On prescribing Ritz values and GMRES residual norms generated by Arnoldi processes

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joint work with

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Outline

- 1. Motivation
- 2. Prescribing convergence behavior for Arnoldi's method
- 3. Prescribing convergence behavior for *both* Arnoldi's method and GMRES



Given a nonsingular matrix and nonzero vector

$$A \in \mathbb{C}^{n \times n}, \quad b \in \mathbb{C}^n,$$

the kth iteration of the Arnoldi orthogonalization process [Arnoldi - 1951] (without breakdown) computes the decomposition

$$AV_k = V_{k+1}\tilde{H}_k,$$

where the columns of $V_k = [v_1, \ldots, v_k]$ (the Arnoldi vectors) contain an orthogonal basis for the *k*th Krylov subspace

$$\mathcal{K}_k(A,b) \equiv \operatorname{span}\{b, Ab, \dots, A^{k-1}b\}$$

and $\tilde{H}_k \in \mathbb{C}^{(k+1) \times k}$ is rectangular upper Hessenberg; by deleting its last row we get the square matrix

$$H_k = V_k^* A V_k \in \mathbb{C}^{k \times k}.$$



Essentially,

- for eigenpair approximations of A, the Arnoldi method [Arnoldi 1951], [Saad 1980] uses the eigenvalues (so-called Ritz values) and eigenvectors of H_k and the first k Arnoldi vectors,
- for approximate solutions to linear systems Ax = b, the GMRES method [Saad, Schultz 1986] solves least squares problems with \tilde{H}_k and $||b||e_1$ and the first k Arnoldi vectors.
- Both the GMRES and the Arnoldi method are very popular methods that are successful for a large variety of problem classes.
- Nevertheless, convergence behavior of the two methods is not fully understood, analysis is particularly challenging with highly non-normal input matrices.



- Often one tries to use the tools that are successful for analysis of hermitian counterparts of GMRES and Arnoldi like the Conjugate Gradient and the Lanczos method.
- For example, the basic tool for explaining Krylov subspace methods for hermitian linear systems is the eigenvalue distribution.
- However, for GMRES it is known for some time that if GMRES generates a certain residual norm history, the same history can be generated with any nonzero spectrum [Greenbaum, Strakoš - 1994].
- Complemented with the fact that GMRES can generate arbitrary non-increasing residual norms, this gives the result that any non-increasing convergence curve is possible with any nonzero spectrum [Greenbaum, Pták, Strakoš - 1996].
- A complete description of the class of matrices and right hand sides with prescribed convergence and eigenvalues was given in [Arioli, Pták, Strakoš - 1998].



An important tool for hermitian eigenproblems solved with Krylov subspace methods is the following interlacing property:

Consider a tridiagonal Jacobi matrix T_m and its leading principal submatrix T_k for some k < m. If the ordered eigenvalues of T_k are

 $\rho_1^{(k)} < \rho_2^{(k)} < \dots < \rho_k^{(k)},$

then in every open interval between two subsequent eigenvalues

 $(\rho_{i-1}^{(k)}, \rho_i^{(k)}), \quad i = 2, \dots, k,$

there lies at least one eigenvalue of T_m .

This interlacing property enables, among others, to prove the persistence theorem (see [Paige - 1971, 1976, 1980] or [Meurant, Strakoš - 2006]) which is crucial for controlling the convergence of Ritz values in the Lanczos method.



- There are generalizations of the interlacing property to the non-hermitian but normal case [Fan, Pall - 1957], [Thompson- 1966], [Ericsson - 1990], [Malamud - 2005], though a geometric interpretation is difficult.
- There is no interlacing property for the eigenvalues of principal submatrices of general non-normal matrices [de Oliveira 1969], [Shomron, Parlett 2009].
- This makes convergence analysis of the Arnoldi method for non-normal input matrices rather delicate, just as it is for the GMRES method.
- The GMRES and Arnoldi methods being closely related through the Arnoldi process, can we show that arbitrary convergence behavior of Arnoldi is possible?
- By arbitrary behavior we mean arbitrary Ritz values for all iterations (we do not consider eigenvectors). Note that this involves many more conditions than prescribing one residual norm per GMRES iteration.



Notation: Let the *k*th Hessenberg matrix H_k generated in Arnoldi's method have the eigenvalue ρ and normalized eigenvector y,

$$H_k y = \rho y.$$

With the Arnoldi decomposition $AV_k = V_{k+1}\tilde{H}_k$, the Ritz pair

 $\{\rho, V_k y\},\$

i.e. the Ritz value - Ritz vector pair has residual norm

 $||A(V_ky) - \rho(V_ky)|| = ||A(V_ky) - V_kH_ky|| = ||V_{k+1}\tilde{H}_ky - V_kH_ky|| = h_{k+1,k}|e_k^Ty|.$

Often for small $h_{k+1,k}|e_k^T y|$, the Arnoldi method takes $\{\rho, V_k y\}$ as an approximate eigenvalue-eigenvector pair of A. Note that a small value $h_{k+1,k}|e_k^T y|$ needs not imply that ρ is close to a true eigenvalue of A, see e.g. [Chatelin - 1993], [Godet-Thobie - 1993]; convergence analysis cannot be based on this value but focusses instead on the quality of approximate invariant subspaces [Beattie, Embree, Sorensen - 2005].



2. Prescribed convergence for Arnoldi's method

Theorem 1 [DT, Meurant - 2012]. Let the set

$$\mathcal{R} = \{ \qquad \rho_1^{(1)}, \\ (\rho_1^{(2)}, \rho_2^{(2)}), \\ \vdots \\ (\rho_1^{(n-1)}, \dots, \rho_{n-1}^{(n-1)}), \\ (\lambda_1, \dots, \lambda_n) \},$$

represent any choice of n(n+1)/2 complex Ritz values and denote by $C^{(k)}$ the companion matrix of the polynomial with roots $\rho_1^{(k)}, \ldots, \rho_k^{(k)}$, i.e.

$$C^{(k)} = \begin{pmatrix} 0 & \dots & 0 & -\alpha_0 \\ 1 & 0 & \dots & 0 & -\alpha_1 \\ & \ddots & & \vdots & \vdots \\ & & & 1 & -\alpha_{k-1} \end{pmatrix}, \qquad \prod_{j=1}^k (z - \rho_j^{(k)}) = z^k + \sum_{j=0}^{k-1} \alpha_j z^j.$$



If we define the unit upper triangular matrix $U(\mathcal{S})$ through

$$U(S) = I_n - \begin{bmatrix} 0 & C^{(1)}e_1 & \vdots & & \vdots \\ & 0 & C^{(2)}e_2 & & \vdots \\ & & 0 & & \\ & & & C^{(n-1)}e_{n-1} \\ & & & & 0 \end{bmatrix},$$

then the upper Hessenberg matrix

$$H(\mathcal{R}) = U(\mathcal{S})^{-1}C^{(n)}U(\mathcal{S})$$

has the spectrum $\lambda_1, \ldots, \lambda_n$ and its *k*th leading principal submatrix has spectrum

$$\rho_1^{(k)}, \dots, \rho_k^{(k)}, \qquad k = 1, \dots, n-1.$$

It has unit subdiagonal.

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Proof: The $k \times k$ leading principal submatrix of $H(\mathcal{R})$ is

$$\begin{bmatrix} I_k, 0 \end{bmatrix} H(\mathcal{R}) \begin{bmatrix} I_k \\ 0 \end{bmatrix} = \begin{bmatrix} I_k, 0 \end{bmatrix} U(\mathcal{S})^{-1} C^{(n)} U(\mathcal{S}) \begin{bmatrix} I_k \\ 0 \end{bmatrix}$$
$$= \begin{bmatrix} U_k^{-1}, \tilde{u}_{k+1}, \dots, \tilde{u}_n \end{bmatrix} \begin{bmatrix} 0 \\ U_k \\ 0 \end{bmatrix} = \begin{bmatrix} U_k^{-1}, \tilde{u}_{k+1} \end{bmatrix} \begin{bmatrix} 0 \\ U_k \end{bmatrix},$$

where U_k denotes the $k \times k$ leading principal submatrix of U(S) and \tilde{u}_j denotes the vector of the first k entries of the jth column of $U(S)^{-1}$ for j > k. Its spectrum is also the spectrum of the matrix

$$U_k[U_k^{-1}, \tilde{u}_{k+1}] \begin{bmatrix} 0\\ U_k \end{bmatrix} U_k^{-1} = [I_k, U_k \tilde{u}_{k+1}] \begin{bmatrix} 0\\ I_k \end{bmatrix},$$

which is a companion matrix with last column $U_k \tilde{u}_{k+1}$.

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2. Prescribed convergence for Arnoldi's method

From

$$e_{k+1} = U_{k+1}U_{k+1}^{-1}e_{k+1} = \begin{bmatrix} U_k & -C^{(k)}e_k \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \tilde{u}_{k+1} \\ 1 \end{bmatrix} = \begin{bmatrix} U_k\tilde{u}_{k+1} - C^{(k)}e_k \\ 1 \end{bmatrix}$$

we obtain $U_k \tilde{u}_{k+1} = C^{(k)} e_k$. \Box

Remark: The matrix

$$H(\mathcal{R}) = U(\mathcal{S})^{-1}C^{(n)}U(\mathcal{S}).$$

is the *unique* upper Hessenberg matrix $H(\mathcal{R})$ with the prescribed spectrum and Ritz values and the entry one along the subdiagonal (see also [Parlett, Strang -2008] where $H(\mathcal{R})$ is constructed in a different way).

Note that U(S) transforms the matrix $C^{(n)}$ with all Ritz values zero to the matrix $H(\mathcal{R})$ with prescribed Ritz values. It is composed of (columns of) companion matrices and we will call U(S) the Ritz value companion transform.



Thus the Ritz values generated in the Arnoldi method can exhibit any convergence behavior: Apply the Arnoldi method to the pair

 $\{H(\mathcal{R}), e_1\}$

where $H(\mathcal{R})$ has the desired Ritz values. Then the method generates the Hessenberg matrix $H(\mathcal{R})$ itself.

Question: Can the same prescribed Ritz values be generated with positive entries other than one on the subdiagonal?

For $\sigma_1, \sigma_2, \ldots, \sigma_{n-1} > 0$ consider the diagonal similarity transformation

 $H \equiv \operatorname{diag}\left(1, \sigma_1, \sigma_1 \sigma_2, \dots, \Pi_{j=1}^{n-1} \sigma_j\right) H(\mathcal{R}) \left(\operatorname{diag}\left(1, \sigma_1, \sigma_1 \sigma_2, \dots, \Pi_{j=1}^{n-1} \sigma_j\right)\right)^{-1}.$

Then the subdiagonal of *H* is $\sigma_1, \ldots, \sigma_{n-1}$ and all leading principal submatrices of *H* are similar to corresponding leading principal submatrices of $H(\mathcal{R})$.



This immediately leads to a parametrization of the matrices and initial Arnoldi vectors that generate a given set of Ritz values \mathcal{R} :

Theorem 2 [DT, Meurant - 2012]. Assume we are given a set of tuples

$$\mathcal{R} = \{ \qquad \rho_1^{(1)}, \\ (\rho_1^{(2)}, \rho_2^{(2)}), \\ \vdots \\ (\rho_1^{(n-1)}, \dots, \rho_{n-1}^{(n-1)}), \\ (\lambda_1, \dots, \lambda_n) \},$$

of complex numbers and n-1 positive real numbers

$$\sigma_1,\ldots,\sigma_{n-1}.$$

If A is a matrix of order n and b a nonzero n-dimensional vector, then the following assertions are equivalent:



- 1. The Hessenberg matrix generated by the Arnoldi method applied to A and initial Arnoldi vector b has eigenvalues $\lambda_1, \ldots, \lambda_n$, subdiagonal entries $\sigma_1, \ldots, \sigma_{n-1}$ and $\rho_1^{(k)}, \ldots, \rho_k^{(k)}$ are the eigenvalues of its kth leading principal submatrix for all $k = 1, \ldots, n-1$.
- 2. The matrix A and initial vector b are of the form

$$A = V D_{\sigma} U(S)^{-1} C^{(n)} U(S) D_{\sigma}^{-1} V^*, \qquad b = ||b|| V e_1,$$

where V is unitary, U(S) is the Ritz value companion transform,

$$D_{\sigma} = \operatorname{diag}(1, \sigma_1, \sigma_1 \sigma_2, \dots, \prod_{j=1}^{n-1} \sigma_j),$$

and $C^{(n)}$ is the companion matrix of the polynomial with roots $\lambda_1, \ldots, \lambda_n$.

This also shows how little on the quality of the Ritz value ρ needs be said by

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

Any distance from ρ to the spectrum of A is possible with any value of $h_{k+1,k}!$ J. Duintjer Tebbens, G. Meurant



Counterintuitive example 1: Convergence of interior Ritz values only:

$$\mathcal{R} = \{ 3, \\ (3,3), \\ (2,3,4), \\ (3,3,3,3), \\ (1,2,3,4,5) \}.$$

This gives the unit upper Hessenberg matrix

$$H(\mathcal{R}) = U(\mathcal{S})^{-1}C^{(5)}U(\mathcal{S}) = \begin{bmatrix} 3 & 0 & 0 & 0 & 0 \\ 1 & 3 & 1 & 0 & 1 \\ & 1 & 3 & -1 & 0 \\ & & 1 & 3 & 5 \\ & & & 1 & 3 \end{bmatrix}$$



Thus these Ritz values are generated by the Arnoldi method applied to

$$A = V \operatorname{diag}\left(1, \sigma_{1}, \sigma_{1} \sigma_{2}, \dots, \Pi_{j=1}^{n-1} \sigma_{j}\right) \begin{bmatrix} 3 & 0 & 0 & 0 & 0 \\ 1 & 3 & 1 & 0 & 1 \\ & 1 & 3 & -1 & 0 \\ & & 1 & 3 & 5 \\ & & & 1 & 3 \end{bmatrix} \operatorname{diag}\left(1, \sigma_{1}, \sigma_{1} \sigma_{2}, \dots, \Pi_{j=1}^{n-1} \sigma_{j}\right)^{-1} V^{*},$$

with initial vector $b = Ve_1$ and for any unitary V and positive values $\sigma_1, \ldots, \sigma_{n-1}$.

This is not a highly non-normal example, for instance with $\sigma_i \equiv 1$:

 $||A|| ||A^{-1}|| = 9.7137,$

and the eigenvector basis W of A has condition number

 $||W|| ||W^{-1}|| = 4.8003.$



Counterintuitive example 2: We can prescribe the "diverging" Ritz values

$$\mathcal{R} = \left\{ \begin{array}{cc} 1, \\ (0,2), \\ (-1,1,3), \\ (-2,0,2,4), \\ (1,1,1,1,1) \right\}, \end{array}$$
with $H(\mathcal{R}) = U(\mathcal{S})^{-1}C^{(5)}U(\mathcal{S}) = \begin{bmatrix} 1 & 1 & 0 & -3 & 0 \\ 1 & 1 & 3 & 0 & -31 \\ 1 & 1 & 3 & 0 & -31 \\ 1 & 1 & 1 & 6 & 0 \\ & & 1 & 1 & -10 \\ & & & 1 & 1 \end{bmatrix}.$

They are generated by Arnoldi applied to $A = VH(\mathcal{R})V^*$, $b = Ve_1$ for unitary V.



The same "diverging" Ritz values are generated with the exponentially decreasing values 2^{-1} , 2^{-2} , 2^{-3} and 2^{-4} on the subdiagonal of the Hessenberg matrix:

$$A = V \begin{bmatrix} 1 & 2 & 0 & -192 & 0 \\ 0.5 & 1 & 12 & 0 & -15872 \\ 0.25 & 1 & 48 & 0 \\ 0.125 & 1 & -160 \\ 0.0625 & 1 \end{bmatrix} V^*, \quad b = ||b|| Ve_1.$$

Then the rounded residual norms $||A(V_k y) - \rho(V_k y)|| = h_{k+1,k}|e_k^T y|$ seem to indicate convergence:

{

 $\frac{1}{2},$ (0.1118, 0.1118), (0.011, 0.0052, 0.011), (0.0006, 0.0001, 0.0001, 0.0006) }.



Starting with initial guess $x_0 = 0$, GMRES iterates x_k minimize the residual norm,

$$\|b - Ax_k\| = \min \|b - As\|$$
 over all $s \in \mathcal{K}_k(A, b)$.

Writing x_k in the Arnoldi basis,

$$x_k = V_k y_k \in \mathcal{K}_k(A, r_0),$$

and using the Arnoldi decomposition $AV_k = V_{k+1}\tilde{H}_k$, we see that the residual norm is

$$\begin{aligned} |b - Ax_k|| &= \|b - AV_k y_k\| = \|V_{k+1}\|b\|e_1 - AV_k y_k\| \\ &= \|V_{k+1}(\|b\|e_1 - \tilde{H}_k y_k)\| = \min_{y \in \mathbb{C}^k} \|\|b\|e_1 - \tilde{H}_k y\|. \end{aligned}$$

Thus the residual norms generated by the GMRES method are fully determined by the Hessenberg matrix \tilde{H}_k and ||b||.



- We have seen that the subdiagonal entries of \tilde{H}_k can be chosen arbitrarily, for any prescribed Ritz values in the *k*th iteration.
- Hence there is a chance we can modify the behavior of GMRES while maintaining the prescribed Ritz values.

Example from earlier: Consider the prescribed 'diverging' Ritz values

$$\mathcal{R} = \{ \begin{array}{c} 1, \\ (0,2), \\ (-1,1,3), \\ (-2,0,2,4), \\ (1,1,1,1,1) \}, \end{array}$$

and the prescribed subdiagonal entries of the generated Hessenberg matrix

$$\sigma_1 = 2^{-1}, \quad \sigma_2 = 2^{-2}, \quad \sigma_3 = 2^{-3}, \quad \sigma_4 = 2^{-4}.$$



The corresponding GMRES convergence curve is

$$||r^{(0)}|| = 1, ||r^{(1)}|| = \sqrt{\frac{1}{5}}, ||r^{(2)}|| = \sqrt{\frac{1}{5}}, ||r^{(3)}|| = 0.0052, ||r^{(4)}|| = 0.0052.$$

Question: Can we force any GMRES convergence speed with arbitrary Ritz values by modifying the subdiagonal entries?

Not any, because there is a relation between GMRES stagnation and zero Ritz values: A singular Hessenberg matrix corresponds to stagnation in the parallel GMRES process, see [Brown - 1991]. In our example we have

$$\rho_1^{(1)} = 1, \quad \|r^{(1)}\| = \frac{1}{\sqrt{5}}$$

$$(\rho_1^{(2)}, \rho_2^{(2)}) = (0, 2), \quad \|r^{(2)}\| = \frac{1}{\sqrt{5}}$$

$$(\rho_1^{(3)}, \rho_2^{(3)}, \rho_3^{(3)}) = (-1, 1, 3), \quad \|r^{(3)}\| = 0.0052$$

$$(\rho_1^{(4)}, \rho_2^{(4)}, \rho_3^{(4)}, \rho_4^{(4)}) = (-2, 0, 2, 4), \quad \|r^{(4)}\| = 0.0052$$



However, this is the only restriction Ritz values put on GMRES residual norms:

Theorem 3 [DT, Meurant - 2012]. Consider a set of tuples of complex numbers

$$\mathcal{R} = \{ \qquad \rho_1^{(1)}, \\ (\rho_1^{(2)}, \rho_2^{(2)}), \\ \vdots \\ (\rho_1^{(n-1)}, \dots, \rho_{n-1}^{(n-1)}), \\ (\lambda_1, \dots, \lambda_n) \},$$

such that $(\lambda_1, \ldots, \lambda_n)$ contains no zero number and *n* positive numbers

 $f(0) \ge f(1) \ge \dots \ge f(n-1) > 0,$

such that the k-tuple $(\rho_1^{(k)},\ldots,\rho_k^{(k)})$ contains a zero number if and only if

$$f(k-1) = f(k).$$



Let A be a square matrix of size n and let b be a nonzero n-dimensional vector. The following assertions are equivalent:

1. The GMRES method applied to A and right-hand side b with zero initial guess yields residuals $r^{(k)}$, k = 0, ..., n - 1 such that

$$||r^{(k)}|| = f(k), \quad k = 0, \dots, n-1,$$

A has eigenvalues

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

and

$$ho_1^{(k)},\ldots,
ho_k^{(k)}$$

are the Ritz values generated at the *k*th iteration for k = 1, ..., n - 1.



2. The matrix A and right hand side b are of the form

$$A = V \operatorname{diag}(f(0), D_c^{-*}) U(\mathcal{S})^{-1} C^{(n)} U(\mathcal{S}) \operatorname{diag}(f(0)^{-1}, D_c^{*}) V^{*}, \qquad b = \|b\| V e_1,$$

where V is a unitary matrix, U(S) is the Ritz value companion transform for \mathcal{R} and $C^{(n)}$ is the companion matrix of the polynomial with roots $\lambda_1, \ldots, \lambda_n$. D_c is a nonsingular diagonal matrix such that

$$R_h^{-T}\hat{h} = -f(0)^2 D_c c,$$

$$\hat{h} = [\eta_1, \dots, \eta_{n-1}]^T, \qquad \eta_k = (f(k-1)^2 - f(k)^2)^{1/2},$$

 R_h being the upper triangular factor of the Cholesky decomposition

$$R_h^T R_h = I - \frac{\hat{h}\hat{h}^T}{f(0)^2},$$

and c is the first row of $U(\mathcal{S})$ without its diagonal entry.

Note we exhausted all freedom modulo unitary transformation.

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Example: Standardly converging Ritz values and 'nearly stagnating' GMRES:

$$\mathcal{R} = \{ 5, \\ (1,5), \\ (1,4,5), \\ (1,3,4,5), \\ (1,2,3,4,5) \}, \\ |r^{(0)}|| = 1, \quad ||r^{(1)}|| = 0.9, \quad ||r^{(2)}|| = 0.8, \quad ||r^{(3)}|| = 0.7, \quad ||r^{(4)}|| = 0.6, \quad ||r^{(5)}|| = 0 \quad \text{gives} \\ A = V \begin{bmatrix} 5 & 0 & 0 & 0 & 0 \\ 10.3237 & 1 & 0 & 0 & 0 \\ 10.3237 & 1 & 0 & 0 & 0 \\ 0.8458 & 4 & 0 & 0 \\ 3.312 & 3 & 0 \\ 2.4169 & 2 \end{bmatrix} \\ V^*, \qquad b = ||b|| Ve_1.$$



Again, this is not a highly non-normal example:

 $||A|| ||A^{-1}|| = 28.9498,$

and the eigenvector basis W of A has condition number

 $\|W\|\|W^{-1}\| = 57.735.$

The residual norms $||A(V_k y) - \rho(V_k y)|| = h_{k+1,k} |e_k^T y|$ for the Ritz pairs are

10.3237,(0.8458, 0.7886),(0.8987, 3.312, 2.0509),(0.9906, 2.4169, 2.3137, 1.7303).

respectively, i.e. they give misleading information.



Conclusions and future work:

- There is no interlacing property for the Hessenberg matrices in the Arnoldi method.
- The Ritz values generated in the Arnoldi method can behave arbitrarily badly.
- Convergence of Ritz values need not say anything about the behavior of GMRES residual norms (zero Ritz values excepted). For close to normal matrices, the opposite has been suggested [van der Vorst, Vuik - 1993].
- Extension to harmonic Ritz values which determine the GMRES polynomials?
- It is desirable to have similar results for popular restarted versions of GMRES and the Arnoldi method (see e.g. the failure of restarted Arnoldi with exact shifts explained in [Embree - 2009]).



For more details see:DUINTJER TEBBENS J, MEURANT G: Any Ritz value behavior is possible for Arnoldi and for GMRES, SIMAX vol. 33 no. 3, pp 958–978, 2012, available at www.cs.cas.cz/duintjertebbens/duintjertebbens_pub.html

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