SIAM J. SCI. COMPUT.
Vol. 24, No. 1, pp. 20–37

GMRES WITH DEFLATED RESTARTING*

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Abstract. A modification is given of the GMRES iterative method for nonsymmetric systems of linear equations. The new method deflates eigenvalues using Wu and Simon's thick restarting approach [*SIAM J. Matrix Anal. Appl.*, 22 (2000), pp. 602–616]. It has the efficiency of implicit restarting but is simpler and does not have the same numerical concerns. The deflation of small eigenvalues can greatly improve the convergence of restarted GMRES. Also, it is demonstrated that using harmonic Ritz vectors is important because then the whole subspace is a Krylov subspace that contains certain important smaller subspaces.

Key words. linear equations, GMRES, deflation, implicit restarting

AMS subject classifications. 65F10, 15A06

PII. S1064827599364659

1. Introduction.

We develop a new version of GMRES [38, 35] for solving large systems of linear equations. It deflates eigenvalues using the thick restarting technique given by Wu and Simon in [48] for the Lanczos eigenvalue method. Deflation can significantly improve the convergence of restarted GMRES, and it helps robustness by allowing the solution of many tough problems that have small eigenvalues.

The new method, called GMRES with deflated restarting or GMRES-DR, is mathematically equivalent to the method GMRES with eigenvectors [23] and to two methods in [25], including implicitly restarted GMRES. Thus this paper could be titled, "Yet another equivalent deflated GMRES method." However, the new approach has the efficiency of implicit restarting but is simpler and does not have the numerical concerns. Thus it should be a useful improvement.

In the next section, we discuss deflation for Krylov methods, including some previous approaches and results. Section 3 presents the new method, including a variant that removes approximate eigenvectors from the Krylov subspace. Then, in section 4, numerical examples are given that illustrate some points, including the importance of having Krylov subspaces with approximate eigenvectors as starting vectors.

2. Deflation in Krylov methods.

2.1. The importance of deflation.

It is well known that the convergence of Krylov subspace methods for linear equations depends to a large degree on the distribution of eigenvalues. (There are exceptions [15, 29].) And if there are small eigenvalues, then removing or deflating them can greatly improve the convergence rate. Likewise, for the problem of computing an eigenvalue, deflating nearby eigenvalues is helpful. One way that eigenvalues can be deflated is for the corresponding eigenvectors to be in the subspace. Once a Krylov subspace grows big enough, some deflation occurs automatically [46, 30]. However, restarted methods may not develop a large enough Krylov subspace for this automatic deflation, and convergence then suffers

*Received by the editors November 29, 1999; accepted for publication (in revised form) November 12, 2001; published electronically May 20, 2002. This work was supported by the National Science Foundation under grant NSF-CCR-9522612 and by the Baylor University Sabbatical Program.
http://www.siam.org/journals/sisc/24-1/36465.html
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accordingly. Also, even if approximate eigenvectors do develop that are accurate enough for deflation, they help only for that cycle and may need to be redeveloped after a restart. Some recent approaches deflate restarted Krylov methods. These are mentioned next for both eigenvalues and linear equations.

2.2. Deflation in restarted methods. In eigenvalue computations for small matrices, deflation of eigenvalues that have completely converged is a natural part of the procedure [32]. However, with large matrices and the Rayleigh–Ritz procedure [32, 33], computation of a particular eigenvector can be assisted by other eigenvectors even if they are not fully converged. And these other approximate eigenvectors do not have to be extremely accurate before the benefits of the deflation can be noticed. Thus it is common in non-Krylov Rayleigh–Ritz methods such as Davidson's method [8, 18, 26, 22, 28, 41, 39, 42] and subspace iteration [32, 33, 43, 16] to keep several eigenvector approximations in the subspace, even if only one is being concentrated on at a time. This can improve convergence, especially for difficult problems with close eigenvalues.

Deflation is more difficult for restarted Krylov methods because the natural way to restart is with only one vector. Block methods with additional storage and expense are possible [33]. A different approach is given in the implicitly restarted Arnoldi (IRA) method [40, 19, 24]. In this paper, when we refer to IRA, it means the approach using "exact shifts." (The unwanted Ritz values are used as shifts for the QR iteration.) IRA effectively restarts the Arnoldi for eigenvalues method [1, 33] with several approximate eigenvectors. Thus deflation can occur. In [23], deflation is added to restarted GMRES for linear equations by augmenting the Krylov subspace with approximate eigenvectors. The method is called GMRES with eigenvectors or GMRES-E. Likewise, Arnoldi for eigenvalues is augmented in [24] for a method that is mathematically equivalent to IRA at the end of each cycle. See [7, 36, 37] for more on augmenting Krylov subspaces.

In another approach to deflating GMRES, Kharchenko and Yeremin [17] build a preconditioner for the matrix using approximate eigenvectors, and Erhel, Burrage, and Pohl [13] develop a different preconditioner. Both of these approaches use approximate eigenvectors generated during only one GMRES cycle. (They may use several sets of vectors thus generated.) This is improved upon by Burrage and Erhel [4] with a method called DEFLATION that keeps working on the approximate eigenvectors outside of GMRES. DEFLATION combines its previous approximate eigenvectors with new ones from each cycle of GMRES.

Methods by Baglama et al. [2], Le Calvez and Molina [6], and the method in [25] all combine GMRES with implicit restarting. That way they can efficiently improve eigenvectors in the subspace. Baglama et al. [2] also build a preconditioner once the approximate eigenvectors are ready to be taken out of the subspace. The method in [25] is called GMRES-IR. It is mathematically equivalent to GMRES-E at the end of each cycle. These implicitly restarted GMRES methods are somewhat complicated and have stability problems associated with IRA. Stability of IRA is addressed by Lehoucq [19] and Lehoucq and Sorensen in [20] but not without additional complication. Lehoucq and Sorensen's locking and purging can also be used for the implicitly restarted GMRES methods and is implemented by Le Calvez and Molina. For eigenvalues problems, the complications that have been mentioned for IRA motivate the development by Wu and Simon [48] of a method for symmetric eigenproblems called thick-restart Lanczos. It is mathematically equivalent to the symmetric IRA approach, and it has about the same efficiency as IRA without the drawbacks. In this paper, we develop a corresponding new deflated version of restarted GMRES. First we

look in the next subsection at some needed details about some of the deflated Krylov methods. See [12] for more on deflated GMRES methods, including discussion of a related approach by De Sturler [10].

2.3. Keeping the subspace a Krylov subspace. In this subsection, we look at how an augmented subspace can still be a Krylov subspace. Notationally, we let m be the maximum dimension of the subspace and k be the number of approximate eigenvectors retained at a restart. Also, we let (θ_i, y_i) be a Ritz pair. Harmonic Ritz pairs [21, 31, 39, 27] are denoted as $(\tilde{\theta}_i, \tilde{y}_i)$. Let v_i be an Arnoldi vector from the Arnoldi recurrence [33]:

$$\begin{aligned} AV_m &= V_m H_m + h_{m+1,m} v_{m+1} e_m^T \\ &= V_{m+1} \bar{H}_m. \end{aligned} \tag{2.1}$$

Note that H_m denotes an m by m matrix, while $\bar{H}_m$ is $m+1$ by m. The ith coordinate vector is e_i. We refer to each pass through the Arnoldi iteration between restarts as one "cycle."

It was shown in [40] that when the Arnoldi method for eigenvalues is implicitly restarted with unwanted Ritz values as the shifts, the new initial vector is a combination of the desired Ritz vectors. And as given in [24] (see also [42]), the first k vectors of the new subspace are all combinations of the desired Ritz vectors. Thus the subspace

$$Span\{y_1, y_2, \ldots, y_k, v_{m+1}, Av_{m+1}, A^2 v_{m+1}, A^3 v_{m+1}, \ldots, A^{m-k-1} v_{m+1}\} \tag{2.2}$$

is the IRA subspace and is a Krylov subspace. Note that v_{m+1} is the last Arnoldi vector from the previous cycle of Arnoldi but from [40] it is also the $k+1$ Arnoldi vector in the new cycle. It is also shown in [24] that subspace (2.2) is equivalent to

$$Span\{y_1, y_2, \ldots, y_k, Ay_i, A^2 y_i, A^3 y_i, \ldots, A^{m-k} y_i\} \tag{2.3}$$

for each i such that $1 \leq i \leq k$. Thus subspace (2.2) contains Krylov subspaces with each Ritz vector as the starting vector.

In a restarted GMRES method, let r_0 be the residual vector from the previous cycle or, equivalently, the right-hand side for the new cycle. The subspace used in GMRES-E [23] is

$$Span\{r_0, Ar_0, A^2 r_0, A^3 r_0, \ldots, A^{m-k-1} r_0, \tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_k\}. \tag{2.4}$$

Thus approximate eigenvectors in the form of harmonic Ritz vectors are tacked on at the end of the Krylov subspace. It appears that putting them at the beginning would destroy the Krylov subspace. (If r_0 is orthogonalized against the harmonic Ritz vectors, then the next step of multiplying that vector by A appears to give an entirely different vector than just Ar_0.) However, as shown in [25] (see also [12]), the approximate eigenvectors can go first. This was implemented in GMRES-IR (following the approach for IRA). The approximate eigenvectors are combined in the right way so that there is an Arnoldi recurrence that can then be extended. In fact, subspace (2.4) is a Krylov subspace, though not with r_0 as the starting vector. The key is that the approximate eigenvectors are correctly chosen to be harmonic Ritz vectors. Subspace (2.4) is equivalent to

$$Span\{\tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_k, A\tilde{y}_i, A^2 \tilde{y}_i, A^3 \tilde{y}_i, \ldots, A^{m-k} \tilde{y}_i\}, \tag{2.5}$$

for $1 \leq i \leq k$, so it contains Krylov subspaces with each of the harmonic Ritz vectors as starting vectors.

In Wu and Simon's thick-restart Lanczos method [48], the Ritz vectors are put in front in a simpler way. They are not combined and are not part of an Arnoldi iteration. However, they can still be extended into the Krylov subspace (2.2). The first k orthonormal basis vectors are different, but the whole subspace is the same.

3. GMRES with deflated restarting. We look at Wu and Simon's approach to restarting [48], but for the nonsymmetric case, and we adapt it for solving linear equations. The new approach is called GMRES-DR, for GMRES with deflated restarting. We felt that name best describes what the method is trying to accomplish, although actually the term "deflated restarting" could be applied to all the approaches mentioned in subsection 2.2. The FOM version will be called FOM-DR, and it computes regular Ritz values while solving linear equations.

3.1. GMRES-DR. The first cycle of GMRES-DR is standard GMRES with r_0 being the residual vector computed. At the end of the cycle, the k desired harmonic Ritz vectors are computed. We let V be the orthonormal matrix whose columns span the subspace. For the second cycle, the first k columns of V are formed by orthonormalizing the harmonic Ritz vectors. Then r_0 is orthogonalized against them to form v_{k+1}. From there, the rest of V can be generated with the usual Arnoldi approach.

Note that this procedure does generate the Krylov subspace (2.4); see subsection 3.3. GMRES-DR gives the same results as GMRES-IR at every iteration (not counting forming the first k columns of V), and it is mathematically equivalent to GMRES-E at the end of each cycle. We next give the algorithm. Note that because the first $k+1$ vectors of the new V are formed from the previous subspace, the orthonormalization can be done with short vectors of length m or $m+1$. However, it has been noticed that for numerical reasons, v_{k+1} needs to be reorthogonalized. We have tested this successfully with no further reorthogonalization, but it seems likely that there are cases where more reorthogonalization is needed. In the algorithm that follows, we assume that the harmonic Ritz values are distinct. (See [25] for a little discussion of the nondistinct harmonic Ritz value case.) We also assume there are at least k finite harmonic Ritz values.

GMRES-DR

1. *Start.* Choose m, the maximum size of the subspace, and k, the desired number of approximate eigenvectors. Choose an initial guess x_0 and compute $r_0 = b - Ax_0$. The recast problem is $A(x - x_0) = r_0$. Let $v_1 = r_0/||r_0||$ and $\beta = ||r_0||$.
2. *First cycle.* Apply standard GMRES(m): generate V_{m+1} and $\bar{H}_m$ with the Arnoldi iteration, solve $\min||c - \bar{H}_m d||$ for d, where $c = \beta e_1$, and form the new approximate solution $x_m = x_0 + V_m d$. Let $\beta = h_{m+1,m}$, $x_0 = x_m$, and $r_0 = b - Ax_m$. Then compute the k smallest (or others, if desired) eigenpairs $(\tilde{\theta}_i, \tilde{g}_i)$ of $H_m + \beta^2 H_m^{-T} e_m e_m^T$. (The $\tilde{\theta}_i$ are harmonic Ritz values; see [31] or [27, p. 40] for this formula.)
3. *Orthonormalization of first k vectors.* Orthonormalize $\tilde{g}_i$'s, first separating into real and imaginary parts if complex, in order to form an m by k matrix P_k. (It may be necessary to adjust k in order to make sure both parts of complex vectors are included.)
4. *Orthonormalization of $k+1$ vector.* First extend $p_1, \ldots, p_k$ (the columns of

P_k) to length $m+1$ by appending a zero entry to each. Then orthonormalize the vector $c - \bar{H}_m d$ against them to form p_{k+1}. Note $c - \bar{H}_m d$ is the length $m+1$ vector corresponding to the GMRES residual vector. P_{k+1} is $m+1$ by $k+1$.

5. *Form portions of new H and V using the old H and V.* Let $\bar{H}_k^{new} = P_{k+1}^T \bar{H}_m P_k$ and $V_{k+1}^{new} = V_{m+1} P_{k+1}$. Then let $\bar{H}_k = \bar{H}_k^{new}$ and $V_{k+1} = V_{k+1}^{new}$.
6. *Reorthogonalization of $k+1$ vector.* Orthogonalize v_{k+1} against the earlier columns of the new V_{k+1}.
7. *Arnoldi iteration.* Apply the Arnoldi iteration from this point to form the rest of V_{m+1} and $\bar{H}_m$. Let $\beta = h_{m+1,m}$.
8. *Form the approximate solution.* Let $c = V_{m+1}^T r_0$ and solve $\min||c - \bar{H}_m d||$ for d. Let $x_m = x_0 + V_m d$. Compute the residual vector $r = b - Ax_m = V_{m+1}(c - \bar{H}_m d)$. Check $||r|| = ||c - \bar{H}_m d||$ for convergence and proceed if not satisfied.
9. *Eigenvalue computations.* Compute the k smallest (or others, if desired) eigenpairs $(\tilde{\theta}_i, \tilde{g}_i)$ of $H_m + \beta^2 H_m^{-T} e_m e_m^T$.
10. *Restart.* Let $x_0 = x_m$ and $r_0 = r$. Go to 3.

At each cycle after the first, a recurrence somewhat similar to the Arnoldi recurrence (2.1) is generated:

$$AV_m = V_{m+1} \bar{H}_m, \tag{3.1}$$

where $\bar{H}_m$ is upper-Hessenberg, *except* for a full leading $k+1$ by $k+1$ portion. Note that Schur vectors can be computed in steps 2 and 9 instead of eigenvectors.

We now look briefly at how the expense and storage of GMRES-DR compares to some previous methods. The main potential advantage of GMRES-DR compared to regular restarted GMRES is in the convergence, but it also does need only $m-k$ matrix-vector products per cycle while GMRES(m) uses m. GMRES-DR can be implemented with about the same length n storage as GMRES(m). GMRES-E is a little higher in both expense and storage than GMRES-DR. About k extra vectors of length n are normally used for GMRES-E.

GMRES-DR has about the same storage and expense requirements as GMRES-IR. The advantage of GMRES-DR is in the simplicity of the algorithm, compared to GMRES-IR. There is no QR iteration and no need for locking and purging to maintain stability, as is done for IRA and in Le Calvez and Molina's version of implicitly restarted GMRES [6]. Experiments are given in section 5 showing potential problems for GMRES-IR without lock and purge. GMRES-DR has no difficulties on the same examples. For more, see [44] in which Stewart shows stability of related eigenvalue methods.

3.2. FOM-DR. The main changes for an FOM version are that the small system of linear equations $H_m d = c$, with $c = V_m^T r_0 = \beta e_{k+1}$, is solved in step 8 instead of the small least squares problem, and the eigenvectors of H_m are computed in step 9. (This gives regular Ritz vectors instead of harmonic ones.) Step 2 is similarly changed. Also, the $k+1$ column of P_{k+1} in step 4 is just e_{m+1} with no orthonormalization. (The reorthogonalization in step 6 is still needed.)

3.3. The whole subspace is a Krylov subspace. As mentioned in subsection 2.3, it has been shown that the subspaces for GMRES-DR and FOM-DR are Krylov subspaces [25]. However, the proofs involved implicit restarting. Here we give more direct proofs.

We let λ be a scalar variable and let

$$\omega_i(\lambda) = \prod_{\substack{l=1 \\ l \neq i}}^{k} (\theta_l - \lambda).$$

LEMMA 3.1. *Let $\theta_1, \theta_2, \ldots, \theta_k$ be distinct scalars. Then for $0 \leq j \leq k-2$,*

$$\sum_{i=1}^{k} \frac{\theta_i^j}{\omega_i(\theta_i)} = 0.$$

Proof. Using the technique of partial fractions,

$$\frac{\lambda^j}{\omega_1(\lambda)} = \sum_{i=2}^{k} \frac{\theta_i^j}{\pi_i} \cdot \frac{1}{\theta_i - \lambda},$$

where

$$\pi_i = \prod_{\substack{l=2 \\ l \neq i}}^{k} (\theta_l - \theta_i).$$

Letting $\lambda = \theta_1$ and using $\theta_i - \theta_1 = -(\theta_1 - \theta_i)$ gives

$$\frac{\theta_1^j}{\omega_1(\theta_1)} = -\sum_{i=2}^{k} \frac{\theta_i^j}{\omega_i(\theta_i)},$$

and, with rearranging, we have the desired result. ∎

THEOREM 3.2. *Suppose we have a subspace $\mathcal{S} = Span\{y_1, y_2, \ldots, y_k, v\}$, with the property that*

$$Ay_i - \theta_i y_i = \gamma_i v, \tag{3.2}$$

for $\theta_1, \ldots, \theta_k$ distinct and for some nonzero γ_i's. Then $\mathcal{S}$ is a Krylov subspace.

Proof. We will construct a basis for the Krylov subspace. Let the starting vector be

$$s = \sum_{i=1}^{k} \frac{1}{\gamma_i \omega_i(\theta_i)} y_i,$$

with ω_i defined as above. Then for $j < k$, $A^j s$ is a combination of the y_i's. Specifically, we claim that

$$A^j s = \sum_{i=1}^{k} \frac{\theta_i^j}{\gamma_i \omega_i(\theta_i)} y_i$$

for $j < k$. To show this inductively, we assume that

$$A^{j-1} s = \sum_{i=1}^{k} \frac{\theta_i^{j-1}}{\gamma_i \omega_i(\theta_i)} y_i.$$

Multiplying both sides by A and then using (3.2) on the next step,

$$\begin{aligned} A^j s &= \sum_{i=1}^{k} \frac{\theta_i^{j-1}}{\gamma_i \omega_i(\theta_i)} A y_i \\ &= \sum_{i=1}^{k} \frac{\theta_i^{j-1}}{\gamma_i \omega_i(\theta_i)} (\theta_i y_i + \gamma_i v) \\ &= \sum_{i=1}^{k} \frac{\theta_i^{j}}{\gamma_i \omega_i(\theta_i)} y_i + \sum_{i=1}^{k} \frac{\theta_i^{j-1}}{\omega_i(\theta_i)} v \\ &= \sum_{i=1}^{k} \frac{\theta_i^{j}}{\gamma_i \omega_i(\theta_i)} y_i, \end{aligned}$$

where Lemma 3.1 is used for the last step. Thus we have our claim.

We have shown so far that $Span\{y_1, y_2, \ldots, y_k\} = Span\{s, As, \ldots, A^{k-1}s\}$ and thus is a Krylov subspace. Multiplying $A^{k-1}s$ by A and using (3.2), we can see that $A^k s$ is a combination of the y_i's and v. Thus $Span\{y_1, \ldots, y_k, v\} = Span\{s, As, \ldots, A^k s\}$. That completes the proof. ∎

The next two theorems are mostly corollaries of this last one. They give the results for GMRES-DR and FOM-DR.

THEOREM 3.3. *The subspace used by GMRES-DR is the subspace* (2.4) *and is a Krylov subspace.*

Proof. The harmonic Ritz residual vectors are defined as $A\tilde{y}_i - \tilde{\theta}_i \tilde{y}_i$, and they are all multiples of the GMRES residual vector [25]. Thus we have (3.2) with $v = r_0$ and with $\tilde{\theta}_i$ and $\tilde{y}_i$ in place of θ_i and y_i. Using Theorem 3.2, $Span\{\tilde{y}_1, \tilde{y}_2, \ldots \tilde{y}_k, r_0\}$ is a Krylov subspace. As usual, let $v_1, \ldots, v_{k+1}$ be the orthonormal basis for this subspace. GMRES-DR adds to this basis with an Arnoldi process, so it clearly generates a Krylov subspace. We next show that this subspace is (2.4).

The vector v_{k+2} comes from orthonormalizing Av_{k+1}.

$$\begin{aligned} Av_{k+1} &= A(\text{a combination of } r_0 \text{ and } \tilde{y}_i\text{'s}) \\ &= \text{a combination of } Ar_0 \text{ and } A\tilde{y}_i\text{'s} \\ &= \text{a combination of } Ar_0,\ r_0, \text{ and } \tilde{y}_i\text{'s}, \end{aligned}$$

using (3.2) on the last step. Thus $Span\{v_1, v_2, \ldots, v_{k+2}\} = Span\{\tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_k, r_0, Ar_0\}$. Continuing for several more steps shows that the subspace generated is $Span\{\tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_k, r_0, Ar_0, \ldots, A^{m-k-1}r_0\}$. ∎

Similarly, the subspace for FOM-DR is a Krylov subspace. Here we let r_0 be the FOM residual vector. The Ritz residual vectors are multiples of the FOM residual vector (and of v_{m+1}). Thus (3.2) holds with $v = r_0$, and the following result can be shown.

THEOREM 3.4. *$Span\{r_0, Ar_0, A^2r_0, \ldots, A^{m-k-1}r_0, y_1, y_2, \ldots, y_k\}$ is the subspace used by FOM-DR, and it is a Krylov subspace.*

3.4. Computing eigenvalues. The methods GMRES-DR and FOM-DR allow us to solve linear equations and compute eigenvalues at the same time. The eigenvalue portion of FOM-DR is equivalent to IRA. It is a nonsymmetric version of the thick-restart Lanczos given in [48]. GMRES-DR has a harmonic or interior eigenvalue version.

In step 9 of GMRES-DR, the harmonic Ritz vectors are not actually formed. However, if more eigenvector information is desired, they could be computed. Also their Rayleigh quotients could be determined. (See the ρ values in [21, 27].) The corresponding residual vectors are $A\tilde{y}_i - \rho_i \tilde{y}_i$, where ρ_i is the Rayleigh quotient of $\tilde{y}_i$. The eigenvector residual norms given in section 5 use this formula and thus are not the same as norms of the harmonic residual vectors that were mentioned in the proof of Theorem 3.3.

3.5. Deflating with eigenvectors removed from the subspace. In this subsection, we propose a method that removes approximate eigenvectors from the GMRES process. They are still used to deflate eigenvalues after being removed, but now the deflation is done in between cycles of standard restarted GMRES. This approach is an alternative to methods in [17, 13, 2, 4] which take approximate eigenvectors from GMRES and use them to build a preconditioner for the matrix. Here, instead of modifying the matrix, we deflate the eigenvalues with a projection over the fixed set of approximate eigenvectors. We call this approach GMRES-Proj. And the overall method of first applying GMRES-DR until approximate eigenvectors are developed and then using GMRES-Proj is called GMRES-DR/GMRES-Proj.

GMRES-Proj has cycles of GMRES alternating with a projection phase. We now look at some of the details. At the point that the switch is done from GMRES-DR to GMRES-Proj and the approximate eigenvectors are removed from the GMRES process, fix V_{k+1}^{pr} to be the matrix V_{k+1}^{new} in step 5 of the GMRES-DR algorithm. The superscript of V_{k+1}^{pr} denotes projection. Also let $\bar{H}_k^{pr}$ be the matrix $\bar{H}_k^{new}$ at that point. Then the key recurrence is

$$AV_k^{pr} = V_{k+1}^{pr} \bar{H}_k^{pr},$$

where $\bar{H}_k^{pr}$ is a $k+1$ by k full matrix and V_k^{pr} has columns that span the set of approximate eigenvectors. Note that we are required to save only the $k+1$ vectors of length n from V_{k+1}^{pr} and the small matrix $\bar{H}_k^{pr}$. We use the Galerkin projection [35] $(V_k^{pr})^T A V_k^{pr} (V_k^{pr})^T (x - x_0) = (V_k^{pr})^T r_0$, which becomes the small linear equations problem $H_k^{pr} d = c$, where $c = (V_k^{pr})^T r_0$.

Galerkin Projection between GMRES Cycles

1. Let the current approximate solution be x_0 and the current system of equations be $A(x - x_0) = r_0$.
2. Solve $H_k^{pr} d = c$, where $c = (V_k^{pr})^T r_0$.
3. The new approximate solution is $x_k = x_0 + V_k^{pr} d$.
4. The new residual vector is $r_k = r_0 - A V_k^{pr} d = r_0 - V_{k+1}^{pr} \bar{H}_k^{pr} d$.

We also mention the MINRES projection.

MINRES Projection between GMRES Cycles

Same as Galerkin, except:

2. Solve $\min ||c - \bar{H}_k^{pr} d||$, where $c = (V_{k+1}^{pr})^T r_0$.

The Galerkin projection is used in the experiments at the end of the next section. It worked better when projecting with poor eigenvector approximations, but a case has also been noticed for a slowly converging problem where the MINRES projection is better. Thus further study is needed on this.

Possible other future developments for GMRES-DR/GMRES-Proj include determining when to perform the switch to the GMRES-Proj approach, based on accuracy

of approximate eigenvectors. Also, work is needed to determine how frequently the projection needs to be done. In the examples in the next section, the projection is used in between every cycle of GMRES, but this is not generally necessary.

And, finally, we mention that GMRES-Proj can be used for solving problems with multiple right-hand sides. The approximate eigenvectors generated for the first right-hand side can be used to efficiently deflate eigenvalues while solving the other right-hand sides.

4. Numerical experiments. The first example has a preconditioned matrix from a real application. Other examples attempt to illustrate points about stability, about the importance of having certain Krylov subspaces, and about whether initial approximate eigenvectors are useful. Then GMRES-Proj is tested.

4.1. Some comparisons.

Example 1. We test GMRES-DR on the oil reservoir simulation matrix Saylor4 from the Harwell-Boeing Sparse Matrix Collection [11]. The matrix has dimension 3564 and is fairly sparse with an average of 6.3 nonzeros per row. The preconditioner is incomplete factorization with permutations but no fill-in (Matlab's luinc(A,'0')). While the matrix is actually symmetric, the preconditioning changes this to a nonsymmetric problem. The other methods are unrestarted full GMRES, restarted GMRES, QMR [14], and Bi-CGSTAB [45]. GMRES-DR(15,5) has $m = 15$ and $k = 5$ (subspaces are dimension 15, including five approximate eigenvectors), while GMRES(15) refers to standard restarted GMRES with subspaces of size 15. The right-hand side has normally distributed random elements. The initial guess x_0 is the zero vector.

Figure 4.1 has residual norms plotted against the number of matrix-vector products. GMRES-DR(15,5) competes well with full GMRES for this example and is much better than GMRES(15). Removing the five smallest eigenvalues makes a big difference. (The six smallest eigenvalues of the preconditioned matrix are 0.00077, 0.011, 0.041, 0.089, 0.095, 0.11, and the largest is about 1.8.) GMRES-DR is also better than QMR in terms of matrix-vector products. However, QMR is competitive in expense: the Matlab flop count for GMRES-DR is 23.6 million and is 23.4 million for QMR. Meanwhile, BiCGSTAB with its transpose-free approach uses only 16.4 million flops. Finally, we mention that while FOM-DR is not included in the figure, its results are almost the same as for GMRES-DR.

A full comparison of the various deflated GMRES methods mentioned in section 2 is beyond the scope of this paper. (See [12] for some theoretical comparisons.) However, in the next two examples, we will compare with the DEFLATION method of Burrage and Erhel [4]. Their approach is relatively simple, and they report favorable results in [4].

Example 2. We first compare GMRES-DR with DEFLATION using the preconditioned Saylor4 matrix from Example 1. GMRES-DR has $m = 15$ and $k = 5$, and DEFLATION uses a GMRES subspace of dimension 15 for the first cycle and subspaces of dimension 10 for the subsequent cycles. After the first GMRES cycle, five approximate eigenvectors are used to build a preconditioner for the matrix. After each of the other GMRES cycles, five approximate eigenvectors are removed from the subspace and combined with previous approximate eigenvectors using a small harmonic Rayleigh–Ritz procedure. Five new approximate eigenvectors are formed. Performance of the two methods is fairly similar. Figure 4.2 has the result for the solution of the linear equations and has the residual norms for the smallest approximate eigenpair. The linear equations residual norms are computed at every iteration, while the eigenvalue calculation is done only at the end of each cycle. The slightly

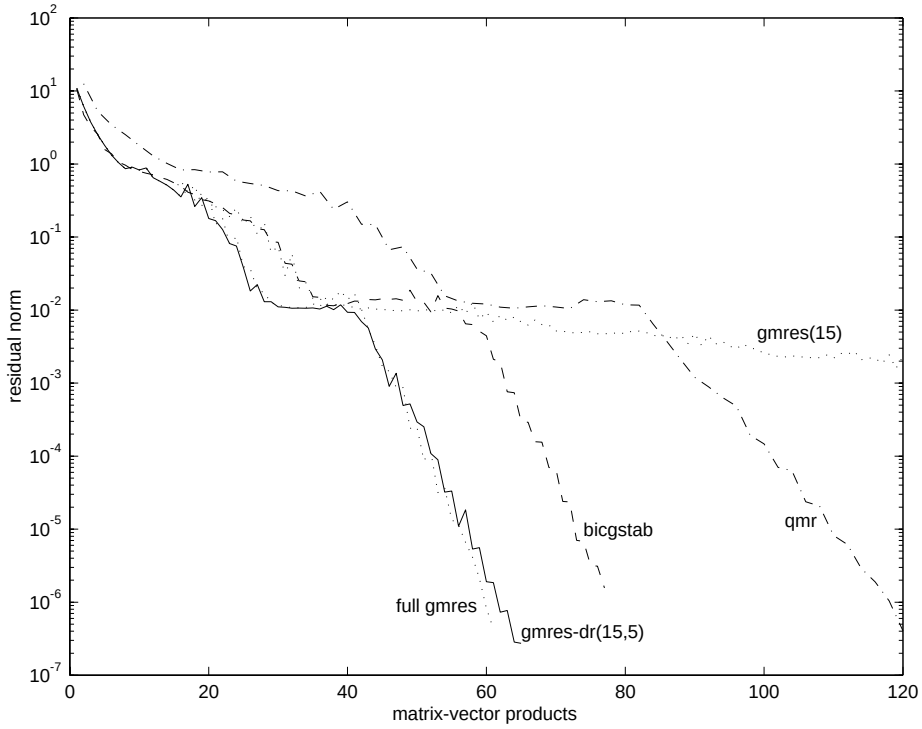

FIG. 4.1. *Comparison of convergence for the preconditioned Saylor4 matrix.*

better performance of GMRES-DR in solving the linear equations can probably be explained by its much better determination of the smallest eigenpair. DEFLATION is not able to develop as good approximations to the eigenvalues, probably because it does not keep the eigenvectors in the Krylov subspace. Nevertheless, however, the approximate eigenvectors for the DEFLATION method are accurate enough to be helpful for the convergence of the linear equations.

Example 3. In this example, we use a matrix with small eigenvalues that must be deflated before the linear equations can be accurately solved. The matrix is bidiagonal with entries 0.01, 0.1, 1, 2, 3, 4, ..., 997, 998 on the main diagonal and 1's on the super diagonal. The right-hand side has all 1's. No preconditioner is used. GMRES-DR has $m = 25$ and $k = 6$, and DEFLATION similarly uses six approximate eigenvectors to precondition and builds subspaces of dimension 19 (after the first cycle). GMRES-DR reaches residual norm of $4.2e-8$ after 16 cycles, while DEFLATION has residual norm of $1.2e-5$ at the same point. DEFLATION gets to $2.2e-8$ at 19 cycles. Thus, again, the performance of GMRES-DR is a little better, but DEFLATION is able to determine tough eigenvalues to enough accuracy to be a fairly effective method.

4.2. Instability of GMRES-IR. Two examples are given where instability in the QR algorithm causes problems in the GMRES-IR method. This is not surprising, given the investigation of IRA in [20]. The first example has a desired eigenvalue that converges too fast. The second has an undesired eigenvalue that is outstanding.

Example 4. The first matrix is diagonal with entries $1, 2, 3, 4, \ldots, 999, 10^5$. The right-hand side has all 1's. Tests are done in double precision on a Vax computer. We run GMRES-IR(10,2), but, instead of using the two smallest, we retain the har-

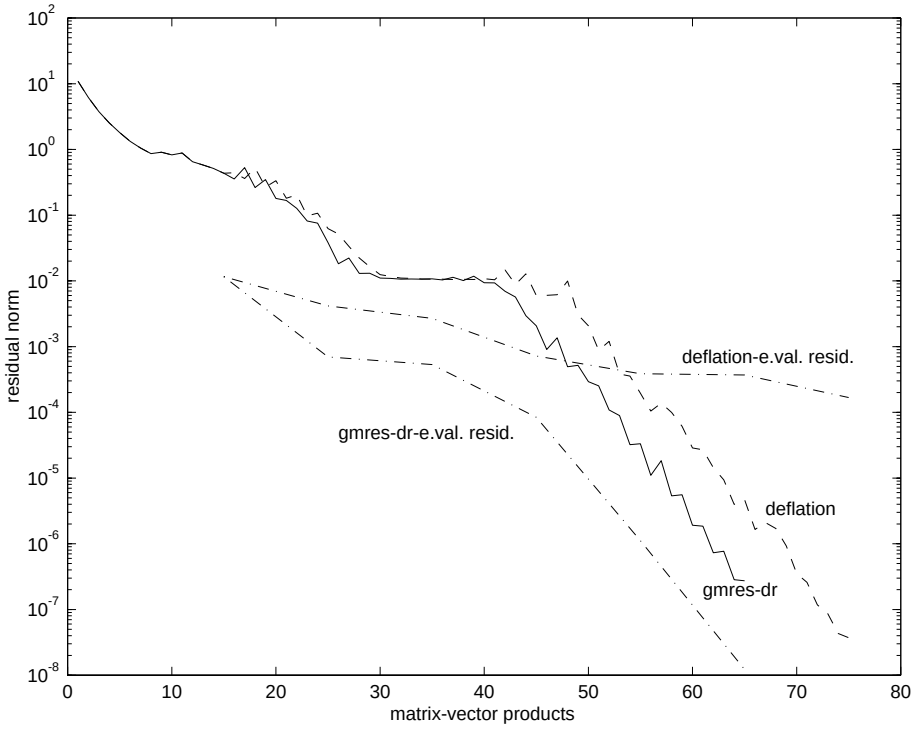

FIG. 4.2. *Linear equations and eigenvalue residuals for GMRES-DR and DEFLATION.*

monic Ritz vectors corresponding to the smallest and the largest harmonic Ritz values. Convergence is quick towards the big eigenvalue, since it is 100 times larger than the others. Eventually, numerical problems set in and the residual norm for the linear equations stalls out at 0.3e-2. The technique of locking is needed [20].

Example 5. The next matrix is the same except the last entry is 10^9 instead of 10^5. This time GMRES-IR(20,3) is used, and only the smallest harmonic Ritz pairs are retained. The residual norm stalls at 0.1e-2. Locking and purging [20, 6] are needed for this case. The problem does not seem severe, since it took an extremely large eigenvalue to cause it. However, large eigenvalues can result from preconditioning.

We note that GMRES-DR was also tested and does not have stability problems for these examples. As mentioned earlier, stability of related eigenvalue methods is shown in [44].

4.3. Importance of Krylov subspaces. Chapman and Saad note in [7, Figure 1] that GMRES-E works much better with harmonic Ritz vectors than with regular Ritz vectors. However, it turns out that this is not because the harmonic Ritz vectors are necessarily better than regular Ritz vectors. We think the important thing is to have certain Krylov subspaces. As mentioned earlier, GMRES-DR uses harmonic Ritz vectors so that the whole subspace (subspace (2.4)) is a Krylov subspace, and the subspace contains the smaller Krylov subspaces with each harmonic Ritz vector as the starting vector in (2.5). Likewise, the FOM-DR method keeps its whole subspace as a Krylov subspace by using regular Ritz vectors and has Krylov subspaces with each Ritz vector as the starting vector. However, if the wrong approximate eigenvectors are chosen, these properties are lost. Most importantly, the equivalence of subspace (2.5)

to subspace (2.4) will no longer hold. Of course, it is not the case that only Krylov subspaces can be effective. However, in this situation, keeping these Krylov subspace properties seems to be important for developing good eigenvectors.

The GMRES-E and FOM-E methods allow any choice for approximate eigenvectors, so we can compare the right choices with the wrong ones. Four methods are compared:

1. GMRES-E-Harm (GMRES-E with choice of harmonic Ritz vectors).
2. FOM-E-Ritz (FOM-E with choice of regular Ritz vectors).
3. GMRES-E-Ritz (GMRES-E with choice of regular Ritz vectors).
4. FOM-E-Harm (FOM-E with choice of harmonic Ritz vectors).

The first two methods listed are equivalent at the end of each cycle to GMRES-DR and FOM-DR. The last two methods choose the wrong approximate eigenvectors. We expect the wrong choice to have more of an effect on the solution of the eigenvalue problem than on the linear equations. The linear equations algorithms still have a Krylov subspace of dimension $m - k$, but the eigenvalue algorithms lose their Krylov subspaces with the approximate eigenvector as the starting vector. However, if the accuracy of the approximate eigenvectors is significantly affected, that can in turn slow convergence for the linear equations.

Example 6. Two examples will be given. This first one has everything the same as in Example 1. Figure 4.3 gives a comparison of the linear equations residual norms for the four methods and then a plot of the residual norm for the smallest Ritz value (regular or harmonic) with each method. The residual vectors for the harmonic Ritz

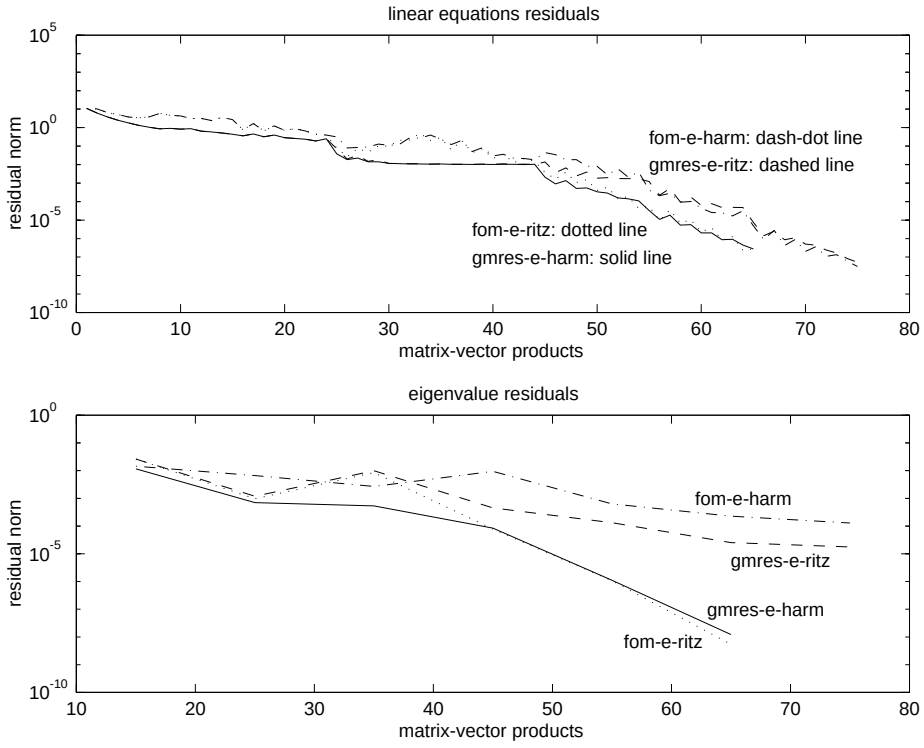

FIG. 4.3. *Comparing whole subspace Krylov vs. not Krylov; Saylor*4 *matrix.*

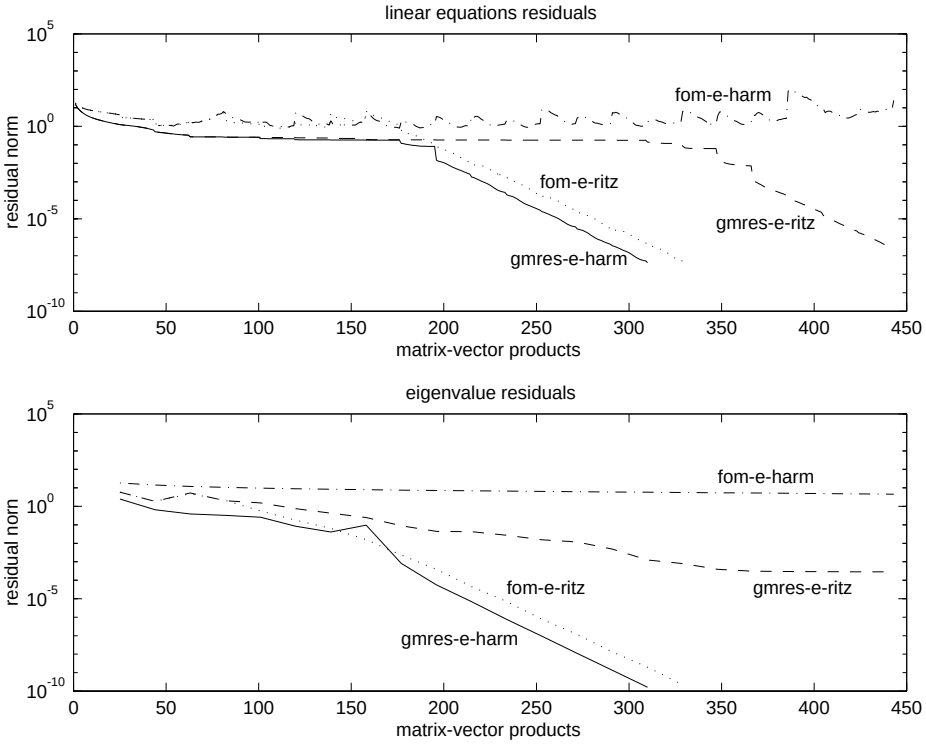

FIG. 4.4. *Comparing whole subspace Krylov vs. not Krylov; bidiagonal matrix.*

vectors are as defined in subsection 3.4. The linear equations have a value plotted at every iteration, while the eigenvalue residual norms are computed only at the end of a cycle. As expected, there is significant loss of eigenvector accuracy for the two methods that do not have the whole Krylov subspace. However, the approximate eigenvectors do become accurate enough to help with convergence of the linear equations. The convergence of the linear equations slows compared to the other methods but not to a large degree. Computing the small eigenvalues is tougher in the next problem.

Example 7. The bidiagonal matrix from Example 3 is used. All the methods have $m = 25$ and $k = 6$. Figure 4.4 shows that GMRES-E-Ritz has significant loss of performance compared with the harmonic choice. Meanwhile, FOM-E-Harm never converges. Without Krylov subspaces built from the harmonic Ritz vectors, the eigenvectors do not become accurate enough to help solve the linear equations. Thus having subspace (2.5) can be crucial.

Looking back at Examples 2 and 3, they give further evidence for this point. DEFLATION does not have subspace (2.5) and does not find the eigenpairs as accurately.

4.4. Initial approximate eigenvectors. It might be expected that GMRES-E would be better than GMRES-DR in the case where there are initial approximate eigenvectors available. They could help convergence of GMRES-E from the beginning, while GMRES-DR would have to generate approximations from scratch. In fact, it was suggested in [24] that for the case of initial approximations, the eigenvalue method corresponding to GMRES-E (called Arnoldi with eigenvectors) has an advantage over

the IRA method. Initial eigenvector approximations are likely to be available in some situations, including when deflation methods are used for nonlinear problems or multiple right-hand sides problems. However, putting in initial vectors will cause some of the Krylov properties to be lost. Here we investigate whether the initial vectors really are useful for solving linear equations.

Example 8. The matrix and starting vector are the same as in Example 3. The first row of Table 4.1 corresponds to GMRES-DR, so there are no initial vectors. The other rows are for the GMRES-E method using harmonic Ritz vectors with $m = 25$ and $k = 6$. Each test uses six initial vectors y_i with 1.0 in the ith position and $\epsilon * randn$ in the other positions, where $randn$ is a random number distributed Normal(0,1). GMRES-DR has $m = 19$ for the first cycle and $m = 25$ for the other cycles. This makes it correspond closer to GMRES-E with initial vectors because the Krylov subspaces with r_0 as starting vector (see the first part of subspace (2.4)) are always dimension 19 for both methods. GMRES-DR also has $k = 6$. The columns of Table 4.1 give the value of ϵ, the residual norm for the smallest approximate eigenvalue after the first cycle, the number of matrix-vector products to improve the linear equations residual norm by a factor of 10^{-5}, and the residual norm for the smallest approximate eigenvalue after the last cycle.

The results seem to divide into three cases, depending on the accuracy of the initial vectors. With $\epsilon = 1$ to $\epsilon = 10^{-2}$, the initial vectors are poor approximate eigenvectors, and they do not help solve the linear equations. However, what is interesting is that the method appears to ignore the initial vectors. The performance is about the same as in GMRES-DR. Probably, after the first cycle, the subspaces used are almost the same as if no initial vectors had been provided, and, if so, then the whole subspaces contain subspaces almost the same as (2.5).

With medium accuracy in the initial vectors, $\epsilon = 10^{-3}$ to about $\epsilon = 10^{-5}$, the solution of the linear equations improves a little. Apparently, however, as the initial vectors become useful, the method deviates significantly from GMRES-DR and then perhaps the whole subspaces no longer approximately contain subspaces (2.5). In any event, the eigenvalue approximations do not become as accurate. In fact, while the approximate eigenvectors for $\epsilon \geq 10^{-2}$ keep improving, convergence stalls out for $\epsilon \leq 10^{-3}$ at the level of accuracy shown in the last column of the table. However, this

TABLE 4.1
Effect of the accuracy of initial vectors; bidiagonal matrix.

ϵ	Eig. res. norm after cycle 1	Mvp's for lin.eq.'s	Eig. res. norm after last cycle
no init.	4.3	245	3.3e-7
1	4.4	247	1.1e-6
1e-1	4.4	247	1.1e-6
1e-2	4.4	247	1.3e-6
1e-3	4.4	229	1.0e-4
1e-4	2.1	220	1.9e-4
1e-5	1.0	190	4.3e-4
1e-6	3.6e-1	140	1.3e-4
1e-7	5.8e-3	90	2.0e-5
1e-8	2.0e-4	80	1.7e-4
1e-9	1.9e-5	80	1.9e-5
1e-10	1.9e-6	80	1.9e-6

TABLE 4.2
Effect of the accuracy of initial vectors; Saylor4 matrix.

ϵ	Eig. res. norm after cycle 1	Mvp's for lin.eq.'s	Eig. res. norm after last cycle
no init.	3.7e-2	65	9.1e-10
1	3.7e-2	65	2.3e-9
1e-1	3.7e-2	67	2.7e-9
1e-2	3.7e-2	69	1.6e-8
1e-3	3.3e-2	65	3.2e-7
1e-4	6.0e-3	65	1.1e-6
1e-5	6.0e-4	51	2.4e-6
1e-6	6.0e-5	45	5.8e-5
1e-7	6.0e-6	37	6.0e-6
1e-8	6.0e-7	35	6.0e-7

is accurate enough to deflate and thus assist in solving the linear equations.

Finally, with good initial vectors, ϵ from about 10^{-6} to 10^{-10}, deflation occurs at the beginning and convergence of the linear equations is much faster. The eigenvectors again stall out and may not improve at all after cycle 1.

As a conclusion to this example, it seems that the approximate eigenvectors have to be reasonably accurate before they are helpful. However, on the other hand, using poor approximations is not harmful, as might have been expected.

Example 9. We now do the same experiment as in the previous example but for the Saylor4 matrix. GMRES-E uses $m = 15$ and $k = 5$, while GMRES-DR ("no init.") uses $m = 10$ for the first cycle and $m = 15$ in subsequent ones. The linear equations residual norm is improved by a factor of 10^{-8} this time. The initial vectors for GMRES-E are the approximate eigenvectors from the final cycle of GMRES-DR with every entry perturbed by adding $\epsilon * randn$.

See Table 4.2 for the results. Again GMRES-E can essentially ignore the initial vectors if they are poor and can perform reasonably well. If the initial vectors are fairly accurate, they can be very useful for the linear equations, but there is limited improvement in the accuracy of the eigenvectors.

4.5. Test of removing eigenvectors from subspace. We now test the GMRES-DR/GMRES-Proj method which runs GMRES-DR and then switches to GMRES-Proj. As discussed in subsection 3.5, GMRES-Proj applies cycles of standard restarted GMRES alternating with a projection over the approximate eigenvectors that were generated by GMRES-DR.

Example 10. We again test with the preconditioned Saylor4 matrix. GMRES-DR uses $m = 15$ and $k = 5$. The switch from GMRES-DR to GMRES-Proj is after the fourth cycle. GMRES-Proj uses GMRES(10) with projection over the five approximate eigenvectors. This method converges almost the same as if GMRES-DR is continued. After six cycles, GMRES-DR has residual norm $2.7e-7$ and GMRES-Proj gets to residual norm $3.6e-7$. After eight cycles, GMRES-DR is at $6.5e-11$ and GMRES-Proj has residual norm $7.1e-11$.

Next we try switching to GMRES-Proj after three cycles. The result is not as good because the eigenvectors are not quite accurate enough to be removed at that point. After six cycles, GMRES-Proj gets to residual norm $1.9e-3$ versus $2.7e-7$ for GMRES-DR. The smallest harmonic Ritz value found after three cycles is 0.0111. This approximate eigenvalue is much better after four cycles with 0.000779 compared

TABLE 4.3
The effect of when eigenvectors are removed

Remove after cycle	Harmonic Ritz val.	Mvp's for $rn < 10^{-6}$	Mvp's for $rn < 10^{-8}$
1	0.0241722	438	634
2	0.0111092	872	1304
3	0.0110664	122	162
4	0.0007785	63	74
5	0.0007707	62	74
6	0.0007707	62	74
no switch	0.0007707	62	73

to the true eigenvalue of 0.0007707. The significant improvement in this approximate eigenvalue from cycle 3 to cycle 4 makes a difference in the convergence of the GMRES-Proj method.

Continuing this study of the need for a certain degree of accuracy of the approximate eigenvectors, Table 4.3 gives results with the switch after different cycles. Only the smallest harmonic Ritz value is listed because it is quite small relative to the others and is thus very significant. The harmonic Ritz value gives a better idea of the accuracy of the associated approximate eigenvector than does the eigenvector residual norm (see Figure 4.2) in this case because, after cycles 2 and 3, the smallest harmonic Ritz value approximates the second eigenvalue of the preconditioned matrix. We see from the table that there is not a good approximation to the smallest eigenpair until after cycle 4. The method has difficulty until this reasonably accurate eigenvector is found. It seems that any deflated GMRES method would share this trait of needing at least roughly accurate approximations to the small eigenpairs before it can be effective.

Example 11. We do another test of GMRES-DR/GMRES-Proj with the bidiagonal matrix from Example 5. For GMRES-DR, we use $m = 25$ and $k = 6$ and then GMRES-Proj has GMRES(19) and six approximate eigenvectors for the projection. The switch from GMRES-DR to GMRES-Proj is done after 10 cycles (196 matrix-vector products). The results for GMRES-Proj are similar to those if GMRES-DR is continued. For example, after 16 cycles, GMRES-DR has residual norm $4.2e-8$ and GMRES-Proj gets to $6.0e-8$. However, if the switch is after eight cycles, the approximate eigenvectors are not quite ready and the residual norm of GMRES-Proj reaches only $1.4e-6$ after 16 cycles.

5. Conclusion. GMRES with deflated restarting was introduced. It is a new way of deflating eigenvalues from GMRES that uses the thick restarting idea. It appears to be an effective restarted GMRES approach to solving linear equations. Nested restarted methods [34, 47, 9] might also be worth considering in some cases, particularly for quite sparse matrices. It seems that GMRES-E could more easily be used in a nested method than could GMRES-DR.

The deflation in GMRES-DR makes restarted GMRES more robust and makes it converge much faster for tough problems with small eigenvalues. It thus can compete better with nonrestarted methods such as QMR, and there is not much added expense per iteration compared to standard restarted GMRES. Matrix-vector products are even saved for the first k vectors of the subspace.

Examples were given that illustrate the remarkable fact that if a Krylov subspace is augmented with the right choice of approximate eigenvectors (harmonic Ritz vec-

tors for GMRES), then the whole subspace is a Krylov subspace, and this subspace contains smaller Krylov subspaces with each harmonic Ritz vector as starting vector. Better performance results.

Also mentioned was a method called GMRES-Proj, which deflates eigenvalues outside of the Krylov subspace. GMRES-Proj is less expensive than the methods that use approximate eigenvectors to build a preconditioner, but further testing and comparison with these other approaches is needed.

Even though we claimed that GMRES-DR has the advantages of GMRES-IR without the drawbacks, GMRES-IR may still have some uses. For example, there are many possible choices in the shifts used in the implicit restarting, all of which lead to Krylov subspaces. Leja points are one choice that has been used in implictly restarted Lanczos [5, 3].

Acknowledgments. The author wishes to thank Eugene Tidmore and Jeff Mitchell for the proof of Lemma 3.1 and the referees for their several careful readings and many suggestions for improvements.

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