On using (harmonic) Ritz values to precondition restarted GMRES

Jurjen Duintjer Tebbens

joint work with

Gérard Meurant

Institute of Computer Science,
Academy of Sciences of the Czech Republic

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Motivation

We consider the solution of linear systems

$$\mathbf{A}x = b$$

where $\mathbf{A} \in \mathbb{C}^{n\times n}$ is **non-normal and nonsingular**, by the Generalized Minimal Residual (GMRES) method [Saad & Schultz 1986].

As this is a Krylov subspace method based on long recurrences, we will focuss on restarted GMRES; GMRES(m) will denote GMRES restarted after every mth iteration.

Without loss of generality, $\|b\| = 1$, $x_0 = 0$.

Mathematical properties of GMRES

Optimality property

The kth residual norm satisfies

$$\|r_k\| = \min_{x \in \mathcal{K}_k(\mathbf{A}, b)} \|b - Ax\|,$$

where the minimization is over all elements of the kth Krylov subspace,

$$\mathcal{K}_k(\mathbf{A}, b) \equiv \text{span}\{b, \mathbf{A}b, \ldots, \mathbf{A}^{k-1}b\}.$$

- Residual norms do not increase, but they can stagnate in GMRES(m)
- Residuals can be written as polynomials in A,

  $$r_k = p(A)b \qquad \text{with} \qquad \|r_k\| = \min_{p \in \pi_k} \|p(A)b\|,$$

  where π_k is the set of polynomials of degree k taking the value one in the origin.

Mathematical properties of GMRES

Influence of spectral properties

Let the Jordan normal form of A be

$$A = XJX^{-1},$$

then the kth residual norm can be written as

$$\|r_k\| = \min_{p \in \pi_k} \|Xp(J)X^{-1}b\|.$$

This shows that the convergence of GMRES, measured by the residual norm, depends on

- the eigenvalues contained in J
- the eigenvectors (or principal vectors with non-diagonalizable input matrices) contained in X
- components of the right-hand side in the eigenvector basis.

The next classical result shows that convergence needs not depend on the eigenvalues alone:

Theorem 1 **[Greenbaum & Pták & Strakoš 1996]** *Let*

$$\|b\| = f_0 \geq f_1 \geq f_2 \cdots \geq f_{n-1} > 0$$

be **any** *non-increasing sequence of real positive values and let*

$$\lambda_1, \ldots, \lambda_n$$

be **any** *set of nonzero complex numbers. Then there exists a class of matrices $A \in \mathbb{C}^{n \times n}$ and right-hand sides $b \in \mathbb{C}^n$ such that the residual vectors $r^{(k)}$ generated by GMRES method satisfy*

$$\|r^{(k)}\| = f_k, \quad 0 \leq k \leq n, \quad \text{and} \quad \text{spectrum}(A) = \{\lambda_1, \ldots, \lambda_n\}.$$

We recently extended this result with the fact that GMRES convergence needs not be dependent on Ritz values either, except that a zero Ritz value implies stagnation:

Theorem 2 **[DT & Meurant 2012]** *In addition to the assumptions of Theorem 1, let also* $n(n-1)/2$ *Ritz values*

$$\begin{array}{ccccc} & & & \theta_1^{(1)}, & \\ & & \theta_1^{(2)}, & \theta_2^{(2)}, & \\ & & \dots & , & \\ & \theta_1^{(n-1)}, & \dots & , & \theta_{n-1}^{(n-1)}, \\ \lambda_1, & \dots\dots\dots & & , & \lambda_n \quad , \end{array}$$

be given and assume that $f_{k-1} = f_k$ *if and only if there is a zero Ritz value for the* k*th iteration.*

Then there exists a class of matrices $A \in \mathbb{C}^{n\times n}$ and right-hand sides $b \in \mathbb{C}^n$ such that the residual vectors $r^{(k)}$ generated by GMRES method satisfy

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and GMRES generates in the kth iteration (for all $k \le n$) the Ritz values

$$\theta_1^{(k)}, \dots, \theta_k^{(k)}.$$

Mathematical properties of GMRES

Influence of Ritz values

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and GMRES generates in the kth iteration (for all $k \le n$) the Ritz values

$$\theta_1^{(k)}, \ldots, \theta_k^{(k)}.$$

- Thus, in every iteration, we can prescribe the Ritz values and simultaneously the GMRES residual norm. Note this does not contradict the result that converging Ritz values cause super-linear convergence of close to normal systems [van der Vorst & Vuik 1993].
- This also shows that the Arnoldi method for eigenproblems can generate arbitrary Ritz values in all intermediate iterations.

Consequences for restarted GMRES?

- It seems possible to prescribe the harmonic Ritz values in the Arnoldi method as well [Meurant, personal communication].
- Prescribing GMRES residual norms and harmonic Ritz values *simultaneously* is unlikely to be possible – harmonic Ritz values are the roots of the GMRES polynomials $r_k = p(A)b$.

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Many acceleration techniques for restarted GMRES rely on spectral information gained from Ritz values or harmonic Ritz values. The purpose of this talk is:

- To investigate whether eigenvalues and Ritz values can be prescribed in restarted GMRES as well.
- To point out possible consequences for preconditioning and other popular acceleration strategies for GMRES(m).

Outline

The parametrization for full GMRES

Here is how one can prescribe Ritz values and residual norms in full GMRES [DT & Meurant 2013]:

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- To force the desired eigenvalues, H will be of the form

$$H = U^{-1}CU, \qquad U \text{ nonsingular upper triangular,}$$

where C is the companion matrix for the prescribed spectrum.

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- To force the desired residual norms, the first row g^T of U has entries

$$g_1 = \frac{1}{f(0)}, \qquad g_k = \frac{\sqrt{f(k-2)^2 - f(k-1)^2}}{f(k-2)f(k-1)}, \qquad k = 2, \ldots, n.$$

The parametrization for full GMRES

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$$U = \begin{bmatrix} & g^T & \\ 0 & T & \end{bmatrix}$$

has entries satisfying

$$\prod_{i=1}^{k}(\lambda - \rho_i^{(k)}) = g_{k+1} + \sum_{i=1}^{k} t_{i,k}\lambda^i.$$

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Is prescribing these values possible in restarted GMRES ?

Generalization for restarted GMRES

Prescribing residual norms in restarted GMRES was considered in the paper [Vecharinsky & Langou 2011]. It assumes a rather special situation in GMRES(m):

1. During every restart cycle, all residual norms stagnate except for the very last iteration inside the cycle.
2. In this very last iteration it is assumed that the residual norm is strictly decreasing.

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2. In this very last iteration it is assumed that the residual norm is strictly decreasing.

Theorem 3 [Vecharinsky & Langou 2011]. *Let n complex nonzero numbers $\lambda_1, \ldots, \lambda_n$ and k positive decreasing numbers*

$$f(0) > f(1) > \cdots > f(k-1) > 0,$$

be given. With the assumptions 1. and 2. above, let the very last residual at the end of the jth cycle be denoted by $\bar{r}_j$. If $km < n$, then:

Generalization for restarted GMRES

- There exists a matrix A of order n with a right hand side such that GMRES(m) generates residual norms at the end of cycles satisfying

$$\|\bar{r}_j\| = f(j), \qquad j = 0, 1, \ldots, k.$$

- The matrix A has the eigenvalues $\lambda_1, \ldots, \lambda_n$.

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In fact, to prescribe all residual norms and all Ritz values in GMRES(m), it suffices that $(m+1) \times m$ Hessenberg matrices of the individual restart cycles have the form described before, i.e. that the kth Hessenberg matrix is

$$\hat{H}_m^{(k)} = \begin{bmatrix} g_1^{(k)} & \ldots & g_{m+1}^{(k)} \\ 0 & T_m^{(k)} & \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ I_m \end{bmatrix} \begin{bmatrix} g_1^{(k)} & \ldots & g_m^{(k)} \\ 0 & T_{m-1}^{(k)} & \end{bmatrix},$$

where $g^{(k)}$ determines the convergence curve and the columns of T_{m-1} determine the Ritz values.

Generalization for restarted GMRES

First, we assume restart cycles do not stagnate in their last iteration.

Theorem 5 **[DT & Meurant 2013?]** *Let*

$$\hat{H}_m^{(1)}, \ldots, \hat{H}_m^{(k)} \in \mathbb{C}^{(m+1)\times m}$$

be k unreduced upper Hessenberg matrices with positive subdiagonal and let $km < n$. If $A \in \mathbb{C}^{n\times n}$ is a matrix and $b \in \mathbb{C}^n$ a nonzero vector, the following assertions are equivalent:

1. *The kth cycle of GMRES(m) applied to A and b does not stagnate in its last iteration and generates the Hessenberg matrix $\hat{H}_m^{(k)}$.*

2. *The matrix A and the vector b have the form*

$$A = VHV^*, \qquad b = Ve_1,$$

where V is unitary, H is upper Hessenberg and the columns $(k-1)m+1$ till km corresponding to the kth cycle are of the form:

Generalization for restarted GMRES

$$H \left[e_{(k-1)m+1}, \ldots, e_{km} \right] = \begin{bmatrix} & (\prod_{i=2}^{k-1} \zeta_1^{(i)}) z^{(1)} e_1^T \hat{H}_m^{(k)} \\ & \vdots \\ \vdots & \\ & \zeta_1^{(k-1)} z^{(k-2)} e_1^T \hat{H}_m^{(k)} \\ \hat{h}^{(k)} & z^{(k-1)} e_1^T \hat{H}_m^{(k)} \begin{bmatrix} 0 \\ I_{m-1} \end{bmatrix} \\ 0 & \begin{bmatrix} 0 & I_m \end{bmatrix} \hat{H}_m^{(k)} \begin{bmatrix} 0 \\ I_{m-1} \end{bmatrix} \\ 0 & 0 \end{bmatrix}, \quad \textit{where}$$

Generalization for restarted GMRES

$$z^{(i)} = \left(I_{m+1} - \hat{H}_m^{(i)}(\hat{H}_m^{(i)})^\dagger\right)e_1 / \left\|\left(I_{m+1} - \hat{H}_m^{(i)}(\hat{H}_m^{(i)})^\dagger\right)e_1\right\|, \quad 1 \leq i \leq k-1,$$

$$\hat{h}^{(k)} = [\hat{h}_1^{(k)}, \ldots, \hat{h}_{m+1}^{(k)}]^T = \frac{1}{\zeta_{m+1}^{(k-1)}}\left(h_{1,1}^{(k)} z^{(k-1)} - \hat{H}_m^{(k-1)}[\zeta_1^{(k-1)}, \ldots, \zeta_m^{(k-1)}]^T\right)$$

and

$$\hat{h}_{m+2}^{(k)} = \frac{h_{2,1}^{(k)}}{\zeta_{m+1}^{(k-1)}}.$$

Thus we know how to generate, by the right choice of columns of H, arbitrary Hessenberg matrices during *all* restarts. Therefore we may prescribe not only GMRES residual norms *inside* cycles and Ritz values but also other values (singular values, harmonic Ritz values ...).

Generalization for restarted GMRES

Remark: Note that prescribing k restarts under the condition $km < n$ means that in the parametrization of the matrix A and the vector b,

$$A = VHV^*, \qquad b = \|b\| V e_1,$$

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Now we allow stagnation at the end of the cycles. Demonstrating this case in detail for the first two cycles, let their residuals be denoted as

$$\begin{aligned} r_0^{(1)} = b, r_1^{(1)}, \quad \ldots \quad, r_m^{(1)}, \\ r_0^{(2)} = r_m^{(1)}, r_1^{(2)}, \quad \ldots \quad, r_m^{(2)}. \end{aligned}$$

Generalization for restarted GMRES

Let m iterations of the initial cycle give the Arnoldi decomposition

$$AV_m^{(1)} \quad = \quad V_{m+1}^{(1)} \hat{H}_m^{(1)}, \quad V_{m+1}^{(1)^*} V_{m+1}^{(1)} = I_{m+1}.$$

The m iterations of the second cycle give the Arnoldi decomposition

$$AV_m^{(2)} = V_{m+1}^{(2)} \hat{H}_m^{(2)}, \quad V_{m+1}^{(2)^*} V_{m+1}^{(2)} = I_{m+1}, \quad V_{m+1}^{(2)} e_1 = \frac{r_m^{(1)}}{\|r_m^{(1)}\|} \equiv V_{m+1}^{(1)} z^{(1)}.$$

The vector $z^{(1)}$ is

$$z^{(1)} = \left(I_{m+1} - \hat{H}_m^{(1)} (\hat{H}_m^{(1)})^\dagger\right) e_1 / \left\| \left(I_{m+1} - \hat{H}_m^{(1)} (\hat{H}_m^{(1)})^\dagger\right) e_1 \right\|.$$

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How do we construct the columns of H ? We know that the columns $1, \ldots, m$ of H are

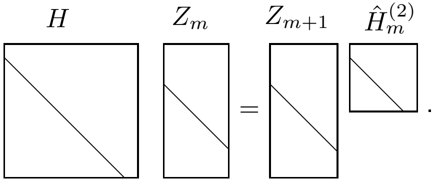
$$H\begin{bmatrix} I_m \\ 0 \end{bmatrix} = \begin{bmatrix} \hat{H}_m^{(1)} \\ 0 \end{bmatrix}.$$

Generalization for restarted GMRES

Lemma 1. *The matrix $\hat{H}_m^{(2)}$ is the Hessenberg matrix generated by m iterations of Arnoldi with input matrix H and initial vector $\begin{bmatrix} z^{(1)T} & 0 \end{bmatrix}^T$, i.e.*

$$HZ_m = Z_{m+1}\hat{H}_m^{(2)}, \quad Z_{m+1}e_1 = \begin{bmatrix} z^{(1)} \\ 0 \end{bmatrix}, \quad Z_{m+1}^* Z_{m+1} = I_{m+1}. \quad (1)$$

Can we construct the columns $m+1, m+2, \ldots, 2m$ of H such that (1) is satisfied with a prescribed Hessenberg matrix $\hat{H}_m^{(2)}$? This will depend on the number of non-zeroes in $\begin{bmatrix} z^{(1)T} & 0 \end{bmatrix}^T$ because

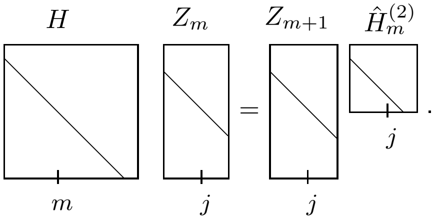


Generalization for restarted GMRES

Lemma 2. *Let $r_m^{(1)} = V_{m+1}^{(1)} z^{(1)}$. Then for an integer j the last $j-1$ entries of $z^{(1)}$ are zero if and only if the last j residual norms are equal, i.e.*

$$\|r_0^{(1)}\| \geq \|r_1^{(1)}\| \geq \cdots \geq \|r_{m-j}^{(1)}\| > \|r_{m-j+1}^{(1)}\| = \cdots = \|r_m^{(1)}\|.$$

Then the Arnoldi decomposition $HZ_m = Z_{m+1}\hat{H}_m^{(2)}$ looks like



Generalization for restarted GMRES

Therefore, with $j-1$ stagnation steps at the end of the first restart cycle:

- the first $j-1$ columns of the Hessenberg matrix of the second cycle $\hat{H}_m^{(2)}$ are fully determined by $\hat{H}_m^{(1)}$ and $z^{(1)}$ - they cannot be prescribed.
- We can also prove that the first row of $\hat{H}_m^{(2)}$ is zero on its first $j-1$ positions, i.e. they correspond to iterations with stagnation!

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- We can also prove that the first row of $\hat{H}_m^{(2)}$ is zero on its first $j-1$ positions, i.e. they correspond to iterations with stagnation!

Corollary *If the last $j-1$ residual norms stagnate in the initial cycle, i.e.*

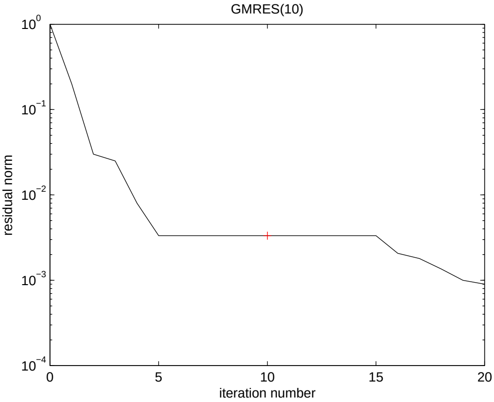
$$\|r_0^{(1)}\| \geq \|r_1^{(1)}\| \geq \cdots \geq \|r_{m-j}^{(1)}\| > \|r_{m-j+1}^{(1)}\| = \cdots = \|r_m^{(1)}\|$$

then the first $j-1$ residual norms stagnate in the second cycle,

$$\|r_0^{(2)}\| = \|r_1^{(2)}\| = \cdots = \|r_{j-1}^{(2)}\|.$$

Hence stagnation in one cycle is literally mirrored in the next cycle!

Generalization for restarted GMRES



Outline

Acceleration of restarted GMRES

The previous results have a number of theoretical implications for strategies to accelerate restarted GMRES like preconditioning.

Any convergence speed of GMRES(m) is possible with any spectrum, therefore:

- A preconditioner that clusters eigenvalues needs not accelerate GMRES(m).
- Additional spectral information is necessary to guarantee acceleration.
- An important example is constraint preconditioning, where the few distinct eigenvalues (e.g. 1 and $(1 \pm \sqrt(5)/2)$ of the preconditioned matrix belong to small Jordan blocks. Then in exact arithmetic GMRES terminates at a very low iteration number (possibly smaller than m). Still this does not say anything on convergence *speed*.

Acceleration of restarted GMRES

Stagnation at the end of one cycle is mirrored in the beginning of the next cycle, therefore:

- Obviously, it is not a good idea to do a standard restart with stagnation at the end of the current cycle
- This may be the moment to modify (adapt) the preconditioner to change the Krylov subspaces one projects onto
- Acceleration with Krylov subspace recycling (see e.g. [de Sturler 1996, 1999], [Parks & de Sturler & Mackey & Johnson & Maiti 2006]) should avoid the subspaces that cause stagnation.
- Stagnation at the end of a cycle may be a strong motivation to adapt any acceleration technique.

Acceleration of restarted GMRES

We now focuss on spectral acceleration techniques (often called deflation techniques, but deflation needs not exploit spectral quantities, see, e.g. [Nabben & Vuik 2004, 2006, 2008]):

- The suspicion is that outlying eigenvalues, mostly eigenvalues close to zero, hamper convergence
- Eigenvalue approximations are obtained from the Ritz or harmonic Ritz values generated during the GMRES(m) process
- The corresponding eigenvectors (or invariant subspaces) are used to eliminate the influence of convergence hampering eigenvalues
- This can be done through preconditioning, augmentation of the Krylov subspaces, projecting away invariant subspaces or a combination of these.

Here is a very incomplete list of proposed strategies and literature:

Acceleration of restarted GMRES

Spectral acceleration techniques for restarted GMRES include:

- Augmentation of Krylov subspaces: [Morgan 1995], [Le Calvez & Molina 1999], [Morgan 2000], [Morgan 2002], [Chapman & Saad 1997]
- Preconditioning: [Kharchenko & Yeremin 1995], [Erhel & Burrage & Pohl 1996], [Baglama & Calvetti & Golub & Reichel 1998], [Frank & Vuik 2001], [Carpentieri & Duff & Giraud 2003], [Loghin & Ruiz & Touhami 2006], [Carpentieri & Giraud & Gratton 2007], [Giraud & Gratton & Martin 2007], [Giraud & Gratton & Pinel & Vasseur 2010]
- Analysis and overviews: [Saad 1997], [Burrage & Erhel 1998], [Eiermann & Ernst & Schneider 2000], [Saad 2000], [Simoncini & Szyld 2007], [Yeung & Tang & Vuik 2010], [Gaul & Gutknecht & Liesen & Nabben 2013]

Acceleration of restarted GMRES

These techniques are very beneficial in a large variety of applications. Nevertheless, our results show that in theory

- Ritz values need not converge to any eigenvalues (small or not) at all
- The same appears to hold for harmonic Ritz values
- It may even be problematic to assess the quality of Ritz values; e.g. the standard residual norm

$$\|A(V_k y) - \rho(V_k y)\| = h_{k+1,k}|e_k^T y|$$

  for a Ritz value/Ritz vector $\{\rho, V_k y\}$ pair needs not be indicative [Godet-Thobie 1993], [DT & Meurant 2012].
- Thus it may be hard to get accurate approximations of eigenvalues close to zero.

Acceleration of restarted GMRES

Suppose we did succeed in finding eigenvalues close to zero and in eliminating their influence on GMRES(m), does this accelerate the solution process ?

- We showed any convergence speed of GMRES(m) is possible with any spectrum
- Therefore, eigenvalues close to zero need not hamper convergence at all
- The argument suggesting small eigenvalues hamper convergence is:
  - At termination, the GMRES polynomial is zero at the eigenvalues and one in the origin.
  - Therefore, if an eigenvalue is close to zero, such a polynomial may be hard to build.

Note that we showed that a zero Ritz value does imply stagnation.

Outline

Conclusions and future work

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  - Can our results be used to build more powerful preconditioners?
  - Are comparable results possible for Krylov subspace methods with short recurrences (Bi-CG, Bi-CGStab,...)?
  - What can be said for GMRES(m) after iteration number n ?

Related papers

- A. Greenbaum and Z. Strakoš, [Matrices that generate the same Krylov residual spaces, IMA Vol. Math. Appl., 60 (1994), pp. 95–118.]
- A. Greenbaum, V. Pták and Z. Strakoš, [Any nonincreasing convergence curve is possible for GMRES, SIMAX, 17 (1996), pp. 465–469.]
- M. Arioli, V. Pták and Z. Strakoš, [Krylov sequences of maximal length and convergence of GMRES, BIT, 38 (1996), pp. 636–643.]
- J. Duintjer Tebbens and G. Meurant, [Any Ritz value behavior is possible for Arnoldi and for GMRES, SIMAX, 33 (2012), pp. 958–978.]
- J. Duintjer Tebbens and G. Meurant, [Prescribing the behavior of early terminating GMRES and Arnoldi iterations, Numer. Algorithms, online first February 2013]

Thank you for your attention!