INVERSE SUBSPACE PROBLEMS WITH APPLICATIONS*

SILVIA NOSCHESE† AND LOTHAR REICHEL‡

Abstract. Given a square matrix A, the inverse subspace problem is concerned with determining a closest matrix to A with a prescribed invariant subspace. When A is Hermitian, the closest matrix may be required to be Hermitian. We measure distance in the Frobenius norm and discuss applications to Krylov subspace methods for the solution of large-scale linear systems of equations and eigenvalue problems as well as to the construction of blurring matrices. Extensions that allow the matrix A to be rectangular and applications to Lanczos bidiagonalization, as well as to the recently proposed subspace-restricted singular value decomposition method for the solution of linear discrete ill-posed problems, also are considered.

Key words. matrix nearness problem, Lanczos method, Arnoldi method, modified singular value decomposition, Lanczos bidiagonalization, ill-posed problem, blurring matrix.

1. Introduction. We investigate properties of several iterative and direct solution methods for linear systems of equations, eigenvalue problems, and linear discrete ill-posed problems by considering how they relate to inverse subspace problems. Given a matrix $A \in \mathbb{C}^{n\times n}$, the inverse subspace problem is concerned with determining a closest matrix with a prescribed invariant subspace $\mathcal{V} \subseteq \mathbb{C}^n$ of dimension $p \leq n$. We will measure the size of matrices $A \in \mathbb{C}^{m\times n}$ with the Frobenius norm

$$\|A\|_F := \sqrt{\langle A, A\rangle},$$

where the inner product is defined by

$$\langle A, B\rangle := \mathrm{Trace}(B^H A), \qquad A, B \in \mathbb{C}^{m\times n},$$

with the superscript ^{H} denoting transposition and complex conjugation.

Thus, we are interested in solving

$$\rho(A, \mathcal{V}) := \min_{M\in\mathbb{C}^{n\times n}} \{\|M - A\|_F \, : \, M\mathcal{V} \subseteq \mathcal{V}\}. \tag{1.1}$$

The quantity $\rho(A, \mathcal{V})$ is the backward error of $\mathcal{V}$ when this space is considered an approximate invariant subspace of the matrix A. In particular, when $\dim(\mathcal{V}) = 1$, the solution of (1.1) is the closest matrix M to A with a prescribed eigenvector. The problem (1.1) as well as the other inverse subspace problems considered in this paper have been discussed by Sun [15] who provided proofs for unitarily invariant matrix norms. Our focus on the Frobenius norm allows us to present much simpler proofs. Bounds in terms of the Frobenius norm are interesting in applications, because this norm is easy to compute.

Let $\mathcal{M} \subset \mathbb{C}^{n\times n}$ denote a subspace of matrices with a desired structure. Then the structured inverse subspace problem is to determine a solution to the minimization problem

$$\rho_{\mathcal{M}}(A, \mathcal{V}) := \min_{M\in\mathcal{M}} \{\|M - A\|_F \, : \, M\mathcal{V} \subseteq \mathcal{V}\}. \tag{1.2}$$

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†Dipartimento di Matematica "Guido Castelnuovo", SAPIENZA Università di Roma, P.le A. Moro, 2, I-00185 Roma, Italy. E-mail: noschese@mat.uniroma1.it. Research supported by a grant from SAPIENZA Università di Roma.

‡Department of Mathematical Sciences, Kent State University, Kent, OH 44242, USA. E-mail: reichel@math.kent.edu. Research supported in part by NSF grant DMS-1115385.

Here $\rho_{\mathcal{M}}(A,\mathcal{V})$ is the structured backward error of $\mathcal{V}$. We will let $\mathcal{M}$ be the set of Hermitian matrices.

We apply the inverse subspace problems (1.1) and (1.2) to the Arnoldi and Lanczos methods, respectively. These are popular Krylov subspace methods for the solution of large-scale linear systems of equations and for the computation of a few desired eigenvalues and associated eigenvectors of a large sparse symmetric or nonsymmetric matrix; see, e.g., Saad [13, 14] for discussions of these methods. Both the Arnoldi and Lanczos methods determine low-rank approximations of a large matrix A. These low-rank matrices have a Krylov subspace as an invariant subspace. We are interested in whether there are matrices much closer to A with the same invariant subspace, and if so, how they can be constructed. Moreover, we describe an application to the construction of blurring matrices. These matrices model atmospheric, motion, or other blur and are used in image deblurring methods. The standard construction of blurring matrices yields boundary artifacts. These artifacts can be suppressed by requiring that the blurring matrix satisfies (1.1) or (1.2) for a suitable subspace $\mathcal{V}$.

We also are concerned with the inverse singular subspace problem for matrices $A \in \mathbb{C}^{m\times n}$ that may be rectangular. Let $\mathcal{U} \subseteq \mathbb{C}^m$ and $\mathcal{V} \subseteq \mathbb{C}^n$ be linear spaces of dimension $p \leq \min\{m,n\}$ and consider the matrix nearness problem

$$\rho(A,\mathcal{U},\mathcal{V}) := \min_{M\in\mathbb{C}^{m\times n}} \{\|M-A\|_F \,:\, M\mathcal{V}\subseteq\mathcal{U},\ M^H\mathcal{U}\subseteq\mathcal{V}\}. \tag{1.3}$$

We refer to the linear spaces $\mathcal{U}$ and $\mathcal{V}$ as left and right singular subspaces of the matrix M. This problem sheds light on the performance of the Lanczos bidiagonalization method for computing a low-rank approximation of A. Partial Lanczos bidiagonalization is commonly applied to determine approximations of a few singular values and associated singular vectors of a large matrix (see, e.g., [1, 2, 8, 11]) or to compute an approximate solution of a large least-squares problem; see Björck [3]. We are interested in how close the low-rank approximation of A determined by a few steps of the Lanczos bidiagonalization method is to the closest matrix to A with the same right and left singular Krylov subspaces, and how this closest matrix can be constructed.

The minimization problem (1.3) also is applied to investigate an available solution method, and to derive a new one, for discrete ill-posed problems of the form

$$\min_{x\in\mathbb{C}^n} \|Ax-b\| \tag{1.4}$$

with a very ill-conditioned, possibly singular, matrix $A \in \mathbb{C}^{m\times n}$. Here $\|\cdot\|$ denotes the Euclidean vector norm. This kind of problems arise when one would like to determine the cause of an observed effect, such as in inverse problems; see Engl et al. [4] and Hansen [5] for discussions. In these applications, the vector $b \in \mathbb{C}^m$ represents available data and typically is contaminated by an error stemming from measurement inaccuracies. Straightforward solution of (1.4) generally gives useless results due to a large propagated error in the computed solution. The severe error propagation is caused by the error in b and the ill-conditioning of A. Round-off errors introduced during the solution process also may contribute to the error in the computed solution. A popular approach to reduce the error propagation for small to medium-sized problems is to compute the singular value decomposition (SVD) of A, and approximate A by a matrix A_k of (low) rank k obtained by setting all but the largest k singular values of A to zero. The solution x_k of minimal Euclidean norm of the least-squares problem obtained when replacing A by A_k in (1.4) is then used as an approximate solution of (1.4). This approach to determine an approximate solution of (1.4) is known as the truncated SVD (TSVD) method. The rank k is a parameter, which determines how much the matrix A is modified before solution. The choice of k is important for the quality of the computed approximate solution of (1.4). A too large value of k gives an unnecessarily large propagated error in x_k, while a too small value may result in a computed approximate solution x_k of poor quality, because A_k is a poor approximation of A. We refer to Engl et al. [4] and Hansen [5] for discussions on many solution methods for linear discrete ill-posed problems, including the TSVD method.

There are situations when no choice of the regularization parameter k gives a satisfactory approximate solution of (1.4), because the subspaces of right singular vectors of A associated with the k largest singular values are not well suited to represent the desired solution for any value of k small enough to avoid severe propagation of the error in b. The subspace-restricted SVD (SRSVD) method described in [10] is designed to remedy this situation. This method allows a user to choose vectors to be in the solution subspace and, thereby, makes it possible to include vectors that represent known important features of the desired solution. For instance, it may be known that the solution is a smooth almost linearly increasing function. Then it can be beneficial to include vectors that can represent a linear function in the solution subspace. The matrix nearness problem (1.3) sheds light on the SRSVD method. Our analysis suggests a modification of this method.

This paper is organized as follows. In Section 2, we discuss inverse subspace problems for general square matrices as well as for Hermitian matrices, and describe applications to the decompositions determined by the Arnoldi and Lanczos methods, as well as to the construction of blurring matrices. The inverse singular subspace problem for a rectangular matrix is discussed in Section 3, where we also consider applications to the decompositions computed by the Lanczos bidiagonalization method. Section 4 applies the inverse singular subspace problem to the SRSVD method for the solution of linear discrete ill-posed problems, and Section 5 presents a few computed examples. Concluding remarks can be found in Section 6.

Throughout this paper I_p denotes the identity matrix of order p, and $I_{p,q}$ is the leading principal $p \times q$ submatrix of $I_{\max\{p,q\}}$. The vector e_j denotes the jth axis vector of appropriate dimension and $\mathcal{R}(M)$ stands for the range of the matrix M.

2. Matrices with specified invariant subspace. This section discusses the inverse subspace problems (1.1) and (1.2), and describes applications to the Arnoldi and Lanczos methods. Let $A \in \mathbb{C}^{n\times n}$ and let $p \leq n$ be the dimension of the invariant subspace spanned by the orthonormal columns of the matrix $V \in \mathbb{C}^{n\times p}$. The following proposition shows that

$$M := (I_n - VV^H)A(I_n - VV^H) + VV^H A \tag{2.1}$$

is the orthogonal projection of A onto the subspace $\mathcal{B}$ of matrices B with invariant subspace $\mathcal{V}$, i.e., $B\mathcal{V} \subseteq \mathcal{V}$. In particular, M is the closest matrix to A in $\mathcal{B}$, i.e., M solves (1.1).

PROPOSITION 2.1. *Consider the matrix $M \in \mathbb{C}^{n\times n}$ defined by (2.1). The following properties hold:*

1. *$M \in \mathcal{B}$;*
2. *if $A \in \mathcal{B}$, then $M \equiv A$;*
3. *if $B \in \mathcal{B}$, then $\langle A - M, B\rangle = 0$.*

Proof. We have $MV = V \cdot V^H AV$, which shows the first property. The second property implies that there is a matrix $S \in \mathbb{C}^{p\times p}$ such that $AV = VS$, from which it follows that

$$M = A - AVV^H + VV^H AVV^H = A,$$

because

$$VV^H AVV^H = VV^H VSV^H = VSV^H = AVV^H,$$

where we have used the fact that $V^H V = I_p$. Finally, since for any $B \in \mathcal{B}$, there is a matrix $D \in \mathbb{C}^{p\times p}$ such that $BV = VD$, we obtain

$$\begin{aligned} &\mathrm{Trace}(AVV^H B^H - VV^H AVV^H B^H) \\ &= \mathrm{Trace}(AVD^H V^H - VV^H AVD^H V^H) \\ &= \mathrm{Trace}(AVD^H V^H) - \mathrm{Trace}(AVD^H V^H VV^H) = 0, \end{aligned}$$

where the last equality follows from the cyclic property of the trace and by $V^H V = I_p$. ∎

The backward error (1.1) satisfies

$$\rho(A, \mathcal{V}) = \sqrt{\mathrm{Trace}(V^H A^H (I_n - VV^H)AV)}. \tag{2.2}$$

This can be seen by observing that for the matrix (2.1), it holds

$$\mathrm{Trace}((A - M)^H (A - M)) = \mathrm{Trace}(VV^H A^H AVV^H - VV^H A^H VV^H AVV^H),$$

and by applying the cyclic property of the trace, we obtain

$$\mathrm{Trace}(VV^H A^H (I_n - VV^H)AVV^H) = \mathrm{Trace}(V^H A^H (I_n - VV^H)AV).$$

Sun [15, Theorem 2.1] showed that the matrix (2.1) solves (1.1) in any unitarily invariant norm as well as (2.2). Our proof using the Frobenius norm is much simpler.

We turn to the structured inverse subspace problem (1.2). Let $A \in \mathbb{C}^{n\times n}$ be Hermitian and let the matrix V and subspace $\mathcal{V}$ be defined as above. The following proposition shows that the matrix

$$M = (I_n - VV^H)A(I_n - VV^H) + VV^H AVV^H \tag{2.3}$$

is the orthogonal projection of A onto the subspace $\mathcal{B}$ of the Hermitian matrices B with invariant subspace $\mathcal{V}$. It follows that the matrix (2.3) solves (1.2).

PROPOSITION 2.2. *Let the matrix $M \in \mathbb{C}^{n\times n}$ be defined by (2.3). The following properties hold:*

1. *$M \in \mathcal{B}$;*
2. *if $A \in \mathcal{B}$, then $M \equiv A$;*
3. *if $B \in \mathcal{B}$, then $\langle A - M, B\rangle = 0$.*

Proof. The matrix (2.3) is Hermitian. The first property therefore follows from $MV = V \cdot V^H AV$. To show the second property, we first note that there is a Hermitian matrix $S \in \mathbb{C}^{p\times p}$ such that $AV = VS$. Using the relations

$$AVV^H = VV^H A = VSV^H, \qquad VV^H AVV^H = VV^H VSV^H = VSV^H,$$

we obtain

$$M = A - AVV^H - VV^H A + 2VV^H AVV^H = A.$$

The third property can be shown by first noting that

$$\operatorname{Trace}((A-M)B) = \operatorname{Trace}(AVV^HB + VV^HAB) - 2\operatorname{Trace}(VV^HAVV^HB).$$

By assumption there is a Hermitian matrix $D \in \mathbb{C}^{p\times p}$ depending on B such that $BV = VD$ and $V^HB = DV^H$. Therefore,

$$\begin{aligned}
\operatorname{Trace}(AVV^HB + VV^HAB) &= \operatorname{Trace}(AVDV^H) + \operatorname{Trace}(AVDV^H),\\
\operatorname{Trace}(VV^HAVV^HB) &= \operatorname{Trace}(VV^HAVDV^H) = \operatorname{Trace}(AVDV^H),
\end{aligned}$$

where we have used the cyclic property of the trace. The desired result now follows. $\square$

One can show similarly as (2.2) that the quantity (1.2) satisfies

$$\rho_{\mathcal{M}}(A,\mathcal{V}) = \sqrt{2\operatorname{Trace}(V^HA(I_n - VV^H)AV)}. \tag{2.4}$$

Let the matrix A be Hermitian, let $\widetilde{M}$ denote the matrix in (2.1), and let $\widehat{M}$ be its orthogonal projection onto the subspace of the Hermitian matrices, i.e., $\widehat{M} = (\widetilde{M} + \widetilde{M}^H)/2$. Let M be defined by (2.3). It follows from (2.2) and (2.4) that

$$\|A - M\|_F = \sqrt{2}\|A - \widetilde{M}\|_F. \tag{2.5}$$

Moreover, direct computations show that

$$\begin{aligned}
\widetilde{M} - A &= (M - \widetilde{M})^H,\\
A - M &= 2(A - \widehat{M}).
\end{aligned} \tag{2.6}$$

The reason for the relations (2.5) and (2.6) is that $A - \widetilde{M}$ and $M - \widetilde{M}$ are legs and $A - M$ is the hypotenuse of the isosceles right triangle with vertices A, $\widetilde{M}$, and M. The relation (2.5) stems from the fact that the length of the hypotenuse is $\sqrt{2}$ times the length of a leg.

We finally consider the determination of the closest matrix $B \in \mathbb{C}^{n\times n}$ to A whose eigenvectors are the columns of a given unitary matrix $V \in \mathbb{C}^{n\times n}$. Then $B = V\Lambda V^H$ for a diagonal matrix Λ. Minimizing $\|A-B\|_F$ is equivalent to minimizing $\|V^HAV - \Lambda\|_F$. The minimum is achieved when Λ is the diagonal part of V^HAV. Therefore, the matrix that minimizes $\|A-B\|_F$ is given by

$$M = V\operatorname{diag}(V^HAV)V^H.$$

Notice that M reduces to A if the columns of V are eigenvectors of A.

The inverse subspace problems (1.1) and (1.2) provide insight into the decompositions determined by the Arnoldi and Lanczos methods. We first consider the former. The Arnoldi method when applied to a matrix $A \in \mathbb{C}^{n\times n}$ with initial unit vector $v_1 \in \mathbb{C}^n$ generically yields after $p \ll n$ steps the Arnoldi decomposition

$$AV_p = V_{p+1}H_{p+1,p}, \tag{2.7}$$

where the matrix $V_{p+1} = [v_1, v_2, \ldots, v_{p+1}] \in \mathbb{C}^{n\times(p+1)}$ has orthonormal columns that span the Krylov subspace

$$\mathcal{K}_{p+1}(A, v_1) = \operatorname{span}\{v_1, Av_1, \ldots, A^pv_1\},$$

the matrix $H_{p+1,p} = [h_{j,k}] \in \mathbb{C}^{(p+1)\times p}$ is of upper Hessenberg form, and $V_p \in \mathbb{R}^{n\times p}$ consists of the first p columns of V_{p+1}; see, e.g., Saad [13] for details. When the last subdiagonal entry, $h_{p+1,p}$, of $H_{p+1,p}$ vanishes, the decomposition (2.7) becomes

$$AV_p = V_p H_p,$$

where H_p denotes the leading $p \times p$ submatrix of $H_{p+1,p}$. Then $\mathcal{R}(V_p) = \mathcal{K}_p(A, v_1)$ is an invariant subspace of A. This situation is rare. Generically, $h_{p+1,p} \neq 0$ and the solution (2.1) of the inverse subspace problem (1.1) helps us determine the distance of A to the closest matrix with invariant subspace $\mathcal{R}(V_p) = \mathcal{K}_p(A, v_1)$.

PROPOSITION 2.3. *The distance in the Frobenius norm between a given matrix $A \in \mathbb{C}^{n\times n}$ and its orthogonal projection onto the subspace of the matrices having the invariant subspace $\mathcal{R}(V_p)$, i.e., the distance between A and the matrix M defined by (2.1) with $V = V_p$, is given by*

$$\|A - M\|_F = |h_{p+1,p}|, \tag{2.8}$$

where $h_{p+1,p}$ is the last subdiagonal entry of the matrix $H_{p+1,p}$ determined by (2.7).

Proof. The results follows by substituting (2.7) into the the right-hand side of (2.2). In detail, one has

$$\begin{aligned}
&\mathrm{Trace}(V^H A^H (I_n - VV^H)AV)) \\
&= \mathrm{Trace}(H_{p+1,p}^H H_{p+1,p} - H_{p+1,p}^H I_{p+1,p} I_{p,p+1} H_{p+1,p}) \\
&= \mathrm{Trace}(H_{p+1,p}^H H_{p+1,p}) - \mathrm{Trace}(H_p^H H_p) \\
&= \|H_{p+1,p}\|_F^2 - \|H_p\|_F^2 = |h_{p+1,p}|^2.
\end{aligned}$$

□

We next show that the closest matrix M to A in Proposition 2.3 generally is not the matrix

$$A_p = V_p H_p V_p^H \tag{2.9}$$

of rank at most p determined by p steps of the Arnoldi method.

PROPOSITION 2.4. *Let the matrices V_p and H_p be determined by p steps of the Arnoldi method with initial vector v_1, cf. (2.7), and let A_p be defined by (2.9). Then*

$$\|A - A_p\|_F = \sqrt{\|A\|_F^2 - \|H_p\|_F^2}. \tag{2.10}$$

Proof. We have that

$$\|A - V_p H_p V_p^H\|_F^2 = \|A\|_F^2 - 2\,\mathrm{Trace}(V_p^H A^H V_p H_p) + \|H_p\|_F^2$$

and

$$\mathrm{Trace}(V_p^H A^H V_p H_p) = \mathrm{Trace}(H_{p+1,p}^H V_{p+1}^H V_p H_p) = \|H_p\|_F^2,$$

where the matrices V_{p+1} and $H_{p+1,p}$ are defined by (2.7). The relation (2.10) follows. □

Thus, Proposition 2.3 gives the lower bound $|h_{p+1,p}|$ for the distance (2.10), which may be much larger than the lower bound. This is illustrated in Section 5.

When computing an approximation of an invariant subspace associated with the, say, p largest eigenvalues of a large matrix $A \in \mathbb{C}^{n\times n}$ by the Arnoldi or restarted Arnoldi methods, one seeks to determine a decomposition (2.7) such that the entry $h_{p+1,p}$ of the matrix $H_{p+1,p}$ is of small magnitude. Proposition 2.3 shows that then there is a matrix $M \in \mathbb{C}^{n\times n}$ of distance $|h_{p+1,p}|$ from A with the invariant subspace $\mathcal{R}(V_p)$. However, by (2.10) the orthogonal projection A_p of A onto $\mathcal{R}(V_p)$ determined by the Arnoldi or restarted Arnoldi methods may be much further from A than $|h_{p+1,p}|$. A reason for this is that A_p is of rank at most p, while the matrix M may be of much larger rank.

We turn to the situation when the matrix A is Hermitian. Then the Arnoldi method simplifies to the Lanczos method, and the Arnoldi decomposition (2.7) becomes the Lanczos decomposition

$$AV_p = V_{p+1}T_{p+1,p}. \tag{2.11}$$

Thus, the matrix V_{p+1} has orthonormal columns, the first p of which form the matrix V_p. Moreover, $T_{p+1,p} = [t_{j,k}] \in \mathbb{C}^{(p+1)\times p}$ is tridiagonal with the Hermitian leading $p \times p$ principal submatrix T_p. When the last subdiagonal entry of the matrix $T_{p+1,p}$ vanishes, the decomposition (2.11) becomes $AV_p = V_pT_p$.

Proposition 2.5. *The distance in the Frobenius norm between a given Hermitian matrix $A \in \mathbb{C}^{n\times n}$ and its orthogonal projection onto the subspace of Hermitian matrices having the invariant subspace $\mathcal{R}(V_p)$, i.e., the distance between A and the matrix M defined by (2.3) with $V = V_p$, is given by*

$$\|A - M\|_F = \sqrt{2}|t_{p+1,p}|, \tag{2.12}$$

where $t_{p+1,p}$ is the last subdiagonal entry of the matrix $T_{p+1,p}$ defined by (2.11).

Proof. Using (2.11), one can rewrite the matrix in the right-hand side of (2.4) as

$$V^HA(I_n - VV^H)AV = V^HAAV - V^HAVV^HAV = t_{p+1,p}^2 e_p e_p^T.$$

The relation (2.12) now follows. □

Analogously to the situation when the Arnoldi method is applied, the matrix M of Proposition 2.5 generally is not the approximation $A_p = V_pT_pV_p^H$ of A determined by p steps of the Lanczos method. We have that similarly to Proposition 2.4,

$$\|A - A_p\|_F = \sqrt{\|A\|_F^2 - \|T_p\|_F^2}. \tag{2.13}$$

The quantity $\sqrt{2}|t_{p+1,p}|$ furnishes a lower bound for the right-hand side and may be much smaller than (2.13). Similar comments to those following the proof of Proposition 2.4 apply.

Remark 2.1. *We have seen that the approximation $A_p = V_pV_p^HAV_pV_p^H$ of A determined by p steps of the Arnoldi method generally is farther away from A than the matrix M of Propositions 2.3. The matrix A_p is close to M when $A(I_n - V_pV_p^H)$ is small. Similarly, the approximation determined by p steps of the Lanczos method when A is Hermitian is close to the matrix M of Proposition 2.5 when $(I_n - V_pV_p^H)A(I_n - V_pV_p^H)$ is small. Let us consider the latter case. In order to clarify the importance of the information given by the matrix M, assume that we are interested in approximations of the eigenvalues of largest magnitude of A. Let the eigenvalues be ordered according to $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$. When $\|A - A_p\|_F$ in (2.13) is close*

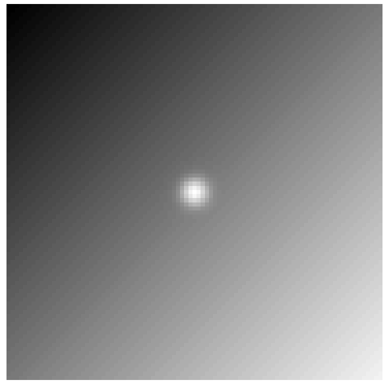

Fig. 2.1. *Exact image.*

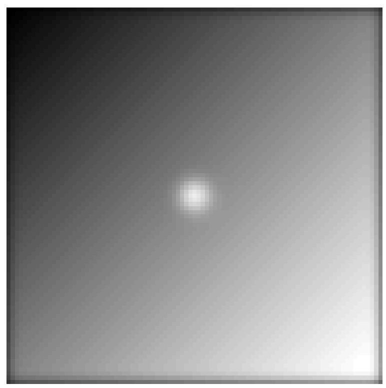

Fig. 2.2. *Image blurred by blurring matrix (2.14).*

to $\|A - M\|_F$ in (2.12), the Frobenius norm of the $(n-p)$-rank Hermitian matrix $M - A_p = (I_n - V_p V_p^H)A(I_n - V_p V_p^H)$ is small. This implies that the first p Ritz values of A approximate p eigenvalues that are much larger than the remaining $n-p$ eigenvalues, since $\|[\lambda_{p+1}, \ldots, \lambda_n]\| \approx \|M - A_p\|_F$. If, on the other hand, the ratio $\|A - A_p\|_F / \|A - M\|_F \gg 1$, then further steps of the Lanczos method are required in order to find all large eigenvalues.

We conclude this section with a brief discussion on the construction of blurring matrices. This is an essential step in image deblurring methods. An insightful discussion on image restoration is provided by Hansen et al. [7]. Consider the 91×91-pixel image shown in Figure 2.1, which shows the superposition of a Gaussian and a linear function. The pixel values for this image, ordered column wise, determine the vector $x \in \mathbb{R}^{8281}$. In image deblurring problems, Figure 2.1 is not available. Instead a blurred version of this image and a model of the blur are known, and our computational task is to reconstruct the image of Figure 2.1. The blur model defines a blurring matrix. Blur may be caused by inaccurate camera settings, motion of the object, or the atmosphere in astronomical imaging. Atmospheric blur typically is modeled by an exponential point spread function. A common approach to construct a matrix that models atmospheric blur is to define a symmetric block Toeplitz matrix with Toeplitz

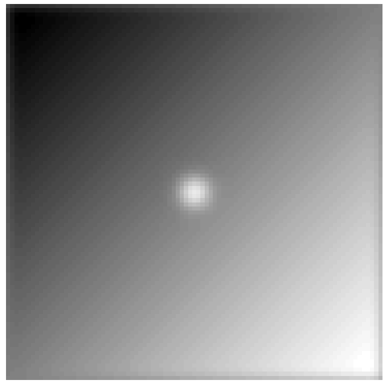

FIG. 2.3. *Image blurred by blurring matrix M obtained by solving an inverse subspace problem for the matrix (2.14).*

blocks,

$$A = (2\pi\sigma^2)^{-1} T \otimes T, \tag{2.14}$$

where T is a Toeplitz matrix and $\otimes$ denotes the Kronecker product.

In our computed example T is a 91×91 symmetric banded Toeplitz matrix, whose first row is given by `[exp(-((0:band-1).^2)/(2*sigma^2)); zeros(1,n-band)]` (using MATLAB notation). The parameter `band` is the half-bandwidth of the matrix T and the parameter $\sigma =$ `sigma` controls the effective width of the underlying Gaussian point spread function

$$h(x, y) = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right),$$

which models the blurring. We let `band` $= 16$ and `sigma` $= 1.5$. A representation of the available blurred image is given by $b := Ax$ and is displayed by Figure 2.2. An approximation of the deblurred image x is determined by computing an approximate solution of $Ax = b$. The solution of this system generally requires regularization, because the blurring matrix is numerically singular. The computation of a restoration x from b is discussed in [9]. In the present paper, we are concerned with the boundary artifacts of Figure 2.2. The darkness of the blurred image close to the boundary depends on that the matrix A is finite-dimensional and, therefore, pixels close to the boundary are treated differently from pixels in the interior of the image; see Ng and Plemmons [12] for a nice discussion and illustrations of boundary effects.

An application of the blurring matrix (2.14) to the vector $e = [1, 1, \ldots, 1]^T$, which represents constant uniform light, gives the same value at all pixels sufficiently far away from the boundary. To secure that the blurring matrix gives an image with the same pixel values at every pixel, we replace the matrix (2.14) by the matrix M, defined by (2.3) with $\mathcal{V} = \text{span}\{e\}$. The blurred image $b' := Mx$ is depicted by Figure 2.3. The boundary artifacts in Figure 2.3 are less noticeable than in Figure 2.2. We therefore propose that symmetric blurring matrices be constructed by solving the inverse subspace problem (1.2). Nonsymmetric blurring matrices can be determined analogously.

3. Matrices with specified left and right singular vectors. This section discusses the inverse singular subspace problem (1.3), and describes an application to the Lanczos bidiagonalization method. Let $A \in \mathbb{C}^{m\times n}$ and let the matrices $U \in \mathbb{C}^{m\times p}$ and $V \in \mathbb{C}^{n\times p}$, for some $p \le \min\{m, n\}$, have orthonormal columns. Let $M \in \mathbb{C}^{m\times n}$ solve (1.3) with $\mathcal{U} = \mathcal{R}(U)$ and $\mathcal{V} = \mathcal{R}(V)$. There are matrices $S_1, S_2 \in \mathbb{C}^{p\times p}$ such that

$$MV = US_1, \qquad M^H U = VS_2.$$

Introduce the polar decomposition $S_1 = QD$, where $Q \in \mathbb{C}^{p\times p}$ is unitary and $D \in \mathbb{C}^{p\times p}$ is Hermitian positive semidefinite. The columns of the matrix $U' = UQ$ also form an orthonormal basis for $\mathcal{U}$ and

$$MV = U'D, \qquad M^H U' = VD. \tag{3.1}$$

The left-hand side equality is immediate. The right-hand side equality follows from the facts that $M^H U' = VS_2Q$ and $D = (U')^H MV$. Therefore, $S_2Q = V^H M^H U' = ((U')^H MV)^H = D^H = D$.

The following proposition shows that the matrix

$$M = (I_m - UU^H)A(I_n - VV^H) + UU^H AVV^H \tag{3.2}$$

is the orthogonal projection of A onto the subspace $\mathcal{B}$ of the matrices $B \in \mathbb{C}^{m\times n}$ such that $B\mathcal{V} \subseteq \mathcal{U}$ and $B^H\mathcal{U} \subseteq \mathcal{V}$, where $\mathcal{U} = \mathcal{R}(U)$ and $\mathcal{V} = \mathcal{R}(V)$. Therefore, the matrix (3.2) solves (1.3).

Proposition 3.1. *Consider the matrix $M \in \mathbb{C}^{m\times n}$ defined in (3.2). The following properties hold:*

1. *$M \in \mathcal{B}$;*
2. *if $A \in \mathcal{B}$, then $M \equiv A$;*
3. *if $B \in \mathcal{B}$, then $\langle A - M, B\rangle = 0$.*

Proof. The first property follows immediately from (3.2). We have

$$MV = U \cdot U^H AV, \qquad M^H U = V \cdot V^H A^H U.$$

To show the second property, we first note that the matrix (3.2) is independent of which orthonormal bases of the spaces $\mathcal{U}$ and $\mathcal{V}$ are represented by the columns of the matrices U and V, respectively. Analogously to (3.1), there are orthonormal bases determined by the columns of suitable matrices U and V such that $AV = US$ and $A^H U = VS$ for a Hermitian positive semidefinite matrix $S \in \mathbb{C}^{p\times p}$. Using these matrices to define (3.2), we obtain

$$M = A - AVV^H - UU^H A + 2UU^H AVV^H = A - 2USV^H + 2USV^H = A.$$

We turn to the third property. Let $B \in \mathcal{B}$ and let the matrices $U \in \mathbb{C}^{m\times p}$ and $V \in \mathbb{C}^{n\times p}$ have orthonormal columns that span $\mathcal{U}$ and $\mathcal{V}$, respectively, and are such that $BV = UD$ and $B^H U = VD$ for a Hermitian positive semidefinite matrix $D \in \mathbb{C}^{p\times p}$. We then obtain

$$\mathrm{Trace}((A - M)B^H) = \mathrm{Trace}(AVV^H B^H + UU^H AB^H) - 2\,\mathrm{Trace}(UU^H AVV^H B^H).$$

The third property now is a consequence of the identities

$$\begin{aligned}\mathrm{Trace}(AVV^H B^H + UU^H AB^H) &= \mathrm{Trace}(AVDU^H) + \mathrm{Trace}(VDU^H A),\\ \mathrm{Trace}(UU^H AVV^H B^H) &= \mathrm{Trace}(UU^H AVDU^H) = \mathrm{Trace}(U^H AVD)\end{aligned}$$

and the cyclic property of the trace. □

When $m = n$ and $U = V$, the matrix (3.2) reduces to the matrix (2.3), and Proposition 3.1 reduces to Proposition 2.2. Moreover, when $p = 1$, the minimization problem (1.3) reduces to determining the closest matrix $M \in \mathbb{C}^{n\times n}$ to A with prescribed left and right singular vectors u and v, respectively.

The backward error (1.3) can be expressed as

$$\rho(A,\mathcal{U},\mathcal{V}) = \sqrt{\mathrm{Trace}(V^H A^H A V + U^H A(I_n - 2VV^H)A^H U)}. \tag{3.3}$$

This can be shown analogously to (2.2).

We turn to an application of these results to decompositions determined by Lanczos bidiagonalization. When $p \ll \min\{m, n\}$ steps of the Lanczos bidiagonalization method are applied to the matrix A with initial unit vector $u_1 \in \mathbb{C}^m$, we obtain generically the decompositions

$$AV_p = U_{p+1}C_{p+1,p}, \qquad A^H U_p = V_p C_p^H, \tag{3.4}$$

where the matrix $U_{p+1} \in \mathbb{C}^{m\times(p+1)}$ with $U_{p+1}e_1 = u_1$ has orthonormal columns that span the Krylov subspace $\mathcal{K}_{p+1}(AA^H, u_1)$, the columns of $V_p \in \mathbb{C}^{n\times p}$ form an orthonormal basis for $\mathcal{K}_p(A^H A, A^H u_1)$, the matrix $U_p \in \mathbb{C}^{n\times p}$ is made up of the p first columns of U_{p+1}, and $C_{p+1,p} = [c_{j,k}] \in \mathbb{C}^{(p+1)\times p}$ is a lower bidiagonal matrix. Moreover, C_p is the leading $p \times p$ submatrix of $C_{p+1,p}$. The decompositions (3.4) simplify to

$$AV_p = U_p C_p, \qquad A^H U_p = V_p C_p^H,$$

when the last subdiagonal entry, $c_{p+1,p}$, of $C_{p+1,p}$ vanishes. In this situation

$$A^H A\mathcal{R}(V_p) \subset \mathcal{R}(V_p), \qquad AA^H\mathcal{R}(U_p) \subset \mathcal{R}(U_p). \tag{3.5}$$

Thus, $\mathcal{R}(V_p)$ and $\mathcal{R}(U_p)$ are invariant subspaces of $A^H A$ and AA^H, respectively.

The relations (3.5) hold, in particular, when the columns of U_p are left singular vectors of A and the columns of V_p the associated right singular vectors. Many methods for computing approximations of a few right and left singular vectors of a large matrix determine a sequence of decompositions of the form (3.4) for judiciously chosen initial vectors u_1; see, e.g., [1, 2, 8, 11]. The above results allow us to determine the distance of A to the closest matrix with left and right singular vectors in $\mathcal{R}(U_p)$ and $\mathcal{R}(V_p)$, respectively. We also provide an expression for the distance between A and the approximation $U_p C_p V_p^H$.

PROPOSITION 3.2. *The distance in the Frobenius norm between a given matrix $A \in \mathbb{C}^{m\times n}$ and its projection onto the subspace of matrices $B \in \mathbb{C}^{m\times n}$ such that $BV_p \subseteq \mathcal{R}(U_p)$ and $B^H U_p \subseteq \mathcal{R}(V_p)$, i.e., its distance to the matrix $M \in \mathbb{C}^{m\times n}$ defined by (3.2) with $U = U_p$ and $V = V_p$, is given by*

$$\|A - M\|_F = |c_{p+1,p}|,$$

where $c_{p+1,p}$ is the last subdiagonal entry of the matrix $C_{p+1,p}$ determined by (3.4).

Proof. The proposition follows by substituting the decompositions (3.4) into the right-hand side of (3.3). In detail, we have

$$\begin{aligned}
&\mathrm{Trace}(AV_pV_p^H A^H + AA^H U_p U_p^H - 2AV_pV_p^H A^H U_p U_p^H) \\
&= \mathrm{Trace}(C_{p+1,p}^H C_{p+1,p} - I_{p,p+1}C_{p+1,p}C_p^H) \\
&= \mathrm{Trace}(C_{p+1,p}^H C_{p+1,p}) - \mathrm{Trace}(C_p^H C_p) \\
&= \|C_{p+1,p}\|_F^2 - \|C_p\|_F^2 = |c_{p+1,p}|^2.
\end{aligned}$$

□

The following result is analogous to Proposition 2.4.

PROPOSITION 3.3. *Let the matrices U_p, V_p, and C_p be determined by p steps of the Lanczos bidiagonalization process with initial vector u_1; cf. (3.4). Then*

$$\|A - U_p C_p V_p^H\|_F = \sqrt{\|A\|_F^2 - \|C_p\|_F^2}.$$

Proof. The decompositions (3.4) and the cyclic property of the trace yield

$$\begin{aligned}
&\|A - U_p C_p V_p^H\|_F^2 \\
&= \|A\|_F^2 - \mathrm{Trace}(A^H U_p C_p V_p^H + V_p C_p^H U_p^H A - V_p C_p^H U_p^H U_p C_p V_p^H) \\
&= \|A\|_F^2 - \mathrm{Trace}(V_p^H V_p C_p^H C_p + C_p V_p^H V_p C_p^H - V_p C_p^H C_p V_p^H) \\
&= \|A\|_F^2 - \|C_p\|_F^2.
\end{aligned}$$

□

REMARK 3.1. *The approximation of A determined by p steps of the Lanczos bidiagonalization is close to the matrix M of Proposition 3.2 when $(I_m - U_p U_p^H)A(I_n - V_p V_p^H)$ is small. In particular, a small entry $c_{p+1,p}$ of the bidiagonal matrix $C_{p+1,p}$ in (3.4) does not guarantee that the matrix $U_p C_p V_p^H$ is close to A.*

4. Application to the solution of discrete ill-posed problems. Denote the unknown error in the vector b in (1.4) by $\hat{e}$ and let $\hat{b}$ be the unavailable error-free data vector associated with b, i.e., $b = \hat{b} + \hat{e}$. We would like to determine an approximation of the solution $\hat{x}$ of minimal Euclidean norm of the least-squares problem obtained by replacing b by $\hat{b}$ in (1.4).

For many discrete ill-posed problems (1.4), the TSVD method, outlined in Section 1, performs fairly well. However, it is often beneficial, and for some problems essential, to incorporate knowledge of the desired solution $\hat{x}$ into the solution process. The SRSVD method, described in [10], allows a user to modify the SVD of A and include vectors in the decomposition that are deemed useful. Let the matrices $U = [u_1, u_2, \ldots, u_p] \in \mathbb{C}^{m \times p}$ and $V = [v_1, v_2, \ldots, v_p] \in \mathbb{C}^{n \times p}$ have orthonormal columns. The SRSVD method allows a user to prescribe that all solution-subspaces of dimension at least p contain the subspace $\mathcal{R}(V)$, and that all range-subspaces of dimension at least p contain $\mathcal{R}(U)$. The dimension p is in applications typically chosen to be small; see [10] for illustrations.

The matrices in the SRSVD method described in [10] are determined by first computing the SVD of $(I_m - UU^H)A(I_n - VV^H)$. Some manipulations then give a decomposition of A whose solution and range subspaces of dimensions larger than or equal p contain $\mathcal{R}(V)$ and $\mathcal{R}(U)$, respectively; see [10] for details. However, the decomposition determined in this manner is not the matrix closest to A with the property that all solution subspaces and all range subspaces of dimensions larger than or equal to p contain $\mathcal{R}(V)$ and $\mathcal{R}(U)$, respectively.

Section 3 suggests a new approach to define a subspace-restricted SVD. Let the matrix M be given by (3.2). Then we obtain the decomposition

$$A = \tilde{U}\tilde{\Sigma}\tilde{V}^H + UU^H A + AVV^H - 2UU^H AVV^H,$$

where $\tilde{U}\tilde{\Sigma}\tilde{V}^H$ is a singular value decomposition of M. Since

$$\tilde{U}^H U = \left[\ I_p \mid O_{p\times(m-p)}\ \right]^T, \quad V^H \tilde{V} = \left[\ I_p \mid O_{p\times(n-p)}\ \right],$$

-6	-5	-4	-3	-2	-1
21.9197	21.9197	21.9197	21.9197	21.9202	21.9352
70.6939	70.6939	70.6940	70.6942	70.6971	70.7867

TABLE 5.1

Example 5.1: Ratios between the distances (2.10) and (2.8) for tridiagonal Toeplitz matrices (5.1). The top row shows k, the middle and last rows the ratios for matrices of order $n = 100$ and $n = 1000$, respectively.

where $O_{r\times s}$ denotes the null matrix of size $r \times s$, we can express $S = \tilde{U}^H A\tilde{V}$ as

$$\tilde{\Sigma} + \left[\begin{array}{c} U^H A \\ \hline O_{(m-p)\times n} \end{array}\right] + \left[\begin{array}{c|c} AV & O_{m\times(n-p)} \end{array}\right] - 2\left[\begin{array}{c|c} U^H AV & O_{p\times(n-p)} \\ \hline O_{(m-p)\times p} & O_{(m-p)\times(n-p)} \end{array}\right].$$

Hence,

$$A = \tilde{U}S\tilde{V}^H$$

is a subspace-restricted SVD such that the solution-subspaces of dimension $k \leq p$ are given by $\text{span}\{v_1, v_2, \ldots, v_k\}$; the associated range-subspaces are $\text{span}\{u_1, u_2, \ldots, u_k\}$. The trailing $m-p$ rows and $n-p$ columns of S are identical with the corresponding rows and columns of $\tilde{\Sigma}$. Computed examples with this SRSVD method are reported in Section 5.

5. Numerical examples. The first example illustrates the bounds of Section 2 for the Arnoldi decomposition. The subsequent example shows the performance of the method proposed in Section 4 for the solution of discrete ill-posed problems. All computations were carried out in MATLAB with about 15 significant decimal digits.

Example 5.1. Consider tridiagonal Toeplitz matrices A defined by

$$L_k = \frac{1}{4}\begin{bmatrix} 2 & -1 & & & & 0 \\ -10^k & 2 & -1 & & & \\ & -10^k & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & -1 \\ 0 & & & & -10^k & 2 \end{bmatrix} \in \mathbb{R}^{n\times n}, \quad k = -6, \ldots, -1. \tag{5.1}$$

Table 5.1 reports the ratios between the distance (2.10) and the lower bound $|h_{p+1,p}|$ in (2.8) for $p = 5$ steps of the Arnoldi method for matrices L_k, $k = -6, -5, \ldots, -1$. Ratios for $n = 100$ (middle row) and $n = 1000$ (last row) are displayed. The first row shows the value of k. We used an initial vector v_1 with normally distributed entries with zero mean, scaled so that $\|v_1\| = 1$, for Arnoldi's method. The columns of the matrices V_{p+1} in the Arnoldi decompositions (3.4) were reorthogonalized. For both $n = 100$ and $n = 1000$, and for all values of k, the lower bounds $|h_{6,5}|$ were about 1. Table 5.1 shows the closest matrix M_k to L_k in the Frobenius norm with invariant subspace $\mathcal{R}(V_5)$ to be much closer to L_k than the low-rank approximation (2.9) determined by the Arnoldi method. The distance between the matrix (2.9) and M_k is large: it is about 21.8 [about 70.5] for $n = 100$ [$n = 1000$], for all values of k; cf. Remark 2.1. $\square$

The following example compares the modification of the TSVD described in Section 4 with that in [10].

x_6	y_4^1	y_2^2	z_5^1	z_1^2	w_5^1	w_3^2
$2.9 \cdot 10^{-1}$	$1.4 \cdot 10^{-1}$	$3.9 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$3.9 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$1.2 \cdot 10^{-2}$

TABLE 5.2

Example 5.2: Relative errors in computed solutions of a discretization of the integral equation (5.2) using the standard truncated SVD method and subspace-restricted variants.

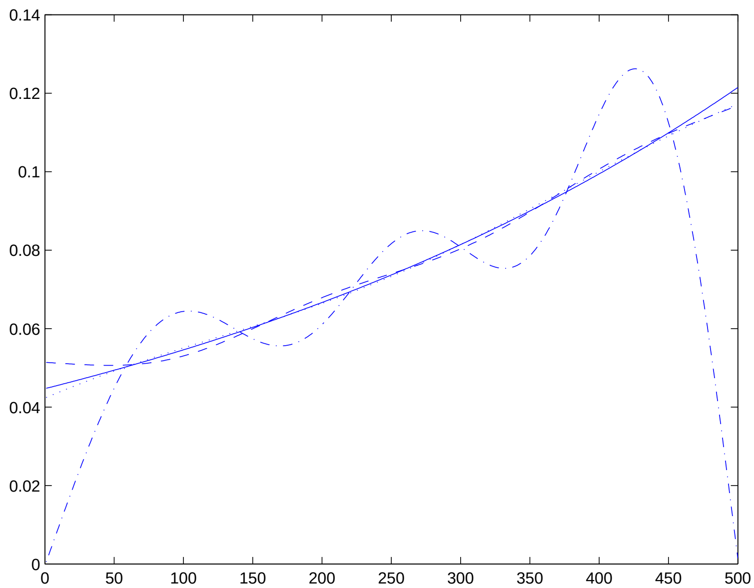

FIG. 5.1. *Example 5.2: Exact solution (solid curve) and approximate solutions determined by TSVD (dash-dotted curve), TSRSVD (dashed curve) and the subspace-restricted SVD of the present paper (dotted curve). The truncation index is determined by the discrepancy principle.*

Example 5.2. We consider the Fredholm integral equation of the first kind

$$\int_0^1 K(s,t)x(t)dt = \mathrm{e}^s + (1-\mathrm{e})s - 1, \qquad 0 \leq s \leq 1, \tag{5.2}$$

whose kernel is the Green's function for the second derivative

$$K(s,t) = \begin{cases} s(t-1), & s < t, \\ t(s-1), & s \geq t. \end{cases}$$

Discretization of (5.2) is carried out by a Galerkin method with orthonormal box functions as test and trial functions using the MATLAB function deriv2 from [6]. This function yields the symmetric matrix $A \in \mathbb{R}^{500\times 500}$ and a scaled approximation $\hat{x} \in \mathbb{R}^{500}$ of the solution $x(t) = \exp(t)$. The error-free right-hand side vector is computed as $\hat{b} = A\hat{x}$. The entries of the error vector $\hat{e}$ in b are normally distributed with zero mean, and scaled to correspond to a specified noise level $\varepsilon = \|\hat{e}\|/\|\hat{b}\|$. We use the truncated SVD method to compute an approximate solution of the discrete problem. The truncation index k is determined with the aid of the discrepancy principle, i.e., we choose $k \geq 0$ to be the smallest integer such that the residual norm satisfies

$$\|Ax_k - b\| \leq \gamma\varepsilon\|\hat{b}\|,$$

where $\gamma > 1$ is a user-supplied constant. In the present example, $\varepsilon = 0.01$ and we set $\gamma = 1.1$. The first column of Table 5.2 reports the relative error in the approximate TSVD solution x_6, where $k = 6$ is given by the discrepancy principle.

Consider the dimension $p = 1$ [$p = 2$] and let the matrix V with orthonormal column[s] contain the discretization of the constant function [constant and linear functions]. The second [third] column of Table 5.2 reports the relative error in the solution y_4^1 [y_2^2] determined by the truncated generalized singular value decompositio (TGSVD) of the matrix pair $\{A, I - VV^H\}$, where $k = 4$ [$k = 2$] is given by the discrepancy principle. The approximate solution z_5^1 [z_1^2] is determined by the truncated SRSVD (TSRSVD) method in [10]; see the fourth [fifth] column of Table 5.2. The TSRSVD method determines a truncation index k similarly as the TSVD method; see Section 1 for an outline of the latter.

We compare these results with the solution w_5^1 [w_3^2] given by the truncated subspace-restricted SVD proposed in Section 4. We choose the subspaces V as above and, since the matrices A and M are symmetric and the eigenvalues are non-positive, we set $U = -V$. The fifth [sixth] column of Table 5.2 reports the case $p = 1$ [$p = 2$].

Figure 5.1 displays the exact solution, the approximate TSVD solution x_6, and the approximate solutions obtained with the subspace-restricted methods (z_1^2 by the TSRSVD in [10] and w_3^2 by our method), where V contains an orthonormal basis for the linear functions. $\Box$

6. Conclusion. This paper is concerned with the distance between a matrix and the closest matrix with a given invariant subspace or the closest matrix with given subspaces of left and right singular vectors. The distance formulas shed light on the Arnoldi, Lanczos, and Lanczos bidiagonalization methods. They also suggest a new method for the solution of discrete ill-posed problems. Computed examples illustrate the competitiveness of the new method proposed. Finally, they suggest a novel approach to determine blurring matrices for image deblurring problems.

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