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Analysis of acceleration strategies for restarted minimal residual methods

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Abstract

We provide an overview of existing strategies which compensate for the deterioration of convergence of minimum residual (MR) Krylov subspace methods due to restarting. We evaluate the popular practice of using nearly invariant subspaces to either augment Krylov subspaces or to construct preconditioners which invert on these subspaces. In the case where these spaces are exactly invariant, the augmentation approach is shown to be superior. We further show how a strategy recently introduced by de Sturler for truncating the approximation space of an MR method can be interpreted as a controlled loosening of the condition for global MR approximation based on the canonical angles between subspaces. For the special case of Krylov subspace methods, we give a concise derivation of the role of Ritz and harmonic Ritz values and vectors in the polynomial description of Krylov spaces as well as of the use of the implicitly updated Arnoldi method for manipulating Krylov spaces.

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1. Introduction

When Krylov subspace methods are employed for approximating the solution of large sparse or structured linear systems of equations

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

their stable implementation requires the construction of orthonormal bases of spaces which increase in dimension with each iteration step.

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If the operator A is Hermitian, or if the notion of orthogonality is suitably modified (see [3]), then these bases can be generated by short recurrence formulas, and this is the key to the efficiency of such widely used methods as CG, MINRES, BCG and QMR (see the monographs of Saad [18] and Greenbaum [9] for an exposition of these methods). For non-Hermitian A, however, a result of Faber and Manteuffel [6] implies that the construction of such bases which are orthonormal with respect to a *given* inner product generally involves orthogonalization against all previously generated vectors, as in algorithms such as FOM, GCR and GMRES. When the resulting storage and computation requirements make these methods impractical, they are often modified to compute an approximation with respect to a space of affordable size, after which the algorithm is *restarted* using the current approximation as the initial guess. Since restarting usually results in slower convergence (or the loss thereof altogether), much recent work has been devoted to compensating for the loss of information that occurs upon restarting by retaining a judiciously chosen part of the previously generated space.

We distinguish two fundamental strategies in existing work: One lies in identifying a subspace $\mathscr{U}$ which slows convergence, approximating this space and eliminating its influence from the iteration process. We shall refer to such a procedure as *deflation*. Such "problematic" subspaces are often identified as eigenspaces of A associated with eigenvalues of small magnitude, but other spaces may sometimes be better suited. Examples of this approach are the augmentation method introduced by Morgan [13,14] and analyzed by Saad [19,20] and Chapman and Saad [2]. Another device for eliminating $\mathscr{U}$ from the iteration is to introduce a preconditioner which inverts the orthogonal section of A onto $\mathscr{U}$, as proposed by Erhel et al. [5], Baglama et al. [1] and, with certain modifications, by Kharchenko and Yeremin [10]. The second fundamental strategy consists of identifying the essential orthogonality constraints by comparing angles between subspaces and maintaining orthogonality only against the most important subspace of a given dimension. Such a strategy is proposed by de Sturler [26].

The main intent of this paper is to provide an abstract framework which permits a uniform presentation as well as a comparison of these methods. Although proposed originally in association with Krylov subspace methods, these approaches can all be applied in the case of completely general correction spaces, as we show in Sections 2.3 and 2.4. In the Krylov subspace case, much emphasis has been placed on the approximation properties of invariant or nearly invariant correction spaces, particularly so in connection with augmentation strategies. We present several results which attempt to shed light on exactly when nearly invariant subspaces are useful. We also show that Krylov spaces can never contain invariant subspaces without being themselves invariant; similarly, an invariant space cannot contain a Krylov space without also containing the associated smallest invariant Krylov space. However, we show that augmenting by invariant subspaces does eliminate the components of the resulting residual in this space.

Since none of the results we shall derive are restricted to the finite-dimensional case, the setting of a separable Hilbert space $\mathscr{H}$ with inner product $(\cdot,\cdot)$ and associated norm $\|\cdot\|$ is the most natural, and we assume that A in (1) is a bounded linear operator.

Section 2 reviews the basic theory of iterative subspace correction methods for solving (1), which are based on the minimal residual (MR) and orthogonal residual (OR) approaches. We highlight the fundamental role of the angles between correction and approximation spaces as introduced in [3]. In addition, the necessary orthogonality relations are described, which must hold for the MR approximation with respect to two arbitrary subspaces to yield the MR approximation with respect

to the sum of these spaces, and it is shown how these orthogonality relations may be relaxed in an optimal way.

Section 3 reviews the implications of using Krylov spaces with regard to the simplification of the algorithms and the advantages of the polynomial representation of the residuals. We include new, much simplified derivations of the role of Ritz and harmonic Ritz values and vectors of A as well as how the recently developed implicitly restarted Arnoldi method can be used to restart the Arnoldi process without additional matrix–vector multiplications.

Section 4 discusses possible strategies for augmenting Krylov spaces and derives some results showing the limitations for augmenting Krylov spaces to obtain A-invariant subspaces. The remainder of Section 4 gives an overview of the most popular restart algorithms, beginning with restarted GMRES itself, for which we give a surprising example for which GMRES with longer restart lengths actually displays slower convergence than for shorter restart lengths. Next, the augmentation algorithm of Morgan is presented, and a new, much simplified proof is given that the augmented Krylov spaces are themselves Krylov spaces. In addition, we show that, at least in the case of exactly invariant subspaces, the augmentation approach is superior to the preconditioning algorithms of Erhel et al. [5] and Baglama et al. [1]. Finally, the optimal truncation algorithm of de Sturler is presented as an implementation of the selective orthogonalization strategy of Section 2.4.

2. Minimal and orthogonal residual methods

2.1. Definitions and basic theory

Given an initial guess $\boldsymbol{x}_0$ for the solution of (1) together with the associated residual vector $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$ and a sequence of nested *correction spaces* in $\mathscr{H}$,

$$\{\boldsymbol{0}\} = \mathscr{C}_0 \subset \mathscr{C}_1 \subset \mathscr{C}_2 \subset \cdots \subset \mathscr{C}_m \subset \mathscr{C}_{m+1} \subset \cdots$$

(for notational convenience, we assume that $\dim \mathscr{C}_m = m$), all methods we shall consider lead to iterates of the form $\boldsymbol{x}_m = \boldsymbol{x}_0 + \boldsymbol{c}_m$ with $\boldsymbol{c}_m \in \mathscr{C}_m$. They differ in the way the corrections $\boldsymbol{c}_m$ are selected from $\mathscr{C}_m$.

For the mth MR iterate $\boldsymbol{x}_m^{\mathrm{MR}} = \boldsymbol{x}_0 + \boldsymbol{c}_m^{\mathrm{MR}}$, the correction $\boldsymbol{c}_m^{\mathrm{MR}}$ is chosen from $\mathscr{C}_m$ to satisfy

$$\|\boldsymbol{b} - A\boldsymbol{x}_m^{\mathrm{MR}}\| = \|\boldsymbol{r}_0 - A\boldsymbol{c}_m^{\mathrm{MR}}\| = \min_{\boldsymbol{c}\in\mathscr{C}_m} \|\boldsymbol{r}_0 - A\boldsymbol{c}\|, \tag{2}$$

or equivalently, such that $A\boldsymbol{c}_m^{\mathrm{MR}}$ is the best approximation to $\boldsymbol{r}_0$ from the mth *approximation space* $\mathscr{W}_m := A\mathscr{C}_m$. As A is invertible, $\boldsymbol{c}_m^{\mathrm{MR}}$ and $\boldsymbol{x}_m^{\mathrm{MR}}$ are uniquely defined; specifically, they are characterized by

$$\boldsymbol{r}_m^{\mathrm{MR}} = \boldsymbol{b} - A\boldsymbol{x}_m^{\mathrm{MR}} = \boldsymbol{r}_0 - A\boldsymbol{c}_m^{\mathrm{MR}} \perp \mathscr{W}_m. \tag{3}$$

To define the OR iterates we introduce the *residual spaces*

$$\mathscr{V}_{m+1} := \operatorname{span}\{\boldsymbol{r}_0\} + \mathscr{W}_m, \quad m \geqslant 0, \tag{4}$$

the name of which derives from the fact that the residual $\boldsymbol{b} - A\boldsymbol{x}$ lies in the space $\operatorname{span}\{\boldsymbol{r}_0\} + A\mathscr{C}_m = \mathscr{V}_{m+1}$ whenever $\boldsymbol{x} = \boldsymbol{x}_0 + \boldsymbol{c}$, $\boldsymbol{c} \in \mathscr{C}_m$. We now set $\boldsymbol{x}_m^{\mathrm{OR}} = \boldsymbol{x}_0 + \boldsymbol{c}_m^{\mathrm{OR}}$ with $\boldsymbol{c}_m^{\mathrm{OR}} \in \mathscr{C}_m$ such that

$$\boldsymbol{r}_m^{\mathrm{OR}} = \boldsymbol{b} - A\boldsymbol{x}_m^{\mathrm{OR}} = \boldsymbol{r}_0 - A\boldsymbol{c}_m^{\mathrm{OR}} \perp \mathscr{V}_m. \tag{5}$$

In contrast to the MR approximation, the OR iterate may not exist for every m; when it does exist, which is the case if and only if $\mathscr{H} = \mathscr{W}_m \oplus \mathscr{V}_m^{\perp}$ (see [3, Proposition 2.2]), then it is uniquely determined.

Clearly, the mth MR approximant $\boldsymbol{x}_m^{\mathrm{MR}}$ as well as the mth OR approximation $\boldsymbol{x}_m^{\mathrm{OR}}$ coincide with the exact solution of (1) if and only if $A^{-1}\boldsymbol{r}_0 \in \mathscr{C}_m$ or equivalently, if and only if $\boldsymbol{r}_0 \in \mathscr{W}_m$. If such an index m exists we define

$$L := \min\{m : \boldsymbol{x}_m^{\mathrm{MR}} = A^{-1}\boldsymbol{b}\} = \min\{m : \boldsymbol{x}_m^{\mathrm{OR}} = A^{-1}\boldsymbol{b}\} \tag{6}$$

and otherwise set $L := \infty$. Alternative characterizations of the termination index L are

$$L = \min\{m : \boldsymbol{r}_0 \in \mathscr{W}_m\} = \min\{m : \mathscr{W}_m = \mathscr{V}_m\} = \min\{m : \mathscr{V}_m = \mathscr{V}_{m+1}\}. \tag{7}$$

The most popular implementations of both MR and OR methods rely on orthonormal bases $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}\}$ of the residual spaces $\mathscr{V}_{m+1}$ generated inductively by orthonormalizing $A\boldsymbol{c}_m$ against a (previously constructed) orthonormal basis $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m\}$ of $\mathscr{V}_m$ using the (modified) Gram–Schmidt algorithm. Here $\boldsymbol{c}_m$ is an arbitrary vector from $\mathscr{C}_m \setminus \mathscr{C}_{m-1}$ and $\boldsymbol{v}_1 = \boldsymbol{r}_0/\beta$ with $\beta := \|\boldsymbol{r}_0\|$. As long as $A\boldsymbol{c}_m \notin \mathscr{V}_m$, a new orthonormal vector $\boldsymbol{v}_{m+1}$ is generated and we may proceed to the next step. If, however, $A\boldsymbol{c}_m \in \mathscr{V}_m$, which is equivalent to $A\boldsymbol{c}_m \in \operatorname{span}\{\boldsymbol{r}_0, A\boldsymbol{c}_1, \ldots, A\boldsymbol{c}_{m-1}\}$, then the algorithm terminates in step m. Since $A\boldsymbol{c}_1, \ldots, A\boldsymbol{c}_m$ are linearly independent (because A is invertible), we see from (6) that $A\boldsymbol{c}_m \in \mathscr{V}_m$ is equivalent to $m = L$. In summary: The Gram–Schmidt process is well defined up to the last step, in which $\boldsymbol{x}_L^{\mathrm{MR}} = \boldsymbol{x}_L^{\mathrm{OR}} = A^{-1}\boldsymbol{b}$.

With $C_m := [\boldsymbol{c}_1 \boldsymbol{c}_2 \cdots \boldsymbol{c}_m]$ and $V_{m+1} := [\boldsymbol{v}_1 \boldsymbol{v}_2 \cdots \boldsymbol{v}_{m+1}]$, the first m orthonormalization steps establish the following Arnoldi-type decomposition of A:

$$AC_m = V_{m+1}\tilde{H}_m = V_m H_m + \eta_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{u}_m^{\mathrm{T}}, \tag{8}$$

(for $m = L$, we have $AC_L = V_L H_L$), where $\tilde{H}_m = [\eta_{j,k}] \in \mathbb{C}^{(m+1)\times m}$ is an upper Hessenberg matrix and $H_m := [I_m \quad \boldsymbol{0}]\tilde{H}_m \in \mathbb{C}^{m\times m}$ is the square matrix obtained by deleting the last row of $\tilde{H}_m$. The entries of $\tilde{H}_m$ are given by $\eta_{j,k} = (A\boldsymbol{c}_k, \boldsymbol{v}_j)$, $1 \leqslant k \leqslant j \leqslant m$, and $\eta_{k+1,k} = \|A\boldsymbol{c}_k - \sum_{j=1}^{k}\eta_{j,k}\boldsymbol{v}_j\| \geqslant 0$, with equality holding if and only if $k = L$. In other words, $\tilde{H}_m$ is an unreduced upper Hessenberg matrix (and hence of full rank m) as long as $m < L$. For $m = L$, $AC_L = V_L H_L$ implies that H_L is nonsingular because A is invertible and both C_L and V_L have rank L.

With respect to the orthonormal basis[1] V_{m+1} of $\mathscr{V}_{m+1}$, the vector $\boldsymbol{r}_0 = \beta\boldsymbol{v}_1 = V_{m+1}\beta\boldsymbol{u}_1^{(m+1)}$ has the coordinates $\beta\boldsymbol{u}_1^{(m+1)}$ ($\boldsymbol{u}_1^{(m+1)} \in \mathbb{C}^{m+1}$ denotes the first unit vector), while the approximation space $\mathscr{W}_m = A\mathscr{C}_m$ is represented by the column space of $\tilde{H}_m$. Consequently,

$$\min_{\boldsymbol{c}=C_m\boldsymbol{y}\in\mathscr{C}_m} \|\boldsymbol{r}_0 - A\boldsymbol{c}\| \quad \text{and} \quad \min_{\boldsymbol{y}\in\mathbb{C}^m} \|\beta\boldsymbol{u}_1^{(m+1)} - \tilde{H}_m\boldsymbol{y}\|_2$$

are equivalent problems ($\|\cdot\|_2$ denotes the Euclidean norm in $\mathbb{C}^{m+1}$).

For $\boldsymbol{x}_m^{\mathrm{MR}} = \boldsymbol{x}_0 + C_m\boldsymbol{y}_m^{\mathrm{MR}}$, condition (2) therefore leads to the least-squares problem

$$\|\beta\boldsymbol{u}_1^{(m+1)} - \tilde{H}_m\boldsymbol{y}_m^{\mathrm{MR}}\|_2 = \min_{\boldsymbol{y}\in\mathbb{C}^m} \|\beta\boldsymbol{u}_1^{(m+1)} - \tilde{H}_m\boldsymbol{y}\|_2. \tag{9}$$

Representing the OR iterate as $\boldsymbol{x}_m^{\mathrm{OR}} = \boldsymbol{x}_0 + C_m\boldsymbol{y}_m^{\mathrm{OR}}$, the Galerkin condition $\boldsymbol{r}_m^{\mathrm{OR}} \perp \mathscr{V}_m$ (cf. (5)) similarly leads to the linear system

$$\boldsymbol{0} = [I_m \quad \boldsymbol{0}](\beta\boldsymbol{u}_1^{(m+1)} - \tilde{H}_m\boldsymbol{y}_m^{\mathrm{OR}}) = \beta\boldsymbol{u}_1^{(m)} - H_m\boldsymbol{y}_m^{\mathrm{OR}}.$$

[1] For convenience we shall identify a basis $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m\}$ with its representation as the row vector $V_m = [\boldsymbol{v}_1 \cdots \boldsymbol{v}_m]$.

It can be shown (see [3, Remark 4.2]) that nonsingularity of H_m is equivalent to the existence of the OR approximation $\boldsymbol{x}_m^{\mathrm{OR}}$.

The orthonormal basis $\{\boldsymbol{v}_1,\ldots,\boldsymbol{v}_m,\boldsymbol{v}_{m+1}\}$ of the residual space $\mathscr{V}_{m+1}$ is the key to a simple representation of the quantities related to the OR approximation. For instance, $\boldsymbol{r}_m^{\mathrm{OR}}$ is a scalar multiple of $\boldsymbol{v}_{m+1}$, as follows immediately from $\mathscr{V}_{m+1}\ni\boldsymbol{r}_m^{\mathrm{OR}}\perp\mathscr{V}_m=\operatorname{span}\{\boldsymbol{v}_1,\ldots,\boldsymbol{v}_m\}$. Since $\boldsymbol{r}_m^{\mathrm{MR}}\perp\mathscr{W}_m$ (see (3)), an orthonormal basis $\{\hat{\boldsymbol{v}}_1,\ldots,\hat{\boldsymbol{v}}_m,\tilde{\boldsymbol{v}}_{m+1}\}$ of $\mathscr{V}_{m+1}$ with the analogous property with regard to the MR approximation should fulfill the condition $\operatorname{span}\{\hat{\boldsymbol{v}}_1,\ldots,\hat{\boldsymbol{v}}_m\}=\mathscr{W}_m$.

It was already noted by Paige and Saunders [16] that the construction of such a basis derives from the computation of a QR decomposition of $\tilde{H}_m$. Indeed, if

$$Q_m\tilde{H}_m=\begin{bmatrix}R_m\\ \boldsymbol{0}\end{bmatrix} \tag{10}$$

with $Q_m\in\mathbb{C}^{(m+1)\times(m+1)}$ unitary and $R_m\in\mathbb{C}^{m\times m}$ upper triangular (and nonsingular since $\tilde{H}_m$ has full rank), then

$$[\hat{V}_m\ \tilde{\boldsymbol{v}}_{m+1}]=[\hat{\boldsymbol{v}}_1\ \cdots\ \hat{\boldsymbol{v}}_m\ \tilde{\boldsymbol{v}}_{m+1}]:=V_{m+1}Q_m^{\mathrm{H}} \tag{11}$$

forms an orthonormal basis of $\mathscr{V}_{m+1}$. Moreover,

$$AC_m=V_{m+1}\tilde{H}_m=V_{m+1}Q_m^{\mathrm{H}}\begin{bmatrix}R_m\\ \boldsymbol{0}\end{bmatrix}=[\hat{V}_m\ \tilde{\boldsymbol{v}}_{m+1}]\begin{bmatrix}R_m\\ \boldsymbol{0}\end{bmatrix}=\hat{V}_mR_m \tag{12}$$

shows that $\hat{V}_m$ constitutes a basis of $\mathscr{W}_m=A\mathscr{C}_m$.

On the other hand, using the QR factorization (10) the least-squares problem (9) can be rewritten as

$$\begin{aligned}\min_{\boldsymbol{y}\in\mathbb{C}^m}\|\beta\boldsymbol{u}_1^{(m+1)}-\tilde{H}_m\boldsymbol{y}\|_2&=\min_{\boldsymbol{y}\in\mathbb{C}^m}\left\|Q_m^{\mathrm{H}}\left(\beta Q_m\boldsymbol{u}_1^{(m+1)}-\begin{bmatrix}R_m\\ \boldsymbol{0}\end{bmatrix}\boldsymbol{y}\right)\right\|_2\\ &=\min_{\boldsymbol{y}\in\mathbb{C}^m}\left\|\beta Q_m\boldsymbol{u}_1^{(m+1)}-\begin{bmatrix}R_m\\ \boldsymbol{0}\end{bmatrix}\boldsymbol{y}\right\|_2=\min_{\boldsymbol{y}\in\mathbb{C}^m}\left\|\begin{bmatrix}\beta\boldsymbol{q}_m-R_m\boldsymbol{y}\\ \beta q_{m+1,1}^{(m)}\end{bmatrix}\right\|_2,\end{aligned}$$

where $[\boldsymbol{q}_m^{\mathrm{T}}\ q_{m+1,1}^{(m)}]^{\mathrm{T}}=Q_m\boldsymbol{u}_1^{(m+1)}$ ($\boldsymbol{q}_m\in\mathbb{C}^m$) denotes the first column of Q_m. The unique solution of the above least-squares problem is $\boldsymbol{y}_m^{\mathrm{MR}}=\beta R_m^{-1}\boldsymbol{q}_m$ and the associated least-squares error is given by $\|\boldsymbol{r}_m^{\mathrm{MR}}\|=\beta|q_{m+1,1}^{(m)}|$.

A QR factorization of $\tilde{H}_m$ (and simultaneously the basis $[\hat{V}_m\ \tilde{\boldsymbol{v}}_{m+1}]$) can be computed inductively. The matrices Q_m, $m=1,2,\ldots,L-1$, are usually constructed as products of Givens rotations

$$Q_m=G_m\begin{bmatrix}Q_{m-1}&\boldsymbol{0}\\ \boldsymbol{0}&1\end{bmatrix}=G_m\begin{bmatrix}G_{m-1}&\boldsymbol{0}\\ \boldsymbol{0}&1\end{bmatrix}\begin{bmatrix}G_{m-2}&O\\ O&I_2\end{bmatrix}\cdots\begin{bmatrix}G_1&O\\ O&I_{m-1}\end{bmatrix} \tag{13}$$

where, for $k=1,2,\ldots,m$,

$$G_k:=\begin{bmatrix}I_{k-1}&\boldsymbol{0}&\boldsymbol{0}\\ \boldsymbol{0}&c_k&s_k\mathrm{e}^{-\mathrm{i}\phi_k}\\ \boldsymbol{0}&-s_k\mathrm{e}^{\mathrm{i}\phi_k}&c_k\end{bmatrix}\quad(c_k,s_k\geqslant 0,c_k^2+s_k^2=1,\phi_k\in\mathbb{R})$$

(for the choice of c_k, s_k and ϕ_k see, e.g., [3]).

In view of (11) we have

$$[\hat{V}_m\ \tilde{\boldsymbol{v}}_{m+1}]=V_{m+1}Q_m^{\mathrm{H}}=[V_m\ \boldsymbol{v}_{m+1}]\begin{bmatrix}Q_{m-1}^{\mathrm{H}}&\boldsymbol{0}\\ \boldsymbol{0}&1\end{bmatrix}G_m^{\mathrm{H}}=[\hat{V}_{m-1}\ \tilde{\boldsymbol{v}}_m\ \boldsymbol{v}_{m+1}]G_m^{\mathrm{H}},$$

i.e., with $\tilde{\boldsymbol{v}}_1 = \boldsymbol{v}_1$,

$$\hat{\boldsymbol{v}}_m = c_m \tilde{\boldsymbol{v}}_m + s_m \mathrm{e}^{-\mathrm{i}\phi_m} \boldsymbol{v}_{m+1},$$
$$\tilde{\boldsymbol{v}}_{m+1} = -s_m \mathrm{e}^{\mathrm{i}\phi_m} \tilde{\boldsymbol{v}}_m + c_m \boldsymbol{v}_{m+1}$$

for $m = 1, 2, \ldots, L-1$. For ease of notation, we further set $\hat{\boldsymbol{v}}_L := \tilde{\boldsymbol{v}}_L$.

Expressions for the entries of the unitary matrices $Q_m = [q_{k,j}^{(m)}]_{1 \leqslant k,j \leqslant m+1}$ can be obtained by forming the products of the Givens matrices in (13). For the first column, this yields

$$q_{k,1}^{(m)} = c_k \prod_{j=1}^{k-1} [-s_j \mathrm{e}^{\mathrm{i}\phi_j}] \quad (1 \leqslant k \leqslant m), \quad q_{m+1,1}^{(m)} = \prod_{j=1}^{m} [-s_j \mathrm{e}^{\mathrm{i}\phi_j}],$$

which immediately leads to the following result (cf. [3, Proposition 4.7]):

Proposition 2.1. *For the MR and OR residual vectors of index $m = 1, 2, \ldots, L-1$ there holds*:

$$\boldsymbol{r}_m^{\mathrm{MR}} = \beta q_{m+1,1}^{(m)} \tilde{\boldsymbol{v}}_{m+1} = \beta \prod_{j=1}^{m} [-s_j \mathrm{e}^{\mathrm{i}\phi_j}] \tilde{\boldsymbol{v}}_{m+1},$$
$$\boldsymbol{r}_m^{\mathrm{OR}} = -\beta \frac{s_m}{c_m} \mathrm{e}^{\mathrm{i}\phi_m} q_{m,1}^{(m-1)} \boldsymbol{v}_{m+1} = \frac{\beta}{c_m} \prod_{j=1}^{m} [-s_j \mathrm{e}^{\mathrm{i}\phi_j}] \boldsymbol{v}_{m+1},$$
$$\boldsymbol{r}_{m-1}^{\mathrm{MR}} - \boldsymbol{r}_m^{\mathrm{OR}} = \frac{\beta}{c_m} q_{m,1}^{(m-1)} \hat{\boldsymbol{v}}_m = \frac{\beta}{c_m} \prod_{j=1}^{m-1} [-s_j \mathrm{e}^{\mathrm{i}\phi_j}] \hat{\boldsymbol{v}}_m.$$

Proposition 2.1 shows that the *convergence history* of an MR method (and, in essence, also of an OR method) is completely determined by the entries in the first column of the matrices Q_m. To emphasize this point we assume a finite termination index L and note that the matrix H_L possesses the QR factorization $Q_{L-1} H_L = R_L$. Now $\boldsymbol{r}_0 \in \mathscr{W}_L$ (cf. (6)) can be represented as a linear combination of the orthonormal basis $\{\hat{\boldsymbol{v}}_1, \hat{\boldsymbol{v}}_2, \ldots, \hat{\boldsymbol{v}}_L\}$ of $\mathscr{W}_L$, $\boldsymbol{r}_0 = \beta V_L \boldsymbol{u}_1 = \beta V_L Q_{L-1}^{\mathrm{H}} Q_{L-1} \boldsymbol{u}_1 = \beta \hat{V}_L Q_{L-1} \boldsymbol{u}_1$, or equivalently, $\boldsymbol{r}_0 = \beta \sum_{j=1}^{L} q_{j,1}^{(L-1)} \hat{\boldsymbol{v}}_j = \beta \sum_{j=1}^{L} q_{j,1}^{(j)} \hat{\boldsymbol{v}}_j$ (where we set $q_{L,1}^{(L)} := q_{L,1}^{(L-1)}$). This equation states that, up to the factor β, the first column of the matrix Q_{L-1} contains the Fourier coefficients of the expansion of $\boldsymbol{r}_0$ with respect to the basis $\hat{V}_L$ of $\mathscr{W}_L$. The MR correction $\boldsymbol{c}_m^{\mathrm{MR}}$ is selected such that $A\boldsymbol{c}_m^{\mathrm{MR}}$ is the best approximation to $\boldsymbol{r}_0$ from $\mathscr{W}_m$, i.e.,

$$A\boldsymbol{c}_m^{\mathrm{MR}} = \beta \sum_{j=1}^{m} q_{j,1}^{(j)} \hat{\boldsymbol{v}}_j \quad \text{and} \quad \boldsymbol{r}_m^{\mathrm{MR}} = \boldsymbol{r}_0 - A\boldsymbol{c}_m^{\mathrm{MR}} = \beta \sum_{j=m+1}^{L} q_{j,1}^{(j)} \hat{\boldsymbol{v}}_j.$$

2.2. The angle connection

We saw in Proposition 2.1 that the sines and cosines of the Givens rotations used to construct the QR decomposition of $\tilde{H}_m$ completely determine the residuals of both the MR and the OR approach. In this section, we recall that these sines and cosines are not merely artifacts of the computational scheme but are the sines and cosines of the angles between $\mathscr{W}_m$ and $\mathscr{V}_m$, i.e., between the mth approximation and the mth residual space.

By

$$\varphi_m := \angle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, A\mathscr{C}_m) = \angle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \mathscr{W}_m) \quad (m = 1, 2, \ldots, L),$$

we denote the angle between $\boldsymbol{r}_{m-1}^{\mathrm{MR}}$ and $A\mathscr{C}_m = \mathscr{W}_m$.[2] Note that $0 < \varphi_m \leqslant \pi/2$ for $m = 1, 2, \ldots, L-1$, but $\varphi_L = 0$ because $\boldsymbol{r}_{L-1}^{\mathrm{MR}} \in \mathscr{V}_L = \mathscr{W}_L$.

The following relations are fundamental for our later investigations (for a proof, see [3, Section 2]).

Theorem 2.2. *For $m = 2, 3, \ldots, L$, there holds*

$$\sin\varphi_m = \frac{\sin\angle(\boldsymbol{r}_0, \mathscr{W}_m)}{\sin\angle(\boldsymbol{r}_0, \mathscr{W}_{m-1})} = \sin\angle(\mathscr{V}_m, \mathscr{W}_m),$$

where $\angle(\mathscr{V}_m, \mathscr{W}_m)$ denotes the largest canonical angle between the spaces $\mathscr{V}_m$ and $\mathscr{W}_m$.[3] *For the case of $m = 1$, we have $\mathscr{V}_1 = \mathrm{span}\{\boldsymbol{r}_0\}$ and thus $\sin\varphi_1 = \sin\angle(\mathscr{V}_1, \mathscr{W}_1)$. In addition, there holds*

$$\sin\angle(\boldsymbol{r}_0, \mathscr{W}_m) = \sin\varphi_1 \sin\varphi_2 \cdots \sin\varphi_m \quad (m = 1, 2, \ldots, L).$$

Moreover, the quantities c_m and s_m which define the Givens rotations G_m of (13) *are given by*

$$c_m = \cos\varphi_m \quad \textit{and} \quad s_m = \sin\varphi_m \quad (m = 1, 2, \ldots, L-1).$$

As a consequence of these assertions, we cite from [3, Section 3] how the vectors involved in the MR and OR approximations are related.

Theorem 2.3. *With $s_m = \sin\angle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, A\mathscr{C}_m)$ and $c_m = \cos\angle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, A\mathscr{C}_m)$ the MR and OR approximations with respect to the correction spaces $\mathscr{C}_m$ satisfy*

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = s_m\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\| = s_1 s_2 \ldots s_m\|\boldsymbol{r}_0\|, \tag{14}$$

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = c_m\|\boldsymbol{r}_m^{\mathrm{OR}}\|, \tag{15}$$

$$\boldsymbol{x}_m^{\mathrm{MR}} = s_m^2\boldsymbol{x}_{m-1}^{\mathrm{MR}} + c_m^2\boldsymbol{x}_m^{\mathrm{OR}} \quad \textit{and} \quad \boldsymbol{r}_m^{\mathrm{MR}} = s_m^2\boldsymbol{r}_{m-1}^{\mathrm{MR}} + c_m^2\boldsymbol{r}_m^{\mathrm{OR}}. \tag{16}$$

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[2] For the reader's convenience, we recall that the angle between a nonzero vector $\boldsymbol{x} \in \mathscr{H}$ and a subspace $\mathscr{U} \subset \mathscr{H}$, $\mathscr{U} \neq \{\boldsymbol{0}\}$, is defined by

$$\cos\angle(\boldsymbol{x}, \mathscr{U}) = \sup_{\boldsymbol{0}\neq\boldsymbol{u}\in\mathscr{U}} \cos\angle(\boldsymbol{x}, \boldsymbol{u}) = \sup_{\boldsymbol{0}\neq\boldsymbol{u}\in\mathscr{U}} \frac{|(\boldsymbol{x}, \boldsymbol{u})|}{\|\boldsymbol{x}\|\,\|\boldsymbol{u}\|}.$$

If $\mathscr{U}$ is finite dimensional this angle is also given by $\cos\angle(\boldsymbol{x}, \mathscr{U}) = \|P_{\mathscr{U}}\boldsymbol{x}\|/\|\boldsymbol{x}\|$, where $P_{\mathscr{U}}$ denotes the orthogonal projection onto $\mathscr{U}$, and consequently, $\angle(\boldsymbol{x}, \mathscr{U}) = 0$ if and only if $\boldsymbol{x} \in \mathscr{U}$. Moreover, $\sin\angle(\boldsymbol{x}, \mathscr{U}) = \|(I - P_{\mathscr{U}})\boldsymbol{x}\|/\|\boldsymbol{x}\|$, and consequently, $\angle(\boldsymbol{x}, \mathscr{U}) = \pi/2$ if and only if $\boldsymbol{x} \perp \mathscr{U}$.

[3] Given orthonormal bases $\{\boldsymbol{v}_j\}_{j=1}^m$ and $\{\boldsymbol{w}_j\}_{j=1}^m$ of two m-dimensional subspaces $\mathscr{V}$ and $\mathscr{W}$, then the cosines of the canonical angles between $\mathscr{V}$ and $\mathscr{W}$ are the singular values of the matrix of inner products $[(\boldsymbol{v}_j, \boldsymbol{w}_k)] \in \mathbb{C}^{m\times m}$. For later use, we remark that the sine of the largest canonical angle between the spaces $\mathscr{V}$ and $\mathscr{W}$ of equal dimension is given by $\|(I - P_{\mathscr{V}})P_{\mathscr{W}}\|$ (cf. [23, Theorem 4.37]).

For later use, we mention another important relation

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = \sin \angle(\boldsymbol{r}_0, A\mathscr{C}_m)\|\boldsymbol{r}_0\|, \tag{17}$$

which follows from (14) and Theorem 2.2.

In view of $s_m = \|\boldsymbol{r}_m^{\mathrm{MR}}\|/\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|$, i.e., $c_m = \sqrt{1 - \|\boldsymbol{r}_m^{\mathrm{MR}}\|^2/\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}$, (15) and (16) are easily rewritten as

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = \sqrt{1 - \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}}\,\|\boldsymbol{r}_m^{\mathrm{OR}}\|,$$

$$\boldsymbol{x}_m^{\mathrm{OR}} = \frac{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2 - \|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}\boldsymbol{x}_m^{\mathrm{MR}} - \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2 - \|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}\boldsymbol{x}_{m-1}^{\mathrm{MR}}.$$

As can be seen from the last two equations, the OR approximation and residual can easily be computed from the corresponding MR quantities. Moreover, since the latter can always be computed in a stable fashion, this is the preferable way of computing these quantities. (An exception is, of course, the Hermitian positive-definite case, in which the OR quantities may be computed stably and at lower expense than their MR counterparts by the classical method of conjugate gradients.)

2.3. Multiple subspace correction

Various recently developed enhancements of the basic MR and OR schemes presented above are based on introducing additional subspace corrections aside from those associated with the stepwise increasing correction spaces. Existing approaches include generating such auxiliary projections from spectral information on the operator A gained during the iteration process or from additional inner iteration or restart cycles. In addition, time and storage constraints often make it necessary to form these projections only approximately, while at the same time keeping this approximation as effective as possible. To better describe and compare these new developments, we first formulate the basic projection steps required to combine two subspace corrections and then, in Section 2.4, discuss how subspace information may be quantified in order to construct effective approximate projections.

Consider an initial approximation $\boldsymbol{x}_0$ to the solution of (1) for which we seek the MR approximation $\boldsymbol{x}_0 + \boldsymbol{c}$ with $\boldsymbol{c}$ selected from the correction space $\mathscr{C}$. We assume $\mathscr{C}$ to be the direct sum $\mathscr{C} = \mathscr{C}_1 \oplus \mathscr{C}_2$ of two spaces $\mathscr{C}_1$ and $\mathscr{C}_2$, and our goal is to obtain the MR approximation as the result of two separate projection steps involving $\mathscr{C}_1$ and $\mathscr{C}_2$, respectively. This task is equivalent to finding the best approximation $\boldsymbol{w} = A\boldsymbol{c} \in \mathscr{W} = A\mathscr{C} = \mathscr{W}_1 \oplus \mathscr{W}_2$ to $\boldsymbol{r}_0$, where $\mathscr{W}_j := A\mathscr{C}_j$, $j = 1, 2$.

If, in a first step, we obtain the best approximation $\boldsymbol{w}_1 = P_{\mathscr{W}_1}\boldsymbol{r}_0$ in $\mathscr{W}_1$, then the best approximation in $\mathscr{W}$ is obtained by introducing the orthogonal complement $\mathscr{Z} := \mathscr{W} \cap \mathscr{W}_1^{\perp}$ of $\mathscr{W}_1$ in $\mathscr{W}$, in terms of which $\mathscr{W}$ has the direct *and orthogonal* decomposition $\mathscr{W} = \mathscr{W}_1 \oplus \mathscr{Z}$. The global best approximation is now given by

$$\boldsymbol{w} := P_{\mathscr{W}}\boldsymbol{r}_0 = (P_{\mathscr{W}_1} + P_{\mathscr{Z}})\boldsymbol{r}_0 = P_{\mathscr{W}_1}\boldsymbol{r}_0 + P_{\mathscr{Z}}(I - P_{\mathscr{W}_1})\boldsymbol{r}_0. \tag{18}$$

The last expression shows that the contribution from the second projection consists of the orthogonal projection onto $\mathscr{Z}$ of the error $(I - P_{\mathscr{W}_1})\boldsymbol{r}_0$ of the first approximation.

Expressing all spaces in terms of $\mathscr{C}_1$ and $\mathscr{C}_2$ and noting that $\mathscr{Z} = (I - P_{A\mathscr{C}_1})A\mathscr{C}_2$, we conclude that the correction $\boldsymbol{c}$ associated with the residual approximation $\boldsymbol{w}$ satisfies

$$A\boldsymbol{c} = \boldsymbol{w} = P_{A\mathscr{C}_1}\boldsymbol{r}_0 + P_{(I-P_{A\mathscr{C}_1})A\mathscr{C}_2}(I - P_{A\mathscr{C}_1})\boldsymbol{r}_0.$$

The global correction is thus of the form $\boldsymbol{c} = \boldsymbol{c}_1 + \boldsymbol{d}$, where

$$A\boldsymbol{c}_1 = P_{A\mathscr{C}_1}\boldsymbol{r}_0, \tag{19}$$

$$A\boldsymbol{d} = P_{(I-P_{A\mathscr{C}_1})A\mathscr{C}_2}(I - P_{A\mathscr{C}_1})\boldsymbol{r}_0. \tag{20}$$

The solution $\boldsymbol{c}_1$ of (19) is simply the MR solution of the equation $A\boldsymbol{c} = \boldsymbol{r}_0$ with respect to the correction space $\mathscr{C}_1$. To obtain a useful representation of $\boldsymbol{d}$, we note that the right-hand side of (20) may be viewed as the MR approximation with respect to $\mathscr{C}_2$ of the equation

$$(I - P_{A\mathscr{C}_1})A\boldsymbol{c} = (I - P_{A\mathscr{C}_1})\boldsymbol{r}_0. \tag{21}$$

Lemma 2.4. *The operator $(I - P_{A\mathscr{C}_1})A$ restricted to $\mathscr{C}_2$ is a bijection from $\mathscr{C}_2$ to $\mathscr{Z}$.*

Proof. The assertion follows by showing that the operator in question is one-to-one: $(I - P_{A\mathscr{C}_1})A\tilde{\boldsymbol{c}} = \boldsymbol{0}$ for $\tilde{\boldsymbol{c}} \in \mathscr{C}_2$ implies $A\tilde{\boldsymbol{c}} \in A\mathscr{C}_1 \cap A\mathscr{C}_2 = \{\boldsymbol{0}\}$. □

The solution $\boldsymbol{d}$ of (20) yielding the second component of the combined correction $\boldsymbol{c}$ may thus be obtained by first determining the MR solution $\boldsymbol{c}_2$ of (21) and then evaluating

$$\boldsymbol{d} = A^{-1}(I - P_{A\mathscr{C}_1})A\boldsymbol{c}_2 = \boldsymbol{c}_2 - A^{-1}P_{A\mathscr{C}_1}A\boldsymbol{c}_2. \tag{22}$$

Lemma 2.5. *The operator $P := A^{-1}(I - P_{A\mathscr{C}_1})A$ restricted to $\mathscr{C}_2$ is the oblique projection onto $A^{-1}\mathscr{Z}$ along $\mathscr{C}_1$.*

Proof. The projection property follows immediately upon squaring P. Since A is nonsingular, $\mathrm{null}(P) = A^{-1}\mathscr{W}_1 = \mathscr{C}_1$ and $\mathrm{range}(P) = A^{-1}(A\mathscr{C}_1)^{\perp}$. Restricted to $\mathscr{C}_2$, the range reduces to the preimage under A of the orthogonal complement of $A\mathscr{C}_1$ with respect to $A\mathscr{C}_2$, i.e., $A^{-1}\mathscr{Z}$. □

At first glance, the evaluation of $\boldsymbol{d}$ as given in (22) appears to require a multiplication by A as well as the solution of another equation involving A with a right-hand side from $A\mathscr{C}_1$, in addition to the computation of the two projections. In fact, we show how $\boldsymbol{d}$ can be calculated inexpensively using quantities generated in the course of the two MR approximation steps.

Assume $\mathscr{C}_1$ has dimension m and that $C_m^{(1)} = [\boldsymbol{c}_1^{(1)} \cdots \boldsymbol{c}_m^{(1)}]$ denotes a basis of $\mathscr{C}_1$. The MR approximation $\boldsymbol{c}_1$ has the coordinate representation $\boldsymbol{c}_1 = C_m^{(1)}\boldsymbol{y}_1$ with $\boldsymbol{y}_1 \in \mathbb{C}^m$. We write the associated Arnoldi-type decomposition (8) as $AC_m^{(1)} = V_{m+1}^{(1)}\tilde{H}_m^{(1)}$. The QR decomposition $Q_m^{(1)}\tilde{H}_m^{(1)} = R_m^{(1)}$ (cf. (10)) makes available the Paige–Saunders basis $\hat{V}_m^{(1)}$ (cf. (11)), which forms an orthonormal basis of $A\mathscr{C}_1$. Note also that, in view of relation (12), there holds

$$A^{-1}\hat{V}_m^{(1)} = C_m^{(1)}R_m^{-1}. \tag{23}$$

The orthogonal projection $P_{A\mathscr{C}_1}$ may be expressed in terms of $\hat{V}_m^{(1)}$ as $\hat{V}_m^{(1)}[\hat{V}_m^{(1)}]^*$, (for $V = [\boldsymbol{v}_1 \cdots \boldsymbol{v}_m]$, $W = [\boldsymbol{w}_1 \cdots \boldsymbol{w}_m]$, we denote by VW^* the linear operator $\boldsymbol{x} \mapsto \sum_{j=1}^{m}(\boldsymbol{x}, \boldsymbol{w}_j)\boldsymbol{v}_j$) and, denoting the residual

of the first MR approximation by $\boldsymbol{r}_1 := \boldsymbol{r}_0 - A\boldsymbol{c}_1$, Eq. (21) may be written

$$(I - \hat{V}_m^{(1)}[\hat{V}_m^{(1)}]^*)A\boldsymbol{c} = \boldsymbol{r}_1.$$

The Arnoldi-type decomposition associated with Eq. (21) in terms of the basis $C_k^{(2)} = [\boldsymbol{c}_1^{(2)} \cdots \boldsymbol{c}_k^{(2)}]$ of the correction space $\mathscr{C}_2$ is given by

$$(I - \hat{V}_m^{(1)}[\hat{V}_m^{(1)}]^*)AC_k^{(2)} = V_{k+1}^{(2)}\tilde{H}_k^{(2)} \tag{24}$$

with the associated MR approximation $\boldsymbol{c}_2 = C_k^{(2)}\boldsymbol{y}_2$, for some $\boldsymbol{y}_2 \in \mathbb{C}^k$. The solution $\boldsymbol{d}$ of (20) as given in (22) can now be expressed as

$$\begin{aligned}\boldsymbol{d} &= \boldsymbol{c}_2 - A^{-1}P_{A\mathscr{C}_1}A\boldsymbol{c}_2 = C_k^{(2)}\boldsymbol{y}_2 - A^{-1}\hat{V}_m^{(1)}[\hat{V}_m^{(1)}]^*AC_k^{(2)}\boldsymbol{y}_2 \\ &= C_k^{(2)}\boldsymbol{y}_2 - C_m^{(1)}[R_m^{(1)}]^{-1}([\hat{V}_m^{(1)}]^*AC_k^{(2)})\boldsymbol{y}_2,\end{aligned}$$

which shows that the action of A^{-1} in (22) is effected by the inverse of the (small) triangular matrix $R_m^{(1)}$. We further observe that the evaluation of $A\boldsymbol{c}_2$ in (22) is accomplished through the $m \times k$ matrix $[\hat{V}_m^{(1)}]^*AC_k^{(2)}$, which is available at no extra cost as a by-product of the orthogonalization process carried out in the second MR step to obtain (24). In fact, (23) and (24) can be combined to yield the global decomposition

$$A[\, C_m^{(1)} \;\; C_k^{(2)} \,] = [\, \hat{V}_m^{(1)} \;\; V_{k+1}^{(2)} \,] \begin{bmatrix} R_m^{(1)} & [\hat{V}_m^{(1)}]^*AC_k^{(2)} \\ O & \tilde{H}_k^{(2)} \end{bmatrix} \tag{25}$$

with respect to $\mathscr{C}$. We summarize the coordinate representation of these two successive projections as

Theorem 2.6. *The MR approximation of the solution of $A\boldsymbol{c} = \boldsymbol{r}_0$ with respect to the correction space $\mathscr{C} = \mathscr{C}_1 \oplus \mathscr{C}_2$ is given by*

$$\boldsymbol{c} = C_m^{(1)}\boldsymbol{y}_1 + C_k^{(2)}\boldsymbol{y}_2 + C_m^{(1)}[R_m^{(1)}]^{-1}([\hat{V}_m^{(1)}]^*AC_k^{(2)})\boldsymbol{y}_2,$$

where the coefficient vectors $\boldsymbol{y}_1 \in \mathbb{C}^m$ and $\boldsymbol{y}_2 \in \mathbb{C}^k$ solve the least-squares problems

$$\| \|\boldsymbol{r}_0\|\boldsymbol{u}_1^{(m+1)} - \tilde{H}_m^{(1)}\boldsymbol{y}_1\|_2 \to \min_{\boldsymbol{y}_1 \in \mathbb{C}^m}, \quad \| \|\boldsymbol{r}_1\|\boldsymbol{u}_1^{(k+1)} - \tilde{H}_k^{(2)}\boldsymbol{y}_2\|_2 \to \min_{\boldsymbol{y}_2 \in \mathbb{C}^k}$$

and the matrices $C_m^{(1)}$, $C_k^{(2)}$, $\hat{V}_m^{(1)}$, $R_m^{(1)}$, $\tilde{H}_m^{(1)}$, and $\tilde{H}_k^{(2)}$ as well as the vector $\boldsymbol{r}_1$ are defined above.

2.4. Incomplete orthogonalization

The MR approximation applied to Eq. (21) in effect maintains orthogonality of the basis vectors of the residual space $\mathscr{V}_2$ against $\mathscr{W}_1 = A\mathscr{C}_1$. Computationally, this is manifested in the generation of the $m \times k$ matrix $(\hat{V}_m^{(1)})^*AC_k^{(2)}$ during the orthonormalization process (cf. (25)). In order to reduce the cost of both the storage of $\hat{V}_m^{(1)}$ and the work involved in the orthogonalization, we now consider performing the MR approximation to the solution of (21) only approximately in the sense that orthogonality is maintained only against a subspace of $\mathscr{W}_1$ of fixed dimension. When faced with the choice of such a subspace against which one can afford to maintain orthogonality, one possible

criterion is to select that space which results in the greatest reduction of the residual norm after the second MR approximation. Such an approach was proposed by de Sturler [25], and will be further described in Section 4.5.

As in Section 2.3, consider the MR approximation with respect to the correction space $\mathscr{C} = \mathscr{C}_1 \oplus \mathscr{C}_2$. The global MR approximation (18) consists of an MR approximation with respect to $\mathscr{C}_1$ followed by a second projection involving the orthogonal complement $\mathscr{Z} := (I - P_{\mathscr{W}_1})\mathscr{W}_2$ of $\mathscr{W}_1 = A\mathscr{C}_1$ with respect to $\mathscr{W}_2 = A\mathscr{C}_2$. The simplest approach of completely omitting the orthogonalization involved in constructing $P_{\mathscr{Z}}$ results in the combined approximation

$$\tilde{\boldsymbol{w}} := P_{\mathscr{W}_1}\boldsymbol{r}_0 + P_{\mathscr{W}_2}(I - P_{\mathscr{W}_1})\boldsymbol{r}_0,$$

in place of (18). This is the standard way of restarting an MR algorithm. Besides the two extremes of complete orthogonalization against $\mathscr{W}_1$ or none at all, it is also possible to orthogonalize against only a subspace $\tilde{\mathscr{W}}_1 \subset \mathscr{W}_1$ of dimension $\ell < m$, which brings up the problem of determining $\tilde{\mathscr{W}}_1$ such that, if orthogonality of the residual space $\mathscr{V}_2$ of the second MR approximation is maintained against $\tilde{\mathscr{W}}_1$, this results in the smallest residual norm over all ℓ-dimensional subspaces of $\mathscr{W}_1$.

The solution of this problem is greatly facilitated by a judicious choice of bases: Let $W_m^{(1)} = [\boldsymbol{w}_1^{(1)} \cdots \boldsymbol{w}_m^{(1)}]$ and $W_k^{(2)} = [\boldsymbol{w}_1^{(2)} \cdots \boldsymbol{w}_k^{(2)}]$ denote biorthogonal orthonormal bases of $\mathscr{W}_1$ and $\mathscr{W}_2$ ordered such that the (diagonal) $m \times k$ matrix $\Gamma := [W_m^{(1)}]^* W_k^{(2)}$ has nonincreasing nonnegative entries $\gamma_1, \ldots, \gamma_{\min\{m,k\}}$. The numbers γ_j are the cosines of the canonical angles between the spaces $\mathscr{W}_1$ and $\mathscr{W}_2$ (cf. [23, Chapter 4.5]) and therefore lie between zero and one. In addition, the assumption $\mathscr{C}_1 \cap \mathscr{C}_2 = \{\boldsymbol{0}\}$ along with the nonsingularity of A implies $\mathscr{W}_1 \cap \mathscr{W}_2 = \{\boldsymbol{0}\}$ and therefore each γ_j is strictly less than one.

An orthogonal basis of $\mathscr{Z}$ is given by $\hat{Z}_k := (I - W_m^{(1)}[W_m^{(1)}]^*)W_k^{(2)}$, and we set $\hat{Z}_k^* \hat{Z}_k = I - \Gamma^{\mathrm{H}}\Gamma =: \Sigma^2 \in \mathbb{C}^{k \times k}$, where $\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_k)$ with

$$\sigma_j = \begin{cases} \sqrt{1 - \gamma_j^2}, & 1 \leqslant j \leqslant \min\{k, m\}, \\ 1, & \text{otherwise}, \end{cases}$$

in view of which $Z_k := \hat{Z}_k \Sigma^{-1}$ is an orthonormal basis of $\mathscr{Z}$. Denoting $Z_k = [\boldsymbol{z}_1 \cdots \boldsymbol{z}_k]$, the following theorem expresses the effect of complete orthogonalization versus none at all:

Theorem 2.7. *In the notation introduced above and with* $\boldsymbol{r}_1 := (I - P_{\mathscr{W}_1})\boldsymbol{r}_0$, *there holds*

$$(P_{\mathscr{W}_2} - P_{\mathscr{Z}})\boldsymbol{r}_1 = \sum_{j=1}^{\min\{k,m\}} (\boldsymbol{r}_1, \boldsymbol{z}_j)\gamma_j(\sigma_j \boldsymbol{w}_j^{(1)} - \gamma_j \boldsymbol{z}_j), \tag{26}$$

$$\|(P_{\mathscr{W}_2} - P_{\mathscr{Z}})\boldsymbol{r}_1\|^2 = \sum_{j=1}^{\min\{k,m\}} \gamma_j^2 |(\boldsymbol{r}_1, \boldsymbol{z}_j)|^2. \tag{27}$$

Proof. Taking note of $\boldsymbol{r}_1 \perp \mathscr{W}_1$ and $W_k^{(2)} = Z_k \Sigma + W_m^{(1)} \Gamma$, we obtain

$$\begin{aligned} (P_{\mathscr{W}_2} - P_{\mathscr{Z}})\boldsymbol{r}_1 &= (W_k^{(2)}[W_k^{(2)}]^* - Z_k Z_k^*)\boldsymbol{r}_1 \\ &= ((Z_k \Sigma + W_m^{(1)}\Gamma)(Z_k \Sigma + W_m^{(1)}\Gamma)^* - Z_k Z_k^*)\boldsymbol{r}_1 \\ &= (W_m^{(1)}\Gamma\Sigma - Z_k \Gamma^{\mathrm{H}}\Gamma) Z_k^* \boldsymbol{r}_1, \end{aligned}$$

which is a reformulation of (26). Taking norms and noting $\mathscr{W}_1 \perp \mathscr{Z}$ as well as $\gamma_j^2 + \sigma_j^2 = 1$ yields (27):

$$\|(P_{\mathscr{W}_2} - P_{\mathscr{Z}})\boldsymbol{r}_1\|^2 = (Z_k^* \boldsymbol{r}_1)^*(\Sigma \Gamma^{\mathrm{H}} \Gamma \Sigma + (\Gamma^{\mathrm{H}}\Gamma)^2)(Z_k^* \boldsymbol{r}_1) = \|\Gamma Z_k^* \boldsymbol{r}_1\|_2^2. \qquad \square$$

We see that the difference between the two projections depends on the $\mathscr{Z}$-components of the approximation error $\boldsymbol{r}_1$ remaining after the first projection weighted by the corresponding cosines γ_j of the canonical angles between $\mathscr{W}_1$ and $\mathscr{W}_2$. Whenever $\gamma_j = 0$, the projection onto $\mathscr{W}_2$ would already have produced the correct component in the direction $\boldsymbol{z}_j$, whereas in case $\gamma_j = 1$ the associated basis vectors $\boldsymbol{w}_j^{(1)}$ and $\boldsymbol{w}_j^{(2)}$ are collinear and $P_{\mathscr{W}_2}$ would have yielded no component in direction $\boldsymbol{z}_j$.

To consider the case of incomplete orthogonalization, let $\tilde{\mathscr{W}}_1 \subset \mathscr{W}_1$ with $\dim \tilde{\mathscr{W}}_1 = \ell < m$. By orthogonalizing the basis of $\mathscr{W}_2$ against $\tilde{\mathscr{W}}_1$, we construct the orthogonal projection onto $\tilde{\mathscr{Z}} := (\tilde{\mathscr{W}}_1 \oplus \mathscr{W}_2) \cap \tilde{\mathscr{W}}_1^{\perp}$, which, applied to $\boldsymbol{r}_1$, yields the difference between $P_{\mathscr{W}_1}\boldsymbol{r}_0$ and the best approximation of $\boldsymbol{r}_0$ in $\tilde{\mathscr{W}}_1 \oplus \mathscr{W}_2$.

Theorem 2.8. *Of all ℓ-dimensional subspaces $\tilde{\mathscr{W}}_1 \subset \mathscr{W}_1$, that which minimizes $\|(P_{\tilde{\mathscr{Z}}} - P_{\mathscr{Z}})(I - P_{\mathscr{W}_1})\boldsymbol{r}_0\|$ over all $\boldsymbol{r}_0 \in \mathscr{H}$ is given by $\tilde{\mathscr{W}}_1 = \operatorname{span}\{\boldsymbol{w}_1^{(1)}, \ldots, \boldsymbol{w}_\ell^{(1)}\}$, and results in*

$$\|(P_{\tilde{\mathscr{Z}}} - P_{\mathscr{Z}})(I - P_{\mathscr{W}_1})\boldsymbol{r}_0\| = \|(P_{\tilde{\mathscr{Z}}} - P_{\mathscr{Z}})\boldsymbol{r}_1\| = \sum_{j=\ell+1}^{\min\{k,m\}} \gamma_j^2 |(\boldsymbol{r}_1, \boldsymbol{z}_j)|^2.$$

Proof. Any orthonormal basis $\tilde{W}_\ell^{(1)} = [\tilde{\boldsymbol{w}}_1 \cdots \tilde{\boldsymbol{w}}_\ell]$ of $\tilde{\mathscr{W}}_1$ has the form $\tilde{W}_\ell^{(1)} = W_m^{(1)} Q_1$ with a matrix $Q_1 \in \mathbb{C}^{m \times \ell}$ consisting of the first ℓ columns of a unitary $m \times m$ matrix $Q = [Q_1\, Q_2]$. We obtain a basis of $\tilde{\mathscr{Z}}$ by orthogonalizing $W_k^{(2)}$ against $\tilde{W}_\ell^{(1)}$:

$$\begin{aligned}
\hat{Z}_\ell &:= (I - \tilde{W}_\ell^{(1)}[\tilde{W}_\ell^{(1)}]^*)W_k^{(2)} = W_k^{(2)} - W_m^{(1)} Q_1 Q_1^{\mathrm{H}} \Gamma \\
&= (Z_k \Sigma + W_k^{(2)} \Gamma) - W_m^{(1)} Q_1 Q_1^{\mathrm{H}} \Gamma = Z_k \Sigma + W_m^{(1)}(I - Q_1 Q_1^{\mathrm{H}})\Gamma \\
&= Z_k \Sigma + W_m^{(1)} Q_2 Q_2^{\mathrm{H}} \Gamma.
\end{aligned}$$

Because of $0 \leqslant \gamma_j < 1$ the Hermitian matrix

$$\hat{Z}_\ell^* \hat{Z}_\ell = \Sigma^2 + \Gamma^{\mathrm{H}} Q_2 Q_2^{\mathrm{H}} \Gamma = I - \Gamma^{\mathrm{H}} Q_1 Q_1^{\mathrm{H}} \Gamma =: S^2$$

is positive definite and therefore possesses a square root S, by means of which we obtain an orthonormal basis of $\tilde{\mathscr{Z}}$ as $Z_\ell := \hat{Z}_\ell S^{-1}$. Again recalling $\boldsymbol{r}_1 \perp \mathscr{W}_1$, we obtain for the difference of the two projections

$$\begin{aligned}
(P_{\tilde{\mathscr{Z}}} - P_{\mathscr{Z}})\boldsymbol{r}_1 &= (Z_\ell Z_\ell^* - Z_k Z_k^*)\boldsymbol{r}_1 \\
&= (Z_k(\Sigma S^{-2}\Sigma - I) + W_m^{(1)}(Q_2 Q_2^{\mathrm{H}} \Gamma S^{-2} \Sigma)) Z_k^* \boldsymbol{r}_1. \qquad (28)
\end{aligned}$$

From the definition of S^2, we have

$$\Sigma S^{-2} \Sigma = (\Sigma^{-1} S^2 \Sigma^{-1})^{-1} = (I + \Sigma^{-1} \Gamma^{\mathrm{H}} Q_2 Q_2^{\mathrm{H}} \Gamma \Sigma^{-1})^{-1} =: (I + MM^{\mathrm{H}})^{-1}$$

with $M = \Sigma^{-1} \Gamma^{\mathrm{H}} Q_2$. We thus obtain

$$\Sigma S^{-2} \Sigma - I = (I + MM^{\mathrm{H}})^{-1} - I = -MM^{\mathrm{H}}(I + MM^{\mathrm{H}})^{-1}$$

as well as $Q_2Q_2^{\mathrm{H}}\Gamma S^{-2}\Sigma = Q_2M^{\mathrm{H}}(I+MM^{\mathrm{H}})^{-1}$, which we insert in (18) to obtain

$$\|(P_{\tilde{\mathscr{Z}}}-P_{\mathscr{Z}})\boldsymbol{r}_1\|^2 = (Z_k^*\boldsymbol{r}_1)[(I+MM^{\mathrm{H}})^{-1}MM^{\mathrm{H}}](Z_k^*\boldsymbol{r}_1). \tag{29}$$

This expression is minimized for all $\boldsymbol{r}_1$ – hence also for all $\boldsymbol{r}_0$ – by choosing Q_1 to minimize the largest eigenvalue of the Hermitian matrix $(I+MM^{\mathrm{H}})^{-1}MM^{\mathrm{H}}$ or, equivalently, that of $MM^{\mathrm{H}} = \Sigma^{-1}\Gamma^{\mathrm{H}}(I-Q_1Q_1^{\mathrm{H}})\Gamma\Sigma^{-1}$. The entries γ_j/σ_j of the $m\times k$ diagonal matrix $\Gamma\Sigma^{-1}$ are nonincreasing, hence the minimum occurs for

$$Q_1 = \begin{bmatrix} I_\ell \\ O \end{bmatrix}$$

and the assertion follows by inserting the resulting choice of M in (29). □

3. Corrections selected from Krylov spaces

The overwhelming majority of subspace correction methods for solving linear systems of equations employ correction spaces of a particularly simple structure known as *Krylov spaces* (or *Krylov subspaces*), which are defined by

$$\mathscr{K}_m := \mathscr{K}_m(A,\boldsymbol{r}_0) := \operatorname{span}\{\boldsymbol{r}_0, A\boldsymbol{r}_0, \ldots, A^{m-1}\boldsymbol{r}_0\}. \tag{30}$$

In this section we survey some of the ramifications of this choice. Section 3.1 discusses the advantages of using Krylov spaces, recalls their description in terms of polynomial spaces and states some technical lemmata. In Sections 3.2 and 3.3 we derive the polynomial counterparts of the OR and MR residual vectors and express their zeros as Ritz and harmonic Ritz values of A, respectively. Finally, we describe the implicitly restarted Arnoldi process of Sorensen [22] for later use as a technique for manipulating Krylov spaces.

3.1. Why Krylov subspaces?

One regard in which (30) is a reasonable choice for a correction space is that it enables the successive generation of the sequence $\{\mathscr{C}_m\}$ using only matrix–vector multiplication by A, an operation which is inexpensive for sparse or structured matrices. Moreover, note that $\mathscr{C}_m = \mathscr{K}_m(A,\boldsymbol{r}_0)$ results in the residual space (cf. (4))

$$\mathscr{V}_{m+1} = \operatorname{span}\{\boldsymbol{r}_0\} + A\mathscr{C}_m = \operatorname{span}\{\boldsymbol{r}_0\} + A\mathscr{K}_m = \mathscr{K}_{m+1},$$

i.e., the residual space $\mathscr{V}_{m+1}$ of index $m+1$ coincides with the correction space $\mathscr{C}_{m+1}$ of the next iteration, obviating the need to store two separate bases. This effectively halves the storage requirements of algorithms which are based on orthonormal bases of the residual spaces. As another consequence, the Arnoldi-type decomposition (8) now becomes a proper Arnoldi decomposition

$$AV_m = V_{m+1}\tilde{H}_m = V_mH_m + \eta_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{u}_m^{\mathrm{T}},$$

which identifies H_m as the *orthogonal section* of A onto $\mathscr{K}_m$, i.e., it represents the linear map $A_{\mathscr{K}_m} := P_{\mathscr{K}_m}A|_{\mathscr{K}_m} : \mathscr{K}_m \to \mathscr{K}_m$ with respect to the basis V_m.

Whether or not Krylov spaces are well suited as correction spaces will, as shown before, depend on the behavior of the angles $\angle(\mathscr{K}_m, A\mathscr{K}_m)$ as m approaches ∞. There are classes of problems

for which this behavior is very favorable. An example where the angles actually tend to zero, which, in view of (14), implies superlinear convergence of the MR and OR approximants, is given by second-kind Fredholm equations (cf. [3, Theorem 6.12]). On the other hand, there are matrix problems of dimension n for which $\angle(\mathscr{K}_m, A\mathscr{K}_m) = \pi/2$ $(m = 1, 2, \ldots, n-1)$, i.e., no Krylov subspace method is able to improve the initial residual until the very last step.

Finally, the theoretical investigation of Krylov subspace methods is greatly facilitated by the intimate connection between a Krylov space and an associated space of polynomials, as can be seen from the representation

$$\mathscr{K}_m(A, \boldsymbol{r}_0) = \{q(A)\boldsymbol{r}_0 : q \in \mathscr{P}_{m-1}\} \quad (m = 1, 2, \ldots),$$

where $\mathscr{P}_m$ denotes the space of all complex polynomials of degree at most m. The linear map

$$\mathscr{P}_{m-1} \ni q \mapsto q(A)\boldsymbol{r}_0 \in \mathscr{K}_m(A, \boldsymbol{r}_0)$$

is thus always surjective, but fails to be an isomorphism if and only if there exists a nonzero polynomial $q \in \mathscr{P}_{m-1}$ with $q(A)\boldsymbol{r}_0 = \boldsymbol{0}$. If such a polynomial exists (e.g., if A has finite rank) then there also exists a (unique) monic polynomial $c = c_{A,\boldsymbol{r}_0}$ of minimal degree for which $c(A)\boldsymbol{r}_0 = \boldsymbol{0}$, which is usually called the *minimal polynomial of* $\boldsymbol{r}_0$ *with respect to* A. It is easy to see that the degree of c equals the smallest integer m for which $\mathscr{K}_m = \mathscr{K}_{m+1}$ and thus coincides with the index L introduced in (6) (cf. also (7)),

$$\begin{aligned} L &= \min\{m \in \mathbb{N}_0 : \mathscr{K}_m = \mathscr{K}_{m+1}\} = \min\{m \in \mathbb{N}_0 : A^{-1}\boldsymbol{r}_0 \in \mathscr{K}_m\} \\ &= \min\{\deg q : q \text{ monic and } q(A)\boldsymbol{r}_0 = \boldsymbol{0}\}. \end{aligned} \tag{31}$$

In other words, $\mathscr{P}_{m-1}$ and $\mathscr{K}_m$ are isomorphic linear spaces if and only if $m \leqslant L$.

The positive-semidefinite sesquilinear form

$$(p, q) := (p(A)\boldsymbol{r}_0, q(A)\boldsymbol{r}_0) \qquad \left(p, q \in \mathscr{P}_\infty := \bigcup_{m \geqslant 0} \mathscr{P}_m\right) \tag{32}$$

is therefore positive definite when restricted to $\mathscr{P}_{L-1}$ and hence defines an inner product on this space. We will use the same notation $(\cdot, \cdot)$ for this inner product as for its counterpart on $\mathscr{H}$, as well as for derived quantities such as its induced norm $\|\cdot\| := (\cdot, \cdot)^{1/2}$ and the orthogonality relation $\perp$.

Since every vector $\boldsymbol{x} \in \boldsymbol{x}_0 + \mathscr{K}_m$ is of the form $\boldsymbol{x} = \boldsymbol{x}_0 + q_{m-1}(A)\boldsymbol{r}_0$ for some $q_{m-1} \in \mathscr{P}_{m-1}$, the corresponding residual $\boldsymbol{r} = \boldsymbol{b} - A\boldsymbol{x}$ can be written

$$\boldsymbol{r} = \boldsymbol{r}_0 - Aq_{m-1}(A)\boldsymbol{r}_0 = p_m(A)\boldsymbol{r}_0, \quad \text{where } p_m(\zeta) := 1 - \zeta q_{m-1}(\zeta) \in \mathscr{P}_m.$$

Note that the *residual polynomial* p_m satisfies the normalization condition $p_m(0) = 1$. Later in this section we will characterize the residual polynomials which belong to the OR and MR iterates as well as their zeros.

First, however, we provide three lemmata for later use. The first recalls a well-known (see, e.g., [15]) consequence of the Arnoldi decomposition $AV_m = V_m H_m + \eta_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{u}_m^{\mathrm{T}}$ of A (see (8)), the second states the conditions under which a Krylov space can have A-invariant subspaces. The third lemma shows that the orthogonal complement of a Krylov space with respect to an A-invariant subspace is itself a Krylov space.

Lemma 3.1. *For every polynomial* $q(\zeta) = \alpha_m\zeta^m + \cdots + \alpha_1\zeta + \alpha_0 \in \mathscr{P}_m$, *there holds*

$$q(A)\boldsymbol{r}_0 = \beta V_m q(H_m)\boldsymbol{u}_1 + \alpha_m\beta \prod_{j=1}^{m} \eta_{j+1,j}\boldsymbol{v}_{m+1},$$

where $\boldsymbol{u}_1 \in \mathbb{C}^m$ *denotes the first unit vector. In particular,* $q(A)\boldsymbol{r}_0 = \beta V_m q(H_m)\boldsymbol{u}_1$ *for every* $q \in \mathscr{P}_{m-1}$.

Lemma 3.2. *A Krylov space* $\mathscr{K}_m(A, \boldsymbol{r}_0)$ *contains an A-invariant subspace if and only if it is itself A-invariant.*

Proof. If $\mathscr{U} \subset \mathscr{K}_m(A, \boldsymbol{r}_0)$ is A-invariant, it must contain an eigenvector $\boldsymbol{z}$ of A. As an element of $\mathscr{K}_m$, $\boldsymbol{z}$ has a representation $\boldsymbol{z} = q_{m-1}(A)\boldsymbol{r}_0$ in terms of a nonzero polynomial q_{m-1} of degree at most $m-1$. Moreover, if λ denotes the eigenvalue of A associated with $\boldsymbol{z}$ and $p(\zeta) := (\zeta - \lambda)q_{m-1}(\zeta)$, then $p(A)\boldsymbol{r}_0 = \boldsymbol{0}$ and hence the degree of the minimal polynomial $c_{A,\boldsymbol{r}_0}$ of $\boldsymbol{r}_0$ with respect to A is at most m. Consequently $L = \deg c_{A,\boldsymbol{r}_0} \leqslant m$ and $\mathscr{K}_m$ is A-invariant (cf. (31)). □

Lemma 3.3. *Let* $\mathscr{U}$ *be an A-invariant subspace,* $\mathscr{T} = \mathscr{U}^\perp$ *its orthogonal complement and set* $A_{\mathscr{T}} := P_{\mathscr{T}}AP_{\mathscr{T}}$. *Then there holds for* $m = 1, 2, \ldots$

$$P_{\mathscr{T}}\mathscr{K}_m(A, \boldsymbol{r}_0) = \mathscr{K}_m(P_{\mathscr{T}}A, P_{\mathscr{T}}\boldsymbol{r}_0) = \mathscr{K}_m(A_{\mathscr{T}}, P_{\mathscr{T}}\boldsymbol{r}_0)$$

and

$$P_{\mathscr{T}}A\mathscr{K}_m(A, \boldsymbol{r}_0) = P_{\mathscr{T}}A\mathscr{K}_m(P_{\mathscr{T}}A, P_{\mathscr{T}}\boldsymbol{r}_0) = A_{\mathscr{T}}\mathscr{K}_m(A_{\mathscr{T}}, P_{\mathscr{T}}\boldsymbol{r}_0).$$

Proof. We have $P_{\mathscr{T}}AP_{\mathscr{U}} = O$, because $\mathscr{U}$ is A-invariant, and therefore

$$P_{\mathscr{T}}A = P_{\mathscr{T}}AP_{\mathscr{U}} + P_{\mathscr{T}}AP_{\mathscr{T}} = P_{\mathscr{T}}AP_{\mathscr{T}}.$$

An obvious induction now shows that for $k = 1, 2, \ldots$

$$P_{\mathscr{T}}A^k\boldsymbol{r}_0 = [P_{\mathscr{T}}A]^k\boldsymbol{r}_0 = [P_{\mathscr{T}}AP_{\mathscr{T}}]^k\boldsymbol{r}_0,$$

which proves the assertions. □

With regard to the notation used in Lemma 3.3, we remark that so far in this paper $A_{\mathscr{T}}$ has denoted the orthogonal section $P_{\mathscr{T}}A|_{\mathscr{T}}$ of A onto $\mathscr{T}$. We henceforth identify $P_{\mathscr{T}}AP_{\mathscr{T}}$ with $A_{\mathscr{T}}$ since $P_{\mathscr{T}}AP_{\mathscr{T}} = P_{\mathscr{T}}A|_{\mathscr{T}}$ on $\mathscr{T}$ and $P_{\mathscr{T}}AP_{\mathscr{T}} = O$ on $\mathscr{T}^\perp$.

3.2. OR residual polynomials

We first investigate the residual polynomials associated with the OR approach: $\boldsymbol{r}_m^{\mathrm{OR}} = p_m^{\mathrm{OR}}(A)\boldsymbol{r}_0$. The condition $\boldsymbol{r}_m^{\mathrm{OR}} \perp \mathscr{K}_m$ translates to $p_m^{\mathrm{OR}} \perp \mathscr{P}_{m-1}$, i.e., p_m^{OR} is an orthogonal polynomial of degree m (normalized to satisfy $p_m^{\mathrm{OR}}(0) = 1$). This also follows from the fact that $\boldsymbol{r}_m^{\mathrm{OR}}$ is a scalar multiple of $\boldsymbol{v}_{m+1}$, the last element of the orthonormal basis $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m, \boldsymbol{v}_{m+1}\}$ of $\mathscr{K}_{m+1}$ (cf. Section 2.1): The basis vector $\boldsymbol{v}_{m+1} \in \mathscr{K}_{m+1} \setminus \mathscr{K}_m$ has the form $\boldsymbol{v}_{m+1} = v_m(A)\boldsymbol{r}_0$ for some polynomial v_m of *exact* degree m, and p_m^{OR} must be a scalar multiple of v_m. Next, $\boldsymbol{v}_{m+1} \perp \mathscr{K}_m$, i.e., $v_m \perp \mathscr{P}_{m-1}$, and $\|\boldsymbol{v}_{m+1}\| = \|v_m\| = 1$ show that v_m is an orthonormal polynomial of degree m. We arrive at $p_m^{\mathrm{OR}} = v_m/v_m(0)$, a normalization which is, of course, only possible if v_m does not vanish at the origin.

The close relation of v_m to the characteristic polynomial of the Hessenberg matrix H_m will show that $v_m(0)=0$ is equivalent to H_m being singular: We know that $\boldsymbol{v}_{m+1}=v_m(A)\boldsymbol{r}_0$ spans the one-dimensional space $\mathscr{K}_{m+1}\cap\mathscr{K}_m^{\perp}$. If, on the other hand, $h_m(\zeta):=\det(\zeta I-H_m)\in\mathscr{P}_m$ denotes the characteristic polynomial of H_m, then by Lemma 3.1 and the Cayley–Hamilton theorem

$$(h_m(A)\boldsymbol{r}_0,\boldsymbol{v}_k)=\beta(V_m h_m(H_m)\boldsymbol{u}_1,\boldsymbol{v}_k)+\beta\prod_{j=1}^{m}\eta_{j+1,j}(\boldsymbol{v}_{m+1},\boldsymbol{v}_k)=0 \tag{33}$$

($k=1,2,\ldots,m$). In other words, $\boldsymbol{v}=h_m(A)\boldsymbol{r}_0$ belongs to $\mathscr{K}_{m+1}\cap\mathscr{K}_m^{\perp}$ and is therefore a scalar multiple of $\boldsymbol{v}_{m+1}$. We have thus shown that the polynomials v_m and h_m can differ only by a scalar factor. We summarize these observations in

Proposition 3.4. *The characteristic polynomial h_m of the Hessenberg matrix H_m is the (unique) monic orthogonal polynomial of degree m with respect to the inner product* (32). *The mth OR iterate exists if and only if $h_m(0)\neq 0$ and, in this case, the corresponding residual polynomial is given by $p_m^{\mathrm{OR}}=h_m/h_m(0)$.*

We next consider the zeros of p_m^{OR} or, equivalently, the eigenvalues of $H_m=V_m^*AV_m$, the orthogonal section $A_{\mathscr{K}_m}$ of A onto $\mathscr{K}_m$. Its eigenvalues θ_j, where

$$H_m\boldsymbol{y}_j=\theta_j\boldsymbol{y}_j \qquad \text{with } \boldsymbol{y}_j\in\mathbb{C}^m,\ \|\boldsymbol{y}_j\|_2=1 \tag{34}$$

are called the *Ritz values* of A (with respect to $\mathscr{K}_m$), while $\boldsymbol{z}_j:=V_m\boldsymbol{y}_j$ are the associated *Ritz vectors*.

As the eigenvalues of the nonderogatory matrix H_m, Ritz values have geometric multiplicity one. In case θ_j has algebraic multiplicity $k_j>1$, we denote by $\boldsymbol{y}_j^{(0)}=\boldsymbol{y}_j,\boldsymbol{y}_j^{(1)},\ldots,\boldsymbol{y}_j^{(k_j-1)}$ the principal vectors of H_m which belong to the eigenvalue θ_j, so that

$$H_m\boldsymbol{y}_j^{(\ell)}=\theta_j\boldsymbol{y}_j^{(\ell)}+\boldsymbol{y}_j^{(\ell-1)} \quad (\ell=1,\ldots,k_j-1)$$

and define $\boldsymbol{z}_j^{(0)}:=V_m\boldsymbol{y}_j^{(0)}$ *and* $\boldsymbol{z}_j^{(\ell)}:=V_m\boldsymbol{y}_j^{(\ell)}$ as the associated Ritz vectors.

Although all our conclusions remain valid in this more general case, we will assume in the remaining sections that H_m has m distinct eigenvalues to avoid the (notational) complication of requiring principal vectors.

The Ritz vectors constitute a basis of $\mathscr{K}_m$, and their residual vectors with regard to the eigenvalue problem (34) are given by

$$\begin{aligned}A\boldsymbol{z}_j-\theta_j\boldsymbol{z}_j=AV_m\boldsymbol{y}_j-\theta_jV_m\boldsymbol{y}_j&=V_mH_m\boldsymbol{y}_j+\eta_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{u}_m^{\mathrm{T}}\boldsymbol{y}_j-\theta_jV_m\boldsymbol{y}_j\\&=\eta_{m+1}(\boldsymbol{u}_m^{\mathrm{T}}\boldsymbol{y}_j)\boldsymbol{v}_{m+1}.\end{aligned} \tag{35}$$

This implies $A\boldsymbol{z}_j-\theta_j\boldsymbol{z}_j\perp\mathscr{K}_m$, which is the commonly used definition of Ritz values and Ritz vectors. We also observe that $(A-\theta_jI)\boldsymbol{z}_j\in\operatorname{span}\{\boldsymbol{v}_{m+1}\}=\operatorname{span}\{h_m(A)\boldsymbol{r}_0\}$ for every eigenvalue θ_j of H_m. As an element of $\mathscr{K}_m$, each Ritz vector $\boldsymbol{z}_j$ can be represented as $\boldsymbol{z}_j=z_j(A)\boldsymbol{r}_0$ with a polynomial $z_j\in\mathscr{P}_{m-1}$. Eq. (35) now implies $(\zeta-\theta_j)z_j(\zeta)=\tau_jh_m(\zeta)$ with $\tau_j\in\mathbb{C}\setminus\{0\}$, which we express as

$$z_j(\zeta)=\tau_j\frac{h(\zeta)}{\zeta-\theta_j}.$$

Proposition 3.5. *Let*

$$h_m(\zeta) = \prod_{j=1}^{J} (\zeta - \theta_j)^{k_j} \quad (\theta_i \neq \theta_j \text{ for } i \neq j)$$

denote the characteristic polynomial of H_m. The Ritz vectors $\boldsymbol{z}_j^{(\ell)}$ ($\ell = 0, \ldots, k_j - 1$) of A with respect to $\mathscr{K}_m(A, \boldsymbol{r}_0)$ have the form

$$\boldsymbol{z}_j^{(\ell)} = z_j^{(\ell)}(A)\boldsymbol{r}_0, \quad \text{where } z_j^{(\ell)}(\zeta) = h_m(\zeta) \sum_{i=0}^{\ell} \frac{\tau_{j,i}}{(\zeta - \theta_j)^{i+1}}$$

is a polynomial of exact degree $m-1$. Moreover, there holds

$$(A - \theta_j I)^{\ell+1} \boldsymbol{z}_j^{(\ell)} \in \operatorname{span}\{\boldsymbol{v}_{m+1}\} = \operatorname{span}\{h_m(A)\boldsymbol{r}_0\} = \operatorname{span}\{\boldsymbol{r}_m^{\mathrm{OR}}\},$$

where the last equality assumes that the mth OR iterate is defined.

3.3. MR residual polynomials

We now turn to the investigation of the residual polynomials p_m^{MR} associated with the MR residuals $\boldsymbol{r}_m^{\mathrm{MR}} = p_m^{\mathrm{MR}}(A)\boldsymbol{r}_0$. Obviously, these polynomials possess the following minimization property:

$$\|p_m^{\mathrm{MR}}\| = \min\{\|p\| : \deg p \leqslant m,\ p(0) = 1\}.$$

The condition $\boldsymbol{r}_m^{\mathrm{MR}} \perp A\mathscr{K}_m$ translates to $p_m^{\mathrm{MR}} \perp \zeta\mathscr{P}_{m-1}$, from which we deduce the *reproducing property* (36) of the MR residual polynomials: For any $q(\zeta) = q(0) + \sum_{j=1}^{m} \alpha_j \zeta^j \in \mathscr{P}_m$, there holds

$$(q, p_m^{\mathrm{MR}}) = (q(0), p_m^{\mathrm{MR}}) + \left(\sum_{j=1}^{m} \alpha_j \zeta^j, p_m^{\mathrm{MR}} \right) = q(0)(1, p_m^{\mathrm{MR}})$$

and because this identity is valid in particular for $q = p_m^{\mathrm{MR}}$ yielding $\|p_m^{\mathrm{MR}}\|^2 = p_m^{\mathrm{MR}}(0)(1, p_m^{\mathrm{MR}}) = (1, p_m^{\mathrm{MR}})$, we obtain

$$(q, p_m^{\mathrm{MR}}) = q(0)\|p_m^{\mathrm{MR}}\|^2 \quad \text{for all } q \in \mathscr{P}_m. \tag{36}$$

The coefficients of p_m^{MR} with respect to the orthonormal basis $\{v_0, v_1, \ldots, v_m\}$ of $\mathscr{P}_m$ are thus given by

$$(p_m^{\mathrm{MR}}, v_j) = \overline{v_j(0)}\|p_m^{\mathrm{MR}}\|^2$$

which, in view of $\|p_m^{\mathrm{MR}}\|^2 = \sum_{j=0}^{m} |v_j(0)|^2 \|p_m^{\mathrm{MR}}\|^4$, results in the expansion

$$p_m^{\mathrm{MR}}(\zeta) = \frac{\sum_{j=0}^{m} \overline{v_j(0)} v_j(\zeta)}{\sum_{j=0}^{m} |v_j(0)|^2} \tag{37}$$

(note that the denominator $\sum_{j=0}^{m} |v_j(0)|^2 \geqslant |v_0(0)|^2$ is always positive since v_0 is a nonzero constant). Furthermore, this representation shows that, since the polynomials v_j are of exact degree j, p_m^{MR} will have degree m if and only if $v_m(0) \neq 0$, i.e., if the OR polynomial of degree m exists. Otherwise $p_m^{\mathrm{MR}} = p_{m-1}^{\mathrm{MR}} = \cdots = p_k^{\mathrm{MR}}$ and $\deg p_m^{\mathrm{MR}} = k$, if k is the largest index less than m for which $v_k(0) \neq 0$.

To characterize the zeros of the MR residual polynomials in an analogous manner as for the OR residual polynomials, we begin by identifying them as the eigenvalues of an orthogonal section of A^{-1} onto the Krylov space

$$\mathscr{K}_m(A^{-1}, A^m \boldsymbol{r}_0) = \operatorname{span}\{A^m \boldsymbol{r}_0, A^{m-1}\boldsymbol{r}_0, \ldots, A\boldsymbol{r}_0\} = A\mathscr{K}_m(A, \boldsymbol{r}_0).$$

We denote the associated Arnoldi decomposition by

$$A^{-1}W_m = W_{m+1}\tilde{G}_m = W_m G_m + \gamma_{m+1,m}\boldsymbol{w}_{m+1}\boldsymbol{u}_m^{\mathrm{T}},$$

in which $\tilde{G}_m = [\gamma_{j,k}] \in \mathbb{C}^{(m+1)\times m}$ is an upper Hessenberg matrix, G_m the associated square Hessenberg matrix obtained by deleting the last row of $\tilde{G}_m$ and $W_{m+1} = [\boldsymbol{w}_1 \ \ldots \ \boldsymbol{w}_{m+1}]$ is an orthonormal basis of $\mathscr{K}_{m+1}(A^{-1}, A^m\boldsymbol{r}_0) = \mathscr{K}_{m+1}(A, \boldsymbol{r}_0)$. If we invoke Lemma 3.1 applied to this Arnoldi decomposition, we obtain

$$q(A^{-1})A^m\boldsymbol{r}_0 = W_m q(G_m)\beta_m \boldsymbol{u}_1^{\mathrm{T}} + \alpha_m\beta_m \prod_{j=1}^{m}\gamma_{j+1,j}\boldsymbol{w}_{m+1}$$

for any polynomial $q(\zeta) = \alpha_m\zeta^m + \cdots + \alpha_1\zeta + \alpha_0 \in \mathscr{P}_m$, where $\beta_m = \|A^m\boldsymbol{r}_0\|$. Denoting by g_m the characteristic polynomial of G_m, we conclude just as in (33) that

$$(g_m(A^{-1})A^m\boldsymbol{r}_0, \boldsymbol{w}_k) = 0, \quad k = 1, \ldots, m$$

and that $\boldsymbol{w} := g_m(A^{-1})A^m\boldsymbol{r}_0$ belongs to

$$\mathscr{K}_{m+1}(A^{-1}, A^m\boldsymbol{r}_0) \cap \mathscr{K}_m(A^{-1}, A^m\boldsymbol{r}_0)^{\perp} = \mathscr{K}_{m+1}(A, \boldsymbol{r}_0) \cap (A\mathscr{K}_m(A, \boldsymbol{r}_0))^{\perp}.$$

By virtue of its inclusion in the latter space, we conclude that the vector $\boldsymbol{w}$ is a scalar multiple of the MR residual vector $\boldsymbol{r}_m^{\mathrm{MR}}$. Moreover, we observe that $\hat{g}_m(\zeta) := g_m(\zeta^{-1})\zeta^m$ is a polynomial in ζ of degree at most m, which is sometimes denoted as the *reversed polynomial* of g_m since it is obtained from g_m by reversing the order of the coefficients. Since $\boldsymbol{w} = \hat{g}_m(A)\boldsymbol{r}_0$ and $\boldsymbol{r}_m^{\mathrm{MR}} = p_m^{\mathrm{MR}}(A)\boldsymbol{r}_0$ are collinear, the same is true for the associated polynomials. Furthermore, since the characteristic polynomial g_m is monic, it follows that $\hat{g}_m$ has value one at zero, and therefore that $\hat{g}_m$ coincides with p_m^{MR}. The desired zeros of p_m^{MR} thus coincide with those of $\hat{g}_m$, which are easily seen to be the reciprocals of the zeros of g_m, which in turn are the eigenvalues of G_m. Since this matrix is not readily available, we instead derive a matrix which is similar to G_m and therefore has the same characteristic polynomial.

Departing from $AV_m = \hat{V}_m R_m$ (cf. (12)), where $\hat{V}_m$ denotes the Paige–Saunders basis of $A\mathscr{K}_m(A, \boldsymbol{r}_0)$ and R_m is the triangular factor in the QR-factorization of $\tilde{H}_m$, we obtain

$$\begin{aligned} A^{-1}\hat{V}_m &= V_m R_m^{-1} = V_{m+1}\begin{bmatrix} R_m^{-1} \\ \boldsymbol{0} \end{bmatrix} = V_{m+1}Q_m^{\mathrm{H}}Q_m\begin{bmatrix} R_m^{-1} \\ \boldsymbol{0} \end{bmatrix} \\ &= [\hat{V}_m \quad \tilde{\boldsymbol{v}}_{m+1}]Q_m\begin{bmatrix} R_m^{-1} \\ \boldsymbol{0} \end{bmatrix} =: [\hat{V}_m \quad \tilde{\boldsymbol{v}}_{m+1}]\tilde{F}_m \\ &= \hat{V}_m F_m + \tilde{\boldsymbol{v}}_{m+1}\boldsymbol{f}_m^{\mathrm{T}} \quad \text{with } \tilde{F}_m \text{ partitioned as } \tilde{F}_m = \begin{bmatrix} F_m \\ \boldsymbol{f}_m^{\mathrm{T}} \end{bmatrix}. \end{aligned} \tag{38}$$

We note that both $\hat{V}_m$ and W_m are orthonormal bases of the same space $A\mathscr{K}_m$, which implies a relation of the form $\hat{V}_m = W_m T$ with a unitary matrix $T \in \mathbb{C}^{m\times m}$. Therefore,

$$F_m = \hat{V}_m^* A^{-1}\hat{V}_m = T^{\mathrm{H}}G_m T$$

and F_m is similar to G_m. The zeros $\tilde{\theta}_j$ of p_m^{MR} are therefore the reciprocals of the eigenvalues of F_m, determined by

$$\frac{1}{\tilde{\theta}_j}\hat{\boldsymbol{y}}_j = F_m\hat{\boldsymbol{y}}_j = [I_m \quad \boldsymbol{0}]Q_m\begin{bmatrix} R_m^{-1} \\ \boldsymbol{0} \end{bmatrix}\hat{\boldsymbol{y}}_j = [I_m \quad \boldsymbol{0}]Q_m\begin{bmatrix} I_m \\ \boldsymbol{0} \end{bmatrix}R_m^{-1}\hat{\boldsymbol{y}}_j =: \hat{Q}_m R_m^{-1}\hat{\boldsymbol{y}}_j,$$

or equivalently, as solution of the generalized eigenvalue problem

$$R_m\tilde{\boldsymbol{y}}_j = \tilde{\theta}_j\hat{Q}_m\tilde{\boldsymbol{y}}_j, \quad \tilde{\boldsymbol{y}}_j := R_m^{-1}\hat{\boldsymbol{y}}_j.$$

The matrix $\hat{Q}_m$ is obtained by deleting the last row and column of Q_m, which, by (13), yields

$$\hat{Q}_m = \begin{bmatrix} I_{m-1} & \boldsymbol{0} \\ \boldsymbol{0} & c_m \end{bmatrix} G_{m-1}\begin{bmatrix} G_{m-2} & \boldsymbol{0} \\ \boldsymbol{0} & 1 \end{bmatrix}\cdots\begin{bmatrix} G_1 & O \\ O & I_{m-2} \end{bmatrix}.$$

Eq. (38) shows that F_m represents the orthogonal section of A^{-1} onto $A\mathscr{K}_m$ with respect to $\hat{V}_m$. Its eigenvalues $1/\tilde{\theta}_j$ are therefore the Ritz values of A^{-1} with respect to this space, and thus satisfy

$$\boldsymbol{0} = \hat{V}_m^*\left(A^{-1}\hat{V}_m\hat{\boldsymbol{y}}_j - \frac{1}{\tilde{\theta}_j}\hat{V}_m\hat{\boldsymbol{y}}_j\right) = \hat{V}_m^*\left(A^{-1}\hat{\boldsymbol{z}}_j - \frac{1}{\tilde{\theta}_j}\hat{\boldsymbol{z}}_j\right)$$

with Ritz vectors $\hat{\boldsymbol{z}}_j := \hat{V}_m\hat{\boldsymbol{y}}_j$, which, upon multiplication by $\tilde{\theta}_j$, substituting $A^{-1}\hat{V}_m = V_m R_m^{-1}$ and multiplication by R_m^{H}, becomes

$$\boldsymbol{0} = R_m^{\mathrm{H}}\hat{V}_m^*(AV_m R_m^{-1}\hat{\boldsymbol{y}}_j - \tilde{\theta}_j V_m R_m^{-1}\hat{\boldsymbol{y}}_j) = (AV_m)^*(A\tilde{\boldsymbol{z}}_j - \tilde{\theta}_j\tilde{\boldsymbol{z}}_j), \tag{39}$$

where $\tilde{\boldsymbol{z}}_j := V_m\tilde{\boldsymbol{y}}_j = V_m R_m^{-1}\hat{\boldsymbol{y}}_j = A^{-1}\hat{\boldsymbol{z}}_j$. Vectors $\tilde{\boldsymbol{z}}_j$ and numbers $\tilde{\theta}_j$ which satisfy (39) are called *harmonic Ritz vectors and values* with respect to A and $\mathscr{K}_m$ (cf. [15]). A better known characterization of these quantities is

$$(AV_m)^*V_m\tilde{\boldsymbol{y}}_j = \frac{1}{\tilde{\theta}_j}(AV_m)^*AV_m\tilde{\boldsymbol{y}}_j, \quad \text{i.e., } H_m^{\mathrm{H}}\tilde{\boldsymbol{y}}_j = \frac{1}{\tilde{\theta}_j}\tilde{H}_m^{\mathrm{H}}\tilde{H}_m\tilde{\boldsymbol{y}}_j.$$

That this formulation gives rise to the same set of eigenvalues can be seen from the similarity transformation

$$(\tilde{H}_m^{\mathrm{H}}\tilde{H}_m)^{-1}H_m^{\mathrm{H}} = [R_m^{-1} \quad \boldsymbol{0}]Q_m\begin{bmatrix} I_m \\ \boldsymbol{0} \end{bmatrix} = R_m^{-1}[I_m \quad \boldsymbol{0}]Q_m\begin{bmatrix} R_m^{-1} \\ \boldsymbol{0} \end{bmatrix}R_m = R_m^{-1}F_m R_m.$$

The harmonic Ritz vectors lie in $\mathscr{K}_m$ and, in view of (39), satisfy

$$(A - \tilde{\theta}_j I)\tilde{\boldsymbol{z}}_j \perp A\mathscr{K}_m.$$

In other words, $(A-\tilde{\theta}_j I)\tilde{\boldsymbol{z}}_j \in \mathscr{K}_{m+1}\cap(A\mathscr{K}_m)^{\perp} = \mathrm{span}\{\boldsymbol{r}_m^{\mathrm{MR}}\}$ and therefore, if the polynomials $\tilde{z}_j \in \mathscr{P}_{m-1}$ are defined by $\tilde{\boldsymbol{z}}_j = \tilde{z}_j(A)\boldsymbol{r}_0$, there holds

$$\tilde{z}_j(\zeta) = \tau_j\frac{p_m^{\mathrm{MR}}(\zeta)}{\zeta - \tilde{\theta}_j} = \tau_j\frac{\hat{g}_m(\zeta)}{\zeta - \tilde{\theta}_j} \tag{40}$$

for some normalization factor $\tau_j \neq 0$.

Remark. Polynomials which possess the reproducing property (36) are called *kernel polynomials*. Their role in Krylov subspace methods was first explored by Stiefel [24] in the Hermitian case and later extended to the non-Hermitian case by Freund [8,7] (see also [11]).

3.4. The implicitly restarted Arnoldi process

When manipulating Krylov subspaces, the following fundamental task often arises: given a Krylov space $\mathscr{K}_m(A,\boldsymbol{v}_1)$ which is not A-invariant, along with the associated Arnoldi factorization

$$AV_m = V_m H_m + \eta_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{u}_m^{\mathrm{T}} \quad (\eta_{m+1,m} \neq 0) \tag{41}$$

and given an arbitrary vector $\boldsymbol{v} \in \mathscr{K}_{m-1}(A,\boldsymbol{v}_1)$, generate the Arnoldi factorization associated with $\mathscr{K}_p(A,\boldsymbol{v})$, i.e., using $\boldsymbol{v}$ as the initial vector, with p as large as possible *without* performing additional multiplications with A. The technique which accomplishes this task is known as the *implicitly restarted Arnoldi* (*IRA*) process and is due to Sorensen [22].

As a member of $\mathscr{K}_{m-1}$, $\boldsymbol{v}$ has the representation $\boldsymbol{v} = q_{k-1}(A)\boldsymbol{v}_1$ with q_{k-1} of exact degree $k-1$, $1 \leqslant k < m$. In other words, $\boldsymbol{v} \in \mathscr{K}_k \setminus \mathscr{K}_{k-1}$. We will show that $p = m-k$ is maximal and the resulting Arnoldi factorization has the form

$$A\check{V}_p = \check{V}_p\check{H}_p + \check{\eta}_{p+1,p}\check{\boldsymbol{v}}_{p+1}\boldsymbol{u}_p^{\mathrm{T}} \tag{42}$$

with $\check{\boldsymbol{v}}_1 = \boldsymbol{v}/\|\boldsymbol{v}\|$. That $p = m-k$ holds should not come as a surprise because the construction of factorization (41) requires m multiplications by A, whereas $\boldsymbol{v}$ can be computed by only $k-1$ matrix–vector products. Exactly $p+1 = m-k+1$, i.e., the number of the 'remaining' multiplications by A are needed to construct (42) in the conventional way.

We assume the polynomial q_{k-1} is given in factored form $q_{k-1}(\zeta) = \prod_{j=1}^{k-1}(\zeta-\theta_j)$, as this is how it is used in the IRA method. The arguments that follow remain valid upon multiplying by a nonzero factor, so we may, without loss of generality, assume q_{k-1} to be monic. It is obviously sufficient to show how decomposition (42) can be established in the case $k=2$, i.e., if $\boldsymbol{v} = (A-\theta I)\boldsymbol{v}_1$. Polynomials of higher degree can then be handled by repeated application of the procedure below.

Each step of the IRA method is based on one step of the shifted QR algorithm. Following Sorensen [22, p. 363], we begin by subtracting θV_m on both sides of the Arnoldi decomposition (41)

$$(A-\theta I)V_m = V_m(H_m - \theta I) + \eta_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{u}_m^{\mathrm{T}},$$

then form the QR factorization of $H_m - \theta I$,

$$(A-\theta I)V_m = V_m QR + \eta_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{u}_m^{\mathrm{T}}, \tag{43}$$

multiply by Q from the right,

$$(A-\theta I)V_m Q = (V_m Q)(RQ) + \eta_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{u}_m^{\mathrm{T}}Q,$$

and add $\theta V_m Q$ on both sides to obtain

$$A(V_m Q) = (V_m Q)(RQ + \theta I) + \eta_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{u}_m^{\mathrm{T}}Q. \tag{44}$$

We rewrite (44) to introduce some extra notation:

$$A[\check{\boldsymbol{v}}_1 \quad \dots \quad \check{\boldsymbol{v}}_{m-1} \quad \boldsymbol{v}_m^+] = [\check{\boldsymbol{v}}_1 \quad \dots \quad \check{\boldsymbol{v}}_{m-1} \quad \boldsymbol{v}_m^+]\begin{bmatrix}\check{H}_{m-1} & * \\ \eta^+\boldsymbol{u}_{m-1}^{\mathrm{T}} & *\end{bmatrix} + \eta_{m+1,m}\boldsymbol{v}_{m+1}[0 \quad \dots \quad 0 \quad q_{m,m-1} \quad q_{m,m}],$$

where we have made use of the fact that

$$RQ + \theta I = \begin{bmatrix}\check{H}_{m-1} & * \\ \eta^+\boldsymbol{u}_{m-1}^{\mathrm{T}} & *\end{bmatrix} \in \mathbb{C}^{m\times m}$$

is again an upper Hessenberg matrix due to the upper Hessenberg form of Q. We note in passing that, in case θ happens to be an eigenvalue of H_m (and only then), the last row of R is zero (and only the last row since H_m is nonderogatory) and therefore $\eta^+ = 0$.

We now omit the last column in (44), giving

$$A[\check{\boldsymbol{v}}_1 \quad \dots \quad \check{\boldsymbol{v}}_{m-1}] = [\check{\boldsymbol{v}}_1 \quad \dots \quad \check{\boldsymbol{v}}_{m-1}]\check{H}_{m-1} + (\eta^+ \boldsymbol{v}_m^+ + \eta_{m+1,m} q_{m,m-1} \boldsymbol{v}_{m+1})\boldsymbol{u}_{m-1}^{\mathrm{T}},$$

which, setting $\check{\eta}_{m,m-1} := \|\eta^+ \boldsymbol{v}_m^+ + \eta_{m+1,m} q_{m,m-1} \boldsymbol{v}_{m+1}\|$, becomes

$$A\check{V}_{m-1} = \check{V}_{m-1}\check{H}_{m-1} + \check{\eta}_{m,m-1}\check{\boldsymbol{v}}_m \boldsymbol{u}_{m-1}^{\mathrm{T}}. \tag{45}$$

Theorem 3.6. *With the notation introduced above, the decomposition* (45) *is an Arnoldi factorization of A with respect to the Krylov space $\mathscr{K}_{m-1}(A, (A - \theta I)\boldsymbol{v}_1)$.*

Proof. Since Q is unitary, it follows that the elements of $\check{V}_{m-1} = [\check{\boldsymbol{v}}_1 \quad \dots \quad \check{\boldsymbol{v}}_{m-1}]$ are orthonormal as the first $m-1$ elements of $V_m Q$. Next, the vector

$$\check{\boldsymbol{v}}_m = (\eta^+ \boldsymbol{v}_m^+ + \eta_{m+1,m} q_{m,m-1} \boldsymbol{v}_{m+1})/\check{\eta}_{m,m-1}$$

has unit norm and is orthogonal to $\check{\boldsymbol{v}}_1, \dots, \check{\boldsymbol{v}}_{m-1}$ since $\boldsymbol{v}_m^+$, as the last element $V_m Q$, is orthogonal to the previous elements $\check{\boldsymbol{v}}_1, \dots, \check{\boldsymbol{v}}_{m-1}$ and since $\boldsymbol{v}_{m+1}$ is orthogonal to V_m and hence also to $V_m Q$. That the new first basis vector $\check{\boldsymbol{v}}_1$ is a multiple of $(A - \theta I)\boldsymbol{v}_1$ follows by equating the first vector on both sides of (43). It remains to show that the Hessenberg matrix $\check{H}_{m-1}$ is unreduced. If $\check{\eta}_{k+1,k} = 0$ for some $k < m$, then this would imply that $\mathscr{K}_k(A, \check{\boldsymbol{v}}_1)$ is a proper A-invariant subspace of $\mathscr{K}_m(A, \boldsymbol{v}_1)$, which, in view of Lemma 3.2, contradicts the assumption $\eta_{m+1,m} \neq 0$. □

As mentioned previously, decomposition (42) involving a new starting vector $\check{\boldsymbol{v}}_1 = q_{k-1}(A)\boldsymbol{v}_1$ is effected by $k-1$ steps of the procedure outlined above. For later use, we note that the associated Krylov space is given by

$$\mathscr{K}_p(A, \check{\boldsymbol{v}}_1) = \{r(A)q_{k-1}(A)\boldsymbol{v}_1 : r \in \mathscr{P}_{p-1}\} \subset \mathscr{K}_{p+k-1}(A, \boldsymbol{v}_1).$$

4. Augmentation strategies and some algorithmic realizations

Up to this point we have not yet considered the question of how to construct suitable correction spaces $\mathscr{C}_m$ for a given initial approximation $\boldsymbol{x}_0$ to the solution of a linear system (1). In practice, this task usually arises in the following form. Given a correction space $\mathscr{C}$, select vectors $\boldsymbol{a}_1, \dots, \boldsymbol{a}_k$ such that the *augmented* correction space $\tilde{\mathscr{C}} := \mathscr{C} + \operatorname{span}\{\boldsymbol{a}_1, \dots, \boldsymbol{a}_k\}$ has better correction properties.

We first specify the (obvious) meaning of phrases such as 'well-suited correction space', 'better correction properties', etc. Let $\mathscr{C} \subset \mathscr{H}$ be a finite-dimensional subspace and denote by $\boldsymbol{r}^{\mathrm{MR}}$ the residual vector of the MR approximation with respect to the correction space $\mathscr{C}$. Whether or not $\mathscr{C}$ is well suited as a correction space, i.e., whether or not $A\mathscr{C}$ contains an acceptable approximation to $\boldsymbol{r}_0$, depends, in view of $\|\boldsymbol{r}^{\mathrm{MR}}\| = \sin \angle(\boldsymbol{r}_0, A\mathscr{C})\|\boldsymbol{r}_0\|$ (cf. (17)), only on the size of the angle $\varphi := \angle(\boldsymbol{r}_0, A\mathscr{C})$. $\mathscr{C}$ is optimal, i.e., $\boldsymbol{r}^{\mathrm{MR}} = \boldsymbol{0}$ if and only if $\varphi = 0$. The worst case is that in which the optimal correction from $\mathscr{C}$ is the null vector (i.e., $\boldsymbol{r}^{\mathrm{MR}} = \boldsymbol{r}_0$), and this occurs precisely for $\varphi = \pi/2$, or equivalently, for $\boldsymbol{r}_0 \perp A\mathscr{C}$.

In Section 4.1 we comment on two general strategies for augmenting correction spaces, the first of which adds nearly A-invariant subspaces to the correction space, whereas the second adds approximate solution of residual equations. Subsequently we survey and compare existing algorithms in which the ideas and strategies developed in the previous sections have been realized.

4.1. General augmentation strategies

It has often been suggested, primarily in the context of Krylov subspace methods, that it is a desirable goal that the correction space $\mathscr{C}$ be either nearly A-invariant or contain a nearly A-invariant subspace, usually spanned by a few approximate eigenvectors of A. Clearly, if a given correction space $\mathscr{C}$ which contains the initial residual $\boldsymbol{r}_0$ – as do e.g. all Krylov spaces – is exactly A-invariant, then $\varphi = 0$ and the MR approximation with respect to $\mathscr{C}$ yields the exact solution. If only a subspace $\mathscr{U}$ of $\mathscr{C}$ is A-invariant, or nearly so in the sense that it lies at a small angle to its image under A, Proposition 4.1 shows that the MR residual with respect to $\mathscr{C}$ then has a small component in the direction of $\mathscr{U}$.

Proposition 4.1. *Given a correction space $\mathscr{C}$, let $\mathscr{U} \subset \mathscr{C}$ denote a subspace such that* $\sin \angle(A\mathscr{U}, \mathscr{U}) \leqslant \varepsilon$. *Then the MR residual $\boldsymbol{r}^{\mathrm{MR}}$ with respect to $\mathscr{C}$ satisfies $\|P_{\mathscr{U}} \boldsymbol{r}^{\mathrm{MR}}\| \leqslant \varepsilon \|\boldsymbol{r}_0\|$.*

Proof. The assertion follows from $P_{\mathscr{U}} \boldsymbol{r}^{\mathrm{MR}} = P_{\mathscr{U}}(I - P_{A\mathscr{C}})\boldsymbol{r}_0$ and $\|P_{\mathscr{U}}(I - P_{A\mathscr{C}})\| \leqslant \|P_{\mathscr{U}}(I - P_{A\mathscr{U}})\| = \sin \angle(A\mathscr{U}, \mathscr{U}) \leqslant \varepsilon$. □

In particular, if $\mathscr{C}$ contains an exactly invariant subspace $\mathscr{U}$, then the MR approximation removes the components of the initial residual in the direction of $\mathscr{U}$ completely. Of course, this may only be of limited use if $\|(I - P_{\mathscr{U}})\boldsymbol{r}_0\| / \|\boldsymbol{r}_0\|$ is large, i.e., if $\mathscr{U}$ does not contain a good approximation of $\boldsymbol{r}_0$. In short, the existence of A-invariant subspaces of $\mathscr{C}$ per se need not be beneficial.

In Lemma 3.2 we already proved that if $\mathscr{C} = \mathscr{K}_m(A, \boldsymbol{r}_0)$ is a Krylov space, then it cannot contain an A-invariant subspace $\mathscr{U}$ unless $\mathscr{K}_m(A, \boldsymbol{r}_0)$ is itself A-invariant, i.e., $\mathscr{K}_m(A, \boldsymbol{r}_0) = \mathscr{K}_L(A, \boldsymbol{r}_0)$. Obviously, augmenting $\mathscr{K}_m(A, \boldsymbol{r}_0)$ by $\operatorname{span}\{A^m \boldsymbol{r}_0, \ldots, A^{L-1} \boldsymbol{r}_0\}$ leads to the new correction space $\mathscr{K}_L(A, \boldsymbol{r}_0)$ which is A-invariant. We now show that there is no 'faster' way to augment $\mathscr{K}_m(A, \boldsymbol{r}_0)$ to an A-invariant space.

Proposition 4.2. *Let $\tilde{\mathscr{C}}$ be an A-invariant subspace containing $\mathscr{K}_m(A, \boldsymbol{r}_0)$. Then $\tilde{\mathscr{C}}$ contains $\mathscr{K}_L(A, \boldsymbol{r}_0)$.*

Proof. By $\mathscr{U}_0 := \cap\{\mathscr{U} : \mathscr{U} \text{ is an } A\text{-invariant subspace with } \mathscr{K}_m \subseteq \mathscr{U}\}$ we denote the smallest A-invariant subspace containing $\mathscr{K}_m$. By definition, $\mathscr{U}_0 \subseteq \mathscr{K}_L$. On the other hand, since $\mathscr{U}_0$ contains $\boldsymbol{r}_0$ and is invariant under A, it must contain also $A^m \boldsymbol{r}_0$ for very $m = 0, 1, \ldots$, i.e., $\mathscr{K}_L \subseteq \mathscr{U}_0$. □

Proposition 4.2 should not lead to the conclusion that it is useless to augment a Krylov subspace $\mathscr{C} = \mathscr{K}_m$ by an A-invariant subspace $\mathscr{U}$. After all, by Proposition 4.1 the MR residual with respect to $\tilde{\mathscr{C}} = \mathscr{C} + \mathscr{U}$ contains no component in the direction of $\mathscr{U}$. We show next that the MR approach with respect to the augmented space $\tilde{\mathscr{C}}$ yields an MR approximation with respect to another Krylov subspace, associated with a 'smaller' linear system.

Lemma 4.3. *Let* $\tilde{\boldsymbol{r}}^{\mathrm{MR}}$ *denote the* MR *residual with respect to* $\tilde{\mathscr{C}} = \mathscr{K}_m(A, \boldsymbol{r}_0) + \mathscr{U}$, *where* $\mathscr{U}$ *is an* A*-invariant subspace. Set further* $\mathscr{T} := \mathscr{U}^{\perp}$, $A_{\mathscr{T}} := P_{\mathscr{T}} A P_{\mathscr{T}}$ *and, finally, let* $\boldsymbol{r}^{\mathrm{MR}}$ *be the residual of the* MR *approximation for* $A_{\mathscr{T}}\boldsymbol{x} = P_{\mathscr{T}}\boldsymbol{r}_0$ *with respect to the correction space* $\mathscr{K}_m(A_{\mathscr{T}}, P_{\mathscr{T}}\boldsymbol{r}_0)$. *Then there holds*

$$\tilde{\boldsymbol{r}}^{\mathrm{MR}} = \boldsymbol{r}^{\mathrm{MR}} \quad \textit{or, equivalently } P_{\mathscr{U}}\tilde{\boldsymbol{r}}^{\mathrm{MR}} = \boldsymbol{0} \quad \textit{and} \quad P_{\mathscr{T}}\tilde{\boldsymbol{r}}^{\mathrm{MR}} = \boldsymbol{r}^{\mathrm{MR}}.$$

Proof. As in Section 2.3 we split the computation of $\tilde{\boldsymbol{r}}^{\mathrm{MR}}$ into two subtasks and write (using that $\mathscr{U}$ is A-invariant)

$$\tilde{\boldsymbol{r}}^{\mathrm{MR}} = (I - P_{\mathscr{U}})\boldsymbol{r}_0 - P_{\mathscr{Z}}(I - P_{\mathscr{U}})\boldsymbol{r}_0 = (I - P_{\mathscr{Z}})P_{\mathscr{T}}\boldsymbol{r}_0,$$

where $\mathscr{Z} = (I - P_{\mathscr{U}})A\mathscr{K}_m(A, \boldsymbol{r}_0) = A\mathscr{K}_m(A, \boldsymbol{r}_0) \cap \mathscr{T} \subseteq \mathscr{T}$, whereby $P_{\mathscr{U}}P_{\mathscr{Z}} = O$. This implies $P_{\mathscr{U}}\tilde{\boldsymbol{r}}^{\mathrm{MR}} = \boldsymbol{0}$ (a fact we could also have deduced directly from Proposition 4.1).

Since $P_{\mathscr{T}}A\mathscr{K}_m(A, \boldsymbol{r}_0) = A_{\mathscr{T}}\mathscr{K}_m(A_{\mathscr{T}}, P_{\mathscr{T}}\boldsymbol{r}_0)$ (cf. Lemma 3.3),

$$\tilde{\boldsymbol{r}}^{\mathrm{MR}} = (I - P_{P_{\mathscr{T}}A\mathscr{K}_m(A,\boldsymbol{r}_0)})P_{\mathscr{T}}\boldsymbol{r}_0 = (I - P_{A_{\mathscr{T}}\mathscr{K}_m(A_{\mathscr{T}},P_{\mathscr{T}}\boldsymbol{r}_0)})P_{\mathscr{T}}\boldsymbol{r}_0,$$

identifying $\tilde{r}^{\mathrm{MR}}$ as the residual of the MR approximation for $A_{\mathscr{T}}\boldsymbol{x} = P_{\mathscr{T}}\boldsymbol{r}_0$ with respect to the Krylov space $\mathscr{K}_m(A_{\mathscr{T}}, P_{\mathscr{T}}\boldsymbol{r}_0)$. □

A different strategy for enriching correction spaces is common for many inner–outer iteration schemes and based on the following trivial observation: Suppose that, for a given correction space $\mathscr{C}$ and associated residual space $\mathscr{V} = \operatorname{span}\{\boldsymbol{r}_0\} + A\mathscr{C}$, we are able to solve $A\boldsymbol{c} = \boldsymbol{r}$ for some $\boldsymbol{r} \in \mathscr{V}$. Such an $\boldsymbol{r}$ has a representation $\boldsymbol{r} = \boldsymbol{r}_0 - A\tilde{\boldsymbol{c}}$ with $\tilde{\boldsymbol{c}} \in \mathscr{C}$, and therefore, by virtue of

$$A\boldsymbol{c} = \boldsymbol{r} = \boldsymbol{r}_0 - A\tilde{\boldsymbol{c}}, \quad \text{i.e.,} \quad \boldsymbol{r}_0 = A(\boldsymbol{c} + \tilde{\boldsymbol{c}}),$$

we see that the augmented correction space $\tilde{\mathscr{C}} = \mathscr{C} + \operatorname{span}\{\boldsymbol{c}\}$ contains the exact correction. In practice, since solving $A\boldsymbol{c} = \boldsymbol{r}$ is generally as difficult as the original problem, one applies an inexpensive approximate solution method to this auxiliary problem, yielding a vector $\boldsymbol{c}$ satisfying $A\boldsymbol{c} = \boldsymbol{r} + \boldsymbol{h}$ and consequently, $\|\tilde{\boldsymbol{r}}^{\mathrm{MR}}\| \leqslant \|\boldsymbol{h}\|$ for the MR residual with respect to $\tilde{\mathscr{C}}$.

The FGMRES algorithm of Saad [17], which is the natural generalization of GMRES to the case of an arbitrary correction space, was originally introduced as a technique that enlarges the correction space at each step by an approximate solution of such a residual equation. In [17], this is achieved by selecting the new correction direction $\boldsymbol{c}_{m+1}$ as the result of a preconditioning step applied to the most recent basis vector $\boldsymbol{v}_{m+1}$ of the residual space $\mathscr{V}_{m+1}$, which may be viewed as an approximate solution of the equation $A\boldsymbol{c} = \boldsymbol{v}_{m+1}$.

A similar approach is taken in the GMRESR (which stands for GMRES Recursive) method of van der Vorst and Vuik [27]. In each step of GMRESR, the new correction vector $\boldsymbol{c}_{m+1}$ is chosen as the approximate solution of the equation $A\boldsymbol{c} = \boldsymbol{r}_m$ obtained by a given number of GMRES steps, where $\boldsymbol{r}_m$ is the residual of the MR approximation using the current correction space $\mathscr{C}_m$. This method was improved upon by de Sturler [25], who observed that, by enforcing orthogonality of the approximation space of the inner GMRES iteration, one can obtain as a result of the inner GMRES iteration the best approximation of $\boldsymbol{r}_0$ from the sum of the inner and outer approximation spaces as described in Section 2.3. In other words, the inner iteration consists of GMRES applied to Eq. (21). The resulting inner–outer iteration scheme is called GCRO.

4.2. Restarted GMRES

In general, the implementation of OR and MR methods require computing and storing at least one orthonormal basis of a space which grows in dimension with each step. A result of Faber and Manteuffel [6] shows that this considerable computational effort can be avoided essentially only for self-adjoint A. It is therefore not surprising that the necessity of truncating or restarting in practical implementations of MR and OR methods is as old as these methods themselves (cf. [21,4]). The most widely used algorithm is GMRES(m), the restarted version of GMRES, which uses a Krylov space of dimension m. One *cycle* of GMRES(m) for solving (1) with initial residual $\boldsymbol{r}_0$ consists of generating the Krylov space $\mathscr{K}_m(A,\boldsymbol{r}_0)$, forming the MR approximation with respect to the correction space $\mathscr{C}=\mathscr{K}_m(A,\boldsymbol{r}_0)$ and repeating this process using the resulting residual as the initial residual for the next cycle until a stopping criterion is satisfied.

In the terminology of Section 2, two consecutive cycles of GMRES(m) consist of two MR approximations with respect to the correction spaces

$$\mathscr{C}_1=\mathscr{K}_m(A,\boldsymbol{r}_0) \quad \text{and} \quad \mathscr{C}_2=\mathscr{K}_m(A,\boldsymbol{r}_m),$$

where $\boldsymbol{r}_m$ denotes the residual of the MR approximation computed in the first cycle. No orthogonalization of the residual space $\mathscr{V}_2$ against the approximation space $A\mathscr{C}_1$ is performed in the second cycle, and thus, in general, the approximation after the second cycle is no longer the MR approximation with respect to $\mathscr{C}_1+\mathscr{C}_2$. Besides this inexact approximation, it may also happen that the sum is not direct. In the extreme case there holds $\boldsymbol{r}_m=\boldsymbol{r}_0$ after the first cycle, so that the second cycle constructs the identical Krylov space (as do all subsequent cycles) and no progress is made, a phenomenon known as *stalling*.

Proposition 4.4. *For two consecutive cycles of* GMRES(m) *with initial residual* $\mathbf{r}_0$, *there holds*

$$\mathscr{K}_m(A,\boldsymbol{r}_0)\oplus\mathscr{K}_m(A,\boldsymbol{r}_m)=\mathscr{K}_{2m}(A,\boldsymbol{r}_0) \tag{46}$$

if and only if no stagnation occurs in the last step of the first cycle.

Proof. By definition, $\mathscr{K}_m(A,\boldsymbol{r}_m)=\{q(A)\,p_m^{\mathrm{MR}}(A)\boldsymbol{r}_0 : q\in\mathscr{P}_{m-1}\}$, where p_m^{MR} denotes the MR polynomial of the last step of the first cycle, and this shows that (46) holds if and only if p_m^{MR} has degree m. Representation (37) of p_m^{MR} shows that this is equivalent with $v_m(0)\neq 0$, which is equivalent to stagnation at step m. □

One of the more common misconceptions regarding GMRES(m) is that a method with larger restart length m applied to the same problem will converge at least as fast as the method with smaller m. A simple counterexample[4] is provided by the 3×3 system

$$A\boldsymbol{x}=\boldsymbol{b}, \qquad A=\begin{bmatrix}1&0&0\\1&1&0\\0&1&1\end{bmatrix}, \qquad \boldsymbol{b}=\begin{bmatrix}-1\\1\\1\end{bmatrix}$$

[4] The authors would like to thank E. de Sturler for pointing out this phenomenon reporting a similar observation in the context of a discrete convection–diffusion problem.

with initial guess $x_0 = \mathbf{0}$. Two cycles of GMRES(2) applied to this example result in a residual norm of $\|r_4^{(2)}\| = 4/15 = 0.26\ldots$, whereas four cycles of GMRES(1), which involve the same number of matrix–vector multiplications, yields $\|r_4^{(1)}\| = 0.057\ldots$. The gap between GMRES(1) and GMRES(2) widens further in subsequent iteration steps, e.g., $\|r_{18}^{(1)}\|_2 = 1.6\ldots 10^{-12}$, whereas $\|r_{18}^{(2)}\|_2 = 3.9\ldots 10^{-5}$. Even more surprising in this example is that $\|r_{10}^{(1)}\|_2 < \|r_{20}^{(2)}\|_2$, showing that ten cycles of GMRES(1) have reduced the residual further than ten cycles of GMRES(2). By expanding this example to the analogous matrix for higher dimensions n one can observe that GMRES(m) is ultimately slower for this system than GMRES($m-1$) for $m = 2, \ldots, n-1$.

4.3. Deflation by augmentation

The first algorithm which attempts to improve the restarted GMRES method by augmenting the Krylov space is due to Morgan [14]. This approach selects a fixed number of approximate eigenvectors of A to add to the Krylov space of the following cycle, as motivated, e.g., by Lemma 4.3. Since the emphasis of [13] is on cases in which the eigenvalues close to the origin limit the convergence rate the most – as is the case, e.g., for the so-called model problem of the discrete Laplacian on the unit cube – harmonic Ritz vectors are chosen as the eigenvector approximations, since, as argued in [12], harmonic Ritz values tend to approximate eigenvalues close to zero more accurately than classical Ritz values.

Each step except the first consists of forming the MR approximation with respect to a correction space $\mathscr{C} = \mathscr{C}_1 + \mathscr{C}_2$ with $\mathscr{C}_1 = \mathscr{K}_m(A, r_0)$ and $\mathscr{C}_2 = \operatorname{span}\{\tilde{z}_1, \ldots, \tilde{z}_k\}$. The vectors $\tilde{z}_1, \ldots, \tilde{z}_k$ are the harmonic Ritz vectors associated with the k harmonic Ritz values $\tilde{\theta}_1, \ldots, \tilde{\theta}_k$ of A with respect to the previous correction space which are closest to the origin. Since no eigenvector information is available in the first cycle, the first correction space is chosen simply as $\mathscr{C} = \mathscr{K}_{m+k}(A, r_0)$.

As subsequently shown by Morgan [14], there is a less expensive implementation of this approach. Consider the MR approximation with initial residual r_0 with respect to the $(m+k)$-dimensional Krylov space $\mathscr{K}_{m+k}(A, r_0)$. As shown in Section 3.3, the associated residual vector has the representation

$$r_{m+k}^{\mathrm{MR}} = p_{m+k}^{\mathrm{MR}}(A) r_0, \quad \text{where } p_{m+k}^{\mathrm{MR}}(\zeta) = \prod_{j=1}^{m+k} \left(1 - \frac{\zeta}{\tilde{\theta}_j}\right).$$

We denote by q_m the polynomial whose zeros are the harmonic Ritz values $\tilde{\theta}_{k+1}, \ldots, \tilde{\theta}_{k+m}$, i.e., those largest in modulus.

Theorem 4.5. *The correction space $\mathscr{C}$ of Morgan's method is itself a Krylov space, namely*

$$\mathscr{C} = \mathscr{K}_m(A, r_{m+k}) + \operatorname{span}\{\tilde{z}_1, \ldots, \tilde{z}_k\} = \mathscr{K}_{m+k}(A, q_m(A) r_0). \tag{47}$$

Proof. The rightmost member of (47) can be represented as

$$\mathscr{K}_{m+k}(A, q_m(A) r_0) = \{r(A) q_m(A) r_0 : r \in \mathscr{P}_{m+k-1}\}.$$

On the other hand, by (40), the harmonic Ritz vectors may be represented in terms of polynomials as $\tilde{\boldsymbol{z}}_j = \tilde{z}_j(A)\boldsymbol{r}_0$ with

$$\tilde{z}_j(\zeta) = \frac{p^{\mathrm{MR}}_{m+k}(\zeta)}{\zeta - \tilde{\theta}_j} = q_m(\zeta) \prod_{\substack{\ell=1 \\ \ell \neq j}}^{k} \left(1 - \frac{\zeta}{\tilde{\theta}_\ell}\right),$$

whereas $\boldsymbol{r}^{\mathrm{MR}}_{m+k} = p^{\mathrm{MR}}_{m+k}(A)\boldsymbol{r}_0$, with

$$p^{\mathrm{MR}}_{m+k}(\zeta) = q_m(\zeta) \prod_{\ell=1}^{k} \left(1 - \frac{\zeta}{\tilde{\theta}_\ell}\right).$$

Therefore, the correction space of Morgan's method may be characterized as

$$\mathscr{C} = \{q_m(A)q(A)\boldsymbol{r}_0 : q \in \mathscr{Q}\},$$

where the polynomial space $\mathscr{Q}$ is given by

$$\begin{aligned}\mathscr{Q} &:= \prod_{\ell=1}^{k} \left(1 - \frac{\zeta}{\tilde{\theta}_\ell}\right) \mathscr{P}_{m-1} + \operatorname{span}\left\{ \prod_{\substack{\ell=1 \\ \ell \neq j}}^{k} \left(1 - \frac{\zeta}{\tilde{\theta}_\ell}\right) : j = 1 \ldots, k \right\} \\ &= \prod_{\ell=1}^{k} \left(1 - \frac{\zeta}{\tilde{\theta}_\ell}\right) \mathscr{P}_{m-1} + \mathscr{P}_{k-1} = \mathscr{P}_{m+k-1},\end{aligned}$$

where the middle equality follows from the fact that $\tilde{\theta}_1, \ldots, \tilde{\theta}_k$ are distinct. □

Eq. (47) shows that $\mathscr{C}$ can be generated by applying the IRA method to $\mathscr{K}_{m+k}(A, \boldsymbol{r}_0)$, using $\tilde{\theta}_{k+1}, \ldots, \tilde{\theta}_{m+k}$ as shifts, to obtain $\mathscr{K}_k(A, q_m(A)\boldsymbol{r}_0)$. The space $\mathscr{C}$ is then obtained after m further steps of the Arnoldi process. This approach is computationally less expensive in that k fewer matrix–vector multiplications with A are required.

As also noted by Morgan, an analogous method can be used to augment the Krylov space in conjunction with an OR iteration. In this case, however, Ritz values and vectors must be used in place of harmonic Ritz values/vectors, as the Ritz values are the zeros of the OR residual polynomial.

4.4. Deflation by preconditioning

The methods of the next class also attempt to utilize spectral information gained during the course of the iteration to accelerate convergence. Instead of augmenting the Krylov space, however, these methods use this information to construct preconditioners which can be improved as more accurate spectral information becomes available. Such an approach was proposed by Erhel et al. [5].

To motivate this approach, assume $\mathscr{U}$ is an A-invariant subspace of dimension k with orthonormal basis U, i.e.,

$$AU =: UA_U, \qquad A_U \in \mathbb{C}^{k \times k}.$$

Note that A_U is the specific representation of the orthogonal section $A_{\mathscr{U}}$ with respect to the basis U. Denoting by T an orthonormal basis of the orthogonal complement $\mathscr{T} = \mathscr{U}^{\perp}$, we can represent the

action of A as

$$A[U \quad T] = [U \quad T] \begin{bmatrix} A_U & U^*AT \\ O & T^*AT \end{bmatrix}.$$

Under the assumption that k is small, it is feasible to solve systems involving A_U directly, and thus to precondition by M defined as

$$M[U \quad T] = [U \quad T] \begin{bmatrix} A_U & O \\ O & I \end{bmatrix} \tag{48}$$

at each step of the iteration. The resulting right-preconditioned operator is then

$$AM^{-1}[U \quad T] = [U \quad T] \begin{bmatrix} I & U^*AT \\ O & T^*AT \end{bmatrix}, \quad \text{i.e.,} \quad AM^{-1} = P_{\mathscr{U}} + AP_{\mathscr{T}}. \tag{49}$$

We want to compare this approach with Morgan's method of augmenting the Krylov space $\mathscr{K}_m(A, \boldsymbol{r}_0)$ by the A-invariant subspace $\mathscr{U}$.

Theorem 4.6. *Let $\boldsymbol{r}_m^M$ denote the MR residual with respect to the correction space $\mathscr{U} + \mathscr{K}_m(A, \boldsymbol{r}_0)$, where $\mathscr{U}$ is an A-invariant subspace, and let $\boldsymbol{r}_m^E$ denote the MR residual with respect to the correction space $\mathscr{K}_m(AM^{-1}, \boldsymbol{r}_0)$ resulting from preconditioning A from the right by M as defined in* (48). *Then there holds*

$$0 = \|P_{\mathscr{U}}\boldsymbol{r}_m^M\| \leqslant \|P_{\mathscr{U}}\boldsymbol{r}_m^E\| \quad \text{and} \quad \|P_{\mathscr{T}}\boldsymbol{r}_m^M\| \leqslant \|P_{\mathscr{T}}\boldsymbol{r}_m^E\|, \tag{50}$$

in particular, $\|\boldsymbol{r}_m^M\| \leqslant \|\boldsymbol{r}_m^E\|$. If, in addition, also $\mathscr{T} = \mathscr{U}^{\perp}$ is A-invariant, then, $P_{\mathscr{U}}\boldsymbol{r}_0 = \boldsymbol{0}$ implies $\boldsymbol{r}_m^E = \boldsymbol{r}_m^M$.

Proof. The left set of inequalities in (50) follow from $P_{\mathscr{U}}\boldsymbol{r}_m^M = \boldsymbol{0}$ which was proved in Lemma 4.3.

We next recall that $A_{\mathscr{T}} = P_{\mathscr{T}}AP_{\mathscr{T}}$ is the orthogonal section of A onto $\mathscr{T}$ (cf. the remark following Lemma 3.3). Since $\boldsymbol{r}_m^E = \boldsymbol{r}_0 - AM^{-1}\boldsymbol{c}$, for some $\boldsymbol{c} \in \mathscr{K}_m(AM^{-1}, \boldsymbol{r}_0)$ we obtain using (49)

$$P_{\mathscr{T}}\boldsymbol{r}_m^E = P_{\mathscr{T}}\boldsymbol{r}_0 - P_{\mathscr{T}}AM^{-1}\boldsymbol{c} = P_{\mathscr{T}}\boldsymbol{r}_0 - P_{\mathscr{T}}AP_{\mathscr{T}}\boldsymbol{c} = P_{\mathscr{T}}\boldsymbol{r}_0 - A_{\mathscr{T}}P_{\mathscr{T}}\boldsymbol{c}.$$

Moreover, $AM^{-1}\mathscr{U} = \mathscr{U}$ together with Lemma 3.3 yield

$$P_{\mathscr{T}}\boldsymbol{c} \in P_{\mathscr{T}}\mathscr{K}_m(AM^{-1}, \boldsymbol{r}_0) = \mathscr{K}_m(P_{\mathscr{T}}AM^{-1}, P_{\mathscr{T}}\boldsymbol{r}_0) = \mathscr{K}_m(A_{\mathscr{T}}, P_{\mathscr{T}}\boldsymbol{r}_0).$$

The last two statements show that $P_{\mathscr{T}}\boldsymbol{r}_m^E$ is of the form $P_{\mathscr{T}}\boldsymbol{r}_0 - A_{\mathscr{T}}\tilde{\boldsymbol{c}}$ with $\tilde{\boldsymbol{c}} \in \mathscr{K}_m(A_{\mathscr{T}}, P_{\mathscr{T}}\boldsymbol{r}_0)$. On the other hand, by Proposition 4.3 there holds

$$\|\boldsymbol{r}_m^M\| = \min_{\boldsymbol{c} \in \mathscr{K}_m(A_{\mathscr{T}}, P_{\mathscr{T}}\boldsymbol{r}_0)} \|P_{\mathscr{T}}\boldsymbol{r}_0 - A_{\mathscr{T}}\boldsymbol{c}\|,$$

i.e., $\|\boldsymbol{r}_m^M\|$ minimizes all expressions of this form, yielding the right inequality of (50).

Next, assuming $A\mathscr{T} = \mathscr{T}$, (49) implies $AM^{-1}\boldsymbol{r}_0 = A_{\mathscr{T}}\boldsymbol{r}_0$ for $\boldsymbol{r}_0 \in \mathscr{T}$, and thus $\mathscr{K}_m(AM^{-1}, \boldsymbol{r}_0) = \mathscr{K}_m(A_{\mathscr{T}}, P_{\mathscr{T}}\boldsymbol{r}_0)$, which shows that in this case both methods minimize over the same space, hence $\boldsymbol{r}_m^E = \boldsymbol{r}_m^M$. □

We note that the assumption $P_{\mathscr{U}}\boldsymbol{r}_0 = \boldsymbol{0}$ is not restrictive, as the preconditioner is built upon the premise that A_U is easily invertible. Since $P_{\mathscr{U}}\boldsymbol{r}_0 = \boldsymbol{0}$ by no means implies that $P_{\mathscr{U}}\boldsymbol{r}_m^E = \boldsymbol{0}$, it cannot be guaranteed that $\|\boldsymbol{r}_m^E\| = \|\boldsymbol{r}_m^M\|$ even for such a special choice of initial residual unless $A\mathscr{T} = \mathscr{T}$.

The availability of an (exactly) A-invariant subspace $\mathscr{U}$, on the other hand, is an assumption that can rarely be satisfied in practice. In such a case, one can nonetheless still define the preconditioner as above, where now $A_U := U^*AU$ represents the orthogonal section of A onto $\mathscr{U}$, resulting in

$$AM^{-1}[U\ T] = [U\ T]\begin{bmatrix} I & U^*AT \\ T^*AUA_U^{-1} & T^*AT \end{bmatrix},$$

based on the heuristic argument that $T^*AUA_U^{-1}$ will be small whenever $\mathscr{U}$ is nearly A-invariant. Such nearly A-invariant spaces are obtained as the span of selected Ritz or harmonic Ritz vectors determined from Krylov spaces generated during previous cycles. In practice it is common to suitably scale A_U in the preconditioner M (see [7]).

Baglama et al. [1] propose a similar algorithm, which preconditions by (48) from the left, leading—again under the assumption that $\mathscr{U}$ is exactly A-invariant—to the preconditioned operator

$$M^{-1}A[U\ T] = [U\ T]\begin{bmatrix} I & A_U^{-1}U^*AT \\ O & T^*AT \end{bmatrix},$$

$$M^{-1}A = P_{\mathscr{U}} + AP_{\mathscr{T}} + (A^{-1} - I)P_{\mathscr{U}}AP_{\mathscr{T}}.$$

The MR correction of the left-preconditioned system is the solution of the minimization problem

$$\|M^{-1}\boldsymbol{r}_m^B\| = \min\{\|M^{-1}(\boldsymbol{r}_0 - AM^{-1}\boldsymbol{c})\| : \boldsymbol{c} \in \mathscr{K}_m(AM^{-1}, \boldsymbol{r}_0)\}$$

(cf. [18, p. 255]).

From (48), it is evident that

$$M^{-1} = A^{-1}P_{\mathscr{U}} + P_{\mathscr{T}}$$

and, consequently, if $A\mathscr{U} = \mathscr{U}$,

$$P_{\mathscr{T}}M^{-1}\boldsymbol{v} = P_{\mathscr{T}}\boldsymbol{v} \quad \text{for all } \boldsymbol{v}.$$

These are the essential ingredients for showing that Proposition 4.6 holds in exactly the same way with $\boldsymbol{r}_m^E$ in place of $\boldsymbol{r}_m^B$.

The construction of an approximately invariant subspace $\mathscr{U}$ is accomplished in [1] by employing the IRA process (cf. Section 3.4).

Kharchenko and Yeremin [10] suggest another adaptive right preconditioner $\tilde{M}$ constructed as follows: After each GMRES cycle the Ritz values and the corresponding left[5] and right Ritz vectors of A with respect $\mathscr{K}_m$ are extracted. The aim is to obtain a preconditioner such that the extremal eigenvalues of A, which are approximated by the Ritz values, are translated to one (or at least to a small cluster around one).

The extremal Ritz values are partitioned into, say, k subsets Θ_j of nearby Ritz values. For each Θ_j, a rank-one transformation of the form $I + \boldsymbol{v}_j\tilde{\boldsymbol{v}}_j^*$ is constructed, where $\boldsymbol{v}_j$ and $\tilde{\boldsymbol{v}}_j$ are linear combinations of the associated right and left Ritz vectors. These linear combinations are chosen to translate simultaneously all Ritz values of Θ_j into a small cluster around one, while satisfying certain stability criteria. One preconditioning step now consists of successive multiplication by these rank-one matrices, i.e.,

$$\tilde{M}^{-1} = (I + \boldsymbol{v}_1\tilde{\boldsymbol{v}}_1^*)\dots(I + \boldsymbol{v}_k\tilde{\boldsymbol{v}}_k^*) = I + [\boldsymbol{v}_1 \dots \boldsymbol{v}_k][\tilde{\boldsymbol{v}}_1 \dots \tilde{\boldsymbol{v}}_k]^*.$$

[5] Left Ritz vectors are defined by $A^*\tilde{\boldsymbol{z}}_j - \bar{\theta}_j\tilde{\boldsymbol{z}}_j \perp \mathscr{K}_m$ and can be obtained from the left eigenvectors of H_m.

For the last equality we have made use of the fact that $\tilde{\boldsymbol{v}}_j^* \boldsymbol{v}_i = 0$ for $i \neq j$, since all eigenvalues of H_m have geometric multiplicity one. Note that, if Θ_j has a small diameter and the Ritz values contained in Θ_j are good approximations of eigenvalues of A, then $\boldsymbol{v}_j$ and $\tilde{\boldsymbol{v}}_j$ are approximate right and left eigenvectors of A. It can be shown that the statement made in Theorem 4.6 also holds for this preconditioning approach.

4.5. Optimal truncation

The methods of the preceding sections were based on restarting an MR iteration once the correction space has reached a given dimension m, and attempted to compensate for the attendant loss of information by augmenting or preconditioning. The methods discussed in this section are related to the former in that they also attempt to retain information contained in the current correction space – in this case orthogonality constraints – which is deemed most useful for convergence.

In place of restarting, the basic scheme underlying this class of methods is a *truncated* MR iteration, in which, as soon as the correction space has reached a maximal dimension m, only a subset of the most recent m basis vectors of the correction space is retained, or equivalently, one or more of these basis vectors is periodically discarded during the iteration. In [26] de Sturler proposes a scheme for selectively discarding subspaces rather than individual basis vectors. This selection process, however, does not rely on spectral or invariant subspace information, but rather on angles between subspaces.

To discard a subspace of dimension ℓ, the subspace selection scheme proposed by de Sturler compares two approximation spaces $\mathcal{W}_1$ and $\mathcal{W}_2$ associated with correction spaces $\mathcal{C}_1$ and $\mathcal{C}_2$. It assumes the availibility of an orthonormal basis $W_m^{(1)} = [\boldsymbol{w}_1^{(1)}, \ldots, \boldsymbol{w}_m^{(1)}]$ of $\mathcal{W}_1$, an *arbitrary* basis $\hat{W}_k^{(2)} = [\hat{\boldsymbol{w}}_1^{(2)}, \ldots, \hat{\boldsymbol{w}}_k^{(2)}]$ of $\mathcal{W}_2$ as well as a factorization

$$(I_k - W_m^{(1)}[W_m^{(1)}]^*)\hat{W}_k^{(2)} = Z_k R$$

with $Z_k = [\boldsymbol{z}_1, \ldots, \boldsymbol{z}_k]$, $Z_k^* Z_k = I_k$ and $R \in \mathbb{C}^{k\times k}$ nonsingular and upper triangular. After computing the singular value decomposition

$$([W_m^{(1)}]^* \hat{W}_k^{(2)})(Z_k^* \hat{W}_k^{(2)})^{-1} = X \Xi \hat{Y}^{\mathrm{H}}, \tag{51}$$

the subspace of $\mathcal{W}_1$ to be retained is chosen as that spanned by the vectors $W_m^{(1)}[\boldsymbol{x}_1 \cdots \boldsymbol{x}_\ell]$, where the vectors $\boldsymbol{x}_j$ are the left singular vectors associated with the ℓ largest singular values. The following proposition relates this choice to the results of Section 2.4.

Proposition 4.7. *With the above notation under the assumption* $\mathcal{W}_1 \cap \mathcal{W}_2 = \{\mathbf{0}\}$, *the singular values appearing in* (51) *are the cotangents of the canonical angles between the spaces* $\mathcal{W}_1$ *and* $\mathcal{W}_2$.

Proof. Let $W_k^{(2)}$ denote an *orthonormal* basis of $\mathcal{W}_2$ such that $\hat{W}_k^{(2)} = W_k^{(2)} S$ with a nonsingular matrix $S \in \mathbb{C}^{k\times k}$. Then the cosines of the canonical angles between $\mathcal{W}_1$ and $\mathcal{W}_2$ are the singular values of $[W_m^{(1)}]^* W_k^{(2)}$, and we write the associated singular value decomposition as $[W_m^{(1)}]^* W_k^{(2)} = X \Gamma Y^{\mathrm{H}}$ with a diagonal matrix $\Gamma \in \mathbb{R}^{m\times k}$ and the unitary matrices $X \in \mathbb{C}^{m\times m}$ and $Y \in \mathbb{C}^{k\times k}$. From

$$\begin{aligned} Z_k R &= (I_k - W_m^{(1)}[W_m^{(1)}]^*)\hat{W}_k^{(2)} = (I_k - (W_m^{(1)}X)(W_m^{(1)}X)^*)(W_k^{(2)}Y)Y^{\mathrm{H}}S \\ &= [(W_k^{(2)}Y) - (W_m^{(1)}X)\Gamma]Y^{\mathrm{H}}S, \end{aligned}$$

we obtain $Z_k = [(W_k^{(2)}Y) - (W_m^{(1)}X)\Gamma]Y^{\mathrm{H}}SR^{-1}$ and therefore, defining the diagonal matrix $\Sigma \in \mathbb{R}^{k\times k}$ by $I_k - \Gamma^{\mathrm{H}}\Gamma = \Sigma^2$, there results

$$I_k = Z_k^* Z_k = (SR^{-1})^{\mathrm{H}} Y\Sigma^2 Y^{\mathrm{H}}(SR^{-1}) = (\Sigma Y^{\mathrm{H}}SR^{-1})^{\mathrm{H}}\Sigma Y^{\mathrm{H}}SR^{-1}$$

which reveals that the $k \times k$ matrix $\Sigma Y^{\mathrm{H}}SR^{-1}$ is also unitary. Note that, in view of $\mathcal{W}_1 \cap \mathcal{W}_2 = \{\mathbf{0}\}$, none of the cosines in Γ are one, hence Σ is nonsingular. Now, inserting

$$[W_m^{(1)}]^* \hat{W}_k^{(2)} = [W_m^{(1)}]^* W_k^{(2)} S = X\Gamma Y^{\mathrm{H}} S,$$

$$Z_k^* \hat{W}_k^{(2)} = (SR^{-1})^{\mathrm{H}} Y[(W_k^{(2)}Y)^* - \Gamma^{\mathrm{H}}(W_m^{(1)}X)^*]W_k^{(2)}S = (SR^{-1})^{\mathrm{H}} Y\Sigma^2 Y^{\mathrm{H}} S$$

can express the singular value decomposition (51) as

$$([W_m^{(1)}]^* \hat{W}_k^{(2)})(Z_k^* \hat{W}_k^{(2)})^{-1} = X(\Gamma\Sigma^{-1})(\Sigma Y^{\mathrm{H}}SR^{-1}),$$

which reveals that its singular values are indeed the cotangents of the angles between $\mathcal{W}_1$ and $\mathcal{W}_2$. □

The proof also shows that the left singular vectors of (51) coincide with those of $[W_m^{(1)}]^* W_k^{(2)}$, hence the selection scheme discards that subspace of $\mathcal{W}_1$ which lies at the largest canonical angles with $\mathcal{W}_2$. As shown in Section 2.4, this choice yields the greatest possible residual reduction when replacing the approximation space $\mathcal{W}_1 + \mathcal{W}_2$ by $\tilde{\mathcal{W}}_1 + \mathcal{W}_2$ with $\tilde{\mathcal{W}}_1$ a subspace of $\mathcal{W}_1$ of dimension $\dim\mathcal{W}_1 - k$.

In [26] de Sturler applies this scheme to a GMRES cycle of length m in order to determine which directions of the s-dimensional Krylov subspace $\mathcal{K}_s(A, \boldsymbol{r}_0)$, $s < m$, are most important for convergence in the sense that maintaining orthogonality against these directions upon restarting after the first s steps results in the greatest residual reduction. The subspaces to be compared are thus $A\mathcal{K}_s(A, \boldsymbol{r}_0)$ and $A\mathcal{K}_{m-s}(A, \boldsymbol{r}_s)$. The subspace comparison in this case is particularly inexpensive, as both spaces lie in $\mathcal{K}_m(A, \boldsymbol{r}_0)$, for which the Arnoldi process has computed an orthonormal basis. Hence, the angle computations can be performed in the coordinate space with respect to this basis, and therefore involve only small matrices. For details, we refer to [26].

This subspace selection scheme is further used in [26] to improve the inner-outer iteration algorithm GCRO (see Section 4.1). The resulting method, named GCROT, uses the subspace selection scheme specialized to GMRES to transfer several vectors from the inner to the outer approximation space after each inner iteration cycle. In addition, once the outer approximation space exceeds a maximal dimension, it is truncated by comparing it against the inner approximation space in the manner outlined above.

5. Concluding remark

Having described all these improvements of restarted GMRES of course raises the question of which method one should use in practice. Some of the theoretical statements we have made in this paper required simplifying assumptions which seldom hold in practice. Our results can be viewed

as a mathematical justification of why and how these methods work, but need to be supplemented by thorough numerical investigations for realistic applications to yield a complete comparison.

We can, however, make the following statement independently of any numerical evidence: None of the techniques presented here can replace an effective preconditioning strategy, but can sometimes dramatically improve the performance of restarted GMRES when applied to a properly preconditioned linear system.

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