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A KRYLOV–SCHUR ALGORITHM FOR LARGE EIGENPROBLEMS*

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Abstract. Sorensen's implicitly restarted Arnoldi algorithm is one of the most successful and flexible methods for finding a few eigenpairs of a large matrix. However, the need to preserve the structure of the Arnoldi decomposition on which the algorithm is based restricts the range of transformations that can be performed on the decomposition. In consequence, it is difficult to deflate converged Ritz vectors from the decomposition. Moreover, the potential forward instability of the implicit QR algorithm can cause unwanted Ritz vectors to persist in the computation. In this paper we introduce a general Krylov decomposition that solves both problems in a natural and efficient manner.

Key words. large eigenproblem, Krylov sequence, Arnoldi algorithm, Krylov decomposition, restarting, deflation

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1. Introduction and background.

In this paper we are going to describe an alternative to the Arnoldi method that resolves some difficulties with its implicitly restarted version. To understand the difficulties and their solution requires a detailed knowledge of the Arnoldi process. We therefore begin with a survey, which will also serve to set the notation for this paper.

Let A be a matrix of order n and let u_1 be a vector of 2-norm one. Let $u_1, u_2, u_3, \ldots$ be the result of sequentially orthogonalizing the Krylov sequence $u_1, Au_1, A^2u_1, \ldots$. In 1950, Lanczos [6] showed that if A is Hermitian then the vectors u_i satisfy a three-term recurrence of the form

$$\beta_k u_{k+1} = A_k u_k - \alpha_k u_k - \beta_{k-1} u_{k-1}, \tag{1.1}$$

a recursion that in principle allows the economical computation of the u_j.

There is an elegant representation of this recursion in matrix terms. Let

$$U_k = (u_1 \;\; u_2 \;\; \cdots \;\; u_k)$$

be the matrix formed from the Lanczos vectors u_j. Then there is a tridiagonal matrix T formed from the α's and β's in (1.1) such that

$$AU_k = U_k T_k + \beta_k u_{k+1} \mathbf{e}_k^{\mathrm{T}}, \tag{1.2}$$

where $\mathbf{e}_k$ is the vector whose last component is one and whose other components are zero. From the orthogonality of the u_j, it follows that T_k is the Rayleigh quotient

$$T_k = U_k^{\mathrm{H}} A U_k.$$

We will call (1.2) a Lanczos decomposition.

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Lanczos appreciated the fact that even for comparatively small k the matrix T_k could contain accurate approximations to the eigenvalues of A. When this happens, the column space $\mathcal{U}_k$ of U_k will usually contain approximations to the corresponding eigenvectors. Such an approximation—call it z—can be calculated by computing a suitable eigenpair (μ, w) of T_k and setting $z = U_k w$. This process is called the Rayleigh–Ritz method; μ is called a Ritz value and z a Ritz vector.

In 1951, Arnoldi [1], building on Lanczos's work, showed that if A is non-Hermitian, then the Lanczos decomposition becomes

$$AU_k = U_k H_k + \beta_k u_{k+1} \mathbf{e}_k^{\mathrm{T}}, \tag{1.3}$$

where H_k is upper Hessenberg. We will call (1.3) an Arnoldi decomposition. Once again, H_k may contain accurate approximations to the eigenvalues of A, especially those on the periphery of the spectrum of A. Moreover, approximations to the eigenvectors may be obtained by the natural generalization of the Rayleigh–Ritz process.

Arnoldi decompositions are essentially unique. Specifically, if H_k is unreduced—that is, if its subdiagonal elements are nonzero—then up to scaling of the columns of U_{k+1} and the rows and columns of H_k, the decomposition is uniquely determined by the space spanned by U_{k+1}.[1] In particular, the Krylov subspace of an unreduced Arnoldi decomposition has a unique starting vector.

Since H_k is not tridiagonal, the Arnoldi vectors do not satisfy a three-term recurrence. To compute u_{k+1} all the columns of U_k must be readily available. If n is large, these vectors will soon consume all available storage, and the process must be restarted. The problem then becomes how to choose a new u_1 that does not discard the information about the eigenvectors contained in $\mathcal{U}_k$. There have been several proposals, whose drawbacks have been nicely surveyed by Morgan [11].

In 1992, Sorensen [14] suggested an elegant way to use the QR algorithm to restart the Arnoldi process. Specifically, suppose we have an Arnoldi decomposition

$$AU_m = U_m H_m + \beta_m u_{m+1} \mathbf{e}_m^{\mathrm{T}} \tag{1.4}$$

of order m that cannot be further expanded because of lack of storage. For some fixed k, choose $m-k$ shifts $\kappa_1, \ldots, \kappa_{m-k}$ and use them to perform $m-k$ steps of the implicitly shifted QR algorithm on the Rayleigh quotient H_m. The effect is to generate an orthogonal matrix Q such that $Q^{\mathrm{H}} H_m Q$ is upper Hessenberg. Then from (1.4)

$$A(U_m Q) = (U_m Q) Q^{\mathrm{H}} H_m Q + \beta_m u_{m+1} \mathbf{e}_m^{\mathrm{T}} Q$$

or

$$A\tilde{U}_m = \tilde{U}_m \tilde{H}_m + u_{m+1} c^{\mathrm{H}}.$$

Sorensen then observed that the structure of Q is such that the first $k-1$ components of c are zero. Consequently, if we let $\tilde{H}_k$ be the leading principal submatrix of $\tilde{H}_m$ of order k and set

$$\beta_k \tilde{u}_{k+1} = \tilde{\gamma}_k u_{m+1} + \tilde{h}_{k+1,k} u_{k+1}, \tag{1.5}$$

then

$$A\tilde{U}_k = \tilde{U}_k \tilde{H}_k + \tilde{u}_{k+1} e_k^{\mathrm{T}}$$

[1] This fact is a direct consequence of the implicit Q theorem, which says that if $H = Q^{\mathrm{H}} A Q$ is an unreduced Hessenberg matrix then Q is determined by its first or last column. See [4, Theorem 7.4.2].

is an Arnoldi decomposition of order k. This process of truncating the decomposition is called implicit restarting.

A second key observation of Sorensen suggests a rationale for choosing the shifts. Specifically, if $p(t) = (t - \kappa_1 I) \cdots (t - \kappa_{m-k} I)$, then

$$\tilde{u}_1 = \frac{p(A)u_1}{\|p(A)u_1\|}.$$

It follows that if we choose the shifts to lie in the part of the spectrum that we are not interested in then the implicit restart process deemphasizes these very eigenvalues.

Each iteration of Sorensen's algorithm consists of two stages: an expansion stage, in which the decomposition is expanded until it is inconvenient to go further, and a contraction or purging stage, in which unwanted parts of the spectrum are suppressed. The contraction phase has two variants. In the exact variant, the shifts are taken to be unwanted eigenvalues of H_m. If, for example, we were concerned with stability, we might choose to retain only the eigenvalues with largest real parts. In the other, more general variant, the shifts are not necessarily eigenvalues of H_m. For example, they might be the zeros of a Chebyshev polynomial spanning an ellipse containing unwanted eigenvalues.

The implicitly restarted Arnoldi algorithm has been remarkably successful and has been implemented in the widely used ARPACK package [9]. However, the method has two important drawbacks.

First, for the exact restart procedure to be effective the unwanted Ritz values μ must be moved to the end of H_m, so that the Rayleigh quotient has the form illustrated below for $k = 3$ and $m = 6$:

$$\begin{pmatrix} h & h & h & h & h & h \\ h & h & h & h & h & h \\ 0 & h & h & h & h & h \\ 0 & 0 & 0 & \mu & h & h \\ 0 & 0 & 0 & 0 & \mu & h \\ 0 & 0 & 0 & 0 & 0 & \mu \end{pmatrix}. \tag{1.6}$$

If H_m is unreduced—that is, if the elements of its first subdiagonal are nonzero—then mathematically H_m must have the form (1.6). In the presence of rounding error, however, the process can fail (for a treatment of this phenomenon, see [17]). This has lead Lehoucq and Sorensen to propose an elaborate method for permanently ridding the decomposition of persistent unwanted Ritz values [8].

The second problem is to move converged Ritz values μ to the beginning of H_k, so that it assumes the form illustrated below:

$$\begin{pmatrix} \mu & h & h & h & h & h \\ 0 & \mu & h & h & h & h \\ 0 & 0 & h & h & h & h \\ 0 & 0 & h & h & h & h \\ 0 & 0 & 0 & h & h & h \\ 0 & 0 & 0 & 0 & h & h \end{pmatrix}.$$

When the converged Ritz values are thus deflated (or locked), one does not have to update the Arnoldi u_1 and u_2 in the Arnoldi decomposition. Lehoucq and Sorensen have proposed a complicated deflation algorithm.

Most of the complications in the purging and deflating algorithms come from the need to preserve the structure of the Arnoldi decomposition (1.3)—in particular, to preserve the Hessenberg form of the Rayleigh quotient and the zero structure of the vector $\mathbf{e}_k$. The purpose of this paper is to show that if we relax the definition of an Arnoldi decomposition, we can solve the purging and deflating problems in a natural and efficient way. Since the method is centered about the Schur decomposition of the Rayleigh quotient, we will call the method the Krylov–Schur method.

The decompositions and algorithms proposed in this paper are not without precursors. Fokkema, Sleijpen, and van der Vorst [3] explicitly use Schur vectors to restart the Jacobi–Davidson algorithm. Stathopoulos, Saad, and Wu [15] point out that because the unprecondition Jacobi–Davidson algorithm is equivalent to the Arnoldi algorithm, one can also use Schur vectors to restart the latter. Lehoucq [7] has used Schur vectors in the deflation process in [8]. Closer to home, for symmetric matrices Wu and Simon [18] exhibit what might be called a Krylov-spectral decomposition, a special case of our Krylov–Schur decomposition to be introduced later. Finally, Morgan [12] has applied an orthogonal Krylov decomposition to the problem of restarting GMRES. What distinguishes our approach is the explicit introduction of general Krylov decompositions whose subspaces are invariant under certain formal operations—operations that can be used to derive and analyze new algorithms.

In the next section we introduce Krylov decompositions and, in particular, the Krylov–Schur decomposition, which lies at the heart of our method. Section 3 treats the Krylov–Schur method and its relation to the implicitly restarted Arnoldi method. In section 4 we treat the numerical stability of the combined steps. In section 5 we show how to deflate vectors and subspaces from a Krylov decomposition. In section 6 we compare the work done by the implicitly restarted Arnoldi and the Krylov–Schur methods. We end with some general comments. Throughout this paper $\|\cdot\|$ will denote the vector and matrix 2-norm, and $\|\cdot\|_{\mathrm{F}}$ will denote the Frobenius norm (see [16, section 1.4.1]).

2. Krylov decompositions. The structure of an Arnoldi decomposition restricts the operations we can perform on its Rayleigh quotient. The following definition introduces a less constraining decomposition.

DEFINITION 2.1. *A* Krylov decomposition of order k *is a relation of the form*

$$AU_k = U_k B_k + u_{k+1} b_{k+1}^{\mathrm{H}}, \tag{2.1}$$

where B_k is of order k and the columns of $(U_k \;\; u_{k+1})$ are independent. The columns of $(U_k \;\; u_{k+1})$ are called the basis *for the decomposition, and they span the* space *of the decomposition. If the basis is orthonormal, we say the decomposition is orthonormal. The matrix B_k is called the* Rayleigh quotient *of the decomposition.*

This definition removes practically all the restrictions imposed on an Arnoldi decomposition. The vectors of the decomposition are not required to be orthonormal and the vector b_{k+1} and the matrix B_k are allowed to be arbitrary. Nonetheless, we shall see that the relation (2.1) is sufficient to insure that $(U_k \;\; u_{k+1})$ is a basis for a Krylov subspace.

The name "Rayleigh quotient" is appropriate for the matrix B_k. For if $(V_k \;\; v_{k+1})^{\mathrm{H}}$ is a left inverse of $(U_k \;\; u_{k+1})$, then $B_k = V_k^{\mathrm{H}} A U_k$. In particular, if $(\mu, U_k w)$ is an eigenpair of A, then (μ, w) is an eigenpair of B_k. Thus the Rayleigh–Ritz procedure extends to Krylov decompositions.

The subspaces of Krylov decompositions are closed under two classes of transformations: translation and similarity. The first allows us to change the vector u_k. The

second allows us to change the pair (B_k, U_k) along with b_{k+1}^{H}. In what follows we will drop subscripts in k and write our Krylov decomposition in the form $AU = UB + ub^{\mathrm{H}}$.

To introduce the operation of translation, let

$$\gamma\tilde{u} = u - Ug,$$

where $\gamma \neq 0$. Then it is easily verified that

$$AU = U(B + gb^{\mathrm{H}}) + \tilde{u}b^{\mathrm{H}},$$

where $\tilde{b}^{\mathrm{H}} = \gamma b^{\mathrm{H}}$, is a Krylov decomposition with the same space as the original. This gives us considerable freedom to replace u by linear combinations of u and U, although the fact that $\gamma \neq 0$ implies that the vector $\tilde{u}$ always contains some component along u. In particular, we can choose $\tilde{u}$ so that $\|\tilde{u}\| = 1$ and $U^{\mathrm{H}}\tilde{u} = 0$.

To introduce similarity transformations, let W be nonsingular. Then

$$A(UW^{-1}) = (UW^{-1})(WBW^{-1}) + u(b^{\mathrm{H}}W^{-1}) \equiv A\tilde{U} = \tilde{U}\tilde{B} + u\tilde{b}^{\mathrm{H}}$$

is a Krylov decomposition whose space is the same as the original. Because the Rayleigh quotient of the new decomposition is similar to that of the old, we say that the two decompositions are similar.[2]

We will say that two Krylov decompositions related by a sequence of translations and similarities are *equivalent*. We are now going to show that any Krylov decomposition is equivalent to an Arnoldi decomposition. Since the space of an Arnoldi decomposition is a (possibly restarted) Krylov subspace, the result justifies the name Krylov decomposition.

THEOREM 2.2. *Let*

$$AU = UB + ub^{\mathrm{T}} \tag{2.2}$$

be a Krylov decomposition of order k. Then (2.2) is equivalent to an Arnoldi decomposition. If the Hessenberg part of the Arnoldi decomposition is unreduced, the Arnoldi decomposition is essentially unique.

Proof. The reduction, which is constructive, proceeds in four stages.

1. By a similarity transformation, orthogonalize the columns of U.
2. By a translation, transform u so that it is of norm one and is orthogonal to $\mathcal{R}(U)$.
3. By a unitary similarity transformation, reduce b to a multiple of $\mathbf{e}_k$.
4. Finally, by a unitary similarity reduce B to Hessenberg form. The reduction is performed rowwise by Householder transformations beginning with the last row, as illustrated in the following Wilkinson diagram:

$$\begin{pmatrix} b & b & b & b & b \\ b & b & b & b & b \\ b^3 & b & b & b & b \\ b^2 & b^2 & b & b & b \\ b^1 & b^1 & b^1 & b & b \end{pmatrix}.$$

[2] A referee has pointed out that these two types of transformations can be combined. Specifically, we say that the Arnoldi decompositions $AU = UB + ub^{\mathrm{T}}$ and $AV = VB + vb^{\mathrm{T}}$ are equivalent if there is a nonsingular matrix $\tilde{W} = \left(\begin{smallmatrix} W & g \\ 0 & \gamma \end{smallmatrix}\right)$ such that $(V\ v) = (U\ u)\tilde{W}$. With $W = I$ we obtain a translation; with $g = 0$ and $\gamma = 1$ we obtain a similarity.

The final reduction to Hessenberg form does not introduce nonzero elements into the first $k-1$ components of b, so that the result of this algorithm is an Arnoldi decomposition. The uniqueness in the unreduced case follows from the uniqueness of unreduced Arnoldi decompositions. □

The proof of Theorem 2.2 illustrates the power of translations and similarities to bring a Krylov decomposition into a useful form without losing the Krylov subspace property. In particular, any Krylov decomposition corresponds to an *orthonormal Krylov decomposition* in which the columns of the basis are orthonormal. (From here on, all our Krylov decompositions will be orthonormal.) Further, we can reduce the Rayleigh quotient to Schur form. The resulting *Krylov–Schur* decomposition is the basis of the main algorithm in this paper, to which we now turn.

3. The Krylov–Schur method. A step of the Krylov–Schur method begins and ends with a Krylov–Schur decomposition of the form

$$AU_k = U_k S_k + u_{k+1} b_{k+1}^{\mathrm{H}},$$

where the letter S (for Schur) stresses the triangularity of the Rayleigh quotient. It will be more convenient to work with the equivalent factored form

$$AU_k = U_{k+1} \hat{S}_k,$$

where

$$\hat{S}_k = \begin{pmatrix} S_k \\ b_{k+1}^{\mathrm{H}} \end{pmatrix}.$$

Like the implicitly restarted Arnoldi method the Krylov–Schur method consists of an expansion phase, in which the underlying Krylov sequence is extended, and a contraction phase, in which the unwanted Ritz values are purged from the decomposition. We will treat each in turn.

The expansion proceeds as in the usual Arnoldi algorithm: the vector Au_{k+1} is orthogonalized against U_{k+1} and normalized to give u_{k+2}, after which S_{k+1} is formed from S_k. The following pseudocode implements this procedure. We assume that U_{k+1} and $\hat{S}_k$ are contained in arrays U and S.

$$\begin{aligned} &1.\ v = A * U[:, k+1], \\ &2.\ w = U^{\mathrm{H}} * v, \\ &3.\ v = v - U * w, \\ &4.\ \nu = \|v\|_2, \\ &5.\ U = (U\ \ v/\nu), \\ &6.\ \hat{S} = \begin{pmatrix} \hat{S} & w \\ 0 & \nu \end{pmatrix}. \end{aligned} \tag{3.1}$$

Note that in a working implementation we would have to reorthogonalize to insure that the vector v is orthogonal to the column space of U to working accuracy (see [16, Algorithm 4.1.13]).

After this process the array $\hat{S}$ has the form illustrated below for $k = 3$:

$$\begin{pmatrix} s & s & s & h \\ 0 & s & s & h \\ 0 & 0 & s & h \\ b & b & b & h \\ 0 & 0 & 0 & h \end{pmatrix}.$$

Here the s's stand for the elements of the original S_k and the b's for the elements of b_{k+1}. The process may be repeated. After $m-k$ steps, the array S has the form illustrated below for $k = 3$ and $m = 6$:

$$\begin{pmatrix} s & s & s & h & h & h \\ 0 & s & s & h & h & h \\ 0 & 0 & s & h & h & h \\ b & b & b & h & h & h \\ 0 & 0 & 0 & h & h & h \\ 0 & 0 & 0 & 0 & h & h \\ 0 & 0 & 0 & 0 & 0 & h \end{pmatrix}. \tag{3.2}$$

At this point the Rayleigh quotient, which resides in $S[1{:}m, 1{:}m]$, is reduced to Schur form to give the Arnoldi–Schur decomposition

$$AU_m = U_m S_m + u_{m+1} b_{m+1}^{\mathrm{H}}. \tag{3.3}$$

This reduction to Schur form begins with a reduction of the Rayleigh quotient to Hessenberg form, and some minor savings can be obtained at this stage by taking advantage of the structure illustrated in (3.2). Although (3.3) suggests that we are computing the entire decomposition, including U_m, in fact it will be more efficient to defer the computation of the columns of U_m until later. We will return to this point in section 6.

We now turn to the problem of purging the unwanted Ritz values from the Krylov–Schur decomposition (3.3)—the contraction phase of the method. The key is the observation that a Krylov–Schur decomposition can be truncated at any point. Specifically, if we partition a Krylov–Schur decomposition in the form

$$A(U_1 \ U_2) = (U_1 \ U_2) \begin{pmatrix} S_{11} & S_{12} \\ 0 & S_{22} \end{pmatrix} + u(b_1^{\mathrm{H}} \ b_2^{\mathrm{H}}), \tag{3.4}$$

then

$$AU_1 = U_1 S_{11} + u b_1^{\mathrm{H}}$$

is also a Krylov–Schur decomposition. Thus the purging problem can be solved by moving the unwanted Ritz values into the southeast corner of the Rayleigh quotient and truncating the decomposition.

The process of using unitary similarities to move eigenvalues around in a Schur form has been well studied. The current front-running algorithm [2], which has been implemented in the LAPACK routine `xTREXC`, is quite reliable—far more so than implicit QR. Consequently, our deflation algorithm consists of little more than moving the unwanted Ritz values, which are visible on the diagonals of S_m, to the southeast corner of the Rayleigh quotient and truncating the decomposition.

The following theorem shows just what a combined expansion and contraction step produces.

THEOREM 3.1. *Let*

$$\mathbb{P} := AU = UH + \beta u \mathbf{e}_k^{\mathrm{T}}$$

be an unreduced Arnoldi decomposition and let

$$\mathbb{Q} := AV = VS + u b^{\mathrm{H}}$$

be an equivalent Krylov–Schur form. Suppose that an implicitly restarted Arnoldi cycle is performed on $\mathbb{P}$ and a Krylov–Schur cycle is performed on $\mathbb{Q}$. If the same Ritz values are discarded in both and those Ritz values are distinct from the other Ritz values, then the resulting decompositions are equivalent.

Proof. We must show that the subspaces associated with the final results are the same. First note that the expansion phase results in equivalent decompositions. In fact, since $\mathcal{R}(U) = \mathcal{R}(V)$ and in both cases we are orthogonalizing the same Krylov sequence, the vectors $u_{k+1} \ldots u_{m+1}$ and $v_{k+1}, \ldots, v_{m+1}$ are the same up to multiples of modulus one.

Now assume that both algorithms have gone through the expansion phase and have moved the unwanted Ritz values to the end of the decomposition. At this point denote the first decomposition by

$$\hat{\mathbb{P}} := A\hat{U} = \hat{U}\hat{H} + \hat{\beta}\hat{u}\mathbf{e}_m^{\mathrm{T}}$$

and the second by

$$\hat{\mathbb{Q}} := A\hat{V} = \hat{V}\hat{S} + \hat{u}\hat{b}^{\mathrm{H}}.$$

Note that for both methods, the final truncation leaves the vector $\hat{u}$ unaltered. Since $\hat{V} = \hat{U}W$ for some unitary W, we have

$$\hat{S} = \hat{V}^{\mathrm{H}}A\hat{V} = W^{\mathrm{H}}\hat{U}^{\mathrm{H}}A\hat{U}W = W^{\mathrm{H}}\hat{H}W.$$

Thus $\hat{H}$ and $\hat{S}$ are similar and have the same Ritz values. Thus it makes sense to say that both methods reject the same Ritz values.

Let P be the unitary transformation applied to the Rayleigh quotient in $\hat{\mathbb{P}}$, and let Q be the one applied to the Rayleigh quotient of $\hat{\mathbb{Q}}$. Then we must show that the subspaces spanned by $\hat{U}P[:, 1{:}k]$ and $\hat{V}Q[:, 1{:}k]$ are the same. For brevity, set $P_k = P[:, 1{:}k]$ and $Q_k = Q[:, 1{:}k]$.

By construction $\mathcal{R}(P_k)$ is the eigenspace $\mathcal{P}$ of Schur vectors of $\hat{H}$ corresponding to the retained Ritz values. Likewise, $\mathcal{R}(Q_k)$ is the eigenspace $\mathcal{Q}$ of Schur vectors of $\hat{S}$ corresponding to the retained Ritz values. By hypothesis these eigenspaces are simple and hence are the same. Since $W^{\mathrm{H}}\hat{S}W = \hat{H}$, the matrix $W^{\mathrm{H}}\hat{P}_k$ spans $\mathcal{Q}$. Hence there is a unitary matrix R such that $Q_k = W^{\mathrm{H}}P_kR$. We then have

$$\hat{V}Q_k = \hat{U}WW^{\mathrm{H}}P_kR = \hat{U}P_kR.$$

It follows that $\hat{V}Q_k$ and $\hat{U}P_k$ span the same subspace. ∎

The import of this theorem is that no matter how you perform the expansion and contraction, mathematically you end up with a decomposition that has been filtered through the polynomial $(t - \mu_1) \ldots (t - \mu_{m-k})$. However, the procedure based on the Krylov–Schur form is numerically more reliable than the one based on implicit restarting.

4. Numerical stability. We now briefly consider the numerical stability of the algorithm. From standard techniques of rounding error analysis it can be shown that as the Krylov–Schur algorithm proceeds, the computed Krylov decompositions satisfy

$$AU = UB + ub^{\mathrm{H}} + R, \tag{4.1}$$

where $\|R\|/\|A\|$ is of the order of the rounding unit and grows slowly. If U is computed with reorthogonalization in the expansion phase, $U^{\mathrm{H}}U = I + F$, where $\|F\|$ is the order

of the rounding unit and also grows slowly. The following theorem shows that we can throw the residual error R back on the matrix A.

THEOREM 4.1. *Let* (4.1) *be satisfied and assume that* U *is of full rank. Let* $E = -RU^\dagger$, *where* $U^\dagger = (U^{\mathrm{H}}U)^{-1}U^{\mathrm{H}}$ *is the pseudoinverse of* U. *Then*

$$(A+E)U = UB + ub^{\mathrm{H}}, \tag{4.2}$$

and

$$\frac{\|R\|}{\|U\|} \leq \|E\| \leq \|R\|\|U^\dagger\|.$$

The lower bound holds for any matrix E *satisfying* (4.2).

Proof. The equation (4.2) is established by direct verification. The upper bound follows from taking norms in the definition of E. On the other hand, if E is any matrix satisfying (4.2), then $EU = -R$, and $\|R\| \leq \|E\|\|U\|$, which establishes the lower bound. □

Since U is nearly orthonormal, $\|U\|$ and $\|U^\dagger\|$ are near one. Hence the theorem shows that the computed generalized Arnoldi decomposition is an exact decomposition of a matrix near A. In this sense the Krylov–Schur algorithm (as well as the implicitly restarted Arnoldi algorithm) is backward stable.

5. Deflation and convergence. We now turn to the problem of deflating converged vectors from an orthonormal Krylov decomposition. We shall see later that if the concern is with a single Ritz vector then the deflation is easy. However, we can also use Krylov decompositions to deflate approximate eigenvectors or eigenspaces that are not obtained by a Rayleigh–Ritz procedure. Moreover, dependencies among the vectors to be deflated can cause the deflation procedure to require smaller residuals in the individual vectors. Consequently, we give a general analysis that covers both of these points.

We say a Krylov decomposition has been deflated if it can be partitioned in the form

$$A(U_1\ U_2) = (U_1\ U_2)\begin{pmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{pmatrix} + u(0\ b_2^{\mathrm{H}}).$$

When this happens, we have $AU_1 = U_1B_{11}$, so that U_{11} spans an eigenspace of A.

There are two advantages to deflating a converged eigenspace. First, by freezing it at the beginning of the Krylov decomposition we insure that the remaining space of the decomposition remains orthogonal to it. In particular, this gives algorithms the opportunity to compute more than one independent eigenvector corresponding to a multiple eigenvalue.

The second advantage of the deflated decomposition is that we can save operations in the contraction phase of an Arnoldi or Krylov–Schur cycle. The expansion phase does not change, and we end up with a decomposition of the form

$$A(U_1\ U_2\ U_3) = (U_1\ U_2\ U_3)\begin{pmatrix} B_{11} & B_{12} & B_{13} \\ 0 & B_{22} & B_{23} \\ 0 & B_{23} & B_{33} \end{pmatrix} + \beta u\mathbf{e}_m^{\mathrm{T}}.$$

Now since B_{11} is uncoupled from the rest of the Rayleigh quotient, we can apply all subsequent transformations exclusively to the eastern part the Rayleigh quotient and

to $(U_2\ U_3)$. If the order of B_{11} is small, the savings will be marginal; but as its size increases during the course of the algorithm, the savings become significant.

Of course, we will never have an exact eigenspace in our decompositions. Instead we will have a basis, say UW, for an approximate eigenspace and an approximation representation M of A on that subspace. The following theorem relates the norm of the residual $A(UW) - (UW)M$ to the quantities in the decomposition we must set to zero in order to deflate.

THEOREM 5.1. *Let*

$$AU = UB + ub^{\mathrm{H}} \tag{5.1}$$

be an orthonormal Krylov decomposition, and let $(M, Z) = (M, UW)$ *be given with* U *and* W *orthonormal. Let* $(W\ W_\perp)$ *be unitary, and set*

$$\tilde{B} = \begin{pmatrix} W^{\mathrm{H}} \\ W_\perp^{\mathrm{H}} \end{pmatrix} B(W\ W_\perp) = \begin{pmatrix} \tilde{B}_{11} & \tilde{B}_{12} \\ \tilde{B}_{21} & \tilde{B}_{22} \end{pmatrix}$$

and

$$\tilde{b}^{\mathrm{H}} = b^{\mathrm{H}}(W\ W_\perp) = (\tilde{b}_1^{\mathrm{H}}\ \tilde{b}_2^{\mathrm{H}}).$$

Then

$$\|AZ - ZM\|_{\mathrm{F}}^2 = \|\tilde{B}_{21}\|_{\mathrm{F}}^2 + \|\tilde{b}_1\|_{\mathrm{F}}^2 + \|\tilde{B}_{11} - M\|_{\mathrm{F}}^2, \tag{5.2}$$

where $\|\cdot\|_{\mathrm{F}}$ *denotes the Frobenius norm.*

Proof. From (5.1) we have $AZ - ZM = UBW - UWM + ub^{\mathrm{H}}W$. If we set

$$(\tilde{U}_1\ \tilde{U}_2) = (Z\ \tilde{U}_2) = U(W\ W_\perp),$$

then

$$\begin{aligned} AZ - ZM &= U(W\ W_\perp)\left[\begin{pmatrix} W^{\mathrm{H}} \\ W_\perp^{\mathrm{H}} \end{pmatrix} B(W\ W_\perp)\begin{pmatrix} I \\ 0 \end{pmatrix} - \begin{pmatrix} I \\ 0 \end{pmatrix} M\right] \\ &\quad + ub^{\mathrm{H}}(W\ W_\perp)\begin{pmatrix} I \\ 0 \end{pmatrix} \\ &= (\tilde{U}_1\ \tilde{U}_2)\begin{pmatrix} \tilde{B}_{11} - M \\ \tilde{B}_{21} \end{pmatrix} + u\tilde{b}_1^{\mathrm{H}}. \end{aligned}$$

The theorem now follows on taking norms. □

To see the consequences of this theorem, suppose that $AZ - ZM$ is small, and, using $(W\ W_\perp)$, we transform the Krylov decomposition $AU - UB = ub^{\mathrm{H}}$ to the form

$$A(\tilde{U}_1\ \tilde{U}_2) = (\tilde{U}_1\ \tilde{U}_2\ u)\begin{pmatrix} \tilde{B}_{11} & \tilde{B}_{12} \\ \tilde{B}_{21} & \tilde{B}_{22} \\ \tilde{b}_1^{\mathrm{H}} & \tilde{b}_2^{\mathrm{H}} \end{pmatrix}. \tag{5.3}$$

Then by (5.2)

$$\left\|\begin{pmatrix} \tilde{B}_{21} \\ \tilde{b}_1^{\mathrm{H}} \end{pmatrix}\right\|_{\mathrm{F}} \leq \|AZ - ZM\|_{\mathrm{F}}, \tag{5.4}$$

with equality if and only if M is the Rayleigh quotient $W^{\mathrm{H}}BW$. Thus if the residual norm $\|AZ - ZM\|_{\mathrm{F}}$ is sufficiently small, we may set $\tilde{B}_{21}$ and $\tilde{b}_1$ to zero to get the deflated

$$A(\tilde{U}_1\ \tilde{U}_2) \cong (\tilde{U}_1\ \tilde{U}_2)\begin{pmatrix}\tilde{B}_{11} & \tilde{B}_{12}\\ 0 & \tilde{B}_{22}\end{pmatrix} + u(0\ b_2^{\mathrm{H}}). \tag{5.5}$$

The deflation procedure that leads to (5.5) is backwards stable. If we restore the quantities that were zeroed in forming (5.5), we get the following relation:

$$A(\tilde{U}_1\ \tilde{U}_2) = (\tilde{U}_1\ \tilde{U}_2)\begin{pmatrix}\tilde{B}_{11} & \tilde{B}_{12}\\ 0 & \tilde{B}_{22}\end{pmatrix} + u(0\ b_2^{\mathrm{H}}) + \tilde{U}_2\tilde{B}_{21} + u\tilde{b}_1^{\mathrm{H}}.$$

If we write this decomposition in the form

$$A\tilde{U} = \tilde{U}\breve{B} + u\breve{b}^{\mathrm{H}} + R, \quad \text{where} \quad R = \tilde{U}_2\tilde{B}_{21} + u\tilde{b}_1^{\mathrm{H}},$$

then

$$\|R\|_{\mathrm{F}} \le \|AZ - ZM\|_{\mathrm{F}}.$$

If we now set $E = R\tilde{U}^{\mathrm{H}}$, then $(A+E)\tilde{U} = \tilde{U}\breve{B} + u\breve{b}^{\mathrm{H}}$. We may summarize these results in the following theorem.

THEOREM 5.2. *Under the hypotheses of Theorem* 5.1, *write the deflated decomposition* (5.5) *in the form*

$$A\tilde{U} \cong \tilde{U}\breve{B} + u\breve{b}^{\mathrm{H}}.$$

Then there is an E *satisfying*

$$\|E\|_{\mathrm{F}} \le \|AZ - ZM\|_{\mathrm{F}} \tag{5.6}$$

such that

$$(A+E)\tilde{U} = \tilde{U}\breve{B} + u\breve{b}^{\mathrm{H}}.$$

Equality holds in (5.6) *if and only if* M *is the Rayleigh quotient* $Z^{\mathrm{H}}AZ = W^{\mathrm{H}}BW$.

Because backward stability is commonly used to determine convergence, Theorems 5.1 and 5.2 suggest how one might combine convergence testing and deflation. Given an approximate pair (M, UW), we transform to the tilde form as in Theorem 5.1 and compute the backward error that would result from deflation. If this is small enough compared with A, we deem the pair to have converged and deflate.[3]

In practice we will seldom encounter a converging subspace unless it is a 2-dimensional subspace corresponding to a complex eigenvalue in a real Schur decomposition. Instead we will be confronted with converged, normalized Ritz pairs $(\mu_i, \hat{z}_i)$ $(i = 1, \ldots, p)$ of one kind or another, and the vectors in these pairs cannot be guaranteed to be orthogonal. If we arrange the vectors in a matrix $\hat{Z}$ and set $\hat{M} = \operatorname{diag}(\mu_1, \ldots, \mu_p)$, the residual $\hat{R} = A\hat{Z} - \hat{Z}\hat{M}$ must be small because the individual residuals are small.

[3] If the concern is with eigenvalues that are small compared with $\|A\|_{\mathrm{F}}$, we may have to demand a smaller backward error to get accurate results. For more, see the discussion of convergence in [13].

The deflation procedure requires an orthonormal basis for the approximate eigenspace in question, which is given by the QR factorization

$$\hat{Z} = ZT \tag{5.7}$$

of $\hat{Z}$. Unfortunately, the residual for Z becomes

$$R = \hat{R}T^{-1} = A\hat{Z}T^{-1} - \hat{Z}\hat{M}T^{-1} = AZ - ZM,$$

where $M = T\hat{M}T^{-1}$. If the columns of $\hat{Z}$ are nearly dependent, $\|T^{-1}\|$ will be large, and the residual may be magnified—perhaps to the point where the deflation cannot be performed safely. The effects of dependency on a different deflation algorithm have also been noted in [8].

It may seem paradoxical that we could have, say, two vectors each of which we can deflate but which taken together cannot be deflated. The resolution of this paradox is to remember that we are not deflating two vectors but the subspace spanned by them. If the vectors are nearly dependent, they must be very accurate to determine their common subspace accurately.

As we have mentioned, the deflation procedure is not confined to eigenpairs calculated by a Rayleigh–Ritz procedure. For example, it can be used to deflate harmonic Ritz vectors [10] or refined Ritz vectors [5]. However, if Ritz vectors are the concern, there is an easy way to deflate them in the Krylov–Schur method. After a cycle of the algorithm, let the current decomposition have the form

$$A(U_1\ U_2) = (U_1\ U_1)\begin{pmatrix} S_{11} & S_{12} \\ 0 & S_{22} \end{pmatrix} + u(0\ b_2^{\mathrm{H}}).$$

Here U_1 represents a subspace that has already been deflated, and S_{22} is the Schur form that remains after the contraction phase.

In this decomposition, to deflate the Ritz pair corresponding to the $(1,1)$-element of S_{22} we must set the first component of b_2 to zero. Consequently, all we have to do to deflate is to verify that that component satisfies our deflation criterion. If some other diagonal element of S_{22} is the candidate for deflation, we can exchange it into the $(2,2)$-position and test as above.

6. Assessment. In comparing the Krylov–Schur algorithm with the implicitly restarted Arnoldi algorithm, we must distinguish the sources of work in the algorithms. The first is the multiplication of a vector by A. Since A will usually be sparse, the cost of this product is unpredictable in general, but it is reasonable to assume that it forms a significant part—perhaps the dominant part—of the computation.

The second source of work is the expansion of the decompositions from one of order k to one of order m. It is easily seen from (3.1) that the work is $2n(m^2 - k^2)$ floating-point adds and multiplies, assuming reorthogonalization is performed. This count is the same for both algorithms.

In the contraction step, both algorithms must transform the Rayleigh quotient and accumulate the transformations in U. For efficiency, we do not accumulate the transformations in U as they are generated but instead accumulate them in an $m \times m$ matrix Q and then compute the new U_k in the form

$$U_m Q[:, 1{:}k]. \tag{6.1}$$

If $n \gg m$, the last step will dominate the transformations applied to the Rayleigh quotient and their accumulation in Q.

For the Krylov–Schur method we must compute the Schur decomposition of the Rayleigh quotient and transform the triangular factor. This means that Q will be full, and the final accumulation step (6.1) will require nkm floating-point additions and multiplications.

For the implicitly restarted Arnoldi we must also compute the Schur decomposition of the Rayleigh quotient H_m. But it is used only to determine the shifts, which are applied directly to H_m. The structure of the transformations is such that $Q[:, 1{:}k]$ is zero below its $m-k$ subdiagonal. This means that the operation count for (6.1) is $nmk - \frac{1}{2}k^2$ additions and multiplication.

To put things together, if $m = 2k$ and reorthogonalization is performed during the expansion, the Krylov–Schur algorithm has an operation count of $7nk^2$ whereas implicitly restarted Arnoldi has an operation count of $6\frac{1}{2}nk^2$. Thus implicitly restarted Arnoldi is marginally superior to Arnoldi–Schur when it comes to accumulation of transformations. Against this must be set the fact that Krylov–Schur deflates in an inexpensive and natural manner and does not require a special routine for purging.

7. Concluding remarks. The Krylov–Schur method admits variations. An important one is based on the observation that we can truncate a Krylov decomposition at any point where the Rayleigh quotient is block triangular [see (3.4)]. This means that when A is real we can work with real Schur forms of the Rayleigh quotient and avoid the necessity of complex arithmetic. The algorithm for exchanging eigenvalues mentioned above will also move the 2×2 blocks of the real Schur form so that the contraction phase proceeds as usual. In deflation, the block in question is moved to the position just after the previously deflated eigenvalues and blocks, and two components of b are tested. An unusual feature of complex eigenvectors is that they may fail to deflate, not because they are dependent on other deflated vectors, but because the real and imaginary parts of their eigenvectors are not sufficiently independent.

When A is Hermitian, the Krylov–Schur method becomes a restarted Lanczos algorithm—in fact the algorithm of Wu and Simon [18]. The Rayleigh quotient is diagonal, so that reordering of the eigenvalues reduces to simple permutations. Moreover, because the eigenvectors of the Rayleigh quotient are orthogonal, a Ritz pair with a small residual norm ϵ will deflate with backward error of order ϵ.

Since the Krylov–Schur method works explicitly with the eigenvalues of the Rayleigh quotient, it is an exact-shift method. Nonetheless, it stands ready to help the general shift method to deflate Ritz pairs and to get rid of unwanted pairs. One simply computes a Krylov–Schur form of the current decomposition and performs the procedures described above. Theorem 2.2 assures us that we can then return to a pure Arnoldi decomposition.

In fact Theorem 2.2 is really the heart of the matter. It allows us to operate freely on the Rayleigh quotient with the knowledge that we are always attached to a Krylov sequence. It is hoped that this freedom will find other applications.

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