Can restarted GMRES exhibit any nonincreasing convergence curve ?

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GAMM Workshop on Applied and Numerical Linear Algebra, Liblice, September 4, 2012.

Outline

1. Prescribed convergence behavior for full GMRES.

2. Prescribed convergence behavior for restarted GMRES.

1. Prescribed convergence for full GMRES

Throughout we will consider a system of linear algebraic equations

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

with a non-hermitian nonsingular matrix to be solved by the GMRES method. Starting with $x_0 = 0$, the kth GMRES iterate x_k minimizes the residual norm,

$$\|r_k\| = \|b - Ax_k\| = \min \|b - As\| \quad \text{over all} \quad s \in \mathcal{K}_k(A, b) \equiv \text{span}\{b, Ab, \ldots, A^{k-1}b\}.$$

We denote the underlying Arnoldi decomposition as

$$AV_k = V_{k+1}\hat{H}_k, \qquad \text{where} \quad V_{k+1}^* V_{k+1} = I_{k+1}$$

and $\hat{H}_k \in \mathbb{C}^{(k+1)\times k}$ is upper Hessenberg. If we write $x_k = V_k y_k \in \mathcal{K}_k(A, r_0)$, then

$$\|r_k\| = \|b - AV_k y_k\| = \|V_{k+1}\|b\|e_1 - AV_k y_k\| = \|V_{k+1}(\|b\|e_1 - \hat{H}_k y_k)\| = \min_{y\in\mathbb{C}^k} \left\| \|b\|e_1 - \hat{H}_k y \right\|,$$

i.e. the residual norm is fully determined by the Hessenberg matrix $\hat{H}_k$.

1. Prescribed convergence for full GMRES

It is known since 1994 [Greenbaum, Strakoš], that if a GMRES convergence curve is generated by some matrix and right hand side $\{A, b\}$, the same curve can be generated by a pair $\{C, d\}$ where the matrix C has arbitrary nonzero spectrum.

In 1996, Greenbaum, Pták and Strakoš complemented this result by showing that any non-increasing convergence curve is possible with any nonzero spectrum.

Finally, in 1998, Arioli, Pták and Strakoš closed this series of papers with a parametrization of the pairs $\{A, b\}$ generating arbitrary Arnoldi behavior:

Theorem 1*[Arioli, Pták and Strakoš - 1998]. Let n complex nonzero numbers $(\lambda_1, \ldots, \lambda_n)$ and n positive numbers*

$$f(0) \geq f(1) \geq \cdots \geq f(n-1) > 0,$$

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

1. Prescribed convergence for full GMRES

1. *The matrix* A *has the eigenvalues* $\lambda_1, \ldots, \lambda_n$, *and the GMRES method applied to* A *and right-hand side* b *with zero initial guess yields residuals* $r^{(k)},\ k = 0, \ldots, n-1$ *such that*

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

2. *The pair* $\{A, b\}$ *is of the form*

$$A = W \begin{bmatrix} h & \begin{matrix} R \\ 0 \end{matrix} \end{bmatrix} \begin{bmatrix} 0 & -\alpha_0 \\ I_{n-1} & \vdots \\ & -\alpha_{n-1} \end{bmatrix} \begin{bmatrix} h & \begin{matrix} R \\ 0 \end{matrix} \end{bmatrix}^{-1} W^*, \qquad b = Wh,$$

where W *is a unitary matrix,* R *is a nonsingular upper triangular matrix of order* $n-1$,

$$h = [\eta_1, \ldots, \eta_n]^T, \qquad \eta_k = \sqrt{f(k-1)^2 - f(k)^2}, \quad k < n, \quad \eta_n = f(n-1)$$

1. Prescribed convergence for full GMRES

and $\alpha_0, \ldots, \alpha_{n-1}$ *are the coefficients of the polynomial* $q(\lambda)$ *with roots* $\lambda_1, \ldots, \lambda_n$,

$$q(\lambda) = (\lambda - \lambda_1) \cdots (\lambda - \lambda_n) = \lambda^n + \sum_{j=0}^{n-1} \alpha_j \lambda^j.$$

The previous parametrization contains the unitary matrix $W = [w_1, w_2, \ldots, w_n]$ representing an orthogonal basis of the Krylov *residual* space $A\mathcal{K}_n(A, r_0)$,

$$\text{span}\{w_1, w_2, \ldots, w_n\} = \text{span}\{Ab, A^2 b, \ldots, A^n b\}.$$

From [DT, Meurant - 2012] we easily obtain an alternative parametrization working with a unitary matrix $V = [v_1, v_2, \ldots, v_n]$ representing an orthogonal basis of the Krylov space $\mathcal{K}_n(A, r_0)$,

$$\text{span}\{v_1, v_2, \ldots, v_n\} = \text{span}\{b, Ab, \ldots, A^{n-1} b\} :$$

1. Prescribed convergence for full GMRES

Theorem 2 [DT, Meurant]. *Let n complex nonzero numbers $(\lambda_1, \ldots, \lambda_n)$ and n positive numbers*

$$f(0) \geq f(1) \geq \cdots \geq f(n-1) > 0,$$

be given. 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 matrix A has the eigenvalues $\lambda_1, \ldots, \lambda_n$, and the GMRES method applied to A and right-hand side b with zero initial guess yields residuals $r^{(k)},\ k = 0, \ldots, n-1$ such that*

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

1. Prescribed convergence for full GMRES

2. *The pair $\{A, b\}$ is of the form*

$$A = V \begin{bmatrix} & g^T & \\ 0 & & T \end{bmatrix}^{-1} \begin{bmatrix} 0 & -\alpha_0 \\ I_{n-1} & \vdots \\ & -\alpha_{n-1} \end{bmatrix} \begin{bmatrix} & g^T & \\ 0 & & T \end{bmatrix} V^*, \quad b = f(0) V e_1,$$

where V is a unitary matrix, T is nonsingular upper triangular of size $n-1$,

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

and $\alpha_0, \ldots, \alpha_{n-1}$ are the coefficients of the polynomial $q(\lambda)$ with roots $\lambda_1, \ldots, \lambda_n$,

$$q(\lambda) = (\lambda - \lambda_1) \cdots (\lambda - \lambda_n) = \lambda^n + \sum_{j=0}^{n-1} \alpha_j \lambda^j.$$

2. Prescribed convergence 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) (GMRES restarted after every mth iteration):

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.

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

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

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

2. Prescribed convergence for restarted GMRES

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

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

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

In this talk we try to generalize the result of Vecharinsky and Langou. First we wish to

1. eliminate the condition that during every restart cycle, all residual norms stagnate except for the very last iteration inside the cycle, i.e. we wish to prescribe residual norms inside restart cycles,
2. but we keep the condition that the residual norm in the last iteration of every cycle is strictly decreasing.

2. Prescribed convergence for restarted GMRES

The system matrix A and right hand side b that we construct will be parametrized as

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

where H is unreduced upper Hessenberg and V is unitary. We will investigate what entries H must have in order to prescribe the residual norms in restarted GMRES.

For the moment we focus on prescribing residual norms in the initial and in the second restart cycle. Let their residuals be denoted as

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

2. Prescribed convergence for restarted GMRES

Let m iterations of the initial cycle give the Arnoldi decomposition

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

The m iterations of the second cycle give the Arnoldi decomposition

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

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

Then we know that the columns $1, \ldots, m$ of H are

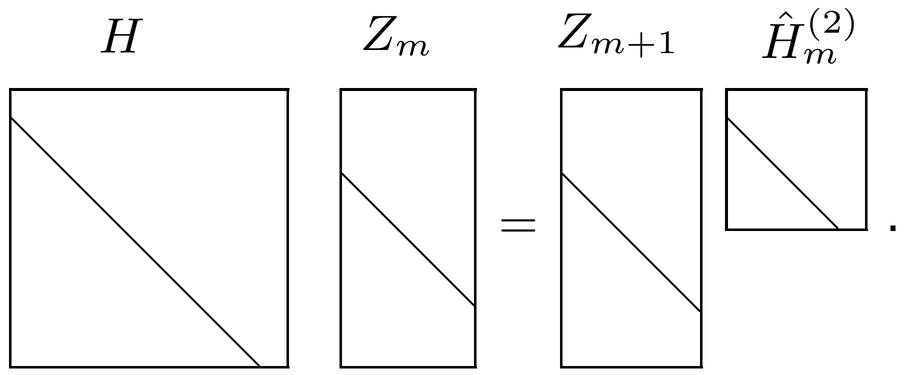
$$H \begin{bmatrix} I_m \\ 0 \end{bmatrix} = \begin{bmatrix} \hat{H}_m^{(1)} \\ 0 \end{bmatrix}.$$

2. Prescribed convergence 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.*

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

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



2. Prescribed convergence for restarted GMRES

Lemma 2. *Let* $r_m^{(1)} = V_{m+1}^{(1)} z^{(1)}$. *Then the last* $j-1$ *entries of* $z^{(1)}$ *are zero, i.e.*

$$e_i^T z^{(1)} = 0, \qquad i = m+3-j, \ldots, m+1$$

for an integer j *if and only if the last* j *residual norms are equal, i.e.*

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

Hence with our assumption that the residual norm in the last iteration of every cycle is strictly decreasing, we always have $e_{m+1}^T z^{(1)} \neq 0$. By choosing appropriately the columns $m+1, m+2, \ldots$ of H such that

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

we can force the Hessenberg matrix $\hat{H}_m^{(2)}$ to have prescribed entries.

2. Prescribed convergence for restarted GMRES

Theorem 4. *Let $A \in \mathbb{C}^{n \times n}$ be a matrix, $b \in \mathbb{C}^n$ be a nonzero vector and $\hat{H}_m^{(1)}, \hat{H}_m^{(2)} \in \mathbb{C}^{(m+1)\times m}$ be unreduced upper Hessenberg matrices with positive subdiagonal. The following assertions are equivalent.*

1. *The initial cycle of GMRES(m) applied to A and b does not stagnate in its last iteration and generates the Hessenberg matrix $\hat{H}_m^{(1)}$ and the second cycle generates the Hessenberg matrix $\hat{H}_m^{(2)}$.*

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

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

where V is unitary and H is upper Hessenberg and its first $2m$ columns are:

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$$H \begin{bmatrix} I_{2m} \\ 0 \end{bmatrix} = \begin{bmatrix} \hat{H}_m^{(1)} & \vdots & z^{(1)} e_1^T \hat{H}_m^{(2)} \begin{bmatrix} 0 \\ I_{m-1} \end{bmatrix} \\ 0 & \hat{h}^{(2)} & \\ 0 & 0 & \begin{bmatrix} 0 & I_m \end{bmatrix} \hat{H}_m^{(2)} \begin{bmatrix} 0 \\ I_{m-1} \end{bmatrix} \\ 0 & 0 & 0 \end{bmatrix},$$

with $z^{(1)} = \left(I_{m+1} - \hat{H}_m^{(1)}(\hat{H}_m^{(1)})^\dagger\right) e_1 / \left\| \left(I_{m+1} - \hat{H}_m^{(1)}(\hat{H}_m^{(1)})^\dagger\right) e_1 \right\|$ *and the vector* $\hat{h}^{(2)} = [\hat{h}_1^{(2)}, \ldots, \hat{h}_{m+2}^{(2)}]^T$ *having the entries*

$$\begin{bmatrix} \hat{h}_1^{(2)} \\ \vdots \\ \hat{h}_{m+1}^{(2)} \end{bmatrix} = \frac{1}{\zeta_{m+1}^{(1)}} \left(h_{1,1}^{(2)} z^{(1)} - \hat{H}_m^{(1)} \begin{bmatrix} \zeta_1^{(1)} \\ \vdots \\ \zeta_m^{(1)} \end{bmatrix} \right), \quad \hat{h}_{m+2}^{(2)} = \frac{h_{2,1}^{(2)}}{\zeta_{m+1}^{(1)}}.$$

2. Prescribed convergence for restarted GMRES

This result can be easily generalized for k restart cycles, as long as $k \cdot m < n$.

Theorem 5. *Let $A \in \mathbb{C}^{n\times n}$ be a matrix, $b \in \mathbb{C}^n$ be a nonzero vector and let for $k \cdot m < n$,*

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

be k unreduced upper Hessenberg matrices with positive subdiagonal. 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*

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

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

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

where

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

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

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 can prescribe not only GMRES residual norms, but also Ritz values and other values (singular values, harmonic Ritz values ...). For residual norms we obtain:

2. Prescribed convergence for restarted GMRES

Corollary. *The residual vectors for the kth restart cycle $r_0^{(k)}, \dots, r_m^{(k)}$ satisfy*

$$\|r_i^{(k)}\| = f(i),\ i = 0, \dots, m$$

if and only if the initial residual of the cycle has norm $f(0)$ and the generated Hessenberg matrix is of the form

$$\hat{H}_m^{(k)} = \begin{bmatrix} g_1^{(k)} & \dots & g_{m+1}^{(k)} \\ 0 & T_m^{(k)} & \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ I_m \end{bmatrix} \begin{bmatrix} g_1^{(k)} & \dots & g_m^{(k)} \\ 0 & T_{m-1}^{(k)} & \end{bmatrix} \in \mathbb{C}^{(m+1)\times m}$$

for a nonsingular upper triangular matrix $T_m^{(k)}$ of size m with leading principal submatrix $T_{m-1}^{(k)}$ of size $m-1$ and

$$g_1^{(k)} = \frac{1}{f(0)}, \qquad g_i^{(k)} = \frac{\sqrt{f(i-2)^2 - f(i-1)^2}}{f(i-2)f(i-1)}, \qquad i = 2, \dots, m.$$

2. Prescribed convergence 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,

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

we prescribe km residual norms and we put conditions on the first km columns of H only. The last column can be chosen arbitrarily. It can be checked, that any nonzero spectrum of A is possible with an appropriate choice of the last column.

Now we come to the case of stagnation at the end of the cycles. For the first two cycles, recall that the Hessenberg matrix $\hat{H}_m^{(2)}$ of the second cycle satisfies

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

and that for the entries of $z^{(1)}$ we have:

2. Prescribed convergence for restarted GMRES

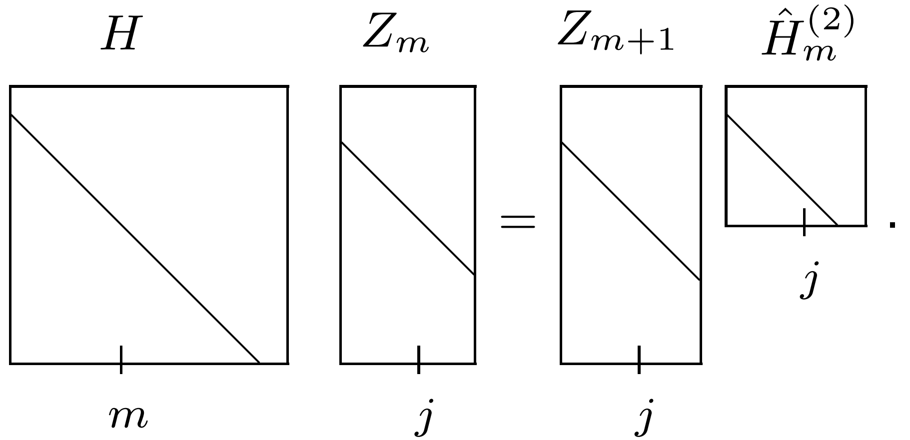
The last $j-1$ entries of $z^{(1)}$ are zero,

$$e_i^T z^{(1)} = 0, \qquad i = m+3-j, \ldots, m+1,$$

if and only if the last j residual norms of the first cycle are equal,

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

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



2. Prescribed convergence 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!

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

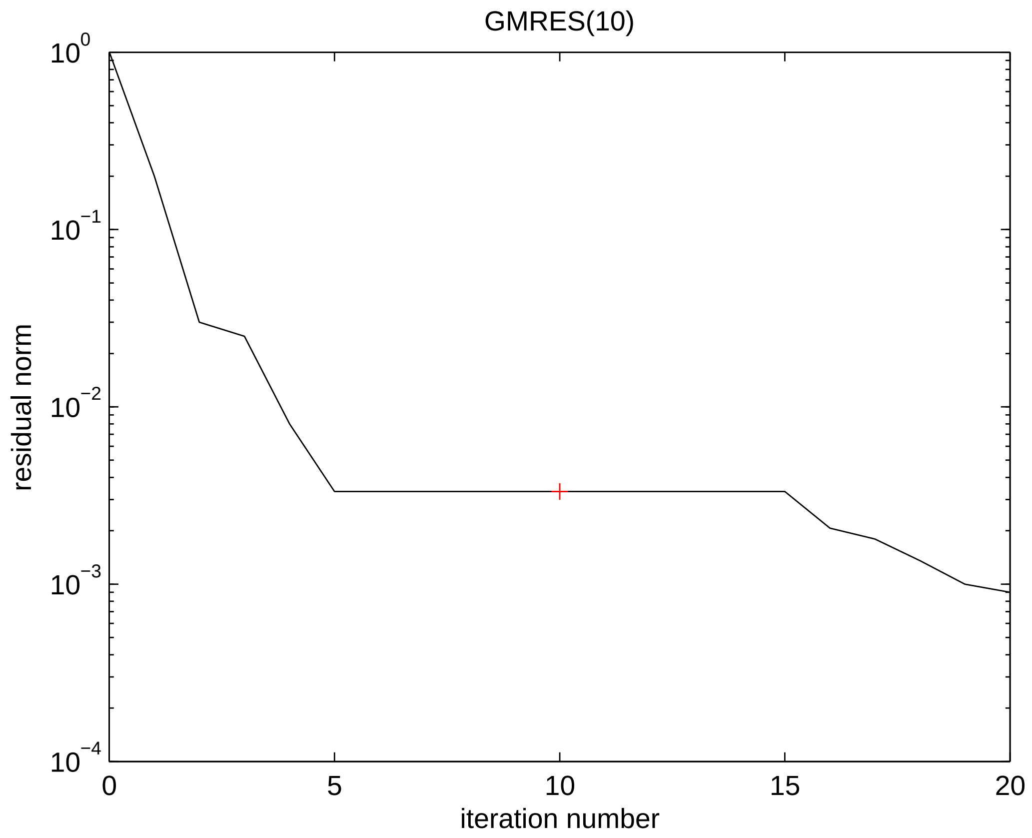
$$\|r_0^{(1)}\| \geq \|r_1^{(1)}\| \geq \cdots \geq \|r_{m-j}^{(1)}\| > \|r_{m-j+1}^{(1)}\| = \cdots = \|r_m^{(1)}\|$$

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!

2. Prescribed convergence for restarted GMRES



2. Prescribed convergence for restarted GMRES

Summarizing our results, under the assumption $km < n$, we showed that:

- Any non-increasing convergence curve is possible for restarted GMRES with any nonzero spectrum if there is no stagnation at the end of any cycle.

- With prescribed stagnation at the end of one cycle, we must prescribe stagnation at the beginning of the next cycle.

Future work includes:

- What can be said about the case $km \geq n$?

- Consequences for restarted Arnoldi (recall we can prescribe Ritz values instead of residual norms)

Thank you for your attention!

Supported by projects numbers M100301201 and IAA100300802 of the grant agency of the Academy of Sciences of the Czech Republic.