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Marcel Schweitzer

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ANY CYCLE-CONVERGENCE CURVE IS POSSIBLE FOR RESTARTED FOM*

MARCEL SCHWEITZER[†]

Abstract. We investigate the possible convergence behavior of the restarted full orthogonalization method (FOM) for non-Hermitian linear systems Ax = b. For the (restarted) GMRES method, it is known that any decreasing sequence of residual norms is possible independent of the eigenvalues of the matrix A. For FOM, however, similar results are not known by now. This note complements the result for restarted GMRES by showing that *any* sequence of residual norms is possible for restarted FOM by a simple construction. An implication of this result is that for every prescribed set of eigenvalues, there exists a matrix A with these eigenvalues for which the restarted Arnoldi method for approximating f(A)b diverges when f is a Stieltjes function.

Key words. linear systems, restarted Krylov subspace methods, full orthogonalization method, restarted Arnoldi method for matrix functions

AMS subject classifications. 65F10, 65F50, 65F60

1. Introduction. For solving a linear system

with a large, sparse, non-Hermitian matrix $A \in \mathbb{C}^{n \times n}$ and a vector $\mathbf{b} \in \mathbb{C}^n$ one often uses a *Krylov subspace method*. One possible choice is the *full orthogonalization method (FOM)*; see, e.g., [9, 11]. Given an Arnoldi decomposition

(1.2)
$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^H,$$

where the columns of $V_m = [v_1 | \cdots | v_m] \in \mathbb{C}^{n \times m}$ form an orthonormal basis of the *m*th Krylov subspace $\mathcal{K}_m(A, \mathbf{b}) = \operatorname{span}\{\mathbf{b}, A\mathbf{b}, \ldots, A^{m-1}\mathbf{b}\}$, the matrix $H_m \in \mathbb{C}^{m \times m}$ is unreduced upper Hessenberg and $\mathbf{e}_m \in \mathbb{C}^m$ denotes the *m*th canonical unit vector, one computes the *m*th FOM iterate for the linear system (1.1) as

(1.3)
$$\boldsymbol{x}_m = \|\boldsymbol{b}\|_2 V_m H_m^{-1} \boldsymbol{e}_1,$$

provided that H_m is non-singular. The FOM iterate x_m is characterized by the variational condition

$$(1.4) b - Ax_m \perp \mathcal{K}_m(A, b).$$

Note that the decomposition (1.2) is unique up to scaling of the columns of V by scalars of modulus one (and scaling of the corresponding entries of H_m ; see, e.g., [12, Theorem 1.3]. Therefore, if the subdiagonal entries of H_m are prescribed to be real and positive (as it always is the case when (1.2) is computed by the Arnoldi process), the decomposition is unique.

For larger values of m, the computational cost of constructing the orthonormal basis v_1, \ldots, v_m (as each basis vector has to be orthogonalized against each previous vector) as well as the cost for computing $H_m^{-1}e_1$ grows. In addition, all basis vectors v_i need to be stored to evaluate (1.3). For Hermitian A, these problems do not occur because short recurrences for the basis vectors can be used (which also translate into short recurrences for the iterates x_m), leading to the *conjugate gradient method* (*CG*) [8] when A is positive definite. In the

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[†]Department of Mathematics, Bergische Universität Wuppertal, 42097 Wuppertal, Germany, schweitzer@math.uni-wuppertal.de

M. SCHWEITZER

non-Hermitian case, a typical remedy is *restarting*. After a fixed (small) number m of steps, one computes a first approximation

$$m{x}_m^{(1)} = \|m{b}\|_2 V_m^{(1)} \left(H_m^{(1)}
ight)^{-1}m{e}$$

and then uses the fact that the error $d_m^{(1)} = x^* - x_m^{(1)}$ (where x^* is the exact solution of (1.1)) satisfies the residual equation

(1.5)
$$Ad_m^{(1)} = r_m^{(1)}, \text{ where } r_m^{(1)} = b - Ax_m^{(1)},$$

so that $d_m^{(1)}$ can be approximated by another *m* steps of FOM for the linear system (1.5) without need to store the quantities $V_m^{(1)}$, $H_m^{(1)}$ related to the first restart cycle. The resulting approximation $\tilde{d}_m^{(1)}$ is then used as an additive correction to the iterate $x_m^{(1)}$ from the the first cycle, i.e.,

$$oldsymbol{x}_m^{(2)} = oldsymbol{x}_m^{(1)} + \widetilde{oldsymbol{d}}_m^{(1)}$$

In the same way, further restart cycles can be performed until the resulting iterate $x_m^{(k)}$ fulfills a prescribed stopping criterion (e.g., a residual norm below some given tolerance). In the following we refer to the resulting iterative method as restarted FOM or FOM(m).

While FOM(m) is simple to understand and implement, it is not at all clear whether the iterates $x_m^{(k)}$ will converge to x^* for $k \to \infty$, even when all iterates are defined (i.e., $H_m^{(k)}$ is non-singular for all k). In the case that A is hermitian positive definite, convergence of restarted FOM (i.e., restarted CG) can easily be proven based on the standard error bound obtained from bounding the CG polynomial by Chebyshev polynomials [9], but as restarting the CG iteration is not necessary due to the availability of short recurrences, this result is of no practical interest. In this paper we show that in the non-Hermitian case, any behavior of restarted FOM (convergence, divergence or stagnation) can occur, independent of the spectrum of A, showing that a convergence analysis for restarted FOM based exclusively on eigenvalue information is not possible in general. This is a direct analogon to similar results concerning (restarted) GMRES [6, 13, 14], the only difference being that due to the minimizing property of GMRES (see, e.g., [10]) the convergence curve always has to be nonincreasing. The remainder of this note is organized as follows. In Section 2, we present our main result and its constructive proof. In Section 3 we discuss the implications of our result for the approximation of f(A)b, the action of a matrix function on a vector, by the restarted Arnoldi method, which is more commonly used in practice. Concluding remarks are given in Section 4.

2. Any cycle-convergence curve is possible for restarted FOM. For the sake of simplicity, we only consider the case of constant restart length m across all restart cycles, keeping in mind that the result below generalizes straight-forwardly to the case of q varying restart lengths $m_i, i = 1, ..., q$ as long as $m_1 + m_2 + \cdots + m_q \leq n$.

THEOREM 2.1. Let $q, m, n \in \mathbb{N}$ with $m \le n-1$ and $q \le \frac{n}{m}$, let $r_1, \ldots, r_q \in \mathbb{R}_+$ be given with $r_1, \ldots, r_{q-1} > 0$ and $r_q \ge 0$ and let $\mu_1, \ldots, \mu_n \in \mathbb{C} \setminus \{0\}$. Then there exist a matrix $A \in \mathbb{C}^{n \times n}$ with spec $(A) = \{\mu_1, \ldots, \mu_n\}$ and a vector $\mathbf{b} \in \mathbb{C}^n$ such that the residuals $\mathbf{r}_m^{(1)}, \ldots, \mathbf{r}_m^{(q)}$ generated by q cycles of FOM(m) for $A\mathbf{x} = \mathbf{b}$ satisfy

$$\|\boldsymbol{r}_{m}^{(j)}\|_{2} = r_{j} \text{ for } j = 1, \dots, q.$$

The proof of Theorem 2.1 is constructive in nature and based on investigating properties of matrices of the form

(2.1)
$$A(\boldsymbol{d}, \boldsymbol{s}) = \begin{bmatrix} d_1 & 0 & \cdots & 0 & s_n \\ s_1 & d_2 & 0 & \cdots & 0 \\ 0 & s_2 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & d_{n-1} & 0 \\ 0 & \cdots & 0 & s_{n-1} & d_n \end{bmatrix}$$

defined by the two vectors $d, s \in \mathbb{C}^n$.

Due to the simple structure of these matrices, we can explicitly give the results of m steps of FOM for this matrix when started with a (multiple of a) canonical unit vector.

PROPOSITION 2.2. Let $A(d, s) \in \mathbb{C}^{n \times n}$ be of the form (2.1), let $m \le n - 1$, $\xi_0 \in \mathbb{C}$ with $|\xi_0| = 1$ and let e_i denote the *i*th canonical unit vector. Then the basis V_{m+1} generated by m steps of FOM for A(d, s) and $\xi_0 e_i$ is given by

$$V_{m+1} = [\xi_0 e_i, \xi_1 e_{i+1}, \dots, \xi_m e_{i+m}]$$

(where, like everywhere in the following, for ease of notation, the indices are to be understood cyclically, i.e., $e_{n+1} := e_1, e_{n+2} := e_2, \ldots$) with $\xi_j = \frac{s_{i+j-1}\xi_{j-1}}{|s_{i+j-1}|}, j = 1, \ldots, m$. The corresponding upper Hessenberg matrix is given by

$$H_m = \begin{bmatrix} d_i & 0 & \cdots & 0 & 0 \\ |s_i| & d_{i+1} & 0 & \cdots & 0 \\ 0 & |s_{i+1}| & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & d_{i+m-1} & 0 \\ 0 & \cdots & 0 & |s_{i+m-1}| & d_{i+m} \end{bmatrix}, \quad h_{m+1,m} = |s_{i+m}|.$$

Proof. The result follows by direct verification of the Arnoldi relation (1.2). Using Proposition 2.2, one easily proves the following result.

PROPOSITION 2.3. Let the assumptions from Proposition 2.2 hold. Then the residual generated by m steps of FOM is given by

(2.2)
$$\boldsymbol{r}_m = (-1)^m \xi_m \frac{|s_i \cdot s_{i+1} \cdots s_{i+m-1}|}{d_i \cdot d_{i+1} \cdots d_{i+m-1}} \boldsymbol{e}_{i+m},$$

and the corresponding residual norm therefore satisfies

$$\|\boldsymbol{r}_m\|_2 = \left|\frac{s_{i+1}\cdots s_{i+m}}{d_{i+1}\cdots d_{i+m}}\right|.$$

Proof. The FOM residual satisfies $r_m = -h_{m+1,m} \| \boldsymbol{b} \| \left(\boldsymbol{e}_m^H H_m^{-1} \boldsymbol{e}_1 \right) \boldsymbol{v}_{m+1}$; see [9]. In our setting we have

$$\|\boldsymbol{b}\| = 1, \quad h_{m+1,m} = |s_{i+m}|, \quad \boldsymbol{v}_{m+1} = \xi_m \boldsymbol{e}_{i+m},$$

and the lower left entry $e_m^H H_m^{-1} e_1$ of H_m^{-1} is $\frac{|s_{i+1}|\cdots|s_{i+1m-1}|}{d_{i+1}\cdots d_{i+m}}$ due to the simple, bidiagonal structure of H_m .

M. SCHWEITZER

Due to Proposition 2.3, given a sequence r_1, \ldots, r_q as in Theorem 2.1, one just needs to choose the coefficient vectors d, s such that they satisfy

$$s_{1} \cdot s_{2} \cdots s_{m} = r_{1} \cdot d_{1} \cdot d_{2} \cdots d_{m}$$

$$s_{m+1} \cdot s_{m+2} \cdots s_{2m} = \frac{r_{2}}{r_{1}} \cdot d_{m+1} \cdot d_{m+2} \cdots d_{2m}$$

$$\vdots \qquad = \qquad \vdots$$

$$(2.3) \qquad s_{(q-1)m+1} \cdot s_{(q-1)m+2} \cdots s_{qm} = \frac{r_{q}}{r_{q-1}} \cdot d_{(q-1)m+1} \cdot d_{(q-1)m+2} \cdots d_{qm}$$

and the corresponding FOM iteration for A(d, s) and $b = e_1$ will exactly produce the residual norm sequence r_1, \ldots, r_q . As each coefficient d_i, s_i appears exactly once in (2.3), one immediately sees that, even if d is already fixed to some prescribed values, such a choice is always possible. We will now show how to prescribe the eigenvalues of A(d, s) by a careful choice of d.

The characteristic polynomial of A(d, s) from (2.1) is given by

$$\chi_{A(d,s)}(\lambda) = (\lambda - d_1) \cdots (\lambda - d_n) + (-1)^{n+1} s_1 \cdots s_n$$

To eliminate the dependence of the characteristic polynomial on s, note that for qm = n, it follows from multiplying all equations in (2.3) that

$$(2.4) s_1 \cdots s_q = r_q \cdot d_1 \cdots d_q.$$

If qm < n, the coefficients s_{qm+1}, \ldots, s_n can always be chosen such that, for given values of d_{mq+1}, \ldots, d_n , (2.4) still holds. Therefore we may rewrite the characteristic polynomial of a matrix A(d, s) generating the desired convergence curve as

(2.5)
$$\chi_{A(d,s)}(\lambda) = (\lambda - d_1) \cdots (\lambda - d_n) + (-1)^{n+1} r_q \cdot d_1 \cdots d_n.$$

Prescribing the eigenvalues of A(d, s) therefore means choosing the values d_1, \ldots, d_n such that the zeros of (2.5) are exactly μ_1, \ldots, μ_n . This can be done as follows. For given μ_1, \ldots, μ_n , there exist coefficients $\beta_{n-1}, \ldots, \beta_0$ such that

$$(\lambda - \mu_1) \cdots (\lambda - \mu_n) = \lambda^n + \beta_{n-1}\lambda^{n-1} + \cdots + \beta_1\lambda + \beta_0$$

The construction used in the following breaks down if $r_q = 1$ as dividing by $1 - r_q$, but without loss of generality we can assume that $r_q \neq 1$; If $r_q = 1$, choose $\alpha \notin \{0, 1\}$, replace all r_i with αr_i and start the FOM iteration with right hand side $\frac{1}{\alpha}e_1$. Then the prescribed residual norms r_1, \ldots, r_q will be generated, but we circumvent our problem as a division by $1 - \alpha r_q \neq 0$ is performed.

We choose the components d_i of d as the n roots of the polynomial

$$\lambda^n + \beta_{n-1}\lambda^{n-1} + \cdots + \beta_1\lambda + \widetilde{\beta}_0 \text{ with } \widetilde{\beta}_0 = (-1)^n \frac{\beta_0}{1 - r_q}$$

which exist due to the fundamental theorem of algebra. With this choice of d_1, \ldots, d_n we have

$$\chi_{A(d,s)}(\lambda) = \lambda^n + \beta_{n-1}\lambda^{n-1} + \dots + \beta_1\lambda + \tilde{\beta}_0 + (-1)^{n+1}r_q \cdot d_1 \cdots d_n$$
$$= \lambda^n + \beta_{n-1}\lambda^{n-1} + \dots + \beta_1\lambda + \frac{\beta_0}{1 - r_q} - r_q \frac{\beta_0}{1 - r_q}$$
$$= \lambda^n + \beta_{n-1}\lambda^{n-1} + \dots + \beta_1\lambda + \beta_0 \left(\frac{1}{1 - r_q} - \frac{r_q}{1 - r_q}\right)$$
$$= \lambda^n + \beta_{n-1}\lambda^{n-1} + \dots + \beta_1\lambda + \beta_0.$$

Therefore, A(d, s) has the desired eigenvalues, which concludes the proof of Theorem 2.1. Also note that this construction implies that all $d_i \neq 0$, so that all Hessenberg matrices $H_m^{(k)}$ are non-singular and all Arnoldi approximations are defined.

Due to the structure of the matrices A(d, s) from (2.1), the unrestarted Arnoldi method behaves the same as the restarted variant (apart from the *n*th iteration), so that the result also directly transfers to the case of unrestarted FOM, where the residual norm after each iteration can be prescribed.

COROLLARY 2.4. Let $n \in \mathbb{N}$, $1 \leq q \leq n$, $r_1, \ldots, r_{q-1} \in \mathbb{R}_+$, $r_q = 0$ and let $\mu_1, \ldots, \mu_n \in \mathbb{C} \setminus \{0\}$. Then there exist a matrix $A \in \mathbb{C}^{n \times n}$ with $\operatorname{spec}(A) = \{\mu_1, \ldots, \mu_n\}$ and a vector $\mathbf{b} \in \mathbb{C}^n$ such that the residuals r_j generated by j steps of FOM for $A\mathbf{x} = \mathbf{b}$ satisfy

$$\|\boldsymbol{r}_{j}\|_{2} = r_{j}$$
 for $j = 1, \ldots, q$.

The proof of Corollary 2.4 is almost identical to the one of Theorem 2.1 apart from the fact that r_n must be the zero vector due to the finite termination property of unrestarted FOM.

3. Approximating f(A)b by restarted Arnoldi. Restarted FOM is rarely used in practice (although there exist situations were it is considered useful, e.g., when solving families of shifted linear systems; see [11]) as restarted GMRES is typically the method of choice for non-Hermitian linear systems, but the (restarted) Arnoldi method for approximating f(A)b, the action of a matrix function on a vector, see, e.g., [1, 3, 5], can be interpreted as implicitly performing (restarted) FOM for families of shifted linear systems if the function f has an integral representation involving a resolvent function. This is, e.g., the case for *Stieltjes functions* [2, 7] defined by the Riemann–Stieltjes integral

$$f(z) = \int_0^\infty \frac{1}{t+z} \,\mathrm{d}\alpha(t),$$

where α is a monotonically increasing, positive function. Examples of Stieltjes functions include $f(z) = z^{-\alpha}$ for $\alpha \in (0, 1]$ or $f(z) = \log(1 + z)/z$. One can show that the restarted Arnoldi approximation (after k cycles with restart length m) for f(A)b when f is a Stieltjes function is given as

$$\boldsymbol{f}_m^{(k)} = \int_0^\infty \boldsymbol{x}_m^{(k)}(t) \,\mathrm{d}\alpha(t),$$

where $\boldsymbol{x}_{m}^{(k)}(t)$ denotes the iterate obtained by applying k cycles of FOM(m) to the shifted linear system

$$(A+tI)\boldsymbol{x}(t) = \boldsymbol{b}$$

with initial guess 0; see [3,4]. Therefore, if the FOM(m) iterates $\mathbf{x}_m^{(k)}(t)$ for $t \in (t_0, t_1)$ with $t_0 < t_1$ and $\mu(t_0) < \mu(t_1)$ diverge, the restarted Arnoldi method for approximating $f(A)\mathbf{b}$ will not converge either. As

$$A(d, s) + tI = A(d + t\mathbf{1}, s)$$
 with $\mathbf{1} = (1, ..., 1)^{H}$

the results from Section 2 also hold for these shifted matrices, so that by (2.2) the residual norm after k steps of FOM(m) for the system $(A + tI)\mathbf{x}(t) = \mathbf{e}_1$ is given by

$$\|\boldsymbol{r}_{m}^{(k)}(t)\|_{2} = \|\boldsymbol{r}_{m}^{(k-1)}(t)\|_{2} \cdot \left|\frac{s_{km+1} \cdot s_{km+2} \cdots s_{(k+1)m}}{(d_{km+1}+t) \cdot (d_{km+2}+t) \cdots (d_{(k+1)m}+t)}\right|.$$

M. SCHWEITZER

As $d_i \neq 0$ for all *i*, the function $||\mathbf{r}_m(t)||_2$ is continuous on an interval $[0, \tilde{t}_1)$ with $\tilde{t}_1 > 0$. Therefore, if the residual norms for $A\mathbf{x} = \mathbf{e}_1$ are prescribed to be increasing, i.e.,

$$\left|\frac{s_{km+1} \cdot s_{km+2} \cdots s_{(k+1)m}}{d_{km+1} \cdot d_{km+2} \cdots d_{(k+1)m}}\right| > 1$$

there exists $0 < t_1 \leq \tilde{t}_1$ such that

$$\frac{s_{km+1} \cdot s_{km+2} \cdots s_{(k+1)m}}{(d_{km+1+t}) \cdot (d_{km+2}+t) \cdots (d_{(k+1)m}+t)} > 1 \text{ for } t \in [0, t_1).$$

Note that, due to the simple structure of the matrices A(d, s), if the norm of the FOM(m) residuals increases in the first q cycles, this increase will continue in later cycles (if qm < n, the coefficients s_{qm+1}, \ldots, s_n have to be chosen suitably), so that the method will indeed diverge. Note that if t_0 , the left endpoint of the support of α , is greater than zero the same construction applies by prescribing increasing residual norms for the system $(A+t_0I)x = b$. We summarize this result in the following corollary.

COROLLARY 3.1. Let f be a Stieltjes function, $m, n \in \mathbb{N}$ and let $\mu_1, \ldots, \mu_n \in \mathbb{C} \setminus \mathbb{R}_-$. Then there exist a matrix $A \in \mathbb{C}^{n \times n}$ and a vector $\mathbf{b} \in \mathbb{C}^n$ such that $\operatorname{spec}(A) = \{\mu_1, \ldots, \mu_n\}$ and the iterates of the restarted Arnoldi method with restart length m do not converge to $f(A)\mathbf{b}$.

Corollary 3.1 shows that a convergence analysis for the restarted Arnoldi method for matrix functions is not possible without additional assumptions on A or f and can not be based on eigenvalue information alone. In [4], a convergence analysis of the restarted Arnoldi method for A Hermitian positive definite and f a Stieltjes function is given in which it is proven that the method always converges to f(A)b, independent of the restart length m.

A more general class of matrices than the class of Hermitian positive definite matrices is the class of normal matrices with field of values in the right half plane (i.e., normal, *positive real* matrices). As we were only concerned with eigenvalues until now and our construction in general leads to non-normal matrices, one might suspect that for normal or positive real matrices, it might also be possible to prove convergence of restarted FOM/Arnoldi. However, by choosing A(d, s) with $d_i = d, s_i = s, i = 1, ..., n$ with suitably chosen values s > d, one can construct normal, positive real matrices for which Arnoldi's method for f(A)b diverges; cf. Section 7 in [4]. Therefore, the authors in [4] propose a restarted algorithm based on interpolation in harmonic Ritz values (which reduces to restarted GMRES in the linear system case, i.e., for $f(z) = z^{-1}$) for which convergence for matrices with spectrum in the right half plane can be proven (thus generalizing a well-known result for restarted GMRES).

4. Conclusions. We have shown that (and how) it is possible to construct a matrix $A \in \mathbb{C}^{n \times n}$ with arbitrary non-zero eigenvalues and a vector $b \in \mathbb{C}^n$ such that the norms of the residuals from the first $q \leq \frac{n}{m}$ cycles of FOM(m) attain any desired values, indicating that convergence analysis of FOM(m) based on eigenvalue information is not possible for non-Hermitian A. As corollaries, we proved that the result also generalizes to FOM without restarts and that for any prescribed eigenvalues there exists a matrix $A \in \mathbb{C}^{n \times n}$ with these eigenvalues and $b \in \mathbb{C}^n$ such that the restarted Arnoldi method for f(A)b does not converge (when f is a Stieltjes function).

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CONVERGENCE OF RESTARTED FOM

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