The roots of GMRES polynomials need not influence GMRES residual norms

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joint work with

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Outline

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1. Eigenvalues and convergence of Krylov subspace methods
2. Some recent results
3. Harmonic Ritz values

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Eigenvalues and convergence of Krylov subspace methods

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- eigenvalues close to zero hamper convergence,
- clustering of eigenvalues stimulates convergence.

Eigenvalues and convergence of Krylov subspace methods

For instance, in the MINRES method, residual norms satisfy the minimization property

$$\|r_k\| = \min_{p \in \pi_k} \|p(A)b\|, \qquad \pi_k \text{ the degree } k \text{ polynomials with } \pi_k(0) = 1.$$

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Thus residual norms are fully determined by two quantities:

1. eigenvalues,
2. components of the right-hand side in the eigenvector basis.

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- $$\frac{\|x - x_k\|_A}{\|x - x_0\|_A} \leq 2\left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1}\right)^k$$

  for the CG method.

Eigenvalues and convergence of Krylov subspace methods

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$$\|r_k\|^2 = \frac{\sum_{I_{k+1}} \left[\prod_{j=1}^{k+1} \gamma_{i_j}\right] \prod_{\substack{i_1 \le i_\ell < i_j \le i_{k+1} \\ i_\ell, i_j \in I_{k+1}}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}{\sum_{I_k} \left[\prod_{j=1}^{k} \gamma_{i_j} |\lambda_{i_j}|^2\right] \prod_{\substack{i_1 \le i_\ell < i_j \le i_k \\ i_\ell, i_j \in I_k}} |\lambda_{i_j} - \lambda_{i_\ell}|^2},$$

where $\gamma_{i_j} = |e_{i_j}^T c|^2$, $c = W^* b$ and $\sum_{I_k}$ denote summation over all possible sets I_k of k indices $i_1, i_2, \ldots, i_k$ such that $1 \le i_1 < \cdots < i_k \le n$.

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Theorem [Greenbaum, Pták & Strakoš, 1996]. *Let*

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

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

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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 the GMRES method applied to A and b satisfy

$$\|r_k\|_2 = f_k, \quad 0 \leq k \leq n, \quad \text{and} \quad \text{eig}(A) = \{\lambda_1, \ldots, \lambda_n\}.$$

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- To force GMRES residual norms $f(0) \geq \cdots \geq f(n-1) > 0$, the first row g^T of U can be chosen as

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

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Summarizing,

$$A = V \begin{bmatrix} & g^T & \\ 0 & & T \end{bmatrix}^{-1} C \begin{bmatrix} & g^T & \\ 0 & & T \end{bmatrix} V^*, \qquad b = Ve_1,$$

for some non-singular, upper triangular matrix $T \in \mathbb{C}^{(n-1)\times(n-1)}$.

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Thus for assessing the quality of a preconditioner $\mathcal{P}$ when GMRES is applied to

$$\mathcal{P}Ax = \mathcal{P}b, \qquad \mathcal{P}A \quad \text{non-symmetric},$$

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For instance in constraint preconditioning, the fact that spec($\mathcal{P}A$) is, say,

$$\text{spec } (\mathcal{P}A) = \{1, \frac{1}{2} \pm \frac{\sqrt{(5)}}{2}\}$$

does not suffice to guarantee fast convergence of GMRES when $\mathcal{P}A$ is non-symmetric. What is needed additionally, is the fact that the eigenvalues have belong to Jordan blocks of small size.

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Practical examples with a tridiagonal matrix where it is hard to explain GMRES convergence based on eigenvalue distribution are given by for instance some convection-diffusion model problems that have been studied by many authors, e.g. [Fischer, Ramage, Sylvester & Wathen, 1999], [Ernst, 2000], [Elman & Ramage, 2001, 2002], [Liesen & Strakoš, 2005]:

Eigenvalues and convergence of Krylov subspace methods

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With Streamline Upwind Petrov Galerkin discretization (SUPG) [Brooks & Hughes, 1979], the coefficient matrix A is of the form

$$A_{i,j} = \nu\langle\nabla\phi_j, \nabla\phi_i\rangle + \langle w\cdot\nabla\phi_j, \phi_i\rangle + \frac{\delta\, h}{\|w\|}\langle w\cdot\nabla\phi_j, w\cdot\nabla\phi_i\rangle,$$

where $0 < \delta < 1$ and $\langle\cdot,\cdot\rangle$ denotes the L^2 inner product on Ω.

Eigenvalues and convergence of Krylov subspace methods

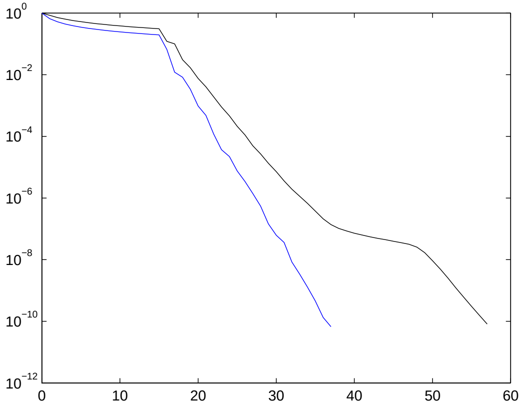

Figure : GMRES residual norms for the convection-diffusion problem with SUPG stabilization parameters $\delta = 0.7$ (blue) and $\delta = 0.2$ (black).

Eigenvalues and convergence of Krylov subspace methods

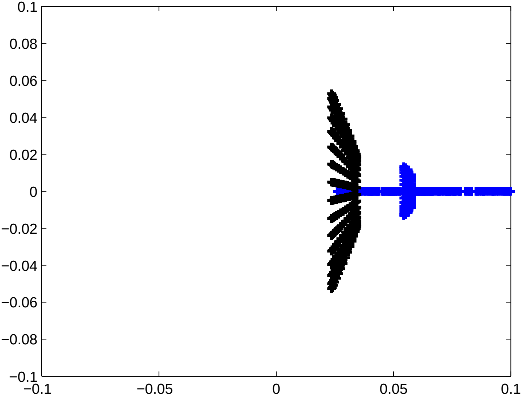

Figure : Spectra of system matrices for the convection-diffusion problem with SUPG stabilization parameters $\delta = 0.7$ (blue) and $\delta = 0.2$ (black).

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- In the CG method for Hermitian positive definite matrices, 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].

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- An analogue result for the GMRES method suggests a similar phenomenon provided A is close to normal - the involved bounds contain $\kappa(W)$ [van der Vorst & Vuik, 1993].

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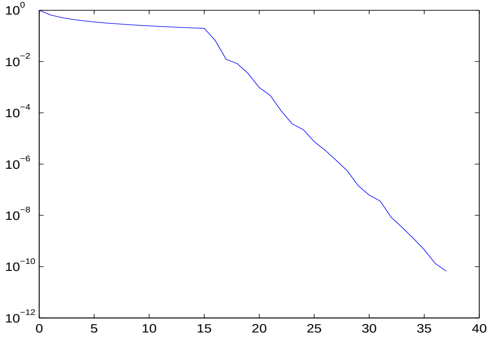
For the higly non-normal case, let us consider the convection-diffusion problem with SUPG stabilization parameter $\delta = 0.7$.

Eigenvalues and convergence of Krylov subspace methods



GMRES residual norms for the convection-diffusion problem with SUPG stabilization parameters $\delta = 0.7$.

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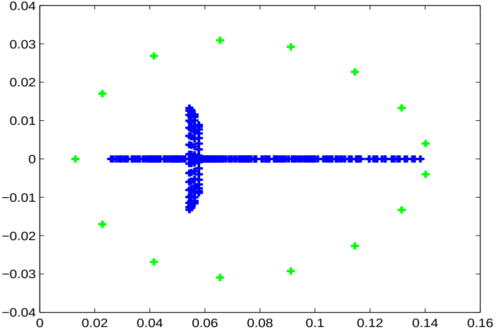
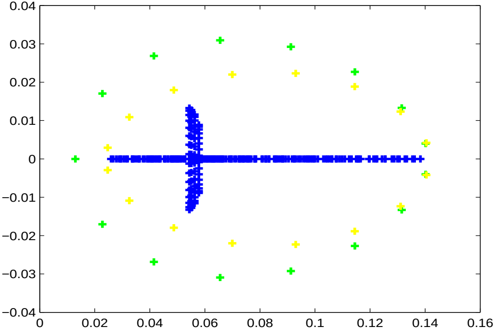


Blue: Eigenvalues of $A \in \mathbb{R}^{256\times 256}$. Green: Ritz values at iteration 15.

Eigenvalues and convergence of Krylov subspace methods



Blue: Eigenvalues of $A \in \mathbb{R}^{256\times 256}$. Yellow: Ritz values at iteration 16.

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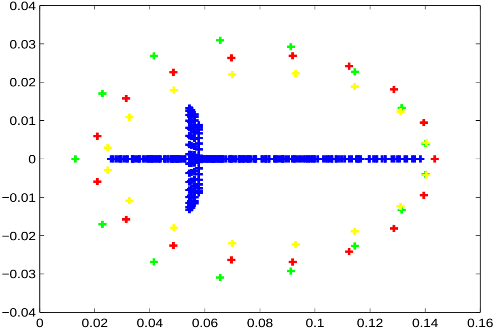

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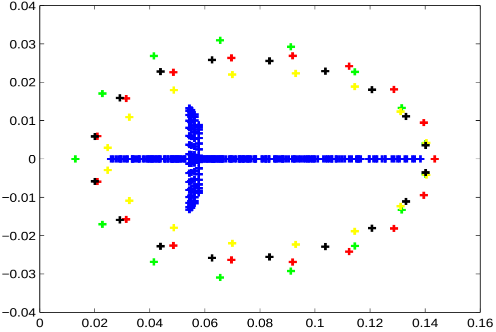

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- What do we know about the relation between Ritz value convergence and GMRES convergence for general non-normal matrices ?
- Do similar results exist for Krylov subspace methods for non-normal matrices other than GMRES?

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Some recent results

An analogue of the Greenbaum, Pták, Strakoš theorem for the FOM method is straightforward using the relation

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- To force FOM residual norms $f(0), \ldots, f(n-1)$, $f(i) > 0$, the first row g^T of U can be chosen as

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In fact, even if V is not orthogonal, but in some Krylov subspace method $KU = V$ holds, the first row of U gives the residual norm of the Krylov subspace method working with V. For example, when V is bi-orthogonal to a basis for $\mathcal{K}(A^*, s)$, it gives Bi-CG residual norms:

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where C is the companion matrix for the prescribed spectrum and where the first row g^T of U has entries
$$g_k = \frac{1}{f(k-1)}, \quad k = 1, \ldots, n,$$
if $f(0), \ldots, f(n-1)$, $f(i) > 0$ are the prescribed Bi-CG residual norms.

Some recent results

It can be shown that tridiagonal T allowing the decomposition

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can be found by applying a Bi-Lanczos process to C [DT & Meurant, 2016].

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The same can be done for the OR/MR pair of methods Hessenberg/CMRH based on Hessenberg LU factorization [Sadok, 1999], [Heyouni & Sadok, 1998] .

In fact, it can be done for any Krylov subspace method for non-normal matrices that is classified as a OR or MR-type method.

Some recent results

In the parametrization for GMRES/FOM

$$A = V \begin{bmatrix} & g^T & \\ 0 & & T \end{bmatrix}^{-1} C \begin{bmatrix} & g^T & \\ 0 & & T \end{bmatrix} V^*, \qquad b = Ve_1,$$

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In the GMRES and FOM methods it can be used to prescribe all Ritz values:

To force at iteration k the Ritz values $\rho_1^{(k)} \dots \rho_k^{(k)}$, $k = 1, \dots, n-1$, the entries $t_{i,k}$ in the kth column of T must satisfy

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

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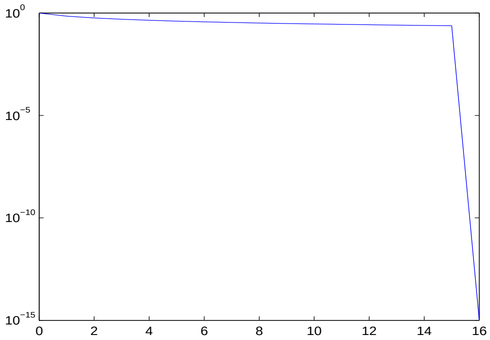
But many deflation methods use instead harmonic Ritz values.

Let us illustrate with a small 1D convection-diffusion problem.

Some recent results



GMRES residual norms for a 1D convection-diffusion problem.

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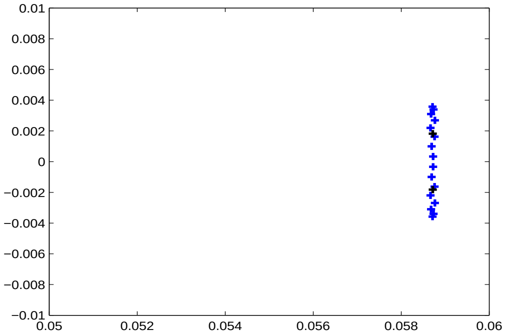

Blue: Eigenvalues of $A \in \mathbb{R}^{16\times 16}$. Black: Ritz values at iteration 2.

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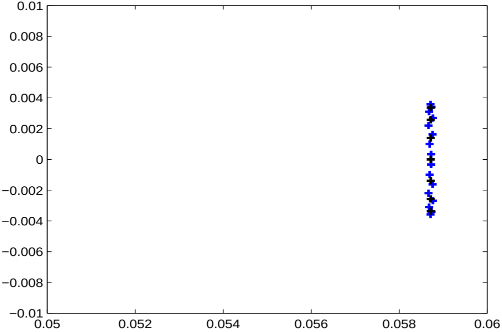
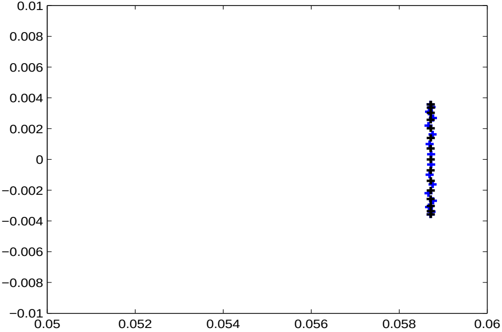


Blue: Eigenvalues of $A \in \mathbb{R}^{16\times 16}$. Black: Ritz values at iteration 7.

Some recent results



Blue: Eigenvalues of $A \in \mathbb{R}^{16\times 16}$. Black: Ritz values at iteration 15.

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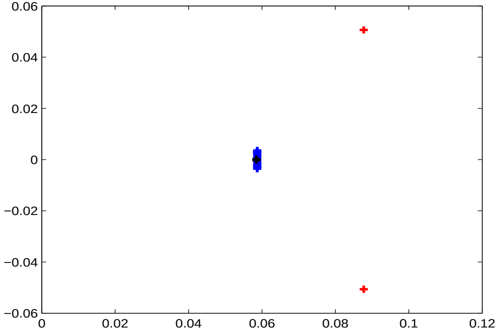

Blue: Eigenvalues of $A \in \mathbb{R}^{16\times 16}$. Black: Ritz values at iteration 2. Red: Harmonic Ritz values at iteration 2.

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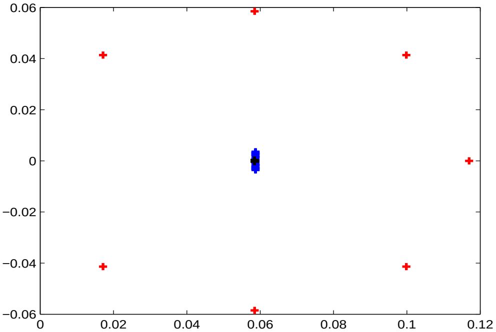

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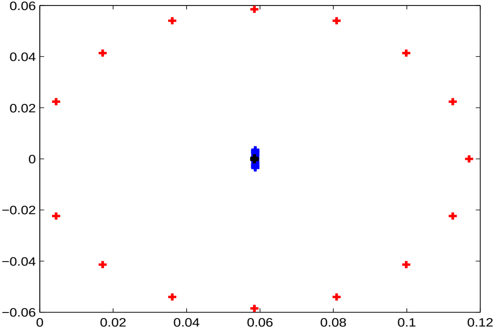

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Red: Harmonic Ritz values at iteration 15.

Outline

Harmonic Ritz values

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If at the kth iteration, GMRES generates residual vector r_k and harmonic Ritz values $\theta_1^{(k)}, \ldots, \theta_k^{(k)}$, then

$$\|r_k\| = \|p_k(A)b\|,$$

where

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

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Thus a close relation might be expected.

Harmonic Ritz values

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Theorem ([Du, DT & Meurant, 2017?])

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

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

If GMRES stagnates from step $k+1$ *to step* $k+m$ *, 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 at step* $k+i$ *is*

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

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

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If H_k is the kth leading principal submatrix of H, the harmonic Ritz values are the eigenvalues of

$$\hat{H}_k = H_k + h_{k+1,k}^2 H_k^{-*} e_k e_k^T.$$

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We have the following relation between the companion matrices for H_k and $\hat{H}_k$:

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Thus with $\hat{C}^{(k)}$ prescribed, we can attempt to construct $U^{(k)}$ while keeping the first row of U fixed.

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1. $u_{1,1} = 1$
2. If $f(k) < f(k-1)$, let $\theta_1^{(k)}, \ldots, \theta_k^{(k)}$ be the roots of the polynomial $z^k + \beta_{k-1} z^{k-1} + \cdots + \beta_1 z + \beta_0$.

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\begin{aligned}
u_{1,k+1} &= \frac{\beta_0}{|\beta_0|} \sqrt{1/f(k)^2 - 1/f(k-1)^2}, \\
u_{k+1,k+1} &= \frac{1/f(k)^2 - 1/f(k-1)^2 + e_1^T U_k U_k^* e_1}{|\beta_0| \sqrt{1/f(k)^2 - 1/f(k-1)^2}}, \\
u_{j,k+1} &= \beta_{j-1} u_{k+1,k+1} - \frac{e_j^T U_k U_k^* e_1}{\bar{u}_{1,k+1}}, \quad j = 2, \ldots, k.
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$$\begin{aligned} u_{1,k+1} &= \frac{\beta_0}{|\beta_0|} \sqrt{1/f(k)^2 - 1/f(k-1)^2}, \\ u_{k+1,k+1} &= \frac{1/f(k)^2 - 1/f(k-1)^2 + e_1^T U_k U_k^* e_1}{|\beta_0| \sqrt{1/f(k)^2 - 1/f(k-1)^2}}, \\ u_{j,k+1} &= \beta_{j-1} u_{k+1,k+1} - \frac{e_j^T U_k U_k^* e_1}{\bar{u}_{1,k+1}}, \quad j = 2, \ldots, k. \end{aligned}$$
3. If $f(k) = f(k-1)$, let $u_{1,k+1} = 0$, $u_{k+1,k+1} > 0$ and $u_{j,k+1}$, $j = 2, \ldots, k$ arbitrary complex.

Conclusion

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

Thank you for your attention.

Related publications

- A. Greenbaum, V. Pták and Z. Strakoš, Any nonincreasing convergence curve is possible for GMRES, **SIAM J. Matrix Anal. Appl.**, 17 (1996), pp. 465–469.
- M. Arioli, V. Pták and Z. Strakoš, Krylov sequences of maximal length and convergence of GMRES, **BIT Num. Maths.**, 38 (1996), pp. 636–643.
- J. Duintjer Tebbens and G. Meurant, Any Ritz value behavior is possible for Arnoldi and for GMRES, **SIAM J. Matrix Anal. Appl.**, 33 (2012), pp. 958–978.
- J. Duintjer Tebbens and G. Meurant, Prescribing the behavior of early terminating GMRES and Arnoldi iterations, **Numer. Algorithms**, 65 (2014), pp. 69–90.
- J. Duintjer Tebbens, G. Meurant, H. Sadok and Z. Strakoš, On investigating GMRES convergence using unitary matrices, **Lin. Alg. Appl.**, 450 (2014), pp. 83–107.
- G. Meurant and J. Duintjer Tebbens, The role eigenvalues play in forming GMRES residual norms with non-normal matrices, **Numer. Algorithms**, 68 (2015), pp. 143–165.
- J. Duintjer Tebbens and G. Meurant, On the convergence of QOR and QMR Krylov methods for solving nonsymmetric linear systems, **BIT Num. Maths.**, 56 (2016), pp. 77–97.