

PERTURBED ARNOLDI FOR COMPUTING MULTIPLE EIGENVALUES

MARK EMBREE[†], THOMAS H. GIBSON[‡], KEVIN MENDOZA[§], AND RONALD B. MORGAN[¶]

Abstract. fill in abstract

Key words. eigenvalues, multiple eigenvalues, Arnoldi, rank-one matrices

AMS subject classifications. 65F15, 15A18

1. Introduction. We wish to compute multiple eigenvalues of large, sparse matrices. The goal is to determine the multiplicity and compute both eigenvalues and eigenvectors. The matrix can be either symmetric or nonsymmetric, but here we do not try to take advantage of symmetry.

There are a variety of applications for which multiple eigenvalues appear. Some examples are in structural design [18], properties of graphs [6], and integral equations [11]. Also, with Krylov methods for singular matrices [5], a low rank null space corresponding to a multiple eigenvalue at 0 can potentially be removed.

The Arnoldi algorithm [2, 16, 19, 13, 15, 17], a Krylov subspace method, is the standard for computing eigenvalues and eigenvectors of a nonsymmetric matrix. In theory, a Krylov subspace can contain only one eigenvector from each eigenspace, so it cannot find multiple eigenvalues. However, roundoff error generally causes multiple eigenvalues and all associated eigenvectors to eventually appear. So one option is to wait for this to happen. Block methods [8, 9, 12, 4, 14, 23, 3] can also be used. Another way is to restart at some point with a new vector and do a combination [10, 20, 15].

We propose a new method that slightly perturbs the matrix in order to split multiple eigenvalues. Applying Arnoldi to the perturbed matrix can produce the desired multiple copies of an eigenvalue and the associated eigenvectors.

((Should we give references here for a perturbation splitting multiple eigenvalues??)) The perturbing of the matrix causes some loss of accuracy in the eigenvalue and eigenvector computations. This error may be acceptable. However if not, we give a method using one or a few rank-one perturbations that allows for improvement of the approximate eigenpairs in a second phase.

Section 2 has background on methods that will be used or extended in the paper. Section 3 examines the approach of waiting for roundoff error. Section 4 has implementation of the method that uses diagonal perturbation to separate multiple eigenvalues. Comparisons are given with other methods. Rank-one perturbations are applied in Section 5.

*The fourth author was supported by the National Science Foundation Computational Mathematics Program under grant DMS-1418677 and by the Baylor University Sabbatical Program.

[†]Department of Mathematics, Virginia Tech, Blacksburg, VA 24061 (embree@vt.edu).

[‡]Department of Mathematics, Baylor University, Waco, TX 76798-7328 (Thomas.Gibson@baylor.edu).

[§]Department of Mathematics, Baylor University, Waco, TX 76798-7328 (Kevin.Mendoza@baylor.edu).

[¶]Department of Mathematics, Baylor University, Waco, TX 76798-7328 (Ronald.Morgan@baylor.edu).

2. Background.

2.1. Restarted Arnoldi. Sorensen's implicitly restarted Arnoldi [19] is standard for computing eigenvalues and eigenvectors of large nonsymmetric matrices. At every cycle it uses the subspace

$$\text{Span}\{y_1, y_2, \dots, y_k, r, Ar, A^2r, A^3r, \dots, A^{m-k-1}r\}. \quad (2.1)$$

where $\{y_1, y_2, \dots, y_k\}$ are Ritz vectors computed at the end of the previous cycle and r is the v_{m+1} vector from previous cycle and is a multiple of the residual vectors for each of these Ritz vectors. This subspace is equivalent [13] to

$$\text{Span}\{y_1, y_2, \dots, y_k, Ay_i, A^2y_i, A^3y_i, \dots, A^{m-k}y_i\},$$

for each y_i . So the subspace contains a Krylov subspace with each Ritz vector as starting vector. Potentially all k Ritz pairs can converge together. A simpler method that is mathematically equivalent to implicitly restarted Arnoldi at the end of each cycle is given in [13]. Wu and Simon [22] (see also [1]) give the symmetric case of a similar method that puts the approximate eigenvectors at the beginning of the subspace instead of the end. This approach is in [15] for the nonsymmetric case, and this is the version of restarted Arnoldi that we will use. A harmonic Rayleigh-Ritz version is also given in [15], but here we use the regular Rayleigh-Ritz version which is equivalent to implicitly restarted Arnoldi. The algorithm for this is given next. At the restart, an orthonormal basis is formed for $\text{Span}\{y_1, y_2, \dots, y_k, r\}$ in V_{k+1}^{new} . Then this is built out to an orthonormal basis for subspace (2.1) with the Arnoldi iteration as the cycle proceeds.

Restarted Arnoldi(m,k)

1. *Start:* Choose m , the maximum size of the subspace, and k , the number of approximate eigenvectors that are retained from one cycle to the next. Also pick nev , the desired number of eigenpairs. Normally $k > nev$. Choose an initial vector v_1 of unit length.
2. *Arnoldi iteration:* Apply the Arnoldi iteration from the current point to generate the Arnoldi-like recurrence $AV_m = V_{m+1}H_{m+1,m}$. The current point is either from v_1 if it is the first cycle or from v_{k+1} on the other cycles. Here $H_{m+1,m}$ is upper-Hessenberg for the first cycle and for the others it is upper-Hessenberg except for a full leading $k+1$ by $k+1$ portion.
3. *Small eigenvalue problem:* Compute the k appropriate eigenpairs (θ_i, g_i) , with g_i normalized, of $H_{m,m}$. The θ_i are the Ritz values.
4. *Check convergence:* Residual norms can be computed using $\|r_i\| \equiv \|Ay_i - \theta_1 y_i\| = h_{m+1,m} * |g_{m,i}|$. If all desired nev eigenpairs have acceptable residual norm, then stop, first computing eigenvectors, if desired, as $y_i = V_m g_i$. Otherwise continue. The next step begins the restart.
5. *Orthonormalization of first k short vectors:* Orthonormalize g_i 's, for $1 \leq i \leq k$, first separating into real and imaginary parts if complex, in order to form a real m by k matrix P_k . Both parts of complex vectors need to be included, so temporarily reduce k by 1 if necessary (or k can be increased by 1).
6. *Form P :* Extend the columns of P_k , called p_1, \dots, p_k , to length $m+1$ by appending a zero to each, then set $p_{m+1} = e_{m+1}$, the $(m+1)$ st coordinate vector of length $m+1$. Let $P_{m+1,k+1}$ be the $m+1$ by $k+1$ matrix with p_i 's as columns.

7. *Form portions of new H and V using the old H and V :* Let $H_{k+1,k}^{new} = P_{k+1}^T H_{m+1,m} P_k$ and $V_{k+1}^{new} = V_{m+1} P_{m+1,k+1}$. Then let $H_{k+1,k} = H_{k+1,k}^{new}$ and $V_{k+1} = V_{k+1}^{new}$.
8. *Reorthogonalization of long $k + 1$ vector:* Orthogonalize v_{k+1} against the earlier columns of the new V_{k+1} . Go to step 2.

Full reorthogonalization is generally used with Arnoldi eigenvalue methods. All experiments here do use this in Step 2 of the algorithm. For Step 3 of this implementation of Arnoldi, it is important to use the 'nobalance' option in versions of Matlab and LINPACK older than 2015. Large errors can be introduced by the balancing (another option is to lock in eigenvectors once they converge [15]).

2.2. Block Arnoldi. ((hyphenate as in Block-Arnoldi or not???)

Block Arnoldi [17] generates a Krylov subspace for each of several starting vectors and puts the basis vectors together to form one overall subspace. In exact arithmetic, block methods can find multiple eigenvalues of multiplicity up to the block size. The disadvantage is that if the overall subspace size is limited by restarting, then the smaller Krylov subspaces of a block method can slow convergence.

For our restarted block Arnoldi tests, we use a version from [14] with regular Ritz vectors; see [3] for a more sophisticated implementation. This method computes Ritz vectors at the time of a restart that are used in the next cycle along with the several Krylov subspaces. We omit the detailed implementation, but do give the subspace. Let the block size be p . Let the maximum size of subspace be m and the number of Ritz vectors saved at the restart be k . Also, let $d = (m - k)/p$, which is the dimension of each individual Krylov subspace. We arrange m , k and p so that d is an integer, but the method can be adjusted if it is not. The subspace in the case of this d being an integer is

$$\text{Span}\{y_1, y_2, \dots, y_k, r_1, r_2, \dots, r_p, Ar_1, Ar_2, \dots, Ar_p, A^2r_1, A^2r_2, \dots, A^2r_p, \dots, A^{d-1}r_1, A^{d-1}r_2, \dots, A^{d-1}r_p, \},$$

where r_1, \dots, r_p are the vectors v_{m+1}, \dots, v_{m+p} from the previous cycle (residual vectors for all of the Ritz pairs are linear combinations of these vectors). The method is called Block Arnoldi(m,k,p).

3. Roundoff Error Approach. The first method for finding multiple eigenvalues is the simple approach of waiting for roundoff error to produce them. This method is not ideal, because the eigenvalues appear one at a time. Also, it is hard to know how long to keep going in case more copies may appear. However, waiting for roundoff error can work reasonably well, and we look at how this happens. Experiments in this section use unrestarted Arnoldi, but roundoff seems to work very similarly for restarted Arnoldi.

Example 1. The matrix is from finite difference discretization of the two-dimensional Laplacian on the unit square. The discretization size is $h = 1/51$ on each side, so the dimension of the matrix is $n = 2500$. The smallest 10 eigenvalues are 0.00759, then a double eigenvalue at 0.0190, single at 0.0303 and three doubles of 0.0378, 0.0492 and 0.0642. The starting vector for unrestarted Arnoldi is generated random Normal(0,1). Figure 3.1 has a plot of the 10 smallest Ritz values at each iteration. By about iteration 180, all Ritz values have settled into place. However, there is a disturbance beginning at iteration 263 as a new value appears and quickly works its way down to

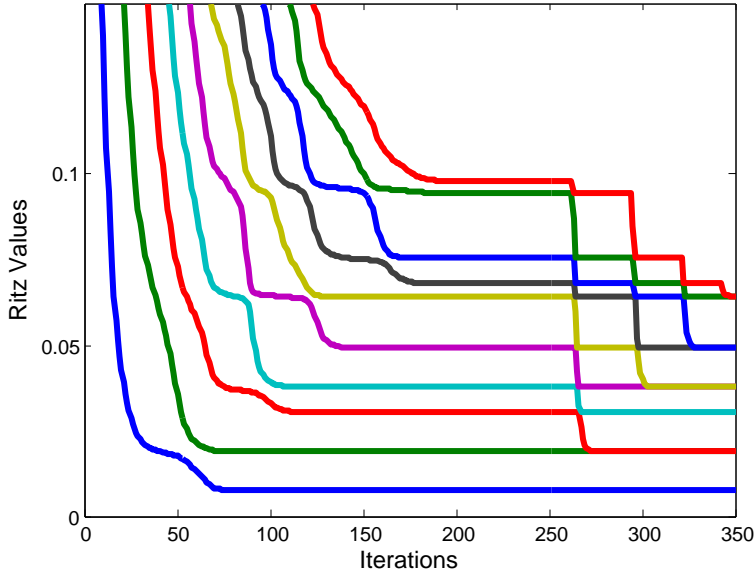


FIG. 3.1. *Non-restarted Arnoldi with the 10 smallest Ritz values plotted at each iteration. Matrix is 2-D Laplacian with $n = 2500$. By iteration 350, there are approximations to all 10 of the smallest eigenvalues, including 4 double eigenvalues.*

join the second eigenvalue as the second copy of this double value. This second copy reaches three significant digits of accuracy by iteration 274. At iteration 295, another new value comes into the picture as one of the 10 smallest Ritz values and it moves down to join the second double eigenvalue 0.0378. By iteration 350, the first four double eigenvalues all have been joined by second copies. The second copy of the first double is now accurate to 13 significant digits and the fourth double has just attained three digits. So Arnoldi with waiting for roundoff error is successful at finding these double eigenvalues.

We continue the example by looking at how the smallest double eigenvalue converges. The solid line in Figure 3.2 shows convergence of the first copy with the residual norm plotted against the iteration. At the same time, we look at how round-off error brings about the second copy. We compute the eigenvector corresponding to the second copy by finding the vector in the eigenspace that is orthogonal to the first copy eigenvector. We measure how much of this second eigenvector is in the Krylov subspace. The dashed line has the norm of the projection of this eigenvector onto the Krylov subspace. This component of the second eigenvector in the Krylov subspace starts at $6.e - 17$ and increases at approximately the same rate that the residual norm for the first copy is improving. It seems that the Krylov subspace is working on both copies equally, even though one is submerged for now. Once this component hits around 1, the 2nd copy appears as a Ritz value. The convergence of this approximation is shown by plotting the residual norm with the dash-dotted line. The convergence rate for this second copy matches the eventual rate for first copy. The first copy initially converges slowly, but demonstrates superlinear convergence [21] once approximations to nearby eigenpairs are accurate enough and then are essentially deflated from the spectrum. Since the second copy appears later, it can have the faster convergence from its start.

Next, Figure 3.3 gives similar graphs for the sixth set of double eigenvalues, the

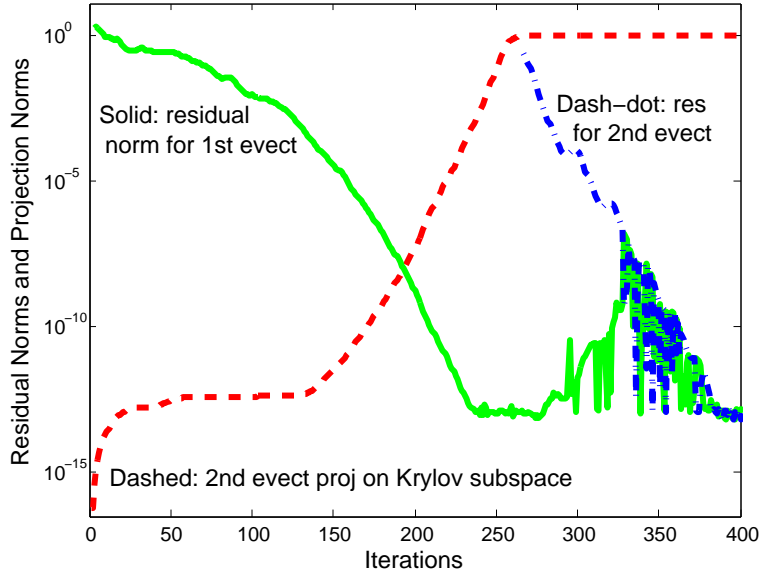


FIG. 3.2. Non-restarted Arnoldi with convergence shown for both eigenvectors of a multiple eigenvalue, plus norm of the projection of the second eigenvector onto the Krylov subspace. Matrix is 2-D Laplacian with $n = 2500$. Find first double eigenvalue (2nd and 3rd eigenvalues).

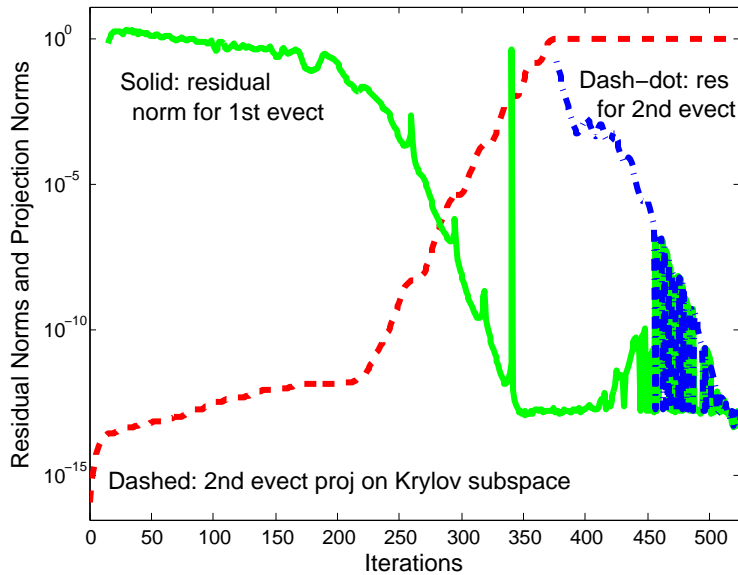


FIG. 3.3. Non-restarted Arnoldi with convergence shown for both eigenvectors of a multiple eigenvalue, plus norm of the projection of the second eigenvector onto the Krylov subspace. Matrix is 2-D Laplacian with $n = 2500$. Find sixth set of double eigenvalues (14th and 15th eigenvalues).

overall 14th and 15th eigenvalues. The convergence is slower initially because this double eigenvalue is further to the interior of the spectrum. Again, the appearance of the second copy in the Krylov subspace roughly matches the convergence of the first copy. Then later, the convergence of the second copy is similar to the later stage convergence of the first.

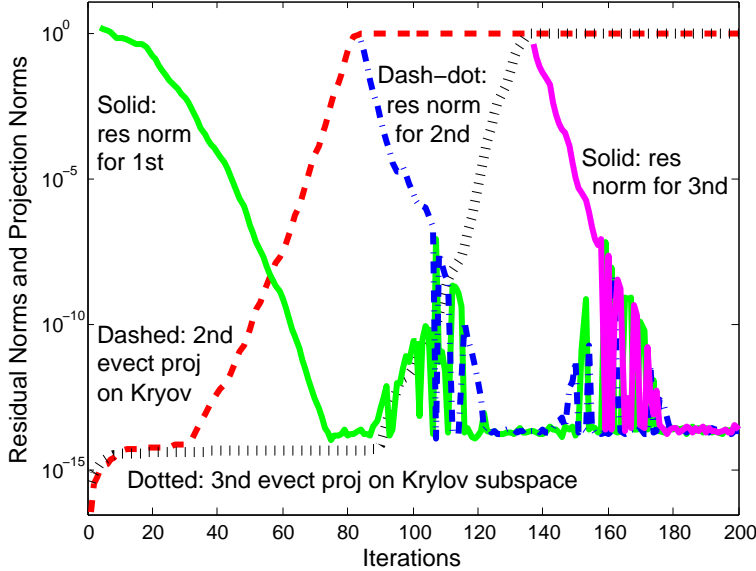


FIG. 3.4. *Non-restarted Arnoldi with convergence shown for the three eigenvectors of a triple eigenvalue, plus norms of the projections of the second and third eigenvectors onto the Krylov subspace. Matrix is 3-D Laplacian with $n = 3375$. Find first triple eigenvalue (2nd, 3rd and 4th eigenvalues).*

Example 2. We now consider a matrix from the three-dimensional Laplacian on the unit cube. We have $h = 1/16$, so the matrix is size $n = 3375$. Figure 3.4 has a plot similar to the last two figures, but for the smallest triple eigenvalue, the second through fourth overall eigenvalues. Note that the second and third copies of this eigenvalue develop one at a time. The component of the third eigenvector in the subspace is shown with a dotted line, and it does not start its rise until after the second copy has appeared as a Ritz value.

4. Diagonal Perturbations. We investigate perturbing the matrix with the goal of separating multiple eigenvalues. In this section, we add a random diagonal perturbation to the matrix. The new matrix that is used for the Arnoldi iteration is $A + P$, where we let $P = \sigma * E$ with E a norm one diagonal matrix. E has diagonal elements generated random $\text{Normal}(0,1)$, then the matrix is normed to 1 (simply divide all the diagonal elements by the maximum one).

Example 3. We use the same matrix as in Example 1 and apply unrestarted Arnoldi to the perturbed matrix with $\sigma = 10^{-4}$. Figure 4.1 has a plot similar to that in Figure 3.1, however, the multiple eigenvalues appear sooner. The second copy of the smallest double eigenvalue reaches 3 significant digits at iteration 188 instead of 274 for the unperturbed Arnoldi in Example 1. One can see that the double eigenvalue has separated because the two values that are calculated are first 0.01895216 and then 0.01895335. The double eigenvalue of the unperturbed matrix is at 0.01895232. Figure 4.1 also shows that the other double eigenvalues are determined faster with the perturbation. For instance, the fourth double eigenvalue corresponds to the 9th and 10th overall eigenvalues, and the second copy gets to 3 significant digits at iteration 274 compared to 350 with the unperturbed matrix.

We now switch to restarted Arnoldi in order to have a more realistic method. Results are fairly similar in both how extra copies appear and in how much the

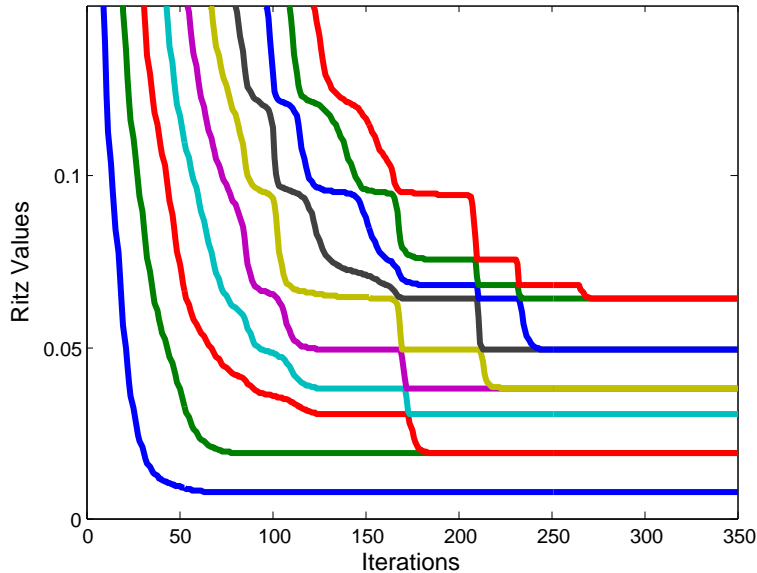


FIG. 4.1. Non-restarted Arnoldi with diagonal perturbation with $\sigma = 1.e - 4$. The 10 smallest Ritz values are plotted at each iteration. Matrix is 2-D Laplacian with $n = 2500$. Around iteration 270, there are approximations to all 10 of the smallest eigenvalues, including the 4 double eigenvalues.

perturbation quickens the appearance.

Example 4. We use a larger 2-D Laplacian matrix of size $n = 40,000$ and compare restarted Arnoldi methods. We use Arnoldi(33,15) and $nev = 10$. So 10 eigenvalues are desired, but 15 Ritz vectors are saved at the restart and then the subspace is built out to dimension 33 before restarting. Four figures are given. The first is Figure 4.2 with the Ritz values for the unperturbed matrix. We now plot against cycles instead of iterations. The first cycle has 33 iterations and subsequent ones have 18 iterations, so the 200 cycles shown corresponds to 3615 iterations. Figure 4.3 shows Ritz values for the perturbed Arnoldi method with $\sigma = 10^{-4}$. Then Figure 4.4 has block-Arnoldi(33,15,2) which restarts with 15 Ritz vectors, then builds out to dimension 33 using block size of $p = 2$ (the first cycle uses $m = 34$ so that it is divisible by p). The block approach has the first copy of double eigenvalues show up slower than waiting for roundoff, but the second copy comes faster, soon after the first. However, this second copy then converges slower. This is due to the smaller Krylov subspaces used by the block method (the block method has Krylov subspaces of dimension nine with each Ritz vector as starting vector, instead of a Krylov subspace of dimension 18 for non-block Arnoldi(33,15)). Figure 4.5 has all three methods for finding the fourth double eigenvalue (the ninth and tenth eigenvalues overall). The plot has the ninth and tenth Ritz values plotted. Note these are not initially the best approximations to the desired eigenvalue; double copies to smaller double eigenvalues need to show up first. This plot shows that the second copy comes first for the perturbed Arnoldi, significantly before either block or waiting for roundoff.

While a perturbation of the matrix helps find multiple eigenvalues faster, the results have limited accuracy as eigenpairs of the original matrix. The next example looks at the relationship between the amount of perturbation, and both when the second copy appears and the accuracy that the eigenvalues and eigenvectors attain.

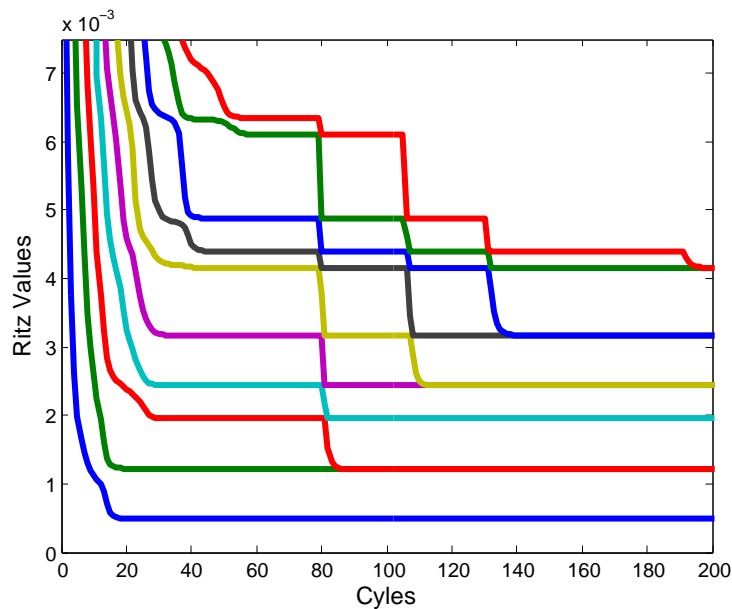


FIG. 4.2. *Restarted Arnoldi(33,15), no perturbation. The 10 smallest Ritz values plotted at each cycle. Matrix is 2-D Laplacian with $n = 40,000$.*

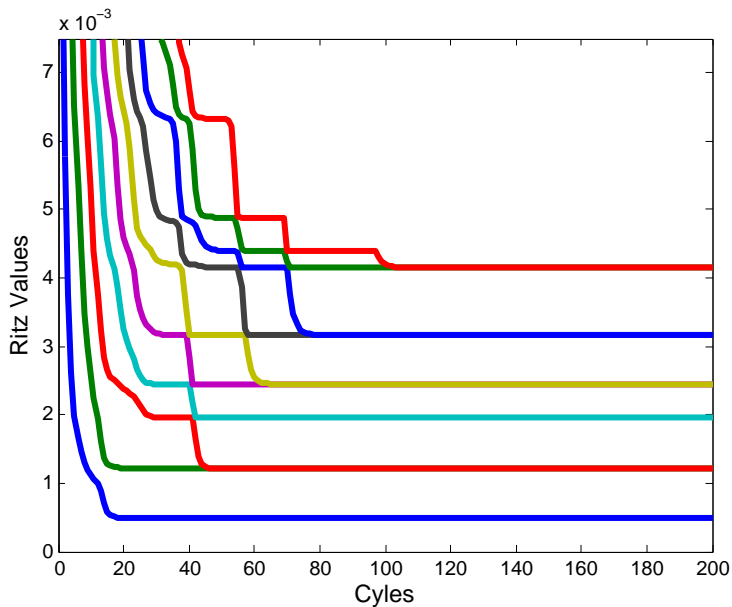


FIG. 4.3. *Restarted Arnoldi(33,15) with diagonal perturbation with $\sigma = 1.e-4$. The 10 smallest Ritz values plotted at each cycle. Matrix is 2-D Laplacian with $n = 40,000$.*

Example 5. The 2-D Laplacian matrix of dimension 40,000 is used again. We use perturbed Arnoldi(33,15) with several values of σ and compare against unperturbed and block Arnoldi. For all methods, we plot the residual norm with respect to A . For perturbed Arnoldi, these residual norms plateau once they reach a level at which the perturbation keeps the Ritz vector from improving as an eigenvector of A . The residual norms with respect to the perturbed matrix keep improving, but are not

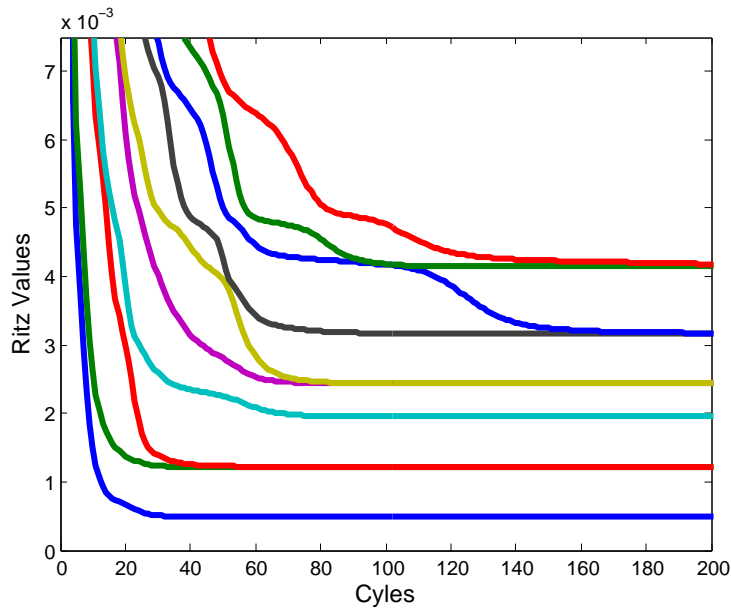


FIG. 4.4. Block Arnoldi(33,15,2). The 10 smallest Ritz values plotted at each cycle. Matrix is 2-D Laplacian with $n = 40,000$.

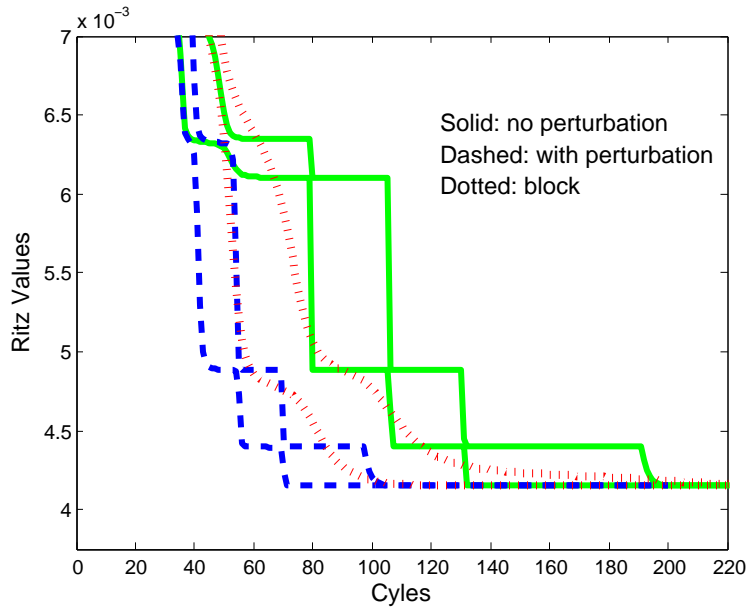


FIG. 4.5. Compare nonrestarted, perturbed and block. Ninth and 10th Ritz values are plotted (so the fourth double eigenvalue). Matrix is 2-D Laplacian with $n = 40,000$.

shown on the plot. Figure 4.6 shows the residual norms for the second copy of the fourth double eigenvalue. It is clear that as σ increases, the copies appear faster, but the eventual accuracy decreases. Arnoldi with no perturbation is slower to find the second copy, but it does reach higher accuracy, residual norm below 10^{-13} (not shown on graph). The residual norm of the second copy for the block method converges much slower than for the other methods.

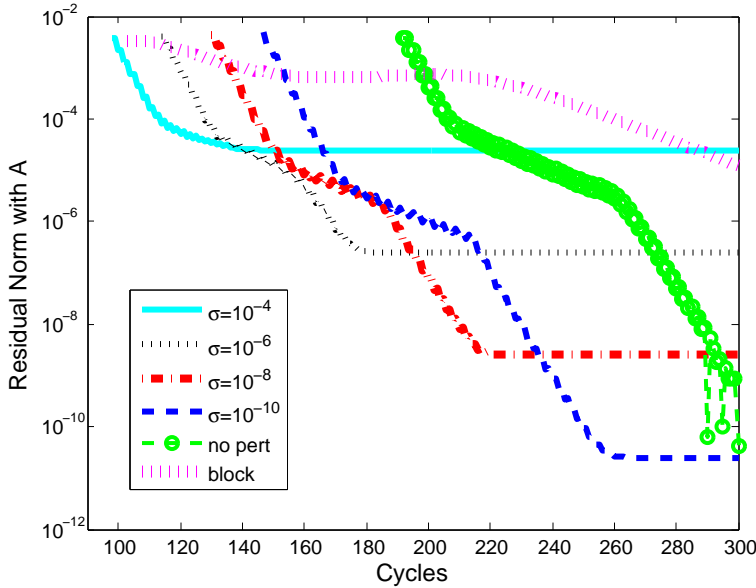


FIG. 4.6. Restarted Arnoldi(33,15) with varying diagonal perturbations σ . The residual norm for the 10th smallest eigenvalue is plotted at each cycle. This shows the convergence of the second copy of the fourth double eigenvalue. No perturbation and block approach are also plotted. Matrix is 2-D Laplacian with $n = 40,000$.

Next we find multiple eigenvalues including a sextuple eigenvalue.

Example 6. We now go back to the 3-D Laplacian on the unit cube, but this time discretize to get a matrix of size $n = 50^3 = 125,000$. There are triple eigenvalues, but there is also a sextuple eigenvalue that corresponds to the overall twelfth through seventeenth eigenvalues. We use Arnoldi(38,20) to compute the first 17 eigenpairs to residual norms below 10^{-4} . Waiting for roundoff error takes 223 cycles. With diagonal perturbation of size $\sigma = 10^{-4}$, 98 cycles are needed. Block Arnoldi(38,20,6) uses 383 cycles. Perturbed Arnoldi is particularly effective for this example because of the high multiplicity and the lower accuracy required. Block Arnoldi is at a disadvantage, because of the problem being fairly difficult so that larger Krylov subspaces are helpful. The subspaces of size 38 developed by Block Arnoldi(38,20,6) have 20 Ritz vectors from the previous cycle and six Krylov subspaces of dimension only three. In fact, if the problem is made more difficult by increasing the matrix size to $n = 75^3 = 421,875$, then regular Arnoldi and perturbed Arnoldi both almost double in the number of cycles, 444 and 193 respectively. Meanwhile, Block Arnoldi goes up 132 percent to 887.

5. Rank-one and Low Rank Perturbations. The diagonal perturbation in the previous section can find multiple eigenvalues faster. However the accuracy is limited. We now discuss a method that perturbs in a different way so that the accuracy can be improved. First we consider the case of double eigenvalues. In [7], a method is given that first finds eigenpairs of a matrix, then computes them for a rank-one update of the matrix. Here this approach will be used, but the first phase will have a rank-one perturbation of the desired matrix, then the second phase will have the desired matrix, which is of course a rank-one change from the first phase.

The first phase uses matrix $\hat{A} = A + \sigma st^T$, where s and t are random unit vectors.

If $z_1 \dots z_{nbuf}$ are eigenvectors of \hat{A} , then the subspace

$$Span\{z_1, z_2, \dots, z_{nbuf}, s, As, A^2s, A^3s, \dots, A^{m-nbuf-1}s\} \quad (5.1)$$

is a Krylov subspace for A . It can be used to start the Arnoldi iteration with A in the second phase. See [7] for more details. So we can generate Ritz vectors using Arnoldi with \hat{A} , and if they are accurate enough, forward them to a second Arnold phase that improves them as eigenvectors of A .

In the algorithm, there is an extra parameter to choose. Since only accurate vectors can be sent from the first phase to the second, we probably do not want to send all k Ritz vectors. However, we may want more than nev of them, in order to have a buffer. So let $nbuf$ be the number of Ritz vectors sent from the first phase to the second phase. Here $k \geq nbuf \geq nev$.

We next give the algorithm for the case of double eigenvalues. For higher multiplicity, one starts with several rank-one perturbations added to A and then removes one for each subsequent phase.

Rank-one perturbed Arnoldi for finding double eigenvalues.

1. *Setup:* Choose m, k, nev and $rtol$ as in the restarted Arnoldi algorithm. Also choose $nbuf =$ number of Ritz vectors that are forwarded from the first to the second phase. Pick random vectors s and t of norm 1; we let $t = s$. Choose the norm of the perturbation σ .
2. *First Phase: Arnoldi iteration with \hat{A} :* Apply restarted Arnoldi(m, k) with matrix $\hat{A} = A + \sigma st^T$. Let $\|r_1\|, \dots, \|r_{nbuf}\|$ be residual norms of the first $nbuf$ Ritz pairs. Let z_1, \dots, z_{nbuf} be the Ritz vectors. Stop the Arnoldi iteration when the norm of the vector with entries $\|r_1\|, \dots, \|r_{nbuf}\|$ is less than $rtol$.
3. *Second Phase: Arnoldi iteration with A :* Begin a restarted Arnoldi iteration with the first cycle using subspace (5.1). Stop when the residual norms of the first nev Ritz pairs are below $rtol$.

THEOREM 5.1. *For a multiple eigenvalue with corresponding eigenspace of dimension mul , only one of the eigenvalues is changed by a rank-one perturbation of the matrix. The eigenspace corresponding to the unchanged eigenvalues is a subset of the original eigenspace.*

((add proof ?))

This theorem shows that for finding double eigenvalues, a rank-one perturbation is sufficient. However, for triple eigenvalues, two rank-ones are needed, and so on.

Example 8. The matrix is the Laplacian matrix of dimension $n = 40,000$. We again use Arnoldi(33,15). We let the desired accuracy be residual norm below 10^{-8} . We still have $numev = 10$, but let $nbuf = 11$. So there are 10 desired eigenvalues, counting doubles doubly, but we move 11 from the first phase into the second. We let s be generated random Normal(0,1) and then normed to one. The vector t is set equal to s so that the perturbation is symmetric. We first use $\sigma = 10^{-2}$. Figure 5.1 shows the residual norm convergence for the 10 smallest Ritz values. These residual norms are with respect to A even though \hat{A} is the matrix used for the first Arnoldi iteration. The first phase takes 166 cycles until the convergence test in the algorithm is achieved. Note that most of the residuals plateau, because the perturbed matrix gives inaccurate eigenvectors for the original matrix. However, four of the residual norms do converge to high accuracy. These correspond to one copy of each double eigenvalue. This is in accordance with Theorem 5.1, which says that the Rank-1 perturbation does not

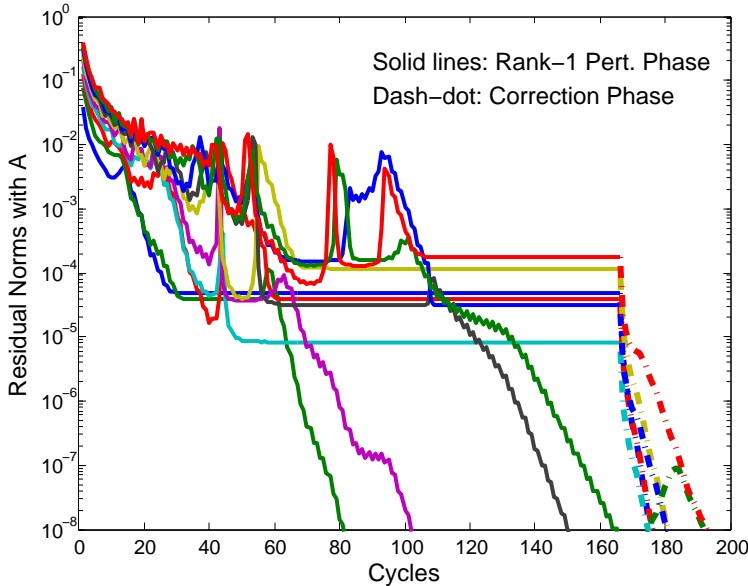


FIG. 5.1. Rank-1 Perturbed Arnoldi(33,15) with $\sigma = 1.e - 2$ followed by the Arnoldi correction phase. Matrix is 2-D Laplacian with $n = 40,000$.

TABLE 5.1

Perturbation of the first and fourth pairs of double eigenvalues.

σ	3rd eigenvalue	10th eigenvalue
0	0.00122137091776	0.00415167062026
10^{-4}	0.00122137091791	0.00415167062462
10^{-2}	0.00122137240153	0.00415171358000
1	0.00122520512527	0.00422933250928

change one eigenpair of a double. The second phase starts at cycle 167 and all residual norms converge by cycle 193. The convergence is rapid because we are able to run an Arnoldi iteration. Also, for this phase we already have approximations to nearby eigenvalues, so they are essentially deflated from the spectrum and the eigenvalues that are trying to converge are essentially well separated.

Now we look at results with several values of σ . Figure 5.2 shows the residual norms for the second copy of the fourth double eigenvalue (the tenth eigenvalue). The σ values are 10^{-6} , 10^{-4} , 10^{-2} and 1. As sigma increases, the first phase goes faster, because the formerly double eigenvalues are more separated. Table 5.1 shows original and perturbed values of the second copies of the first and fourth double eigenvalues (the 3rd and 10th overall eigenvalues). With the larger σ 's, the second phase has more work to do. The approximate eigenvectors are less accurate at the beginning of the second phase due to the greater perturbation in the first phase. Interestingly, the eventual results are fairly insensitive to the choice of σ . The number of cycles needed for residual norm below 10^{-8} is similar for this large range of perturbations.

The rank-one perturbation method with $\sigma = 10^{-2}$ uses 193 cycles to reach residual norm of 10^{-8} . We now compare to the other methods in this paper. Diagonally perturbed Arnoldi with $\sigma = 10^{-8}$ does reach this accuracy at cycle 212. So diagonal perturbation is not far behind rank-one, but as seen in Figure 4.6, the σ must be chosen more carefully. Using unperturbed Arnoldi and waiting for roundoff error is

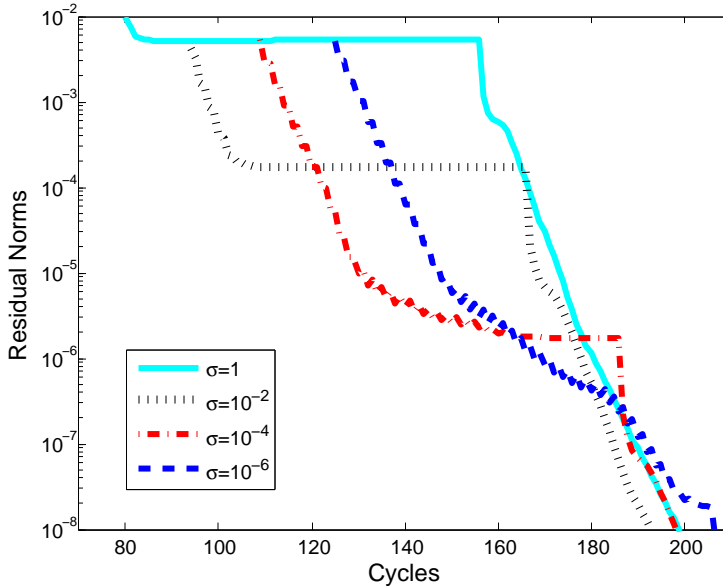


FIG. 5.2. Rank-1 Perturbed Arnoldi(33,15) with different sigma values, $\sigma = 1$, $\sigma = 1.e - 2$, $\sigma = 1.e - 4$, $\sigma = 1.e - 6$ followed by the Arnoldi correction phase. Matrix is 2-D Laplacian with $n = 40,000$.

tricky. If one sets the residual norm tolerance for 10^{-8} , the method will stop at 174 cycles with 10 eigenvalues determined to the specified accuracy. However, only the first three doubles have been found. If one continues the iteration, then eventually get the fourth double to residual norm accuracy of 10^{-8} at cycle 288. Block Arnoldi(33,15,2) takes 451 cycles.

Next for less accuracy with residual norm tolerance of 10^{-5} , the rank-one perturbation method with $\sigma = 10^{-2}$ needs 137 cycles. This is less than it looks like on Figure 5.2, because the first phase can be terminated earlier. Diagonally perturbed Arnoldi with $\sigma = 10^{-6}$ hits this mark at cycle 152. Meanwhile, unperturbed Arnoldi requires 238 cycles and again faces the issue of potentially being terminated too early, both after cycle 94 and after 151. Block Arnoldi takes 304 cycles to reach this residual norm tolerance.

Example 9. We now go back to the 3-D Laplacian matrix from Example 6. We use Arnoldi(33,15) in order to compute the ten smallest eigenvalues (a single and three triples) to accuracy of residual norm below 10^{-8} . For rank-one perturbations, we let $\sigma = 10^{-2}$, and diagonal perturbation uses $\sigma = 10^{-8}$. The rank-one approach uses three phases, because there are triple eigenvalues. The total cycles are 62, 50 for the first phase and six each for the next two phases. Unlike for computing double eigenvalues in the previous example, diagonal perturbation is marginally better with 59 cycles. Perhaps diagonal perturbation has an advantage as the multiplicity increases. Meanwhile, waiting for roundoff is a little slower at 69 cycles and Block-Arnoldi(33,15,3) is much slower with 165 cycles.

Example 10. We now consider computing the double eigenvalues of the nonsymmetric matrix RDB1250L from Matrix Market. Here $n = 1250$. The 11 smallest eigenvalues in magnitude are two copies each of -0.307994, -0.308311, -0.314221, -0.320983 and -0.338745 and then a single eigenvalue -0.341567. This multiple eigenvalue problem is fairly difficult because the smallest eigenvalues in magnitude are not

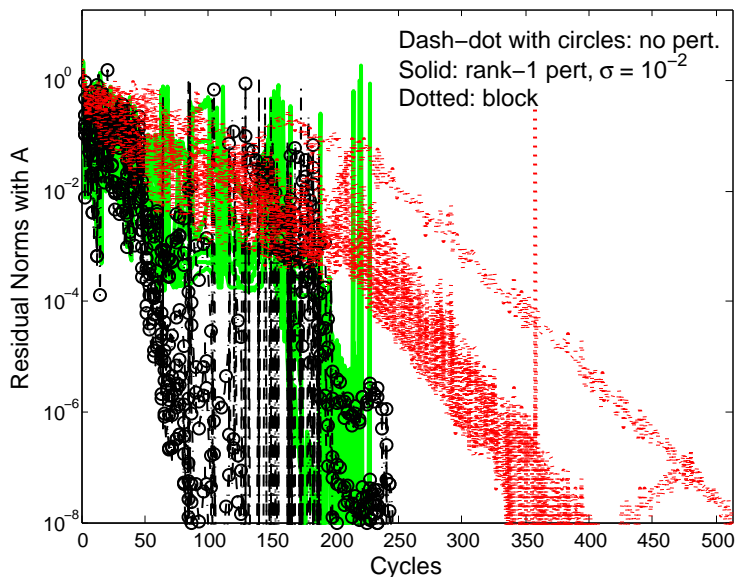


FIG. 5.3. Rank-1 Perturbed Arnoldi(33,15) with $\sigma = 1.e - 2$ followed by the Arnoldi correction phase, compared against no perturbation and block-Arnoldi. Matrix is RDB1250L. Residual norms for the smallest 10 Ritz values in magnitude are shown.

only double, they are close to each other. Also there are complex eigenvalues above and below these small eigenvalues that can cause spurious Ritz values near the origin. The smallest two pairs are particularly close. Also note that the 11th eigenvalue is very close to the double just smaller in magnitude. Therefore it is important for the convergence of this double to also have an approximation to the 11th eigenvector.

We first test Arnoldi(33,15) with both wait for roundoff and rank-one perturbation and Block Arnoldi(33,15,2). For the perturbation, we let $\sigma = 1.e - 2$, $nbuf = 11$, and again $s = t$ even though the matrix is nonsymmetric. The residual norms for the smallest 10 Ritz values are shown in Figure 5.3. It takes 228 cycles for the rank-1 perturbation method to converge versus 246 for unperturbed and 513 for block.

We next simulate a more difficult problem by limiting the size of the overall subspace. We apply versions of Arnoldi(16,6) in order to find the two smallest doubles. We let $nev = 4$ and $nbuf = 4$. This test will demonstrate that Arnoldi with no perturbation is trickier to use than with a rank-one perturbation. Watching the residual norms in Figure 5.4, it initially looks like Arnoldi with no perturbation is much more successful. The residual norms for the four smallest in magnitude Ritz values all converge to high accuracy. This is because the method has not yet detected the second copies of the double eigenvalues. The method must be forced to run way past the point at which it seems to have converged, until finally after 2000 cycles, the second copies start to show up. Meanwhile, rank-one perturbed Arnoldi has been struggling with the second copies and so the residual norms with respect to A have taken much longer to become accurate, even for the first copies that are not changed by the rank-one perturbation. The residual norms with respect to \hat{A} are accurate enough after 3601 cycles to switch to the second phase, then 450 more cycles are needed to converge to residual norms with respect to A below 10^{-8} . So the cycle total is 4051. This compares to 7041 cycles for unperturbed Arnoldi. However, the main point is that it is difficult to know when to stop the unperturbed Arnoldi, because it seems

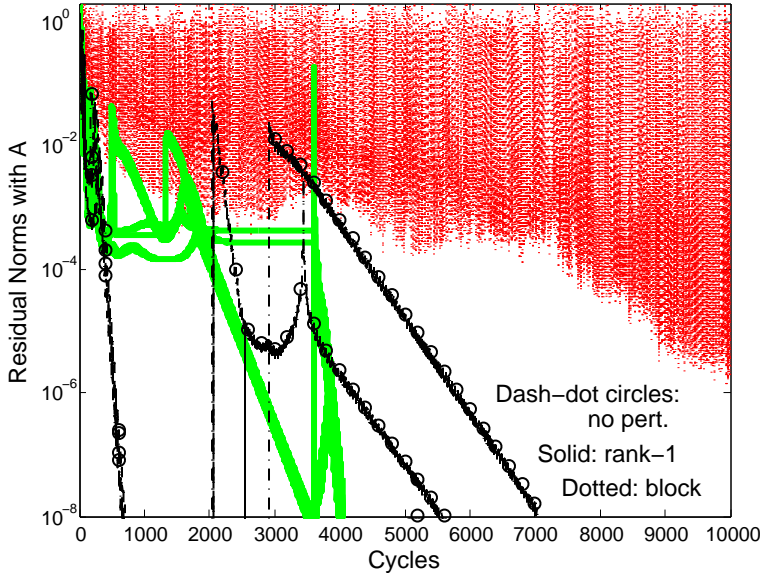


FIG. 5.4. Rank-1 Perturbed Arnoldi(16,6) with $\sigma = 1.e - 2$ followed by the Arnoldi correction phase, compared against no perturbation and block-Arnoldi. Matrix is RDB1250L. Residual norms for the smallest 4 Ritz values in magnitude are shown.

to have converged after 695 cycles and appears to do little from then until cycle 2059 when the first second copy materializes. We finally mention that the subspaces here are too small for block-Arnoldi to succeed. We ran it to 40,000 cycles, and it showed no sign of converging to both double eigenvalues.

6. Conclusion. Regular Arnoldi is a surprisingly viable method for finding multiple eigenvalues, though one does need to wait for roundoff error to help find the extra copies. Diagonally perturbing a matrix can help expose the multiple eigenvalues faster, however it does limit the accuracy. With rank-one perturbations, higher accuracy can be found. These new methods can be better than a block approach for difficult problems.

All the methods in this paper require some degree of specification of the multiplicity that we are looking for. Block methods need the block-size specified and the rank-one perturbation method needs to know the number of rank-one perturbations to use. Unperturbed Arnoldi may need to know the multiplicity to look for so that it does not terminate too early. The same is true for the diagonally perturbed Arnoldi. The last two methods may be best for the case of not knowing the multiplicity. And between the two, diagonally perturbed Arnoldi is less likely to be terminated before multiple eigenvalues have appeared.

REFERENCES

- [1] A. M. Abdel-Rehim, R. B. Morgan, D. A. Nicely, and W. Wilcox. Deflated and restarted symmetric Lanczos methods for eigenvalues and linear equations with multiple right-hand sides. *SIAM J. Sci. Comput.*, 32:129–149, 2010.
- [2] W. E. Arnoldi. The principle of minimized iterations in the solution of the matrix eigenvalue problem. *Quart. Appl. Math.*, 9:17–29, 1951.
- [3] J. Baglama. Augmented block Householder Arnoldi method. *Linear Algebra Appl.*, 429:2315–2334, 2008.

- [4] J. Baglama, D. Calvetti, and L. Reichel. IRBL: An implicitly restarted block Lanczos method for large-scale Hermitian eigenproblems. *SIAM J. Sci. Comput.*, 24:16501677, 2003.
- [5] D. Calvetti, B. Lewis, and L. Reichel. On the choice of subspace for iterative methods for linear discrete ill-posed problems. *Int. J. Appl. Math. Comput. Sci.*, 11:10691092, 2001.
- [6] D. M. Cvetković, M. Doob, and H. Sachs. *Spectra of Graphs*. Academic Press, New York, NY, 1979.
- [7] M. Embree and R. B. Morgan. Krylov methods for eigenvalues and linear equations with rank-one updated matrices. technical report, 2016.
- [8] G. H. Golub and R. Underwood. The block Lanczos method for computing eigenvalues. In John Rice, editor, *Mathematical Software III*, pages 364–377. Academic Press, New York, 1977.
- [9] R. G. Grimes, J. L. Lewis, and H. D. Simon. A shifted block Lanczos algorithm for solving sparse symmetric generalized eigenproblems. *SIAM J. Matrix Anal.*, 15:228272, 1994.
- [10] Z. Jia. Arnoldi type algorithms for large unsymmetric multiple eigenvalue problems. *J. Comput. Math.*, 17:257–274, 1999.
- [11] K. Q. Lan. Multiple eigenvalues for singular Hammerstein integral equations with applications to boundary value problems. *J. Comput. Appl. Math.*, 189:109–119, 2006.
- [12] R. B. Lehoucq and K. J. Maschhoff. Implementation of an implicitly restarted block Arnoldi method. Technical Report MCS-P649-0297, Argonne National Laboratory, Argonne, IL, 1997.
- [13] R. B. Morgan. On restarting the Arnoldi method for large nonsymmetric eigenvalue problems. *Math. Comp.*, 65:1213–1230, 1996.
- [14] R. B. Morgan. Restarted block-GMRES with deflation of eigenvalues. *Appl. Numer. Math.*, 54:222–236, 2005.
- [15] R. B. Morgan and M. Zeng. A harmonic restarted Arnoldi algorithm for calculating eigenvalues and determining multiplicity. *Linear Algebra Appl.*, 415:96–113, 2006.
- [16] Y. Saad. Variations on Arnoldi’s method for computing eigenvalues of large unsymmetric matrices. *Linear Algebra Appl.*, 34:269–295, 1980.
- [17] Y. Saad. *Numerical Methods for Large Eigenvalue Problems, 2nd Edition*. SIAM, Philadelphia, PA, 2011.
- [18] A.P. Seyranian, E. Lund, and N. Olhoff. Multiple eigenvalues in structural optimization problems. *Structural Optimization*, 8:207–227, 1994.
- [19] D. C. Sorensen. Implicit application of polynomial filters in a k -step Arnoldi method. *SIAM J. Matrix Anal. Appl.*, 13:357–385, 1992.
- [20] D. C. Sorensen. Deflation for implicitly restarted Arnoldi methods. Technical Report TR98-12, Rice University, Houston, Texas, 1998.
- [21] A. van der Sluis and H. A. van der Vorst. The rate of convergence of conjugate gradients. *Numer. Math.*, 48:543–560, 1986.
- [22] K. Wu and H. Simon. Thick-restart Lanczos method for symmetric eigenvalue problems. *SIAM J. Matrix Anal. Appl.*, 22:602 – 616, 2000.
- [23] Y. Zhou and Y. Saad. Block Krylov-Schur method for large symmetric eigenvalue problems. *Numer. Algor.*, 47:341–359, 2008.