell+1} + \alpha I_{\ell+1} \right)^{-3} I_{q,\ell+1} U_{\ell+1}^* V_{n,\ell+1}^* y_n^\delta, \tag{4.28}$$

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 (4.27). 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

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

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

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

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

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

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,

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

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This shows (4.27). Equation (4.28) now follows by substituting (4.23) into (4.27). □

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 (4.27) easily can be evaluated.

COROLLARY 4.9. *Let the conditions in Section 2 hold and choose n according to (2.8). Assume that $1 \leq \ell \leq n$ is large enough so that (4.14) has a solution, which we denote by $\hat{\alpha}$. Consider the regularized solution $x^{\delta}_{\hat{\alpha},n,\ell}$, defined by (4.4) with $\alpha = \hat{\alpha}$, an element in $\mathcal{X}_n$. Assume that the conditions of Corollary 4.6 hold. Then*

$$\|\hat{x} - x^{\delta}_{\hat{\alpha},n,\ell}\|_{\mathcal{X}} \leq C'\|\hat{x}\|^{l/(k+l)}_{\mathcal{H}^k}\delta^{k/(k+l)} + \mathcal{O}(\delta^{2/3}) \quad as \quad \delta \searrow 0 \tag{4.29}$$

for a suitable constant $C' > 0$ with the parameter l the same as in (2.6).

Proof. Let $x_n \in \mathcal{X}_n$ be the minimal-norm solution (2.2) of (2.1) with n chosen according to (2.8). Then we obtain by the triangle inequality and (2.9) that

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

Now considering x_n and $x^{\delta}_{\hat{\alpha},n,\ell}$ elements in $\mathbb{R}^n$, we obtain from (2.5) that

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

The inequality (4.29) 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 [11] and Neubauer [13], 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.

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	$1.67 \cdot 10^{-1}$	$3.23 \cdot 10^{-4}$

TABLE 5.1

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	$1.14 \cdot 10^{-1}$	4.44	$2.13 \cdot 10^{-1}$	$4.20 \cdot 10^{-4}$
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 5.2

Example 5.1: The phillips *test problem. The noise level (5.3) is 0.1%.*

Example 5.1. Consider the Fredholm integral equation of the first kind discussed by Phillips [16],

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

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

$$x(t) = \begin{cases} 1 + \cos\left(\frac{\pi t}{3}\right), & |t| < 3, \\ 0, & |t| \geq 3, \end{cases} \tag{5.2}$$

$$\kappa(s,t) = x(s-t),$$

$$y(s) = (6 - |s|)\left(1 + \frac{1}{2}\cos\left(\frac{\pi s}{3}\right)\right) + \frac{9}{2\pi}\sin\left(\frac{\pi|s|}{3}\right).$$

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. A related 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 zero mean, that models "noise," to y_n. The noise vector e_n is scaled to correspond to a prescribed

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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 5.1 displays the approximation error

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

cf. (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 5.1 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 5.1.

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 5.1 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 5.1 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 5.1 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 5.2, which shows results for noise level 0.1%. The α-values of Table 5.2 are smaller than of Table 5.1, as can be expected. Moreover, the relative errors $\|x_{\alpha,n,\ell}^\delta - x_n\|_2 / \|x_n\|$ reported in Table 5.2 are smaller than the corresponding errors of Table 5.1.

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 5.3 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 5.1. 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. $\square$

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 [7]. 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

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 5.3

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

n	ℓ	h_ℓ	α	$\frac{\|x_{\alpha,n,\ell}^\delta - x_n\|_2}{\|x_n\|_2}$	$\frac{\|x_{\alpha,n,\ell}^\delta - x_{\alpha,n}^\delta\|_2}{\|x_n\|_2}$
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 5.4

Example 5.2: The phillips *test problem. The noise level* (5.3) *is 1%.*

the exact solution (5.2). Since the matrix A_n is symmetric, the Arnoldi process (Algorithm (1)) simplifies to the Lanczos process. Table 5.4 is analogous to Table 5.1 and shows results for the noise level (5.3) 1%. Results for noise level 0.1% are displayed in Table 5.5, which is analogous to Table 5.2. Due to the diffent scaling of matrices and right-hand side 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 computed approximation $x_{\alpha,n,\ell}^\delta$ for $n = 2000$, $\ell = 30$, and $\nu = 1 \cdot 10^{-2}$, are shown in Figure 5.1. $\square$

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

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

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 [7] and gives a nonsymmetric matrix $A_n \in \mathbb{R}^{n,n}$ and

n	ℓ	h_ℓ	α	$\dfrac{\|x^\delta_{\alpha,n,\ell}-x_n\|_2}{\|x_n\|_2}$	$\dfrac{\|x^\delta_{\alpha,n,\ell}-x^\delta_{\alpha,n}\|_2}{\|x_n\|_2}$
1000	20	$1.76\cdot10^{-2}$	$8.73\cdot10^{-1}$	$8.02\cdot10^{-2}$	$2.16\cdot10^{-14}$
1000	30	$5.40\cdot10^{-3}$	$3.55\cdot10^{-1}$	$4.73\cdot10^{-2}$	$5.05\cdot10^{-14}$
1000	40	$2.40\cdot10^{-3}$	$2.21\cdot10^{-1}$	$3.66\cdot10^{-2}$	$8.52\cdot10^{-14}$
2000	20	$1.75\cdot10^{-2}$	$8.71\cdot10^{-1}$	$8.01\cdot10^{-2}$	$2.91\cdot10^{-14}$
2000	30	$5.39\cdot10^{-3}$	$3.55\cdot10^{-1}$	$4.73\cdot10^{-2}$	$6.63\cdot10^{-14}$
2000	40	$2.22\cdot10^{-3}$	$2.14\cdot10^{-1}$	$3.60\cdot10^{-2}$	$1.09\cdot10^{-13}$
4000	20	$1.76\cdot10^{-2}$	$8.73\cdot10^{-1}$	$8.03\cdot10^{-2}$	$4.45\cdot10^{-14}$
4000	30	$5.78\cdot10^{-3}$	$3.73\cdot10^{-1}$	$4.86\cdot10^{-2}$	$9.99\cdot10^{-14}$
4000	40	$2.57\cdot10^{-3}$	$2.31\cdot10^{-1}$	$3.74\cdot10^{-2}$	$1.63\cdot10^{-13}$

TABLE 5.5

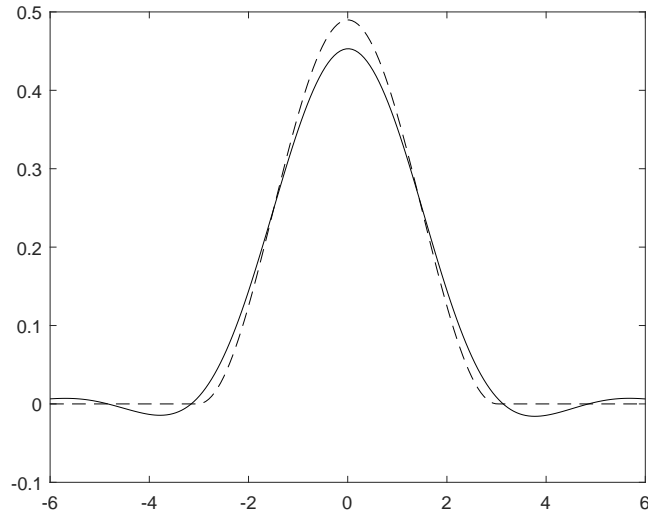*Example 5.2: The* phillips *test problem. The noise level* (5.3) *is 0.1%.*

FIG. 5.1. *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* $\nu=1\%$.

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 $y_n^\delta \in \mathbb{R}^n$, 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 5.6. 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 5.6 is 3.23 and the smallest one for all matrices is about $1\cdot10^{-13}$.

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	$3.16 \cdot 10^{-4}$	$1 \cdot 10^{-3}$	$2.00 \cdot 10^{-3}$	$1.86 \cdot 10^{-1}$	$4.36 \cdot 10^{-4}$

TABLE 5.6

Example 5.3: The baart *test problem for $\ell = 10$, three sizes n, and two noise levels ν.*

We remark that since the singular values of A decrease expoeontially with their index number, the condition (2.6) 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. $\square$

6. Conclusion. 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 example illustrate the theory.

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