Do Ritz values influence the behavior of restarted GMRES?

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joint work with

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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,

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

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

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

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

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* $n(n-1)/2$ *complex values*

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

be given and assume that $f_{k-1} = f_k$ *if and only if*

$$0 \in \{\theta_1^{(k)}, \dots, \theta_k^{(k)}\}.$$

Mathematical properties of GMRES

Influence of Ritz values

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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- Thus, in every iteration, we can prescribe the Ritz values and simultaneously the GMRES residual norm.
- 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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The purpose of this talk is:

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

Outline

1. Prescribing residual norms and Ritz values in GMRES(m)
2. Without stagnation at the end of cycles
3. Allowing stagnation at the end of cycles
4. Brief discussion
5. Conclusions

The parametrization for full GMRES

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$$A = VHV^*, \qquad H \text{ upper Hessenberg.}$$

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

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 $\lambda_1, \dots, \lambda_n$ 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.

Outline

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

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

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

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: Prescribing k restarts under the condition $km < n$ means that in the parametrization

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

we put conditions on the first $km < n$ columns of H only. The last column can be chosen arbitrarily. It can be checked (see, e.g., [Parlett & Strang 2008], that any nonzero spectrum of A is possible with an appropriate choice of the last column.

Outline

Generalization for restarted GMRES

Let m iterations of the initial cycle give the Arnoldi decomposition

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

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The m iterations of the second cycle give the Arnoldi decomposition

$$AV_m^{(2)} = V_{m+1}^{(2)}\hat{H}_m^{(2)}, \quad V_{m+1}^{(2)^*}V_{m+1}^{(2)} = I_{m+1},$$

where if $r_m^{(1)}$ is the residual vector at the end of the first cycle,

$$V_{m+1}^{(2)}e_1 = \frac{r_m^{(1)}}{\|r_m^{(1)}\|} \equiv V_{m+1}^{(1)}z^{(1)}.$$

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

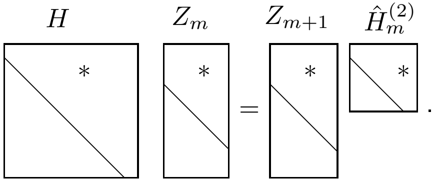
$$H\begin{bmatrix} I_m \\ 0 \end{bmatrix} = \begin{bmatrix} \hat{H}_m^{(1)} \\ 0 \end{bmatrix}.$$

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

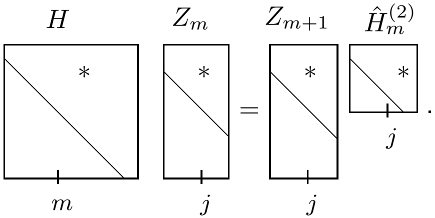


Generalization for restarted GMRES

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

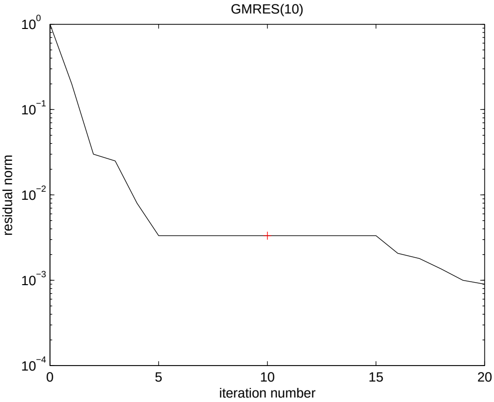
$$\|r_0^{(1)}\| \geq \|r_1^{(1)}\| \geq \cdots \geq \|r_{m-j}^{(1)}\| > \|r_{m-j+1}^{(1)}\| = \cdots = \|r_m^{(1)}\|$$

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

Preconditioning restarted GMRES

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

Any convergence speed of restarted GMRES 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 of the preconditioned matrix belong to small Jordan blocks.

Acceleration of restarted GMRES

Our results also have consequences for 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.

Acceleration of restarted GMRES

Any nonzero Ritz values can be generated by restarted GMRES, therefore:

- There is no guarantee that spectral acceleration techniques will find good approximate eigenvalues from Ritz values.
- The same appears to hold for harmonic Ritz values
- Additionally, and again, any convergence speed of GMRES(m) is possible with any spectrum
- Therefore, eigenvalues close to zero need not hamper convergence at all

Note that we showed that a zero Ritz value *does* imply stagnation. At the end of a cycle it even also implies stagnation at the beginning of the next cycle.

Outline

Conclusions and future work

- Any prescribed non-stagnating residual norms and nonzero Ritz values are possible for the first n iterations of restarted GMRES, with any spectrum of A.

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- Many spectral acceleration techniques are very efficient in practice, but lack a sound theoretical explication for their success.

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  - 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!