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RESEARCH ARTICLE

Pseudoeigenvector bases and deflated GMRES for highly nonnormal matrices†

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Summary

Pseudoeigenvalues have been extensively studied for highly nonnormal matrices. This paper focuses on the corresponding pseudoeigenvectors. The properties and uses of pseudoeigenvector bases are investigated. It is shown that pseudoeigenvector bases can be much better conditioned than eigenvector bases. We look at the stability and the varying quality of pseudoeigenvector bases. Then applications are considered including the exponential of a matrix. Several aspects of GMRES convergence are looked at, including why using approximate eigenvectors to deflate eigenvalues can be effective even when there is not a basis of eigenvectors.

KEYWORDS

eigenvalues, deflation, GMRES, linear equations, nonnormal matrices pseudoeigenvalues

1 | INTRODUCTION

Pseudoeigenvalues have been studied extensively (see previous work[1–5]) for nonnormal matrices and for stability of differential equations and other applications. Here, we study the associated pseudoeigenvectors. They have been looked at before[6–8] but not as extensively studied as pseudoeigenvalues. In particular, pseudoeigenvectors have not been used to analyze generalized minimal residual (GMRES) convergence.

Pseudoeigenvectors of a matrix can be thought of as the eigenvectors of a nearby matrix. We define ϵ-pseudoeigenvectors as follows:

Definition 1. Let A be an n by n matrix. Let E be any matrix such that $\|E\| = \epsilon$. Then the eigenvectors of $A + E$ are defined to be ϵ-pseudoeigenvectors of A. The n associated eigenvalues are ϵ-pseudoeigenvalues of A.

Note the usual definition of ϵ-pseudoeigenvalues includes eigenvalues of all matrices with perturbation of norm less than ϵ (or less than or equal to). Here, we choose only ones associated with perturbations of norm equal to ϵ.

We observe that there are many ϵ-pseudoeigenvectors even for a fixed value of ϵ. There is a different set for each choice of E. For a particular perturbation matrix E, the set of ϵ-pseudoeigenvectors will usually have n linearly independent elements.

When the pseudoeigenvectors from a specific perturbation E form a basis for R^n (as they generally will), we call this a pseudoeigenvector basis. Such a basis can be useful when there is not a good basis made up of eigenvectors, as is the case when the eigenvector basis is highly ill-conditioned or when the Jordan canonical form of A is non-diagonal. In this paper, we will analyze and apply pseudoeigenvector bases.

One important application is the GMRES[9] method for solving large nonsymmetric systems of linear equations. Convergence of GMRES for highly nonnormal matrices is a difficult topic. Some aspects have been studied.[10–17] Pseudoeigenvalues have been used to analyze GMRES convergence.[1,5,18,19] Here, we analyze with pseudoeigenvector bases.

Deflated GMRES methods (see previous work[20–29]) can be an improvement over regular restarted GMRES when the matrix has small eigenvalues that slow the convergence. One particular deflated GMRES method called GMRES-DR[26] is a restarted GMRES method that augments the Krylov subspace with approximate eigenvectors. The convergence can often be

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improved, because the approximate eigenvectors essentially remove or deflate out the eigenvalues once they are accurate enough. It is not clear that such a deflated method will be helpful for highly nonnormal matrices, because removing some eigenvalues is of dubious value when the eigenvalues do not control the convergence. We will give examples showing that deflated GMRES can nevertheless be effective for highly nonnormal matrices and will offer an explanation.

Section 2 shows that pseudoeigenvector bases can be better conditioned than the original eigenvector basis. It is also observed that the conditioning can vary for pseudoeigenvector bases with the same size perturbation, and an example is given with what appears to be a nearly optimal basis. Section 3 considers stability of pseudoeigenvector bases. The rest of the paper has some examples of applications of pseudoeigenvector bases. Section 4 has the exponential of a matrix. Tortoise and the Hare convergence of GMRES[13] is in Section 5. Application to general GMRES convergence is in Section 6, while Section 7 has deflated GMRES.

2 | CONDITIONING OF PSEUDOEIGENVECTOR BASES

2.1 | A pseudoeigenvector basis can be better conditioned

In this section, we demonstrate that for a nonnormal matrix A, pseudoeigenvector bases can be better conditioned than the original eigenvector basis. Here, the measure of the conditioning of a basis stored as columns of X is $\kappa(X) = \|X\|\|X^{-1}\|$. It is certainly possible for a perturbation to not improve conditioning of eigenvectors (e.g., if $E = \epsilon I$). However, the structure of many matrices of interest causes their eigenvectors to be very ill-conditioned and allows perturbations to improve them. Davies[8] has an investigation into this same topic, including a formula for evaluating the accuracy of an approximate diagonalization of the form $A + E = XDX^{-1}$.

Here, we norm all eigenvectors and pseudoeigenvectors to one. The norming of vectors can effect the conditioning of a basis, but unit norms give results that are near to the optimal.[30]

An obvious case for improvement is when the matrix is not diagonalizable, and so there is not a basis of eigenvectors. We use such a matrix for the first example.

Example 1. As one of the test matrices in this paper, we let A be the bidiagonal matrix with 1's in all the diagonal and superdiagonal positions. So the matrix is made up of one large Jordan block. Figure 4 has plots of two sets of 10^{-2}-pseudoeigenvalues for this matrix of size $n = 100$ and real perturbations. However, here, we have $n = 500$, and we use complex perturbation matrices E of norm ϵ. They are formed by filling an n by n matrix N with entries that have real part generated randomly with normal (0,1) distribution and imaginary part generated the same way. Then E is set to $(\frac{\epsilon}{\|N\|}) * N$, and the eigenvectors of $A + E$ are computed. These are an ϵ-pseudoeigenvector basis for A. With a perturbation matrix of norm 10^{-8}, the condition number for the pseudoeigenvector basis is $2.1*10^{10}$, while with $\epsilon = 10^{-4}$, the condition number is $1.6*10^{6}$. There is a trade-off: as the perturbation becomes larger, the conditioning of the pseudoeigenvector basis gets better, but this basis has eigenvectors for a matrix further from the original one.

Next, we consider highly nonnormal matrices that are diagonalizable. In our testing, the conditioning of the eigenvectors can usually be improved with a perturbation. We give a Toeplitz matrix example. Experiments with some other Toeplitz matrices give similar results; some have even more highly ill-conditioned eigenvectors and some less.

Example 2. The Butterfly matrix from Trefethen et al.[5] has zeros on the main diagonal, superdiagonal with all -i's, the diagonal above that has 1's, the subdiagonal has i's, and the diagonal below has -1's. We let $n = 100$ and 500. For $n = 100$, the eigenvector basis for the matrix is ill-conditioned with condition number equal to $1.8*10^{9}$. This is shown in Figure 1 as the horizontal dashed line. The dots in the figure show the conditioning of the pseudoeigenvector bases that result from perturbing the matrix with random, complex matrices of increasing norm. We see that perturbing the matrix improves the conditioning of the eigenvectors starting with perturbation matrices of norm 10^{-8}. The pseudoeigenvector basis is significantly better conditioned for larger perturbation matrices such as with norm 10^{-4} or 10^{-2}. Next, the Butterfly matrix of size $n = 500$ is considered. The condition number for the matrix of eigenvectors is now $2.5*10^{19}$. This is shown on Figure 1 with the horizontal solid line. Of course, this is the computed condition number of a computed matrix of eigenvectors and is unlikely to be accurate. Even with a small perturbations, the conditioning improves dramatically. It is interesting that the relationship on the log–log plot between

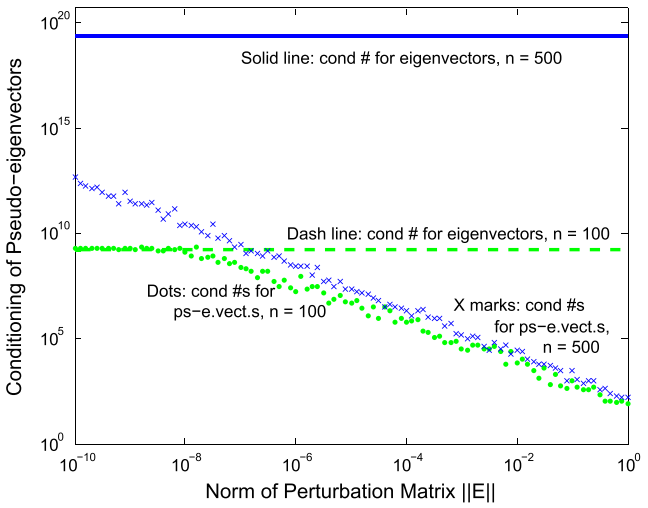

FIGURE 1 Conditioning of pseudoeigenvector bases for the butterfly matrix

the norm of the perturbation matrix and the condition number of the basis of pseudoeigenvectors is almost linear. If the perturbation matrices are instead just scaled versions of the same random matrix, then the dots fall even closer to a straight line. Davies'[8] formula for evaluating a pseudoeigenvector basis is $\sigma = \kappa * \epsilon_0 + \|E\|$, where κ is the conditioning of the pseudoeigenvector basis and ϵ_0 is machine epsilon. Lower σ indicates a better basis. For this example, with $n = 500$, the lowest σ is about 10^{-7} at $\epsilon = \|E\| = 10^{-7}$.

2.2 | Quality of pseudoeigenvector bases

We consider better conditioned bases to be of better quality. In this subsection, we show that even for a fixed ϵ, it is possible for some ϵ-pseudoeigenvector bases to be significantly better than others. We will concentrate on Jordan block matrices such as the one used in Example 1, and will give a conjecture on the optimal pseudoeigenpairs for this matrix.

Example 3. We consider the 2 by 2 version of the Jordan block matrix in Example 1. We generate 1,000 different real perturbation matrices of norm 10^{-3} and look at the conditioning of the resulting pseudoeigenvector bases. It is surprising how much this conditioning varies. There is over two orders of magnitude difference between the highest condition number $4.5*10^3$ and the lowest of $3.2*10^1$. Figure 2 has a log–log plot of the condition numbers versus the distance between the two pseudoeigenvalues for each perturbation. The better conditioned pseudoeigenvector bases occur when the pseudoeigenvalues are more separated. It is interesting how consistent this relationship is; in fact, it is linear on this log–log plot. The slope is negative one. This means that the condition number is inversely proportional to the distance between pseudoeigenvalues. We also note that if instead complex perturbations are used, then there is not as much variance in the conditioning. The range is from $2.4*10^2$ down to $3.2*10^1$.

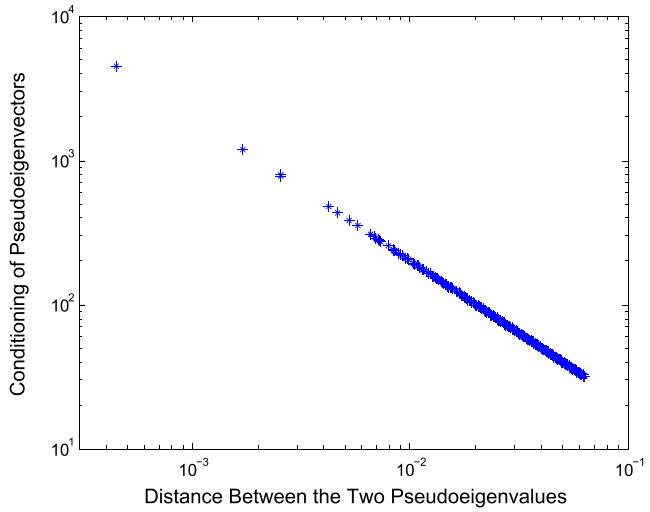

FIGURE 2 Condition of pseudoeigenvector basis as a function of distance between pseudoeigenvalues for 2 by 2 matrix

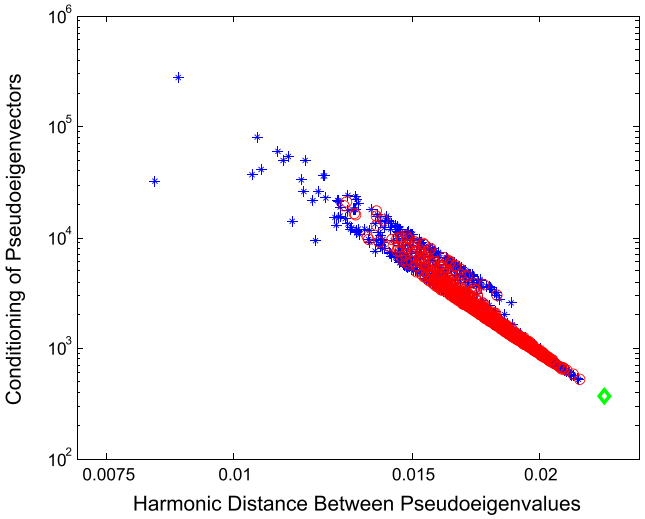

FIGURE 3 Condition of pseudoeigenvector basis as a function of distances between pseudoeigenvalues for 7 by 7 matrix

However, if these complex perturbation results are plotted as in Figure 2, the points fall on the same line. It has been noted before that complex perturbations can give a wider spread on the pseudoeigenvalues,[5] and as we have seen here, bigger spread means better conditioning.

We next consider the 7 by 7 version of this matrix. Again we use perturbations of norm 10^{-3}. Figure 3 has the conditioning of the pseudoeigenvectors plotted against the harmonic distance between the pseudoeigenvalues (this is the reciprocal of the sum of the reciprocals of all of the distances). This is done for 1,000 real perturbations (asterisks) and 1,000 complex perturbations (circles). The diamond on the graph is for a perturbation of 10^{-3} in the (7,1) position; this is discussed in the next example. The points in this log–log plot are not linear as they were for the 2 by 2 case, but most of the values do fall in a band. The complex perturbations follow the same pattern as the real ones but do not have the higher conditioned outliers. We also tried 100 by 100 matrices but did not see a relationship between conditioning and harmonic distance.

We next look at structured perturbations. These have been considered before for the pseudoeigenvalues; see Trefethen et al.[5] and its references.

Example 4. We consider a specific perturbation for the Jordan block matrix. Let E be the matrix that is all zeros except for a positive entry of size ϵ in the $(n,1)$ position. Then the eigenvalues of the perturbed matrix are

$$1 + \sqrt[n]{\epsilon} exp\left(i\frac{2k\pi}{n}\right), \quad k = 0, 1, \ldots, n-1.$$

The pseudoeigenvalues are on a circle of radius $\sqrt[n]{\epsilon}$ around the point (1,0). So the pseudoeigenvalues are well spaced. The condition number of the pseudoeigenvector basis is $\epsilon^{\frac{1}{n}-1}$.[31] For more on perturbations of Jordan blocks, see Moro et al.[6] For the case of the 7 by 7 matrix with an $\epsilon = 10^{-3}$

perturbation in the (7,1) entry, the condition number is $3.7*10^2$. This compares to values between $5*10^2$ and $3*10^5$ for the 2,000 real and complex perturbations in the previous example. For a Jordan block matrix of size $n = 500$, with 100 random real perturbations and 100 random complex, the minimum pseudoeigenvector bases condition number is $5.0*10^4$ and the maximum is $2.1*10^6$. Meanwhile, for the special $(n,1)$ entry perturbation, the condition number is $9.9*10^2$. So this gives a significant improvement in the conditioning of the pseudoeigenvector basis. We conjecture that this is a nearly optimal perturbation for the Jordan block matrix. Perhaps this will help in finding good pseudoeigenvector bases for other structured matrices.

Example 5. Consider the 3 by 3 matrix with ones on the main diagonal, a 10 in the (1,2) position and a 1 in the (1,3) position and zeros elsewhere. Experimentally, the best perturbation appears to be an ϵ in the (2,1) position.

For some other 3 by 3 matrices, we tested two approaches to finding a good perturbation. One way is to test the 18 perturbations that add plus or minus ϵ to an entry. The second way tests thousands of random perturbations. The two approaches give about the same best conditioned pseudoeigenvector bases. So a simple way of finding a nearly optimal basis may be possible in some cases.

3 | STABILITY OF PSEUDOEIGENVECTOR BASES

For a basis of pseudoeigenvectors to be useful, it would help if there is some stability relative to the choice of E. This means that using a different E of similar norm will not change everything about the basis. We know that there are limits to this stability, because we have just observed in the previous section that pseudoeigenvector bases can vary significantly in quality. More specifically, putting an ϵ perturbation in the $(n,1)$ entry of the Jordan block gives significantly different eigenvectors than putting the perturbation in the $(1,n)$ entry. However, we now investigate what can be shown about stability of pseudoeigenvectors.

Example 6. We again use the Jordan block matrix from Example 1. Here, we have $n = 100$ and let $\epsilon = 10^{-2}$. The perturbation matrices E are formed by filling an n by n matrix N with real entries generated randomly with normal(0,1) distribution, then multiplying by $\frac{\epsilon}{||N||}$. Figure 4 has the pseudoeigenvalues of A that come from two different choices of E, called E_1 and E_2. There is a similarity in the general appearance, but some variation in the exact placement of the pseudoeigenvalues. We next look at how much a pseudoeigenvector corresponding to the smallest pseudoeigenvalue changes with a different perturbation. Let $\{\zeta, x_1\}$ be the eigenpair of $A + E_1$ with smallest eigenvalue. Figure 5 gives the sine of the angle between x_1 and the subspace spanned by the first k eigenvectors of $A + E_2$, ordered by distance of their

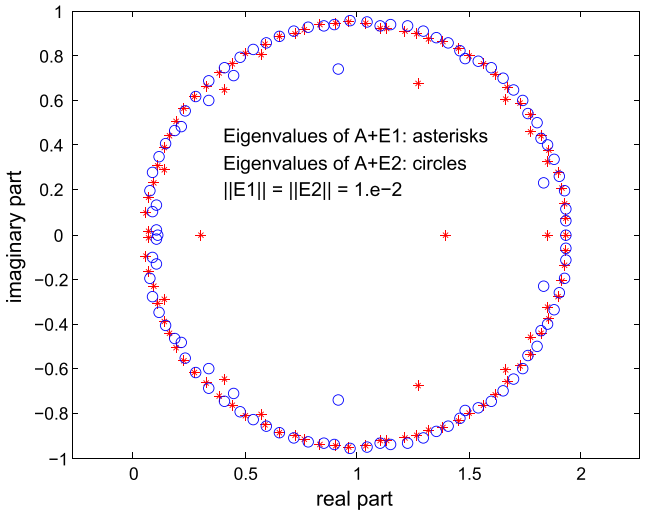

FIGURE 4 Pseudoeigenvalues of A from two different perturbations $A + E$

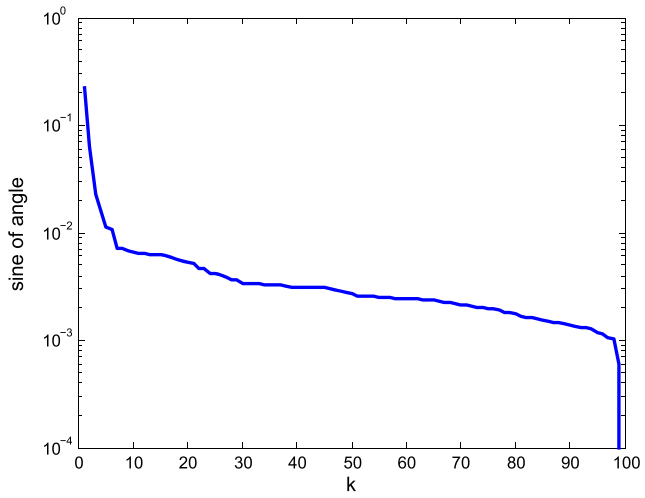

FIGURE 5 Sines of angles between smallest eigenvector of $A + E_1$ and the best approximation from the span of the first k eigenvectors of $A + E_2$ (Eigenvectors of $A + E_2$ are ordered by distance of the corresponding eigenvalue from the smallest eigenvalue of $A + E_1$)

corresponding eigenvalue from ζ. This is also $\|(I - P_k)x_1\|$, for P_k the orthogonal projector onto the subspace spanned by the first k eigenvectors of $A + E_2$. The sine is well below one even for $k = 1$ and goes below 10^{-2} for $k = 7$. So we see that x_1 is mostly in the subspace spanned by the first few pseudoeigenvectors associated with perturbation E_2.

The following theorem relates small singular values of shifted matrices to pseudoeigenvalues. It shows that if $A - \gamma I$ has a small singular value σ, then A has γ as an ϵ-pseudoeigenvalue for a small ϵ, specifically $\epsilon = \sigma$. The right singular vector is the pseudoeigenvector. It follows a standard result (such as in Trefethen et al.,[5] Chapter 2).

Theorem 1. If (σ,v,u) is a singular triplet of $A - \gamma I$, then v is an σ-pseudoeigenvector of A, with associated σ-pseudoeigenvalue γ.

Somewhat conversely, we can show that an ϵ-pseudoeigenvector is composed mostly of singular vectors corresponding to small singular values of a shifted matrix. This indicates that the pseudoeigenvector is somewhat stable. For this pseudoeigenvalue, a corresponding pseudoeigenvector is composed mostly of these singular vectors regardless of the E.

Theorem 2. Assume that $\{\zeta,x\}$ is an ϵ-pseudoeigenpair of A, and let E be the associated perturbation matrix so that $(A+E)x = \zeta x$ with $||E|| = \epsilon$. Let the singular value decomposition of $A-\zeta I$ be $(A-\zeta I)V = U\Sigma$. Let $x = Vg$, so that the elements of g give the coefficients of the expansion of x in terms of the basis of right singular vectors. Then

$$||\Sigma g|| \leq \epsilon.$$

Proof.

$$\begin{aligned} ||\Sigma g|| &= ||U\Sigma g|| \\ &= ||(A-\zeta I)Vg|| \\ &= ||((A+E-\zeta I)x - Ex|| \\ &= ||Ex|| \\ &\leq \epsilon. \end{aligned}$$

□

Note that $||\Sigma g||$ is the norm of the vector with ith component $\sigma_i g_i$. If ϵ is small, then for each i, either the ith singular value is small or the component of x in that direction is small. Thus, x is made up of mostly singular vectors associated with small singular values.

The next theorem has a similar purpose. It gives a condition so that if two ϵ-pseudoeigenvalues are nearly equal but come from different choices of E, then the associated ϵ-pseudoeigenvectors are close to each other.

Theorem 3. Suppose we have two choices of E, say $E1$ and $E2$, both of norm equal to ϵ, and they give rise to ϵ-pseudoeigenvalues ζ and τ respectively. Let the associated unit length ϵ-pseudoeigenvectors be $x1$ and $x2$, so $(A+E1)x1 = \zeta x1$ and $(A+E2)x2 = \tau x2$. Let the singular values of the matrix $A-\zeta I+E1$ be $\sigma_1,\ldots,\sigma_n$, ordered from largest to smallest. While $\sigma_n = 0$, we assume σ_{n-1} is not zero. Then

$$sin\angle(x1,x2) \leq \frac{2\epsilon + |\zeta-\tau|}{\sigma_{n-1}}.$$

Proof. Since $(A+E1-\zeta I)x1 = 0$ and $(A+E2-\tau I)x2 = 0$,

$$(A+E1-\zeta I)d = f + (\zeta-\tau)x_2, \tag{1}$$

where $d = x1 - x2$ and $f = (E2-E1)x2$. Note that $||f|| \leq 2\epsilon$.

Using the singular value decomposition, $A+E1-\zeta I = U\Sigma V^T$, where U and V are orthogonal and the singular values are ordered with σ_n being smallest. Because $A-\zeta I+E1$ is singular, $\sigma_n = 0$ and $v_n = x1$. Expanding $x2$ in terms of the basis of right singular vectors, $x2 = \sum_{i=1}^{n}\beta_i v_i$. Then $cos\angle(x1,x2) = \beta_n$ and

$$sin\angle(x1,x2) = \sqrt{\sum_{i=1}^{n-1}|\beta_i|^2}. \tag{2}$$

Next, $d = (1-\beta_n)v_n - \sum_{i=1}^{n-1}\beta_i v_i$. From (1), $f + (\zeta-\tau)x_2 = U\Sigma V^T d = 0 - \sum_{i=1}^{n-1}\beta_i\sigma_i u_i$. Then $||f+(\zeta-\tau)x_2|| \geq \sigma_{n-1}\sqrt{\sum_{i=1}^{n-1}|\beta_i|^2}$, and using Equation 2, $sin\angle(x1,x2) \leq \frac{||f+(\zeta-\tau)x2||}{\sigma_{n-1}} \leq \frac{2\epsilon+|\zeta-\tau|}{\sigma_{n-1}}$.

□

So if there is some separation of the small singular values of $A-\zeta I+E1$, and ϵ is small, then pseudoeigenvectors of near pseudoeigenvalues from two different perturbations of A are close to each other.

We next move to applications of pseudoeigenvector bases.

4 | EXPONENTIAL OF A MATRIX

We apply an idea of Davies[8] that illustrates how pseudoeigenvectors can be used to compute matrix functions. Davies finds fractional powers of a matrix.

A well-known way of computing the exponential of a matrix is to find the eigenvalue decomposition $A = Z\Lambda Z^{-1}$. Then

$$e^A = Ze^{\Lambda}Z^{-1}. \tag{3}$$

However, this does not work well when the eigenvectors are ill-conditioned. A pseudoeigenvector decomposition can be substituted. If $A+E = Z\Lambda Z^{-1}$, then $e^A \approx Ze^{\Lambda}Z^{-1}$. We are not advocating this as a good way to compute the matrix exponential, but we will show that the pseudoeigenvector basis can give better results than the eigenvector basis. Also, pseudoeigenvectors may be worth considering for large matrices.

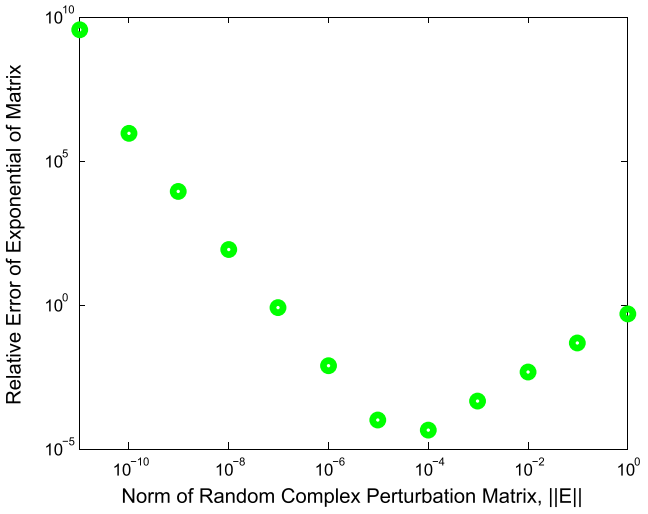

FIGURE 6 Relative difference between exponential of matrix using a pseudoeigenvalue decomposition and the Matlab result

Example 7. We use the butterfly matrix from Example 2, except all the diagonal elements are changed from 0 to 1.9. The size is $n = 500$. We first compute the eigendecomposition using the Matlab 'eig' command and use it in formula (3). We compare with the answer Matlab gives with its 'expm' command and compute the relative difference (the difference divided by Matlab's answer). The eigenvalue decomposition formula differs by an enormous relative amount of $3.3*10^{17}$. Next, we use the pseudoeigenvalue decomposition. The matrix is perturbed with a random complex matrix of varying norm, and then the eigendecomposition is computed and used in formula (3). Figure 6 has a plot of the relative difference between the results and Matlab's 'expm' answer. The least relative difference is $4.4*10^{-5}$ with an ϵ of 10^{-4}, but every ϵ gives a big improvement over using the unperturbed eigenvalue decomposition.

For large matrices, Matlab's matrix exponential function may not be practical. Using a few pseudoeigenvectors is a possibility. To show this, we attempt to compute the exponential of the inverse of the same butterfly matrix. We do not use a larger matrix so that the accuracy can be checked. Iterative methods such as Arnoldi are needed to find the pseudoeigenvectors of a large matrix, but here, we use Matlab's 'eig'. We let E be a complex random normal perturbation matrix of norm 10^{-10} and compute the five smallest eigenvalues of $A + E$ and the corresponding right and left eigenvectors. These are then used in the formula

$$e^{A^{-1}} \approx \sum_{i=1}^{5} z_i e^{\frac{1}{\lambda_i}} w_i,$$

where λ_i are the pseudoeigenvalues and z_i and w_i are corresponding right and left eigenvectors of the perturbed matrix. The result is surprisingly good considering only five pseudoeigenvalues are used. The relative difference is $3.3*10^{-2}$ between the approximation and the full matrix result computed by Matlab's 'expm' . This compares to $9.9*10^{5}$ for the same computation but with five eigenvalues and associated right and left eigenvectors of the unperturbed matrix. Next, we try the computation with a perturbation of norm 10^{-6}, and the result is much worse than with the 10^{-10} perturbation. Using again five pseudoeigenvalues, the relative difference is $5.0*10^{7}$. So while this example shows some potential, it also points out the need for further study.

5 | TORTOISE AND THE HARE CONVERGENCE OF RESTARTED GMRES

We now consider the linear equations problem $Ax = b$ and give an example showing how a pseudoeigenvector basis can be of assistance in analyzing convergence of restarted GMRES. Normally, with restarted GMRES, the more frequent the restarts, the slower the convergence. Tortoise and the Hare[13,32] refers to the phenomenon of faster convergence with more frequent restarts. The pseudoeigenvector basis will help in explaining this behavior. It also helps show why there can be superlinear convergence.

Example 8. The matrix A is the same as in Example 1, except the size is $n = 20$. The right-hand side is set to all ones and then normed to one. We apply both GMRES(1) and GMRES(3), and the (1,1) panel of Figure 7 shows the convergence. Because GMRES(1) converges in fewer iterations than GMRES(3), this is an example of Tortoise and the

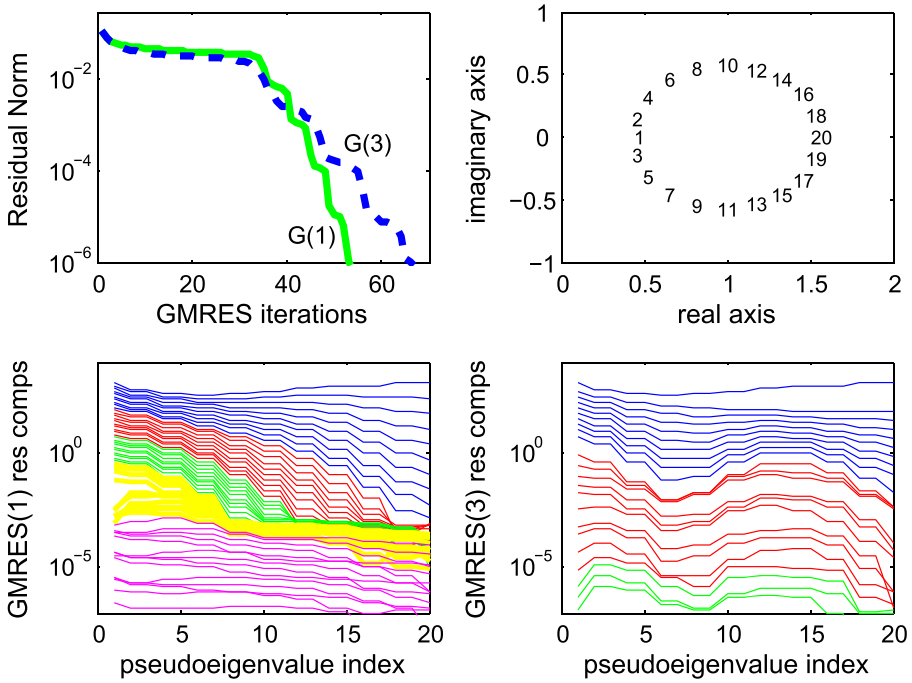

FIGURE 7 Tortoise and the Hare GMRES convergence with pseudoeigenvector components

Hare convergence. We perturb the matrix with an random real matrix of norm $\epsilon = 10^{-4}$ and compute the eigenvectors to give a pseudoeigenvector basis for the original matrix. The (1,2) panel shows the corresponding pseudoeigenvalues numbered in order of magnitude. The two lower panels show the components of the residual vectors at the beginning of each GMRES cycle expanded in terms of the pseudoeigenvectors. GMRES(1) takes 54 iterations and thus 54 cycles to reach residual norm below 10^{-6}. So there are 54 curves shown in the (2,1) panel for the residual components of GMRES(1), and they move mostly downward as the iteration proceeds. GMRES(3) takes 69 iterations or 23 cycles, and there are 23 curves shown in the (2,2) panel of the figure. We see that GMRES(1) works first on the larger components and meanwhile the overall residual norm plateaus. GMRES(1) next works on the middle-sized components. Then when it finally gets around to reducing the small components, the convergence is rapid. This shows why there is superlinear convergence for GMRES(1): the method is working all along, but only after all regions of the pseudospectrum have been dealt with does the residual norm convergence show this. Now with GMRES(3), the cubic polynomials tend to concentrate in a couple of regions, and the residual norm components take on a somewhat cubic shape. GMRES(3) is working too hard in some areas and not enough in others. Results are similar with other right-hand sides and other perturbations, so it seems that GMRES(3) is prone to this cubic-shape behavior. This analysis does not completely explain the convergence but is does show that using a pseudoeigenvector basis gives some insight.

6 | CONVERGENCE OF GMRES FOR HIGHLY NONNORMAL MATRICES

The standard convergence bound for GMRES is not always meaningful for highly nonnormal matrices because of a term involving the condition number of an eigenvector basis. We will use a basis of pseudoeigenvectors to establish a different convergence result for GMRES, which may sometimes be more useful. In this estimate, there is a trade-off between the value of ϵ used and the conditioning of the basis. For small ϵ, the basis may be ill-conditioned. For larger ϵ, another factor in the bound grows.

Estimate 1. Assume there is a basis for C^n made up of a set of ϵ-pseudoeigenvectors of A. Let the pseudoeigenvectors be $w_1, \ldots, w_n$, and let W be the matrix with these vectors as columns. Let the associated ϵ-pseudoeigenvalues be $\zeta_1, \ldots, \zeta_n$. If the current problem is $A(x - x_0) = r_0$, then after a cycle of restarted GMRES(m), the new residual vector satisfies

$$||r|| \leq \left(\kappa(W) \min_{q(0)=1, deg(q)\leq m} \max_{i=1,\ldots,n} |q(\zeta_i)| + B(\epsilon) \right) ||r_0||.$$

Here, $B(\epsilon)$ indicates a term bounded by an unknown multiple of ϵ that depends on the polynomial q and on $\kappa(W)$.

Proof. Let Λ be the diagonal matrix with the ζ_i's on the diagonal. Then $A + E = W\Lambda W^{-1}$. Next, for q a polynomial, $q(A) = q(A+E) + B(\epsilon) = q(W\Lambda W^{-1}) + B(\epsilon) = Wq(\Lambda)W^{-1} + B(\epsilon)$. Therefore,

$$\begin{aligned} ||r|| &= \min_{q(0)=1, deg(q)\leq m} ||q(A)r_0|| \\ &= \min_{q(0)=1, deg(q)\leq m} ||Wq(\Lambda)W^{-1}r_0|| + B(\epsilon)||r_0|| \\ &\leq \kappa(W) \min_{q(0)=1, deg(q)\leq m} ||q(\Lambda)||||r_0|| + B(\epsilon)||r_0|| \\ &\leq \left(\kappa(W) \min_{q(0)=1, deg(q)\leq m} \max_{i=1,\ldots,n} |q(\zeta_i)| + B(\epsilon) \right) ||r_0|| \end{aligned}$$

□

For a matrix with no basis of eigenvectors or highly ill-conditioned basis of eigenvectors, using a pseudoeigenvector basis and the associated pseudoeigenvalues may be more instructive about convergence.

Example 9. We use two matrices similar to the one from Example 1, but the entries on the main diagonal are now all 1.02 for the first matrix and 1.10 for the second one. Both are size $n = 500$. The right-hand sides are the same random vector. Convergence is shown in Figure 8. For the case of diagonal elements 1.02, non-restarted GMRES improves the residual norm by a factor of $2.1*10^{-4}$ in 300 iterations. For the other matrix, GMRES converges by a factor of $1.3*10^{-9}$ in 200 iterations. We consider the convergence estimate $\kappa(Z)(a/c)^{300}$,[14] where $\kappa(Z)$ is the condition number for the pseudoeigenvector basis and where a is the radius and c is the center of a circle containing the ϵ-pseudospectrum. We use a random real perturbation of norm ϵ for finding pseudoeigenvalues and the pseudoeigenvector basis. The smallest magnitude pseudoeigenvalue is used for the estimate of the radius a. See Tables 1 and 2 for the conditioning of the pseudoeigenvector basis and for the convergence estimate. We notice that we get better convergence estimates with larger values of ϵ, at least up to 10^{-2}. This shows that for this example, the basis of pseudoeigenvectors is more useful for larger ϵ. The basis becomes better conditioned as ϵ increases.

TABLE 1 Breakdown of a GMRES convergence bound

ϵ	$\kappa(Z)$	$(a/c)^{300}$	Convergence estimate	Improved convergence estimate
10^{-8}	1.3e+10	8.5e − 9	1.1e+2	4.0
10^{-6}	1.2e+8	1.4e − 7	1.6e+1	0.64
10^{-4}	1.0e+6	1.8e − 6	1.9	0.10
10^{-3}	9.4e+4	7.6e − 6	0.72	0.041
10^{-2}	8.2e+3	9.5e − 5	0.78	0.016
10^{-1}	6.8e+2	1.7e − 3	1.2	0.0066

Note. Matrix with $Diag = 1.02$. Residual improves by factor of 2.1e − 4 in 300 GMRES iterations.

TABLE 2 Breakdown of a GMRES convergence bound

ϵ	$\kappa(Z)$	$(a/c)^{200}$	Convergence estimate	Improved convergence estimate
10^{-6}	1.2e+8	7.3e − 12	8.8e − 4	2.0e − 5
10^{-4}	1.0e+6	4.1e − 11	4.3e − 5	1.2e − 6
10^{-3}	9.4e+4	1.1e − 10	1.1e − 5	3.3e − 7
10^{-2}	8.2e+3	5.7e − 10	4.7e − 6	8.3e − 8
10^{-1}	6.8e+2	4.0e − 9	2.7e − 6	2.1e − 8

Note. Matrix with $Diag = 1.10$. Residual improves by factor of 1.3e − 9 in 200 GMRES iterations.

Next, we do the same calculation with the perturbation of only the $(n,1)$ entry that is mentioned in Section 2.2 The same calculations are done, and only the convergence estimate is given in the last column. This gives estimates that come close to the actual convergence for the larger values of ϵ. However, the estimate may then be losing validity due to a possibly large $B(\epsilon)$ term.

7 | DEFLATED GMRES

Deflated GMRES methods improve the convergence of restarted GMRES by using approximate eigenvectors to remove the effect of some eigenvalues (usually small ones). The eigenvectors can be used to build a preconditioner, or they can be put into the subspace. We will consider the latter approach, specifically the method GMRES with deflated restarting (GMRES-DR)[26] which both solves linear equations and computes eigenvalues and eigenvectors. The GMRES-DR method deflates eigenvalues by computing eigenvectors while it is solving linear equations. At the conclusion of a cycle, it uses its subspace to both update the linear equations solution and compute new approximate eigenvectors. Then for the next cycle, it builds a subspace that is spanned by the approximate eigenvectors and new Krylov vectors. This subspace is

$$Span\{\tilde{y}_1, \tilde{y}_2, \ \dots \ \tilde{y}_k, r_0, Ar_0, A^2r_0, A^3r_0, \ \dots \ , A^{m-k-1}r_0\}, \quad (4)$$

where the $\tilde{y}_i$'s are harmonic Ritz vectors generated by the previous cycle and r_0 is the linear equations residual vector from the previous cycle. GMRES-DR(m,k) has maximum size of subspace m and saves k approximate eigenvectors at the restart. The presence of approximate eigenvectors in the subspace essentially removes or deflates the corresponding eigenvalues. This can vastly improve convergence compared to regular GMRES when there are small eigenvalues.

In this section, we show that deflated GMRES can work for highly nonnormal matrices. We will give examples where it is not clear that there are small eigenvalues and the corresponding eigenvectors that can be deflated. First, an estimate is given that indicates how deflation can potentially work in this situation.

The following estimate shows that the approximate eigenvectors generated by GMRES-DR can be viewed as pseudoeigenvectors and also that the convergence is roughly as if the corresponding pseudoeigenvalues are deflated from the spectrum.

Estimate 2. Let $y_1, \dots, y_k$ be normalized approximate eigenvectors of A with associated approximate eigenvalues $\theta_1, \dots, \theta_k$ and residual vectors $r_i = Ay_i - \theta_i y_i$. Let $Span\{y_1, \dots, y_k, r_0, Ar_0, \dots, A^{m-k-1}r_0\}$ be the subspace for a cycle of an augmented minimum residual Krylov method (such as GMRES-DR). Let $Y = [y_1 \dots y_k]$ and $R = [r_1 \dots r_k]$. Let a QR factorization of Y be $Y = QU$ with Q n by k orthonormal and U k by k upper triangular. Let $E = -RU^{-1}Q^T$ and $\epsilon = \|E\|$. Then we first conclude that $A + E$ has eigenpairs (θ_i, y_i) for $1 \le i \le k$. Let the other eigenpairs be (ξ_i, w_i) for $k + 1 \le i \le n$, and let W be the matrix with $y_1, \dots, y_k$ as the first columns and $w_{k+1}, \dots w_n$ as the other columns. Let the current problem be $A(x - x_0) = r_0$. Then after a cycle, the new residual vector satisfies

$$||r|| \le \kappa(W)\left(\min_{q(0)=1, deg(q) \le m-k} \ \max_{i=k+1, \dots, n} |q(\xi_i)| + B(\epsilon)\right) ||r_0||, \quad (5)$$

with $\epsilon \le \|R\|\kappa(U)$. As in Estimate 6.1, $B(\epsilon)$ indicates a term bounded by an unknown multiple of ϵ.

Proof. It is quick to show that the (θ_i, y_i)'s are pseudoeigenpairs. Let e_i denote the ith coordinate vector. Then, for $1 \le i \le k$,

$$\begin{aligned}(A + E)y_i &= Ay_i - RU^{-1}Q^T y_i \\ &= Ay_i - RU^{-1}Q^T Ye_i \\ &= \theta_i y_i + r_i - RU^{-1}Q^T QUe_i \\ &= \theta_i y_i + r_i - r_i \\ &= \theta_i y_i.\end{aligned}$$

Next, we prove the bound on ϵ, using that Y has normalized columns so the norm of U is bounded below by 1:

$$\begin{aligned}\epsilon = ||E|| = ||RU^{-1}Q^T|| = ||RU^{-1}|| \le ||R||||U^{-1}|| \\ \le ||R||||U^{-1}||||U|| = ||R||\kappa(U).\end{aligned}$$

Finally, let $\xi_i = \theta_i$ for $1 \le i \le k$, and let Ξ be the diagonal matrix with the ξ_i's on the diagonal. Let $r_0 = \Sigma_{i=1}^k \beta_i y_i + \Sigma_{i=k+1}^n \beta_i w_i$. After a cycle of GMRES-DR, let the approximate solution be $\hat{x} = \Sigma_{i=1}^k \gamma_i y_i + p(A)r_0$, for p a polynomial of degree $m - k - 1$. Then the new residual vector is $r = r_0 - A\hat{x} = r_0 - \Sigma_{i=1}^k \gamma_i Ay_i - Ap(A)r_0 = -\Sigma_{i=1}^k \gamma_i Ay_i + q(A)r_0$, where $q(\alpha) \equiv 1 - \alpha p(\alpha)$.

Next, as in the proof of Estimate 6.1, $q(A) = Wq(\Xi)W^{-1} + B(\epsilon)$. In the next equation, the minimum is over all choices of γ_i's and polynomials q satisfying the given conditions.

$$\begin{aligned}||r|| &= \min_{q(0)=1, deg(q) \le m-k} || - \Sigma_{i=1}^k \gamma_i Ay_i + q(A)r_0|| \\ &= \min_{q(0)=1, deg(q) \le m-k} || - \Sigma_{i=1}^k \gamma_i(\theta_i y_i - Ey_i) \\ &\quad + \Sigma_{i=1}^k \beta_i q(\xi_i)y_i + \Sigma_{i=k+1}^n \beta_i q(\xi_i)w_i + B(\epsilon)r_0||.\end{aligned}$$

We can choose the γ_i's to be any values we want, because the minimum residual will always be as good. Letting $\gamma_i = -\beta_i q(\xi_i)/\theta_i$,

$$||r|| \leq \min_{q(0)=1, deg(q)\leq m-k} || - \Sigma_{i=1}^{k} \frac{\beta_i}{\theta_i} q(\xi_i) E y_i + \Sigma_{i=k+1}^{n} \beta_i q(\xi_i) w_i + B(\epsilon) r_0 ||$$

The β_i's are bounded by $\kappa(W)||r_0||$ and the E terms go into the $B(\epsilon)$:

$$||r|| \leq \kappa(W) \left(\min_{q(0)=1, deg(q)\leq m-k} \max_{i=k+1,\ldots,n} |q(\xi_i)| + B(\epsilon) \right) ||r_0||$$

□

Note the bound in Equation 5 has a max over the polynomial at eigenvalues not including k of them. So these k are deflated from the bound.

The $\kappa(U)$ term in the bound on the size of ϵ is one in the symmetric case. Then the size of ϵ depends on the accuracy of the approximate eigenvectors.

Example 10. Let A be the Jordan block matrix from Example 1. Let $n = 500$ and let the right-hand side have random Normal(0,1) entries. This example is extreme, because there is only one eigenvector and all of the eigenvalues are 1. It is not at all clear that deflating eigenvalues will be helpful, because there are no small eigenvalues. Also, with only one eigenvector, using approximate eigenvectors for deflation is questionable. However, as shown in Figure 9, GMRES-DR is able to effectively deflate eigenvalues and give faster convergence than restarted GMRES. GMRES-DR(40,20) uses 20 approximate eigenvectors to deflate and a Krylov portion of dimension 20. It converges faster than both GMRES(40) and GMRES(20). Notice there is a Tortoise and the Hare effect[13] here for restarted GMRES as $m = 20$ converges faster than $m = 40$.

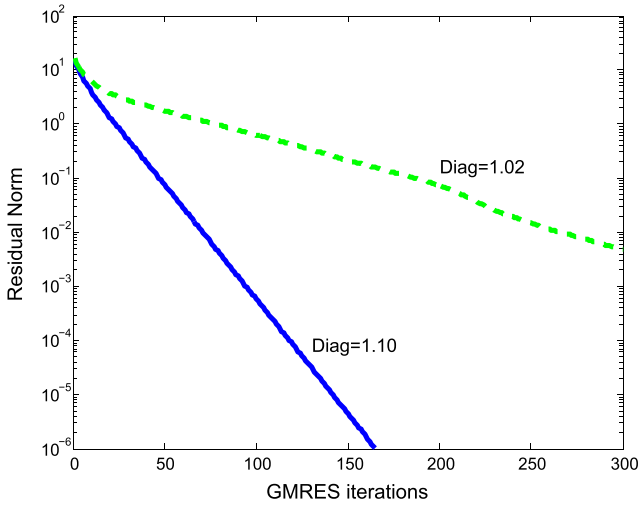

FIGURE 8 Convergence of full GMRES for the two bidiagonal matrices.

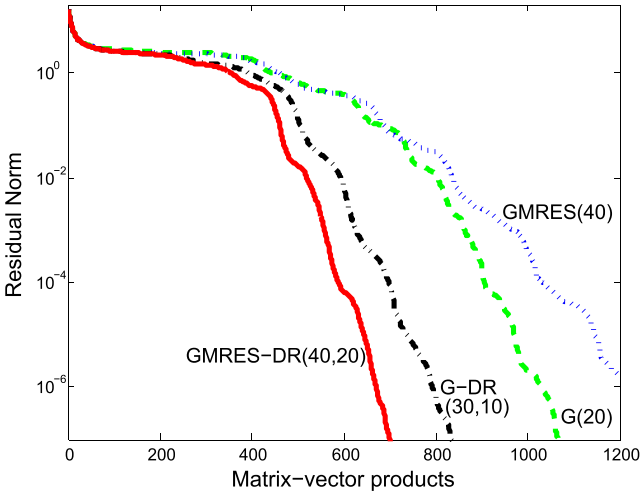

FIGURE 9 GMRES and GMRES-DR for the Jordan block matrix. Deflation of eigenvalues is effective even though there are no small eigenvalues

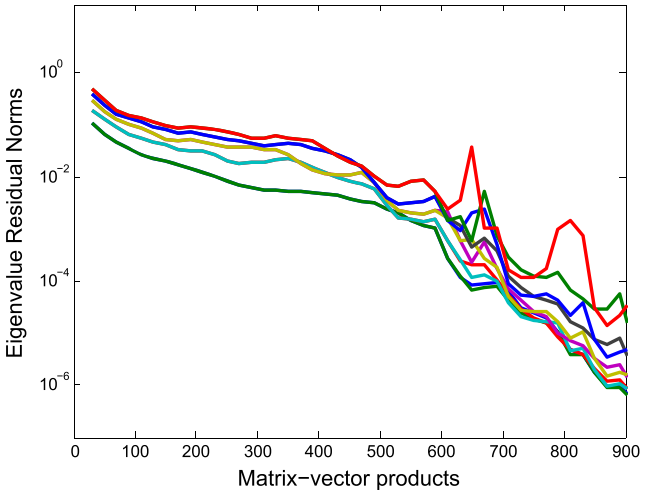

FIGURE 10 Convergence of harmonic Ritz pairs for GMRES-DR(30,10)

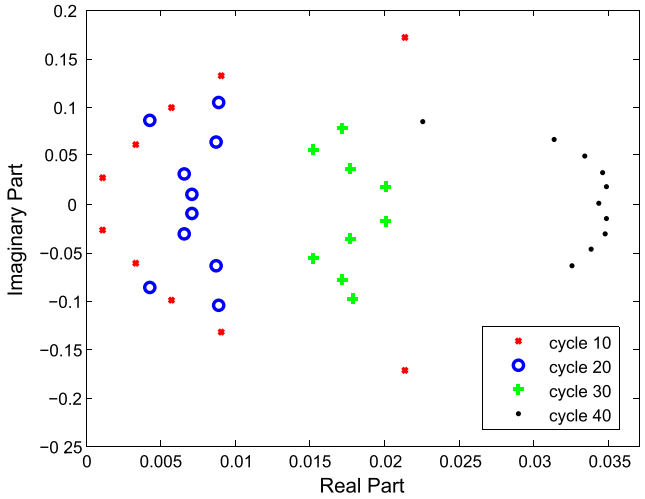

FIGURE 11 Smallest harmonic Ritz values for GMRES-DR(30,10) after cycles 10, 20, 30 and 40

GMRES-DR computes approximate eigenvectors that are also pseudoeigenvectors and deflates the corresponding pseudoeigenvalues, as indicated by Estimate 7.1. Figure 10 shows the residual norms in GMRES-DR(30,10) for the harmonic Ritz pairs that are the approximate eigenpairs. They seem to be converging well. However, in contrast to what is usually observed for matrices with well-conditioned eigenvector matrices, the harmonic Ritz values do not settle down into a regular convergence pattern. Figure 11 shows that they move to the right in the complex plane as they converge. Because the only eigenvalue is at 1.0, it makes sense that approximate eigenvalues would move towards this value as they converge. Figure 12 shows all of the harmonic Ritz values for GMRES-DR(30,10) after cycle 30 and also the values for GMRES(20) for cycle 30. GMRES-DR(30,10) has small pseudoeigenvalues that are deflated out and improve the convergence.

Next, we look at applying a portion of Estimate 7.1 to this situation. We look at the perturbed matrix $A + E$ for $E = -RU^{-1}Q^T$, where the quantities are defined in the estimate. The estimate claims that GMRES-DR convergence goes mostly according to the spectrum of this matrix with k eigenvalues deflated out. Figure 13 shows the smallest eigenvalues of this perturbed matrix after 10 and after 30 cycles of GMRES-DR(40,20). For after 10 cycles, the dots are the eigenvalues of $A + E$, and the asterisks are the 20 smallest harmonic Ritz values. The eigenvalues of $A + E$ that have an asterisk around them are deflated from the spectrum. However, there are some dots close to the origin without asterisks, so the convergence at 10 cycles is still slow (there are 220 matrix-vector products after 10 cycles). After 30 cycles and 620 matrix-vector products, the eigenvalues of $A + E$ are shown with pluses and all of the small ones correspond to harmonic Ritz values, shown with circles. At that point, convergence is very fast because the small eigenvalues of the perturbed matrix are being deflated.

We now run a test that shows that the approximate eigenvectors generated by GMRES-DR are useful for deflating

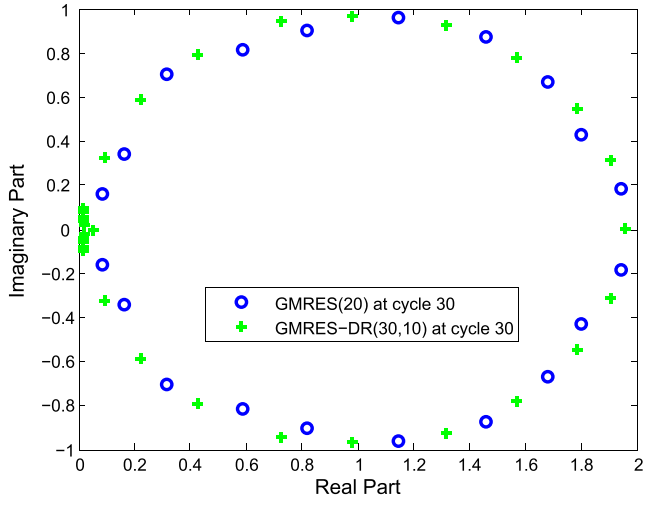

FIGURE 12 Harmonic Ritz values for GMRES(20) and GMRES-DR(30,10) after cycle 30

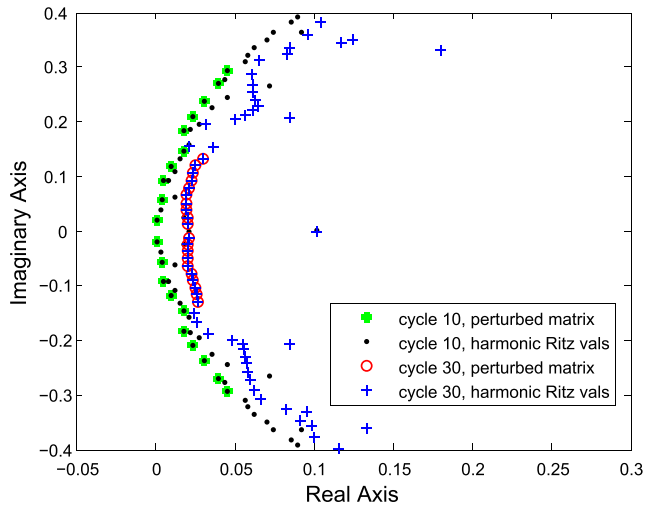

FIGURE 13 Eigenvalues of the perturbed matrix from Estimate 7.1

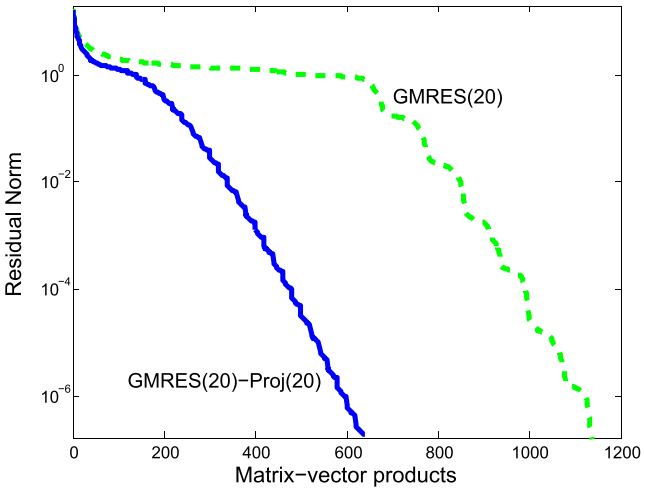

FIGURE 14 Deflation of pseudoeigenvalues for a second right-hand side

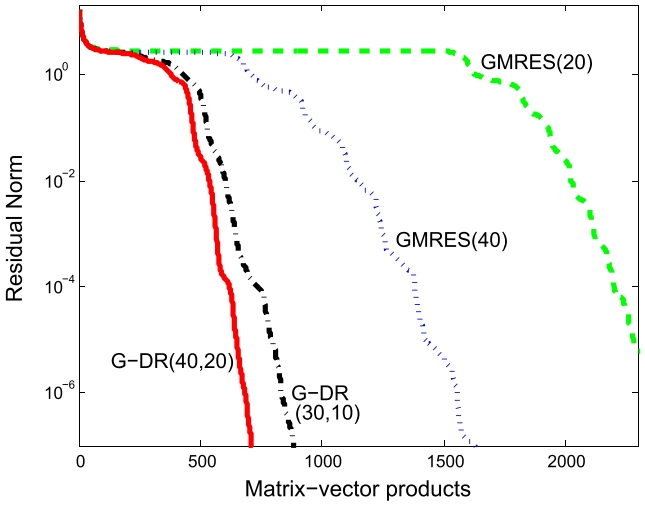

FIGURE 15 GMRES and GMRES-DR for shifted Jordan block matrix with diagonal elements 0.999

eigenvalues for another system of equations with the same matrix and different right-hand side. We take the harmonic Ritz vectors from the end of a run of GMRES-DR(40,20) that goes for 36 cycles or 700 matrix-vector products. Then the GMRES(20)-Proj(20) method[33] is applied. It alternates minimum residual projection over the 20 harmonic Ritz vectors with cycles of GMRES(20). Figure 14 shows the convergence versus regular GMRES(20). The approximate eigenvalues are useful even though they are fixed vectors with fixed harmonic Ritz values instead of the continually moving values used by GMRES-DR. These pseudoeigenvectors are not always as effective in this second right-hand side situation; see the tests in Example 12.

Example 11. We now shift the Jordan block matrix in the previous example to make it more difficult. We slightly change all of the diagonal elements to 0.999 and leave the superdiagonal elements at 1.0. Initially, n is again 500. Figure 15 shows that this shift makes the problem more difficult for restarted GMRES. The small pseudoeigenvalues are shifted closer to the origin by 0.001. Note that the pseudospectra are shift invariant, $\sigma_\epsilon(A + \xi I) = \xi + \sigma_\epsilon(A)$, while harmonic Ritz values are not. With a further shift of diagonal elements to 0.998, the problem is too difficult for GMRES(20) and GMRES(40). They do not converge. Meanwhile GMRES-DR(40,20) works about the same as before. In fact, even with the matrix having diagonal elements of 0.992, GMRES-DR(40,20) converges to relative residual tolerance of 10^{-10} in 920 matrix-vector products versus 760 for the first case of diagonal elements equal to 1.0. However, with diagonal elements of 0.990, GMRES-DR(40,20) also stagnates (interestingly, GMRES-DR(35,15) does converge).

Next, we use different shifts of the original Jordan block matrix and look at how many pseudoeigenvalues need to be deflated in order for GMRES-DR to converge. We use GMRES-DR(20+k,k) for values of k that are multiples of five. We start with a shift of 0.005 that gives diagonal elements of 0.995 and then keep doubling the shift. The size of k needed is given in Table 3 for each shift. This number of pseudoeigenvalues needed for deflation increases as the pseudospectrum is pushed to the left. Results are also given for the

TABLE 3 List of number of pseudoeigenvectors needed for deflation with different shifts

	$n = 500$	$n = 1000$
Shift	k needed	k needed
0	0	0
0.005	10	45
0.01	15	50
0.02	25	55
0.04	35	80
0.08	45	90
0.16	50	100
0.32	60	120
0.64	80	165

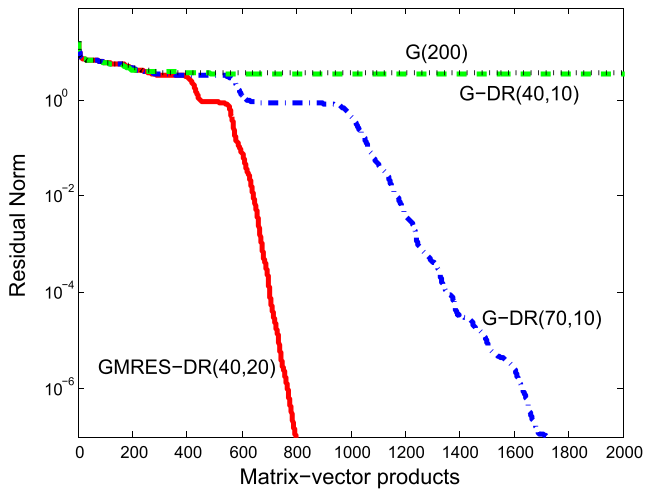

FIGURE 16 GMRES and GMRES-DR for the Butterfly matrix

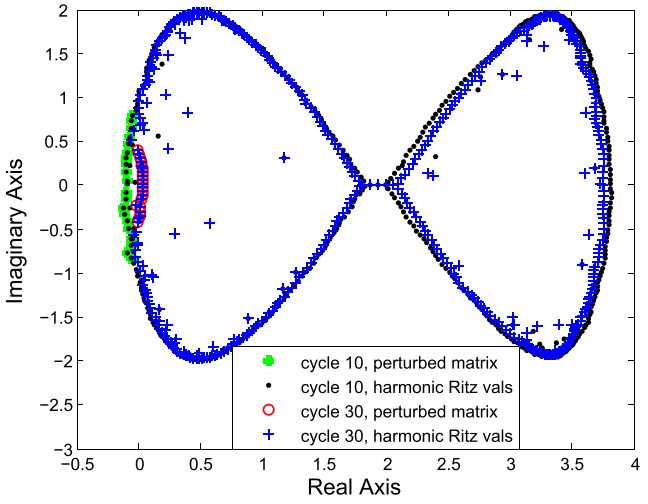

FIGURE 17 Eigenvalues of the perturbed matrix from Estimate 7.1 for the Butterfly matrix

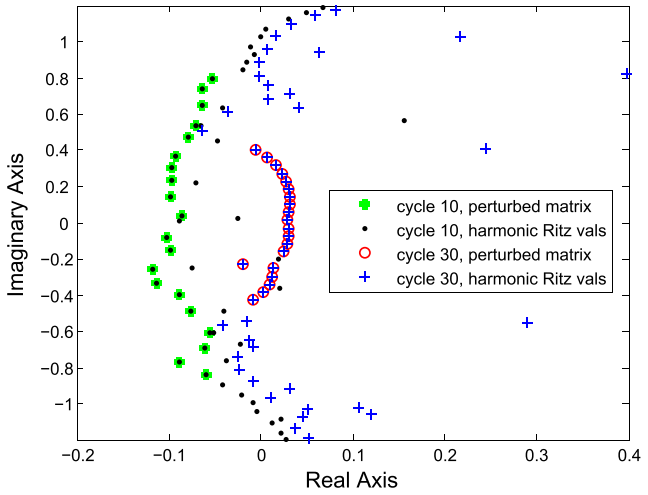

FIGURE 18 Closeup of eigenvalues of the perturbed matrix from Estimate 7.1 for the Butterfly matrix

matrix of twice the size and then many more pseudoeigenvectors need to be deflated. For the larger shifts, about twice as many are needed. It makes sense that the pseudoeigenvalues are packed in about twice as thick for the larger matrix, so more need to be deflated.

Example 12. We next test with the Butterfly matrix from Example 7, so the diagonal elements are again changed from 0 to 1.9, and the size is $n = 500$. The change in diagonal shifts the pseudospectrum from surrounding the origin in the complex plane to just right of the origin (depending on the ϵ). Deflation of eigenvalues is necessary for convergence. Figure 16 shows that deflating 20 pseudoeigenvalues is very effective. Figure 17 has eigenvalues of the perturbed matrix $A + E$ from Estimate 7.1 at the end of 10 cycles and 30 cycles of GMRES-DR(40,20). The closeup in Figure 18 shows the perturbed matrix at cycle 10 has some small eigenvalues that do not correspond to any of the 20 harmonic Ritz values and so are not being deflated. However, by cycle 30, all of the smallest eigenvalues of the perturbed matrix (denoted by pluses) do correspond to harmonic Ritz values. So at that point, there is fast convergence for GMRES-DR(40,20).

Next, we again use pseudoeigenvectors from solving one system to deflate pseudoeigenvalues for a second system with a different right-hand side. We apply GMRES-DR(40,20) for solving the first right-hand side, then deflate the 20 pseudoeigenvectors for GMRES(20)-Proj(20) on the second right-hand side. However, this method does not converge; see Figure 19. Using 30 pseudoeigenvectors is effective. It seems that GMRES-Proj may need more pseudoeigenvectors than GMRES-DR.

Example 13. The next test matrix is a SUPG matrix from previous work[19,34,35] with $n = 2500$ and $\nu = .01$. Figure 20 shows the eigenvalues of the matrix and the pseudoeigenvalues using perturbations with three different values of ϵ. Looking only at the eigenvalues, the problem appears easy, because the eigenvalues are clumped together well away from the origin. How-

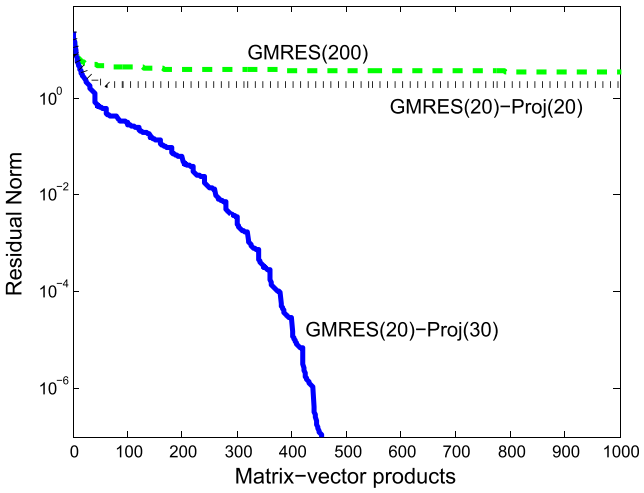

FIGURE 19 Deflation of pseudoeigenvalues for a second right-hand side

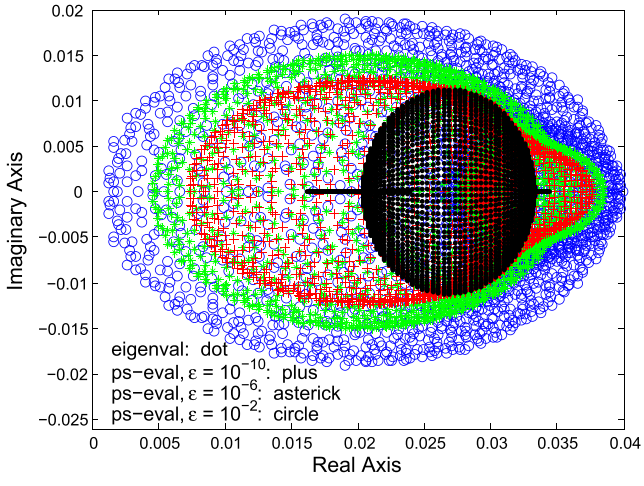

FIGURE 20 Eigenvalues and some pseudoeigenvalues of SUPG matrix

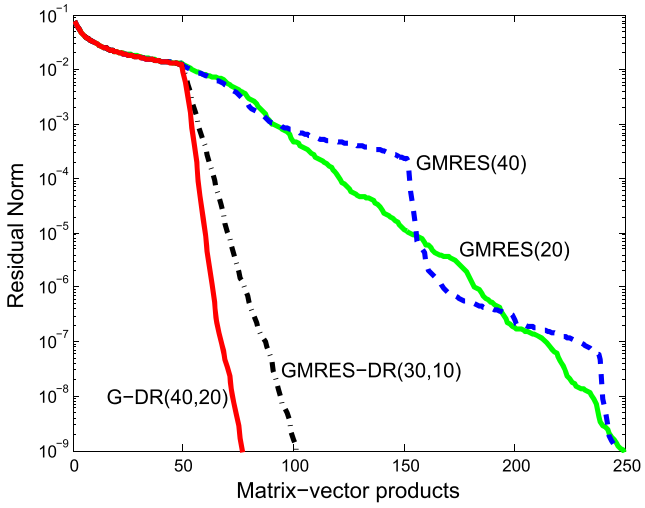

FIGURE 21 GMRES and GMRES-DR for the SUPG matrix Deflation of eigenvalues is effective even though there are no small eigenvalues

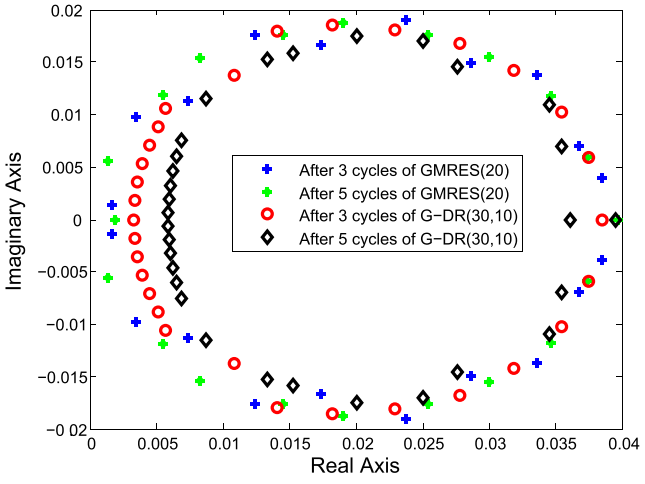

FIGURE 22 Harmonic Ritz values for GMRES(20) and GMRES-DR(30,10) after cycles 3 and 5

ever, the pseudoeigenvalues come close to the origin for the larger values of ϵ, so the problem is not so simple for restarted GMRES. Figure 21 shows that deflating pseudoeigenvectors is very helpful. GMRES-DR(40,20) converges about three times faster than the restarted GMRES runs. The harmonic Ritz values for GMRES(20) and GMRES-DR(30,10) after Cycles 3 and 5 are shown in Figure 22.

8 | CONCLUSION

This paper shows that pseudoeigenvectors can be used to assist understanding of GMRES convergence. In particular, it is explained why deflating eigenvalues can be effective even when the eigenvectors are poorly defined. There is still much to be studied with GMRES convergence and pseudoeigenvectors are one possible tool.

Pseudoeigenvectors are also potentially useful for computations, such as for the matrix exponential. They can perform much better than eigenvectors. They may not be a competitive method with leading approaches for small matrices. However, it is possible that for large matrices, some pseudoeigenvectors can be used for an approximation. These can come from either eigenvectors of a perturbed matrix or from computing eigenvectors of the original matrix with iterative methods.

This paper also looks at aspects of stability and variability of pseudoeigenvector bases and compares them to eigenvector bases for highly nonnormal matrices. While pseudoeigenvector bases for a fixed matrix do vary and some are better than others, some stability can be shown.

Perhaps in the future, pseudoeigenvectors will receive more attention like their companion pseudoeigenvalues.

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