# On the convergence curves that can be generated by restarted GMRES

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joint work with

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# Outline

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- Let

$$U = \begin{bmatrix} & g^T & \\ 0 & T & \end{bmatrix}$$

# The parametrization for full GMRES

- To force the residual norm sequence $f(0) \geq \cdots \geq f(n-1) > 0$, the first row $g^T$ of $U$ has entries

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

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Prescribing residual norms in restarted GMRES was considered in the paper [Vecharinsky & Langou 2011].

# Results for restarted GMRES

The paper assumes a special situation in GMRES(m):

1. During every restart cycle, all residual norms stagnate except for the very last iteration inside the cycle.
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2. In this very last iteration it is assumed that the residual norm is strictly decreasing.

**Theorem 1** [Vecharinsky & Langou 2011]. *Let $k$ positive decreasing numbers*

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

*and $n$ complex nonzero numbers $\lambda_1, \ldots, \lambda_n$ be given. With the assumptions 1. and 2. above, let the very last residual at the end of the $j$th cycle be denoted by $\bar{r}_j$. If $km < n$, then:*

- 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

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

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

# Residual norms inside cycles

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- To generate in the $k$th cycle the residual norms

$$f^{(k)}(0) \geq \cdots \geq f^{(k)}(m),$$

we choose the $k$th Hessenberg matrix of dimension $(m+1) \times m$ is to be of the form

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

where

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

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The constructed matrices and right-hand sides will, as before, have the form

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After $m$ iterations of the initial cycle we wish to have the Arnoldi decomposition

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

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

The $m$ iterations of the second cycle should give the Arnoldi decomposition

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

# Comparison of the first two cycles

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

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

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**Lemma 1.** *If the initial cycle generates residual norms*

$$\|r_0^{(1)}\| \geq \|r_1^{(1)}\| \geq \cdots \geq \|r_m^{(1)}\|$$

*and we define*

$$g_0^{(1)} = 1/\|r_0^{(1)}\|^2, \quad g_i^{(1)} = \sqrt{\frac{1}{\|r_{i-1}^{(1)}\|^2} - \frac{1}{\|r_{i-2}^{(1)}\|^2}}, \quad g^{(1)} \equiv [g_0^{(1)}, \ldots, g_m^{(1)}]^T,$$

*then* $z^{(1)} = g^{(1)}$ *and* $g^{(1)} \perp \hat{H}_m^{(1)} e_i, \quad i = 1, \ldots, m.$

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Here is a relation between the small Hessenberg matrix $\hat{H}_m^{(2)}$ of the second cycle and the large Hessenberg matrix $H$ in the matrix $A = VHV^*$ which we construct:

# Comparison of the first two cycles

**Lemma 2.** *The matrix* $\hat{H}_m^{(2)}$ *is the Hessenberg matrix generated by* $m$ *iterations of the Arnoldi process with input* $H$ *and* $\left[\begin{array}{cc} g^{(1)T} & 0 \end{array}\right]^T$*:*

$$HZ_m = Z_{m+1}\hat{H}_m^{(2)}, \quad Z_{m+1}e_1 = \left[\begin{array}{c} g^{(1)} \\ 0 \end{array}\right], \quad Z_{m+1}^* Z_{m+1} = I_{m+1}. \quad (1)$$

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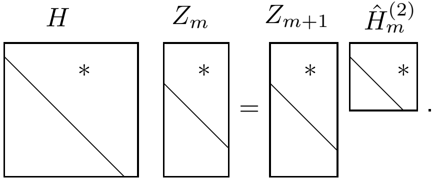
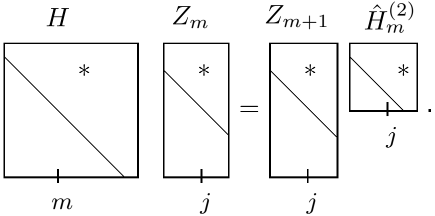
Can we construct the columns $m+1, m+2, \ldots, 2m$ of $H$ such that (1) is satisfied with a prescribed Hessenberg matrix $\hat{H}_m^{(2)}$ an "inverse" Arnoldi problem? This will depend on the number of trailing zeroes in $g^{(1)}$ because the Arnoldi decomposition has the structure



# Stagnation at the end of cycles

Because $g_i^{(1)} = \sqrt{\frac{1}{\|r_{i-1}^{(1)}\|^2} - \frac{1}{\|r_{i-2}^{(1)}\|^2}}$, with $j$ stagnation steps at the end of the first restart cycle, the trailing $j$ entries of $g^{(1)}$, are zero.

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




The first $j$ columns of the Hessenberg matrix of the second cycle $\hat{H}_m^{(2)}$ are fully determined by $\hat{H}_m^{(1)}$ and $g^{(1)}$ - they cannot be prescribed.

# Stagnation at the end of cycles

**Lemma 3** *If the last $j$ residual norms stagnate in the initial cycle, i.e.*

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

*then the first row of $\hat{H}_m^{(2)}$ is zero on positions one till $j$.* Proof: For $i < j$,

$$\begin{aligned} e_1^T \begin{bmatrix} \hat{H}_m^{(2)} \\ 0 \end{bmatrix} e_i &= e_1^T \begin{bmatrix} Z_{m+1}^* H Z_m \\ 0 \end{bmatrix} e_i \\ &= \begin{bmatrix} {g^{(1)}}^* & 0 \end{bmatrix} H Z_m e_i = {g^{(1)}}^* \hat{H}_m^{(1)} \begin{bmatrix} Z_m e_i \\ 0 \end{bmatrix} = 0. \end{aligned}$$

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

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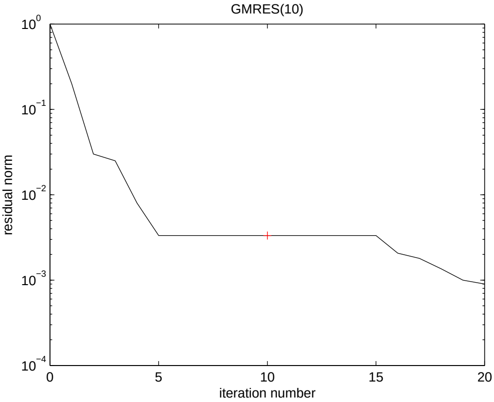
*then the first $j$ residual norms stagnate in the second cycle,*

$$\|r_0^{(2)}\| = \|r_1^{(2)}\| = \cdots = \|r_j^{(2)}\|.$$

# Stagnation at the end of cycles

Hence stagnation in one cycle is literally mirrored in the next cycle and we cannot prescribe any residual norm history!



# Prescribed Hessenberg matrices in GMRES(m)

If we assume no restart cycles stagnate in their last iterations, we can try to solve the "inverse" Arnoldi problem:

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

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This can be done in many ways, depending on the choice of columns of $Z_{m+1}$ (the Arnoldi vectors). Let us consider the most straightforward, "canonical" choice

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Equating the subsequent columns in $HZ_m = Z_{m+1}\hat{H}_m^{(2)}$ gives explicit values for columns $m+1$ till $2m$ of $H$ and leads to:

# Prescribed Hessenberg matrices in GMRES(m)

**Theorem 2** **[DT & Meurant 2014?]** *Let $A \in \mathbb{C}^{n \times n}$ and $b \in \mathbb{C}^n$ and let for $km < n$,*

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

*be $k$ given unreduced upper Hessenberg matrices with positive subdiagonal and nonsingular leading $m \times m$ principal submatrix. Then the $k$th cycle of GMRES(m) applied to $A$ and $b$ generates the Hessenberg matrix*

$$\hat{H}_m^{(k)}$$

*if*

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

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

# Prescribed Hessenberg matrices in GMRES(m)

$$H\left[e_{(k-1)m+1},\ldots,e_{km}\right]=\begin{bmatrix} & \gamma^{(1)}g^{(1)}\hat{h}^T_{(k)} \\ & \vdots \\ \vdots & \\ & \gamma^{(k-1)}g^{(k-1)}\hat{h}^T_{(k)} \\ t^{(k)} & g^{(k)}\hat{h}^T_{(k)} \\ 0 & \begin{bmatrix} 0 & I_m \end{bmatrix}\hat{H}^{(k)}_m\begin{bmatrix} 0 \\ I_{m-1}\end{bmatrix} \\ 0 & 0 \end{bmatrix},\quad \textit{where}$$

$$\hat{h}^T_{(k)}=e_1^T\hat{H}^{(k)}_m\begin{bmatrix} 0 \\ I_{m-1}\end{bmatrix},\quad \gamma^{(\ell)}=\left(\prod_{i=\ell+1}^{k-1} g_1^{(i-1)}\right)\quad \text{and}$$

$$t^{(k)}=\frac{1}{\zeta^{(k-1)}_{m+1}}\left[(h^{(k)}_{1,1}z^{(k-1)}-\hat{H}^{(k-1)}_m[\zeta^{(k-1)}_1,\ldots,\zeta^{(k-1)}_m]^T),h^{(k)}_{2,1}\right]^T.$$

# Prescribed Hessenberg matrices in GMRES(m)

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, but also Ritz values and possibly other values (singular values [Ernst & Eiermann 2001], harmonic Ritz values, etc. ...).

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**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

# Other constructions

- We constructed matrices and right-hand sides yielding a sequence of prescribed Hessenberg matrices if the GMRES process is restarted.
- The construction found the entries of $H$ using the "canonical" choice

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- Other choices lead to different parametrizations, e.g.

$$\tilde{H} = \begin{bmatrix} I_{m+1} & \hat{H}_m^{(1)} S_0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & I_{n-2m-1} \end{bmatrix}^{-1} H \begin{bmatrix} I_{m+1} & \hat{H}_m^{(1)} S_0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & I_{n-2m-1} \end{bmatrix}$$

where $S_1$ is nonsingular upper triangular such that $S_1^* S_1 - I_m$ is positive definite and $S_0$ satisfies $(\hat{H}_m^{(1)} S_0)^* \hat{H}_m^{(1)} S_0 = S_1^* S_1 - I_m$.

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This means the linear systems in Theorem 2 represent the optimal situation for GMRES(m), where restarting is as efficient as running full GMRES.

# Relation with full GMRES

- All constructions give the same behavior of GMRES(m) (it generates the same small Hessenberg matrices)
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This means the linear systems in Theorem 2 represent the optimal situation for GMRES(m), where restarting is as efficient as running full GMRES.
Equivalently, we constructed systems where full GMRES can be computed with short recurrences ...

# Relation with full GMRES

The linear systems in Theorem 2 also enable to construct situations where GMRES(m) converges faster than GMRES(m+i) for some $i > 0$:

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Example: We construct a linear system with

$$A \in \mathbb{R}^{16\times 16}, \quad b \in \mathbb{R}^{16}$$

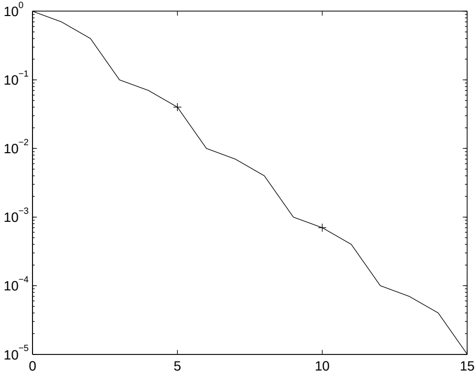
such that GMRES(5) generates the prescribed residual norms

$$\left[\|r_0^{(1)}\|, \|r_1^{(1)}\|, \dots, \|r_5^{(1)}\|\right] = [1, 0.7, 0.4, 0.1, 0.07, 0.04]$$

$$\left[\|r_0^{(2)}\|, \|r_1^{(2)}\|, \dots, \|r_5^{(2)}\|\right] = [0.04, 0.01, 0.007, 0.004, 0.001]$$

$$\left[\|r_0^{(3)}\|, \|r_1^{(3)}\|, \dots, \|r_5^{(3)}\|\right] = [0.001, 7 \cdot 10^{-4}, 4 \cdot 10^{-4}, 10^{-4}, 7 \cdot 10^{-5}]$$

# Example



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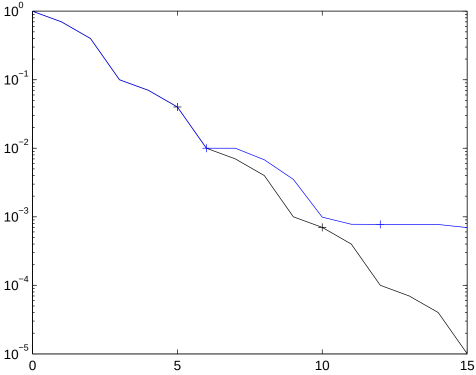

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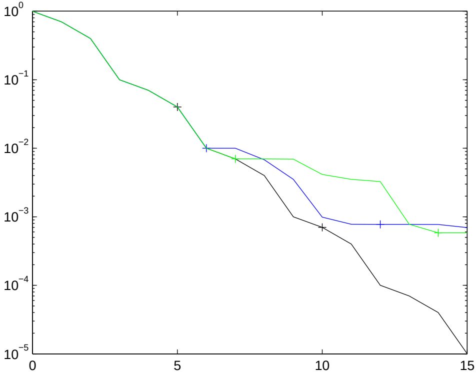

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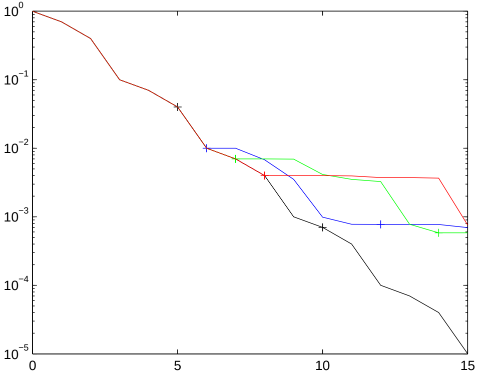

# Outline

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  - Can the sufficiency of shorter restart parameters be detected during the GMRES(m) process ?
  - What can be said for GMRES(m) after iteration number $n$ ?

**Thank you for your attention!**

# 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.]
- E. Vecharinsky and J. Langou, [ Any admissible cycle-convergence behavior is possible for restarted GMRES at its initial cycles, 18 (2011), Num. Lin. Alg. Appl., pp. 499?-511. ]
- 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, 65 (2014), pp. 69–90. ]
- J. Duintjer Tebbens, G. Meurant, H. Sadok and Z. Strakoš, [ On Investigating GMRES Convergence Using Unitary Matrices , 450 (2014), Lin. Alg. Appl., pp. 83–107. ]