Implicitly restarting GMRES and FOM

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February 21, 2016

Abstract

GMRES and FOM are well-known Krylov subspace methods for approximately solving linear systems $Ax = b$. To mitigate the increasing computational complexity and storage costs, these methods are usually repeatedly restarted. However, in an ordinary restart spectral data is dismissed, which can be valuable to improve the speed of convergence. In this article the convergence behaviour is analyzed, and subsequently it is shown how spectral data can be used to implicitly restart GMRES and FOM using the IRAM procedure. Real-life examples are given to confirm the potential of these methods.

1 Krylov subspace methods

In this paper we are interested in solving the linear system

$$A\boldsymbol{x} = \boldsymbol{b}, \tag{1}$$

for $\boldsymbol{x}, \boldsymbol{b} \in \mathbb{C}^n$ and $A \in \mathbb{C}^{n \times n}$ nonsingular. Subspace methods solve Equation (1) approximately by imposing two conditions: $\boldsymbol{x}$ must be extracted from a *search subspace* $\mathcal{V} \subset \mathbb{C}^n$, while its residual $\boldsymbol{b} - A\boldsymbol{x}$ must be perpendicular to a *test subspace* $\mathcal{W} \subset \mathbb{C}^n$. A popular choice for these subspaces is the *Krylov subspace induced by A and $\boldsymbol{b}$ of order k*, which is defined by

$$\mathcal{K}_k(A, \boldsymbol{b}) = \operatorname{span}\{\boldsymbol{b}, A\boldsymbol{b}, A^2\boldsymbol{b}, \ldots, A^{k-1}\boldsymbol{b}\}.$$

Different choices for the search and test subspaces lead to different methods. In this article we study FOM and GMRES, the former imposing the

Galerkin condition $\mathcal{V} = \mathcal{W} = \mathcal{K}_k(A, \boldsymbol{b})$ and the latter imposing the Petrov-Galerkin condition $\mathcal{V} = \mathcal{K}_k(A, \boldsymbol{b})$ while $\mathcal{W} = A\mathcal{K}_k(A, \boldsymbol{b})$.

The order k is iteratively enlarged, and clearly when k gets so large that the Krylov subspace becomes A-invariant, the exact solution to Equation (1) is part of the search subspace. In our analysis we will therefore assume that the dimension of $\mathcal{K}_k(A, \boldsymbol{b})$ always equals k.

As a preliminary note, often an initial guess $\boldsymbol{x}_0$ for Equation (1) is given, so that in practice one often solves the error equation

$$A\boldsymbol{e} = A(\boldsymbol{x} - \boldsymbol{x}_0) = \boldsymbol{b} - A\boldsymbol{x}_0 = \boldsymbol{r}_0 \quad \text{and } \boldsymbol{x} = \boldsymbol{x}_0 + \boldsymbol{e}$$

is approximately solved for $\boldsymbol{e} \in \mathcal{K}_k(A, \boldsymbol{r}_0)$.

1.1 Arnoldi method

A basis for the Krylov subspace $\mathcal{K}_k(A, \boldsymbol{b})$ as given by $\{\boldsymbol{b}, A\boldsymbol{b}, \ldots, A^{k-1}\boldsymbol{b}\}$ is numerically unstable, since the sequence converges to the eigenvector corresponding to the eigenvalue of largest absolute magnitude. Therefore, the vectors will become linearly depedent in finite precision. A more stable alternative is provided by the Arnoldi method, which builds an orthonormal basis for the Krylov subspace. In this section we will not go into detail about the method and implementation itself, but we will stress the relation between Hessenberg matrices and Krylov subspaces through the Arnoldi relation.

Definition 1. *A Hessenberg matrix H is a matrix for which if $H_{ij} = 0$ for all $i > j + 1$.*

Definition 2. *A Hessenberg matrix H is* **unreduced** *if $H_{i+1,i} \neq 0$ for all i.*

Theorem 1. *Given an $n \times k$ orthonormal matrix V_k and a $(k+1) \times k$ matrix $\underline{H}_k$ such that $AV_k = V_{k+1}\underline{H}_k$, then $\underline{H}_k$ is an unreduced Hessenberg matrix $\iff$ $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\}$ is a basis for $\mathcal{K}_k(A, \boldsymbol{v}_1)$, with $\boldsymbol{v}_i$ the ith column of V_k*

Proof. First we prove ($\Rightarrow$): for $k = 1$ we have the relation $A\boldsymbol{v}_1 = h_{11}\boldsymbol{v}_1 + h_{21}\boldsymbol{v}_2$ with $h_{21} \neq 0$, therefore $\boldsymbol{v}_2 \in \mathcal{K}_2(A, \boldsymbol{v}_1)$ and $\boldsymbol{v}_2 \notin \mathcal{K}_1(A, \boldsymbol{v}_1)$. Suppose $\boldsymbol{v}_i \in \mathcal{K}_i(A, \boldsymbol{v}_1)$ and $\boldsymbol{v}_i \notin \mathcal{K}_{i-1}(A, \boldsymbol{v}_1)$, then $\boldsymbol{v}_i = \alpha A^{i-1}\boldsymbol{v}_1 + \boldsymbol{y}$ with $\alpha \neq 0$ and $\boldsymbol{y} \in \mathcal{K}_{i-1}(A, \boldsymbol{v}_1)$. The Arnoldi relation dictates $A\boldsymbol{v}_i = \sum_{j=1}^{i} h_{ji}\boldsymbol{v}_j + h_{i+1,i}\boldsymbol{v}_{i+1}$ with $h_{i+1,i} \neq 0$ and hence $\boldsymbol{v}_{i+1} = \alpha A^i \boldsymbol{v}_1 + A\boldsymbol{y} \in \mathcal{K}_{i+1}(A, \boldsymbol{v}_1)$ and $\boldsymbol{v}_{i+1} \notin \mathcal{K}_i(A, \boldsymbol{v}_0)$. Hence by induction $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\}$ forms a basis for $\mathcal{K}_k(A, \boldsymbol{v}_1)$.

The prove for ($\Leftarrow$) is by construction and defines theoretically the Arnoldi method, so we will not show the details.

□

From time to time it is more convenient to express the *Arnoldi relation* $AV_k = V_{k+1}\underline{H}_k$, by defining $\eta = h_{k+1,k}$ and the matrix H_k as the $k \times k$ upper block of $\underline{H}_k$:

$$\underline{H}_k = \begin{bmatrix} H_k \\ \eta \boldsymbol{e}_k^* \end{bmatrix},$$

with $\boldsymbol{e}_k$ the kth standard basis vector. Then we can also write

$$AV_k = V_k H_k + \eta \boldsymbol{v}_{k+1} \boldsymbol{e}_k^*.$$

2 GMRES and FOM

GMRES and FOM use the Arnoldi method to find an orthonormal basis for a relatively low-dimensional Krylov subspace and exploit the structure of the Hessenberg matrix of the Arnoldi relation to efficiently extract solutions from it.

Let the superscript F correspond to approximate solution of FOM. The Galerkin condition of FOM implies that

$$\begin{aligned} \boldsymbol{r}_0 - A\boldsymbol{x}^F \perp \mathcal{K}_k(A, \boldsymbol{r}_0) \quad & \text{where } \boldsymbol{x}^F \in \mathcal{K}_k(A, \boldsymbol{r}_0) = \mathcal{R}(V_k) \\ \iff V_k^*(\boldsymbol{r}_0 - AV_k\boldsymbol{y}^F) = 0 \quad & \text{with } \boldsymbol{x}^F = V_k\boldsymbol{y}^F. \end{aligned}$$

Note that the Arnoldi relation implies $V_k^* A V_k = H_k$ and that $\boldsymbol{r}_0$ is a multiple of the first column of V_k. Hence the FOM problem reduces to solving

$$H_k \boldsymbol{y}^F = \beta \boldsymbol{e}_1 \quad \text{with } \beta = \|\boldsymbol{r}_0\|_2 . \tag{2}$$

GMRES follows the same line of reasoning, but with the test space being $A\mathcal{K}_k(A, \boldsymbol{r}_0) = \mathcal{R}(AV_k) = \mathcal{R}(V_{k+1}\underline{H}_k)$ and with the superscript G:

$$\begin{aligned} & \boldsymbol{r}_0 - A\boldsymbol{x}^G \perp \mathcal{K}_k(A, \boldsymbol{r}_0) \quad \text{where } \boldsymbol{x}^G \in \mathcal{K}_k(A, \boldsymbol{r}_0) = \mathcal{R}(V_k) \\ & \iff \underline{H}_k^* V_{k+1}^* (\boldsymbol{r}_0 - AV_k\boldsymbol{y}^G) = 0 \quad \text{with } \boldsymbol{x}^G = V_k\boldsymbol{y}^G \\ & \iff \underline{H}_k^* (\beta\boldsymbol{e}_1 - \underline{H}_k\boldsymbol{y}^G) = 0 \\ & \iff \beta\boldsymbol{e}_1 - \underline{H}_k\boldsymbol{y}^G \perp \mathcal{R}(\underline{H}_k). \end{aligned} \tag{3}$$

But Equation (3) is the normal equation, which shows that the low-dimensional GMRES problem is given by solving:

$$\underline{H}_k \boldsymbol{y}^G = \beta \boldsymbol{e}_1 \quad \text{(in least-squares sense)}. \tag{4}$$

This is equivalent to minimizing the residual norm, and also explains the name of GMRES:

$$\min_{\boldsymbol{y}^G} \left\| \beta \boldsymbol{e}_1 - \underline{H}_k \boldsymbol{y}^G \right\|_2 = \min_{\boldsymbol{y}^G} \left\| V_{k+1}(\beta \boldsymbol{e}_1 - \underline{H}_k \boldsymbol{y}^G) \right\|_2 = \min_{\boldsymbol{x}^G \in \mathcal{K}(A, \boldsymbol{r}_0)} \left\| \boldsymbol{r}_0 - A\boldsymbol{x}^G \right\|_2 .$$

Equations (2) and (4) more or less define the FOM and GMRES algorithm: solve these problems at each Arnoldi iteration and stop if satisfied. However, a few improvements can be made.

Theorem 2. *Let $\underline{H}_k$ be unreduced. For every k, there exists a unique $\vec{\boldsymbol{\gamma}}_{k+1} \in N(\underline{H}_k^*)$ such that $\gamma_1 = 1$; and there exists a scalar γ_{k+2} such that $\vec{\boldsymbol{\gamma}}_{k+2} \equiv \begin{bmatrix} \vec{\boldsymbol{\gamma}}_{k+1} \\ \gamma_{k+2} \end{bmatrix} \in N(\underline{H}_{k+1}^*)$.*

Proof. Clearly $\dim N(\underline{H}_k^*) = 1$ as it is upper triangular with an additional column, which shows $\vec{\boldsymbol{\gamma}}_{k+1}$ exists and is unique if $\gamma_1 = 1$. Furthermore, if $\vec{\boldsymbol{\gamma}}_{k+1} \in N(\underline{H}_k^*)$, then due to the Hessenberg structure, it follows that

$$\underline{H}_{k+1}^* \begin{bmatrix} \vec{\boldsymbol{\gamma}}_{k+1} \\ \gamma_{k+2} \end{bmatrix} = \begin{bmatrix} \vec{\boldsymbol{0}} \\ \bar{h}_{1k}\gamma_1 + \cdots + \bar{h}_{kk}\gamma_k + \bar{\eta}\gamma_{k+1} \end{bmatrix}$$

and therefore we set $\gamma_{k+1} \equiv -\frac{1}{\bar{\eta}}(\bar{h}_{1k}\gamma_1 + \cdots + \bar{h}_{kk}\gamma_k)$, which proves the theorem. □

Theorem 2 gives us a tool to determine the GMRES and FOM residual at each Arnoldi iteration, without the need to solve the low-dimensional problems each time. The last equivalence of Equation (3) shows that the GMRES residual $\beta \boldsymbol{e}_1 - \underline{H}_k \boldsymbol{y}^G \in \mathcal{R}(\underline{H}_k)^\perp = N(\underline{H}_k^*)$, so that by Theorem 2 it follows

$$\beta \boldsymbol{e}_1 - \underline{H}_k \boldsymbol{y}^G = \tau \vec{\boldsymbol{\gamma}}_{k+1} \text{ for some } \tau \in \mathbb{C} \tag{5}$$

Multiplying from the left with $\vec{\boldsymbol{\gamma}}_{k+1}^*$ gives us

$$|\beta| = |\tau| \left\| \vec{\boldsymbol{\gamma}}_{k+1} \right\|_2^2, \tag{6}$$

and by taking norms on both sides of Equation (5) and combining the result with Equation (6), the find the follow residual norm of GMRES:

$$\left\|\beta \boldsymbol{e}_1 - \underline{H}_k \boldsymbol{y}^G\right\|_2 = \frac{|\beta|}{\left\|\vec{\boldsymbol{\gamma}}_{k+1}\right\|_2}.$$

Similarly for FOM, we have with y_k^F the kth element of $\boldsymbol{y}^F$

$$\beta \boldsymbol{e}_1 - \underline{H}_k \boldsymbol{y}^F = -\boldsymbol{e}_{k+1} \eta y_k^F \tag{7}$$

since the first k rows contain only zeros. By pre-multiplying with $\vec{\boldsymbol{\gamma}}_{k+1}^*$, we get $\beta = -\bar{\gamma}_{k+1} \eta y_k^F$. Plugging this into Equation (7) and taking norms yields the FOM residual norm as

$$\left\|\beta \boldsymbol{e}_1 - \underline{H}_k \boldsymbol{y}^F\right\|_2 = \frac{|\beta|}{|\gamma_{k+1}|}.$$

Usually we are mostly interested in reducing the relative residual norm $\|\boldsymbol{r}_k\|_2 / \|\boldsymbol{r}_0\|_2$, since an absolute measure is somewhat arbitrary. In that case we can even inspect just $1/\left\|\vec{\boldsymbol{\gamma}}_{k+1}\right\|_2$ for GMRES and $1/|\gamma_{k+1}|$ for FOM.

The final procedures for GMRES and FOM are given in Algorithm 1.

3 Convergence behaviour of FOM and GMRES

Due to the relation between the residuals of GMRES and FOM through the null-space vector $\vec{\boldsymbol{\gamma}}_{k+1}$, it is enough to investigate the convergence behaviour one of the two. However, a more careful study of both GMRES and FOM provides key notions for implicit restarting strategies treated later.

Since the search subspace is $\mathcal{K}_k(A, \boldsymbol{r}_0)$ for both FOM and GMRES, one can express the approximate solution at iteration k as a product of a polynomial q_{k-1} of maximal degree $k-1$ in A and the initial residual $\boldsymbol{r}_0$:

$$\boldsymbol{x}_k = q_{k-1}(A)\boldsymbol{r}_0.$$

Note that the residual at iteration k is therefore a polynomial p_k of maximal degree k:

$$\boldsymbol{r}_k \equiv \boldsymbol{r}_0 - A\boldsymbol{x}_k = (I - Aq_{k-1}(A))\boldsymbol{r}_0 = p_k(A)\boldsymbol{r}_0$$

with the condition that $p_k(0) = 1$. This polynomial is defined as the *residual polynomial* or *FOM/GMRES polynomial*. Clearly every trivial residual polynomial satisfies the the test space criterion, but we will assume that at least

Algorithm 1 GMRES and FOM. The procedure $\textsc{Orth}(A\boldsymbol{v}_k, V_k)$ performs an Arnoldi step, returning an orthonormal vector $\boldsymbol{v}_{k+1} \perp V_k$ and a new column $\boldsymbol{h}_k$ of the Hessenberg matrix.

Input: $A \in \mathbb{R}^{n\times n}$, $\boldsymbol{b} \in \mathbb{R}^{n\times 1}$, $\boldsymbol{x}_0 \in \mathbb{R}^{n\times 1}$ (initial guess), tolerance tol
Output: approximate solution $\boldsymbol{x}_k$
$\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$
$\beta = \|\boldsymbol{r}_0\|_2$
$\boldsymbol{v}_1 = \boldsymbol{r}_0/\beta$
$\gamma_1 = 1$
▷ GMRES or FOM respectively
for $k = 1, 2, \ldots, n$ **while** $\beta/\left\|\boldsymbol{\gamma}_{k+1}\right\|_2 < tol$ **or** $\beta/|\gamma_{k+1}| < tol$ **do**
  $[\boldsymbol{v}_{k+1}, \boldsymbol{h}_k] \leftarrow \textsc{Orth}(A\boldsymbol{v}_k, V_k)$
  $\gamma_{k+1} \equiv -(\bar{h}_{1k}\gamma_1 + \cdots + \bar{h}_{kk}\gamma_k)/\bar{h}_{k+1,k}$
end for
Solve $\boldsymbol{y}^G = \arg\min_{\boldsymbol{y}} \|\beta\boldsymbol{e}_1 - \underline{H}_k\boldsymbol{y}\|_2$ ▷ GMRES
$\boldsymbol{x}_k \equiv \boldsymbol{x}_0 + V_k\boldsymbol{y}^G$
Solve $H_k\boldsymbol{y}^F = \beta\boldsymbol{e}_1$ ▷ FOM
$\boldsymbol{x}_k \equiv \boldsymbol{x}_0 + V_k\boldsymbol{y}^F$

some progress is made in the sense that the residual polynomial is non-trivial. Later we will see that this implies that it has strict degree k.

For further analysis, suppose for the sake of the argument that A is diagonalizable such that $A = X\Lambda X^{-1}$ with $\Lambda_{ii} = \lambda_i$ the eigenvalues of A. Then we have that

$$\|\boldsymbol{r}_k\|_2 = \|p_k(A)\boldsymbol{r}_0\|_2 \leq \|X\|_2 \left\|X^{-1}\right\|_2 \|p_k(\Lambda)\|_2 \|\boldsymbol{r}_0\|_2$$

and by defining the condition number of X as $C(X) = \|X\|_2 \|X^{-1}\|_2$ we get

$$\frac{\|\boldsymbol{r}_k\|_2}{\|\boldsymbol{r}_0\|_2} \leq C(X) \min_{\substack{deg(p_k)=k \\ p_k(0)=1}} \max_{\lambda_i} |p_k(\lambda_i)|.$$

If A is close to normal in the sense that $C(X)$ is close to 1, one can see that the speed of convergence may largely depend on the eigenvalue distribution of A. Also note that when A has an eigenvalue close to 0, it might be particularly hard to find a low degree polynomial such that $p_k(0) = 1$ while $|p(\lambda_i)|$ is small for all i.

To be more precise, it is crucial to investigate the zeros of the residual polynomial for both GMRES and FOM. To this end we introduce (harmonic) Ritz pairs and subsequently show that these and only these form the zeros for respectively GMRES and FOM.

Definition 3. *A pair $(\theta, \boldsymbol{y})$ with $\theta \in \mathbb{C}$ and $\boldsymbol{y} \in \mathbb{C}^n$ not trivial is a Ritz pair of A with respect to $\mathcal{K}_k(A, \boldsymbol{v}_1)$ if $A\boldsymbol{y} - \theta\boldsymbol{y} \perp \mathcal{K}_k(A, \boldsymbol{v}_1)$. If $A\boldsymbol{y} - \theta\boldsymbol{y} \perp A\mathcal{K}_k(A, \boldsymbol{v}_1)$, then $(\theta, \boldsymbol{y})$ is a harmonic Ritz pair.*

Hence ordinary Ritz pairs are solutions to the eigenproblem under the same Galerkin condition as FOM imposes, while harmonic Ritz pairs are solutions to the eigenproblem under the Petrov-Galerkin condition of GMRES.

Theorem 3. *Let $AV_k = V_{k+1}\underline{H}_k$ be the Arnoldi relation. Then $H_k\boldsymbol{y} = \theta\boldsymbol{y}$ $\iff$ $(\theta, V_k\boldsymbol{y})$ is a Ritz pair of A with respect to $\mathcal{K}_k(A, \boldsymbol{v}_1)$.*

Proof. The result follows by working out the Galerkin condition. □

Theorem 4. *Under the same conditions as Theorem 3. Then $(\theta, V_k\boldsymbol{y})$ is a harmonic Ritz pair of A $\iff$ $(\theta, \boldsymbol{y})$ is a solution to the generalized eigenvalue problem*

$$(H_k^* H_k + |\eta|^2 \boldsymbol{e}_k \boldsymbol{e}_k^*)\boldsymbol{y} = \theta H_k^* \boldsymbol{y}$$

Hence, if H_k^* is invertible, $(\theta, \boldsymbol{y})$ is an eigenpair of $H_k + |\eta|^2 \boldsymbol{f}_k \boldsymbol{e}_k^*$ with $\boldsymbol{f}_k = H_k^{-*}\boldsymbol{e}_k$.[1]

Proof. The results follow by straight-forwardly working out the Petrov-Galerkin condition and noting that $\underline{H}_k^*\underline{H}_k = H_k^* H_k + |\eta|^2 \boldsymbol{e}_k \boldsymbol{e}_k^*$. □

For now we will assume that H_k is invertible, so that the harmonic Ritz values can be obtained from solving an ordinary eigenvalue problem. At the end of this section we will briefly discuss the validity of this assumption.

Now we first prove a lemma which is a tool for showing that the zeros of the GMRES and FOM residual polynomial are indeed respectively the harmonic Ritz and ordinary Ritz values.

Lemma 1. *Let p be a monic non-trivial polynomial and H an unreduced $k \times k$ Hessenberg matrix. Then the following statements are equivalent*

[1] A more efficient way to determine the harmonic Ritz values, when one already constructs the null-space vector $\boldsymbol{\gamma}_{k+1}$ is given through $H_k + |\eta|^2 \boldsymbol{f}_k \boldsymbol{e}_k^* = H_k - \frac{\eta}{\gamma_{k+1}} \vec{\boldsymbol{\gamma}}_k \boldsymbol{e}_k^*$

1. $p(H)\boldsymbol{e}_1 = \vec{\mathbf{0}}$
2. *p is the (unique) minimal polynomial of H.*
3. $p^{(j)}(\theta) = 0$ *for all* $\theta \in \sigma(H)$ *and* $j < \mu_H(\theta)$ *with* $\mu_H(\theta)$ *the algebraic multiplicity of* θ

Proof. We will show this briefly. Since H is unreduced, it follows inductively that $H^r_{ij} = 0$ if $i > j+r$ while $H^r_{j+r,j} \neq 0$. Hence the set $\{\boldsymbol{e}_1, H\boldsymbol{e}_1, \ldots, H^{k-1}\boldsymbol{e}_1\}$ is linearly independent and forms a basis for $\mathbb{C}^k = \mathcal{K}_k(H, \boldsymbol{e}_1)$. Therefore $H^k\boldsymbol{e}_1$ can be uniquely written as a linear combination of these basis vectors:

$$H^k\boldsymbol{e}_1 = p_{k-1}(H)\boldsymbol{e}_1$$

with p_{k-1} a polynomial of strict degree $k-1$. Hence $p(H) = H^k - p_{k-1}(H)$ is the unique, non-trivial, monic polynomial of lowest degree for which $p(H)\boldsymbol{e}_1 = \vec{\mathbf{0}}$. Notice that this implies that the minimal polynomial of H has at least degree k. By the Cayleigh-Hamilton theorem it follows that every matrix satisifies its characteristic equation. The characteristic equation is of degree k and by uniqueness of p up to scaling, it must therefore follow that p is the characteristic polynomial of H so that $p(H) = O$ and $p^{(j)}(\theta) = 0$ for all eigenvalues θ of H and $j < m(\theta)$. As a consequence, p must be the minimal polynomial of H as well. □

Lemma 2. *For $j < k$ it holds that $A^jV_k\boldsymbol{e}_1 = V_kH_k^j\boldsymbol{e}_1$*

Proof. Note that $AV_k = (V_kH_k + \eta\boldsymbol{v}_{k+1}\boldsymbol{e}_k^*)$ so that the claim is clearly true for $j = 1$. Suppose $A^{i-1}V_k\boldsymbol{e}_1 = V_kH_k^{i-1}\boldsymbol{e}_1$, then

$$A^iV_k\boldsymbol{e}_1 = V_kH_k^i\boldsymbol{e}_1 + \eta\boldsymbol{v}_{k+1}\boldsymbol{e}_k^*H_k^{i-1}\boldsymbol{e}_1$$

but $\boldsymbol{e}_k^*H_k^{i-1}\boldsymbol{e}_1 = 0$ whenever $i < k$, by using a result from the proof of Lemma 1. □

Theorem 5. *Let θ_i denote the ith Ritz value of A with respect to the Krylov subspace $\mathcal{K}_k(A, \boldsymbol{v}_1)$ of dimension k and let $\mu(\theta_i)$ be the algebraic multiplicity of θ_i. Let p be a polynomial of strict degree k. Then following statements are equivalent:*

- $p(A)\boldsymbol{v}_1 \perp \mathcal{K}_k(A, \boldsymbol{v}_1)$
- $p^{(j)}(\theta_i) = 0$ *for all i and $j < \mu(\theta_i)$*

Proof. Since the polynomial is of degree k, we must treat the last term with care when using Lemma 2. We have

$$V_k^* A^k V_k \boldsymbol{e}_1 = \begin{bmatrix} I \\ \vec{\mathbf{0}}^* \end{bmatrix} \underline{H}_k H_k^{k-1} \boldsymbol{e}_1 = H_k^k \boldsymbol{e}_1$$

and hence by applying Lemma 2 to each term of the polynomial it follows $V_k^* p(A) V_k \boldsymbol{e}_1 = \vec{\mathbf{0}} \iff p(H_k)\boldsymbol{e}_1 = \vec{\mathbf{0}}$. Hence, from Lemma 1 the statement of the theorem follows. □

Theorem 6. *Similarly as in Theorem 5, let θ_i denote the ith harmonic Ritz value of A with respect to $\mathcal{K}_k(A, \boldsymbol{v}_1)$ and let $\mu(\theta_i)$ be its algebraic multiplicity. Let p be a polynomial of strict degree k. Then following statements are equivalent:*

- $p(A)\boldsymbol{v}_1 \perp \mathcal{K}_k(A, \boldsymbol{v}_1)$
- $p^{(j)}(\theta_i) = 0$ *for all* i *and* $j < \mu(\theta_i)$

Proof. Let $p(z) = \sum_{i=0}^{k} \alpha_i z^i$ define the coefficients of p. Note that for $i < k$ we have

$$\underline{H}_k^* V_{k+1}^* A^i V_k \boldsymbol{e}_1 = \underline{H}_k^* V_{k+1}^* V_k H_k^i \boldsymbol{e}_1 = H_k^* H_k^i \boldsymbol{e}_1$$

by application of Lemma 2. Furthermore, it is easy to show that

$$H_k^i \boldsymbol{e}_1 = (H_k + \boldsymbol{w}\boldsymbol{e}_k^*)^i \boldsymbol{e}_1$$

for any k-vector $\boldsymbol{w}$. This gives us all the ingredients to prove the theorem, as the condition $p(A)\boldsymbol{v}_1 \perp A\mathcal{K}_k(A, \boldsymbol{v}_1)$ is equivalent to all the following equations:

$$\begin{aligned} \underline{H}_k^* V_{k+1}^* p(A) V_k \boldsymbol{e}_1 &= \vec{\mathbf{0}}, \\ H_k^* \sum_{i=0}^{k-1} \alpha_i H_k^i \boldsymbol{e}_1 + \alpha_k (H_k^* H_k + |\eta|^2 \boldsymbol{e}_k \boldsymbol{e}_k^*) H_k^{k-1} \boldsymbol{e}_1 &= \vec{\mathbf{0}}, \\ \sum_{i=0}^{k} \alpha_i (H_k + |\eta|^2 H_k^{-*} \boldsymbol{e}_k \boldsymbol{e}_k^*)^i \boldsymbol{e}_1 &= \vec{\mathbf{0}}. \end{aligned}$$

Let $\boldsymbol{f}_k = H_k^{-*} \boldsymbol{e}_k$ as before. Then $p(H_k + |\eta|^2 \boldsymbol{f}_k \boldsymbol{e}_k^*)\boldsymbol{e}_1 = \vec{\mathbf{0}}$. Clearly $H_k + |\eta|^2 \boldsymbol{f}_k \boldsymbol{e}_k^*$ is unreduced since only the last column of H_k is altered, therefore Lemma 1 still applies, and by uniqueness of p up to scaling the statement of the theorem follows. □

Corollary 1. *Let $p^F(z)$ be the FOM polynomial such that $p^F(A)\boldsymbol{r}_0 \perp \mathcal{K}_k(A, \boldsymbol{r}_0)$. Then $p^F(\theta) = 0$ if and only if θ is a Ritz value.*

Corollary 2. *Let $p^G(z)$ be the GMRES polynomial such that $p^F(A)\boldsymbol{r}_0 \perp A\mathcal{K}_k(A, \boldsymbol{r}_0)$. Then $p^F(\theta) = 0$ if and only if θ is a harmonic Ritz value.*

We will also state the following corollary right away, which justifies previous statements about "a" Ritz pair, in the sense that there is indeed just one Ritz vector for each Ritz value.

Corollary 3. *The geometric multiplicity of (harmonic) Ritz values is* 1.

Proof. Let $H = H_k$ in the case of ordinary Ritz values and $H = H_k + |\eta|^2 \boldsymbol{f}_k \boldsymbol{e}_k^*$ in the case of harmonic Ritz values. If the statement of the corollary does not hold, then there exists an eigenvalue θ of H with two Jordan blocks, and hence the degree of the minimal polynomial of H is smaller than k, which contradicts Lemma 1. □

We have assumed that H_k is invertible, so that all Ritz values are nonzero. We want the same for harmonic Ritz values as a last preliminary result.

Theorem 7. *Let $(\theta, \boldsymbol{u})$ be a harmonic Ritz pair of A with respect to $\mathcal{K}_k(A, \boldsymbol{v}_1)$, then $\theta \neq 0$.*

Proof. Since $A\boldsymbol{u} - \theta\boldsymbol{u} \perp \mathcal{R}(AV_k)$ with $\boldsymbol{u} \in \mathcal{R}(V_k)$, it follows $A\boldsymbol{u} - \theta\boldsymbol{u} \perp A\boldsymbol{u}$. Let $\boldsymbol{v} \equiv A\boldsymbol{u}$, then $\|\boldsymbol{v}\|_2^2 = \theta \boldsymbol{u}^* A^* \boldsymbol{u}$ and hence

$$\theta = \frac{\|\boldsymbol{v}\|_2^2}{\boldsymbol{v}^* \boldsymbol{u}} = \frac{\|\boldsymbol{v}\|_2^2}{\boldsymbol{v}^* A^{-1} \boldsymbol{v}}$$

so that $|\theta| \geq \frac{1}{\|A^{-1}\|_2} > 0$. □

From Corollaries 1 and 2 and by Theorem 7 we learn that the residual polynomials of FOM and GMRES are fully determined as

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

with θ_i the ordinary and harmonic Ritz values respectively, so that

$$\boldsymbol{r}_k = \prod_{i=1}^{k} \left(1 - \frac{1}{\theta_i} A\right) \boldsymbol{r}_0.$$

This gives us some key insights into convergence behaviour, since we can now see that (harmonic) Ritz values close to the origin which are not fully converged to an eigenvalue of A, may slow down convergence. However, as soon as a (harmonic) Ritz value θ approximates or "captures" an eigenvalue λ well enough, the components of $\boldsymbol{r}_0$ in the direction of the corresponding eigenvector are effectively removed in the new residual $\boldsymbol{r}_k$. From then on, the speed of convergence is governed by the remaining eigenvalues.

Lastly in this section, we will inspect the strength of our analysis and see if it is solid enough. The key argument is established in the previous paragraph: the (harmonic) Ritz values approximate the eigenvalues of A and then approximately remove the components of the initial residual in the direction of the corresponding eigenvector. To support this claim, we have assumed that the residual polynomials are non-trivial, that H_k is invertible and that A is close to normal in the sense that small perturbations of an eigenvalue result in a small residual of the eigenproblem.

All assumptions are undermined for the normal matrix $A \equiv [\boldsymbol{e}_2, \ldots, \boldsymbol{e}_n, \boldsymbol{e}_1]$ in the problem $A\boldsymbol{x} = \boldsymbol{e}_1$, where H_k is only invertible when $k = n$ and GMRES just obtains $x_k = \boldsymbol{0}$ for $k < n$. However, a good preconditioner resolves these troubles. Lastly, in most real-life linear systems super-linear convergence behaviour in the reduction of the residual norm is observed in FOM and GMRES as soon as (harmonic) Ritz values start to form good approximations to "problematic" eigenvalues close to the origin, verifying the previous analysis.

4 Restart

GMRES and FOM are not particularly suitable as is, since the computational complexity and the required storage in the Arnoldi iteration become unfeasible. Every kth iteration requires the storage of a new n-vector, while orthogonalization requires at least $\mathcal{O}(4kn)$ flops (depending on the chosen method), so that orthogonalization can even overtake the costs of sparse MV-products.

The most common way to circumvent both these problems, is to restart GMRES or FOM after a fixed number of m iterations, construct the best approximation $\boldsymbol{x}_m$ and restart the algorithm with $\boldsymbol{x}_0 \leftarrow \boldsymbol{x}_m$. These algorithms are usually referred to as GMRES(m) or FOM(m). To use more precise terminology, the whole GMRES process up to a restart is called a *cycle* while

a single Arnoldi step is an *iteration*. The *size* of a cycle is the number of iterations from start to restart.

An obvious shortcoming of these restarted variants is that they might lose the superlinear convergence property of ordinary GMRES and FOM when a cycle size is too small. In that case good approximations to eigenvalues close to the origin may never be obtained, resulting in slow reduction of the residual norm, and as a consequence larger computational work due to the vast amount of matrix-vector products.

In an attempt to recover the superlinear convergence behaviour in restarted GMRES and FOM, one can utilize the approximate spectral information in different ways at the end of each cycle. For instance, it can be used to build or improve preconditioners to deflate small eigenvalues, or to augment the Krylov subspace with the approximate eigenvectors. In this article we will explore how to use the approximate spectral data to implicitly restart GMRES and FOM, so that the next cycle of the algorithm starts out with a Krylov subspace which contains the ℓ Ritz vectors of choice. The resulting algorithms are aptly called *thick restarted* GMRES or FOM, or GMRES-IR(m, ℓ) and FOM-IR(m, ℓ) for brevity, similar as to [3].

Before we explore these algorithms, we want to elaborate on the computational costs of obtaining the (harmonic) Ritz values. Note that for both harmonic and ordinary Ritz values we must find the eigenvalues of a Hessenberg matrix, so that the first Hessenberg transformation phase of the shifted QR-algorithm can be ommitted. If the QR-algorithm needs about $\mathcal{O}(k)$ steps to converge, the complexity is approximately $\mathcal{O}(k^3)$. If $n \simeq k^2$, the compexity of obtaining the spectral data is $\mathcal{O}(kn)$, which is proportional to the costs of the last orthogonalization step.

4.1 Shrinking the Krylov subspace

At the end of a cycle of FOM and GMRES we have obtained the Arnoldi relation $AV_k = V_{k+1}\underline{H}_k$, where the columns of V_k form an orthonormal basis for $\mathcal{K}_k(A, \boldsymbol{v}_1)$. We would like to shrink the size of this Krylov subspace, so that we can restart GMRES or FOM with a new Arnoldi relation $A\tilde{V}_\ell = \tilde{V}_{\ell+1}\underline{\tilde{H}}_\ell$ with $\ell < k$, such that $\mathcal{R}(\tilde{V}_\ell) \subset \mathcal{K}_k(A, \boldsymbol{v}_1)$ contains the Ritz vectors corresponding to ℓ selected Ritz values. We will first show that this is indeed possible, subsequently how the smaller Arnoldi relation can be obtained efficiently, and lastly how the GMRES and FOM methods must be changed to incorporate implicit restarts.

Theorem 8. *Let $\mathcal{K}_k(A, \boldsymbol{v}_1)$ be a k-dimensional Krylov subspace and let $(\theta_i, \boldsymbol{u}_i)$ denote the (harmonic) Ritz pairs of A with respect to $\mathcal{K}_k(A, \boldsymbol{v}_1)$ for $i = 1, \ldots, k$ such that multiples are repeated. Define for $1 \leq \ell < k$*

$$\tilde{\boldsymbol{v}}_1 \equiv \prod_{i=\ell+1}^{k} (A - \theta_i I)\boldsymbol{v}_1.$$

Then $\mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1)$ is an ℓ-dimensional Krylov subspace such that for $i = 1, \ldots, \ell$ the pairs $(\theta_i, \boldsymbol{u}_i)$ are the (harmonic) Ritz pairs of A with respect to $\mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1)$.

Proof. It is not hard to see that $\mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1) \subset \mathcal{K}_k(A, \boldsymbol{v}_1)$ and that it has dimension ℓ. Clearly $A\mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1) \subset A\mathcal{K}_k(A, \boldsymbol{v}_1)$ as well. For ease of notation, define the test subspaces $\mathcal{W} = A\mathcal{K}_k(A, \boldsymbol{v}_1)$ and $\tilde{\mathcal{W}} = A\mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1)$ in the case of harmonic Ritz values, while $\mathcal{W} = \mathcal{K}_k(A, \boldsymbol{v}_1)$ and $\tilde{\mathcal{W}} = \mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1)$ in the case of ordinary Ritz values. By Theorems 5 and 6 the first statement of

$$\left[\prod_{i=1}^{k}(A - \theta_i I)\right] \boldsymbol{v}_1 \perp \mathcal{W} \Rightarrow \left[\prod_{i=1}^{\ell}(A - \theta_i I)\right] \tilde{\boldsymbol{v}}_1 \perp \tilde{\mathcal{W}}$$

follows. The implication is due to the fact that $\tilde{\mathcal{W}} \subset \mathcal{W}$. Now by applying Theorems 5 and 6 once more, it follows that the (harmonic) Ritz value of A with respect to $\mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1)$ are indeed $\theta_1, \ldots, \theta_\ell$ with multiples repeated.

Lastly we use Corollary 3, which tells us that each Ritz value corresponds to exactly one Ritz vector. By explicitly constructing this Ritz vector in $\mathcal{K}_k(A, \boldsymbol{v}_1)$, we can show it is contained in $\mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1)$ as well. Define for $j \leq \ell$ the polynomial

$$q_j(z) \equiv \prod_{\substack{i=1 \\ i \neq j}}^{k} (z - \theta_i)$$

Note that $q_j(A)\boldsymbol{v}_1 = q_j(H_k)\boldsymbol{e}_1 \neq \vec{\boldsymbol{0}}$ since q_j is a polynomial of order $k - 1$. Clearly $(A - \theta_j I)q_j(A)\boldsymbol{v}_1 \perp \mathcal{W}$ and hence $\boldsymbol{u}_i = q_j(A)\boldsymbol{v}_1$ is the Ritz vector of A w.r.t. $\mathcal{K}_k(A, \boldsymbol{v}_1)$ corresponding to θ_j. Do the same for the smaller Krylov subspace such that $\tilde{q}_j(z) \equiv \prod_{\substack{i=1 \\ i \neq j}}^{\ell}(z - \theta_i)$ forms the Ritz vector $\tilde{q}_j(A)\tilde{\boldsymbol{v}}_1$ of A with respect to $\mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1)$ corresponding to the Ritz value θ_j. Clearly $\tilde{q}_j(A)\tilde{\boldsymbol{v}}_1 = q_j(A)\boldsymbol{v}_1$ and hence the Ritz vectors coincide. Therefore $\mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1)$ contains the Ritz vectors of A with respect to $\mathcal{K}_k(A, \tilde{\boldsymbol{v}}_1)$ for $\theta_1, \ldots, \theta_\ell$. $\square$

Corollary 4. *If all (harmonic) Ritz values are distinct, then*

$$\mathcal{K}_\ell(A, \tilde{\boldsymbol{v}}_1) = \text{span}\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_\ell\}.$$

Since the zeros of the GMRES polynomial are the harmonic Ritz values, while for the FOM polynomial these are ordinary Ritz values, Theorem 8 naturally leads to preserving harmonic Ritz values in the case of GMRES and ordinary Ritz values in the case of FOM.

Of course an implicit restart implies that we should not form $\tilde{\boldsymbol{v}}_1$ explicitly as it is defined, and an Arnoldi relation for the Krylov subspace it induces must be obtained cheaply as well. To this end, remember that the shifted QR-algorithm applied to a matrix H performs iterations of the shifted power method in the first column of its unitary matrix Q, which implies that it implicitly generates a polynomial in H. By chosing the shifts as the unwanted (harmonic) Ritz values $\theta_{\ell+1}, \ldots, \theta_k$, this can be taken to our advantage. This is exactly what happens in the Implicitly Restarted Arnoldi Method (IRAM) [2].

4.2 IRAM

In the sections that follow we will focus on the transition from one cycle of FOM and GMRES to a new cycle. To distinguish variables between cycles, a tilde '$\sim$' is used to identify the entity in the next cycle.

Theorem 9. *Let $AV_k = V_{k+1}\underline{H}_k$ and $\mu_k, \ldots, \mu_{\ell+1}$ be as in Algorithm 2 and define the polynomial*

$$p(z) = \prod_{i=\ell+1}^{k} (z - \mu_i),$$

then the procedure produces the Arnoldi relation

$$A\tilde{V}_\ell = \tilde{V}_{\ell+1}\underline{\tilde{H}}_k \text{ and } \tilde{\boldsymbol{v}}_1 = \tilde{\tau} p(A)\boldsymbol{v}_1 \quad \text{for some } \tilde{\tau} \in \mathbb{C},$$

where $\tilde{\boldsymbol{v}}_1$ and $\boldsymbol{v}_1$ are the first column of respectively $\tilde{V}_\ell$ and V_k.

Proof. We first factor the Hessenberg matrix $\underline{H}_k - \mu_k \underline{I}_k = \underline{Q}_k R_k$. This can be obtained by applying $k+1$ Givens rotations G_i of size $k+1$ each ith subdiagonal element $\underline{H}_{i+1,i}$, so that $G_k \cdots G_1(\underline{H}_k - \mu_k \underline{I}_k) = [R_k, \vec{0}]^*$. Then define $\underline{Q}_k = \underline{I}_k^* G_1^* \cdots G_k^*$, i.e. the product of Givens rotation with the last

Algorithm 2 Implicitly restarted Arnoldi Method (IRAM). The underlined matrices have one row more than columns, so that $\underline{I}_j$ is I_j with an additional bottom row of zeros. If $\underline{Q}$ is $(j+1) \times j$, then $\underline{Q}'$ denotes the size $j \times (j-1)$ left upper block of $\underline{Q}$.

Given the Arnoldi relation $AV_k = V_{k+1}\underline{H}_k$
Set $U = I_{k+1}$ and $\underline{S}_k = \underline{H}_k$
for $j = k, k-1, \ldots, \ell+1$ **do**
  (1) Select shift μ_j
  (2) Compute QR-factorization of $\underline{S} - \mu_j \underline{I}_j = \underline{Q}R$
  (3) $\underline{S} \leftarrow R\underline{Q}' + \mu_j \underline{I}_{j-1}$
  (4) $U \leftarrow U\underline{Q}$
end for
$\tilde{V}_{\ell+1} \equiv V_{k+1}U$
$\underline{\tilde{H}}_\ell \equiv \underline{S}$

---

column removed. A standard result form the QR-algorithm is that then also $\underline{Q}_k$ is Hessenberg. Next, let $\underline{Q}'_k$ be the left upper $k \times (k-1)$ block of $\underline{Q}_k$, that is

$$\underline{Q}'_k \equiv \underline{I}_k^* \underline{Q}_k \underline{I}_{k-1}. \tag{8}$$

Also define the quantities

$$\underline{H}^+_{k-1} \equiv R_k \underline{Q}'_k + \mu \underline{I}_{k-1} \quad \text{and} \quad V^+_{k-1} \equiv V_k \underline{Q}'_k, \quad V^+_k \equiv V_{k+1}\underline{Q}_k.$$

Since R_k is upper triangular, we have that $\underline{H}^+_{k-1}$ is Hessenberg as well. Furthermore

$$\underline{Q}_k \underline{H}^+_{k-1} = \underline{Q}_k R_k \underline{Q}'_k + \mu \underline{Q}_k \underline{I}_{k-1} = (\underline{H}_k - \mu_k \underline{I}_k)\underline{Q}'_k + \mu \underline{Q}_k \underline{I}_{k-1} = \underline{H}_k \underline{Q}'_k$$

by application of Equation (8). We can use this to construct a new Arnoldi relation

$$AV^+_{k-1} = AV_k \underline{Q}'_k = V_{k+1}\underline{H}_k \underline{Q}'_k = V_{k+1}\underline{Q}_k \underline{H}^+_{k-1} = V^+_k \underline{H}^+_{k-1}. \tag{9}$$

Moreover

$$(A - \mu I_n)V_k = AV_k - \mu V_k = V_{k+1}(\underline{H}_k - \mu \underline{I}_k) = V_{k+1}\underline{Q}_k R_k = V^+_k R_k.$$

If we inspect the first column only, we find due to the fact that R_k is upper triangular that

$$(A - \mu I_n)\boldsymbol{v}_1 = (A - \mu I_n)V_1 \boldsymbol{e}_1 = V^+_k R_k \boldsymbol{e}_1 = r_{11}\boldsymbol{v}^+_1$$

with r_{11} the left upper entry of R_k. Hence $\boldsymbol{v}_1^+$ is a multiple of $(A-\mu I_n)\boldsymbol{v}_1$.

Since we now have the Arnoldi relation of Equation (9) which is reduced by one dimension, we can repeat the argument above inductively and obtain

$$U \equiv \underline{Q}_k \underline{Q}_{k-1} \cdots \underline{Q}_{\ell+1}$$

where $\underline{Q}_i$ is Q of step i of Algorithm 2. Then $U \in \mathbb{C}^{(k+1)\times(\ell+1)}$ is orthonormal and $U' = \underline{I}_k^* \underline{U}_k \underline{I}_{k-1}$, which gives us

$$U\underline{\tilde{H}}_\ell = \underline{H}_k U'.$$

If now $\tilde{V}_\ell \equiv V_k U'$ and $\tilde{V}_{\ell+1} = V_{k+1}U$, then

$$A\tilde{V}_\ell = V_{k+1}\underline{H}_k U' = V_{k+1}U\underline{\tilde{H}}_\ell = \tilde{V}_{\ell+1}\underline{\tilde{H}}_\ell.$$

such that $\tilde{v}_1 = \tilde{\tau} p(A)\boldsymbol{v}_1$. □

Remark. In ordinary FOM and GMRES, V_{k+1} and $\underline{H}_k$ are real if A is real. Using IRAM with complex shifts may result in complex $\tilde{V}_{\ell+1}$ and $\underline{\tilde{H}}_k$. This is not desirable, since complex numbers have double storage demands and increase computational costs. However, since (harmonic) Ritz values are eigenvalues of real matrices, shifts come in conjugate pairs and hence it is possible to perform two shifts at the same time to mitigate the problem.

For ease of discussion, suppose S_1 is square, so that two QR-steps give

$$\begin{aligned} S_1 - \theta I &= Q_1 R_1, \\ S_2 &\equiv R_1 Q_1 + \theta I, \\ S_2 - \bar{\theta} I &= Q_2 R_2, \\ S_3 &\equiv R_2 Q_2 + \bar{\theta} I. \end{aligned}$$

Then its is easily verified that if $Q \equiv Q_1 Q_2$ and $R \equiv R_2 R_1$, it follows

$$(S_1 - \theta I)(S_1 - \bar{\theta} I) = QR \quad \text{and} \quad QS_3 = S_1 Q$$

But $(S_1 - \theta I)(S_1 - \bar{\theta} I) = S_1^2 - 2\Re(\theta) S_1 + |\theta|^2 I$ is real, and hence Q can be chosen real. However, squaring S_1 is expensive. A solution is to compute its first column only, which requires only one MV-product with S_1, and find a Householder reflection $Q_{(0)}$ which makes the vector a multiple of $\boldsymbol{e}_1$:

$$Q_{(0)}(S_1 - \theta I)(S_1 - \bar{\theta} I)\boldsymbol{e}_1 = r_{11}\boldsymbol{e}_1$$

This determines the first column of Q. Apply $Q_{(0)}$ to S_1, which perturbs the Hessenberg structure, and can be restored using k additional Householder reflections $Q_{(1)}, \ldots, Q_{(k)}$, so that in the end $Q = Q_{(0)} \cdots Q_{(k)}$. We will not prove correctness and the details with regard to non-square matrices here, but refer to [1].

4.3 Implicitly restarted FOM

Restarting FOM with the notions of IRAM is manageable but subtle, as we only have to make sure that no high dimensional operations are necessary to solve the projected problem in later cycles. At the end of the first cycle we still solve the same projected problem $H_k \boldsymbol{y} = \beta \boldsymbol{e}_1$ where $\beta = \|\boldsymbol{r}_0\|_2$. In later cycles, we must work with a different right hand side, since $\tilde{\boldsymbol{v}}_1$ is not the initial residual anymore. Note that by using Equation (7) the residual $\boldsymbol{r}_k$ can be written as

$$\boldsymbol{r}_k = -V_{k+1}(\eta y_k^F \boldsymbol{e}_{k+1}) = -\eta y_k^F \boldsymbol{v}_{k+1} \tag{10}$$

Hence the FOM residual is a multiple of the vector $\boldsymbol{v}_{k+1}$. We will now show that this vector is preserved in the IRAM procedure as $\tilde{\boldsymbol{v}}_{\ell+1} = \boldsymbol{v}_k$.

Since the Ritz values are the eigenvalues of H_k and we are using them as shifts, it follows that $H_k - \theta_k I$ is of dimension $k-1$. Hence if $H_k - \theta_k I = Q_o R_o$ is a QR-decomposition such that both Q_o and R_o are of size $k \times k$, then the last row of R_o must contain only zeros. Denote by $\boldsymbol{q}_i$ the ith column of Q_o and by $\boldsymbol{r}_i^*$ the ith row of R_o. Then the full QR-decomposition of the non-square Hessenberg matrix is just one row-swap away:

$$\begin{bmatrix} H - \theta_k I \\ \eta \boldsymbol{e}_k^* \end{bmatrix} = \begin{bmatrix} Q_o & \vec{\boldsymbol{0}} \\ \vec{\boldsymbol{0}}^* & 1 \end{bmatrix} \begin{bmatrix} R_o \\ \eta \boldsymbol{e}_k^* \end{bmatrix} = \begin{bmatrix} \boldsymbol{q}_1 & \cdots & \boldsymbol{q}_{k-1} & \vec{\boldsymbol{0}} & \boldsymbol{q}_k \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{r}_1^* \\ \vdots \\ \boldsymbol{r}_{k-1}^* \\ \eta \boldsymbol{e}_k^* \\ \vec{\boldsymbol{0}}^* \end{bmatrix}. \tag{11}$$

By considering the economical form for Equation (11) we find indeed the decomposition $\underline{H}_k - \theta_k \underline{I}_k = QR$ with Q of size $(k+1) \times k$ and R of size $k \times k$ such that Q has only zeros in its last row and column except for $Q_{k+1,k} = 1$. Therefore we have

$$V_k^+ = V_{k+1} Q = \begin{bmatrix} V_{k-1}^+ & \boldsymbol{v}_{k+1} \end{bmatrix}.$$

By induction it follows that at the end of the IRAM procedure we are left with $\tilde{V}_{\ell+1} = \begin{bmatrix}\tilde{V}_k U' & \boldsymbol{v}_{k+1}\end{bmatrix}$ or more compactly $\tilde{\boldsymbol{v}}_{\ell+1} = \boldsymbol{v}_{k+1}$.

Finally we can show which low-dimensional system we must solve with implicitly restarted FOM and what tricks we can use to determine the norm of the residual without solving the low-dimensional system. At the end of the first cycle of FOM we set $\tilde{\boldsymbol{r}}_0 \leftarrow \boldsymbol{r}_k$ and define

$$\tilde{\beta} \equiv -\eta y_k.$$

Then we continue with FOM starting from $A\tilde{V}_\ell = \tilde{V}_{\ell+1}\underline{\tilde{H}}_\ell$ and obtain the Arnoldi relation $A\tilde{V}_k = \tilde{V}_{k+1}\underline{\tilde{H}}_k$ with $k \geq \ell$. The Galerkin condition of FOM now implies

$$\tilde{\boldsymbol{r}}_k = \tilde{\boldsymbol{r}}_0 - A\tilde{V}_k\tilde{\boldsymbol{y}} = \tilde{V}_{k+1}(\tilde{\beta}\boldsymbol{e}_{\ell+1} - \underline{\tilde{H}}_k\tilde{\boldsymbol{y}}) \perp \mathcal{R}(\tilde{V}_k)$$

for $\tilde{\boldsymbol{y}} \in \mathbb{C}^k$ and hence we must solve

$$\tilde{H}_k\boldsymbol{y} = \tilde{\beta}\boldsymbol{e}_{\ell+1}.$$

Not too much changes with regard to determining the residual norm cheaply, since pre-multiplying

$$\tilde{\beta}\boldsymbol{e}_{\ell+1} - \underline{\tilde{H}}_k\tilde{\boldsymbol{y}} = -\tilde{\eta}\tilde{y}_k\boldsymbol{e}_{k+1}$$

with $\tilde{\boldsymbol{\gamma}}_{k+1}^*$ gives $|\tilde{\beta}\tilde{\gamma}_{\ell+1}| = |\tilde{\eta}\tilde{y}_k\tilde{\gamma}_{k+1}|$, so that

$$\|\tilde{\boldsymbol{r}}_k\|_2 = \left\|\tilde{\beta}\boldsymbol{e}_{\ell+1} - \underline{\tilde{H}}_k\tilde{\boldsymbol{y}}\right\|_2 = \frac{|\tilde{\beta}||\tilde{\gamma}_{\ell+1}|}{|\tilde{\gamma}_{k+1}|}.$$

Lastly, the FOM polynomial changes slightly as the right-hand side has a different structure. Suppose $\boldsymbol{x}_k = q_{k-1}(A)\tilde{\boldsymbol{v}}_1 \in \mathcal{K}(A, \tilde{\boldsymbol{v}}_1)$ with q_{k-1} a polynomial of degree $(k-1)$ is the solution at step k. Since $\tilde{\boldsymbol{r}}_0 = \tilde{\beta}\tilde{\boldsymbol{v}}_{\ell+1} \in \mathcal{K}_k(A, \tilde{\boldsymbol{v}}_1)$, we can still find a polynomial p_k of degree k such that:

$$\tilde{\boldsymbol{r}}_k = \tilde{\boldsymbol{r}}_0 - Aq_{k-1}(A)\tilde{\boldsymbol{v}}_1 = p_k(A)\tilde{\boldsymbol{v}}_1.$$

Therefore, the zeros of the FOM polynomial remain the Ritz values, but the condition $p_k(0) = 1$ is not necessarily the case.

In this section we have only discussed the transition from the first cycle to the second, but note that Equation (10) holds in the second cycle as well, and hence no additional changes have to be made for the following cycles.

4.4 Implicitly restarted GMRES

Implementing IRAM in GMRES is carried out similarly; the trick is to transfer the residual at the end of the first cycle into the second, without working with high dimensional vectors and matrices. The first cycle is still an ordinary GMRES cycle, and by using Equation (5) we find that the GMRES residual at the kth iteration is given as

$$\boldsymbol{r}_k = V_{k+1}(\beta \boldsymbol{e}_1 - \underline{H}_k \boldsymbol{y}) = \tau V_{k+1} \vec{\boldsymbol{\gamma}}_{k+1} \tag{12}$$

for a scalar τ. Note that if $\tilde{\boldsymbol{\gamma}}_{\ell+1} \equiv U^* \vec{\boldsymbol{\gamma}}_{k+1}$, it follows that

$$\tilde{\boldsymbol{\gamma}}_{\ell+1}^* \underline{\tilde{H}}_\ell = \vec{\boldsymbol{\gamma}}_{k+1}^* U \underline{\tilde{H}}_\ell = \vec{\boldsymbol{\gamma}}_{k+1}^* \underline{H}_k U' = \mathbf{0}^*$$

and hence $\tilde{\boldsymbol{\gamma}}_{\ell+1} \in N(\underline{\tilde{H}}_\ell^*)$. Furthermore

$$N(\underline{H}_k^*) = N(\underline{H}_k^* - \bar{\theta}_k \underline{I}_k^*)^\perp = R(\underline{H}_k - \theta_k \underline{I}_k) = R(Q_k)$$

so that by induction $\vec{\boldsymbol{\gamma}}_{k+1} \in R(U)$ and hence $UU^* \vec{\boldsymbol{\gamma}}_{k+1} = \vec{\boldsymbol{\gamma}}_{k+1}$ since it is a projection onto the range of the orthonormal matrix U. This way we get the relation

$$V_{k+1} \vec{\boldsymbol{\gamma}}_{k+1} = V_{k+1} U U^* \vec{\boldsymbol{\gamma}}_{k+1} = \tilde{V}_{\ell+1} \tilde{\boldsymbol{\gamma}}_{\ell+1}.$$

At the start of the following cycle we set $\tilde{\boldsymbol{r}}_0 \leftarrow \boldsymbol{r}_k$, so that the Petrov-Galerkin condition now implies

$$\tilde{\boldsymbol{r}}_k = \tilde{\boldsymbol{r}}_0 - A\tilde{V}_k \tilde{\boldsymbol{y}} = \tilde{V}_{k+1} \left(\begin{bmatrix} \tau \tilde{\boldsymbol{\gamma}}_{\ell+1} \\ \vec{\mathbf{0}} \end{bmatrix} - \underline{\tilde{H}}_k \tilde{\boldsymbol{y}} \right) \perp \mathcal{R}(A\tilde{V}_k)$$

for a vector $\tilde{\boldsymbol{y}} \in \mathbb{C}^k$. As a consequence, the low-dimensional problem we need to solve becomes

$$\underline{\tilde{H}}_k \tilde{\boldsymbol{y}} = \begin{bmatrix} \tau \tilde{\boldsymbol{\gamma}}_{\ell+1} \\ \vec{\mathbf{0}} \end{bmatrix} \quad \text{(in least-squares sense)}.$$

If we update the null-space vector $\tilde{\boldsymbol{\gamma}}_{\ell+1}$ in each iteration equivalently to before, so that $\tilde{\boldsymbol{\gamma}}_{k+1} \in N(\underline{\tilde{H}}_k^*)$, then a cheap look-up for the residual norm at each iteration k is provided by

$$\|\boldsymbol{r}_k\|_2 = \frac{|\tau| \left\|\tilde{\boldsymbol{\gamma}}_{\ell+1}\right\|_2^2}{\left\|\tilde{\boldsymbol{\gamma}}_{k+1}\right\|_2}.$$

Lastly, notice that $\tilde{\boldsymbol{r}}_0 = \tau\tilde{V}_{\ell+1}\boldsymbol{\gamma}_{\ell+1} \in \mathcal{K}_{\ell+1}(A, \tilde{\boldsymbol{v}}_1)$, so that $\tilde{\boldsymbol{r}}_0 = r_\ell(A)\tilde{\boldsymbol{v}}_1$ for a polynomial r_ℓ of degree ℓ. Hence, the GMRES polynomial at iteration $k \geq \ell$ remains determined by

$$\tilde{\boldsymbol{r}}_k = \tilde{\boldsymbol{r}}_k - Aq_{k-1}(A)\tilde{\boldsymbol{v}}_1 = p_k(A)\tilde{\boldsymbol{v}}_1$$

for p_k of degree k, and hence the harmonic Ritz values remain the zeros of the GMRES polynomial.

The only relation unique to the first cycle was expressed in Equation (12), but the result still holds for the second cycle as well. Therefore, all the following cycles can be addressed equivalently as shown in this section.

5 Results

The solution is always fixed as $\boldsymbol{x} = \vec{\mathbf{1}}$ vector and hence the right hand side is determined as $\boldsymbol{b} = A\vec{\mathbf{1}}$. Furthermore, note that if results for GMRES(m, ℓ) or FOM(m, ℓ) are shown for real matrices A, the value ℓ denotes a maximum "thickness" in the sense that the dimension of the Krylov subspace at restart can be smaller than ℓ. This is because conjugate Ritz values are both removed.

5.1 Capturing the eigenvalues

To show the potential of thick restart, we construct a matrix which can be considered hard for restarted GMRES, in the sense that there are many eigenvalues close to the boundary of the convex hull and a few of them close to the origin. Let $A = I + N$ with I the identity and N a matrix whose off-diagonal elements are normally distributed with mean $\mu = 0$ and $\sigma^2 = \frac{1}{n-1}$, so that its convex hull is likely a circle of radius 1 around 1 in the complex plane. Here we pick $n = 100$ for the size of A and the size of a cycle if $m = 20$ iterations. In Figure 1 the eigenspectrum of A is plotted, together with the harmonic Ritz values at the end of the fifth cycle of (thick) restarted GMRES. It is clear that ordinary restarted GMRES does not do a good job at capturing the eigenvalues of A, while thick restarted GMRES generates very good approximations to about seven eigenvalues close to the origin. Notice as well how the harmonic Ritz values come in conjugate pairs, verifying that we indeed work with real matrices. The convergence behaviour for GMRES(20) and GMRES-IR$(20, \ell)$ is shown in Figure 2 as a function of the number of matrix-vector products. One sees that ordinary restarted GMRES makes

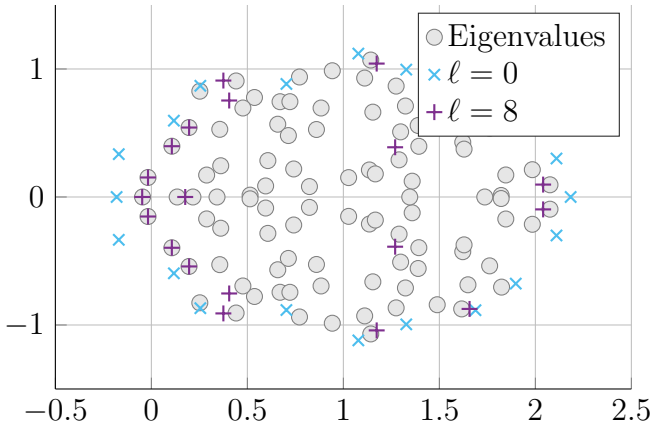

Figure 1: The eigenspectrum of A with Harmonic Ritz values at the fifth cycle of GMRES, with (+) and without (×) thick restart.

no progress after the 70 MV-products, while thick restarted GMRES comes close to the convergence behaviour of full GMRES. Note how for $\ell \in \{1, 2, 3\}$ most significant improvement happens, while for $\ell > 3$ the relative reduction in total MV-products shrinks. This corresponds to the number of eigenvalues close to 0.

5.2 Real world problems

In this section thick restarted GMRES and FOM are applied to a couple matrices from the Matrix Market.

Sherman4. First the `Sherman4` matrix is used, which is real, sparse, 1104×1104 and non-symmetric. The matrix is numerically not very challenging, since it is well-conditioned and positive definite. There is a pair of eigenvalues close to the origin at 0.0307 and 0.0847 and the remaining eigenvalues lie approximately in the interval $[0.2, 67]$. The tolerance for the relative residual is set to 10^{-6} an the size of the cycle is $m = 20$ iterations. In Figure 3 the residual reduction with respect to the previous MV-product is shown, and it is immediately clear that full GMRES shows two major bumps around iterations 15 to 30 and 40 to 60. Inspection of the harmonic Ritz spectrum shows that these bumps correspond with harmonic Ritz values converging to respectively the first and second eigenvalue of A.

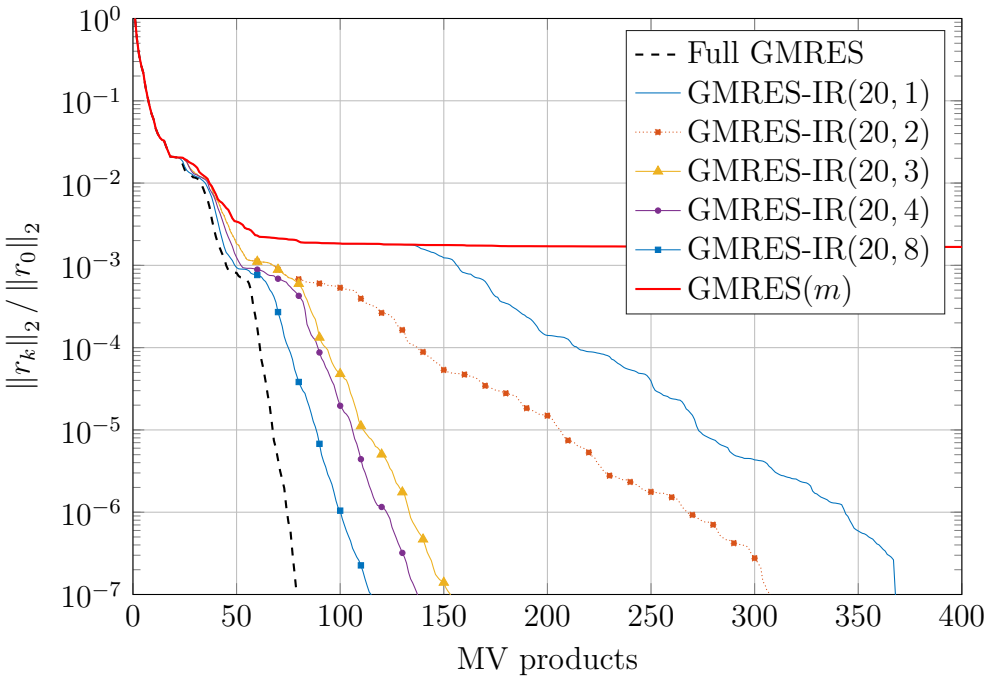

Figure 2: Convergence behaviour of ordinary restarted GMRES, full GMRES and thick restarted GMRES for different values of ℓ

When using ordinary restarted GMRES, the two smallest Ritz values are never captured and as a consequence the convergence behaviour is steadily linearly yet extremely slowly. Implicitly restarted GMRES almost mimics the bumps of full GMRES, but needs about ten MV-products more to capture the second eigenvalue. Clearly the resulting speed of convergence is significantly better than ordinary restarted GMRES.

Table 1: Number of MV-products for the `Sherman4` matrix

Method	MV-products
Full GMRES	106
GMRES-IR(20, 7)	127
FOM-IR(20, 7)	130
GMRES(20)	524
FOM(20)	627
QMRIDR(20)	114

In Table 1 we compare the total number of matrix-vector products necessary to reach the wanted tolerance, and clearly implicitly restarted GMRES and FOM perform very much alike. Also note from the table that the implicit

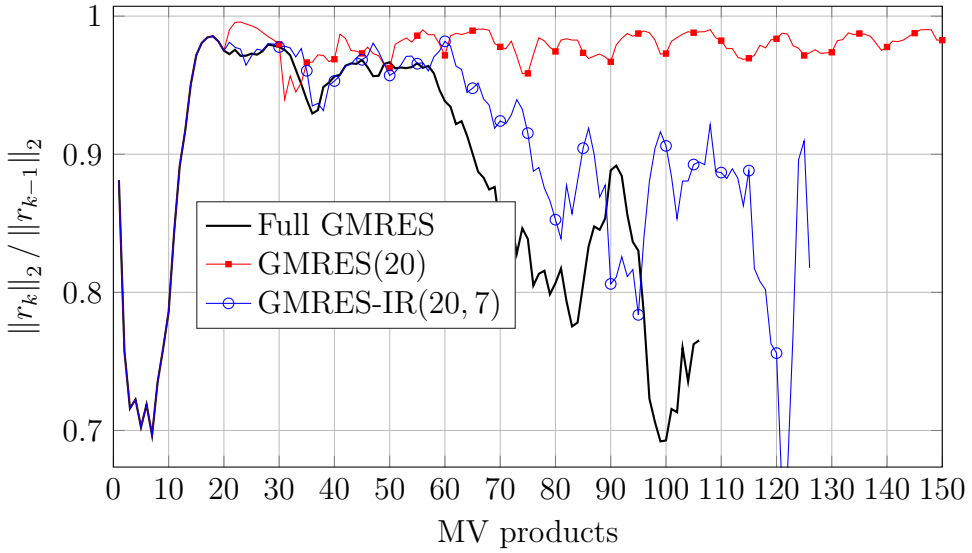

Figure 3: Normed residual reduction per MV-product for the `Sherman4` matrix

restarting strategies can potentially contest with other state of the art techniques such as QMRIDR.

We can also investigate the total number of vector operations necessary for different values of ℓ. We count inner products twice as their complexity is $\mathcal{O}(2n)$ and scalar vector products of $\mathcal{O}(n)$ once. In Table 2 we list both the number of MV-products and the number of vector operations, which shows that although the number of MV-products reduces for larger ℓ, the number of vector operations increases. This is due to the fact that computing $\tilde{V}_{\ell+1} = V_k U$ is slightly more involved for larger ℓ, with respect to a thinner restart with some additional orthogonalization steps. Furthermore, the number of cycles increases if ℓ increases further, which is undesirable, as it requires more costly implicit restarts.

Note that FOM performs much alike GMRES, and that it sometimes requires less vector operations. That can be explained by noting that for FOM we only have to compute the matrix $\tilde{V}_\ell$ since $\tilde{\boldsymbol{v}}_{\ell+1}$ is known at the end of each cycle.

Sherman5. Lastly we inspect the real, non-symmetric `Sherman5` matrix, which has a more challenging size of 3312×3312, a total of 20,793 nonzeros, a worse conditioning of order $\mathcal{O}(10^5)$ and a more problematic eigenspectrum

Method	MV	V	Cycl.	Method	MV	V	Cycl.
Full GMRES	106	22,785	1	Full FOM	109	24,084	1
GMRES(20, 1)	267	13,806	14	FOM(20, 1)	269	13,367	15
GMRES(20, 2)	156	8538	9	FOM(20, 2)	166	8880	10
GMRES(20, 3)	145	8555	9	FOM(20, 3)	149	8431	9
GMRES(20, 4)	138	8844	9	FOM(20, 4)	145	8851	9
GMRES(20, 5)	135	9181	9	FOM(20, 5)	136	8918	9
GMRES(20, 6)	130	9588	9	FOM(20, 6)	132	9322	9
GMRES(20, 7)	127	10,326	10	FOM(20, 7)	129	9925	10
GMRES(20, 8)	127	10,938	10	FOM(20, 8)	130	10,948	11
GMRES(20, 9)	126	11,878	11	FOM(20, 9)	129	11,507	11
GMRES(20, 10)	127	13,068	12	FOM(20, 10)	129	12,547	12

Table 2: Convergence statistics for the `Sherman4` matrix. MV is the number of matrix-vector products, V the number of vector operations and 'Cycl.' the number of restarts.

as well: the origin is near the center of the convex hull and many eigenvalues are relatively close to it. To tackle this problem, a sparse incomplete LU-decomposition is used as a preconditioner to cluster the eigenvalues better around 1. Here $LU \approx A$ is formed using a drop tolerance of 0.3 so that $nnz(L)+nnz(U) = 8317$ is just a fraction of $nnz(A)$. Using left preconditioning, an estimated number of 3000 eigenvalues of $U^{-1}L^{-1}A$ are now clustered in the disc $|1 - z| < 0.5$ in the complex plane, while only few remain close to the origin. This is the situation where one expects implicitly restarted GMRES and FOM to make the difference.

Indeed, when setting the size of the cycle to $m = 20$, the thickness to just $\ell = 4$ and the tolerance to 10^{-6}, the convergence behaviour is as in Figure 4. The bumps in FOM show the entrance of small Ritz values, but notice how the convergence becomes very regular after about 25 MV-products when compared to ordinary restarted FOM. This is an indication that thick restarted FOM captures the smallest eigenvalues better. The number of MV-products is reduced tremendously when using thick restart, which is desirable when using a preconditioner.

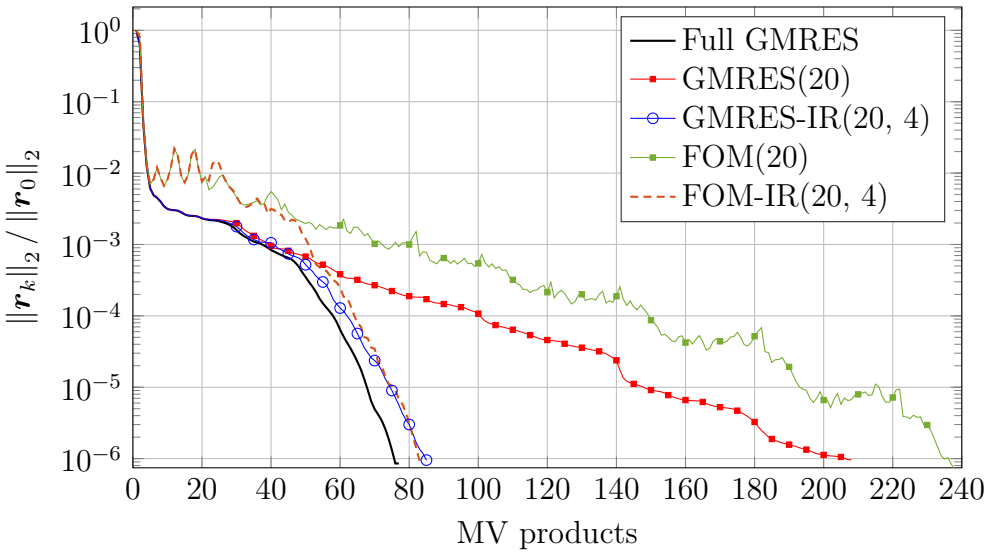

Figure 4: Relative residual as a function of the number of MV-products for the `Sherman5` matrix

6 Conclusion and discussion

In this article it is shown how the (harmonic) Ritz values influence the convergence of GMRES and FOM, and how these values can be utilized to implicitly restart the methods as to retain the superlinear convergence behaviour of full GMRES and FOM. The resulting methods GMRES-IR and FOM-IR show great potential on a few real-life linear systems, and the importance of capturing the eigenvalues closest to the origin is stressed.

In particular, under the assumption that a preconditioner already clusters the eigenvalues of a matrix A around 1 in the complex plane, leaving only a few outliers close to the origin, the implicit restarting strategies can really improve the speed of convergence when using a relatively small thickness ℓ.

An open question remains whether the methods are stable enough for general purpose.

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