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An Improved GMRES Method Augmented with Eigenvectors*

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Abstract: The restarted GMRES method augmented with eigenvectors is a useful method for solving nonsymmetric linear systems, especially the systems with a few of the smallest eigenvalues. But it is difficult to choose the appropriate number of eigenvectors that should be used, so the convergence may be slowed down and the precision could be reduced. This paper presents an improved method which adds the eigenvectors orderly and can be combined with some criterions to decide the proper number of eigenvectors adaptively. The numerical experiments show that this method can give higher precision, less iterates and CPU time.

Key words: GMRES, Krylov subspace method, nonsymmetric systems, eigenvector

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For solving the large nonsymmetric linear equation

$$AX = b \tag{1}$$

GMRES algorithm[1] is commonly used. It uses the Arnoldi algorithm[2,3] to build an orthogonal basis $\{v_1, \cdots, v_k\}$ for the Krylov subspace $\{v_1, Av_1, \cdots, A^{k-1}v_1\}$, with a full orthogonalization process. The best approximate solution is extracted from the subspace in that the norm of the residual vector is minimized.

However, the method becomes much expensive and the storage requirements increase when full orthogolization is used. So we usually use the restarted GMRES method, but during the restarting, some information is lost, the subspace is discarded, and this slows down the convergence, especially when there are a few small eigenvalues.

To remedy this disadvantage, some important information should be retained at the restart[4]. Give an algorithm named 'A Restarted GMRES Method Augmented with Eigenvectors'. It adds to the Krylov subspace some approximation to an invariant subspace associated with a few of the lowest eigenvalues, i.e. it saves approximate eigenvectors of a corresponding to the smallest eigenvalues on magnitude, and adds them to the new subspace. So the convergence could be accelerated, and the minimal property is retained.

But this algorithm also has some disadvantages. For example, the proper number of ap-

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proximate eigenvectors is hard to choose and more or fewer eigenvectors could have poor effects on the convergence. Assume the number of approximate eigenvectors which will be added to the new subspace is k, and the number of the smallest eigenvalues is s. First, if $s<k$ i.e. the number of approximate eigenvectors is smaller than we need, the smallest eigenvalues could not completely be deflated, and the expense could still be high. Second, if $s>k$, i.e. the number of approximate eigenvectors is more than we need, the expense would be higher, and the precision would be reduced because of the round error. Third, we noted that it may be a while before the approximate eigenvectors become very accurate, and an approximate eigenvector can have beneficial effects long before it has attained full accuracy[4]. So it just needs the eigenvectors corresponding to a few number of the smallest eigenvalues that less than k and the precision of them need not to be more accurate. Fourth, in some cases, we maybe can not confirm the k in advance or the eigenvectors are not really needed.

To remedy these poor effects, in this paper we present an improved restarted GMRES method which adds the eigenvectors orderly, and could be combined with criterions to add the approximate eigenvectors or back to standard restarted GMRES after discarding the approximate eigenvectors adaptively.

1 Adding approximate eigenvectors to the subspace orderly

The restarted GMRES algorithm augmented with eigenvectors[4] is useful for some case of system with a few of the smallest eigenvalues, because the convergence of GMRES is related to the condition number and the eigenvalue distribution of A, i.e. the smallest eigenvalues will slow down the convergence. Let P_m be the space of all polynomials of degree$\leqslant m$, σ represent the spectrum of A. These proprieties could be shown by the following theorems:

Theorem 1[1] Suppose that A is diagonalizable so that $A=XDX^{-1}$ and let

$$\varepsilon^{(m)}=\min_{p\in P_m,P(0)=1}\max_{\lambda_i\in\sigma}|p(\lambda_i)| \tag{2}$$

Then the residual norm provided at the m step of GMRES satisfies

$$\|r_{m+1}\|\leqslant K(X)\varepsilon^{(m)}\|r_0\| \tag{3}$$

where $K(X)=\|X\|\|X^{-1}\|$.

Theorem 2[4] Suppose A has spectral decomposition $A=Z\Lambda Z^{-1}$, with all the eigenvalues being real and positive. Assuming that the initial guess x_0 is the zero vector, we have

$$\|r\|/\|b\|\leqslant 2\|Z\|\|Z^{-1}\|*(1-2/(\sqrt{K}+1))^m \tag{4}$$

where $K=\lambda_n/\lambda_1$.

So, if we save the approximate eigenvectors of A corresponding to the smallest eigenvalues in magnitude, and add them to the new subspace. The convergence will be accelerated. This is demonstrated in the following theorem:

Theorem 3[4] Suppose A has spectral decomposition $A=Z\Lambda Z^{-1}$, with all the eigenvalues being real and positive. Assume that the minimum residual solution $\bar{x}$ is extracted from the

subspace Span$\{b, Ab, \cdots, A^{m-1}b, z_1, z_2, \cdots, z_k\}$. where z_i is column of Z. Then

$$\| r \| / \| b \| \leqslant 2 \| Z \| \| Z^{-1} \| (1 - 2/(\sqrt{K_e} + 1))^m \tag{5}$$

where $r = b - A\bar{x}$ is the residual vector, $K_e = \lambda_n / \lambda_{k+1}$.

To avoid the poor effects of the restarted GMRES augmented with eigenvectors listed formerly, we add the eigenvectors corresponding to the smallest eigenvalues orderly, i.e. we add one eigenvector to the subspace at first run, then two in the second run, then three in the third, etc. So, when $s < k$ (s, k as assumed in the beginning paragraph), the new method will soon reach the most proper number of eigenvectors and convergence quickly. When $s > k$, the new method could add up to the number of eigenvectors needed and avoid the possibility of stagnation caused by the rest smallest eigenvalues. Then the convergence bound improves from

$$\| r \| / \| b \| \leqslant 2 \| Z \| \| Z^{-1} \| (1 - 2/(\sqrt{K_e} + 1))^m$$

To

$$\| r \| / \| b \| \leqslant 2 \| Z \| \| Z^{-1} \| (1 - 2/(\sqrt{K_m} + 1))^m$$

Where $K_e = \lambda_n / \lambda_{k+1}$, $K_m = \lambda_n / \lambda_{m+1}$.

So we can roughly compare convergence by comparing $\sqrt{K_m}$ to $\sqrt{K_e}$, i.e. the rate of convergence is roughly $\sqrt{\lambda_{k+1}/\lambda_{m+1}}$ times faster. If there are some negative eigenvalues in the spectrum of A, we could also add all the corresponding negative eigenvectors orderly to the subspace. Using Theorem 1, we have

Corollary 1 Suppose A has spectrum decomposition $A = Z \Lambda Z^{-1}$, with $\lambda_i < 0$, $i \leqslant k$, $0 < \lambda_{k+1} \leqslant \lambda_{k+2} \leqslant \cdots \leqslant \lambda_n$, and the initial x_0 is the zero vector, the minimum residual solution is extracted from the subspace span $\{b, Ab, \cdots, A^{m-1}b, z_1, z_2, \cdots, z_k\}$, where z_i is column of Z, then

$$\| r \| / \| b \| \leqslant 2 \| Z \| \| Z^{-1} \| (1 - 2/(\sqrt{K_e} + 1))^m$$

where $K_e = \lambda_n / \lambda_{k+1}$

Proof: (omitted)

So, by adding all the negative eigenvectors to the subspace, we can get the same convergence as when A is positive definite.

According to the third problem with the early analysis, the approximate eigenvectors can have beneficial effects long before they have attained full accuracy. This is shown in the following theorem for the case of m approximate eigenvectors.

Theorem 4 Suppose A has spectral decomposition $A = Z \Lambda Z^{-1}$, with Λ diagonal. Suppose the GMRES method added eigenvectors orderly used with k approximate eigenvectors $y_1, y_2, \cdots, y_k$. Let $\psi_i \equiv \angle(y_i, z_i)$ and let θ_i be the coefficient of z_i in the expansion of b, then

$$\| r \| \leqslant \| Z \| \| Z^{-1} \| \max_{i=k+1,\cdots,n} | q(\lambda_i) | \| b \| + \sum_{i=1}^{k} \| A \| \tan\psi_i | q(\lambda_i) \| \theta_i | \lambda_i \tag{6}$$

Where q is a polynomial of degree m or less such that $q(0) = 1$, m is the dimension of the original Krylov subspace.

Proof: Any vector from the span$\{b, Ab, \cdots, A^{m-1}b, z_1, z_2, \cdots, z_k\}$ can be written in the form

$$\bar{x} = \sum_{i=1}^{k} a_i y_i + p(A)b \tag{7}$$

where p is a polynomial of degree $m-1$ or less. Expand b in terms of the eigenvectors

$$b = \sum_{i=1}^{n} \theta_i Z_i \tag{8}$$

and define the polynomial q as $q(x)=1-xp(x)$, so q is a polynomial of degree m or less, such that $q(0)=1$. Then we can calculate that

$$r = b - A\bar{x} = -\sum_{i=1}^{k} a_i \lambda_i y_i + q(A)b \tag{9}$$

Decompose $y_i = \cos\psi_i z_i + \sin\psi_i u_i$, where y_i, z_i, and u_i are all unit vectors and $u_i \perp z_i$. Then

$$r = q(A)b - \sum_{i=1}^{k} a_i \lambda_i z_i \cos\psi_i - \sum_{i=1}^{k} a_i \sin\psi_i A u_i =$$

$$\sum_{i=k+1}^{n} \theta_i q(\lambda_i) Z_i + \sum_{i=1}^{k} ((\theta_i q(\lambda_i) - a_i \lambda_i \cos\psi_i) z_i - a_i \sin\psi_i A u_i \tag{10}$$

Pick $a_i = \theta_i q(\lambda_i)/\lambda_i \cos\psi_i$ and use the minimum residual property. Then

$$\| r \| \leqslant \| \sum_{i=k+1}^{n} \theta_i q(\lambda_i) z_i + \sum_{i=1}^{k} ((\theta_i q(\lambda_i) - a_i \lambda_i \cos\psi_i) z_i - a_i \sin\psi_i A u_i \| \leqslant$$

$$\| \sum_{i=k+1}^{n} \theta_i q(\lambda_i) z_i \| + \| \sum_{i=1}^{k} \theta_i q(\lambda_i) \tan\psi_i A u_i / \lambda_i \| \leqslant$$

$$\| Z \| \| Z^{-1} \| \max_{i=k+1,\cdots,m} | q(\lambda_i) | \| b \| + \sum_{i=1}^{k} \| A \| \tan\psi_i | q(\lambda_i) \| \theta_i | / \lambda_i$$

The inaccuracy of the approximate eigenvector causes the second term in the right-hand of (6). Roughly, it appears that this term will not be significant as long as the accuracy of the approximate eigenvector is greater than the amount improvement brought by the polynomial q.

When the eigenvalues are all real by choosing the polynomial q to be a shifted and scaled Chebyshev polynomial that is small over the interval$[\lambda_{k+1}, \lambda_n]$, the (6)can be made more specific.

Corollary 2 Under the assumption in Theorem 5, assume that all the eigenvalues are real and positive, then

$$\| r \| \leqslant \| z \| \| z^{-1} \| (1 - 2/(\sqrt{K_e} + 1))^m \| b \| + \sum_{i=1}^{k} \| A \| \theta_i \tan\psi_i / \lambda_i \tag{11}$$

$$\| r \| \leqslant \| z \| \| z^{-1} \| (1 - 2/(\sqrt{K_e} + 1))^m \| b \| + \sum_{i=1}^{k} \| A \| \tan\psi_i / \lambda_i \tag{12}$$

where $K_e = \lambda_n / \lambda_{k+1}$.

Proof: (omitted)

2 Implementations

To remedy the disadvantage of the GMRES(m) algorithm with eigenvectors, we use the improved method by adding the eigenvectors orderly to the subspace. There are some variations of this algorithm.

First, we could give a fix number k, if the number of eigenvectors added orderly reaches k, then the number of vectors will never add, and behave like the restart GMRES(m) augmented with k eigenvectors.

Second, we add one eigenvector to the subspace at first, then after one iteration, we use criterions to judge if the eigenvector is still beneficial. If not, the next eigenvector will be added, else, no other eigenvector will be added at the next restart. By this means, the eigenvectors will be added until tolerance be satisfied.

Third, because even beneficial eigenvectors may lose their effectiveness once components of the residual vector in the directions of those eigenvectors have been purged. If so, the approximate eigenvectors will be released and the algorithm will go back to the standard restarted GMRES.

The last two varieties of algorithms could be seemed as adaptive procedures, and can be used in the case in which the approximate number of eigenvectors could hardly to predict.

We now define some terminology. Let m be the dimension of the Krylov subspace, and k be the number of eigenvectors used in this iteration step, and $s = m + k$. Let W be n by s matrix whose first m columns are the orthonormalized Arnoldi vectors and whose last k vectors are the approximate eigenvectors y_i, for $i = 1:k$, and let Q be n by $s+1$ matrix whose first $m+1$ columns are Arnoldi vectors and whose last columns are formed by orthogonalizing the vectors Ayi, for $i = 1:k$, against the previous columns of Q.

Then we get

$$AW = Q\bar{H} \tag{13}$$

where $\bar{H}$ is an $(s+1)$by s upper-Hessenberg matrix.

The next step is to solve the minimum residual equation[4]

$$\min_{d \in R^1} \| \| r_0 \| e_1 - \bar{H}d \|_2 \tag{14}$$

the new approximate solution is $\bar{x} = x_0 + Wd$ on the span$\{q_1, q_2, \ldots, q_m, y_1, y_2, \ldots, y_k\}$.

The last step is to find $k+1$ new approximate eigenvectors. As the same as the restart GMRES with eigenvalues[4], we use a version of Rayleigh－Ritz algorithm for solving the reduced problem

$$WT * A * Wg_i = (1/\theta_i) WT * A * AWg_i \tag{15}$$

Let $F = WT * A * W$, $G = WT * AT * AW$, then the reduced eigenvalue problem is the s by s generalized eigenvalue problem

$$Fg_i = (1/\theta_i) Gg_i \tag{16}$$

If we calculate $k+1$ generalized eigenvectors g_i, $i=1,\ldots,k+1$, corresponding to $k+1$ smallest θ_i, then the approximate eigenvector of A is $y_i = Wg_i$, and $Ay_i = AWg_i = Q\overline{H}g_i$. If y_i is complex, the real and imaginary parts are used seperately. From (12), $G = \overline{H}T * QT * Q\overline{H}$. Let $P\overline{H} = R$, where P is orthogonal and R is upper triangular. Then $G = RT * R$. For the generating process of F, G, see [4]. Based on the previous discussion, the implementation is a little difference for the first run, before any restart. Standard GMRES is used, except eigenvectors added orderly at the end . For simplicity, we list the algorithm just for the second and subsequent runs.

3 The Improved Restarted GMRES with Eigenvectors(I-IV)

Algorithm 1:

1. Initial definitions and caculations: The Krylov subspace generated by the Arnoldi process using initial $r_0 = b - Ax_0$. The dimension is m and k is the number of approximate eigenvectors. $s = m + k$, the approximate eigenvectors yi, $i = 1,\cdots,k$. F_{old} has bee generated from the last run. Let $\beta = \| r_0 \|$, $q1 = r_0/\beta$, $w_1 = q_1$, for $i = 1,\cdots,k$, do $W_{m+i} = y_i$; For $j = m+1,\cdots,s$, do $f_{i,j} = g_i * F_{old}\, gi$, $i = m+1,\cdots,s$

2. Arnoldi process:

For $j = 1,2,\ldots,m$ do

$h_{i,j} = (Aq_j, q_i)$, $i = 1,2,\ldots,j$

$$\overline{q}_{i+1} = Aq_i - \sum_{i=1}^{j} h_{i,j}q_i$$

$$h_{j+1,j} = \| \overline{q}_{j+1} \|_2, q_{j+1} = \overline{q}_{j+1}/h_{j+1,j}$$

$$f_{j,i} = h_{i,j}, i = 1,2,\ldots,j$$

$$f_{j,m+i} = (Aq_j, y_i) i = 1,2,\ldots,k$$

If $j < m$ then $w_{j+1} = q_{j+1}$ and $f_{j,j+1} = h_{j+1,j}$

3. Add approximate eigenvectors:

For $j = m+1,\ldots,s$ do

$h_{i,j} = (Aw_j, q_j), i = 1,2,\ldots,j$

$$\overline{q}_{j+1} = Aw_j - \sum_{i=1}^{j} h_{i,j}q_i$$

$$h_{j+1,j} = \| \overline{q}_{j+1} \|_2, q_{j+1} = \overline{q}_{j+1}/h_{j+1,j}$$

$$f_{j,i} = h_{i,,j}, i = 1,2,\ldots,m$$

4. Form the approximate solution:

Solve the minimum problem $\min_{d \in R^s} \| \| r_0 \| e_1 - \overline{H}d \|_2$, then $\overline{x} = x_0 + Wd$

5. Restart:

Compute $r = b - A\overline{x}$ if it satisfies with the residual norm requirement then stop, else let , $r_0 = r, k = k+1$, $x_0 = \overline{x}$

6. Form the new k approximate eigenvectors: Calculate $G = RT * R$. Solve the generalized eigenvalue problem $Fg_i = (1/\theta_i) Gg_i$. For g_i, $i = 1, \ldots, k$ which is the k Ritz vectors corresponding to the smallest θ_i, and separate g_i into real and complex part(if it is complex and treat as two distinct vectors). Then form $y_i = wg_i$ and $Ay_i = Q\overline{H}g_i$, $i = 1, 2, \cdots, k$.

Let Fold = F. Go to 1.

To add the eigenvectors orderly with a maximum number K (the first variety of algorithm). We have little change in Step 5 of Algorithm 1:

Algorithm 2

Steps 1-4 are the same as Algorithm 1.

Step 5. Restart: Compute $r = b\text{-}A\bar{x}$ if it satisfies with the residual norm requirement then stop, else if $k < K$ then $k = k + 1$; else end. Let $x_0 = \bar{x}$, $r_0 = r$.

Step 6 is the same as Algorithm 1.

To add the eigenvector orderly under the criterions (the second variety of the algorithm), we have some change in Step 5 of Algorithm 1.

Algorithm 3

Steps 1-4 are the same as Algorithm 1.

Step 5. Restart:

Compute $r = b\text{-}A\bar{x}$ if it satisfies with the residual norm requirement then stop, else if criterions are satisfied then $k = k + 1$; else end . Let $x_0 = \bar{x}, r_0 = r$. Step 6 is the same as algorithm 1.

To add the eigenvector orderly and discard all the eigenvectors adaptively with some criterions. (the third variety of the algorithm) we have more changes in Algorithm 1.

Algorithm 4

Steps 1-4 are the same as Algorithm 1.

Step 5. Restart :

Compute $r = b - A\bar{x}$ if it satisfies with the residual norm requirement then stop, else , let $x_0 = \bar{x}$, $r_0 = r$. If criterions are satisfied then go to Step 7; else $k = k + 1$, go to Step 6.

Step 6 is the same as Algorithm 1.

Steps 7-9 are the same as the standard restarted GMRES, for using the Krylov subspace of $(m + k)$ dimensions (the precise process is omitted).

Next, we will examine their expense and storage requirements as compared to the GMRES method augmented with eigenvectors.

We consider only the matrix-vector multiplication(mvp) expense. Then, suppose the GMRES method with eigenvectors use k approximate eigvectors. So in each iteration , the algorithm has $(m + 2k)$ mvp, m for Arnoldi process, and $2k$ for generate yi, $Ay_i\, i = 1, 2, \cdots, k$. After n iterations the total expense is $(m + 2k)n$ mvps and corresponding storage requirement is $(m + 2k)$ vectors of length n.

On the other hand, the improved algorithms have different expense while the number of

iteration increase. Suppose the iteration number is n, the number of Krylov vectors is m, and the number of eigenvectors is s. Then the expense of this time of iteration process is $(m+2s)$ mvps. The corresponding storage requirement is $(m+2s)$ vectors of length n.

For Algorithm 1, the expense after n iterations is $n(m+n+1)$mvps (in the situation $s=n$). For Algorithm 2, suppose the maxim number of eigenvectors is s, then the expense is $(m+n+1)n$ if $n\leqslant s$, $(m+2s)n+(1-s)s$ if $n>s$. For Algorithm 3, Suppose in each z_i $(i=1,\cdots,s)$ iterations, the corresponding number of approximate eigenvectors is i, where $n=\sum_{i=1}^{s}Z_i$. The total expense is $(mn+2\sum_{i=1}^{s}iZ_i)$mvps. For Algorithm 4, suppose in $s+1$ steps, the approximate eigenvectors will be discarded, and the algorithm back to standard restarted GMRES with $(m+s)$ Krylov vectors. Then the total expense is $[(m+s)n+s]$ mvps.

For Algorithms 1-3, the storage requirements in the end are $(m+2s)$, however, for Algorithm 4, they are up to $(m+2s)$, then decrease to $(m+s)$ vectors of length n.

3 Examples

At first, we will give some definitions. We denote the standard Full GMRES by FULL(); the standard restarted GMRES with Krylov subspace of m dimension by $R(m)$; the GMRES augmented with k eigenvectors and m Krylov vectors by $E(m, k)$; Algorithm 1 by $N1(m)$, m is the dimension of the Krylov subspace; Algorithm 2 by $N2(m, k)$, k is the maximum number of eigenvectors that can be added; Algorithms 3,4 by $N3(m)$, $N4(m)$ orderly.

In the following examples, the right-hand sides have all entries 1.0. The initial guess x_0 are zero vectors. The first two examples are bidiagonal matrix, with 0.1 in each superdiagonal position. The calculations are done in double precision on PC with Pentium-II CPU, 32M memory.

Example 1 We denote the matrix as A(300,300), which has 0.1,0.2, ,0.9,1,2,...,291 on the main diagonal ,and as mentioned above ,the super diagonal element has 0.1's. It is the case with more numbers of the smallest eigenvalues. For this matrix, we choose $m=20$, and $k=4$(i.e. 20 Krylov vectors and 4 approximate eigenvectors). k was decided by the experience estimate in [4]. The result and the graph of convergence was shown in Table 1 and Fig 1.

Table 1 The numerical results of Example 1

	ITERATIONS	CPU TIME	RESIDUAL
FULL()	201	46.69s	5.836e-011
R(20)	88	24.16s	9.149e-011
E(16,4)	41	13.23s	5.588e-011
*N*2(16,4)	34	10.16s	3.841e-011
*N*1(16)	16	6.37s	5.146e-011

Thus, in the same size of subspace, $E(16,4)$ and $N2(16,4)$ are better than Full GMRES and R(20), and $N2(16,4)$ is better than $E(16,4)$. Based on the same size of Krylov subspace, $N1(16)$ is obviously the best in all the algorithms being compared, because it can add enough eigenvectors adaptively to remove the poor effect caused by the smallest eigenvalues more efficiently than others.

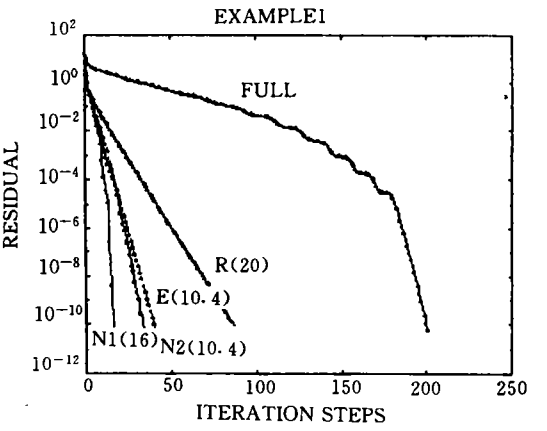

Fig. 1　The convergence curves of Example 1

Example 2　The next matrix has some negative eigenvalues, i.e. it is an indefinite problem. The entries on the main diagonal are: $-5,\cdots,-1,1,\cdots,295$. See Table 2 and graph in Fig. 2 for the computational results.

The results show that under the same size of subspace, the improved algorithm is better than standard restart GMRES, and GMRES augmented with eigevectors. Under the same Krylov subspace, the $N3(16)$ is the most efficiently, and the residual norm is one order of magnitude better, because the eigenvector corresponding to the negative eigenvalues are orderly added and very helpful with the components of the residual were quickly stripped.

Table 2　The numerical results of Example 2

	ITERATIONS	CPU TIME	RESIDUAL
FULL()	150	27.08s	8.188e−011
R(21)	74	24.06s	9.766e−011
E(16,5)	59	17.36s	7.535e−011
*N*2(16,5)	42	12.63s	7.278e−011
*N*1(16)	13	4.72s	4.785e−012

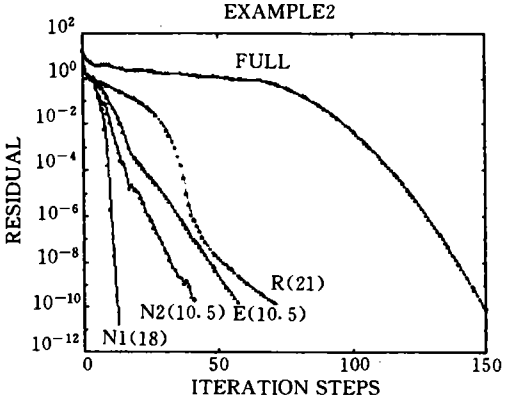

Fig. 2　The convergence curves of Example 2

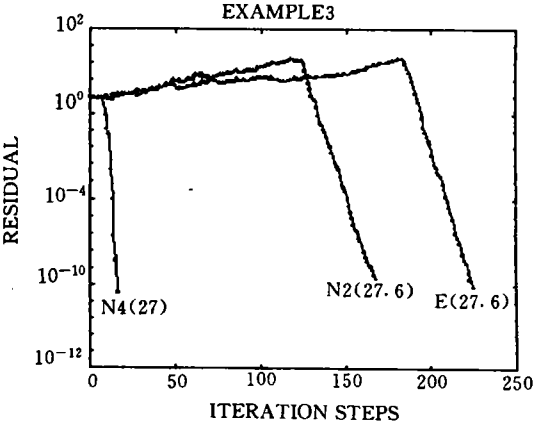

Fig. 3 The convergence curves of Example 3

The previous examples work in the situation that the proper number eigenvectors which should be used can be judged by experience and the method which add approximate eigenvectors corresponding to the smallest eigenvalues to the subspace could be very helpful. But in some case, it doesn't work. For examples, the eigenvalues scatter around the complex plane or the smallest eigenvales are less separated from rest of the spectrum, or there may be not small eigenvalues. To decide the proper number of eignvectors, which should be added under the situation that could hardly be decided by experience, we should give an algorithm that can do this adaptively with some criterions. This algorithm should also helpful to decide whether we should discard the eigenvectors's subspace, when they are no more helpful after some times of iterations or under the situation that adding eigenvectors doesn't helpful. So we use the improved Algorithm 4, with criterions[4]:

$$\| r_m \| - \| r_{m+k} \| < 0.2(\| r_{m+k} \| - \| r_m \|) \tag{17}$$

and

$$-\lg(\varepsilon_n e_1)_{\text{new}} + \lg(\varepsilon_n e_1)_{\text{old}} < 0.1(-\lg \| r_{m+k} \|_{\text{new}} + \lg \| r_{m+k} \|_{\text{old}}) \tag{18}$$

here, r_m(or r_{m+k})is the residual after in m(or $m+k$) iterations,

$$\varepsilon_n e_i = \| Ay_i - \rho_i y_i \| / \| y_i \| \tag{19}$$

is the eigenvector residual norm ,where

$$\rho_i = y_i T * Ay_i / y_i T * y_i = y_i T * F * y_i / y_i T * y_i \tag{20}$$

The next example will show the efficiency of it.

Example 3 Denote the matrix by $A(100,100)$, d is a diagonal matrix with main diagonal elements are 1.0, with β in each supperdiagonal position $\beta = 0.9$. The method that adding eigenvectors is not helpful on this problem.

Under the Krylov subspace with dimension 27, the results and graph is shown in Table 3 and Fig 3. We could see that Algorithm 4 is more efficient than the others.

In addition, Algorithm 4 also efficient in Examples 1 − 3, and we can also compare it with the previous results come from the others algorithm.

Table 3 The numerical results of Example 3

	ITERATIONS	CPU TIME	RESIDUAL
$E(27,6)$	225	106.67s	7.078e−011
$N2(27,6)$	169	79.64s	9.431e−011
$N1(27)$	17	7.63s	3.154e−011

4 Conclusions

Adding approximate eignvectors to the subspace is a useful method to solve some case of large nonsymmetric system especially with a few of smallest eigenvalues. The restarted GMRES method with eigenvectors compute and save fixed number k eigenvectors, and add them to

Krylov subspace. But it has some disadvantages. The improved GMRES algorithm with eigenvectors presents a new thought to add the eigenvectors to the subspace orderly, and could combine some criterions to add eigenvectors or discard them adaptivly. It could efficiently remedy these disadvantage, and raise the converge speed and numerical precision. The numerical examples prove it.

In addition, to make the adaptive procedure more efficiently, we should find more efficient criterions. This problem needs more research.

References

[1] Saad Y, Schyktz M H. GMRES: a generalized minimal residual algorithm for solving nonsymmetric systems. SIAM J Sci Statist Comput, 1986, 7:856~869.

[2] Saad Y. Variations on Arnodi's method for computing eigenelements of large unsymmetric matrics. Lin Algebra Appl, 1980,34:269~295.

[3] Saad Y. Krylov subspace methods for solving large unsymmetric linear systems. Math Comp, 1981,37: 105~126.

[4] Morgan R B. A Restarted GMRES Method Augmented with Eigenvectors. SIAM J Matrix Anal Appl, 1995, 4(16):1 154~1 171.

[5] Morgan R B. Computing interior eigenvalues of large matrices. Linear Algebra Appl, 1991,154~156:289 ~309.

[6] Gui Lizhong, Shu Jiwu. The modified GMRES algorithm for solving large unsymmetric linear systems. J Nanjing Univ, Math Biquart, 1999, 1(16):109~118.

一种改进的利用特征向量的GMRES方法

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摘 要: 利用特征向量的重开始的GMRES方法是一种解非对称线型系统的,特别是解拥有少量极小特征值的非对称线型系统的有效方法,但应采用的恰当的特征向量数目却很难确定.这将可能导致收敛速度的减慢和数值结果的精度降低.给出了一种改进的利用特征向量的GMRES方法,它采用逐次增加特征向量的方法,并可结合特定的收敛准则自适应的确定恰当的特征向量数目.数值结果证明此方法可以得到更高的精度,花费更少的迭代次数和CPU时间.

关键词: GMRES方法, Krylov子空间方法, 非对称系统,特征值