Any admissible harmonic Ritz value set is possible for GMRES

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GMRES

Consider a nonsingular linear system

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{C}^{n \times n}, \quad \mathbf{b} \in \mathbb{C}^{n}.$$

For initial guess $\mathbf{x}_0$, GMRES finds an approximate solution

$$\mathbf{x}_k \in \mathbf{x}_0 + \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$$

by minimizing the Euclidean norm of the residual

$$\mathbf{r}_k := \mathbf{b} - \mathbf{A}\mathbf{x}_k, \qquad \|\mathbf{r}_k\| = \min_{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|,$$

where

$$\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) := \operatorname{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \ldots, \mathbf{A}^{k-1}\mathbf{r}_0\}.$$

GMRES

GMRES residual norms satisfy the minimization property

$$\|\mathbf{r}_k\| = \min_{p(z)\in\mathbb{P}_k, p(0)=1} \|p(\mathbf{A})\mathbf{r}_0\|,$$

where $\mathbb{P}_k$ denotes the set of polynomials with degree $\leq k$.

The residual $\mathbf{r}_k$ can be *uniquely* expressed as

$$\mathbf{r}_k = p_k(\mathbf{A})\mathbf{r}_0, \qquad \deg(p_k) \leq k, \qquad p_k(0) = 1.$$

The polynomial $p_k(z)$ is called GMRES *residual polynomial*.

Eigenvalues and convergence: normal case

Plugging the spectral decomposition $\mathbf{A} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^*$ yields

$$\|\mathbf{r}_k\| = \min_{p(z)\in\mathbb{P}_k, p(0)=1} \|p(\mathbf{A})\mathbf{r}_0\| = \min_{p(z)\in\mathbb{P}_k, p(0)=1} \|p(\mathbf{\Lambda})\mathbf{W}^*\mathbf{r}_0\|.$$

Thus residual norms are fully determined by

- (i) eigenvalues,
- (ii) components of the initial residual in the eigenvector basis.

The previous bound leads to the well-known bound

$$\frac{\|\mathbf{r}_k\|}{\|\mathbf{r}_0\|} \leq \min_{p(z)\in\mathbb{P}_k, p(0)=1} \max_{\lambda\in\Lambda(\mathbf{A})} |p(\lambda)|.$$

The possibly worst convergence rate is decided by the eigenvalue distribution.

Eigenvalues and convergence: nonnormal case

With nonnormal matrices $\mathbf{A}$, convergence need not be governed by spectrum.

Theorem 1 (Greenbaum, Pták & Strakoš, SIMAX 1996)

Let

$$\|\mathbf{r}_0\| = \rho_0 \geq \rho_1 \geq \cdots \geq \rho_{n-1} > 0$$

be any non-increasing sequence of real positive numbers and let

$$\{\lambda_1, \lambda_2, \cdots, \lambda_n\}$$

be any set of nonzero complex numbers. Then there exists a class of matrices $\mathbf{A} \in \mathbb{C}^{n \times n}$ *and initial residuals* $\mathbf{r}_0 \in \mathbb{C}^n$ *such that the residuals* $\mathbf{r}_k$ *generated by* GMRES *satisfy*

$$\|\mathbf{r}_k\| = \rho_k, \quad k = 0 : n-1, \quad \Lambda(\mathbf{A}) = \{\lambda_1, \lambda_2, \cdots, \lambda_n\}.$$

Arnoldi process for the pair $\{\mathbf{A}, \mathbf{r}_0\}$

MGS orthogonalization for the orthonormal basis of $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$

Algorithm: Arnoldi process

$\mathbf{v}_1 = \mathbf{r}_0 / \|\mathbf{r}_0\|$
for $k = 1, 2, 3, \ldots$
  $\mathbf{w} = \mathbf{A}\mathbf{v}_k$
  for $i = 1$ **to** k
    $h_{ik} = \mathbf{v}_i^* \mathbf{w}$
    $\mathbf{w} = \mathbf{w} - h_{ik}\mathbf{v}_i$
  end
  $h_{k+1,k} = \|\mathbf{w}\|$
  $\mathbf{v}_{k+1} = \mathbf{w} / h_{k+1,k}$
end

We call the Arnoldi process *breaks down* if at some step k, an entry $h_{k+1,k} = 0$ is encountered.

Arnoldi relation

We assume that the Arnoldi process for the pair $\{\mathbf{A}, \mathbf{r}_0\}$ does not break down before the nth iteration. Then we have

$$\mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{H}, \quad \mathbf{V} \in \mathbb{C}^{n\times n}, \quad \mathbf{H} \in \mathbb{C}^{n\times n},$$

where $\mathbf{V}^*\mathbf{V} = \mathbf{I}$ and $\mathbf{H}$ is irreducible upper Hessenberg:

$$\mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \cdots & \mathbf{v}_n \end{bmatrix}, \quad \mathbf{H} = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1n} \\ h_{21} & h_{22} & \ddots & \vdots \\ & \ddots & \ddots & \vdots \\ & & h_{n,n-1} & h_{nn} \end{bmatrix}.$$

For $k < n$, let $\mathbf{H}_k$ and $\underline{\mathbf{H}}_k$ denote the upper-left $k \times k$ and $(k+1) \times k$ submatrices of $\mathbf{H}$, respectively. We have

$$\mathbf{H}_k = \mathbf{V}_k^* \mathbf{A} \mathbf{V}_k, \qquad \underline{\mathbf{H}}_k = \mathbf{V}_{k+1}^* \mathbf{A} \mathbf{V}_k,$$

where $\mathbf{V}_k = \begin{bmatrix} \mathbf{v}_1 & \cdots & \mathbf{v}_k \end{bmatrix}$. We use $\mathbf{H}_n = \underline{\mathbf{H}}_n = \mathbf{H}$.

Ritz values and harmonic Ritz values

Ritz values $\{\lambda_j^{(k)}\}_{j=1}^k$: eigenvalues of $\mathbf{H}_k\mathbf{y} = \lambda\mathbf{y}$

Harmonic Ritz values $\{\theta_j^{(k)}\}_{j=1}^k$: eigenvalues of $\underline{\mathbf{H}}_k^*\underline{\mathbf{H}}_k\mathbf{y} = \theta\mathbf{H}_k^*\mathbf{y}$

Remark 1

- *Totally,* $(n+1)n/2$ *Ritz values or harmonic Ritz values.*
- *Both* $\{\lambda_j^{(n)}\}_{j=1}^n$ *and* $\{\theta_j^{(n)}\}_{j=1}^n$ *are eigenvalues of* $\mathbf{A}$.
- *The harmonic Ritz value* $\theta_j^{(k)} \neq 0$ *and could be* ∞.

Lemma 2 (Freund,1992; Cao,1997; etc.)

The unique GMRES *residual polynomial is given by*

$$p_k(z) = \prod_{j=1}^{k}\left(1 - \frac{z}{\theta_j^{(k)}}\right).$$

Ritz values and convergence

- In the CG method for Hermitian positive definite linear systems, a converged Ritz value often implies an accelerated phase of convergence of the **A**-norm of the error, see, e.g., [van der Sluis & van der Vorst, 1986].
- An analogue result for the GMRES method suggests a similar phenomenon provided **A** is close to normal (the involved bounds contain the condition number of the eigenvector matrix). [van der Vorst & Vuik, 1993].

What do we know about the relation between Ritz values and GMRES convergence for general nonnormal matrices?

Any Ritz value behavior is possible with any GMRES residual norm history. [Duintjer Tebbens & Meurant, SIMAX, 2012].

Harmonic Ritz values and convergence

Many deflation methods use harmonic Ritz values to accelerate the convergence of restarted GMRES, see, e.g.,
[Morgan, SISC, 2002],
[Giraud, Gratton, Pinel, & Vasseur, SISC, 2010],
[Agullo, Giraud, & Jing, SIMAX, 2014]

What do we know about the relation between harmonic Ritz values and GMRES convergence for general nonnormal matrices?

Property of harmonic Ritz values

Theorem 3

Let $\Theta^{(k)}$ denote the k-tuple of the harmonic Ritz values:

$$\Theta^{(k)} = (\theta_1^{(k)}, \theta_2^{(k)}, \ldots, \theta_k^{(k)}).$$

If GMRES *applied to* $\{\mathbf{A}, \mathbf{r}_0\}$ *stagnates from step* $k+1$ *to step* $k+m$ $(0 \leq k < k+m \leq n-1)$*, i.e.,*

$$\|\mathbf{r}_k\| = \|\mathbf{r}_{k+1}\| = \cdots = \|\mathbf{r}_{k+m}\|,$$

then, for $i = 1 : m$*, the* $(k+i)$*-tuple of the harmonic Ritz values (regardless of the order)*

$$\Theta^{(k+i)} = (\theta_1^{(k)}, \theta_2^{(k)}, \ldots, \theta_k^{(k)}, \infty, \cdots, \infty).$$

Proof: Follows from $p_k(z) = p_{k+1}(z) = \cdots = p_{k+m}(z)$.

Admissible harmonic Ritz value set

For prescribed GMRES residual norms (without loss of generality, in the sequel, we assume $\|\mathbf{r}_0\| = 1$)

$$1 = \|\mathbf{r}_0\| \geq \|\mathbf{r}_1\| \geq \cdots \geq \|\mathbf{r}_{n-1}\| > \|\mathbf{r}_n\| = 0,$$

we call a set of tuples of nonzero complex numbers

$$\begin{aligned}
\Theta &= \{\Theta^{(1)},\ \Theta^{(2)},\ \ldots,\ \Theta^{(n)}\} \\
&= \{\theta_1^{(1)}, \\
&\quad (\theta_1^{(2)}, \theta_2^{(2)}), \\
&\quad \vdots \\
&\quad (\theta_1^{(n)}, \theta_2^{(n)}, \ldots, \theta_n^{(n)})\}
\end{aligned}$$

an admissible harmonic Ritz value set if $\theta_j^{(n)} \neq \infty$ and the tuples $\{\Theta^{(i)}\}_{i=1}^{n-1}$ satisfy the property in Theorem 3.

Krylov matrix and the companion matrix

Consider QR factorization of the Krylov matrix

$$\mathbf{K} := \begin{bmatrix} \mathbf{r}_0 & \mathbf{A}\mathbf{r}_0 & \cdots & \mathbf{A}^{n-1}\mathbf{r}_0 \end{bmatrix} = \mathbf{V}\mathbf{U}^{-\mathbf{1}},$$

where $\mathbf{U}^{-1}$ is the nonsingular upper triangular matrix representing the change of basis. Let $\mathbf{C}$ be the companion matrix associated with the characteristic polynomial of $\mathbf{A}$, denoted as

$$\mathbf{C} = \begin{bmatrix} \mathbf{0} & -c_0 \\ \mathbf{I}_{n-1} & -\mathbf{c}_{n-1} \end{bmatrix},$$

where

$$\mathbf{c}_{n-1} = \begin{bmatrix} c_1 & c_2 & \cdots & c_{n-1} \end{bmatrix}^{\mathrm{T}}.$$

The monic polynomial with coefficients $c_{n-1}, \cdots, c_0$ has the eigenvalues of $\mathbf{A}$ as roots. We have

$$\mathbf{A}\mathbf{K} = \mathbf{K}\mathbf{C}.$$

Decompositions of $\mathbf{H}$, $\mathbf{H}_k$ and $\underline{\mathbf{H}}_k$

Lemma 4 (DT & Meurant, 2016)

The matrix $\mathbf{H}$ *can be written as* $\mathbf{H} = \mathbf{U}^{-1}\mathbf{C}\mathbf{U}$ *where* $\mathbf{C}$ *is the companion matrix of* $\mathbf{A}$ *and* $\mathbf{U}$ *is upper triangular* $(u_{ii} > 0)$*.*

Lemma 5 (DT & Meurant, 2016)

For $1 \leq k < n$ *the matrices* $\mathbf{H}_k$ *and* $\underline{\mathbf{H}}_k$ *can be written as*

$$\mathbf{H}_k = \mathbf{U}_k^{-1}\mathbf{C}^{(k)}\mathbf{U}_k, \qquad \underline{\mathbf{H}}_k = \mathbf{U}_{k+1}^{-1}\mathbf{E}_{k+1}\begin{bmatrix}\mathbf{U}_k \\ \mathbf{0}_{1\times k}\end{bmatrix},$$

where $\mathbf{U}_k$ *is the upper-left* $k \times k$ *submatrix of* $\mathbf{U}$ *and*

$$\mathbf{C}^{(k)} = \mathbf{E}_k + \begin{bmatrix}\mathbf{0} & \mathbf{U}_k\mathbf{U}^{-1}_{1:k,k+1}\end{bmatrix}, \quad \mathbf{E}_k = \begin{bmatrix}0 & & & \\ 1 & 0 & & \\ & \ddots & \ddots & \\ & & 1 & 0\end{bmatrix}.$$

GMRES residual polynomial companion matrix

Remark 2 (DT & Meurant, 2016)

For $1 \le k < n$, $\mathbf{C}^{(k)}\mathbf{e}_k = -\mathbf{U}_{1:k,k+1}/u_{k+1,k+1}$.

Lemma 6 (Meurant, 2016)

For $1 \le k < n$, *assume that* $\mathbf{H}_k$ *is nonsingular. The matrix*

$$\widehat{\mathbf{H}}_k := \mathbf{H}_k + h_{k+1,k}^2 \mathbf{H}_k^{-*}\mathbf{e}_k\mathbf{e}_k^{\mathrm{T}},$$

whose eigenvalues are the harmonic Ritz values at step k, *can be written as*

$$\widehat{\mathbf{H}}_k = \mathbf{U}_k^{-1}\widehat{\mathbf{C}}^{(k)}\mathbf{U}_k,$$

$\mathbf{U}_k$ *being upper triangular and the companion matrix*

$$\widehat{\mathbf{C}}^{(k)} = \mathbf{C}^{(k)} + \frac{1}{u_{k+1,k+1}^2 \overline{\mathbf{e}_1^{\mathrm{T}}\mathbf{C}^{(k)}\mathbf{e}_k}} \mathbf{U}_k\mathbf{U}_k^*\mathbf{e}_1\mathbf{e}_k^{\mathrm{T}}.$$

GMRES residual norms and U

Theorem 7 (Relation to entries of $\mathbf{U}$)

GMRES *residual norms,* $\|\mathbf{r}_k\|$*, satisfy:*

$$\|\mathbf{r}_k\| = \left(\sum_{l=1}^{k+1} |u_{1l}|^2 \right)^{-1/2} .$$

Corollary 8

For $1 \leq k < n$*,*

$$|u_{1,k+1}| = \sqrt{\frac{1}{\|\mathbf{r}_k\|^2} - \frac{1}{\|\mathbf{r}_{k-1}\|^2}}.$$

Construction of the desired U

Given $\{\rho_k\}_{k=0}^{n-1}$ and an admissible harmonic Ritz value set Θ:
Step $k = 0$**:** Let $u_{11} = 1$.
Step $1 \le k < n$**:** (i) If $\rho_k < \rho_{k-1}$, let $\{\theta_j^{(k)}\}_{j=1}^{k}$ be the roots of the polynomial $z^k + \beta_{k-1}z^{k-1} + \cdots + \beta_1 z + \beta_0$. Let

$$u_{1,k+1} = \frac{\beta_0}{|\beta_0|}\sqrt{1/\rho_k^2 - 1/\rho_{k-1}^2},$$

$$u_{k+1,k+1} = \frac{1}{|\beta_0|\rho_k^2\sqrt{1/\rho_k^2 - 1/\rho_{k-1}^2}},$$

$$u_{j,k+1} = \beta_{j-1}u_{k+1,k+1} - \frac{\mathbf{e}_j^{\mathrm{T}}\mathbf{U}_k\mathbf{U}_k^*\mathbf{e}_1}{\overline{u}_{1,k+1}}, \quad j = 2, \ldots, k.$$

(ii) If $\rho_k = \rho_{k-1}$, let $u_{1,k+1} = 0$, $u_{k+1,k+1}$ be arbitrarily chosen positive real number, and $u_{j,k+1}$ for $j = 2 : k$, be arbitrarily chosen complex numbers.

Construction of the desired pair $\{\mathbf{A}, \mathbf{r}_0\}$

Theorem 9

Given $\{\rho_k\}_{k=0}^{n-1}$ and an admissible harmonic Ritz value set Θ. Let $\mathbf{H} = \mathbf{U}^{-1}\mathbf{C}\mathbf{U}$ where $\mathbf{U}$ is chosen by the previous procedure and $\mathbf{C}$ is the companion matrix with prescribed eigenvalues. GMRES applied to $\{\mathbf{H}, \mathbf{e}_1\}$ generates the residual $\mathbf{r}_k$ with $\|\mathbf{r}_k\| = \rho_k$, and all the prescribed harmonic Ritz values.

General $\{\mathbf{A}, \mathbf{r}_0\}$ can be constructed via the invariance under unitary similarity transformations.

Theorem 10 (Trefethen & Bau, 1997; etc.)

Let GMRES be applied to a matrix $\mathbf{A} \in \mathbb{C}^{n\times n}$ and a vector $\mathbf{r}_0$. If $\mathbf{A}$ is changed to $\mathbf{PAP}^*$ for some unitary matrix $\mathbf{P}$, and $\mathbf{r}_0$ is changed to $\mathbf{P}\mathbf{r}_0$, then the residuals $\{\mathbf{r}_k\}$ change to $\{\mathbf{P}\mathbf{r}_k\}$.

QR factorization: $\mathbf{H} = \mathbf{QR}$

The matrix $\mathbf{Q}$ is unitary irreducible upper Hessenberg.

Lemma 11 (Entries of $\mathbf{Q}$)

Rows 2 through n of the unitary irreducible upper Hessenberg matrix $\mathbf{Q}$ are uniquely determined (up to complex signs) by the first row of $\mathbf{Q}$. Specifically, for $i = 1 : n-1$ and $j = i+1 : n$

$$q_{i+1,i} = \alpha_i \frac{\sqrt{1 - \sum_{l=1}^{i} |q_{1l}|^2}}{\sqrt{1 - \sum_{l=1}^{i-1} |q_{1l}|^2}},$$

$$q_{i+1,j} = -\alpha_i \frac{\overline{q}_{1i} q_{1j}}{\sqrt{1 - \sum_{l=1}^{i-1} |q_{1l}|^2}\sqrt{1 - \sum_{l=1}^{i} |q_{1l}|^2}},$$

where

$$|\alpha_1| = |\alpha_2| = \cdots = |\alpha_{n-1}| = 1.$$

GMRES residual norms and Q:

Lemma 12 (Relation to entries of $\mathbf{Q}$)

GMRES *residual norms,* $\|\mathbf{r}_k\|$*, satisfy:*

$$\|\mathbf{r}_k\| = \left(\sum_{l=k+1}^{n} |q_{1l}|^2\right)^{1/2}, \quad \|\mathbf{r}_k\| = |q_{k+1,k}|\|\mathbf{r}_{k-1}\|.$$

Corollary 13

The entries of the first row of $\mathbf{Q}$*,* q_{1k}*, satisfy*

$$|q_{1k}| = \sqrt{\|\mathbf{r}_{k-1}\|^2 - \|\mathbf{r}_k\|^2}.$$

Remark 3

By Lemma 11 *and Corollary* 13*, given* GMRES *residual norms implies entries of* $\mathbf{Q}$ *are uniquely determined up to complex signs.*

Parameterized inverse eigenvalue problems

By $\mathbf{H} = \mathbf{QR}$, we can rewrite the eigenvalue problem $\mathbf{H}_k\mathbf{y} = \lambda\mathbf{y}$ as

$$\mathbf{Q}_k\mathbf{R}_k\mathbf{y} = \lambda\mathbf{y},$$

where $\mathbf{Q}_k$ and $\mathbf{R}_k$ denote the upper-left $k \times k$ submatrices of $\mathbf{Q}$ and $\mathbf{R}$, respectively. By $\mathbf{H} = \mathbf{QR}$, we have

$$\underline{\mathbf{H}}_k = \underline{\mathbf{Q}}_k\mathbf{R}_k,$$

where $\underline{\mathbf{Q}}_k$ denotes the upper-left $(k+1) \times k$ submatrix of $\mathbf{Q}$. Therefore, we can rewrite the generalized eigenvalue problem $\underline{\mathbf{H}}_k^*\underline{\mathbf{H}}_k\mathbf{y} = \theta\mathbf{H}_k^*\mathbf{y}$ as

$$\mathbf{R}_k\mathbf{y} = \theta\mathbf{Q}_k^*\mathbf{y}.$$

Remark 4

Given the matrix $\mathbf{Q}$, we can determine $\mathbf{R}_k$ column by column according to the prescribed Ritz values or harmonic Ritz values.

Conclusion and future work

Conclusion: Any admissible harmonic Ritz value set is possible for GMRES.

For assessing the quality of a preconditioner $\mathbf{M}$ when GMRES is applied to

$$\mathbf{M}^{-1}\mathbf{A}\mathbf{x} = \mathbf{M}^{-1}\mathbf{b}, \quad \mathbf{M}^{-1}\mathbf{A} \text{ non-normal},$$

the spectrum of $\mathbf{M}^{-1}\mathbf{A}$ alone is not enough for convergence analysis.

- Clustering of eigenvalues does not suffice to guarantee fast convergence for nonnormal case.
- Not either need eigenvalues, Ritz values, and harmonic Ritz values close to zero hamper convergence.

Future work: Attempt to find theoretical reasons for the fact that deflation methods work in spite of these results. Design efficient preconditioners, etc.

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