VECTOR EXTRAPOLATION ENHANCED TSVD FOR LINEAR DISCRETE ILL-POSED PROBLEMS

K. JBILOU*, L. REICHEL†, AND H. SADOK‡

In memory of Gene H. Golub

Abstract. The truncated singular value decomposition (TSVD) is a popular solution method for small to moderately sized linear ill-posed problems. The truncation index can be thought of as a regularization parameter; its value affects the quality of the computed approximate solution. The choice of a suitable value of the truncation index generally is important, but can be difficult without auxiliary information about the problem being solved. This paper describes how vector extrapolation methods can be combined with TSVD, and illustrates that the determination of the proper value of the truncation index is less critical for the combined extrapolation-TSVD method than for TSVD alone. The numerical performance of the combined method suggests a new way to determine the truncation index.

Key words. ill-posed problem, truncated singular value decomposition, vector extrapolation, truncation criterion.

1. Introduction. Gene Golub has made numerous significant contributions to scientific computing. His interests included the SVD and vector extrapolation; see, e.g., [10, 11]. This paper discusses the application of these methods to the solution of linear discrete ill-posed problems.

The use of scalar extrapolation methods in the context of ill-posed problems was pioneered by Brezinski et al. [5]; see also [6] for a recent discussion. We believe the application of vector extrapolation methods to the solution of linear discrete ill-posed problems to be new. For an excellent overview of extrapolation methods; see Brezinski and Redivo Zaglia [4].

We consider the computation of an approximate solution of the system of equations

$$Ax = b \tag{1.1}$$

with a matrix $A \in \mathbb{R}^{m\times n}$ of ill-determined rank, i.e., A has many singular values of different orders of magnitude close to zero. In particular, A is severely ill-conditioned and possibly singular. We describe the method for the situation when $m \geq n$; however, the method also is applicable when $m < n$.

Systems of equations (1.1) with a matrix of ill-determined rank often are referred to as linear discrete ill-posed problems. They arise in science and engineering when one seeks to determine the cause of an observed effect. In these applications, the right-hand side $b \in \mathbb{R}^m$ is obtained from measured data and typically is contaminated by a measurement error $e \in \mathbb{R}^m$.

Let $\hat{b} \in \mathbb{R}^m$ denote the unknown error-free vector associated with b, i.e.,

$$b = \hat{b} + e. \tag{1.2}$$

*Laboratoire de Mathématiques Pures et Appliquées, Université du Littoral, Centre Universtaire de la Mi-Voix, Batiment H. Poincarré, 50 Rue F. Buisson, BP 699, 62228 Calais cedex, France. E-mail: `jbilou@lmpa.univ-littoral.fr`.

†Department of Mathematical Sciences, Kent State University, Kent, OH 44242, USA. E-mail: `reichel@math.kent.edu`.

‡Laboratoire de Mathématiques Pures et Appliquées, Université du Littoral, Centre Universtaire de la Mi-Voix, Batiment H. Poincarré, 50 Rue F. Buisson, BP 699, 62228 Calais cedex, France. E-mail: `sadok@lmpa.univ-littoral.fr`.

We are interested in determining an accurate approximation of the solution $\hat{x}$ of minimal Euclidean norm of the unavailable consistent system of equations

$$Ax = \hat{b}$$

with error-free right-hand side. Thus, $\hat{x} = A^\dagger \hat{b}$, where $A^\dagger$ denotes the Moore-Penrose pseudoinverse of A. Note that due to the error e in b and the ill-conditioning of the matrix A, the vector

$$A^\dagger b = A^\dagger(\hat{b} + e) = \hat{x} + A^\dagger e$$

generally does not furnish a meaningful approximation of $\hat{x}$.

A popular method for computing an approximation of $\hat{x}$ is to use the Truncated Singular Value Decomposition (TSVD), which replaces $A^\dagger$ by a low-rank approximation; see, e.g., Golub and Van Loan [12] or Hansen [14] for discussions. A brief review of this method is provided in Section 2. A difficulty when applying TSVD is to determine a suitable rank of the approximation of $A^\dagger$. The rank, which is equal to the truncation index, can be considered a regularization parameter. Our vector extrapolation enhanced TSVD method provides a new approach to choosing this index. Section 3 describes some known vector extrapolation methods, and Section 4 shows how to apply one of them, the reduced rank extrapolation method, together with TSVD, to the solution of linear discrete ill-posed problems. Section 5 presents some numerical examples and Section 6 contains concluding remarks.

2. TSVD. Introduce the singular value decomposition

$$A = \sum_{j=1}^{n} \sigma_j u_j v_j^T, \tag{2.1}$$

with the singular values σ_j ordered so that

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_\ell > \sigma_{\ell+1} = \ldots = \sigma_n = 0. \tag{2.2}$$

Then

$$Av_j = \sigma_j u_j, \qquad A^T u_j = \sigma_j v_j, \qquad 1 \leq j \leq n,$$

and the matrices $U = [u_1, u_2, \ldots, u_n] \in \mathbb{R}^{m\times n}$ and $V = [v_1, v_2, \ldots, v_n] \in \mathbb{R}^{n\times n}$ have orthonormal columns, see, e.g., [12] for details on the singular value decomposition. In problems of interest to us, several of the smallest nonvanishing singular values are tiny.

For any $1 \leq k \leq \ell$, the rank-k approximation A_k of A is defined by

$$A_k = \sum_{j=1}^{k} \sigma_j u_j v_j^T \tag{2.3}$$

and its Moore-Penrose pseudoinverse is

$$A_k^\dagger = \sum_{j=1}^{k} \sigma_j^{-1} v_j u_j^T. \tag{2.4}$$

Consider, for $1 \le k \le \ell$, the least-squares problem

$$\min_{x\in\mathbb{R}^n} \|A_k x - b\|$$

with minimal-norm solution

$$x_k := A_k^\dagger b = \sum_{j=1}^{k} \frac{u_j^T b}{\sigma_j} v_j. \tag{2.5}$$

Here and throughout this paper $\|\cdot\|$ denotes the Euclidean vector norm or the associated induced matrix norm.

We would like to determine an index k, such that x_k defined by (2.5) is an accurate approximation of $\hat{x}$. For future reference, we let $k_{\rm opt} \ge 1$ be the smallest integer, such that

$$\|x_{k_{\rm opt}} - \hat{x}\| = \min_{k\ge 1} \|x_k - \hat{x}\|. \tag{2.6}$$

When an estimate of the norm of the error e in b is available, the discrepancy principle can be used to determine such an index; see, e.g., [14]. We are concerned with the situation when no estimate of the norm of e is known. Several heuristic methods for choosing a suitable index k in this situation have been proposed in the literature, the most popular of which may be the L-curve criterion discussed by Hansen; see, e.g., [14]. This criterion is based on plotting the points $\{\log(\|Ax_k - b\|), \log(\|x_k\|)\}$, for $k = 1, 2, \ldots$. These points typically lie on an L-shaped curve, referred to as "the L-curve," and k is chosen to be the index of the point closest to the "vertex" of this curve. It is the purpose of the present paper to propose new guidelines, suggested by results for vector extrapolated TSVD, for the selection of a suitable value of the index k.

3. Vector extrapolation methods. The convergence of iterates determined by a slowly convergent iterative process often can be accelerated by extrapolation methods. The most popular vector extrapolation methods are minimal polynomial extrapolation (MPE) by Cabay and Jackson [7], reduced rank extrapolation (RRE) by Eddy [8] and Mesina [19], and modified minimal polynomial extrapolation (MMPE) due to Brezinski [3], Pugachev [20], and Sidi et al. [24]. Convergence analyses of these methods can be found in [21, 23, 24, 25] and recursive implementations are described in [3, 9, 17]. When applied to linearly generated vector sequences, the MPE and RRE methods are mathematically equivalent to the FOM and GMRES Krylov subspace methods, respectively, for the iterative solution of linear systems of equations; see [22]. We remark that vector extrapolation methods also can be applied to determine the solution of nonlinear systems of equations; see [15, 16, 18] for details.

Let $\{s_p\}_{p\ge 0}$ be a sequence of vectors in $\mathbb{R}^n$, and define the first and the second forward differences

$$\Delta s_p := s_{p+1} - s_p \quad \text{and} \quad \Delta^2 s_p := \Delta s_{p+1} - \Delta s_p.$$

When applied to the sequence $\{s_p\}_{p\ge 0}$, the MPE, RRE, and MMPE vector extrapolation methods produce approximations $t_p^{(q)}$ of the limit or antilimit of the s_p as $p \to \infty$ of the form

$$t_q^{(p)} := \sum_{j=0}^{q} \gamma_j^{(q)} s_{p+j}, \tag{3.1}$$

where

$$\sum_{j=0}^{q} \gamma_j^{(q)} = 1 \quad \text{and} \quad \sum_{j=0}^{q} \eta_{ij}\gamma_j^{(q)} = 0, \qquad 0 \le i < q, \tag{3.2}$$

with $\eta_{ij} := (y_{i+1}^{(p)}, \Delta s_{p+j})$ and

$$\begin{array}{lcll} y_{i+1}^{(p)} & := & \Delta s_{p+i} & \text{for MPE,} \\ y_{i+1}^{(p)} & := & \Delta^2 s_{p+i} & \text{for RRE,} \\ y_{i+1}^{(p)} & := & y_{i+1} & \text{for MMPE.} \end{array}$$

Here $\{y_1, y_2, \dots, y_q\}$ is a set of linearly independent vectors in $\mathbb{R}^n$. These vectors often are chosen to be the canonical vectors in some order; see e.g., [17].

Introduce the matrices

$$Y_{q,p} := [y_1^{(p)}, y_2^{(p)}, \dots, y_q^{(p)}], \qquad \Delta^i S_{q,p} := [\Delta^i s_p, \Delta^i s_{p+1}, \dots, \Delta^i s_{p+q-1}], \quad i = 1, 2.$$

Using Schur's formula, $t_q^{(p)}$ can be expressed as

$$t_q^{(p)} = s_p - \Delta S_{q,p}(Y_{q,p}^T \Delta^2 S_{q,p})^{-1} Y_{q,p}^T \Delta s_p,$$

where $t_q^{(p)}$ exists and is unique if and only if $\det(Y_{q,p}^T \Delta^2 S_{q,p}) \neq 0$. The $t_q^{(p)}$ can be computed by algorithms described in [9] for several values of p and q.

Let us introduce new approximations of the limit or anti-limit of the s_p,

$$\tilde{t}_q^{(p)} := \sum_{j=0}^{q} \gamma_j^{(q)} s_{p+j+1}. \tag{3.3}$$

Following [18], we define the generalized residual

$$\tilde{r}(t_q^{(p)}) := \tilde{t}_q^{(p)} - t_q^{(p)}, \tag{3.4}$$

which can be expressed as

$$\tilde{r}(t_q^{(p)}) = \Delta s_p - \Delta^2 S_{q,p}(Y_{q,p}^T \Delta^2 S_{q,p})^{-1}\, Y_{q,p}^T \Delta s_p. \tag{3.5}$$

The above formula shows that $\tilde{r}(t_q^{(p)})$ is the orthogonal projection of Δs_p onto

$$\operatorname{span}\{\Delta^2 s_p, \Delta^2 s_{p+1}, \dots, \Delta^2 s_{p+q-1}\}.$$

When the sequence $\{s_p\}_{p \ge 0}$ is generated linearly, i.e., when

$$s_{p+1} = (I - A)\, s_p + b, \qquad p = 0, 1, \dots\ ,$$

the generalized residuals reduce to the classical residuals,

$$\tilde{r}(t_q^{(p)}) = r(t_q^{(p)}) = b - A\, t_q^{(p)}.$$

Henceforth, we focus on the case when p is kept fixed, and set $p = 0$. For notational convenience, we denote the matrices $\Delta^i S_{q,0}$ by $\Delta^i S_q$, $1 \le i \le 2$, and the vectors $y_q^{(0)}$ and $t_q^{(0)}$ by y_q and t_q, respectively.

The system of equations (3.2) can be written as

$$\left\{\begin{array}{l} \gamma_0^{(q)} + \gamma_1^{(q)} + \ldots + \gamma_q^{(q)} = 1, \\ \gamma_0^{(q)}(y_1, \Delta s_0) + \gamma_1^{(q)}(y_1, \Delta s_1) + \ldots + \gamma_q^{(q)}(y_1, \Delta s_q) = 0, \\ \gamma_0^{(q)}(y_2, \Delta s_0) + \gamma_1^{(q)}(y_2, \Delta s_1) + \ldots + \gamma_q^{(q)}(y_2, \Delta s_q) = 0, \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \gamma_0^{(q)}(y_q, \Delta s_0) + \gamma_1^{(q)}(y_q, \Delta s_1) + \ldots + \gamma_q^{(q)}(y_q, \Delta s_q) = 0. \end{array}\right. \tag{3.6}$$

Let $\beta_i^{(q)} = \gamma_i^{(q)}/\gamma_q^{(q)}$ for $0 \le i \le q$. Then

$$\gamma_i^{(q)} = \frac{\beta_i^{(q)}}{\displaystyle\sum_{i=0}^{q} \beta_i^{(q)}} \quad \text{for } \ 0 \le i < q \quad \text{ and } \quad \beta_q^{(q)} = 1. \tag{3.7}$$

With this notation, the linear system of equations (3.6) becomes

$$\left\{\begin{array}{l} \beta_0^{(q)}(y_1, \Delta s_0) + \beta_1^{(q)}(y_1, \Delta s_1) + \ldots + \beta_{q-1}^{(q)}(y_1, \Delta s_{q-1}) = -(y_1, \Delta s_q), \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \beta_0^{(q)}(y_q, \Delta s_0) + \beta_1^{(q)}(y_q, \Delta s_1) + \ldots + \beta_{q-1}^{(q)}(y_q, \Delta s_{q-1}) = -(y_q, \Delta s_q). \end{array}\right. \tag{3.8}$$

This system can be written in the form

$$(Y_q^T \, \Delta S_{q-1}) \, \beta^{(q)} = -Y_q^T \, \Delta s_q, \tag{3.9}$$

where $\beta^{(q)} = [\beta_0^{(q)}, \beta_1^{(q)}, \ldots, \beta_{q-1}^{(q)}]^T$ and $\Delta S_q = [\Delta s_0, \Delta s_1, \ldots, \Delta s_{q-1}]$.

Assume now that $\gamma_0^{(q)}, \gamma_1^{(q)}, \ldots, \gamma_q^{(q)}$ have been calculated and introduce the new variables

$$\alpha_0^{(q)} = 1 - \gamma_0^{(q)}, \quad \alpha_j^{(q)} = \alpha_{j-1}^{(q)} - \gamma_j^{(q)}, \quad 1 \le j < q, \text{ and } \alpha_{q-1}^{(q)} = \gamma_q^{(q)}, \tag{3.10}$$

so that the vector t_q can be expressed as

$$t_q = s_0 + \sum_{j=0}^{q-1} \alpha_j^{(q)} \Delta s_j = s_0 + \, \Delta S_{q-1} \, \alpha^{(q)}, \tag{3.11}$$

where $\alpha^{(q)} = [\alpha_0^{(q)}, \ldots, \alpha_{q-1}^{(q)}]^T$.

In order to determine the $\gamma_i^{(q)}$, we first have to compute the $\beta_i^{(q)}$ by solving the nonsingular linear system of equations (3.9). Using (3.4) and (3.11), the generalized residual $\tilde{r}(t_q)$ can be expressed as

$$\tilde{r}(t_q) = \sum_{i=0}^{q} \gamma_i^{(q)} \, \Delta s_q = \Delta S_q \, \gamma^{(q)}, \tag{3.12}$$

where $\gamma^{(q)} = [\gamma_0^{(q)}, \ldots, \gamma_q^{(q)}]^T$.

4. Application of RRE to TSVD. In the remainder of this paper, we only consider the application of RRE to the sequence of vectors generated by TSVD, because the MPE method gives the same iterates as TSVD, and MMPE is more expensive than RRE for the present application. In the sequel, we set

$$y_i = \Delta^2 s_{i-1} \text{ for } 1 \le i \le m-2,$$

and consider the sequence $\{s_k\}_{k\ge 0}$ generated by TSVD. Thus,

$$s_0 := 0, \qquad s_k := x_k = A_k^\dagger b = \sum_{j=1}^{k} \frac{u_j^T b}{\sigma_j} v_j = \sum_{j=1}^{k} \delta_j v_j, \tag{4.1}$$

where

$$\delta_j := \frac{u_j^T b}{\sigma_j}, \qquad 1 \le j \le k. \tag{4.2}$$

Thus, we have

$$\Delta s_{k-1} = s_k - s_{k-1} = \delta_k v_k, \tag{4.3}$$

We may assume that $\delta_k \neq 0$, because if this is not the case, then we delete the corresponding member from the sequence (4.1) and compute the next one by keeping the same index notation. The matrix $\Delta S_{k-1} = [\Delta s_0, \ldots, \Delta s_{k-1}]$ can be factored according to

$$\Delta S_{k-1} = [\delta_1 v_1, \ldots, \delta_k v_k] = V_k \operatorname{diag}[\delta_1, \ldots, \delta_k], \tag{4.4}$$

where $V_k = [v_1, \ldots, v_k]$. Moreover, since $\Delta^2 s_{k-1} = \delta_{k+1} v_{k+1} - \delta_k v_k$, we deduce that

$$\Delta^2 S_{k-1} = V_{k+1} \begin{bmatrix} -\delta_1 & & & \\ \delta_2 & -\delta_2 & & \\ & \ddots & \ddots & \\ & & \delta_k & -\delta_k \\ & & & \delta_{k+1} \end{bmatrix}. \tag{4.5}$$

Then using (4.4), we get

$$\Delta^2 S_{k-1}^T \Delta S_{k-1} = \begin{bmatrix} -\delta_1 & & & \\ \delta_2 & -\delta_2 & & \\ & \ddots & \ddots & \\ & & \delta_k & -\delta_k \\ & & & \delta_{k+1} \end{bmatrix}^T V_{k+1}^T \, [\delta_1 \, v_1, \ldots, \delta_k \, v_k].$$

On the other hand, since

$$V_{k+1}^T \, [\delta_1 v_1, \ldots, \delta_k v_k] = \begin{bmatrix} \delta_1 & 0 & \ldots & 0 \\ 0 & \delta_2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \ldots & 0 & \delta_k \\ 0 & 0 & \ldots & 0 \end{bmatrix}, \tag{4.6}$$

it follows that

$$\Delta^2 S_{k-1}^T \Delta S_{k-1} = \begin{bmatrix} -\delta_1^2 & \delta_2^2 & & & \\ & -\delta_2^2 & \delta_3^2 & & \\ & & \ddots & \ddots & \\ & & & -\delta_{k-1}^2 & \delta_k^2 \\ & & & & -\delta_k^2 \end{bmatrix}.$$

Consequently, using (4.3) and (4.4), we obtain

$$\Delta^2 S_{k-1}^T \Delta s_k = [0, \ldots, 0, \delta_{k+1}^2]^T,$$

and it follows that the solution of the linear system

$$\Delta^2 S_{k-1}^T \Delta S_{k-1} \beta^{(k)} = -\Delta^2 S_{k-1}^T \Delta s_k \tag{4.7}$$

is given by

$$\beta_i^{(k)} = \frac{\delta_{k+1}^2}{\delta_{i+1}^2}, \qquad 0 \leq i < k.$$

Therefore

$$\sum_{i=0}^{k} \beta_i^{(k)} = 1 + \sum_{i=0}^{k-1} \frac{\delta_{k+1}^2}{\delta_{i+1}^2} = \delta_{k+1}^2 \sum_{i=0}^{k} \frac{1}{\delta_{i+1}^2}.$$

Using (3.7), we obtain

$$\gamma_j^{(k)} = \frac{\frac{1}{\delta_{j+1}^2}}{\displaystyle\sum_{i=0}^{k} \frac{1}{\delta_{i+1}^2}}, \qquad 0 \leq j \leq k. \tag{4.8}$$

We therefore can compute the scalars $\alpha_0^{(k)}, \ldots, \alpha_{k-1}^{(k)}$ in (3.10) by

$$\alpha_i^{(k)} = \sum_{j=i+1}^{k} \gamma_j^{(k)} = \frac{\displaystyle\sum_{j=i+1}^{k} \frac{1}{\delta_{j+1}^2}}{\displaystyle\sum_{l=0}^{k} \frac{1}{\delta_{l+1}^2}}, \qquad 0 \leq i < k. \tag{4.9}$$

Finally, the extrapolated vector t_k can be determined from

$$t_k = \sum_{j=1}^{k} \alpha_{j-1}^{(k)} \frac{u_j^T b}{\sigma_j} v_j. \tag{4.10}$$

Notice that the application of the RRE method acts as a filter for TSVD with filter factors $f_j^{(k)} = \alpha_{j-1}^{(k)}$, $1 \leq j \leq k$.

We need to evaluate $\|t_{k+1} - t_k\|$ for our stopping criterion. From (4.10) we obtain that

$$t_{k+1} - t_k = \sum_{j=1}^{k} \frac{(\alpha_{j-1}^{(k+1)} - \alpha_{j-1}^{(k)})}{\sqrt{\delta_j}} v_j + \frac{\alpha_k^{(k+1)}}{\sqrt{\delta_{k+1}}} v_{k+1}.$$

Since the vectors v_j, $1 \le j \le k+1$, are orthonormal, it follows that

$$\|t_{k+1} - t_k\| = \sqrt{\sum_{j=1}^{k} \frac{|\alpha_{j-1}^{(k+1)} - \alpha_{j-1}^{(k)}|^2}{\delta_j} + \frac{|\alpha_k^{(k+1)}|^2}{\delta_{k+1}}}.$$

The generalized residual can be written as

$$\tilde{r}(t_k) = \Delta S_k \, \gamma^{(k)} = V_{k+1} \operatorname{diag}\left[\frac{u_1^T b}{\sigma_1}, \ldots, \frac{u_{k+1}^T b}{\sigma_{k+1}}\right] \gamma^{(k)}, \qquad (4.11)$$

where $\gamma^{(k)} = [\gamma_0^{(k)}, \gamma_1^{(k)}, \ldots, \gamma_k^{(k)}]^T$ is given by (4.8). It follows from (4.2) that

$$\|\tilde{r}(t_k)\|^2 = \sum_{i=0}^{k} \delta_{i+1}^2 \left(\gamma_i^{(k)}\right)^2,$$

and by using (4.8), we obtain the simple expression

$$\|\tilde{r}(t_k)\| = \frac{1}{\sqrt{\sum_{j=0}^{k} \frac{1}{\delta_{j+1}^2}}}.$$

Moreover, from the relation (4.8) we also have

$$\|\tilde{r}(t_k)\| = \sqrt{\delta_k^2 \gamma_{k-1}^{(k)}}.$$

For well-posed problems, $\|\tilde{r}(t_k)\|$ decreases to zero as k increases. However, for ill-posed problems with an error in the right-hand side, the $\|\tilde{r}(t_k)\|$ decrease when k increases and is sufficiently small, but for larger values of k, the norm $\|\tilde{r}(t_k)\|$ increases with k. As will be illustrated in the following section, the value of the index k for which the $\|\tilde{r}(t_k)\|$ cease to decrease often gives a good approximation x_k of $\hat{x}$. The RRE-TSVD algorithm is summarized as follows:

Algorithm 1. `The RRE-TSVD algorithm`

- `Compute the SVD of the matrix` A: $[U, \Sigma, V] = svd(A)$.
  `Set` $s_0 = 0$, $s_1 = \frac{u_1^T b}{\sigma_1} v_1$, `and` $t_1 = s_1$, `with`
  $u_i = U(:, i)$ `and` $v_i = V(:, i)$ `for` $i = 1, \ldots, n$.
- `For` $k = 2, \ldots, n$
  1. `Compute` s_k `from` *(4.1)*.
  2. `Compute the` $\gamma_i^{(k)}$ `and` $\alpha_i^{(k)}$ `for` $i = 0, \ldots, k-1$, `using` *(4.8)* `and` *(4.9)*.
  3. `Form the approximation` t_k `by` *(4.10)*.
  4. `If` $\|t_k - t_{k-1}\| / \|t_{k-1}\| < tol$, `stop`.
- *End*

5. Numerical examples. All computations are carried out using MATLAB 7.4 with unit round-off $\epsilon \approx 2 \cdot 10^{-16}$. We used the MATLAB Regularization Tools package [13]. The matrices A and the desired solutions $\hat{x}$ are determined by codes of this package; the assumed unknown error-free right-hand side is given by $\hat{b} := A\hat{x}$. The associated "noisy" right-hand side b is determined by (1.2), where the "noise-vector" e has normally distributed components with zero mean, normalized so that a specific noise-level

$$\nu = \frac{\|e\|}{\|\hat{b}\|}$$

is achieved.

Example 5.1. We illustrate the convergence behavior of the sequences $\{t_k\}_{k\geq 1}$ and $\{\|\tilde{r}(t_k)\|\}_{k\geq 1}$ by considering the integral equation

$$\int_0^{\pi/2} \kappa(s,t)x(t)dt = g(s), \qquad 0 \leq s \leq \pi, \tag{5.1}$$

where

$$\kappa(s,t) = \exp(s\,\cos(t)) \;\text{ and }\; g(s) = 2\sin(s)/s.$$

The solution is given by $x(t) = \sin(t)$. This integral equation is discussed in [1]. We used the MATLAB code baart from [13] to discretize (5.1) by a Galerkin method with 600 orthonormal box functions as test and trial functions. This yields the nonsymmetric matrix $A \in \mathbb{R}^{600\times 600}$ with the condition number $\kappa(A) = 4 \cdot 10^{18}$ computed by MATLAB, where $\kappa(A) := \|A\|\,\|A^{-1}\|$. Thus, A is numerically singular. The vectors $\hat{b}$ and b are determined as described above with noise-level $\nu = 1 \cdot 10^{-2}$.

Figure 5.1 shows the convergence of TSVD and RRE-TSVD. Observe from Figure 5.1 that when k increases and is sufficiently small, the relative error norms

$$\|s_k - \hat{x}\|/\|\hat{x}\| \;\text{ and }\; \|t_k - \hat{x}\|/\|\hat{x}\|$$

decrease; here the s_k are determined by TSVD and the t_k by RRE-TSVD. However, when k is larger than $k_{\text{opt}} = 9$, the error in the s_k increases; the norm of the error in the t_k stagnates at $k = k_{\text{opt}}$; cf. (2.6) for the definition of k_{opt}. The generalized residual norm also stagnates at $k = k_{\text{opt}}$. Hence, stagnation of the generalized residual norm is a practical criterion for selecting a suitable truncation index k for both RRE-TSVD and TSVD.

We remark that the L-curve criterion, as implemented by the MATLAB function l_corner from [13], gives the truncation index $k = 6$. This is not a good choice, as can be seen from Figure 5.1. For many linear discrete ill-posed problems, the L-curve criterion determines a value of the truncation index, which is not close to the optimal one. $\square$

Example 5.2. For this experiment, we generate the nonsymmetric matrix $A \in \mathbb{R}^{1000\times 1000}$ and the desired solution $\hat{x} \in \mathbb{R}^{1000}$ with the code wing from [13]; the condition number of A is larger than $1 \cdot 10^{20}$, i.e., the matrix is numerically singular. The right-hand side b is generated similarly as in Example 5.1 with noise-level $\nu = 1 \cdot 10^{-2}$.

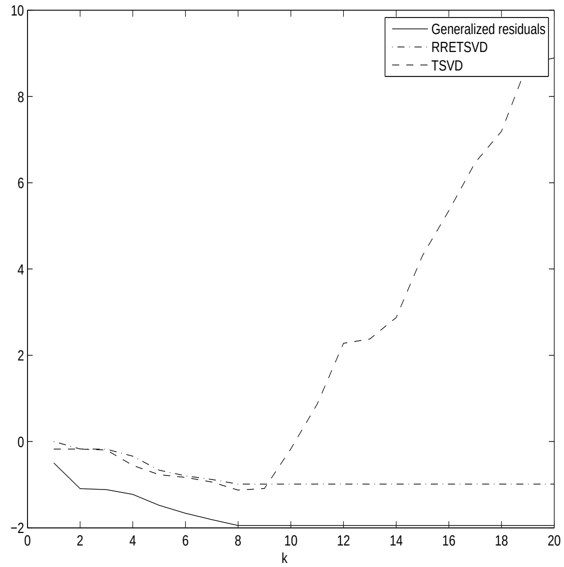

FIG. 5.1. *Example 5.1: The relative errors $\|s_k - \hat{x}\|/\|\hat{x}\|$ for TSVD (dashed graph), the relative errors $\|t_k - \hat{x}\|/\|\hat{x}\|$ for RRE-TSVD (dash-dotted graph), and the norm of the generalized residuals $\|\tilde{r}(t_k)\|$ (solid graph).*

Figure 5.2 compares TSVD and RRE-TSVD. The graphs show the relative error norm versus the truncation index k as well as the norm of the generalized residuals for RRE-TSVD. As can be seen from the figure, the best truncation index is $k_{\rm opt} = 5$ for TSVD. The generalized residual norm $\|\tilde{r}(t_k)\|$ stagnates at $k = 3$. We note that the errors in t_3 and t_5 are about the same. Moreover, t_3 is a good approximation of $\hat{x}$.

The L-curve criterion, as implemented by the function l_corner in [13], determines the truncation index $k = 2$. This is not a good choice. □

Example 5.3. We consider two more examples, *foxgood* and *heat*, from [13]. These linear discrete ill-posed problems are discretized to yield matrices of order 800 and 500, respectively. The desired solutions $\hat{x}$ are provided by the codes *foxgood* and *heat*, and the right-hand sides b are determined similarly as in Example 5.1 with noise level $\nu = 1 \cdot 10^{-2}$.

We detect stagnation of the generalized residuals $\tilde{r}_k$ by computing the quotient $|\|\tilde{r}_{k+1}\| - \|\tilde{r}_k\||/\|\tilde{r}_k\|$ for increasing values of k. Let $\hat{k}$ be the smallest index, such that

$$\frac{|\|\tilde{r}_{\hat{k}+1}\| - \|\tilde{r}_{\hat{k}}\||}{\|\tilde{r}_{\hat{k}}\|} \leq 5 \cdot 10^{-3}. \tag{5.2}$$

We say that stagnation has occurred at $k = \hat{k}$, and use $t_{\hat{k}}$ as approximation of $\hat{x}$. The choice of right-hand side in (5.2) is based on numerical experience; we have found it to give good results for a large number of linear discrete ill-posed problems.

The selection criterion (5.2) formalizes the approach of Examples 5.1 and 5.2. In particular, the use of the criterion (5.2) obviates the need to look at graphs. This criterion is an attractive alternative to other approaches, such as the L-curve criterion, that are used when no information about the norm of the error e in b is available.

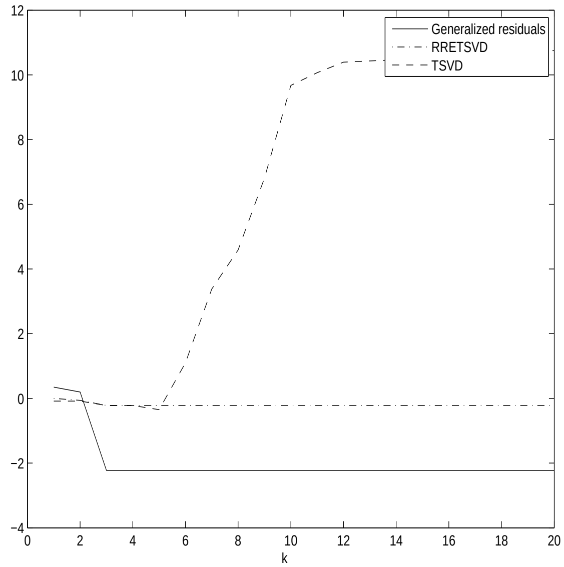

Fig. 5.2. *Example 5.2: The relative errors* $\|s_k - \hat{x}\|/\|\hat{x}\|$ *for TSVD (dashed graph), the relative errors* $\|t_k - \hat{x}\|/\|\hat{x}\|$ *for RRE-TSVD (dash-dotted graph), and the norm of the generalized residuals* $\|\tilde{r}(t_k)\|$ *(solid graph).*

Nevertheless, being a heuristically motivated criterion, which does not explicitly use $\|e\|$, it may fail; see [2] for a discussion. Tables 5.1 and 5.2 show results for *foxgood* and *heat*, respectively.

Table 5.1
foxgood with noise-level $\nu = 1 \cdot 10^{-2}$.

k	$\|t_k - \hat{x}\|/\|\hat{x}\|$	$\|s_k - \hat{x}\|/\|\hat{x}\|$	$\|\|\tilde{r}_{k+1}\| - \|\tilde{r}_k\|\|/\|\tilde{r}_k\|$
4	$4.11 \cdot 10^{-2}$	$6.97 \cdot 10^{-2}$	$1.37 \cdot 10^{-3}$
5	$4.11 \cdot 10^{-2}$	$9.13 \cdot 10^{-2}$	$3.08 \cdot 10^{-4}$

Table 5.1 shows (5.2) to be satisfied for $k = 4$. This is the smallest value of k for which (5.2) holds. Thus, $\hat{k} = 4$ and we use t_4 as an approximation of $\hat{x}$. The error in the approximate solutions s_k determined by TSVD increases with k for $k \geq 4$, while the error in the approximate solutions t_k computed by RRE-TSVD does not change much when k increasae and $k \geq 4$.

Table 5.2
heat with noise-level $\nu = 1 \cdot 10^{-2}$.

k	$\|t_k - \hat{x}\|/\|\hat{x}\|$	$\|s_k - \hat{x}\|/\|\hat{x}\|$	$\|\|\tilde{r}_{k+1}\| - \|\tilde{r}_k\|\|/\|\tilde{r}_k\|$
27	$7.11 \cdot 10^{-2}$	$8.34 \cdot 10^{-2}$	$2.57 \cdot 10^{-3}$
28	$7.11 \cdot 10^{-2}$	$9.68 \cdot 10^{-2}$	$5.18 \cdot 10^{-4}$

Table 5.2 shows (5.2) to be satisfied for $k = 27$ and, indeed, $\hat{k} = 27$. Thus, we use t_{27} as an approximation of $\hat{x}$. Note that the error in t_{28} is about the same as in t_{27}, but the error in s_{28} is larger than the error in s_{27}. Moreover, the error in t_{27} is smaller than the error in s_{27}. $\square$

6. Conclusion. This paper describes how vector extrapolation can be applied together with TSVD. The stagnation point for the generalized residual determined by the extrapolation method typically is a suitable truncation index. The approximate solutions computed by extrapolation generally do not deteriorate in quality when the truncation index is increased. The choice of truncation index therefore is less critical than for TSVD.

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