A new adaptive restart for GMRES(m) method

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Abstract

GMRES(m) is a Krylov subspace method for solving nonsymmetric linear systems of equations. The difficulty of this method lies in choosing the appropriate restart cycle m. We propose a new strategy for the adaptive restart for GMRES(m) which is based on using the difference of the Ritz and harmonic Ritz values. We also report on numerical experiments which show that this new approach is both effective and robust.

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1 Introduction

Consider the problem of solving a linear system of the form

$$A\boldsymbol{x} = \boldsymbol{b}\,, \tag{1}$$

where $A \in \mathcal{C}^{n\times n}$ is a sparse nonsymmetric and nonsingular matrix, and $\mathcal{C}^{n\times n}$ denotes the set of complex matrices of dimension $n \times n$. Such linear systems often arise in scientific computing.

GMRES is one of the Krylov subspace methods for solving (1). It minimizes the residual norm over the Krylov subspace

$$\mathcal{K}_m(A, \boldsymbol{r}_0) = \operatorname{span}\{\boldsymbol{r}_0, A\boldsymbol{r}_0, A^2\boldsymbol{r}_0, \ldots, A^{(m-1)}\boldsymbol{r}_0\}\,, \quad m = 1, 2, \ldots\,, \tag{2}$$

at every step, and $\boldsymbol{r}_0$ is the initial residual vector. In GMRES, the orthonormal basis $(\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m)$ of $\mathcal{K}_m(A, \boldsymbol{r}_0)$ is computed by orthogonalizing the

Krylov basis $\{\boldsymbol{r}_0, A\boldsymbol{r}_0, \ldots, A^{(m-1)}\boldsymbol{r}_0\}$ with Arnoldi process [2]. The computed orthonormal basis form an orthogonal matrix $V_m = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m] \in \mathcal{C}^{n\times m}$. In the Arnoldi process, scalars $h_{i,j}$ are also computed so that the square upper Hessenberg matrix $H_m = (h_{i,j}) \in \mathcal{C}^{m\times m}$ satisfies

$$AV_m = V_m H_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^H = V_{m+1}\bar{H}_m\,, \tag{3}$$

where $\bar{H}_m \in \mathcal{C}^{(m+1)\times m}$ is the matrix H_m supplemented with an extra row $(0, \ldots, 0, h_{m+1,m})$, and $\boldsymbol{e}_m$ is column m of the identity matrix of dimension m. Multiplying (3) by V_m^H from the left, we get

$$V_m^H A V_m = H_m\,. \tag{4}$$

In theory [12], the full GMRES converges before n iterations. But the cost for computing the orthonormal basis of subspace $\mathcal{K}_m(A, \boldsymbol{r}_0)$ increases linearly with the iteration count. According to this drawback, the full GMRES is not practical for large linear systems of equations. In order to reduce the cost of the full GMRES, a restarted version of GMRES, which restarts after each cycle of m iterations, is often used. The restarted version is denoted by GMRES(m). Compared to the full GMRES, GMRES(m) requires less work and storage, but the difficulty lies in choosing the appropriate restart cycle m. Generally, m is selected according to numerical experience. The best way to select m has not yet been established. A number of different approaches of adaptive restart have been proposed [6, 10, 11, 14]. We propose a new adaptive restarting strategy based on using the difference of the Ritz and harmonic Ritz values which is computed from the upper Hessenberg matrices H_m and $\bar{H}_m$.

In Section 2 we briefly describe the Ritz and harmonic Ritz values and their related properties. In Section 3 a new restarting strategy based on exploiting the Ritz and harmonic Ritz values is proposed. This restarting strategy can still work well in preconditioned GMRES(m). As an example, we make use of the preconditioner used in DEFLATED-GMRES(m, k) in Section 4. We also report on some numerical experiments comparing the proposed method with other methods in Section 5. These results show that this new approach is both effective and robust.

2 Ritz and harmonic Ritz values

The Ritz and harmonic Ritz values and vectors are approximate eigenvalues and eigenvectors. Recently, they have been used in a number of modified versions of GMRES(m) to achieve better performance. For example, the harmonic Ritz values and vectors are used in MORGAN(m, k) [8, 9]. We make different use of the Ritz and harmonic Ritz values.

Definition 1 (Ritz values [13]) *If $\mathcal{V}_k$ is a linear subspace of $\mathcal{C}^{n\times n}$, then λ_k is a Ritz value of A with respect to $\mathcal{V}_k$ with Ritz vector $\boldsymbol{u}_k$ when $(A\boldsymbol{u}_k - \lambda_k\boldsymbol{u}_k)\perp\mathcal{V}_k$, $\boldsymbol{u}_k \in \mathcal{V}_k$, $\boldsymbol{u}_k \neq 0$.*

In the context of the GMRES, $\mathcal{V}_k$ is the Krylov subspace $\mathcal{K}_m(A, \boldsymbol{r}_0)$. A Ritz value λ with Ritz vector $\boldsymbol{u} = V_m\boldsymbol{y}_m$, $\boldsymbol{y}_m \in \mathcal{C}^{m\times 1}$, with respect to $\mathcal{K}_m(A, \boldsymbol{r}_0)$ satisfies $(A\boldsymbol{u} - \lambda\boldsymbol{u})\perp\mathcal{K}_m(A, \boldsymbol{r}_0) \Leftrightarrow V_m^H(AV_m\boldsymbol{y}_m - \lambda V_m\boldsymbol{y}_m) = 0$, where V_m is defined in equation (3). Using relation (4), we have $H_m\boldsymbol{y}_m = \lambda\boldsymbol{y}_m$. That is, the eigenvalues of H_m are the Ritz values of A with respect to the Krylov subspace $\mathcal{K}_m(A, \boldsymbol{r}_0)$.

We skip the definition for harmonic Ritz values and vectors, which are found in [13]. In order to compute the harmonic Ritz values from the Krylov subspace $\mathcal{K}_m(A, \boldsymbol{r}_0)$, we use of the following theorem.

Theorem 2 (Sleijpen et al. [13]) *Let $\mathcal{V}_k$ be some k-dimensional subspace. A value $\bar{\lambda}_k \in \mathcal{C}$ is a harmonic Ritz value of A with respect to the subspace $\mathcal{W}_k := A\mathcal{V}_k$ if and only if $A\boldsymbol{u}_k - \bar{\lambda}_k\boldsymbol{u}_k\perp A\mathcal{V}_k$ for some $\boldsymbol{u}_k \in \mathcal{V}_k$, $\boldsymbol{u}_k \neq \boldsymbol{0}$.*

According to this theorem, a harmonic Ritz value $\bar{\lambda}$ with harmonic Ritz vector $\boldsymbol{u} = V_m\boldsymbol{y}_m$, $\boldsymbol{y}_m \in \mathcal{C}^{m\times 1}$, with respect to subspace $A\mathcal{K}_m(A, \boldsymbol{r}_0)$ satisfies

$$(A\boldsymbol{u} - \bar{\lambda}\boldsymbol{u})\perp A\mathcal{K}_m(A, \boldsymbol{r}_0) \Leftrightarrow (AV_m)^H(AV_m\boldsymbol{y}_m - \bar{\lambda}V_m\boldsymbol{y}_m) = 0\,,$$

where V_m is the same as in equation (3). Using equations (3) and (4), we have $\bar{H}_m^H \bar{H}_m \boldsymbol{y}_m = \bar{\lambda} H_m^H \boldsymbol{y}_m$. When H_m is nonsingular, it can be rewritten as $H_m^{-H} \bar{H}_m^H \bar{H}_m \boldsymbol{y}_m = \bar{\lambda} \boldsymbol{y}_m$. That is, the eigenvalues of $H_m^{-H} \bar{H}_m^H \bar{H}_m$ are the harmonic Ritz values of A with respect to subspace $A\mathcal{K}_m(A, \boldsymbol{r}_0)$. Equation (3) allows us to rewrite $H_m^{-H} \bar{H}_m^H \bar{H}_m$ as $H_m + h_{m+1,m}^2 f_m \boldsymbol{e}_m^H$, where $f_m = H_m^{-H} \boldsymbol{e}_m$.

3 An adaptive restarting strategy

To reiterate, we know that

1. the eigenvalues of matrix H_m are the Ritz values with respect to the Krylov subspace $\mathcal{K}_m(A, \boldsymbol{r}_0)$, and
2. the eigenvalues of $H_m + h_{m+1,m}^2 f_m \boldsymbol{e}_m^H$ are the harmonic Ritz values with respect to the subspace $A\mathcal{K}_m(A, \boldsymbol{r}_0)$.

Note that when an invariant Krylov subspace has been found, the harmonic Ritz values equal to the Ritz values, since in this case $h_{m+1,m} = 0$. From Saad et al. [12], GMRES converges when $h_{m+1,m} = 0$. Goossens et al. [5] gave an upper bound of the 2-norm of the second item in $H_m + h_{m+1,m}^2 f_m \boldsymbol{e}_m^H$:

$$\|h_{m+1,m}^2 \boldsymbol{f}_m \boldsymbol{e}_m^H\|_2 \leq \frac{h_{m+1,m}^2}{\sigma_{min}(H_m)} , \tag{5}$$

where $\sigma_{\min}(H_m)$ is the smallest singular value of H_m.

This upper bound shows that the difference between the Ritz and harmonic Ritz values can only be large when $|h_{m+1,m}|$ is large or $\sigma_{min}(H_m)$ is small, which is the case when GMRES stagnates. Goossens et al. suggested that the difference between the Ritz and harmonic Ritz values be used for predicting the stagnation of GMRES [5]. Our main contribution is to put this result to practical use in GMRES(m). That is, we propose an adaptive restarting strategy using this result.

We compute the difference between the maximum Ritz value $\lambda_{\max}$ and the maximum harmonic Ritz value $\bar{\lambda}_{\max}$ per iteration. If it is larger than the one generated from the last iteration, then we restart. Otherwise no restart is carried out. Note that the maximum restart cycle should be specified in view of memory limitations. Minimum restart cycle can be specified too.

Our new method is denoted as RITZ-GMRES($m_{\min}, m_{\max}$), where $m_{\min}$ is the minimum restart cycle and $m_{\max}$ is the maximum restart cycle. Algorithm 1 details the computational scheme. Compared with the classical GMRES(m), extra work for computing $\lambda_{\max}$ and $\bar{\lambda}_{\max}$ is required. But the cost only depends on the dimension of the Krylov subspace, which is small ($\leq m_{\max}$). In Section 5 we show that this new adaptive restart is both effective and robust.

4 Application in preconditioned GMRES(m)

The new restarting strategy proposed in Algorithm 1 can also work well in preconditioned GMRES(m). As an example, we make use of the preconditioning technique used in DEFLATED-GMRES(m, k).

It has been observed that the convergence of GMRES(m) may be slower than the full GMRES. It appears as if the restarting procedure loses the information on the smallest Ritz values [3, 4]. In order to eliminate those smallest Ritz values, a preconditioning technique, named deflation, is used in DEFLATED-GMRES(m, k) [3, 4].

Let $|\lambda_1| \leq |\lambda_2| \leq \cdots \leq |\lambda_n|$ be the Ritz values of A, and $\boldsymbol{u}_i$ be the Ritz vector with respect to λ_i. In DEFLATED-GMRES(m, k), a fixed number l ($l = 1$ in this paper) of Ritz vectors $\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_l$ are pulled out after each

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Algorithm 1: RITZ-GMRES($m_{\min}, m_{\max}$)

Require: ϵ is the tolerance for the residual norm

$i := 0$; convergence:=false;
repeat
  $\boldsymbol{r}_0 := \boldsymbol{b} - A\boldsymbol{x}_0$; $\beta := \|\boldsymbol{r}_0\|_2$; $\boldsymbol{v}_1 := \boldsymbol{r}_0/\beta$;
  $m := 1$;
  while $m \leq m_{\max}$ **do**
    $i := i + 1$;
    $\bar{\boldsymbol{v}} := A\boldsymbol{v}_m$;
    for $j = 1, 2, \ldots, m$ **do**
      $H(j, m) := \boldsymbol{v}^H \bar{\boldsymbol{v}}$;
      $\bar{\boldsymbol{v}} := \bar{\boldsymbol{v}} - H(j, m)\boldsymbol{v}_i$;
    $H(m+1, m) := \|\bar{\boldsymbol{v}}\|_2$;
    $\boldsymbol{v}_{m+1} := \bar{\boldsymbol{v}}/\|\bar{\boldsymbol{v}}\|_2$;
    if $\|\boldsymbol{r}_m\|_2 < \epsilon$ **then**
      convergence:=true; break;
    compute $\boldsymbol{f}_m = H^{-H}\boldsymbol{e}_m$ and $\mathcal{H} = H + H(m+1, m)^2 \boldsymbol{f}_m \boldsymbol{e}_m^H$;
    compute the maximum eigenvalue $\lambda_{\max}$ of H;
    compute the maximum eigenvalue $\bar{\lambda}_{\max}$ of $\mathcal{H}$;
    $D_{\text{cur}} := |\lambda_{\max} - \bar{\lambda}_{\max}|$;
    if ($i > 1$ and $D_{\text{cur}} > D_{\text{pre}}$ and $m \geq m_{\min}$) or $m = m_{\max}$ **then**
      $\boldsymbol{y} = \min_y \|\beta \boldsymbol{e}_1 - H\boldsymbol{y}\|_2$;
      $\boldsymbol{x}_m = \boldsymbol{x}_0 + V_m \boldsymbol{y}$;
      $\boldsymbol{x}_0 := \boldsymbol{x}_m$;
      $D_{\text{pre}} := D_{\text{cur}}$;
      break;
    $D_{\text{pre}} := D_{\text{cur}}$;
    $m := m + 1$;
until convergence

---

restart. They are used to increase an orthonormal matrix U_j. The right preconditioner

$$M^{-1} = I_n + U_j \left(|\lambda_n| T_j^{-1} - I_j \right) U_j^H \,, \quad T_j = U_j^H A U_j \,, \tag{6}$$

is updated after each restart until the dimension of U_j equals a number k. I_n and I_j are the identity matrices with dimension n and j. After preconditioning by (6), the smallest Ritz values $\lambda_1, \ldots, \lambda_j$ are removed.

Now consider applying the restarting strategy proposed in Section 3. As the Ritz values and vectors are already used in DEFLATED-GMRES(m, k), the extra cost of applying the proposed restarting strategy is only the cost for computing the maximum harmonic Ritz value. Since the computed Ritz vectors are not reliable when the dimension of Krylov subspace is too small, we suggest that the adaptive restarting strategy should not be carried out until no Ritz vector is needed any more, in other words, until the dimension of U_j equals to k:

- Run DEFLATED-GMRES($m_{\max}, k$) for the first k/l cycles;
- Run RITZ-GMRES($m_{\min}, m_{\max}$) with preconditioner M^{-1}.

This preconditioned method is denoted as DEFLATED-RITZ($m_{\min}, m_{\max}, k$), where k denotes the maximum dimension of the orthonormal matrix U in (6).

5 Numerical experiments

In this section we provide a few experimental results to show the efficiency of the adaptive restarting strategy proposed in Section 3. At first, we compare RITZ-GMRES($m_{\min}, m_{\max}$) with classical GMRES(m) without preconditioning in Example 5.1. Then, we compare DEFLATED-RITZ($m_{\min}, m_{\max}, k$) with DEFLATED-GMRES(m, k) in Example 5.2.

All experiments have been performed on a Dell PowerEdge 1750 computer (CPU: Intel(R) Xeon(R) 3.00 GHz, OS: Red Hat Linux 9.0, 4 GB main memory), used in single processor mode in double precision. The initial guess $\boldsymbol{x}_0$ is set to zero and the system is scaled so that the initial residual vector has unit length. The tolerance ϵ for the residual norm is set to 10^{-12}. Execution of each method is interrupted if the residual norm does not converge after 20,000 iterations. $m_{\max}$ is set to 50 and $m_{\min}$ is set to 1 in Example 5.1, and 5 in Example 5.2. CLAPACK's routines `dgeev` and `zgeev` are used for the computation of the Ritz and harmonic Ritz values and vectors [1].

5.1 First example

We consider the problem which arises from the 5 point center difference discretization of the elliptic partial differential problem [7] in the unit square region $\Omega = [0,1] \times [0,1]$.

$$\begin{aligned} -u_{xx} - u_{yy} + D((y-1/2)u_x + (x-1/3)(x-2/3)u_y) &= G\,, \\ u|_{\partial\Omega} &= 1 + xy\,, \end{aligned}$$

where G is defined so that $u = 1 + xy$ on Ω. The mesh size h is set to $1/513$. Hence, the dimension of the coefficient matrix is $262,144$. Dh is set to 2^{-3}, 2^{-4}, 2^{-5}, 2^{-6} and 2^{-7}. Table 1 presents the results for various choices of Dh. For each Dh, the shortest computation time is emphasised. From Table 1, see that RITZ-GMRES$(1,50)$ is much more successful than the classical GMRES(m) since it converges for all the Dh. The computation time is much shorter too.

Next we study the real restart cycles of RITZ-GMRES$(1,50)$. Average and maximum values of the real restart cycles are shown in Table 2. From Table 2 see that the real cycles are rather small for all Dh. As an example, we plot all the real restart cycles in Figure 1 for $Dh = 2^{-4}$. Since in this case, the average value of the real restart cycles is about 5 and the maximum value is 27, we compare the convergence of RITZ-GMRES$(1,50)$ to

Table 1: Results for Example 5.1 (T: time(sec) I: iterations)

Dh	2^{-3}		2^{-4}		2^{-5}		2^{-6}		2^{-7}	
Method	I	T	I	T	I	T	I	T	I	T
GMRES(10)	(-5.)	2039	(-5.)	2035	(-5.)	2042	(-5.)	2041	(-4.)	2037
GMRES(20)	(-6.)	3090	(-6.)	3084	(-7.)	3091	(-7.)	3081	(-6.)	3083
GMRES(30)	(-8.)	4138	(-9.)	4133	(-9.)	4135	(-10.)	4126	(-8.)	4131
GMRES(40)	(-10.)	5189	(-11.)	5190	18235	4741	(-11.)	5189	(-11.)	5185
GMRES(50)	(-11.)	6252	(-10.)	6243	11911	3711	14709	4592	19340	6030
RITZ-GMRES(1,50)	18422	*1976*	12063	*1505*	12688	*1621*	13072	*1832*	9380	*1307*

Values in ( ) are $\log_{10} \|\boldsymbol{r}_m\|_2$ if the method does not converge after 20,000 iterations.

Table 2: Restart cycle of RITZ-GMRES$(1, 50)$ for Example 5.1

Dh	2^{-3}	2^{-4}	2^{-5}	2^{-6}	2^{-7}
Average restart cycle	4.77	4.92	5.02	5.85	5.65
Maximum restart cycle	25	27	29	31	28

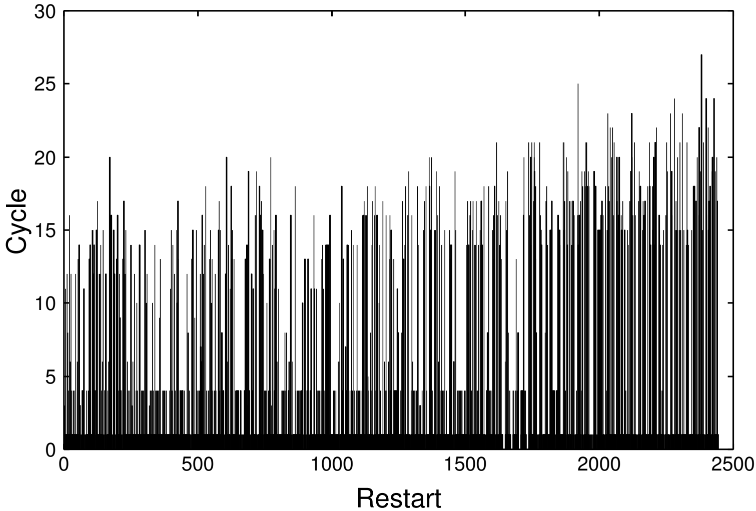

Figure 1: Restart cycle of RITZ-GMRES$(1, 50)$ for Example 5.1 ($Dh = 2^{-4}$)

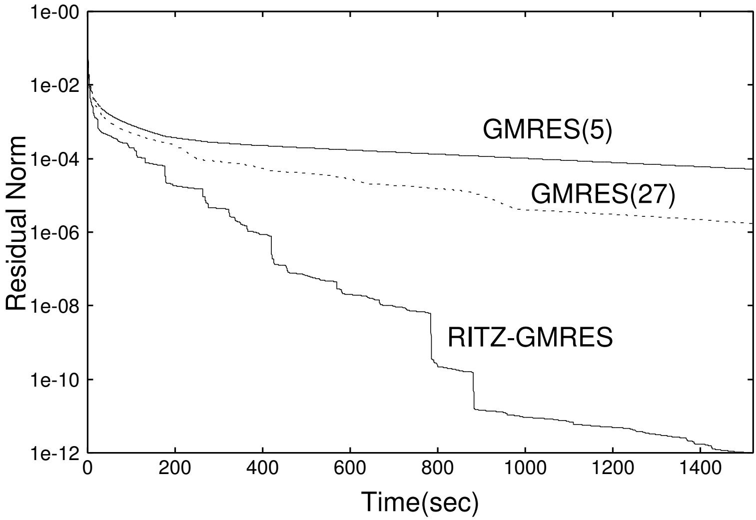

Figure 2: Residual norm versus computation time for Example 5.1 ($Dh = 2^{-4}$)

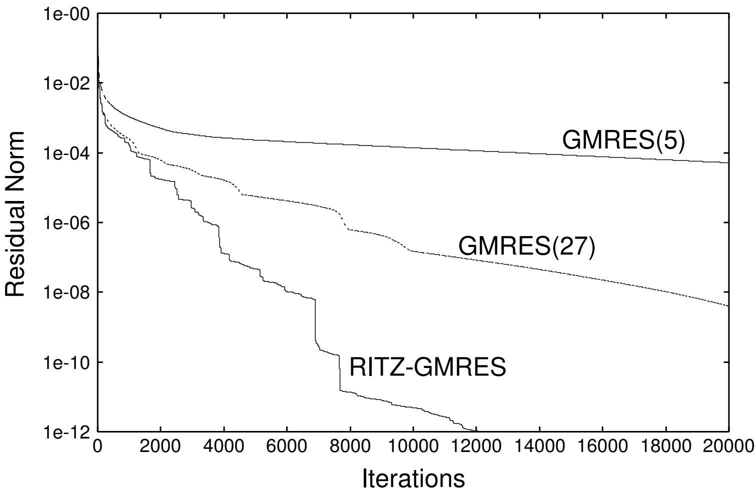

Figure 3: Residual norm versus iterations for Example 5.1 ($Dh = 2^{-4}$)

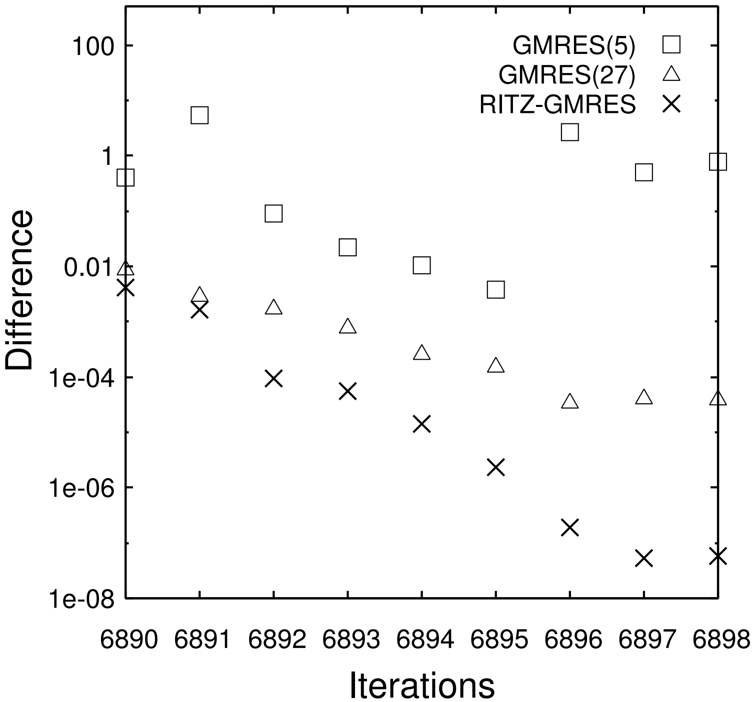

Figure 4: $|\lambda_{\max} - \bar{\lambda}_{\max}|$ near step 6897 for Example 5.1 ($Dh = 2^{-4}$)

GMRES(5) and GMRES(27) in Figures 2 and 3. From Figures 2 and 3, we find that although RITZ-GMRES(1, 50) is more efficient computing the orthonormal basis of the Krylov subspace on the average, it converges faster in terms of both iterative number and computation time. These results show that RITZ-GMRES($m_{\min}, m_{\max}$) is more efficient than the classical GMRES(m).

We also compute all the values of $|\lambda_{\max} - \bar{\lambda}_{\max}|$ in RITZ-GMRES(1, 50), GMRES(5) and GMRES(27) of the first 12,063 iterations since RITZ-GMRES(1, 50) converges after 12,063 iterations. We find that RITZ-GMRES (1, 50) has more small values of $|\lambda_{\max} - \bar{\lambda}_{\max}|$ than the other two methods. In detail, RITZ-GMRES(1, 50) has 1,873 values of $|\lambda_{\max} - \bar{\lambda}_{\max}|$ smaller than 0.000001, and GMRES(27) has only 336 and GMRES(5) has none. We plot the values of

Table 3: Results for Example 5.2

	GMRES(10)	GMRES(20)	GMRES(30)	GMRES(40)	GMRES(50)
Iterations	18619	9430	6419	4947	4088
Time(sec)	680	558	530	524	540

Table 4: Results for Example 5.2 (T: computation time(sec) I: iterations)

Method	k =1		k =2		k =3		k =4	
	I	T	I	T	I	T	I	T
DEFLATED-GMRES(50,k)	3203	414	3057	416	2681	380	2313	344
DEFLATED-RITZ(5,50,k)	5058	393	3363	269	3676	293	2887	236

$|\lambda_{\max} - \bar{\lambda}_{\max}|$ near step 6897 in Figure 4, since RITZ-GMRES$(1, 50)$ converges faster than the other two methods near this step. From Figure 4 see that the values of $|\lambda_{\max} - \bar{\lambda}_{\max}|$ in RITZ-GMRES$(1, 50)$ are smaller than those in GMRES(5) and GMRES(27). This result coincides with the observation that the value of $|\lambda_{\max} - \bar{\lambda}_{\max}|$ can be used to predict the stagnation of the residual norm of GMRES.

5.2 Second example

Next, compare DEFLATED-GMRES(m, k) to DEFLATED-RITZ$(m_{\min}, m_{\max}, k)$. The matrix is a bidiagonal matrix similar to the first example in [8]. We let the matrix have $1 + i$, $2 + 2i$, ..., $16384 + 16384i$ on the main diagonal and $0.1 + 0.1i$ on the super diagonal. The right-hand side has all entries $1.0 + 1.0i$. Although this matrix does not have physical meaning, it is helpful for verifying whether the proposed restarting strategy is efficient for those linear systems whose eigenvalues range over wide width.

Table 3 shows the numerical results for the classical GMRES(m). Whereas Table 4 shows the results for the DEFLATED-GMRES(m, k) and the DEFLATED-RITZ$(m_{\min}, m_{\max}, k)$ for variable k. In DEFLATED-GMRES(m, k), the restart cycle m is set to 50 since the computed Ritz vectors used in preconditioner (6) are not reliable when m is too small. Compare Tables 3 and 4 to see that both DEFLATED-GMRES(m, k) and DEFLATED-RITZ$(m_{\min}, m_{\max}, k)$ work better than the classical GMRES(m) because of preconditioning. From Table 4, also see that DEFLATED-RITZ$(5, 50, k)$ is more successful than DEFLATED-GMRES$(50, k)$. These results show that the new restarting strategy still works well in the preconditioned GMRES(m).

6 Concluding Remark

We proposed a new adaptive restart for GMRES(m) using the difference of the Ritz and harmonic Ritz values. The difference is estimated by the absolute value of the difference of the maximum Ritz value and the maximum harmonic Ritz value. Numerical experiments show that the proposed method can work much better than the classical GMRES(m) with fixed restart cycle. We also apply this restarting strategy to DEFLATED-GMRES(m, k) as an example.

Further research is needed to study the stability of the proposed restarting strategy, including application in other preconditioned GMRES(m) methods, for solving general non-Hermitian linear systems.

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