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ORIGINAL PAPER

Prescribing the behavior of early terminating GMRES and Arnoldi iterations

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Abstract We generalize and extend results of the series of papers by Greenbaum and Strakoš (IMA Vol Math Appl 60:95–118, 1994), Greenbaum et al. (SIAM J Matrix Anal Appl 17(3):465–469, 1996), Arioli et al. (BIT 38(4):636–643, 1998) and Duintjer Tebbens and Meurant (SIAM J Matrix Anal Appl 33(3):958–978, 2012). They show how to construct matrices with right-hand sides generating a prescribed GMRES residual norm convergence curve as well as prescribed Ritz values in all iterations, including the eigenvalues, and give parametrizations of the entire class of matrices and right-hand sides with these properties. These results assumed that the underlying Arnoldi orthogonalization processes are breakdown-free and hence considered non-derogatory matrices only. We extend the results with parametrizations of classes of general nonsingular matrices with right-hand sides allowing the early termination case and also give analogues for the early termination case of other results related to the theory developed in the papers mentioned above.

Keywords Arnoldi process · Early termination · GMRES method · Prescribed GMRES convergence · Arnoldi method · Prescribed Ritz values

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1 Introduction

We consider solving linear systems

$$Ax = b, \tag{1}$$

where A is a nonsingular matrix of order n and b a given nonzero n-dimensional vector with the GMRES algorithm; see [17]. Assuming that GMRES terminates at iteration n, the results of a series of papers by Arioli, Greenbaum, Pták and Strakoš [1, 7, 8] show that for an arbitrary sequence of n prescribed non-increasing residual norms there exists a class of matrices and right-hand sides that gives these residual norms. Moreover, the eigenvalues of those matrices can be chosen freely, showing that GMRES convergence for general matrices need not depend on the eigenvalues of A alone. The last paper [1] of the series shows explicitly how to construct matrices and right-hand sides with prescribed residual norms and eigenvalues, see Theorem 2.1 and Corollary 2.4 in that paper.

The GMRES algorithm is based on the Arnoldi process that generates upper Hessenberg matrices whose eigenvalues are known as Ritz values. In the Arnoldi method (see e.g. [2, 15]), these values are used as approximations of the eigenvalues of A. Based on the results of [1], the authors have shown in [5] that one can construct a class of matrices and right-hand sides with a prescribed residual norm convergence curve and prescribed Ritz values in *every* GMRES iteration, i.e. with in total $n(n+1)/2$ prescribed Ritz values for the first until the nth iteration. This shows that there exists a class of matrices and right-hand sides for which the Ritz values generated in the iterations of the Arnoldi method (or, equivalently, of the GMRES method) can be arbitrary and fully independent of the spectrum. In addition, they need not have any influence on the n residual norms generated in the GMRES method (except when they are zero; in that case GMRES stagnates).

All these results assume that the GMRES or Arnoldi method terminates at the iteration number n. Hence they assume, in particular, that A is non-derogatory and that its minimal polynomial is of degree n. We wish to extend these results to general, possibly derogatory nonsingular matrices with minimal polynomial of any degree smaller than or equal to n. Some popular types of preconditioners, like constraint preconditioners, give preconditioned matrices with minimal polynomials of a low degree, so that in exact arithmetic termination takes place after a few iterations, see, e.g., [9, 14]. It is therefore important to extend the above mentioned results to the early termination case when GMRES or Arnoldi terminates, in exact arithmetic, before iteration n. Note that for practical problems, in particular when n is large, one rarely computes n iterations of an Arnoldi or GMRES process. Often one will stop at a low iteration number with the value of the last subdiagonal entry of the Hessenberg matrix being below a given tolerance. For instance, the aim of most restarted versions of the Arnoldi method, in particular with polynomial filters [18], is to construct restart cycles where the subdiagonal entries of the Hessenberg matrices converge to zero quickly, see, e.g., [3, 10]. If the subdiagonal entry is small enough, this might in some cases correspond to early termination of the Arnoldi orthogonalization process in exact arithmetic.

The conclusion of the paper [1] already mentioned that it is desirable to formulate the parametrizations of matrices and right-hand sides of that paper also for the early termination case. Some aspects of the early termination case related to the minimal polynomial are pointed out in the next to last section of that paper. Results for early termination were also described in the Ph.D. thesis of Liesen [11]; see also [12]. It follows easily from these publications, that if a convergence curve terminating before iteration n is generated by GMRES, then it can also be generated with a matrix with a number of prescribed eigenvalues. However, the authors are not aware of a complete parametrization of all matrices and right-hand sides giving a prescribed non-increasing GMRES convergence curve terminating before or at iteration n and where the input matrix has prescribed eigenvalues. Not either are they aware of results on prescribing Ritz values for the early termination case. The corresponding parametrizations could be useful for theoretical investigations on convergence behavior of variants of the GMRES and Arnoldi methods. In this paper we will give these parametrizations and we also prove some additional properties for the case with early termination similar to those proven in [13] for the case with termination at iteration n.

The contents of the paper are as follows. Section 2 gives a new parametrization of the class of matrices and right-hand sides with a prescribed convergence curve and prescribed Ritz values with termination at iteration k for $k \leq n$. Section 3 generalizes the parametrization given in [1] to the case of early termination and elaborates on the relation to the minimal polynomial of A with respect to b. In Section 4 we prove some properties of the matrices involved in the parametrizations and give an expression for the GMRES iterates.

Throughout the paper we use the same notation as in [1] and [5] and e_i denotes the ith column of the identity matrix of appropriate dimension. The entry on position i, j of a matrix M is denoted as $m_{i,j}$. In this paper we assume exact arithmetic and with “the subdiagonal” and “subdiagonal entries” we will mean the (entries on the) first diagonal under the main diagonal.

2 Prescribed Ritz values and GMRES residual norms with early termination

The Arnoldi orthogonalization process applied to an input matrix $A \in \mathbb{C}^{n\times n}$ with an initial nonzero vector $b \in \mathbb{C}^n$ yields, if it does not terminate before the nth iteration, the so-called Arnoldi decomposition

$$AV = VH, \qquad Ve_1 = b/\|b\|, \quad V^*V = I_n, \tag{2}$$

where $H \in \mathbb{C}^{n\times n}$ is an unreduced upper Hessenberg matrix containing the coefficients of the Arnoldi recursion and $V \in \mathbb{C}^{n\times n}$ is the unitary matrix whose first k columns are basis vectors of the kth Krylov subspace $\mathcal{K}_k(A, b)$ defined as $\mathcal{K}_k(A, b) = \text{span}\{b, Ab, \ldots, A^{k-1}b\}$ for $1 \leq k \leq n$. If the orthogonalization process *does* break down at an iteration number k, $k < n$,this means that $h_{k+1,k} = 0$ and we obtain an Arnoldi decomposition which we will write as

$$AV_{n,k} = V_{n,k}H_k, \qquad V_{n,k}e_1 = b/\|b\|, \quad V_{n,k}^*V_{n,k} = I_k, \tag{3}$$

where $V_{n,k} \in \mathbb{C}^{n\times k}$ and $H_k \in \mathbb{C}^{k\times k}$ is an unreduced upper Hessenberg matrix of order k.

Since GMRES residual norms are invariant under unitary transformation of the linear system, the convergence curve generated by A and b in (2) is identical with the convergence curve generated by $H = V^*AV$ and $\|b\|e_1 = V^*b$. Similarly, the Ritz values in the Arnoldi method applied to A and b are the Ritz values obtained from H and e_1. Thus essentially all information about Ritz values and residual norms is contained in H. And naturally, because every iteration computes a new column of H, all information on the Ritz values and residual norms generated until the kth iteration must be contained in the first k columns of H. Moreover, with termination at iteration number k, the convergence curve and Ritz values generated by A and b in (3) are identical with those generated by H_k and $\|b\|e_1 = V_{n,k}^*b$ because the Hessenberg matrix obtained by applying the Arnoldi process to the pair $(H_k, \|b\|e_1)$ is simply H_k. We will therefore focuss on characterizing the Hessenberg matrices H_k that generate prescribed GMRES residual norms and prescribed Ritz values until the kth iteration. The next proposition shows how to generate prescribed Ritz values. It can be seen as a complement of [5, Proposition 2.1]; its proof is only a slight modification of the proof of [5, Proposition 2.1].

Proposition 1 *Let the set*

$$\begin{aligned}\mathcal{R} = \Big\{&\rho_1^{(1)},\\ &\left(\rho_1^{(2)},\ \rho_2^{(2)}\right),\\ &\vdots\\ &\left(\rho_1^{(k-1)},\ldots,\rho_{k-1}^{(k-1)}\right),\\ &(\lambda_1,\ldots\ldots\ldots,\lambda_k)\Big\}\end{aligned}$$

represent any choice of $k(k+1)/2$ complex Ritz values and H_k be an unreduced upper Hessenberg matrix. The following two assertions are equivalent:

1. *H_k has the spectrum $\lambda_1,\ldots,\lambda_k$ and its jth leading principal submatrix has eigenvalues $\rho_1^{(j)},\ldots,\rho_j^{(j)}$ for all $j = 1,\ldots,k-1$.*
2. *H_k has the form*

$$H_k = \begin{bmatrix} & g^T \\ 0 & T_{k-1}\end{bmatrix}^{-1} C^{(k)} \begin{bmatrix} & g^T \\ 0 & T_{k-1}\end{bmatrix}, \tag{4}$$

where $C^{(k)}$ is the companion matrix of the polynomial with roots $\lambda_1,\ldots,\lambda_k$

$$C^{(k)} = \begin{bmatrix} 0 & -\alpha_0 \\ I_{k-1} & \vdots \\ & -\alpha_{k-1}\end{bmatrix}, \qquad \prod_{j=1}^{k}(\lambda-\lambda_j) = \lambda^k + \sum_{j=0}^{k-1}\alpha_j\lambda^j,$$

the first entry g_1 *of the vector* g *is nonzero and* T_{k-1} *is a nonsingular upper triangular matrix of order* $k-1$ *whose entries satisfy*

$$\prod_{i=1}^{j}\left(\lambda-\rho_i^{(j)}\right)=g_{j+1}+\sum_{i=1}^{j}t_{i,j}\lambda^i$$

for $j=1,\dots,k-1$.

Proof Clearly, H_k in (4) is unreduced upper Hessenberg and its spectrum is $\lambda_1,\dots,\lambda_k$ by the definition of $C^{(k)}$. We will show that the spectrum of the $j\times j$ leading principal submatrix of H_k is $\rho_1^{(j)},\dots,\rho_j^{(j)}$ for $j<k$. Let U be the nonsingular upper triangular matrix

$$\begin{bmatrix} & g^T \\ 0 & T_{k-1}\end{bmatrix}$$

and let U_j denote the $j\times j$ leading principal submatrix of U. Also, for $i>j$, let $\tilde{u}_i$ denote the vector of the first j entries of the ith column of U^{-1}. The spectrum of the $j\times j$ leading principal submatrix of H_k is the spectrum of

$$[I_j,0]\,U^{-1}C^{(k)}U\begin{bmatrix} I_j\\ 0\end{bmatrix}=\begin{bmatrix} U_j^{-1} & \tilde{u}_{j+1} & \dots & \tilde{u}_k\end{bmatrix}\begin{bmatrix} 0\\ U_j\\ 0\\ \vdots\end{bmatrix}=\begin{bmatrix} U_j^{-1} & \tilde{u}_{j+1}\end{bmatrix}\begin{bmatrix} 0\\ U_j\end{bmatrix}.$$

It is also the spectrum of the matrix

$$U_j\begin{bmatrix} U_j^{-1} & \tilde{u}_{j+1}\end{bmatrix}\begin{bmatrix} 0\\ U_j\end{bmatrix}U_j^{-1}=\begin{bmatrix} I_j & U_j\tilde{u}_{j+1}\end{bmatrix}\begin{bmatrix} 0\\ I_j\end{bmatrix},$$

which is a companion matrix with last column $U_j\tilde{u}_{j+1}$. From

$$\begin{aligned}
e_{j+1} &= U_{j+1}U_{j+1}^{-1}e_{j+1}=\begin{bmatrix} & g_{j+1}\\ U_j & t_{1,j}\\ & \vdots\\ 0 & t_{j,j}\end{bmatrix}\begin{bmatrix} U_j^{-1} & \tilde{u}_{j+1}\\ & \\ 0 & 1/t_{j,j}\end{bmatrix}e_{j+1}\\
&=\begin{bmatrix} U_j\tilde{u}_{j+1}+\begin{bmatrix} g_{j+1}/t_{j,j}\\ t_{1,j}/t_{j,j}\\ \vdots\\ t_{j-1,j}/t_{j,j}\end{bmatrix}\\ \\ 1\end{bmatrix},
\end{aligned}$$

we obtain that the entries of $U_j\tilde{u}_{j+1}$ are the coefficients corresponding to λ^0 till λ^{j-1} of the monic polynomial with roots $\rho_1^{(j)},\dots,\rho_j^{(j)}$. If conversely, H_k is unreduced Hessenberg with the given spectrum and Ritz values, then it can always be decomposed in the form (4) by subsequently equating the columns of the equation

$$H_kU^{-1}=U^{-1}C^{(k)}$$

with the first column of U^{-1} being

$$U^{-1}e_1 = \frac{1}{g_1}e_1$$

for some nonzero number g_1. Then the claim follows with the first part of the proof. □

Assume we have given a vector g in (4) with first entry nonzero. According to the previous proposition, if the $(j+1)$st entry of g is nonzero, we can always define the jth column of T_{k-1} such that H_k has prescribed nonzero Ritz values $\rho_1^{(j)}, \ldots, \rho_j^{(j)}$. If the $(j+1)$st entry of g is zero, we can define the jth column of T_{k-1} such that $\rho_1^{(j)}, \ldots, \rho_j^{(j)}$ takes arbitrary values except for at least one zero value. In the next theorem we show that g can be chosen such that it forces any prescribed GMRES residual norms when GMRES is applied to H_k with right hand side $\|b\|e_1$. This immediately gives a parametrization of the class of matrices and right-hand sides such that GMRES terminates at iteration number k and generates residual norms and prescribed Ritz values in all iterations. The only restriction is that a zero Ritz value in some iteration implies a singular Hessenberg matrix and corresponds to stagnation in the parallel GMRES process, see e.g. [4, 6].

Theorem 1 *Consider a set of tuples of complex numbers*

$$\begin{aligned}\mathcal{R} = \Big\{&\rho_1^{(1)},\\ &\left(\rho_1^{(2)},\ \rho_2^{(2)}\right),\\ &\vdots\\ &\left(\rho_1^{(k-1)}, \ldots, \rho_{k-1}^{(k-1)}\right),\\ &(\lambda_1, \ldots\ldots\ldots, \lambda_k)\Big\},\end{aligned}$$

such that $(\lambda_1, \ldots, \lambda_k)$ *contains no zero number and k positive numbers*

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

such that $f(j-1) = f(j)$ *if and only if the j-tuple* $\left(\rho_1^{(j)}, \ldots,\ \rho_j^{(j)}\right)$ *contains a zero number. If A is a matrix of order* $n \geq k$ *and b a nonzero n-dimensional vector, then the following assertions are equivalent:*

1. *The GMRES method applied to A and right-hand side b with zero initial guess terminates at iteration number k and yields residuals* $r^{(j)},\ j = 0, \ldots, k-1$ *such, that*

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

   the spectrum of A contains the eigenvalues $\lambda_1, \ldots, \lambda_k$ *and* $\rho_1^{(j)}, \ldots, \rho_j^{(j)}$ *are the eigenvalues of the jth leading principal submatrix of the generated Hessenberg matrix for all* $j = 1, \ldots, k-1$.

2. *The matrix A and the right-hand side b are of the form*

$$A = V \begin{bmatrix} H_k & B \\ 0 & D \end{bmatrix} V^*, \qquad b = f(0)Ve_1, \tag{5}$$

where V is any unitary matrix and $B \in \mathbb{C}^{k\times(n-k)}$, $D \in \mathbb{C}^{(n-k)\times(n-k)}$ *are submatrices with arbitrary entries. The unreduced upper Hessenberg matrix* H_k *has the form*

$$H_k = \begin{bmatrix} & g^T \\ 0 & T_{k-1} \end{bmatrix}^{-1} C^{(k)} \begin{bmatrix} & g^T \\ 0 & T_{k-1} \end{bmatrix}, \tag{6}$$

with $C^{(k)}$ *being the companion matrix of the polynomial with roots* $\lambda_1, \ldots, \lambda_k$, *with the k-dimensional real vector g being defined as*

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

and with a nonsingular upper triangular matrix T_{k-1} *of order* $k-1$ *whose entries satisfy*

$$\prod_{i=1}^{j}\left(\lambda - \rho_i^{(j)}\right) = g_{j+1} + \sum_{i=1}^{j} t_{i,j}\lambda^i$$

for $j = 1, \ldots, k-1$.

Proof The case $k = 1$ is straightforward, hence we assume $k \geq 2$. We have to show two claims, namely that the generated Hessenberg matrix has the form (6) if and only if we have the prescribed Ritz values (including the eigenvalues $(\lambda_1, \ldots, \lambda_k)$ contained in the spectrum) of the first assertion and if and only if we have the prescribed GMRES residual norms of the first assertion. The first claim follows from Proposition 1: If we have the prescribed Ritz values (including the eigenvalues $(\lambda_1, \ldots, \lambda_k)$), the Hessenberg matrix generated by GMRES applied to A and b must have the form

$$\begin{bmatrix} & g^T \\ 0 & T_{k-1} \end{bmatrix}^{-1} C^{(k)} \begin{bmatrix} & g^T \\ 0 & T_{k-1} \end{bmatrix}$$

and, conversely, the Hessenberg matrix (6) generated by A and b has the prescribed Ritz values.

Let us consider the second claim on GMRES residual norms. We will use the following equivalence. Let $\hat{H}_k$ be the Hessenberg matrix obtained from an Arnoldi process terminating at iteration number k. Then if a QR decomposition $\hat{H}_k = Q_k R_k$ of $\hat{H}_k$ is computed with Givens rotations that zero out the subdiagonal entries of $\hat{H}_k$, the absolute values of the individual rotation parameters define the GMRES residual norms and vice versa. More precisely, if the jth subdiagonal entry was eliminated with Givens cosine c_j and sine s_j, then

$$\|r^{(j)}\| = \|b\| \prod_{i=1}^{j} |s_i| = f(0) \prod_{i=1}^{j} |s_i|, \tag{7}$$

and vice versa, see, e.g., [16, Section 6.5.5, p. 166].

First we prove the implication $2 \rightarrow 1$. If the Arnoldi process generates the decomposition $AV_{n,k} = V_{n,k}H_k$, where $V_{n,k}$ denotes the matrix containing the first k columns of V and where

$$H_k = \begin{bmatrix} g^T \\ 0 \;\, T_{k-1} \end{bmatrix}^{-1} C^{(k)} \begin{bmatrix} g^T \\ 0 \;\, T_{k-1} \end{bmatrix},$$

this means that the jth Krylov residual subspace $A\mathcal{K}_j(A, b)$ is spanned by the vectors $V_{n,k}H_k e_1, \ldots, V_{n,k}H_k e_j$ for all $j \le k$. The same subspace is spanned by the vectors $V_{n,k}H_k \hat{R}_k e_1, \ldots, V_{n,k}H_k \hat{R}_k e_j$ for any nonsingular upper triangular matrix $\hat{R}_k$ of size k. Consequently, the GMRES residual norms obtained with the Arnoldi decomposition $AV_{n,k} = V_{n,k}H_k$ are identical with those obtained when the decomposition is $AV_{n,k} = V_{n,k}H_k\hat{R}_k$. Now consider

$$\hat{R}_k \equiv \begin{bmatrix} g^T \\ 0 \;\, T_{k-1} \end{bmatrix}^{-1} (C^{(k)})^{-1} \begin{bmatrix} g_1 & 0 \\ 0 & T_{k-1} \end{bmatrix} C^{(k)}. \tag{8}$$

It can easily be checked that this matrix is nonsingular upper triangular. Therefore we can also analyze the residual norms obtained when the generated upper Hessenberg matrix is

$$\hat{H}_k \equiv H_k\hat{R}_k = \begin{bmatrix} 1 & -\hat{g}^T/g_1 \\ 0 & I \end{bmatrix} C^{(k)},$$

where $\hat{g} = [g_2, \ldots, g_k]^T$. We do this by investigating the Givens rotations used for a QR decomposition of $\hat{H}_k$. Let us zero out the first subdiagonal entry of the upper Hessenberg matrix $\hat{H}_k$. With $\hat{h}_{1,1} = -g_2/g_1$ and $\hat{h}_{2,1} = 1$ we obtain the Givens cosine and sine satisfying

$$|c_1| = \frac{|g_2/g_1|}{\sqrt{1 + (g_2/g_1)^2}}, \qquad |s_1| = \frac{1}{\sqrt{1 + (g_2/g_1)^2}}.$$

Thus

$$|s_1| = \frac{1}{\sqrt{1 + \frac{f(0)^2 - f(1)^2}{f(1)^2}}} = \frac{f(1)}{f(0)}$$

and with (7) we have $\|r^{(1)}\| = f(1)$ as desired. Now assume $|s_i| = \frac{f(i)}{f(i-1)}$ for $i = 1, \ldots, j$. Then the application of all previous j Givens rotations to the $(j+1)$st column of $\hat{H}_k$, that is to the vector $[-g_{j+2}/g_1, 0, \ldots, 0, 1, 0, \ldots, 0]^T$, yields a vector whose $(j+1)$st entry is $-\prod_{i=1}^{j}(-s_i)g_{j+2}/g_1$ and its $(j+2)$nd entry is 1. Then we obtain the Givens cosine and sine

$$|c_{j+1}| = \frac{\prod_{i=1}^{j}|s_i| g_{j+2}/g_1}{\sqrt{1 + \prod_{i=1}^{j}|s_i|^2 (g_{j+2}/g_1)^2}}, \qquad |s_{j+1}| = \frac{1}{\sqrt{1 + \prod_{i=1}^{j}|s_i|^2 (g_{j+2}/g_1)^2}}.$$

Thus

$$|s_{j+1}| = \left(1 + (g_{j+2}/g_1)^2 \prod_{i=1}^{j} |s_i|^2\right)^{-\frac{1}{2}} = \left(1 + g_{j+2}^2 f(j)^2\right)^{-\frac{1}{2}}$$
$$= \left(1 + \frac{f(j)^2 - f(j+1)^2}{f(j+1)^2}\right)^{-\frac{1}{2}} = \frac{f(j+1)}{f(j)}$$

and with (7) we have $\|r^{(j+1)}\| = f(j+1)$ as desired.

Now consider the implication $1 \to 2$. Let the Arnoldi decomposition generated with A and b be denoted

$$A\hat{V}_{n,k} = \hat{V}_{n,k} H_k.$$

Then the Hessenberg matrix H_k can always be decomposed in the form (4) by subsequently equating the columns of the equation

$$H_k U_k^{-1} = U_k^{-1} C^{(k)}$$

with the first column of U_k^{-1} being

$$U_k^{-1} e_1 = f(0) e_1$$

and by using the partitioning

$$U_k = \begin{bmatrix} & g^T \\ 0 & T_{k-1} \end{bmatrix}$$

of the resulting upper triangular matrix U_k. As seen in the implication $2 \to 1$, the Hessenberg matrix

$$\hat{H}_k \equiv H_k \hat{R}_k = \begin{bmatrix} 1 & -\hat{g}^T/g_1 \\ 0 & I \end{bmatrix} C^{(k)},$$

where $\hat{R}_k$ is as defined in (8), $\hat{g} = [g_2, \ldots, g_k]^T$ and $g_1 = 1/f(0)$, generates the same prescribed residual norms. They imply that the Givens rotations to zero out the subdiagonal of $\hat{H}_k$ satisfy

$$f(0) \prod_{i=1}^{j} |s_i| = f(j), \quad j = 1, \ldots, k-1,$$

see (7). Using the same argument as in the implication $2 \to 1$, we obtain that

$$g_1 = \frac{1}{f(0)}, \qquad |g_j|^2 = \frac{f(j-2)^2 - f(j-1)^2}{f(j-2)^2 f(j-1)^2}, \qquad j = 2, \ldots, k.$$

If D_k is a unitary diagonal matrix such that all entries of the vector g_k^{TD} are positive real and $\hat{V}$ a unitary matrix whose first k columns are the columns of $\hat{V}_{n,k}$, then we can write A as

$$A = \left(\hat{V} \begin{bmatrix} D_k & 0 \\ 0 & I \end{bmatrix}\right) \begin{bmatrix} D_k^* H_k D_k & D_k^* \hat{B} \\ 0 & D \end{bmatrix} \left(\hat{V} \begin{bmatrix} D_k & 0 \\ 0 & I \end{bmatrix}\right)^*$$

and with $V \equiv \hat{V} \begin{bmatrix} D_k & 0 \\ 0 & I \end{bmatrix}$ and $B \equiv D_k^* \hat{B}$ we obtain the claim. □

Theorem 1 gives a complete parametrization of the matrices with right-hand sides generating a prescribed GMRES residual norm history with prescribed Ritz values and allowing the early termination case. Of course, it holds for $k = n$, too. Note that with $k < n$ the system matrix A in (5) is allowed to be singular, because B, D are fully arbitrary. For example, B and D can both be zero matrices. For GMRES terminating at iteration $k < n$, the theorem prescribes not all but only k eigenvalues of A. The remaining eigenvalues can be prescribed additionally by choosing the spectrum of D accordingly.

With Theorem 1 we have a new and rather simple description of the class of matrices and right-hand sides we wish to characterize. The prescribed Ritz values and residual norms are easily recognized in this parametrization. We remark that the parametrization given in [5, Corollary 3.7] and formulated for $k = n$ only, describes the Hessenberg matrices with the same prescribed values in a different manner and could have been used as well. However, it does not clearly give the relation to the prescribed GMRES convergence curve. Yet another parametrization for the same prescribed values and for $k = n$ is given by [5, Theorem 3.6]. In this theorem, it is the prescribed Ritz values that are not easily recognized from the parametrization.

The latter theorem is formulated with the help of orthogonal bases for the Krylov *residual* subspaces $A\mathcal{K}_k(A, b)$, $1 \leq k \leq n$. In contrast, Theorem 1 and [5, Corollary 3.7] express the freedom in prescribing n GMRES residual norms and the Ritz values of all n iterations with a unitary matrix V whose first k columns represent, for all $1 \leq k \leq n$, an orthogonal basis for the Krylov space $\mathcal{K}_k(A, b)$ itself. They are therefore directly linked with the standard implementations of GMRES and Arnoldi which build up orthogonal bases for $\mathcal{K}_k(A, b)$, $k = 1, 2 \ldots.$

3 Early termination and the parametrization of [1]

In this section we address the parametrization formulated in [1]. The authors were concerned with prescribing GMRES residual norms and eigenvalues only, not Ritz values. The central question is how the following parametrization, which is the main result of [1], can be extended to the early termination case.

Theorem 2 (see [1]) *Assume we are given n nonnegative numbers*

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

and n complex numbers $\lambda_1, \ldots, \lambda_n$ *all different from 0. If A is a matrix of order n and b a nonzero n-dimensional vector, then the following assertions are equivalent:*

1. *The spectrum of A is* $\{\lambda_1, \ldots, \lambda_n\}$ *and GMRES applied to A and 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 matrix A is of the form*

$$A = WYC^{(n)}Y^{-1}W^*$$

and $b = Wh$, where W is any unitary matrix, the matrix Y is given by

$$Y = \begin{bmatrix} & R \\ h & \\ & 0 \end{bmatrix} \tag{9}$$

R being any nonsingular upper triangular matrix of order $n-1$, h a vector describing the convergence curve such that

$$\begin{aligned} h &= [\eta_1, \ldots, \eta_n]^T, \qquad \eta_k = \left(f(k-1)^2 - f(k)^2\right)^{1/2}, \quad k < n, \\ \eta_n &= f(n-1), \end{aligned} \tag{10}$$

and $C^{(n)}$ is the companion matrix corresponding to the polynomial $q(\lambda) = \prod_{j=1}^{n}(\lambda - \lambda_j)$.

One of the main ingredients of the proof in [1] for this theorem is a matrix equality related to the characteristic polynomial for A. If we define $K \equiv [b, Ab, \ldots, A^{n-1}b]$, then we have the equality

$$AK = KC^{(n)} \tag{11}$$

for the companion matrix $C^{(n)}$ corresponding to the characteristic polynomial $q(\lambda) = \prod_{j=1}^{n}(\lambda - \lambda_j)$ of A. This is because of $q(A) = 0$, which follows from the Cayley-Hamilton theorem. The proof in [1] essentially uses (11) in combination with the relation $K = WY$, which can be substituted in (11) to give the expression $A = WYC^{(n)}Y^{-1}W^*$ in the second assertion.

In this section we will try to extend Theorem 2 to the early termination case with a proof based on the same type of argumentation. The relation (11) will still hold due to the Cayley-Hamilton theorem, but it will involve rank deficient matrices K. It is then not clear whether an expression similar to $A = WYC^{(n)}Y^{-1}W^*$ can be derived. The rank deficiency might be eliminated by considering the minimal polynomial of A (which is equal to the characteristic polynomial when there is no early termination). If it is of degree ℓ, $\ell < n$, we have

$$AK_{n,\ell} = K_{n,\ell}C^{(\ell)}, \tag{12}$$

where $K_{n,\ell} \equiv [b, Ab, \ldots, A^{\ell-1}b]$ and $C^{(\ell)}$ is the companion matrix for the minimal polynomial of A. In [1, Section 3] it was recalled that there always exists a right hand side b such that GMRES terminates at iteration number ℓ and properties of the components of b in the Jordan canonical vector basis of A were investigated. This led to a characterization of right-hand sides giving Krylov subspaces whose dimension corresponds exactly to the degree of the minimal polynomial of A (called Krylov sequences of maximal length).

Of course, a complete generalization of Theorem 2 to the early termination case cannot exclude the situation where Krylov sequences do not reach maximal length. It is necessary to consider the minimal polynomial of A *with respect to* b, i.e. the polynomial p of minimum degree for which $p(A)b = 0$. GMRES terminates at iteration $k < n$ if and only if the minimal polynomial of A with respect to b has degree k. Then we can write

$$AK_{n,k} = K_{n,k}C_p^{(k)}, \tag{13}$$

where $C_p^{(k)}$ is the companion matrix for the minimal polynomial $p(\lambda)$ of A with respect to b. For our generalization we will use this type of matrix equality. Note that Theorem 1 of the previous section reveals the minimal polynomial of A with respect to b in the early termination case; it is the polynomial with roots $\lambda_1, \ldots, \lambda_k$ which takes the value one at the origin.

In the following theorem we give a direct, brute force generalization of Theorem 2 to the early termination case using an argumentation technique similar to that in the proof of [1, Theorem 2.1 and Proposition 2.4] and based on (13). It may look rather technical and lengthy, but we have chosen this formulation to emphasize all the instances where Theorem 2 is modified and to reveal the different phases leading to a new generalized parametrization. More precisely, we give three equivalent characterizations of early terminating linear systems with prescribed residual norms and spectrum. The first shows the relation with the minimal polynomial q of A. Thus if we prescribe termination at the iteration number corresponding to the degree of q, we obtain a Krylov sequence of maximal length. The second uses the minimal polynomial of A with respect to b, i.e. it uses (13). But as for the first characterization, this does not describe how to construct the matrices A generating a prescribed convergence curve terminating at the kth iteration. It only gives a condition that such a matrix A must satisfy. The last characterization also shows how to construct A. The theorem is formulated in such a way that it enables to prescribe all the distinct eigenvalues of the system matrix.

Theorem 3 *Assume we are given k positive numbers*

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

and m distinct complex numbers $\lambda_1, \ldots, \lambda_m$, all different from 0. The following assertions are equivalent for a matrix A of order n having m distinct eigenvalues and $n \geq k$, $n \geq m$:

1. $\lambda_1, \ldots, \lambda_m$ *are the eigenvalues of A and GMRES applied to A and b with a zero initial guess terminates at iteration number k and yields residuals $r^{(j)}$, $j = 0, \ldots, k-1$ such that*

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

2. *The vector b is of the form $b = W_{n,k}h_k$ where $W_{n,k} \in \mathbb{C}^{n\times k}$ has orthonormal columns and the real vector $h_k = [\eta_1, \ldots, \eta_k]^T$ has the entries*

$$\eta_j = \left(f(j-1)^2 - f(j)^2\right)^{1/2}, \quad 1 \leq j < k, \qquad \eta_k = f(k-1). \tag{14}$$

The matrix A satisfies the equation

$$AW_{n,k}Y_{k,\ell} = W_{n,k}Y_{k,\ell}C^{(\ell)}, \tag{15}$$

where $C^{(\ell)} \in \mathbb{C}^{\ell\times\ell}$ is the companion matrix corresponding to a polynomial

$$q(\lambda) = \Pi_{j=1}^{m}(\lambda - \lambda_j)^{\ell_j}$$

with integers $\ell_j > 0$ *such that* $\sum_{j=1}^{m} \ell_j = \ell \geq k$. *The matrix* $Y_{k,\ell} \in \mathbb{C}^{k \times \ell}$ *is given by*

$$Y_{k,\ell} = \begin{bmatrix} \eta_1 & & \\ \vdots & R_{k-1} & \hat{R} \\ \eta_k & 0 & 0 \end{bmatrix},$$

with R_{k-1} *being a nonsingular upper triangular matrix of order* $k-1$ *and* $\hat{R} \in \mathbb{C}^{k \times (\ell - k)}$ *being the matrix whose columns are given recursively through the relations*

$$\hat{R} e_i = Y_{k,\ell} \left[e_i \ \dots \ e_{i+k-1} \right] \begin{bmatrix} -\beta_0 \\ \vdots \\ -\beta_{k-1} \end{bmatrix}, \quad i = 1, \dots, \ell - k, \tag{16}$$

for coefficients $\beta_0, \dots, \beta_{k-1}$ *of a polynomial* $p(\lambda)$ *of degree* k *of the form*

$$p(\lambda) = \Pi_{j=1}^{m} (\lambda - \lambda_j)^{\tilde{\ell}_j} = \lambda^k + \sum_{j=0}^{k-1} \beta_j \lambda^j, \tag{17}$$

with $0 \leq \tilde{\ell}_j \leq \ell_j$.

3. *The vector* b *is of the form* $b = W_{n,k} h_k$ *with the same notation as in the previous assertion. The matrix* A *has the eigenvalues* $\lambda_1, \dots, \lambda_m$ *and satisfies the equation*

$$A W_{n,k} Y_k = W_{n,k} Y_k C_p^{(k)}, \tag{18}$$

where Y_k *is the principal submatrix of order* k *of* $Y_{k,\ell}$, *that is*

$$Y_k = \begin{bmatrix} h_k & \begin{matrix} R_{k-1} \\ 0 \end{matrix} \end{bmatrix}$$

and $C_p^{(k)}$ *is the companion matrix for the polynomial* $p(\lambda)$ *from* (17),

$$C_p^{(k)} = \begin{bmatrix} 0 & -\beta_0 \\ I_{k-1} & \vdots \\ & -\beta_{k-1} \end{bmatrix}. \tag{19}$$

4. *The vector* b *is of the form* $b = W_{n,k} h_k$ *with the same notation as in the previous assertion. The matrix* A *is of the form*

$$A = W \begin{bmatrix} Y_k C_p^{(k)} Y_k^{-1} & H_{1,2} \\ 0 & H_{2,2} \end{bmatrix} W^* \tag{20}$$

where W *is unitary and its first* k *columns are* $W_{n,k}$, $C_p^{(k)}$ *is the companion matrix for the polynomial* $p(\lambda)$ *from* (17) *(see also* (19)*),* Y_k *is the principal submatrix*

$$Y_k = \begin{bmatrix} h_k & \begin{matrix} R_{k-1} \\ 0 \end{matrix} \end{bmatrix}$$

of order k *of* $Y_{k,\ell}$ *and the union of the spectra of* $C_p^{(k)}$ *and* $H_{2,2}$ *is* $\{\lambda_1, \dots, \lambda_m\}$.

Proof Let us first prove that $1 \rightarrow 2$. Let $q(\lambda)$ be the minimal polynomial of A, $q(\lambda) = \Pi_{j=1}^{m}(\lambda - \lambda_j)^{\ell_j}$ with integers $\ell_j > 0$ such that $\sum_{j=1}^{m} \ell_j = \ell \geq k$, let

$$z = [\zeta_1, \ldots, \zeta_\ell]^T, \quad \text{where} \quad \frac{q(\lambda)}{(-1)^\ell \prod_{j=1}^{m} \lambda_j^{\ell_j}} = 1 - \left(\zeta_1 \lambda + \ldots + \zeta_\ell \lambda^\ell\right)$$

and define $K_{n,\ell} \equiv [b, Ab, \ldots, A^{\ell-1}b]$ and $B_{n,\ell} = [Ab, A^2b, \ldots, A^\ell b]$. From $q(A) = 0$ and $q(A)b = 0$ we get

$$AK_{n,\ell} = K_{n,\ell}C^{(\ell)}, \qquad AB_{n,\ell} = B_{n,\ell}C^{(\ell)}, \qquad b = B_{n,\ell}z. \tag{21}$$

Consider a QR decomposition of $B_{n,\ell}$, $B_{n,\ell} = \tilde{W}\tilde{R}_{n,\ell}$ with $\tilde{W} \in \mathbb{C}^{n\times n}$ unitary and $\tilde{R}_{n,\ell} \in \mathbb{C}^{n\times\ell}$ upper triangular. Because GMRES terminates at the kth iteration, $A^{k+i}b$ is linearly dependent on $Ab, \ldots, A^k b$ for all $i > 0$ and the rows $k+1$ until n of $\tilde{R}_{n,\ell}$ must be zero. The prescribed residual norms imply that

$$b = \tilde{W}\Gamma h, \quad h = \begin{pmatrix} h_k \\ 0 \end{pmatrix}$$

where Γ is a diagonal unitary matrix and h_k is defined by (14), see [7, p. 466]. Define $W \equiv \tilde{W}\Gamma$ and $R_{n,\ell} \equiv \Gamma^* \tilde{R}_{n,\ell}$. Then $b = Wh$ as desired. Furthermore we have

$$WR_{n,\ell}z = B_{n,\ell}z = b = Wh, \quad \text{i.e.} \quad R_{n,\ell}z = h. \tag{22}$$

Then from (21) we have $B_{n,\ell} = AK_{n,\ell} = K_{n,\ell}C^{(\ell)}$, i.e. $K_{n,\ell} = B_{n,\ell}[C^{(\ell)}]^{-1}$. With $B_{n,\ell} = WR_{n,\ell}$ it follows that $K_{n,\ell} = WR_{n,\ell}[C^{(\ell)}]^{-1}$ and with (21) that

$$AWR_{n,\ell}[C^{(\ell)}]^{-1} = \left(WR_{n,\ell}[C^{(\ell)}]^{-1}\right) C^{(\ell)}.$$

Define the matrix $Y_{n,\ell} \in \mathbb{C}^{n\times\ell}$ as $Y_{n,\ell} \equiv R_{n,\ell}[C^{(\ell)}]^{-1}$ and note that $[C^{(\ell)}]^{-1} = \begin{bmatrix} z & \begin{matrix} I_{\ell-1} \\ 0 \end{matrix} \end{bmatrix}$. Because $R_{n,\ell}z = h$, we have $Y_{n,\ell} = [h, R_{n,\ell}e_1, \ldots, R_{n,\ell}e_{\ell-1}]$. However, the rows $k+1$ to n of $Y_{n,\ell}$ must be zero (so are the corresponding rows of $R_{n,\ell}$) and thus $Y_{n,\ell}$ has the form

$$Y_{n,\ell} = \begin{bmatrix} \eta_1 & & \\ \vdots & R_{k-1} & \hat{R} \\ \eta_k & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

where R_{k-1} denotes the leading principal submatrix of order $k-1$ of $R_{n,\ell}$ and $\hat{R} \in \mathbb{C}^{k\times(\ell-k)}$ the remaining nonzero part of $R_{n,\ell}$. Denoting the first k columns of W by $W_{n,k}$ and the first k rows of $Y_{n,\ell}$ by $Y_{k,\ell}$, we have $W_{n,k}Y_{k,\ell} = WY_{n,\ell}$. Then we obtain (15) from

$$\begin{aligned} AW_{n,k}Y_{k,\ell} &= AWY_{n,\ell} = AWR_{n,\ell}[C^{(\ell)}]^{-1} = \left(WR_{n,\ell}[C^{(\ell)}]^{-1}\right) C^{(\ell)} \\ &= WY_{n,\ell}C^{(\ell)} = W_{n,k}Y_{k,\ell}C^{(\ell)}. \end{aligned}$$

Finally, because GMRES terminates at the kth iteration, the minimal polynomial of A with respect to b is a polynomial $p(\lambda)$ of degree k with $p(A)b = 0$ which is a divisor of $q(\lambda)$. If we write $p(\lambda)$ as $p(\lambda) = \lambda^k + \sum_{j=0}^{k-1} \beta_j \lambda^j$ and since h_k denotes the first k entries of h, then with $[b, Ab, \ldots, A^{k-1}b] = W_{n,k} \begin{bmatrix} h_k & \begin{matrix} R_{k-1} \\ 0 \end{matrix} \end{bmatrix}$ we have

$$
\begin{aligned}
A^k b &= -\sum_{j=0}^{k-1} \beta_j A^j b = W_{n,k} \begin{bmatrix} h_k & \begin{matrix} R_{k-1} \\ 0 \end{matrix} \end{bmatrix} \begin{bmatrix} -\beta_0 \\ \vdots \\ -\beta_{k-1} \end{bmatrix} \\
&= W_{n,k} Y_{k,\ell} \begin{bmatrix} e_1 & \ldots & e_k \end{bmatrix} \begin{bmatrix} -\beta_0 \\ \vdots \\ -\beta_{k-1} \end{bmatrix}.
\end{aligned}
$$

Because $A^k b = B_{n,\ell} e_k = W_{n,k} \hat{R} e_1$, this shows the first condition in (16) for $i = 1$. Recursively, for $i = 2, \ldots, \ell - k$, we obtain

$$
\begin{aligned}
A^{k+i-1} b &= A^{i-1}(A^k b) = -\sum_{j=0}^{k-1} \beta_j A^{j+i-1} b \\
&= \begin{bmatrix} b & Ab & \ldots & A^{k-1} b \end{bmatrix} \begin{bmatrix} \vdots \\ 0 \\ -\beta_0 \\ \vdots \\ -\beta_{k-i-1} \end{bmatrix} \\
&\quad - W_{n,k} \left(\beta_{k-i} \hat{R} e_1 + \ldots + \beta_{k-1} \hat{R} e_i \right).
\end{aligned}
$$

Using $A^{k+i-1} b = B_{n,\ell} e_{k+i-1} = W_{n,k} \hat{R} e_i$ one obtains the remaining conditions in (16).

Now, let us consider the implication 2 $\rightarrow$ 3. Denote the eigenpairs of $C^{(\ell)}$ by $\{\lambda_i, y_i\}$ for $i = 1, \ldots, m$. Then

$$
A W_{n,k} Y_{k,\ell} y_i = W_{n,k} Y_{k,\ell} C^{(\ell)} y_i = \lambda_i W_{n,k} Y_{k,\ell} y_i,
$$

hence λ_i is an eigenvalue of A for $i = 1, \ldots, m$ and these m distinct eigenvalues are the only distinct eigenvalues by the assumptions of the theorem. Let us introduce the notation $C_p^{(k)}$ for the companion matrix of the polynomial $p(\lambda)$ in (17) and Y_k for the first k columns of $Y_{k,\ell}$. Then if we equate the first k columns in (15) and $k < \ell$, we obtain

$$
A W_{n,k} Y_k = W_{n,k} Y_{k,\ell} \begin{bmatrix} e_2 & \ldots & e_{k+1} \end{bmatrix} = W_{n,k} Y_k C_p^{(k)}
$$

because of (16). In case $k = \ell$, the polynomials $q(\lambda)$ and $p(\lambda)$ are identical and we also obtain

$$
A W_{n,k} Y_k = W_{n,k} Y_{k,\ell} C^{(\ell)} \begin{bmatrix} e_1 & \ldots & e_k \end{bmatrix} = W_{n,k} Y_{k,\ell} C^{(k)} = W_{n,k} Y_k C_p^{(k)}.
$$

For proving that 3 $\rightarrow$ 4, assume that A satisfies (18). Then for a matrix $\tilde{W} \in \mathbb{C}^{n\times n-k}$ such that $[W_{n,k}, \tilde{W}]$ is unitary, A also satisfies

$$A[W_{n,k}, \tilde{W}]\begin{bmatrix} Y_k & 0 \\ 0 & I_{n-k} \end{bmatrix} = [W_{n,k}, \tilde{W}]\begin{bmatrix} Y_k C_p^{(k)} & W_{n,k}^* A\tilde{W} \\ 0 & \tilde{W}^* A\tilde{W} \end{bmatrix}.$$

With the notation $W \equiv [W_{n,k}, \tilde{W}]$, $H_{1,2} \equiv W_{n,k}^* A\tilde{W}$ and $H_{2,2} \equiv \tilde{W}^* A\tilde{W}$ this immediately gives (20). Assertion 3 also assumes that the distinct eigenvalues of A are $\lambda_1, \ldots, \lambda_m$. Therefore the union of the spectra of $C_p^{(k)}$ and $H_{2,2}$ is $\{\lambda_1, \ldots, \lambda_m\}$.

To prove 4 $\rightarrow$ 1, we first note that by assumption the union of the spectra of $C_p^{(k)}$ and $H_{2,2}$ is $\{\lambda_1, \ldots, \lambda_m\}$ and therefore A has distinct eigenvalues $\{\lambda_1, \ldots, \lambda_m\}$. Now it suffices to show that $W_{n,k}$ is a unitary basis of $A\mathcal{K}_k(A, b)$, see [7, p. 466]. We will prove this again by induction. We have, using (20),

$$\begin{aligned} Ab &= W\begin{bmatrix} Y_k C_p^{(k)} Y_k^{-1} & H_{1,2} \\ 0 & H_{2,2} \end{bmatrix} W^* b = W\begin{bmatrix} Y_k C_p^{(k)} Y_k^{-1} h_k \\ 0 \end{bmatrix} \\ &= W\begin{bmatrix} Y_k e_2 \\ 0 \end{bmatrix} = r_{1,1} w_1. \end{aligned}$$

Now let $A^{j-1}b = W_{n,k} Y_k e_j$ be the induction assumption. Then if $j < k$,

$$\begin{aligned} A^j b &= W\begin{bmatrix} Y_k C_p^{(k)} Y_k^{-1} & H_{1,2} \\ 0 & H_{2,2} \end{bmatrix} W^* W_{n,k} Y_k e_j = W\begin{bmatrix} Y_k C_p^{(k)} Y_k^{-1} Y_k e_j \\ 0 \end{bmatrix} \\ &= W\begin{bmatrix} Y_k e_{j+1} \\ 0 \end{bmatrix} \end{aligned}$$

and we have

$$W\begin{bmatrix} Y_k e_{j+1} \\ 0 \end{bmatrix} = W_{n,k}\begin{bmatrix} R_{k-1} e_j \\ 0 \end{bmatrix}$$

with $r_{j,j} \neq 0$. If $j = k$,

$$\begin{aligned} A^k b &= W\begin{bmatrix} Y_k C_p^{(k)} Y_k^{-1} & H_{1,2} \\ 0 & H_{2,2} \end{bmatrix} W^* W_{n,k} Y_k e_k = W\begin{bmatrix} Y_k C_p^{(k)} Y_k^{-1} Y_k e_k \\ 0 \end{bmatrix} \\ &= W\begin{bmatrix} Y_k C_p^{(k)} e_k \\ 0 \end{bmatrix} \end{aligned}$$

and with the definition (17) of the polynomial p, we have

$$W\begin{bmatrix} Y_k C_p^{(k)} e_k \\ 0 \end{bmatrix} = W_{n,k} Y_k \begin{bmatrix} -\beta_0 \\ \vdots \\ -\beta_{k-1} \end{bmatrix},$$

where the last entry of $Y_k \left[\beta_0, \ldots, \beta_{k-1}\right]^T$ is $\beta_0 \eta_k \neq 0$, see (14). □

The parametrization given by the previous theorem, that is, expression (20), resembles the parametrization of Section 2, that is, expression (5), in particular with respect to the partitioning of the involved Hessenberg matrices. An important difference is, that (20) gives no information on Ritz values before iteration number k. This information might be incorporated, but probably only in a rather complicated, implicit manner as is the case in [5, Theorem 3.6], which holds for termination at iteration n.

Because we do not prescribe all Ritz values, there are more degrees of freedom in (20) than in (5). Let us summarize them. The unitary matrix W in (20) is chosen arbitrarily. The non-singular upper triangular matrix R_{k-1} contained in Y_k is arbitrary. The companion matrix $C_p^{(k)}$ is constructed from an arbitrary polynomial $p(\lambda)$ of degree k whose roots belong to the prescribed distinct eigenvalues. The matrix $H_{1,2}$ is fully arbitrary and $H_{2,2}$ is arbitrary except that its spectrum must guarantee that the union of the spectrum with the roots of $p(\lambda)$ add up to the complete set of prescribed distinct eigenvalues.

4 Some additional properties

In this section we generalize some relations and properties satisfied by the matrices in the parametrization of [1] (see Theorem 1). They also give insight into the relation with the alternative parametrization of Section 2 based on orthogonal bases for Krylov subspaces instead of orthogonal bases for Krylov residual subspaces. Most results were proved in [13] for termination at iteration n. First, in the next two theorems, we prove some relations similar to those in [13, Theorem 3.1]. Throughout the section, k is always a positive integer smaller or equal to n indicating the iteration number when GMRES terminates.

Theorem 4 *The Krylov matrix $K_{n,k} = [b, Ab, \ldots, A^{k-1}b]$ can be factorized as*

$$K_{n,k} = V_{n,k}\hat{U}_k, \tag{23}$$

where $V_{n,k}$ is a matrix whose columns are orthonormal basis vectors of the Krylov subspace $\mathcal{K}_k(A, b)$ and $\hat{U}_k$ is an upper triangular matrix with a real positive diagonal. Moreover,

$$\hat{U}_k = \|b\| \left[\, e_1 \;\; H_k e_1 \;\; \ldots \;\; H_k^{k-1} e_1 \,\right]$$

and

$$\hat{U}_k^{-1} = U_k = \begin{bmatrix} & g^T \\ 0 & T_{k-1} \end{bmatrix}, \tag{24}$$

the entries of the last matrix being defined in Theorem 1 describing the parametrization of Section 2.

Proof We have $b = \|b\| V_{n,k}e_1$. Let us prove that $A^j V_{n,k} = V_{n,k} H_k^j,\ j = 1, \ldots, k-1$. This is true for $j = 1$ since we have $AV_{n,k} = V_{n,k}H_k$. Let us assume that $A^{j-1}V_{n,k} = V_{n,k}H_k^{j-1}$. Then,

$$A^j V_{n,k} = A\left(A^{j-1}V_{n,k}\right) = AV_{n,k}H_k^{j-1} = V_{n,k}H^j.$$

Therefore,

$$K_{n,k} = \left[\, b \;\; Ab \;\; \cdots \;\; A^{k-1}b \,\right] = \|b\| V_{n,k} \left[\, e_1 \;\; H_k e_1 \;\; \cdots \;\; H_k^{k-1} e_1 \,\right].$$

The matrix H_k being upper Hessenberg, one can prove easily that the matrix $\hat{U}_k$ is upper triangular. Moreover, since H_k has a positive first subdiagonal, the diagonal entries of $\hat{U}_k$ are positive. From $AK_{n,k} = K_{n,k}C_p^{(k)}$, we obtain that $H_k\hat{U}_k = \hat{U}_k C_p^{(k)}$. Therefore, $\hat{U}_k$ is the inverse of the upper triangular matrix involved in the factorization of H_k in Theorem 1. □

Equation (24) shows how the QR factorization (23) of the Krylov matrix $K_{n,k}$ is related to the generated Ritz values: The entries of every new column in the inverse of the R factor are the coefficients of a polynomial whose roots are the new Ritz values. A slightly modified result for termination at iteration n is [5, Lemma 3.1].

The next theorem addresses two more factorizations. It expresses the QR factorization of $AK_{n,k}$ in terms of the parametrization given in Theorem 3 and the factorization of the Hessenberg matrix in the alternative parametrization in Theorem 1 reveals several relations to the matrices in Theorem 3.

Theorem 5 *Using the notation of Theorem 3.2, the matrix $AK_{n,k}$ can be factorized as*

$$AK_{n,k} = W_{n,k}\tilde{\mathcal{R}}_k,$$

where the upper triangular matrix $\tilde{\mathcal{R}}_k$ is equal to $Y_k C_p^{(k)}$. The first $k-1$ columns of $\tilde{\mathcal{R}}_k$ are

$$\begin{bmatrix} & R_{k-1} & \\ 0 & \cdots & 0 \end{bmatrix},$$

the matrix R_{k-1} being defined in Theorem 3. The upper Hessenberg matrix H_k of Theorem 1 and Theorem 3 can be factorized as

$$H_k = Q_k \mathcal{R}_k \tag{25}$$

where

$$Q_k = V_{n,k}^* W_{n,k} = \hat{U}_k Y_k^{-1}$$

is upper Hessenberg and such that its first row is $h_k^T/\|h_k\|$. The matrix $\mathcal{R}_k$ is linked to $\tilde{\mathcal{R}}_k$ by

$$\tilde{\mathcal{R}}_k = \mathcal{R}_k \hat{U}_k,$$

the upper triangular matrix $\hat{U}_k$ being defined in Theorem 4.

Proof Using the same notation as in the first part of the proof of Theorem 3, we have

$$B_{n,k} = A\left[\, b \;\; Ab \;\; \cdots \;\; A^{k-1}b \,\right] = AK_{n,k} = WR_{n,k}.$$

The proof of Theorem 3 also shows that $K_{n,k} = W_{n,k}Y_k$. We have $K_{n,k}e_1 = W_{n,k}Y_k e_1 = W_{n,k}h_k = b$ and the equation follows for the remaining columns from the proof of the implication $4 \to 1$. Therefore,

$$\begin{aligned} AK_{n,k} &= WR_{n,k}, \\ &= W_{n,k}\tilde{\mathcal{R}}_k, \\ &= AW_{n,k}Y_k, \\ &= W_{n,k}Y_kC_p^{(k)}, \end{aligned}$$

from (18). This yields $\tilde{\mathcal{R}}_k = Y_kC_p^{(k)}$ and, from the structure of $C_p^{(k)}$, the first $k-1$ columns of $\tilde{\mathcal{R}}_k$ are

$$\begin{bmatrix} & R_{k-1} & \\ 0 & \cdots & 0 \end{bmatrix}.$$

We have

$$H_k = \hat{U}_kC_p^{(k)}\hat{U}_k^{-1}, \quad \hat{U}_k = V_{n,k}^*W_{n,k}Y_k,$$

from $K_{n,k} = V_{n,k}\hat{U}_k = W_{n,k}Y_k$. Let $Q_k = V_{n,k}^*W_{n,k}$ and $\mathcal{R}_k = Y_kC_p^{(k)}\hat{U}_k^{-1}$ which is an upper triangular matrix. Then,

$$H_k = V_{n,k}^*W_{n,k}Y_kC_p^{(k)}U_k^{-1} = Q_k\mathcal{R}_k,$$

and $\mathcal{R}_k\hat{U}_k = \tilde{\mathcal{R}}_k$. Moreover,

$$Q_kY_k = V_{n,k}^*W_{n,k}Y_k = \hat{U}_k.$$

Instead of considering the first row of Q_k, let us look at the first column of $Q_k^* = W_{n,k}^*V_{n,k}$,

$$Q_k^*e_1 = W_{n,k}^*V_{n,k}e_1 = W_{n,k}^*\frac{b}{\|b\|} = \frac{h_k}{\|h_k\|},$$

since $b = W_{n,k}h_k$ and $\|b\| = \|h_k\|$. Therefore, the first row of Q_k is real positive and describes the convergence of GMRES. □

We point out that in contrast with the situation of termination at iteration n, see [13, Theorem 3.1], the matrix Q_k in the factorization (25) of H_k needs not have orthogonal columns and therefore (25) is in general not a QR factorization. However, a unitary matrix can be obtained from Q_k by modifying its last column. The matrix Q_k also reveals relations between R_{k-1}, T_{k-1}, h_k and g. Let us recall the role of these matrices and vectors. The main freedom in forcing a GMRES convergence history according to (20) in Theorem 3 is, apart from the unitary change of variables expressed by W and the irrelevant submatrices $H_{1,2}$ and $H_{2,2}$, given by the upper triangular matrix R_{k-1}. The convergence history is determined by h_k. The analogs of R_{k-1} and h_k of Theorem 3 in the alternative parametrization of Theorem 1 are precisely T_{k-1} and g.

Finally let us consider the GMRES iterates. They can be expressed using the matrices in the parametrization of Section 3.

Theorem 6 *The GMRES iterates x_j, $j < k$ are given by*

$$x_j = W_{n,k} Y_k \begin{bmatrix} R_j^{-1} h_j \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad h_j = \begin{bmatrix} \eta_1 \\ \vdots \\ \eta_j \end{bmatrix},$$

where R_j is the leading principal submatrix of order j of R_{k-1}.

Proof The residual vector r_j at iteration $j < k$ can be written as $r_j = b - u$ where $u \in A\mathcal{K}_j$ yields the minimum

$$\|r_j\| = \min_{u \in A\mathcal{K}_j} \|b - u\|.$$

The solution is given by the orthogonal projection of b on $A\mathcal{K}_j$. But, we have an orthogonal basis of the subspace $A\mathcal{K}_j$ given by the columns of $W_{n,j}$ and the solution can be written as

$$u = W_{n,k} \left[\eta_1 \ \cdots \ \eta_j \ 0 \cdots 0 \right]^T.$$

Since $b = W_{n,k} h_k$ we obtain that the residual vector is

$$r_j = W_{n,k} \left[0 \cdots 0 \ \eta_{j+1} \ \cdots \ \eta_k \right]^T.$$

The corresponding iterate is given by

$$x_j = A^{-1}(b - r_j) = A^{-1} W_{n,k} \left[\eta_1 \ \cdots \ \eta_j \ 0 \cdots 0 \right]^T.$$

From (18) we have $A^{-1} W_{n,k} = W_{n,k} Y_k \left(C_p^{(k)} \right)^{-1} Y_k^{-1}$ and

$$x_j = W_{n,k} Y_k \left(C_p^{(k)} \right)^{-1} Y_k^{-1} \left[\eta_1 \ \cdots \ \eta_j \ 0 \cdots 0 \right]^T.$$

The inverse of the matrix Y_k being

$$Y_k^{-1} = \begin{bmatrix} 0 \ \cdots \ 0 & 1/\eta_k \\ R_{k-1}^{-1} & -R_{k-1}^{-1} h_{k-1}/\eta_k \end{bmatrix},$$

we obtain

$$x_j = W_{n,k} Y_k \left(C_p^{(k)} \right)^{-1} \begin{bmatrix} 0 \\ R_j^{-1} h_j \\ 0 \\ \vdots \\ 0 \end{bmatrix} = W_{n,k} Y_k \begin{bmatrix} R_j^{-1} h_j \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

using the structure of the inverse of the companion matrix. □

Note that $K_{n,k} = W_{n,k} Y_k = V_{n,k} \hat{U}_k$. Hence Theorem 6 explains what are the coordinates of the iterates x_j in the three bases given by $K_{n,k}$, $V_{n,k}$, $W_{n,k}$. It also shows that the GMRES iterates do not depend on the eigenvalues of the matrix A in the sense that, in the parametrization of Section 3, one can change the coefficients of the last column of the companion matrix without changing the iterates.

5 Conclusion

In this paper we have generalized the results proved in [1] and [5] to the case of early termination of the Arnoldi process. We showed how to construct, for such an Arnoldi process, matrices and right-hand sides having a prescribed GMRES residual norm convergence curve as well as prescribed Ritz values at all the iterations. This was done with the help of a novel parametrization in which both the prescribed residual norms and the prescribed Ritz values are easily recognized. We also addressed in detail the original parametrization in [1], which shows how to prescribe residual norms and eigenvalues, and we generalized it with a proof along the same lines as the proof in [1]. In our proof the minimal polynomial of A and the minimal polynomial of A with respect to b play an important role and we elaborated on this issue. Finally, we showed that a number of results for the matrices in the parametrization in [1], some of which appeared in [13], can be generalized to the early termination case, too, and formulated some relations between the different parametrizations that were derived in this paper.

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