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Geometric aspects of the theory of Krylov subspace methods

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The development of Krylov subspace methods for the solution of operator equations has shown that two basic construction principles underlie the most commonly used algorithms: the orthogonal residual (OR) and minimal residual (MR) approaches. It is shown that these can both be formulated as techniques for solving an approximation problem on a sequence of nested subspaces of a Hilbert space, an abstract problem not necessarily related to an operator equation. Essentially all Krylov subspace algorithms result when these subspaces form a Krylov sequence. The well-known relations among the iterates and residuals of MR/OR pairs are shown to hold also in this rather general setting. We further show that a common error analysis for these methods involving the canonical angles between subspaces allows many of the known residual and error bounds to be derived in a simple and consistent manner. An application of this analysis to compact perturbations of the identity shows that MR/OR pairs of Krylov subspace methods converge q-superlinearly when applied to such operator equations.

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CONTENTS

1. Overview

In the past three decades research on Krylov subspace techniques for solving linear systems of equations has brought forth a variety of algorithms and methods so large that even specialists in matrix computations have difficulties keeping up. This situation is all the more confusing for scientists whose main interests lie elsewhere when faced with choosing among the many approaches for solving a linear system, or merely attempting to obtain an overview of the methods and how they are related. This state of affairs applies not only to the methods themselves, but also to many theoretical results obtained time and again for each individual method.

It is our objective in this paper to develop the theory and algorithms on which all Krylov subspace methods are based through several layers of abstraction, proceeding from the most general to the most specific and leading to Krylov subspace methods in the form in which they are currently used. We have found several advantages to this approach. First, by obtaining each result in as general a setting as possible, it is easier to distinguish properties unique to Krylov subspace methods from those which these methods inherit as, say, projection methods or subspace correction methods. We will indeed see that many results on Krylov subspace methods hold in greater generality than usually stated, and that many computational elements of these methods can be translated with little modification to more general methods. Second, our approach emphasizes the common origin of all Krylov subspace methods and we have found this approach an elegant yet simple way of presenting this theory, tying together in a consistent and natural framework many results that are otherwise difficult to relate. Finally, we have found that this way of developing Krylov subspace theory offers a new and insightful perspective and is accessible to any reader familiar with only basic facts about inner product spaces.

In the literature on Krylov subspace techniques for solving linear systems of equations, two principal methods have emerged as the basis for most

algorithms: these are the *minimal residual* (MR) and the *orthogonal residual* (OR) approaches. Both methods select an approximation to the solution of the linear system from a shifted Krylov space. The former does this in such a way that the resulting residual norm is minimized, whereas the latter chooses the approximation such that the associated residual is orthogonal to the Krylov space. The following is a list of the most widely used MR/OR pairs:

- the conjugate residual (CR)/conjugate gradient (CG) methods for Hermitian definite systems (Hestenes and Stiefel 1952)
- the minimal residual method (MINRES)/CG methods for Hermitian indefinite systems (Paige and Saunders 1975)
- the full orthogonalization method (FOM)/generalized minimal residual method (GMRES) for the non-Hermitian case (Saad 1981, Saad and Schultz 1986)
- the biconjugate gradient (BCG)/quasi-minimal residual (QMR) methods (QMR) for non-Hermitian problems (Lanczos 1952, Freund and Nachtigal 1991)
- conjugate gradients squared (CGS)/transpose-free QMR (TFQMR) for non-Hermitian problems (Sonneveld 1989, Freund 1993),

where the last two pairs of methods require us to define orthogonality with respect to a problem-dependent inner product, a matter which will be discussed in detail in Sections 4 and 5.

Expositions of these and other Krylov subspace methods can be found, for instance, in the monographs of Hageman and Young (1981), Axelsson (1994), Bruaset (1995), Fischer (1996), Saad (1996), Greenbaum (1997), Weiss (1997), and Meurant (1999). In addition, there are also several survey papers with differing emphases, among which we mention those of Ashby, Manteuffel and Saylor (1990), Freund, Golub and Nachtigal (1992), Gutknecht (1997), Golub and van der Vorst (1997) and van der Vorst and Saad (2000).

In what follows, $\mathcal{H}$ denotes a Hilbert space with inner product $(\cdot,\cdot)$ and associated norm $\|\cdot\|$. By $A : \mathcal{H} \to \mathcal{H}$, we always denote an invertible bounded linear operator. Krylov subspace methods for solving a linear operator equation

$$A\boldsymbol{x} = \boldsymbol{b} \tag{1.1}$$

begin with an initial approximation $\boldsymbol{x}_0$ of $\boldsymbol{x} = A^{-1}\boldsymbol{b}$ and at each step $m = 1, 2, \ldots$ attempt to construct an improved approximation $\boldsymbol{x}_m = \boldsymbol{x}_0 + \boldsymbol{c}_m$ by adding a correction $\boldsymbol{c}_m$ from the Krylov space

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

of order m with respect to A and the initial residual $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$. The MR approach determines the correction $\boldsymbol{c}_m^{\mathrm{MR}}$ in such a way that the associated residual is minimized, that is,

$$\|\boldsymbol{b} - A\boldsymbol{x}_m^{\mathrm{MR}}\| = \|\boldsymbol{r}_0 - A\boldsymbol{c}_m^{\mathrm{MR}}\| = \min_{\boldsymbol{c}\in\mathcal{K}_m(A,\boldsymbol{r}_0)} \|\boldsymbol{r}_0 - A\boldsymbol{c}\|, \tag{1.2a}$$

while the OR approach determines the correction from the Galerkin condition

$$\boldsymbol{b} - A\boldsymbol{x}_m^{\mathrm{OR}} = \boldsymbol{r}_0 - A\boldsymbol{c}_m^{\mathrm{OR}} \perp \mathcal{K}_m(A, \boldsymbol{r}_0). \tag{1.2b}$$

In contrast to the MR approximation, there are situations where the OR approximation may not exist or may not be uniquely determined and these are discussed below.

The Krylov subspace MR and OR methods are special cases of the more general *subspace correction methods*: given an arbitrary correction space $\mathcal{C}_m$ of dimension m, determine $\boldsymbol{c}_m^{\mathrm{MR}}$ and $\boldsymbol{c}_m^{\mathrm{OR}}$ such that

$$\|\boldsymbol{r}_0 - A\boldsymbol{c}_m^{\mathrm{MR}}\| = \min_{\boldsymbol{c}\in\mathcal{C}_m} \|\boldsymbol{r}_0 - A\boldsymbol{c}\| \tag{1.3a}$$

and

$$\boldsymbol{r}_0 - A\boldsymbol{c}_m^{\mathrm{OR}} \perp \mathcal{V}_m, \tag{1.3b}$$

respectively, for some suitable m-dimensional test space $\mathcal{V}_m$. Letting $\mathcal{W}_m := A\mathcal{C}_m$ denote the image of the correction space under A, we can reformulate (1.3a) and (1.3b) as the task of determining $\boldsymbol{w}_m^{\mathrm{MR}}, \boldsymbol{w}_m^{\mathrm{OR}} \in \mathcal{W}_m$ such that

$$\|\boldsymbol{r}_0 - \boldsymbol{w}_m^{\mathrm{MR}}\| = \min_{\boldsymbol{w}\in\mathcal{W}_m} \|\boldsymbol{r}_0 - \boldsymbol{w}\| \tag{1.4a}$$

and

$$\boldsymbol{r}_0 - \boldsymbol{w}_m^{\mathrm{OR}} \perp \mathcal{V}_m. \tag{1.4b}$$

The solutions of (1.4a) and (1.4b) are, of course, given by the orthogonal projection $\boldsymbol{w}_m^{\mathrm{MR}} = P_{\mathcal{W}_m}\boldsymbol{r}_0$ of $\boldsymbol{r}_0$ onto $\mathcal{W}_m$ and the oblique projection $\boldsymbol{w}_m^{\mathrm{OR}} = P_{\mathcal{W}_m}^{\mathcal{V}_m}\boldsymbol{r}_0$ of $\boldsymbol{r}_0$ onto $\mathcal{W}_m$ orthogonal to $\mathcal{V}_m$, respectively. In view of (1.4a) and (1.4b), the MR and OR approaches consist of approximating $\boldsymbol{r}_0 \in \mathcal{H}$ in the space $\mathcal{W}_m$ by its orthogonal and oblique projections onto $\mathcal{W}_m$.

In the following section we shall determine what can be said about the approximation of an arbitrary element in $\mathcal{H}$ by its orthogonal and oblique projections with respect to given spaces $\mathcal{W}$ and $\mathcal{V}$ of equal (finite) dimension. We then consider such approximations with respect to nested sequences of spaces $\{\mathcal{W}_m\}_{m\geq 0}$ and $\{\mathcal{V}_m\}_{m\geq 0}$ and show that all the well-known relations between Krylov subspace MR and OR approximations and their residuals already hold in this abstract setting of approximation by orthogonal and oblique projection. The source of these relations is thereby seen to lie in the properties of orthogonal and oblique projections on a nested sequence of

subspaces, where the oblique projection is orthogonal to the previous error space (which we shall call residual space to emphasize its Krylov subspace correspondence). In particular, these relations are not restricted to Krylov spaces, or even to solving equations.

In the usual implementations, the Krylov MR/OR approximations are computed by solving a small least-squares problem or linear system, respectively, involving a tridiagonal or Hessenberg matrix at each step. This is done by maintaining a QR factorization of this Hessenberg matrix which is updated at each step using Givens rotations. Due to the Hessenberg structure, only one Givens rotation is required at each step, and the angles of these rotations can be used to characterize the OR and MR residual norms and also to express the iterates and residuals in terms of each other.

In our abstract setting, these relations are derived using only the notion of angles between the spaces which define the orthogonal and oblique projections. The sines and cosines occurring in these expressions are therefore not mere artifacts of the computational scheme for the MR and OR approximations, but have an intrinsic meaning. It is this intrinsic relationship between the orthogonal and oblique projections that is at the root of the often observed close relationship between MR and OR approximations.

We further discuss the relation between MR and quasi-minimal residual (QMR) approximations. The latter is also obtained by solving a least-squares problem in coordinate space, the only difference to the MR approximation being that these coordinates are with respect to a non-orthogonal basis. We show that QMR approximations become MR approximations if only the inner product is appropriately chosen. Again, the QMR approximation can be defined in our abstract setting and then has a structure identical to the MR approximation. This distinction between MR and QMR approximations via different inner products also extends to OR and quasi-orthogonal residual (QOR) approximations; in fact, we show that *essentially any* Krylov subspace method for solving a linear system can be classified as both an MR or OR method by appropriate choice of the inner product.

In Section 2 we cast the MR and OR approximations to the solution of an operator equation as abstract approximation problems or, equivalently, as an orthogonal and oblique projection method, respectively. In contrast to the orthogonal projection, there are situations in which the oblique projection, and hence the OR approximation, may not exist. A useful characterization of the oblique projection as the Moore–Penrose inverse of the product of two orthogonal projections leads to a canonical way of defining an OR approximation in case of such a breakdown. We characterize the conditions under which the oblique projection exists and relate the norm of the oblique projection to the angle between two subspaces.

Section 3 specializes the spaces characterizing the projections to two sequences of closely related nested spaces. It is shown that, under these general

conditions, all the well-known relations among OR/MR pairs such as FOM/GMRES can be derived. These results also elucidate the theory behind residual smoothing techniques.

Section 4 explores the coordinate calculations required to compute the MR and OR approximations with respect to orthogonal and non-orthogonal bases of the underlying spaces. These involve solving least-squares problems and linear systems with a Hessenberg matrix. When a QR-factorization based on Givens rotations is used to solve these problems, the angles characterizing the Givens rotations are identified as the angles between these subspaces. Moreover, it is shown that methods based on non-orthogonal bases can be characterized as MR/OR methods with respect to a different, basis-dependent inner product. We further characterize the QMR and QOR approximations as oblique projections with respect to the original inner product and conclude with a characterization for when the QMR approximation coincides with the MR approximation.

Section 5 specializes the spaces yet further to Krylov subspaces and their images under the operator A. We recover familiar Krylov subspace algorithms and show that our framework covers all Krylov subspace methods.

In Section 6 we show how angles between subspaces may be used to derive known residual and error bounds for MR and OR methods and include an application to compact perturbations of the identity.

Final remarks and conclusions are given in Section 7.

2. Approximations, projections and angles

Here we consider two basic methods for approximating a vector $\boldsymbol{r}_0 \in \mathcal{H}$ by an element $\boldsymbol{w}$ from a subspace $\mathcal{W} \subset \mathcal{H}$ and recall their well-known relations to projections and angles. Although the results in this and the following two sections make no reference to solving equation (1.1), we will, of course, ultimately make this connection. In order to avoid changing notation at that point, however, we adopt the notation and terminology of equation solving from the beginning. Thus we denote the (for now arbitrary) vector to be approximated by $\boldsymbol{r}_0$, since this role will later be played by the residual vector associated with an initial guess $\boldsymbol{x}_0$ for $A^{-1}\boldsymbol{b}$. Similarly, we denote the associated approximation error $\boldsymbol{r}_0 - \boldsymbol{w}$ by $\boldsymbol{r}$, as it will coincide with the residuals $\boldsymbol{r} = \boldsymbol{b} - A(\boldsymbol{x}_0 + \boldsymbol{c}) = \boldsymbol{r}_0 - A\boldsymbol{c}$ of subsequent correction vectors $\boldsymbol{c}$ in the equation-solving context (*i.e.*, $\boldsymbol{w}$ is then of the form $\boldsymbol{w} = A\boldsymbol{c}$).

Given an arbitrary finite-dimensional subspace $\mathcal{W} \subset \mathcal{H}$ and an element $\boldsymbol{r}_0 \in \mathcal{H}$, we define its MR approximation $\boldsymbol{w}^{\mathrm{MR}}$ as the best approximation of $\boldsymbol{r}_0$ from $\mathcal{W}$ and denote by $\boldsymbol{r}^{\mathrm{MR}}$ the associated error

$$\boldsymbol{w}^{\mathrm{MR}} := P_{\mathcal{W}}\boldsymbol{r}_0, \qquad \boldsymbol{r}^{\mathrm{MR}} := \boldsymbol{r}_0 - \boldsymbol{w}^{\mathrm{MR}} = (I - P_{\mathcal{W}})\boldsymbol{r}_0 \perp \mathcal{W},$$

where $P_{\mathcal{W}}$ is the orthogonal projection onto $\mathcal{W}$. The distance between $\boldsymbol{r}_0$

and its best approximation $P_{\mathcal{W}}\boldsymbol{r}_0$ in $\mathcal{W}$ can be described in terms of angles between vectors and subspaces of $\mathcal{H}$. The angle $\measuredangle(\boldsymbol{x},\boldsymbol{y})$ between two nonzero elements $\boldsymbol{x},\boldsymbol{y}\in\mathcal{H}$ is defined by the relation

$$\cos\measuredangle(\boldsymbol{x},\boldsymbol{y}) := \frac{|(\boldsymbol{x},\boldsymbol{y})|}{\|\boldsymbol{x}\|\,\|\boldsymbol{y}\|},$$

which, in view of the Cauchy–Schwarz inequality, uniquely determines the number $\measuredangle(\boldsymbol{x},\boldsymbol{y})\in[0,\pi/2]$. We note here that the natural definition of the angle would replace the modulus in the numerator by the real part; our definition, however, is more appropriate for comparing subspaces (see also the discussion of this issue in Davis and Kahan (1970, p. 9)). Similarly, we define the angle between a nonzero vector $\boldsymbol{x}\in\mathcal{H}$ and a subspace $\mathcal{U}\subset\mathcal{H}$, $\mathcal{U}\neq\{\boldsymbol{0}\}$, as

$$\measuredangle(\boldsymbol{x},\mathcal{U}) := \inf_{\boldsymbol{0}\neq\boldsymbol{u}\in\mathcal{U}}\measuredangle(\boldsymbol{x},\boldsymbol{u}), \quad \textit{i.e.}, \quad \cos\measuredangle(\boldsymbol{x},\mathcal{U}) = \sup_{\boldsymbol{0}\neq\boldsymbol{u}\in\mathcal{U}}\cos\measuredangle(\boldsymbol{x},\boldsymbol{u}).$$

Further, we define the sine of this angle as

$$\sin\measuredangle(\boldsymbol{x},\mathcal{U}) := \sqrt{1-\cos^2\measuredangle(\boldsymbol{x},\mathcal{U})}.$$

The connection between angles and orthogonal projections is given in the following lemma, a proof of which can be found in Wedin (1983), for example.

Lemma 2.1. Let $\mathcal{U}$ be a finite-dimensional subspace of $\mathcal{H}$ and let $P_{\mathcal{U}}$ denote the orthogonal projection onto $\mathcal{U}$. For each $\boldsymbol{x}\in\mathcal{H}$ we have

$$\measuredangle(\boldsymbol{x},\mathcal{U}) = \measuredangle(\boldsymbol{x},P_{\mathcal{U}}\boldsymbol{x}) \tag{2.1}$$

and, as a consequence,

$$\|P_{\mathcal{U}}\boldsymbol{x}\| = \|\boldsymbol{x}\|\cos\measuredangle(\boldsymbol{x},\mathcal{U}), \tag{2.2}$$

$$\|(I-P_{\mathcal{U}})\boldsymbol{x}\| = \|\boldsymbol{x}\|\sin\measuredangle(\boldsymbol{x},\mathcal{U}). \tag{2.3}$$

In light of this result, the distance between $\boldsymbol{r}_0$ and its MR approximation $\boldsymbol{w}^{\mathrm{MR}}$ may be expressed as

$$\|\boldsymbol{r}^{\mathrm{MR}}\| = \|\boldsymbol{r}_0-\boldsymbol{w}^{\mathrm{MR}}\| = \|(I-P_{\mathcal{W}})\boldsymbol{r}_0\| = \|\boldsymbol{r}_0\|\sin\measuredangle(\boldsymbol{r}_0,\mathcal{W}). \tag{2.4}$$

In order to define the OR approximation in this abstract setting we require a further finite-dimensional subspace $\mathcal{V}\subset\mathcal{H}$ to formulate the orthogonality constraint. The OR approximation $\boldsymbol{w}^{\mathrm{OR}}\in\mathcal{W}$ of $\boldsymbol{r}_0$ is then defined by the requirement

$$\boldsymbol{w}^{\mathrm{OR}}\in\mathcal{W}, \qquad \boldsymbol{r}_0-\boldsymbol{w}^{\mathrm{OR}}\perp\mathcal{V}.$$

Of course, since choosing $\mathcal{V}=\mathcal{W}$ yields the MR approximation, the latter is just a special case of the OR approximation. We choose nonetheless to distinguish the two, both for historical reasons and for ease of exposition. Existence and uniqueness of $\boldsymbol{w}^{\mathrm{OR}}$ are summarized in the following result.

Lemma 2.2. If $\mathcal{V}, \mathcal{W}$ are subspaces of the Hilbert space $\mathcal{H}$ and $\boldsymbol{r}_0 \in \mathcal{H}$, then

(a) there exists $\boldsymbol{w} \in \mathcal{W}$ such that $\boldsymbol{r}_0 - \boldsymbol{w} \perp \mathcal{V}$ if and only if $\boldsymbol{r}_0 \in \mathcal{W} + \mathcal{V}^\perp$;

(b) such a $\boldsymbol{w}$ is unique if and only if $\mathcal{W} \cap \mathcal{V}^\perp = \{\boldsymbol{0}\}$.

Thus, a unique OR approximation is defined for any $\boldsymbol{r}_0 \in \mathcal{H}$ whenever $\mathcal{H} = \mathcal{W} \oplus \mathcal{V}^\perp$. In this case $\boldsymbol{w}^{\mathrm{OR}}$ is the *oblique* projection of $\boldsymbol{r}_0$ onto $\mathcal{W}$ *orthogonal to* $\mathcal{V}$ (or, equivalently, along $\mathcal{V}^\perp$), which we denote by $P_{\mathcal{W}}^{\mathcal{V}} : \mathcal{H} \to \mathcal{W}$, and $\boldsymbol{w}^{\mathrm{OR}}$ is characterized by

$$\boldsymbol{w}^{\mathrm{OR}} = P_{\mathcal{W}}^{\mathcal{V}} \boldsymbol{r}_0, \qquad \boldsymbol{r}^{\mathrm{OR}} = \boldsymbol{r}_0 - \boldsymbol{w}^{\mathrm{OR}} = (I - P_{\mathcal{W}}^{\mathcal{V}})\boldsymbol{r}_0 \perp \mathcal{V}.$$

When it exists, the oblique projection $P_{\mathcal{W}}^{\mathcal{V}}$ is given by the Moore–Penrose inverse $(P_{\mathcal{V}} P_{\mathcal{W}})^+$ of $P_{\mathcal{V}} P_{\mathcal{W}}$ (*cf.* Wedin (1983)). This is established in the following two lemmas, the first of which describes the mapping properties of $(P_{\mathcal{V}} P_{\mathcal{W}})^+$.

Lemma 2.3. Given two finite-dimensional subspaces $\mathcal{V}$ and $\mathcal{W}$ of the Hilbert space $\mathcal{H}$, let $S := (P_{\mathcal{V}} P_{\mathcal{W}})^+$ denote the Moore–Penrose inverse of the product of the orthogonal projections onto $\mathcal{W}$ and $\mathcal{V}$. Then S is a projection and we have

$$\operatorname{range}(S) = \mathcal{W} \cap (\mathcal{V} + \mathcal{W}^\perp), \tag{2.5}$$

$$\operatorname{null}(S) = \mathcal{V}^\perp + (\mathcal{W}^\perp \cap \mathcal{V}). \tag{2.6}$$

Proof. The proof of the projection property $S^2 = S$ follows along the lines of Greville (1974, Theorem 1). First, since $P := P_{\mathcal{V}} P_{\mathcal{W}}$ has finite rank, its Moore–Penrose pseudo-inverse $P^+ = S$ exists and satisfies $\operatorname{range}(P^+) = \operatorname{range}(P^*)$, from which it follows that

$$\operatorname{range}(S) \subset \operatorname{range}(P_{\mathcal{W}}), \qquad \operatorname{range}(S^*) \subset \operatorname{range}(P_{\mathcal{V}}),$$

and hence, by the idempotency of $P_{\mathcal{V}}$ and $P_{\mathcal{W}}$,

$$P_{\mathcal{W}} S = S, \qquad S P_{\mathcal{V}} = S,$$

which together imply $S^2 = S P_{\mathcal{V}} P_{\mathcal{W}} S = P^+ P P^+ = P^+ = S$.

Since $\operatorname{range}(S) = \operatorname{range}((P_{\mathcal{V}} P_{\mathcal{W}})^*) = \operatorname{range}(P_{\mathcal{W}} P_{\mathcal{V}})$ and analogously for the null space, it is sufficient to show (2.5) and (2.6) for the operator $P_{\mathcal{W}} P_{\mathcal{V}}$ instead of S. To derive (2.5), note that $\boldsymbol{w} \in \mathcal{W}$ lies in $\operatorname{range}(P_{\mathcal{W}} P_{\mathcal{V}})$ if and only if there exists $\boldsymbol{v} \in \mathcal{V}$ such that $\boldsymbol{v} = \boldsymbol{w} + \boldsymbol{w}_\perp$ for some $\boldsymbol{w}_\perp \in \mathcal{W}^\perp$, which in turn is equivalent to $\boldsymbol{w} \in \mathcal{W} \cap (\mathcal{V} + \mathcal{W}^\perp)$. To see (2.6), note that any $\boldsymbol{x} \in \mathcal{H}$ may be written as $\boldsymbol{x} = (\boldsymbol{w} + \boldsymbol{w}_\perp) + \boldsymbol{v}_\perp$ with $\boldsymbol{w} \in \mathcal{W}$, $\boldsymbol{w}_\perp \in \mathcal{W}^\perp$, $\boldsymbol{v}_\perp \in \mathcal{V}^\perp$, and $\boldsymbol{w} + \boldsymbol{w}_\perp \in \mathcal{V}$. Thus, $\boldsymbol{x} \in \operatorname{null}(P_{\mathcal{W}} P_{\mathcal{V}})$ if and only if $\boldsymbol{w} = \boldsymbol{0}$ or, equivalently, $\boldsymbol{x} \in \mathcal{V}^\perp + (\mathcal{W}^\perp \cap \mathcal{V})$. □

Lemma 2.4. Given two finite-dimensional subspaces $\mathcal{V}$ and $\mathcal{W}$ of the Hilbert space $\mathcal{H}$ such that $\mathcal{H} = \mathcal{W} \oplus \mathcal{V}^\perp$, the oblique projection $P_{\mathcal{W}}^{\mathcal{V}}$ onto $\mathcal{W}$ orthogonal to $\mathcal{V}$ is given by

$$P_{\mathcal{W}}^{\mathcal{V}} = (P_{\mathcal{V}} P_{\mathcal{W}})^+. \tag{2.7}$$

Proof. By the previous lemma, S is a projection and, in view of $\mathcal{V} + \mathcal{W}^\perp = (\mathcal{V}^\perp \cap \mathcal{W})^\perp$, $\mathcal{W}^\perp \cap \mathcal{V} = (\mathcal{W} + \mathcal{V}^\perp)^\perp$, and $\mathcal{H} = \mathcal{W} \oplus \mathcal{V}^\perp$, its range is $\mathcal{W}$ and its null space is $\mathcal{V}^\perp$, which together characterize it as $P_{\mathcal{W}}^{\mathcal{V}}$. □

Remark 2.5. We note that, while the left-hand side of (2.7) exists only under the condition $\mathcal{H} = \mathcal{W} \oplus \mathcal{V}^\perp$, the right-hand side is always defined. Thus, $(P_{\mathcal{V}} P_{\mathcal{W}})^+ \boldsymbol{r}_0$ can be viewed as a natural way of defining an OR approximation in those cases where this direct sum condition fails to hold, a situation sometimes referred to, in the context of Krylov subspace methods, as a *Galerkin breakdown*.

As is to be expected, the error $\boldsymbol{r}^{\mathrm{OR}} = \boldsymbol{r}_0 - P_{\mathcal{W}}^{\mathcal{V}} \boldsymbol{r}_0$ depends on the angles between the subspaces $\mathcal{V}$ and $\mathcal{W}$, which we introduce as follows (*cf.* Golub and Van Loan (1996, Section 12.4.3)): Given two finite-dimensional subspaces $\mathcal{V}$ and $\mathcal{W}$ of $\mathcal{H}$, let $m := \min(\dim \mathcal{V}, \dim \mathcal{W})$. The *canonical* or *principal angles* $\{\theta_j\}_{j=1}^m$ between $\mathcal{V}$ and $\mathcal{W}$ are defined recursively by

$$\cos\theta_j := \max_{\mathbf{0} \neq \boldsymbol{v} \in \mathcal{V}} \max_{\mathbf{0} \neq \boldsymbol{w} \in \mathcal{W}} \frac{|(\boldsymbol{v}, \boldsymbol{w})|}{\|\boldsymbol{v}\| \, \|\boldsymbol{w}\|} =: \frac{|(\boldsymbol{v}_j, \boldsymbol{w}_j)|}{\|\boldsymbol{v}_j\| \, \|\boldsymbol{w}_j\|}$$

subject to $\boldsymbol{v} \perp \boldsymbol{v}_1, \ldots, \boldsymbol{v}_{j-1}$ and $\boldsymbol{w} \perp \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{j-1}$. We further define *the* angle between the spaces $\mathcal{V}$ and $\mathcal{W}$ as the largest canonical angle

$$\measuredangle(\mathcal{V}, \mathcal{W}) := \theta_m.$$

Remark 2.6. If $P_{\mathcal{V}} P_{\mathcal{W}} = \sum_{j=1}^m \sigma_j(\cdot, \boldsymbol{w}_j) \boldsymbol{v}_j$ is a singular value decomposition of $P_{\mathcal{V}} P_{\mathcal{W}}$, then the variational characterization of the singular values,

$$\sigma_j(P_{\mathcal{V}} P_{\mathcal{W}}) = \max_{\boldsymbol{v} \in \mathcal{V}, \boldsymbol{w} \in \mathcal{W}} \frac{|(P_{\mathcal{V}} P_{\mathcal{W}} \boldsymbol{w}, \boldsymbol{v})|}{\|\boldsymbol{w}\| \, \|\boldsymbol{v}\|} =: \frac{|(P_{\mathcal{V}} P_{\mathcal{W}} \boldsymbol{w}_j, \boldsymbol{v}_j)|}{\|\boldsymbol{w}_j\| \, \|\boldsymbol{v}_j\|}$$

subject to $\boldsymbol{v} \perp \boldsymbol{v}_1, \ldots, \boldsymbol{v}_{j-1}$, $\boldsymbol{w} \perp \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{j-1}$ for $j = 1, \ldots, m$ (*cf.* Björck and Golub (1973)), shows immediately that $\cos\theta_j = \sigma_j$. Furthermore, we note that, given any two orthonormal bases $\{\boldsymbol{v}_j\}_{j=1}^{\dim \mathcal{V}}$ and $\{\boldsymbol{w}_j\}_{j=1}^{\dim \mathcal{W}}$ of $\mathcal{V}$ and $\mathcal{W}$, then the cosines of the canonical angles are the singular values of the matrix of inner products $[(\boldsymbol{v}_j, \boldsymbol{w}_k)]_{j=1,\ldots,\dim \mathcal{V}, k=1,\ldots,\dim \mathcal{W}}$ (*cf.* Chatelin (1993)).

Remark 2.7. As a consequence of Remark 2.6, we see that $S = (P_{\mathcal{V}} P_{\mathcal{W}})^+$ can be written as

$$S = \sum_{j=1}^m \sigma_j^+(\cdot, \boldsymbol{v}_j) \boldsymbol{w}_j \quad \text{with} \quad \sigma_j^+ := \begin{cases} 1/\sigma_j, & \text{if } \sigma_j > 0, \\ 0, & \text{otherwise.} \end{cases}$$

In particular, we have

$$\operatorname{range}(S) = \operatorname{span}\{\boldsymbol{w}_j : \sigma_j > 0\}, \qquad \operatorname{null}(S) = \operatorname{span}\{\boldsymbol{v}_j : \sigma_j > 0\}^{\perp}.$$

Thus, we have $\operatorname{range}(S) = \mathcal{W}$ if and only if $\dim(\mathcal{W}) = m$ and $\sigma_j > 0$ for all $j = 1, \ldots, m$. Similarly, $\operatorname{null}(S) = \mathcal{V}^{\perp}$ if and only if $\dim(\mathcal{V}) = m$ and $\sigma_j > 0$ for all $j = 1, \ldots, m$. Consequently, the oblique projection $P_{\mathcal{W}}^{\mathcal{V}}$ exists if and only if $\dim(\mathcal{V}) = \dim(\mathcal{W})$ and $\measuredangle(\mathcal{V}, \mathcal{W}) < \pi/2$.

Remark 2.8. Two further characterizations of the angle between two subspaces, $\mathcal{V}$ and $\mathcal{W}$, are given by

$$\measuredangle(\mathcal{V}, \mathcal{W}) = \max_{\substack{\boldsymbol{v} \in \mathcal{V}, \\ \boldsymbol{v} \neq \boldsymbol{0}}} \measuredangle(\boldsymbol{v}, P_{\mathcal{W}}^{\mathcal{V}} \boldsymbol{v})$$

(see Saad (1982)) and $\sin \measuredangle(\mathcal{V}, \mathcal{W}) = \|P_{\mathcal{V}} - P_{\mathcal{W}}\|$ (*cf.* Chatelin (1993, p. 5)).

Besides the relative position of the spaces $\mathcal{V}$ and $\mathcal{W}$, the error of the OR approximation also depends on the position of $\boldsymbol{r}_0$ with respect to $\mathcal{V}$ and $\mathcal{W}$. In this generality, all we can do to bound the OR approximation error is determine the norm of the complementary projection $I - P_{\mathcal{W}}^{\mathcal{V}}$. For simplicity, since $\mathcal{H} = \mathcal{W} \oplus \mathcal{V}^{\perp}$ for finite-dimensional $\mathcal{V}$ and $\mathcal{W}$ implies $\dim \mathcal{V} = \dim \mathcal{W}$, we assume that both spaces have the same dimension $m < \infty$.

The following result was stated in Saad (1982).

Theorem 2.9. Given two m-dimensional subspaces $\mathcal{V}, \mathcal{W} \subset \mathcal{H}$ of the Hilbert space $\mathcal{H}$ such that $\mathcal{H} = \mathcal{W} \oplus \mathcal{V}^{\perp}$, let $P_{\mathcal{W}}^{\mathcal{V}} : \mathcal{H} \to \mathcal{W}$ denote the oblique projection onto $\mathcal{W}$ orthogonal to $\mathcal{V}$. Then

$$\|I - P_{\mathcal{W}}^{\mathcal{V}}\| = \frac{1}{\cos \measuredangle(\mathcal{V}, \mathcal{W})}. \tag{2.8}$$

Proof. The proof follows from the fact that $\|P\| = \|I - P\|$ for any nontrivial projection operator P in a Hilbert space (*cf.* Kato (1960)). Thus, letting $\sigma_{\min}$ and $\sigma_{\max}$ denote the smallest and largest singular values of an operator, we have

$$\|I - (P_{\mathcal{V}} P_{\mathcal{W}})^{+}\| = \|(P_{\mathcal{V}} P_{\mathcal{W}})^{+}\| = \sigma_{\max}((P_{\mathcal{V}} P_{\mathcal{W}})^{+}) = \frac{1}{\sigma_{\min}(P_{\mathcal{V}} P_{\mathcal{W}})}$$

and the conclusion follows from Remark 2.6. □

Without further assumptions on $\boldsymbol{r}_0$ and the spaces $\mathcal{V}$ and $\mathcal{W}$, all we can say about the error of the OR approximation is

$$\|\boldsymbol{r}^{\mathrm{OR}}\| = \|\boldsymbol{r}_0 - \boldsymbol{w}^{\mathrm{OR}}\| = \|(I - P_{\mathcal{W}}^{\mathcal{V}})\boldsymbol{r}_0\| \leq \frac{\|\boldsymbol{r}_0\|}{\cos \measuredangle(\mathcal{V}, \mathcal{W})}.$$

As an immediate consequence, noting that

$$\boldsymbol{r}^{\mathrm{OR}} = (I - P_{\mathcal{W}}^{\mathcal{V}})\boldsymbol{r}_0 = (I - P_{\mathcal{W}}^{\mathcal{V}})(\boldsymbol{r}_0 - \boldsymbol{w}), \qquad \forall \boldsymbol{w} \in \mathcal{W},$$

we obtain

$$\|\boldsymbol{r}^{\mathrm{OR}}\| \leq \|I - P_{\mathcal{W}}^{\mathcal{V}}\| \inf_{\boldsymbol{w}\in\mathcal{W}} \|\boldsymbol{r}_0 - \boldsymbol{w}\| = \|I - P_{\mathcal{W}}^{\mathcal{V}}\|\, \|\boldsymbol{r}^{\mathrm{MR}}\|,$$

an estimate usually referred to as *Céa's lemma* in connection with projection methods (see, *e.g.*, Brenner and Scott (1994)), which, in view of (2.8), implies

$$\cos\measuredangle(\mathcal{V},\mathcal{W})\, \|\boldsymbol{r}^{\mathrm{OR}}\| \leq \|\boldsymbol{r}^{\mathrm{MR}}\| \leq \|\boldsymbol{r}^{\mathrm{OR}}\|.$$

3. Approximations from nested subspaces

Until now nothing further has been assumed to relate $\mathcal{V}$, $\mathcal{W}$ and $\boldsymbol{r}_0$; hence we were only able to bound the error in the OR approximation in terms of the angle between the spaces $\mathcal{V}$ and $\mathcal{W}$. We will obtain more interesting results in this section by selecting a specific test space $\mathcal{V}$ which differs only slightly from the approximation space $\mathcal{W}$. This choice, however, is still general enough to cover all MR and OR methods, in particular Krylov subspace methods. We now investigate MR and OR approximations on nested sequences of subspaces, which is the setting in which these approximations are used by practical algorithms.

3.1. MR approximations

Consider a sequence of nested subspaces

$$\{\boldsymbol{0}\} = \mathcal{W}_0 \subset \mathcal{W}_1 \subset \cdots \subset \mathcal{W}_{m-1} \subset \mathcal{W}_m \subset \cdots \tag{3.1}$$

of $\mathcal{H}$ and assume for simplicity that $\dim \mathcal{W}_m = m$. Throughout this section, $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$ will always denote an *ascending* orthonormal basis of $\mathcal{W}_m$, that is, one such that $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_j\}$ forms a basis of $\mathcal{W}_j$ for every $j = 1, \ldots, m$. In terms of such a basis, the MR approximation, that is, the best approximation of $\boldsymbol{r}_0 \in \mathcal{H}$ from $\mathcal{W}_m$, can be expressed as the truncated Fourier expansion

$$\boldsymbol{w}_m^{\mathrm{MR}} = P_{\mathcal{W}_m}\boldsymbol{r}_0 = \sum_{j=1}^{m} (\boldsymbol{r}_0, \boldsymbol{w}_j)\boldsymbol{w}_j = \boldsymbol{w}_{m-1}^{\mathrm{MR}} + (\boldsymbol{r}_0, \boldsymbol{w}_m)\boldsymbol{w}_m, \qquad m \geq 1,$$

so that the norm of the associated error $\boldsymbol{r}_m^{\mathrm{MR}} = \boldsymbol{r}_0 - \boldsymbol{w}_m^{\mathrm{MR}}$ is given by

$$\begin{aligned} \|\boldsymbol{r}_m^{\mathrm{MR}}\|^2 = \|(I - P_{\mathcal{W}_m})\boldsymbol{r}_0\|^2 &= \|\boldsymbol{r}_0\|^2 - \sum_{j=1}^{m} |(\boldsymbol{r}_0, \boldsymbol{w}_j)|^2 \\ &= \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2 - |(\boldsymbol{r}_0, \boldsymbol{w}_m)|^2. \end{aligned} \tag{3.2}$$

Relation (3.2) shows that no improvement in the MR approximation results whenever the direction in which $\mathcal{W}_{m-1}$ is enlarged is orthogonal to $\boldsymbol{r}_0$. In

other words,

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| < \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\| \quad \text{if and only if} \quad (\boldsymbol{r}_0, \boldsymbol{w}_m) \neq 0. \tag{3.3}$$

To relate the approximations on successive spaces, note that for $m \geq 1$ we have

$$\boldsymbol{w}_m^{\mathrm{MR}} = \boldsymbol{w}_{m-1}^{\mathrm{MR}} + P_{\mathcal{W}_m} \boldsymbol{r}_{m-1}^{\mathrm{MR}},$$

from which it follows that

$$\boldsymbol{r}_m^{\mathrm{MR}} = \boldsymbol{r}_{m-1}^{\mathrm{MR}} - P_{\mathcal{W}_m} \boldsymbol{r}_{m-1}^{\mathrm{MR}} = (I - P_{\mathcal{W}_m}) \boldsymbol{r}_{m-1}^{\mathrm{MR}}. \tag{3.4}$$

To express successive approximation errors in terms of angles, we note that (3.4) together with (2.3) yields

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = \|(I - P_{\mathcal{W}_m}) \boldsymbol{r}_{m-1}^{\mathrm{MR}}\| = s_m \, \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|, \tag{3.5}$$

where $s_m := \sin \measuredangle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \mathcal{W}_m)$. Note that the sine s_m is also given by (*cf.* (2.4))

$$s_m = \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|} = \frac{\|(I - P_{\mathcal{W}_m}) \boldsymbol{r}_0\|}{\|(I - P_{\mathcal{W}_{m-1}}) \boldsymbol{r}_0\|} = \frac{\sin \measuredangle(\boldsymbol{r}_0, \mathcal{W}_m)}{\sin \measuredangle(\boldsymbol{r}_0, \mathcal{W}_{m-1})}, \tag{3.6}$$

that is, s_m is the sine of the angle between the previous approximation error and $\mathcal{W}_m$ or, equivalently, the quotient of the sines of the angles between $\boldsymbol{r}_0$ and the current and previous approximation spaces. In order for the last three terms in (3.6) to make sense, we assume that $\boldsymbol{r}_0 \notin \mathcal{W}_{m-1}$; otherwise, the approximation problem is solved exactly in the space $\mathcal{W}_{m-1}$ and the larger spaces no longer contribute toward improving the approximation.

In view of (3.2) and (3.5), the corresponding cosine is given by

$$c_m := \sqrt{1 - s_m^2} = \sqrt{1 - \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}} = \frac{|(\boldsymbol{r}_0, \boldsymbol{w}_m)|}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|} \tag{3.7}$$

and we see that an equivalent way of stating (3.3) is

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| < \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\| \quad \text{if and only if} \quad c_m \neq 0. \tag{3.8}$$

An obvious induction applied to (3.5) leads to the error formula

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = s_1 s_2 \cdots s_m \, \|\boldsymbol{r}_0\|, \tag{3.9}$$

from which we see that the sequence of approximations will converge to $\boldsymbol{r}_0$ if and only if the product of sines tends to zero. Moreover, if the numbers s_m themselves tend to zero, the convergence of the MR approximations is superlinear.

3.2. OR approximations

In order to define the OR approximations associated with the nested sequence $\{\mathcal{W}_m\}_{m \geq 0}$, we fix the sequence $\{\mathcal{V}_m\}_{m \geq 1}$ of spaces which define the

orthogonality condition by setting

$$\mathcal{V}_m := \operatorname{span}\{\boldsymbol{r}_0\} + \mathcal{W}_{m-1}, \qquad m = 1, 2, \ldots. \tag{3.10}$$

With this definition of $\mathcal{V}_m$, since the mth OR and MR approximations lie in $\mathcal{W}_m$, the corresponding approximation errors lie in $\mathcal{V}_{m+1}$. Since these errors turn out to be residual vectors in the context of subspace correction methods for solving $A\boldsymbol{x} = \boldsymbol{b}$, we shall refer to $\{\mathcal{V}_m\}_{m\geq 1}$ as the sequence of *residual spaces*.

We first investigate the question of when the OR approximation is well-defined. In view of Remark 2.7, this amounts to checking whether the angle between $\mathcal{V}_m$ and $\mathcal{W}_m$ is strictly less than $\pi/2$. As a consequence of the special choice (3.10) of $\mathcal{V}_m$, it turns out that this angle is the same as $\measuredangle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \mathcal{W}_m)$.

Theorem 3.1. If the spaces $\mathcal{V}_m$ and $\mathcal{W}_m$ are related as in (3.10), then the largest canonical angle between them is given by

$$\measuredangle(\mathcal{V}_m, \mathcal{W}_m) = \measuredangle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \mathcal{W}_m). \tag{3.11}$$

Moreover, the remaining $m-1$ canonical angles between $\mathcal{V}_m$ and $\mathcal{W}_m$ are zero.

Proof. Noting that $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_{m-1}, \widehat{\boldsymbol{w}}_m\}$, with $\widehat{\boldsymbol{w}}_m = \boldsymbol{r}_{m-1}^{\mathrm{MR}}/\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|$, is an orthonormal basis of $\mathcal{V}_m$, we obtain the cosine of the largest canonical angle as the smallest singular value of the matrix

$$\begin{bmatrix} (\boldsymbol{w}_1, \boldsymbol{w}_1) & \ldots & (\boldsymbol{w}_{m-1}, \boldsymbol{w}_1) & (\boldsymbol{w}_m, \boldsymbol{w}_1) \\ \vdots & & \vdots & \vdots \\ (\boldsymbol{w}_1, \boldsymbol{w}_{m-1}) & \ldots & (\boldsymbol{w}_{m-1}, \boldsymbol{w}_{m-1}) & (\boldsymbol{w}_m, \boldsymbol{w}_{m-1}) \\ (\boldsymbol{w}_1, \widehat{\boldsymbol{w}}_m) & \ldots & (\boldsymbol{w}_{m-1}, \widehat{\boldsymbol{w}}_m) & (\boldsymbol{w}_m, \widehat{\boldsymbol{w}}_m) \end{bmatrix} = \begin{bmatrix} I_{m-1} & \boldsymbol{0} \\ \boldsymbol{0} & \frac{(\boldsymbol{w}_m, \boldsymbol{r}_0)}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|} \end{bmatrix}$$

(*cf.* Remark 2.6). Thus the smallest singular value is $|(\boldsymbol{w}_m, \boldsymbol{r}_0)|/\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\| = c_m$ (*cf.* (3.7)) and all remaining singular values are equal to one. □

As an immediate consequence of Theorem 3.1, we obtain the following characterization of when the oblique projection $P_{\mathcal{W}_m}^{\mathcal{V}_m}$ is defined for our specific choice of $\mathcal{V}_m$.

Corollary 3.2. The OR approximation of an arbitrary $\boldsymbol{r}_0 \in \mathcal{H}$ with respect to the sequence of spaces $\mathcal{V}_m$ and $\mathcal{W}_m$ as given by (3.1) and (3.10) is uniquely defined if and only if $(\boldsymbol{r}_0, \boldsymbol{w}_m) \neq 0$, that is, if and only if the MR approximation improves as $\mathcal{W}_{m-1}$ is enlarged to $\mathcal{W}_m$.

Thus the degenerate case in which the OR approximation is not uniquely defined for all $\boldsymbol{r}_0 \in \mathcal{H}$ and for which the MR approximation makes no progress is characterized by $c_m = 0$. We thus tacitly assume $(\boldsymbol{r}_0, \boldsymbol{w}_m) \neq 0$ whenever mentioning the OR approximation of index m.

In many algorithms such as GMRES it is convenient to work also with an ascending basis $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m\}$ of $\mathcal{V}_m$. The following result, which will be used in Section 6.4, relates $\measuredangle(\boldsymbol{r}_0, \boldsymbol{w}_m)$ with $\measuredangle(\boldsymbol{v}_{m+1}, \boldsymbol{w}_m)$.

Lemma 3.3. If the subspaces $\mathcal{V}_m$ and $\mathcal{W}_m$ are related by (3.10) and $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m\}$ and $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$ are ascending orthonormal bases of $\mathcal{V}_m$ and $\mathcal{W}_m$, respectively, then

$$|(\boldsymbol{v}_{m+1}, \boldsymbol{w}_m)| = s_m.$$

In the degenerate case $(\boldsymbol{r}_0, \boldsymbol{w}_m) = 0$, the vectors $\boldsymbol{v}_{m+1}$ and $\boldsymbol{w}_m$ must be collinear.

Proof. From $\boldsymbol{v}_{m+1} \in \operatorname{span}\{\boldsymbol{r}_0, \boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\} \cap \operatorname{span}\{\boldsymbol{r}_0, \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{m-1}\}^\perp$ we conclude $\boldsymbol{v}_{m+1} \in \operatorname{span}\{\boldsymbol{r}_m^{\mathrm{MR}}, \boldsymbol{w}_m\}$ and the assertion follows from the remaining requirements $\|\boldsymbol{v}_{m+1}\| = 1$ and $\boldsymbol{v}_{m+1} \perp \boldsymbol{r}_0$: Using the notation from the proof of Theorem 3.1, we set $\hat{\boldsymbol{w}}_{m+1} := \boldsymbol{r}_m^{\mathrm{MR}}/\|\boldsymbol{r}_m^{\mathrm{MR}}\|$ and note that $\{\hat{\boldsymbol{w}}_m, \boldsymbol{w}_m\}$ form an orthonormal basis of $\operatorname{span}\{\boldsymbol{r}_m^{\mathrm{MR}}, \boldsymbol{w}_m\}$, hence $\boldsymbol{v}_{m+1} = \alpha\hat{\boldsymbol{w}}_m + \beta\boldsymbol{w}_m$ for some coefficients $\alpha, \beta \in \mathbb{C}$. Since $(\boldsymbol{r}_m^{\mathrm{MR}}, \boldsymbol{r}_0) = \|\boldsymbol{r}_m^{\mathrm{MR}}\|^2$, orthogonality of $\boldsymbol{v}_{m+1}$ and $\boldsymbol{r}_0$ yields

$$0 = (\boldsymbol{v}_{m+1}, \boldsymbol{r}_0) = \frac{\alpha}{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}(\boldsymbol{r}_m^{\mathrm{MR}}, \boldsymbol{r}_0) + \beta(\boldsymbol{w}_m, \boldsymbol{r}_0) = \alpha\|\boldsymbol{r}_m^{\mathrm{MR}}\| + \beta(\boldsymbol{w}_m, \boldsymbol{r}_0).$$

The requirement that $\boldsymbol{v}_{m+1}$ have unit norm now gives

$$|\beta|^2 = \left(1 + \frac{|(\boldsymbol{w}_m, \boldsymbol{r}_0)|^2}{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}\right)^{-1} = \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2 + |(\boldsymbol{w}_m, \boldsymbol{r}_0)|^2} = \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2} = s_m^2.$$

Since $\boldsymbol{r}_m^{\mathrm{MR}} \perp \boldsymbol{w}_m$, we now obtain $|(\boldsymbol{v}_{m+1}, \boldsymbol{w}_m)| = |\beta| = s_m$.

If $(\boldsymbol{r}_0, \boldsymbol{w}_m) = 0$ then $|(\boldsymbol{v}_{m+1}, \boldsymbol{w}_m)| = 1$, *i.e.*, $|(\boldsymbol{v}_{m+1}, \boldsymbol{w}_m)| = \|\boldsymbol{v}_{m+1}\|\,\|\boldsymbol{w}_m\|$, which means that these two vectors are collinear. □

3.3. Relations between MR and OR approximations

Recall that $\boldsymbol{r}_0 \in \mathcal{W}_{m-1}$ implies that the MR approximation with respect to the space $\mathcal{W}_{m-1}$ solves the approximation problem exactly. The same is true for the OR approximation, since $\boldsymbol{r}_0 \in \mathcal{W}_{m-1}$ implies $\boldsymbol{r}_0 - \boldsymbol{r}_{m-1}^{\mathrm{OR}} \in \mathcal{W}_{m-1} \cap \mathcal{V}_{m-1}^\perp = \{\boldsymbol{0}\}$, so that the OR approximation solves the problem exactly whenever the MR approximation does. In other words, the assumption $\boldsymbol{r}_0 \notin \mathcal{W}_{m-1}$ is *equivalent* to saying that both $\boldsymbol{r}_{m-1}^{\mathrm{MR}}$ and $\boldsymbol{r}_{m-1}^{\mathrm{OR}}$ are not yet zero.

If we define $\widetilde{\boldsymbol{w}}_m := |(\boldsymbol{w}_m, \boldsymbol{r}_0)|\widehat{\boldsymbol{w}}_m/(\boldsymbol{r}_0, \boldsymbol{w}_m)$, where $\widehat{\boldsymbol{w}}_m = \boldsymbol{r}_{m-1}^{\mathrm{MR}}/\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|$, then $(\boldsymbol{w}_m, \widetilde{\boldsymbol{w}}_m) = c_m$ (*cf.* the proof of Theorem 3.1). Consequently, the sets $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$ and $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_{m-1}, \widetilde{\boldsymbol{w}}_m/c_m\}$ form a pair of *biorthonormal* bases of $\mathcal{W}_m$ and $\mathcal{V}_m$. This fact allows us to express the oblique projection

which determines the OR approximation as the singular value expansion

$$P_{\mathcal{W}_m}^{\mathcal{V}_m} = \sum_{j=1}^{m-1} (\cdot, \boldsymbol{w}_j)\boldsymbol{w}_j + \frac{1}{c_m}(\cdot, \widetilde{\boldsymbol{w}}_m)\boldsymbol{w}_m, \tag{3.12}$$

from which we derive the following expression for the difference of the OR and MR approximations:

$$\begin{aligned} \boldsymbol{w}_m^{\mathrm{OR}} - \boldsymbol{w}_m^{\mathrm{MR}} &= (P_{\mathcal{W}_m}^{\mathcal{V}_m} - P_{\mathcal{W}_m})\boldsymbol{r}_0 = \left[c_m^{-1}(\boldsymbol{r}_0, \widetilde{\boldsymbol{w}}_m) - (\boldsymbol{r}_0, \boldsymbol{w}_m)\right] \boldsymbol{w}_m \\ &= \frac{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2 - |(\boldsymbol{r}_0, \boldsymbol{w}_m)|^2}{(\boldsymbol{w}_m, \boldsymbol{r}_0)}\boldsymbol{w}_m = \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{(\boldsymbol{w}_m, \boldsymbol{r}_0)}\boldsymbol{w}_m. \end{aligned} \tag{3.13}$$

In other words, since the spaces $\mathcal{V}_m$ and $\mathcal{V}_m$ are so closely related, the projection $P_{\mathcal{W}_m}^{\mathcal{V}_m}$ is simply a rank-one modification of $P_{\mathcal{W}_m}$ and this is the essential ingredient of the proof for the following familiar relations.

Theorem 3.4. Given an arbitrary element $\boldsymbol{r}_0 \in \mathcal{H}$, a nested sequence of subspaces $\mathcal{W}_m \subset \mathcal{H}$ of dimension m (*cf.* (3.1)) and a corresponding sequence of error spaces $\mathcal{V}_m$ as defined by (3.10), then the MR and OR approximations of $\boldsymbol{r}_0$ with respect to $\mathcal{W}_m$ and $\mathcal{V}_m$ satisfy

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = s_m \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|, \tag{3.14}$$

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = s_1 s_2 \cdots s_m \|\boldsymbol{r}_0\|, \tag{3.15}$$

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = c_m \|\boldsymbol{r}_m^{\mathrm{OR}}\|, \tag{3.16}$$

$$\|\boldsymbol{r}_m^{\mathrm{OR}}\| = s_1 s_2 \cdots s_m \|\boldsymbol{r}_0\| / c_m, \tag{3.17}$$

where $s_m = \sin \measuredangle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \mathcal{W}_m)$ and $c_m = \cos \measuredangle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \mathcal{W}_m)$.

Proof. Identities (3.14) and (3.15) are merely restatements of (3.5) and (3.9), which have already been proved. Next, from (3.13) we obtain

$$\boldsymbol{r}_m^{\mathrm{MR}} - \boldsymbol{r}_m^{\mathrm{OR}} = \boldsymbol{w}_m^{\mathrm{OR}} - \boldsymbol{w}_m^{\mathrm{MR}} \in \operatorname{span}\{\boldsymbol{w}_m\}, \tag{3.18}$$

and

$$\boldsymbol{w}_m^{\mathrm{OR}} = \boldsymbol{w}_m^{\mathrm{MR}} + \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{(\boldsymbol{w}_m, \boldsymbol{r}_0)}\boldsymbol{w}_m = \boldsymbol{w}_{m-1}^{\mathrm{MR}} + \frac{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}{(\boldsymbol{w}_m, \boldsymbol{r}_0)}\boldsymbol{w}_m, \tag{3.19}$$

where we have used (3.2) for the last equality. Since $\boldsymbol{r}_m^{\mathrm{MR}} \perp \boldsymbol{w}_m$, the Pythagorean identity and (3.2) yield

$$\|\boldsymbol{r}_m^{\mathrm{OR}}\|^2 = \left(1 + \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{|(\boldsymbol{w}_m, \boldsymbol{r}_0)|^2}\right) \|\boldsymbol{r}_m^{\mathrm{MR}}\|^2 = \frac{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}{|(\boldsymbol{w}_m, \boldsymbol{r}_0)|^2} \|\boldsymbol{r}_m^{\mathrm{MR}}\|^2,$$

which, in view of (3.7), gives the error formula

$$\|\boldsymbol{r}_m^{\mathrm{OR}}\| = \frac{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\| \, \|\boldsymbol{r}_m^{\mathrm{MR}}\|}{|(\boldsymbol{w}_m, \boldsymbol{r}_0)|} = \frac{1}{c_m}\|\boldsymbol{r}_m^{\mathrm{MR}}\|$$

for the OR approximation, establishing (3.16) and (3.17). □

In addition to the norm identities contained in Theorem 3.4, it is also possible to relate the MR and OR approximations and their errors, as the next theorem shows.

Theorem 3.5. Under the assumptions of Theorem 3.4, the MR and OR approximations and errors satisfy

$$\boldsymbol{w}_m^{\mathrm{MR}} = s_m^2 \boldsymbol{w}_{m-1}^{\mathrm{MR}} + c_m^2 \boldsymbol{w}_m^{\mathrm{OR}}, \tag{3.20}$$

$$\boldsymbol{r}_m^{\mathrm{MR}} = s_m^2 \boldsymbol{r}_{m-1}^{\mathrm{MR}} + c_m^2 \boldsymbol{r}_m^{\mathrm{OR}}, \tag{3.21}$$

$$\frac{\boldsymbol{w}_m^{\mathrm{MR}}}{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2} = \sum_{j=0}^{m} \frac{\boldsymbol{w}_j^{\mathrm{OR}}}{\|\boldsymbol{r}_j^{\mathrm{OR}}\|^2}, \tag{3.22}$$

$$\frac{\boldsymbol{r}_m^{\mathrm{MR}}}{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2} = \sum_{j=0}^{m} \frac{\boldsymbol{r}_j^{\mathrm{OR}}}{\|\boldsymbol{r}_j^{\mathrm{OR}}\|^2}, \tag{3.23}$$

$$\frac{1}{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2} = \sum_{j=0}^{m} \frac{1}{\|\boldsymbol{r}_j^{\mathrm{OR}}\|^2} = \frac{1}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2} + \frac{1}{\|\boldsymbol{r}_m^{\mathrm{OR}}\|^2}. \tag{3.24}$$

Proof. From (3.19) and $\boldsymbol{w}_m^{\mathrm{MR}} - \boldsymbol{w}_{m-1}^{\mathrm{MR}} = (\boldsymbol{r}_0, \boldsymbol{w}_m)\boldsymbol{w}_m$ we obtain

$$\begin{aligned}
\boldsymbol{w}_m^{\mathrm{OR}} &= \boldsymbol{w}_m^{\mathrm{MR}} + \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{(\boldsymbol{w}_m, \boldsymbol{r}_0)} \frac{1}{(\boldsymbol{r}_0, \boldsymbol{w}_m)} (\boldsymbol{w}_m^{\mathrm{MR}} - \boldsymbol{w}_{m-1}^{\mathrm{MR}}) \\
&= \boldsymbol{w}_m^{\mathrm{MR}} + \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2} \frac{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}{|(\boldsymbol{r}_0, \boldsymbol{w}_m)|^2} (\boldsymbol{w}_m^{\mathrm{MR}} - \boldsymbol{w}_{m-1}^{\mathrm{MR}}) \\
&= \boldsymbol{w}_m^{\mathrm{MR}} + \frac{s_m^2}{c_m^2} (\boldsymbol{w}_m^{\mathrm{MR}} - \boldsymbol{w}_{m-1}^{\mathrm{MR}})
\end{aligned}$$

(*cf.* (3.14) and (3.7)), which implies the relationship (3.20) between the MR and OR approximations and, by way of $s_m^2 + c_m^2 = 1$, the corresponding relationship (3.21) between their errors.

Repeated application of these two formulas leads to

$$\boldsymbol{w}_m^{\mathrm{MR}} = \sum_{j=0}^{m} \tau_{m,j}^2 \boldsymbol{w}_j^{\mathrm{OR}} \qquad \text{and} \qquad \boldsymbol{r}_m^{\mathrm{MR}} = \sum_{j=0}^{m} \tau_{m,j}^2 \boldsymbol{r}_j^{\mathrm{OR}},$$

where $\tau_{m,0} := s_1 s_2 \dots s_m$ and $\tau_{m,j} := c_j s_{j+1} \dots s_m$ $(1 \le j \le m)$. Using (3.14) and (3.16) this can be simplified to

$$\tau_{m,j} = c_j \frac{\|\boldsymbol{r}_{j+1}^{\mathrm{MR}}\|}{\|\boldsymbol{r}_j^{\mathrm{MR}}\|} \frac{\|\boldsymbol{r}_{j+2}^{\mathrm{MR}}\|}{\|\boldsymbol{r}_{j+1}^{\mathrm{MR}}\|} \cdots \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|} = c_j \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_j^{\mathrm{MR}}\|} = \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_j^{\mathrm{OR}}\|},$$

and we obtain (3.22) as well as (3.23). Finally, since the errors $\boldsymbol{r}_j^{\mathrm{OR}}$ are

orthogonal, we have

$$\frac{1}{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2} = \sum_{j=0}^{m} \frac{1}{\|\boldsymbol{r}_j^{\mathrm{OR}}\|^2} = \sum_{j=0}^{m-1} \frac{1}{\|\boldsymbol{r}_j^{\mathrm{OR}}\|^2} + \frac{1}{\|\boldsymbol{r}_m^{\mathrm{OR}}\|^2} = \frac{1}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2} + \frac{1}{\|\boldsymbol{r}_m^{\mathrm{OR}}\|^2},$$

which proves (3.24). Strictly speaking, this proves

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

only under the assumption that all OR approximations $\boldsymbol{w}_1^{\mathrm{OR}}, \ldots, \boldsymbol{w}_m^{\mathrm{OR}}$ exist. But this last equation is merely a reformulation of the Pythagorean identity,

$$1 = s_m^2 + c_m^2 = \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2} + \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_m^{\mathrm{OR}}\|^2}$$

(*cf.* (3.14), (3.16)), requiring only the existence of $\boldsymbol{w}_m^{\mathrm{OR}}$ (besides $\boldsymbol{r}_0 \notin \mathcal{W}_m$). □

Corollary 3.6. In view of

$$s_m = \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|}, \qquad \textit{i.e.,} \quad c_m = \sqrt{1 - \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}},$$

an angle-free formulation of (3.16), (3.20) and (3.21) reads

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

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

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

Of course, the first of these identities, or its reformulation

$$\|\boldsymbol{r}_m^{\mathrm{OR}}\| = \left(1 - \frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}\right)^{-1/2} \|\boldsymbol{r}_m^{\mathrm{MR}}\|,$$

only makes sense if $\boldsymbol{w}_m^{\mathrm{OR}}$ is defined, which is equivalent to $\|\boldsymbol{r}_m^{\mathrm{MR}}\| < \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|$. If $\|\boldsymbol{r}_m^{\mathrm{MR}}\| \approx \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|$ then the factor $(1 - \|\boldsymbol{r}_m^{\mathrm{MR}}\|^2/\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2)^{-1/2}$ will be large and, consequently, $\|\boldsymbol{r}_m^{\mathrm{OR}}\| \gg \|\boldsymbol{r}_m^{\mathrm{MR}}\|$. Conversely, if the MR approximation makes considerable progress in step m, then $(1 - \|\boldsymbol{r}_m^{\mathrm{MR}}\|^2/\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2)^{-1/2} \approx 1$ and $\|\boldsymbol{r}_m^{\mathrm{OR}}\| \approx \|\boldsymbol{r}_m^{\mathrm{MR}}\|$. In the context of Krylov subspace methods, this observation is sometimes referred to as the *peak/plateau phenomenon* of MR/OR approximations (see, *e.g.*, Cullum and Greenbaum (1996)).

Remark 3.7. We close this section by reconsidering the issue of the so-called Galerkin breakdown mentioned in Remark 2.5. Using the biorthonormal bases introduced in (3.12), we obtain the singular value expansion of $P_{\mathcal{V}}P_{\mathcal{W}}$ as

$$P_{\mathcal{V}}P_{\mathcal{W}} = \sum_{j=1}^{m-1} (\cdot, \boldsymbol{w}_j)\boldsymbol{w}_j + c_m(\cdot, \boldsymbol{w}_m)\widetilde{\boldsymbol{w}}_m.$$

If, in view of (2.7), one defines the OR approximation in the degenerate case $c_m = 0$ by $\boldsymbol{w}_m^{\mathrm{OR}} := (P_{\mathcal{V}}P_{\mathcal{W}})^{+}\boldsymbol{r}_0$, then this leads to $\boldsymbol{w}_m^{\mathrm{OR}} = \boldsymbol{w}_{m-1}^{\mathrm{MR}} = \boldsymbol{w}_m^{\mathrm{MR}}$. We thereby arrive at a natural extension of the definition of the OR approximation in the case of a Galerkin breakdown.

3.4. Smoothing algorithms

A *smoothing algorithm* transforms a given sequence $\{\boldsymbol{u}_m\} \subset \mathcal{W}_m$ of approximations to $\boldsymbol{r}_0$ into a new sequence $\{\hat{\boldsymbol{u}}_m\} \subset \mathcal{W}_m$ according to

$$\hat{\boldsymbol{u}}_m := (1 - \alpha_m)\hat{\boldsymbol{u}}_{m-1} + \alpha_m \boldsymbol{u}_m \tag{3.25}$$

($m = 1, 2, \ldots$, $\hat{\boldsymbol{u}}_0 := \boldsymbol{u}_0 = \boldsymbol{0}$). The associated approximation errors $\boldsymbol{r}_m = \boldsymbol{r}_0 - \boldsymbol{u}_m$ and $\hat{\boldsymbol{r}}_m = \boldsymbol{r}_0 - \hat{\boldsymbol{u}}_m$ then satisfy

$$\hat{\boldsymbol{r}}_m = (1 - \alpha_m)\hat{\boldsymbol{r}}_{m-1} + \alpha_m \boldsymbol{r}_m.$$

The intention is that the errors of the transformed sequence should decrease 'more smoothly' than those of the original sequence. Ideally, we would like to have $\hat{\boldsymbol{u}}_m = \boldsymbol{w}_m^{\mathrm{MR}}$ and we shall discuss two smoothing procedures which achieve this goal when applied to $\boldsymbol{u}_m = \boldsymbol{w}_m^{\mathrm{OR}}$, that is, to the sequence of OR approximations.

In *minimal residual smoothing* (*cf.* Weiss (1994), Zhou and Walker (1994) or Gutknecht (1997, Section 17)), the parameter α_m in (3.25) is chosen to minimize the norm of the error $\hat{\boldsymbol{r}}_m = \hat{\boldsymbol{r}}_{m-1} - \alpha_m(\hat{\boldsymbol{r}}_{m-1} - \boldsymbol{r}_m)$ as a function of α_m. In other words, we seek the best approximation $\alpha_m(\hat{\boldsymbol{r}}_{m-1} - \boldsymbol{r}_m)$ from $\mathrm{span}\{\hat{\boldsymbol{r}}_{m-1} - \boldsymbol{r}_m\}$ to $\hat{\boldsymbol{r}}_{m-1}$, which is obtained for

$$\alpha_m^{\mathrm{MR}} := \frac{(\hat{\boldsymbol{r}}_{m-1}, \hat{\boldsymbol{r}}_{m-1} - \boldsymbol{r}_m)}{\|\hat{\boldsymbol{r}}_{m-1} - \boldsymbol{r}_m\|^2}.$$

In an alternative smoothing procedure known as *quasi-minimal residual smoothing* (*cf.* Zhou and Walker (1994) or Gutknecht (1997, Section 17)), the parameter α_m is chosen as

$$\alpha_m^{\mathrm{QMR}} := \frac{\tau_m^2}{\|\boldsymbol{r}_m\|^2} \quad \text{with } \tau_m \text{ such that} \quad \frac{1}{\tau_m^2} = \frac{1}{\tau_{m-1}^2} + \frac{1}{\|\boldsymbol{r}_m\|^2},\ \tau_0 = \|\boldsymbol{r}_0\|.$$

It is easy to see by induction that

$$\tau_m^2 = \frac{1}{\sum_{j=0}^m 1/\|\boldsymbol{r}_j\|^2}, \quad \textit{i.e.}, \quad \alpha_m^{\mathrm{QMR}} = \frac{1/\|\boldsymbol{r}_m\|^2}{\sum_{j=0}^m 1/\|\boldsymbol{r}_j\|^2},$$

and therefore

$$\hat{\boldsymbol{u}}_m = \frac{\sum_{j=0}^m \boldsymbol{u}_j/\|\boldsymbol{r}_j\|^2}{\sum_{j=0}^m 1/\|\boldsymbol{r}_j\|^2} \quad \text{as well as} \quad \hat{\boldsymbol{r}}_m = \frac{\sum_{j=0}^m \boldsymbol{r}_j/\|\boldsymbol{r}_j\|^2}{\sum_{j=0}^m 1/\|\boldsymbol{r}_j\|^2}.$$

The last formula for $\hat{\boldsymbol{u}}_m$ reveals the strategy behind quasi-minimal residual smoothing: $\hat{\boldsymbol{u}}_m$ is a weighted sum of all previous iterates $\boldsymbol{u}_0, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_m$ with weights $(1/\|\boldsymbol{r}_k\|^2)/(\sum_{j=0}^m (1/\|\boldsymbol{r}_j\|^2))$ which are (relatively) large if $\boldsymbol{u}_k$ approximates $\boldsymbol{r}_0$ well and (relatively) small if $\boldsymbol{u}_k$ is a poor approximation to $\boldsymbol{r}_0$.

In general, that is, for an arbitrary sequence $\{\boldsymbol{u}_m\} \in \mathcal{W}_m$, minimal and quasi-minimal residual smoothing will generate different 'smoothed' iterates $\hat{\boldsymbol{u}}_m$. In the case of $\boldsymbol{u}_m = \boldsymbol{w}_m^{\mathrm{OR}}$, however, these two methods are equivalent.

Proposition 3.8. If either the minimal residual or the quasi-minimal residual smoothing algorithm is applied to the sequence of OR approximations $\{\boldsymbol{w}_m^{\mathrm{OR}}\}$ for an element $\boldsymbol{r}_0 \in \mathcal{H}$, then the resulting smoothed sequence consists of the MR approximations $\boldsymbol{w}_m^{\mathrm{MR}}$ for $\boldsymbol{r}_0$ and the associated smoothing parameters are given by $\alpha_m^{\mathrm{MR}} = \alpha_m^{\mathrm{QMR}} = c_m^2$.

Proof. An induction shows that minimal residual smoothing applied to $\boldsymbol{u}_m = \boldsymbol{w}_m^{\mathrm{OR}}$ yields $\hat{\boldsymbol{u}}_m = \boldsymbol{w}_m^{\mathrm{MR}}$ and that, in this case, $\alpha_m^{\mathrm{MR}} = c_m^2$: the assertion is trivial for $m = 1$. Assuming $\hat{\boldsymbol{u}}_{m-1} = \boldsymbol{h}_{m-1}^{\mathrm{MR}}$ for some $m \geq 2$, we see from (3.19) that

$$\hat{\boldsymbol{r}}_{m-1} - \boldsymbol{r}_m = \boldsymbol{r}_{m-1}^{\mathrm{MR}} - \boldsymbol{r}_m^{\mathrm{OR}} = \frac{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}{(\boldsymbol{w}_m, \boldsymbol{r}_0)} \boldsymbol{w}_m$$

and consequently, noting that $\boldsymbol{r}_{m-1}^{\mathrm{MR}} = \boldsymbol{r}_m^{\mathrm{MR}} + (\boldsymbol{r}_0, \boldsymbol{w}_m)\boldsymbol{w}_m$ and $\boldsymbol{r}_m^{\mathrm{MR}} \perp \boldsymbol{w}_m$,

$$(\hat{\boldsymbol{r}}_{m-1}, \hat{\boldsymbol{r}}_{m-1} - \boldsymbol{r}_m) = \left((\boldsymbol{r}_0, \boldsymbol{w}_m)\boldsymbol{w}_m, \frac{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2}{(\boldsymbol{w}_m, \boldsymbol{r}_0)} \boldsymbol{w}_m \right) = \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2.$$

From (3.7) and (3.20), there finally follows

$$\alpha_m^{\mathrm{MR}} = \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2 \frac{|(\boldsymbol{w}_m, \boldsymbol{r}_0)|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^4} = \frac{|(\boldsymbol{w}_m, \boldsymbol{r}_0)|^2}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2} = c_m^2 \quad \text{and} \quad \hat{\boldsymbol{u}}_m = \boldsymbol{w}_m^{\mathrm{MR}}.$$

The analogous assertion for quasi-minimal residual smoothing follows, with (3.22) and (3.23), immediately from the orthogonality of the error vectors $\boldsymbol{r}_m^{\mathrm{OR}}$. □

It should not come as a surprise that, in our setting, a one-dimensional minimization procedure such as minimal residual smoothing yields the best approximation $\boldsymbol{w}_m^{\mathrm{MR}}$, which is the global optimum on $\mathcal{W}_m$. Recall that $\boldsymbol{w}_m^{\mathrm{OR}}$ is already 'nearly optimal' and needs to be corrected only in the direction of $\boldsymbol{w}_m$.

4. Working with coordinates

The results of the previous sections more closely resemble the matrix formulation of familiar Krylov subspace methods once they are formulated in coordinates with respect to suitable bases of the spaces $\mathcal{W}_m$ and $\mathcal{V}_m$. Specifically, the relevant quantities may be represented in terms of bases of either space, and the situation is simplified if either of these bases is orthogonal. The distinction between which bases are used and whether these are orthogonal also results in three fundamental algorithmic approaches on which all Krylov subspace solvers and their generalizations are based. As we show in this section, these three approaches may all be expressed at the abstract level of the preceding two sections, and this serves to isolate the algorithmic features of these approximation methods from issues associated with their use for solving equations, for instance, by Krylov subspace methods.

We shall begin with the simplest formulation in terms of an ascending orthonormal basis of the sequence $\{\mathcal{W}_m\}$ followed by an approach which first generates an ascending orthonormal basis of $\{\mathcal{V}_m\}$ from a not necessarily orthogonal ascending basis of $\{\mathcal{W}_m\}$. It is seen that the familiar relation of these two bases via an unreduced upper Hessenberg matrix in the Krylov subspace context also holds in the abstract setting as a direct consequence of the definition of the sequence of residual spaces (3.10). The third basic approach allows for neither of the two ascending bases to be orthogonal, and it is shown how this case can be made to fit into the MR/OR framework by introducing a new, basis-dependent inner product.

Motivated by this last approach, we show that, when allowing for such a change of inner product, any sequence of approximations in a Hilbert space becomes a sequence of either MR or OR approximations.

4.1. Using an orthonormal basis of $\mathcal{W}_m$

If, for each $m \geq 1$, the vectors $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$ form an orthonormal basis of $\mathcal{W}_m$, then each $\boldsymbol{w} \in \mathcal{W}_m$ possesses the unique representation $\boldsymbol{w} = W_m \boldsymbol{y}$, in which W_m denotes the row vector $W_m := [\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m]$ and $\boldsymbol{y} \in \mathbb{C}^m$ is the coordinate vector of $\boldsymbol{w}$ with respect to this basis. The characterization $\boldsymbol{r}_m^{\mathrm{MR}} = \boldsymbol{r}_0 - W_m \boldsymbol{y}_m^{\mathrm{MR}} \perp \mathcal{W}_m$ then immediately determines the coordinate vector $\boldsymbol{y}_m^{\mathrm{MR}}$ of $\boldsymbol{w}_m^{\mathrm{MR}}$ to be

$$\boldsymbol{y}_m^{\mathrm{MR}} = [(\boldsymbol{r}_0, \boldsymbol{w}_1), \ldots, (\boldsymbol{r}_0, \boldsymbol{w}_m)]^{\top}. \tag{4.1}$$

The coordinate vector $\boldsymbol{y}_m^{\mathrm{OR}}$ of the corresponding OR approximation $\boldsymbol{w}_m^{\mathrm{OR}}$ is given by

$$\boldsymbol{y}_m^{\mathrm{OR}} = [(\boldsymbol{r}_0, \boldsymbol{w}_1), \ldots, (\boldsymbol{r}_0, \boldsymbol{w}_{m-1}), \|\boldsymbol{w}_{m-1}^{\mathrm{MR}}\|^2/(\boldsymbol{w}_m, \boldsymbol{r}_0)]^\top \tag{4.2}$$

since $\boldsymbol{w}_m^{\mathrm{OR}} = \boldsymbol{w}_{m-1}^{\mathrm{MR}} + \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2/(\boldsymbol{w}_m, \boldsymbol{r}_0)\boldsymbol{w}_m$ (*cf.* (3.19)).

4.2. Using an orthonormal basis of $\mathcal{V}_m$

We now drop the orthogonality requirement on the vectors $\boldsymbol{w}_j$, assuming only that the sequence of vectors $\{\boldsymbol{w}_m\}$ forms an ascending basis of the sequence of approximation spaces $\{\mathcal{W}_m\}$. In the same manner, let $\{\boldsymbol{v}_m\}$ form an ascending basis of the corresponding residual spaces space $\mathcal{V}_m$. Since $\mathcal{W}_m \subseteq \operatorname{span}\{\boldsymbol{r}_0\} + \mathcal{W}_m = \mathcal{V}_{m+1}$, we may represent each basis vector $\boldsymbol{w}_k$ as a linear combination of $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{k+1}$,

$$\boldsymbol{w}_k = \sum_{j=1}^{k+1} \eta_{j,k} \boldsymbol{v}_j, \qquad k = 1, \ldots, m,$$

or, more compactly, employing the row vector notation $W_m = [\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m]$ and $V_m := [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m]$, $m = 1, 2, \ldots$,

$$W_m = V_{m+1}\tilde{H}_m = V_m H_m + [\boldsymbol{0}, \ldots, \boldsymbol{0}, \eta_{m+1,m}\boldsymbol{v}_{m+1}], \tag{4.3}$$

where $\tilde{H}_m =: [\eta_{j,k}] \in \mathbb{C}^{(m+1)\times m}$ is an upper Hessenberg matrix and $H_m := [I_m \ \boldsymbol{0}]\tilde{H}_m$ is the square matrix obtained by deleting the last row of $\tilde{H}_m$. Note that as long as $\boldsymbol{r}_0 \notin \mathcal{W}_m$, that is, $\boldsymbol{w}_m \notin \mathcal{V}_m$, we have $\eta_{m+1,m} \neq 0$ and therefore $\operatorname{rank}(\tilde{H}_m) = m$. If $\boldsymbol{r}_0 \in \mathcal{W}_m$ for some index m, we let

$$L := \min\{m : \boldsymbol{r}_0 \in \mathcal{W}_m\} \tag{4.4}$$

be the smallest such index and note that $\mathcal{V}_{L+1} = \mathcal{V}_L = \operatorname{span}\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_L\}$, that is, $W_L = V_L H_L$, implying $\operatorname{rank}(H_L) = \operatorname{rank}(\tilde{H}_L) = L$. If such an index does not exist, we set $L = \infty$. To avoid cumbersome notation we shall concentrate on the case of $L < \infty$, which is the most relevant for practical applications. We note, however, that all our conclusions can be proved in the general case.

For a given sequence $\{\boldsymbol{w}_j\}_{j\geq 1}$, an *orthonormal* sequence of vectors $\{\boldsymbol{v}_j\}_{j\geq 1}$ may be constructed recursively, starting with $\boldsymbol{v}_1 := \boldsymbol{r}_0/\|\boldsymbol{r}_0\|$ and, in view of $\mathcal{V}_{m+1} = \mathcal{V}_m + \operatorname{span}\{\boldsymbol{w}_m\}$, successively orthogonalizing each $\boldsymbol{w}_m$ against the previously generated $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m$:

$$\begin{aligned} \boldsymbol{v}_1 &:= \boldsymbol{r}_0/\beta, \quad \beta := \|\boldsymbol{r}_0\|, \\ \boldsymbol{v}_{m+1} &:= \frac{(I - P_{\mathcal{V}_m})\boldsymbol{w}_m}{\|(I - P_{\mathcal{V}_m})\boldsymbol{w}_m\|}, \qquad m = 1, 2, \ldots, L-1. \end{aligned} \tag{4.5}$$

Of course, this is simply the Gram–Schmidt orthogonalization procedure

applied to the basis $\{\boldsymbol{r}, \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{m-1}\}$ of $\mathcal{V}_m$, and hence in this case the entries in the Hessenberg matrix introduced in (4.3) are given by

$$\eta_{j,m} = (\boldsymbol{w}_m, \boldsymbol{v}_j), \qquad j = 1, \ldots, m+1, \quad m \geq 1.$$

We also note that

$$\eta_{m+1,m} = (\boldsymbol{w}_m, \boldsymbol{v}_{m+1}) = \|(I - P_{\mathcal{V}_m})\boldsymbol{w}_m\| \geq 0 \tag{4.6}$$

with equality holding if and only if $\boldsymbol{w}_m \in \mathcal{V}_m$ or, equivalently, $\boldsymbol{r}_0 \in \mathcal{W}_m$, that is, $m = L$.

We now turn to the determination of the coordinate vectors of the MR and OR approximations with respect to the basis $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$. In the following lemma and in the remainder of the paper, we will employ the notation $\boldsymbol{u}_1^{(m)}$ to denote the first unit coordinate vector of $\mathbb{C}^m$ and omit the superscript when the dimension is clear from the context.

Lemma 4.1. The coordinate vector $\boldsymbol{y}_m^{\mathrm{MR}} \in \mathbb{C}^m$ of the MR approximation $\boldsymbol{w}_m^{\mathrm{MR}}$ with respect to the basis $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$ is the solution of the least-squares problem

$$\|\beta \boldsymbol{u}_1^{(m+1)} - \tilde{H}_m \boldsymbol{y}\|_2 \to \min_{\boldsymbol{y} \in \mathbb{C}^m}, \tag{4.7}$$

whereas the coordinate vector $\boldsymbol{y}_m^{\mathrm{OR}}$ of the OR approximation solves the linear system of equations

$$H_m \boldsymbol{y} = \beta \boldsymbol{u}_1^{(m)}. \tag{4.8}$$

In short,

$$\boldsymbol{y}_m^{\mathrm{MR}} = \beta \tilde{H}_m^{+} \boldsymbol{u}_1^{(m+1)} \quad \text{and} \quad \boldsymbol{y}_m^{\mathrm{OR}} = \beta H_m^{-1} \boldsymbol{u}_1^{(m)},$$

where $\tilde{H}_m^{+} = (\tilde{H}_m^H \tilde{H}_m)^{-1} \tilde{H}_m^H$ is the Moore–Penrose pseudo-inverse of $\tilde{H}_m$.

Proof. The assertions of the lemma become obvious when the relevant quantities are represented in terms of the orthonormal basis $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}\}$ of $\mathcal{V}_{m+1}$. The vector $\boldsymbol{r}_0$ to be approximated possesses the coordinate vector $\beta \boldsymbol{u}_1 \in \mathbb{R}^{m+1}$ and the approximation space $\mathcal{W}_m = \operatorname{span}\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$ is represented by the span of the columns of $\tilde{H}_m$. In other words, if $\boldsymbol{w} \in \mathcal{W}_m$ has the coordinate vector $\boldsymbol{y}$ with respect to $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$, then $\boldsymbol{r} = \boldsymbol{r}_0 - \boldsymbol{w} \in \mathcal{V}_{m+1}$ has the coordinate vector $\beta \boldsymbol{u}_1 - \tilde{H}_m \boldsymbol{y}$ with respect to $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}\}$. More formally, for any $\boldsymbol{w} = W_m \boldsymbol{y} \in \mathcal{W}_m$ ($\boldsymbol{y} \in \mathbb{C}^m$),

$$\boldsymbol{r}_0 - \boldsymbol{w} = \boldsymbol{r}_0 - W_m \boldsymbol{y} = \beta \boldsymbol{v}_1 - V_{m+1} \tilde{H}_m \boldsymbol{y} = V_{m+1}(\beta \boldsymbol{u}_1 - \tilde{H}_m \boldsymbol{y}).$$

As the vectors $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}\}$ are orthonormal, it follows that

$$\|\boldsymbol{r}_0 - \boldsymbol{w}\| = \|\beta \boldsymbol{u}_1 - \tilde{H}_m \boldsymbol{y}\|_2$$

($\|\cdot\|_2$ denoting the Euclidean norm in $\mathbb{C}^{m+1}$). Similarly, $\boldsymbol{r}_0 - \boldsymbol{w} \perp \mathcal{V}_m$

if and only if the first m components of $\beta \boldsymbol{u}_1 - \tilde{H}_m \boldsymbol{y}$ vanish, that is, if $\beta \boldsymbol{u}_1^{(m)} - H_m \boldsymbol{y} = \boldsymbol{0}$. □

Remark 4.2. To determine $\boldsymbol{y}_m^{\mathrm{OR}}$ using Lemma 4.1 we must of course assume that the linear system $H_m \boldsymbol{y} = \beta \boldsymbol{u}_1$ is solvable. But this is equivalent to our previous characterization of the existence of $\boldsymbol{w}_m^{\mathrm{OR}}$, namely that $c_m = \cos \measuredangle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \mathcal{W}_m) \neq 0$ (*cf.* (3.8) and Corollary 3.2), which can be seen as follows. First, note that $\boldsymbol{u}_1^{(m)}$ and the first $m-1$ column vectors of H_m form a basis of $\mathbb{C}^m$ as long as $m \leq L$ (since $\eta_{j+1,j} \neq 0$ for $j = 1, 2, \ldots, L-1$). This implies that $H_m \boldsymbol{y} = \beta \boldsymbol{u}_1$ is consistent, that is, $\boldsymbol{u}_1 \in \mathrm{range}(H_m)$, if and only if H_m is nonsingular.

Next, recall from Remark 2.6 that c_m equals the smallest singular value of the matrix $[(\boldsymbol{v}_j, \hat{\boldsymbol{w}}_k)]_{j,k=1,2,\ldots,m}$, where $\{\hat{\boldsymbol{w}}_1, \hat{\boldsymbol{w}}_2, \ldots, \hat{\boldsymbol{w}}_m\}$ is any orthonormal basis of $\mathcal{W}_m$. We select such an orthonormal basis and represent its elements as linear combinations in the original basis $\{\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_m\}$. In our row vector notation, this leads to a nonsingular matrix $T \in \mathbb{C}^{m \times m}$ with $[\hat{\boldsymbol{w}}_1, \hat{\boldsymbol{w}}_2, \ldots, \hat{\boldsymbol{w}}_m] = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_m]T$. Now,

$$[(\boldsymbol{v}_j, \hat{\boldsymbol{w}}_k)] = T^H \, [(\boldsymbol{v}_j, \boldsymbol{w}_k)] = (H_m T)^H$$

and, consequently, the smallest singular value of $[(\boldsymbol{v}_j, \hat{\boldsymbol{w}}_k)]$ is positive if and only if H_m is nonsingular.

Remark 4.3. In view of (4.3) and the result of Lemma 4.1, the approximations $\boldsymbol{w}_m^{\mathrm{MR}}$ and $\boldsymbol{w}_m^{\mathrm{OR}}$ and their associated errors have the following representations in terms of the basis $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}\}$:

$$\begin{aligned} \boldsymbol{w}_m^{\mathrm{MR}} &= V_{m+1} \tilde{H}_m \tilde{H}_m^{+} \beta \boldsymbol{u}_1^{(m+1)}, & \boldsymbol{r}_m^{\mathrm{MR}} &= V_{m+1} \left(I_{m+1} - \tilde{H}_m \tilde{H}_m^{+} \right) \beta \boldsymbol{u}_1^{(m+1)}, \\ \boldsymbol{w}_m^{\mathrm{OR}} &= V_{m+1} \tilde{H}_m H_m^{-1} \beta \boldsymbol{u}_1^{(m)}, & \boldsymbol{r}_m^{\mathrm{OR}} &= V_{m+1} \left(\begin{bmatrix} I_m \\ \boldsymbol{0} \end{bmatrix} - \tilde{H}_m H_m^{-1} \right) \beta \boldsymbol{u}_1^{(m)}. \end{aligned} \tag{4.9}$$

The last identity shows that the coordinate vector of $\boldsymbol{r}_m^{\mathrm{OR}}$ has a particularly simple form. Introducing the notation $H_m^{-1} = \left[\eta_{j,k}^{[-1]}\right]$, we obtain, for $m < L$,

$$\begin{aligned} \boldsymbol{r}_m^{\mathrm{OR}} &= \beta V_{m+1} \left(\boldsymbol{u}_1^{(m+1)} - \tilde{H}_m H_m^{-1} \boldsymbol{u}_1^{(m)} \right) \\ &= \beta V_{m+1} \left(I_{m+1} - \tilde{H}_m [H_m^{-1} \ \boldsymbol{0}] \right) \boldsymbol{u}_1^{(m+1)} \\ &= \beta V_{m+1} \begin{bmatrix} \boldsymbol{0} \\ -\eta_{m+1,m} \, \eta_{m,1}^{[-1]} \end{bmatrix} = -\beta \eta_{m+1,m} \, \eta_{m,1}^{[-1]} \boldsymbol{v}_{m+1}. \end{aligned}$$

The matrix $I_{m+1} - \tilde{H}_m [H_m^{-1} \ \boldsymbol{0}]$ represents $I - P_{\mathcal{W}_m}^{\mathcal{V}_m}$ restricted to $\mathcal{V}_{m+1}$ with respect to the orthonormal basis $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}\}$. The following lemma,

which was recently obtained by Hochbruck and Lubich (1998), provides a simpler expression for this projection.

Lemma 4.4. Let the vector $\hat{\boldsymbol{w}}_{m+1} \in \mathcal{V}_{m+1} \cap \mathcal{W}_m^{\perp}$ be defined by the condition $(\boldsymbol{v}_{m+1}, \hat{\boldsymbol{w}}_{m+1}) = 1$. Then, for all $\boldsymbol{v} \in \mathcal{V}_{m+1}$, we have

$$(I - P_{\mathcal{W}_m}^{\mathcal{V}_m})\boldsymbol{v} = (\boldsymbol{v}, \hat{\boldsymbol{w}}_{m+1})\boldsymbol{v}_{m+1}. \tag{4.10}$$

Further, the coordinate vector $\hat{\boldsymbol{y}}_{m+1}$ of $\hat{\boldsymbol{w}}_{m+1}$ with respect to $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}\}$ has the form

$$\hat{\boldsymbol{y}}_{m+1} = \begin{bmatrix} \boldsymbol{g}_m \\ 1 \end{bmatrix}, \quad \text{where } \boldsymbol{g}_m \text{ solves} \quad H_m^H \boldsymbol{g}_m = -\eta_{m+1,m}\boldsymbol{u}_m$$

and $\boldsymbol{u}_m$ denotes the last unit coordinate vector in $\mathbb{R}^m$.

Proof. On $\mathcal{V}_{m+1}$, the projection $I - P_{\mathcal{W}_m}^{\mathcal{V}_m}$ is characterized by the two properties

$$\begin{aligned} (I - P_{\mathcal{W}_m}^{\mathcal{V}_m})\boldsymbol{v} &= \boldsymbol{v} && \forall \boldsymbol{v} \in \mathcal{V}_{m+1} \cap \mathcal{V}_m^{\perp} = \operatorname{span}\{\boldsymbol{v}_{m+1}\}, \\ (I - P_{\mathcal{W}_m}^{\mathcal{V}_m})\boldsymbol{v} &= \boldsymbol{0} && \forall \boldsymbol{v} \in \mathcal{V}_{m+1} \cap \mathcal{W}_m, \end{aligned}$$

that is, it is the oblique projection onto $\mathcal{V}_{m+1} \cap \mathcal{V}_m^{\perp}$ orthogonal to $\mathcal{V}_{m+1} \cap \mathcal{W}_m^{\perp}$, both of which are one-dimensional spaces of which $\{\boldsymbol{v}_{m+1}\}$ and $\{\hat{\boldsymbol{w}}_{m+1}\}$ are biorthonormal bases. Thus, (4.10) is the singular value expansion of $I - P_{\mathcal{W}_m}^{\mathcal{V}_m}$ restricted to $\mathcal{V}_{m+1}$.

To determine the coordinate vector $\hat{\boldsymbol{y}}_{m+1}$, we first note that the requirement $(\boldsymbol{v}_{m+1}, \hat{\boldsymbol{w}}_{m+1}) = 1$ implies that its last component is equal to one. Furthermore, $\hat{\boldsymbol{w}}_{m+1} \perp \mathcal{W}_m$ translates to $\hat{\boldsymbol{y}}_{m+1} \in \operatorname{null}(\tilde{H}_m^H)$, since the columns of $\tilde{H}_m$ span the coordinate space of $\mathcal{W}_m$. Letting $\boldsymbol{g}_m \in \mathbb{C}^m$ denote the first m components of $\hat{\boldsymbol{y}}_{m+1}$ and recalling that $\eta_{m+1,m} > 0$, we obtain

$$\boldsymbol{0} = \tilde{H}_m^H \hat{\boldsymbol{y}}_{m+1} = \begin{bmatrix} H_m^H & \eta_{m+1,m}\boldsymbol{u}_m \end{bmatrix} \begin{bmatrix} \boldsymbol{g}_m \\ 1 \end{bmatrix} = H_m^H \boldsymbol{g}_m + \eta_{m+1,m}\boldsymbol{u}_m. \qquad \square$$

The representation (4.10) can be used to obtain another expression for the OR approximation error as follows: by virtue of the inclusion $\mathcal{W}_{m-1} \subset \mathcal{W}_m$, an arbitrary vector $\boldsymbol{w} \in \mathcal{W}_{m-1}$ must lie in the nullspace of $I - P_{\mathcal{W}_m}^{\mathcal{V}_m}$. Furthermore, the difference $\boldsymbol{r}_0 - \boldsymbol{w} \in \operatorname{span}\{\boldsymbol{r}_0\} + \mathcal{W}_{m-1} = \mathcal{V}_m$ has a representation $\boldsymbol{r}_0 - \boldsymbol{w} = V_m \boldsymbol{z}$ with $\boldsymbol{z} \in \mathbb{C}^m$. It follows that

$$\begin{aligned} \boldsymbol{r}_m^{\mathrm{OR}} &= (I - P_{\mathcal{W}_m}^{\mathcal{V}_m})\boldsymbol{r}_0 = (I - P_{\mathcal{W}_m}^{\mathcal{V}_m})(\boldsymbol{r}_0 - \boldsymbol{w}) = (\boldsymbol{r}_0 - \boldsymbol{w}, \hat{\boldsymbol{w}}_{m+1})\boldsymbol{v}_{m+1} \\ &= \left(V_{m+1} \begin{bmatrix} \boldsymbol{z} \\ 0 \end{bmatrix}, V_{m+1} \begin{bmatrix} \boldsymbol{g}_m \\ 1 \end{bmatrix} \right) \boldsymbol{v}_{m+1} = (\boldsymbol{g}_m^H \boldsymbol{z})\, \boldsymbol{v}_{m+1}, \end{aligned} \tag{4.11}$$

and therefore $\|\boldsymbol{r}_m^{\mathrm{OR}}\| = |\boldsymbol{g}_m^H \boldsymbol{z}| \le \|\boldsymbol{g}_m\|_2 \, \|\boldsymbol{z}\|_2$ with equality holding if and only if $\boldsymbol{g}$ and $\boldsymbol{z}$ are collinear. At the same time, as $\boldsymbol{g}_m$ is fixed, equality must occur when $\|\boldsymbol{z}\|_2 = \|\boldsymbol{r}_0 - \boldsymbol{w}\|$ is minimized among all $\boldsymbol{w} \in \mathcal{W}_{m-1}$,

which is the case for $\boldsymbol{w} = \boldsymbol{w}_{m-1}^{\mathrm{MR}}$. As a result, $\|\boldsymbol{r}_m^{\mathrm{OR}}\| = \|\boldsymbol{g}_m\|_2 \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|$ which, in view of (3.14) and (3.16), implies $\|\boldsymbol{g}_m\|_2 = s_m/c_m$, an identity which could also have been derived directly from the definition of $\boldsymbol{g}_m$.

The least-squares problem (4.7) can be solved with the help of a QR decomposition of the Hessenberg matrix $\tilde{H}_m$, which we write as

$$Q_m \tilde{H}_m = \begin{bmatrix} R_m \\ \mathbf{0} \end{bmatrix}, \tag{4.12}$$

with $Q_m \in \mathbb{C}^{(m+1)\times(m+1)}$ unitary ($Q_m^H Q_m = I_{m+1}$) and $R_m \in \mathbb{C}^{m\times m}$ upper triangular. Substituting (4.12) in (4.7) yields

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

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

The following theorem identifies the angles between $\boldsymbol{r}_0$ and $\mathcal{W}_m$ as well as those between the spaces $\mathcal{V}_m$ and $\mathcal{W}_m$ with quantities which occur in the first column of the matrix Q_m.

Theorem 4.5. If, for $m = 1, \ldots, L$, $Q_m = [q_{j,k}^{(m)}]_{j,k=1}^{m+1} \in \mathbb{C}^{(m+1)\times(m+1)}$ is the unitary matrix in the QR decomposition (4.12) of the Hessenberg matrix $\tilde{H}_m$ in (4.3), then

$$\sin \measuredangle(\boldsymbol{r}_0, \mathcal{W}_m) = \left| q_{m+1,1}^{(m)} \right|, \tag{4.13}$$

$$\sin \measuredangle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \mathcal{W}_m) = \sin \measuredangle(\mathcal{V}_m, \mathcal{W}_m) = \left| q_{m+1,1}^{(m)} / q_{m,1}^{(m-1)} \right|. \tag{4.14}$$

Proof. As mentioned earlier (*cf.* the proof of Lemma 4.1) the vector $\boldsymbol{r}_0$ possesses the coordinates $\beta \boldsymbol{u}_1^{(m+1)}$ with respect to the orthonormal basis $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}\}$ of $\mathcal{V}_{m+1}$, whereas $\mathcal{W}_m$ is represented by $\mathrm{range}(\tilde{H}_m) \subset \mathbb{C}^{m+1}$. This implies

$$\measuredangle(\boldsymbol{r}_0, \mathcal{W}_m) = \measuredangle_2(\beta \boldsymbol{u}_1, \mathrm{range}(\tilde{H}_m)) = \measuredangle_2(\boldsymbol{u}_1, \mathrm{range}(\tilde{H}_m)),$$

where the subscript 2 indicates that the last two angles are defined with respect to the Euclidean inner product on $\mathbb{C}^{m+1}$.

The vectors $[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}] Q_m^H$ form another orthonormal basis of $\mathcal{V}_{m+1}$

with respect to which $\boldsymbol{r}_0$ possesses the coordinate vector $\beta Q_m \boldsymbol{u}_1^{(m+1)} =: \beta[\boldsymbol{q}_m^\top, q_{m+1,1}^{(m)}]^\top$, that is, a multiple of the first column of Q_m, and $\mathcal{W}_m$ is represented by $Q_m \tilde{H}_m \boldsymbol{y} = \left[\begin{smallmatrix} R_m \boldsymbol{y} \\ \mathbf{0} \end{smallmatrix}\right]$ ($\boldsymbol{y} \in \mathbb{C}^m$), a subspace of $\mathbb{C}^{m+1}$ which we identify with $\mathbb{C}^m$ because it consists of those vectors from $\mathbb{C}^{m+1}$ whose last component equals zero. Consequently,

$$\measuredangle(\boldsymbol{r}_0, \mathcal{W}_m) = \measuredangle_2(\beta[\boldsymbol{q}_m^\top, q_{m+1,1}^{(m)}]^\top, \mathbb{C}^m) = \measuredangle_2([\boldsymbol{q}_m^\top, q_{m+1,1}^{(m)}]^\top, \mathbb{C}^m)$$

which, in view of (2.3), proves assertion (4.13). Formula (4.14) follows directly from (3.6) and (3.11). □

The matrix Q_m is usually constructed as a product of Givens rotations

$$Q_m = G_m \begin{bmatrix} G_{m-1} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} G_{m-2} & \mathbf{0} \\ \mathbf{0} & I_2 \end{bmatrix} \cdots \begin{bmatrix} G_1 & \mathbf{0} \\ \mathbf{0} & I_{m-1} \end{bmatrix}$$

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

$$G_k := \begin{bmatrix} I_{k-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \tilde{c}_k & \tilde{s}_k e^{-i\phi_k} \\ \mathbf{0} & -\tilde{s}_k e^{i\phi_k} & \tilde{c}_k \end{bmatrix} \qquad (\tilde{c}_k, \tilde{s}_k \geq 0, \tilde{c}_k^2 + \tilde{s}_k^2 = 1, \phi_k \in \mathbb{R}).$$

We briefly explain how these rotations have to be chosen inductively. Assume that we have constructed $G_1, \ldots, G_{m-2}, G_{m-1}$ such that

$$\begin{bmatrix} G_{m-1} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} G_{m-2} & \mathbf{0} \\ \mathbf{0} & I_2 \end{bmatrix} \cdots \begin{bmatrix} G_1 & \mathbf{0} \\ \mathbf{0} & I_{m-1} \end{bmatrix} \tilde{H}_m = \begin{bmatrix} R_{m-1} & \boldsymbol{r} \\ \mathbf{0} & \tau \\ \mathbf{0} & \eta_{m+1,m} \end{bmatrix}.$$

For later use, we rewrite this identity in the form

$$\begin{bmatrix} Q_{m-1} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} H_m \\ 0 \cdots 0 \; \eta_{m+1,m} \end{bmatrix} = \begin{bmatrix} R_{m-1} & \boldsymbol{r} \\ \mathbf{0} & \tau \\ \mathbf{0} & \eta_{m+1,m} \end{bmatrix}. \tag{4.15}$$

Now we set

$$\begin{aligned} \tilde{c}_m &:= \frac{|\tau|}{\sqrt{|\tau|^2 + \eta_{m+1,m}^2}}, \quad \tilde{s}_m := \frac{\eta_{m+1,m}}{\sqrt{|\tau|^2 + \eta_{m+1,m}^2}}, \\ \phi_m &:= \arg(\eta_{m+1,m}) - \arg(\tau) = -\arg(\tau) \end{aligned} \tag{4.16}$$

(recall $\eta_{m+1,m} \geq 0$) and verify by a simple calculation that

$$\begin{bmatrix} I_{m-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \tilde{c}_m & \tilde{s}_m e^{-i\phi_m} \\ \mathbf{0} & -\tilde{s}_m e^{i\phi_m} & \tilde{c}_m \end{bmatrix} \begin{bmatrix} R_{m-1} & \boldsymbol{r} \\ \mathbf{0} & \tau \\ \mathbf{0} & \eta_{m+1,m} \end{bmatrix} = \begin{bmatrix} R_{m-1} & \boldsymbol{r} \\ \mathbf{0} & \rho \\ \mathbf{0} & 0 \end{bmatrix}$$

with $\rho = \sqrt{|\tau|^2 + \eta_{m+1,m}^2}\, e^{-i\phi_m}$.

That the quantities $\tilde{s}_m$ and $\tilde{c}_m$ are indeed the sines and cosines of the angles $\measuredangle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \mathcal{W}_m) = \measuredangle(\mathcal{V}_m, \mathcal{W}_m)$ can be easily seen as follows. Since $q_{m+1,1}^{(m)} = -\tilde{s}_m e^{i\phi_m} q_{m,1}^{(m-1)}$, by Theorem 4.5 we have

$$s_m = \measuredangle(\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \mathcal{W}_m) = |q_{m+1,1}^{(m)} / q_{m,1}^{(m-1)}| = \tilde{s}_m.$$

When describing MR and OR approximations the alternate orthonormal basis of $\mathcal{V}_{m+1}$ which occurred in the proof of Theorem 4.5, and which was already employed by Paige and Saunders (1975), often proves useful: we thus define

$$\hat{V}_{m+1} := [\hat{\boldsymbol{v}}_1^{(m+1)}, \ldots, \hat{\boldsymbol{v}}_{m+1}^{(m+1)}] := V_{m+1} Q_m^H. \tag{4.17}$$

The notation $\hat{\boldsymbol{v}}_1^{(m+1)}, \ldots, \hat{\boldsymbol{v}}_{m+1}^{(m+1)}$ for these new basis vectors is not entirely appropriate, since, as the following proposition shows, all but the last do not change with the index m.

Proposition 4.6. We have

$$[\hat{\boldsymbol{v}}_1^{(m+1)}, \ldots, \hat{\boldsymbol{v}}_m^{(m+1)}, \hat{\boldsymbol{v}}_{m+1}^{(m+1)}] = [\hat{\boldsymbol{v}}_1, \ldots, \hat{\boldsymbol{v}}_m, \tilde{\boldsymbol{v}}_{m+1}],$$

where $\tilde{\boldsymbol{v}}_1 = \boldsymbol{v}_1$, and, for $m = 1, \ldots, L-1$,

$$\begin{aligned} \hat{\boldsymbol{v}}_m &= \quad c_m \tilde{\boldsymbol{v}}_m + s_m e^{i\phi_m} \boldsymbol{v}_{m+1}, \\ \tilde{\boldsymbol{v}}_{m+1} &= -s_m e^{-i\phi_m} \tilde{\boldsymbol{v}}_m + \quad c_m \boldsymbol{v}_{m+1}. \end{aligned}$$

The vectors $\{\hat{\boldsymbol{v}}_1, \ldots, \hat{\boldsymbol{v}}_m, \tilde{\boldsymbol{v}}_{m+1}\}$ form an orthonormal basis of $\mathcal{V}_{m+1}$ such that $\{\hat{\boldsymbol{v}}_1, \ldots, \hat{\boldsymbol{v}}_m\}$ is a basis of $\mathcal{W}_m$. In addition,

$$\boldsymbol{w}_m^{\mathrm{MR}} = \hat{V}_{m+1} \beta \begin{bmatrix} \boldsymbol{q}_m \\ 0 \end{bmatrix} \quad \text{and} \quad \boldsymbol{r}_m^{\mathrm{MR}} = \hat{V}_{m+1} \beta \begin{bmatrix} \mathbf{0} \\ q_{m+1,1}^{(m)} \end{bmatrix}. \tag{4.18}$$

Proof. To prove the first two assertions, we observe

$$\begin{aligned} \hat{V}_{m+1} = V_{m+1} Q_m^H &= [V_m, \boldsymbol{v}_{m+1}] \begin{bmatrix} Q_{m-1}^H & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} G_m^H \\ &= \begin{bmatrix} \hat{V}_m, \boldsymbol{v}_{m+1} \end{bmatrix} \begin{bmatrix} I_{m-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & c_m & -s_m e^{-i\phi_m} \\ \mathbf{0} & s_m e^{i\phi_m} & c_m \end{bmatrix}. \end{aligned}$$

That the first m columns of $\hat{V}_{m+1}$ form a basis of the approximation space $\mathcal{W}_m$ follows from

$$W_m = V_{m+1} \tilde{H}_m = V_{m+1} Q_m^H \begin{bmatrix} R_m \\ \mathbf{0} \end{bmatrix} = [\hat{\boldsymbol{v}}_1, \ldots, \hat{\boldsymbol{v}}_m] \, R_m,$$

which also implies (4.18). □

We summarize the coordinate representations of the MR and OR errors in the following result.

Proposition 4.7. For the MR and OR errors we have

$$\boldsymbol{r}_m^{\mathrm{MR}} = \beta\, q_{m+1,1}^{(m)}\, \tilde{\boldsymbol{v}}_{m+1} = \beta \prod_{j=1}^{m} \left[-s_j e^{i\phi_j}\right] \tilde{\boldsymbol{v}}_{m+1},$$

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

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

Proof. The recursive definition of Q_m allows us to express its entries $q_{k,1}^{(m)}$ explicitly in terms of the quantities s_j and c_j:

$$q_{k,1}^{(m)} = c_k \prod_{j=1}^{k-1} \left[-s_j e^{i\phi_j}\right] \quad (1 \le k \le m), \qquad q_{m+1,1}^{(m)} = \prod_{j=1}^{m} \left[-s_j e^{i\phi_j}\right].$$

This, together with (4.18), proves the first identity.

Next, we recall from Remark 4.3 that $\boldsymbol{r}_m^{\mathrm{OR}} = -\beta\eta_{m+1,m}\, \eta_{m,1}^{[-1]} \boldsymbol{v}_{m+1}$. To eliminate $\eta_{m,1}^{[-1]}$ from this relation, we note that the matrix H_m possesses the QR decomposition (*cf.* (4.15))

$$Q_{m-1} H_m = \begin{bmatrix} R_{m-1} & \boldsymbol{r} \\ \boldsymbol{0} & \tau \end{bmatrix}, \qquad \textit{i.e.,} \quad H_m^{-1} = \begin{bmatrix} R_{m-1}^{-1} & \tilde{\boldsymbol{r}} \\ \boldsymbol{0} & 1/\tau \end{bmatrix} Q_{m-1}, \tag{4.19}$$

which implies $\eta_{m,1}^{[-1]} = q_{m,1}^{(m-1)}/\tau$. Since $\eta_{m+1,m}/\tau = e^{i\phi_m} s_m/c_m$ (*cf.* (4.16)) we conclude $\eta_{m,1}^{[-1]}\eta_{m+1,m} = q_{m,1}^{(m-1)} e^{i\phi_m} s_m/c_m$. This proves the second identity.

The desired representation of $\boldsymbol{r}_{m-1}^{\mathrm{MR}} - \boldsymbol{r}_m^{\mathrm{OR}}$ now follows from $\hat{\boldsymbol{v}}_m = c_m \tilde{\boldsymbol{v}}_m + s_m e^{i\phi_m} \boldsymbol{v}_{m+1}$ (*cf.* Proposition 4.6). □

We note that all relations of Theorem 3.4 connecting the MR and OR approaches can be easily obtained by manipulating the error representations of Proposition 4.7. Indeed, this is essentially how these relations are proven in the literature on Krylov subspace methods. The main difference there is that the occurring sines and cosines result from the Givens rotations needed to construct the QR decomposition of $\tilde{H}_m$, and they have not been identified as the sines and cosines of $\measuredangle(\boldsymbol{r}_0, \mathcal{W}_m)$.

Finally, we observe that the vector $\hat{\boldsymbol{w}}_{m+1}$ introduced in Lemma 4.4 is given by $\tilde{\boldsymbol{v}}_{m+1}/c_m$ in terms of the last vector in the Paige–Saunders basis, so that an equivalent formulation of (4.10) reads

$$\big(I - P_{\mathcal{W}_m}^{\mathcal{V}_m}\big)\boldsymbol{v} = \frac{(\boldsymbol{v}, \tilde{\boldsymbol{v}}_{m+1})}{c_m} \boldsymbol{v}_{m+1} \qquad (\boldsymbol{v} \in \mathcal{V}_{m+1}).$$

4.3. Using arbitrary bases of $\mathcal{W}_m$ and $\mathcal{V}_m$

For practical computations it is desirable that the Hessenberg matrices $\tilde{H}_m$ introduced in (4.3) have small bandwidth. Indeed, if $\tilde{H}_m$ has only k nonvanishing diagonals, namely the ones with indices $-1, 0, 1, \ldots, k-2$ (we follow the standard notation according to which a diagonal has index k if its entries $\eta_{j,\ell}$ are characterized by $\ell - j = k$), then only k diagonals of the upper triangular matrices R_m are nonzero, namely those with indices $k = 0, 1, \ldots, k-1$. This follows easily from the fact that Q_m has lower Hessenberg form. This banded structure of the matrices R_m can then be used to derive k-term recurrence formulas for the coordinate vectors $\boldsymbol{y}_m$ in terms of $\boldsymbol{y}_{m-1}, \boldsymbol{y}_{m-2}, \ldots, \boldsymbol{y}_{m-k+1}$ and for the approximations $\boldsymbol{w}_m$ in terms of $\boldsymbol{w}_{m-1}, \boldsymbol{w}_{m-2}, \ldots, \boldsymbol{w}_{m-k+1}$. (This statement applies to both the MR and the OR approach.) The most important consequence of this observation is that, at each step, only the k previous approximations (or, in other implementations, the last k basis vectors) need to be stored, which means that in this case storage requirements do not increase with m. If we insist on choosing $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_L$ as orthogonal vectors then the Hessenberg matrices will generally not have banded form. The main motivation for giving up orthogonality of the basis of $\mathcal{V}_m$ is therefore to constrain the bandwidth of H_m in order to keep storage requirements low.

As explained at the beginning of Section 4.2, no orthogonality conditions are required to derive the fundamental relationship (4.3)

$$W_m = V_{m+1}\tilde{H}_m = V_m H_m + [\boldsymbol{0}, \ldots, \boldsymbol{0}, \eta_{m+1,m}\boldsymbol{v}_{m+1}].$$

In this section, we assume only that $\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots$ are linearly independent such that $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m\}$ constitutes a basis of $\mathcal{V}_m$ $(m = 1, 2, \ldots, L)$. Just as before, the jth column of the upper Hessenberg matrix $\tilde{H}_m \in \mathbb{C}^{(m+1)\times m}$ contains the coefficients of $\boldsymbol{w}_j \in \mathcal{W}_j \subset \mathcal{V}_{m+1}$ with respect to the basis vectors $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}$. The difference is that, since now the vectors $\boldsymbol{v}_j$ need not be orthogonal, these coefficients can no longer be expressed in terms of the inner product with which $\mathcal{H}$ was originally endowed. We shall see below that we can recover the usual inner product representation by switching to another suitable inner product. Recall from the proof of Lemma 4.1 that, for each $\boldsymbol{w} = W_m\boldsymbol{y} \in \mathcal{W}_m$ $(\boldsymbol{y} \in \mathbb{C}^m)$, the associated error in approximating $\boldsymbol{r}_0$ is represented by

$$\boldsymbol{r} = \boldsymbol{r}_0 - \boldsymbol{w} = \boldsymbol{r} - W_m\boldsymbol{y} = \beta\boldsymbol{v}_1 - V_{m+1}\tilde{H}_m\boldsymbol{y} = V_{m+1}(\beta\boldsymbol{u}_1 - \tilde{H}_m\boldsymbol{y}).$$

Minimizing the norm of $\boldsymbol{r}$ among all $\boldsymbol{w} \in \mathcal{W}_m$ leads as above to the least squares problem

$$\min_{\boldsymbol{y}\in\mathbb{C}^m} \left\| V_{m+1}\big(\beta\boldsymbol{u}_1 - \tilde{H}_m\boldsymbol{y}\big) \right\| = \min_{\boldsymbol{y}\in\mathbb{C}^m} \|\beta\boldsymbol{u}_1 - \tilde{H}_m\boldsymbol{y}\|_{\boldsymbol{v}}, \tag{4.20}$$

in which now $\|\cdot\|_{\boldsymbol{v}}$ denotes the norm induced on the coordinate space with

respect to V_L by the inner product $(\cdot,\cdot)$ given on $\mathcal{H}$. More precisely, if we set for $\boldsymbol{x},\boldsymbol{y}\in\mathbb{C}^L$

$$(\boldsymbol{x},\boldsymbol{y})_{\boldsymbol{v}} := (V_L\boldsymbol{x},V_L\boldsymbol{y}) = \boldsymbol{y}^H M\boldsymbol{x}, \quad \text{where } M := [(\boldsymbol{v}_j,\boldsymbol{v}_k)]\in\mathbb{C}^{L\times L}, \tag{4.21}$$

then $(\cdot,\cdot)_{\boldsymbol{v}}$ is an inner product on $\mathbb{C}^L$ with associated norm

$$\|\cdot\|_{\boldsymbol{v}} = \sqrt{(\cdot,\cdot)_{\boldsymbol{v}}}.$$

At this point one could proceed as in the algorithms which use an orthogonal basis, the only difference being that all inner products in the coordinate space now require knowledge of the Gram matrix M. In particular, the Givens rotations and the matrices Q_m in the QR factorization (4.12) must now be unitary with respect to the inner product $(\cdot,\cdot)_{\boldsymbol{v}}$, that is, they must satisfy $Q_m^H M_m Q_m = I_m$, where $M_m\in\mathbb{C}^{(m+1)\times(m+1)}$ is the $(m+1)$st leading principal submatrix of M. The submatrices M_m, however, *cannot* be computed unless all basis vectors $\boldsymbol{v}_1,\boldsymbol{v}_2,\ldots,\boldsymbol{v}_{m+1}$ are available, and thus any short recurrence for generating these would not result in any storage savings: this is precisely what we wish to avoid.

An alternative was originally proposed by Freund (1992): rather than solving the minimization problem (4.20), we instead solve

$$\min_{\boldsymbol{y}\in\mathbb{C}^m}\|\beta\boldsymbol{u}_1-\tilde{H}_m\boldsymbol{y}\|_2,$$

and, if $\boldsymbol{y}_m^{\mathrm{QMR}}\in\mathbb{C}^m$ denotes the unique solution to this least-squares problem, regard

$$\boldsymbol{w}_m^{\mathrm{QMR}} := W_m\boldsymbol{y}_m^{\mathrm{QMR}}$$

as an approximation of $\boldsymbol{r}_0$. Adhering to the terminology introduced by Freund, we refer to this approach as the *quasi-minimal residual* (QMR) approach. Following the convention in the literature on Krylov subspace methods, we refer to the (coordinate) vector

$$\boldsymbol{s}_m^{\mathrm{QMR}} := \beta\boldsymbol{u}_1-\tilde{H}_m\boldsymbol{y}_m^{\mathrm{QMR}}\in\mathbb{C}^{m+1}$$

as the *quasi-error* of $\boldsymbol{w}_m^{\mathrm{QMR}}$.

We note that, instead of changing the inner product in the coordinate space from $(\cdot,\cdot)_{\boldsymbol{v}}$ to the Euclidean inner product, one could equivalently have replaced the given inner product $(\cdot,\cdot)$ on $\mathcal{V}_L\subseteq\mathcal{H}$ by

$$(\boldsymbol{v},\boldsymbol{w})_V = (V_L\boldsymbol{x},V_L\boldsymbol{y})_V =: \boldsymbol{y}^H\boldsymbol{x} \qquad \forall\boldsymbol{v}=V_L\boldsymbol{x},\boldsymbol{w}=V_L\boldsymbol{y}\in\mathcal{V}_L, \tag{4.22}$$

and proceeded as in the MR algorithm of Section 4.2. The new inner product $(\cdot,\cdot)_V$ thus defined has the property that the basis vectors $\{\boldsymbol{v}_1,\ldots,\boldsymbol{v}_L\}$ are orthonormal. For related work on interpreting QMR approximations as MR approximations in a modified norm see Barth and Manteuffel (1994).

The following assertions are obvious if we keep in mind that, for $\boldsymbol{x},\boldsymbol{y}\in\mathbb{C}^L$,

we have the relations

$$\begin{aligned}(V_L\boldsymbol{x}, V_L\boldsymbol{y})_V &= (V_L\boldsymbol{x}, V_L M^{-1}\boldsymbol{y}) = (V_L M^{-1}\boldsymbol{x}, V_L\boldsymbol{z}) \\ &= (V_L M^{-1/2}\boldsymbol{x}, V_L M^{-1/2}\boldsymbol{y}), \\ (V_L\boldsymbol{x}, V_L\boldsymbol{y}) &= (V_L\boldsymbol{x}, V_L M\boldsymbol{y})_V = (V_L M\boldsymbol{x}, V_L\boldsymbol{y})_V \\ &= (V_L M^{1/2}\boldsymbol{x}, V_L M^{1/2}\boldsymbol{y})_V.\end{aligned} \tag{4.23}$$

As a consequence, we obtain for instance the following result.

Theorem 4.8. The QMR iterates are the MR iterates with respect to the inner product $(\cdot,\cdot)_V$:

$$\|\boldsymbol{r}_m^{\mathrm{QMR}}\|_V = \|\boldsymbol{r}_0 - \boldsymbol{w}_m^{\mathrm{QMR}}\|_V = \min_{\boldsymbol{w}\in\mathcal{W}_m} \|\boldsymbol{r}_0 - \boldsymbol{w}\|_V.$$

In terms of the original norm on $\mathcal{H}$, the MR and QMR errors may be bounded by

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| \le \|\boldsymbol{r}_m^{\mathrm{QMR}}\| \le \sqrt{\kappa_2(M_m)}\,\|\boldsymbol{r}_m^{\mathrm{MR}}\|, \tag{4.24}$$

in which $\kappa_2(M_m)$ denotes the (Euclidean) condition number of the (Hermitian positive definite) matrix M_m. Moreover, we have

$$\|\boldsymbol{r}_m^{\mathrm{QMR}}\| \le \lambda_{\max}^{1/2}(M_m)\|\boldsymbol{s}_m^{\mathrm{QMR}}\|.$$

Proof. Only the second inequality in (4.24) remains to be proved. This follows immediately from

$$\lambda_{\min}^{1/2}(M_m)\,\|\boldsymbol{y}\|_2 \le \|\boldsymbol{y}\|_{\boldsymbol{v}} \le \lambda_{\max}^{1/2}(M_m)\,\|\boldsymbol{y}\|_2 \qquad \forall \boldsymbol{y}\in\mathbb{C}^{m+1}. \qquad \square$$

In view of (4.24) the deviation of the QMR approach from the MR approach is bounded by the condition numbers $\kappa_2(M_m)$, that is, by the ratio of the extremal eigenvalues of M_m. The largest eigenvalue $\lambda_{\max}(M_m)$ is easily controlled: it merely requires choosing the basis vectors $\boldsymbol{v}_m$ to have unit length, that is, $\|\boldsymbol{v}_m\| = 1$ for all m, to ensure $\lambda_{\max}(M_m) \le m+1$ (note that $\lambda_{\max}(M_m) \le \|M_m\|_F := [\sum_{j,k=1}^{m+1}(\boldsymbol{v}_j,\boldsymbol{v}_k)^2]^{1/2} \le [\sum_{j,k=1}^{m+1}\|\boldsymbol{v}_j\|\,\|\boldsymbol{v}_k\|]^{1/2}$). The crucial point is to construct the basis V_m in such a way that $\lambda_{\min}(M_m)$ does not approach zero (or does so only slowly).

Another immediate consequence of (4.23) is as follows.

Proposition 4.9. The QMR error vectors satisfy

$$\boldsymbol{r}_m^{\mathrm{QMR}} \perp \mathcal{U}_m,$$

where $\mathcal{U}_m := \{\boldsymbol{v} = V_{m+1}\boldsymbol{y} \,:\, \boldsymbol{y} = M_m^{-1}\tilde{H}_m\boldsymbol{z} \text{ for some } \boldsymbol{z}\in\mathbb{C}^m\}$ is an m-dimensional subspace of $\mathcal{V}_{m+1}$ ($\mathcal{U}_L = \mathcal{V}_L$ for $m = L$) and orthogonality is understood with respect to the original inner product $(\cdot,\cdot)$ on $\mathcal{H}$. Consequently,

$$\boldsymbol{r}_m^{\mathrm{QMR}} = \left(I - P_{\mathcal{W}_m}^{\mathcal{U}_m}\right)\boldsymbol{r}_0,$$

where $P_{\mathcal{W}_m}^{\mathcal{U}_m}$ denotes the oblique projection onto $\mathcal{W}_m$ orthogonal to $\mathcal{U}_m$.

Proof. Since the QMR approximations are merely the MR approximations with respect to $(\cdot,\cdot)_V$, their errors $\boldsymbol{r}_m^{\mathrm{QMR}} \in \mathcal{V}_{m+1}$ are characterized by

$$\boldsymbol{r}_m^{\mathrm{QMR}} \perp_V \mathcal{W}_m.$$

From this observation and (4.23) both assertions easily follow.

An equally simple proof results from the fact that

$$\boldsymbol{r}_m^{\mathrm{QMR}} = V_{m+1}\left(\beta\boldsymbol{u}_1 - \tilde{H}_m \boldsymbol{y}_m^{\mathrm{QMR}}\right),$$

where $\boldsymbol{y}_m^{\mathrm{QMR}}$ solves the least-squares problem $\|\beta\boldsymbol{u}_1 - \tilde{H}_m\boldsymbol{y}\|_2 \to \min$. In other words,

$$\beta\boldsymbol{u}_1 - \tilde{H}_m\boldsymbol{y}^{\mathrm{QMR}} \perp \mathrm{range}(\tilde{H}_m) \quad \text{or} \quad \beta\boldsymbol{u}_1 - \tilde{H}_m\boldsymbol{y}^{\mathrm{QMR}} \perp_{\boldsymbol{v}} M^{-1}\,\mathrm{range}(\tilde{H}_m).$$

□

Note that the orthogonal complement of $\mathcal{U}_m$ is given by $\mathcal{U}_m^{\perp} = \mathrm{span}\{\boldsymbol{r}_m^{\mathrm{QMR}}\} + \mathcal{V}_{m+1}^{\perp}$, that is, $\mathcal{U}_m^{\perp} \oplus \mathcal{V}_m = \mathcal{H}$ and the oblique projection $P_{\mathcal{W}_m}^{\mathcal{U}_m}$ exists.

We now briefly describe the analogue of the OR approach when using a non-orthogonal basis. In place of seeking $\boldsymbol{y} \in \mathbb{C}^m$ such that

$$0 = \left(V_{m+1}[\beta\boldsymbol{u}_1 - \tilde{H}_m\boldsymbol{y}], \boldsymbol{v}_j\right) = (\beta\boldsymbol{u}_1 - \tilde{H}_m\boldsymbol{y}, \boldsymbol{u}_j)_{\boldsymbol{v}} \qquad (j = 1, 2, \ldots, m),$$

which would lead to $\boldsymbol{r} - W_m\boldsymbol{y} \perp \mathcal{V}_m$ and thereby to a proper OR approximation, we instead determine a coordinate vector $\boldsymbol{y}_m^{\mathrm{QOR}} \in \mathbb{C}^m$ to satisfy

$$0 = (\beta\boldsymbol{u}_1 - \tilde{H}_m\boldsymbol{y}_m^{\mathrm{QOR}}, \boldsymbol{u}_j)_2 \quad (j = 1, 2, \ldots, m),\ \textit{i.e.},\ H_m\boldsymbol{y}_m^{\mathrm{QOR}} = \beta\boldsymbol{u}_1 \quad (4.25)$$

(provided H_m is nonsingular) and thus obtain the corresponding approximants $\boldsymbol{w}_m^{\mathrm{QOR}} := W_m\boldsymbol{y}_m^{\mathrm{QOR}}$. In terms of the inner product $(\cdot,\cdot)_V$ on $\mathcal{V}_L$ these are characterized by

$$\boldsymbol{r}_m^{\mathrm{QOR}} = \boldsymbol{r}_0 - \boldsymbol{w}_m^{\mathrm{QOR}} \perp_V \mathcal{V}_m$$

that is, the QOR iterates are the OR iterates with respect to the inner product $(\cdot,\cdot)_V$. By analogy with Proposition 4.9 we obtain the following result.

Proposition 4.10. The QOR errors satisfy

$$\boldsymbol{r}_m^{\mathrm{QOR}} \perp \mathcal{T}_m,$$

where $\mathcal{T}_m := \{\boldsymbol{v} = V_{m+1}\boldsymbol{y} \in \mathcal{V}_{m+1} : \boldsymbol{y} = M_m^{-1}[\boldsymbol{z}^\top\ 0]^\top \text{ with } \boldsymbol{z} \in \mathbb{C}^m\}$ is an m-dimensional subspace of $\mathcal{V}_{m+1}$ ($\mathcal{T}_L = \mathcal{V}_L$ for $m = L$) and orthogonality is understood with respect to the original inner product $(\cdot,\cdot)$ on $\mathcal{H}$. Consequently,

$$\boldsymbol{r}_m^{\mathrm{QOR}} = \left(I - P_{\mathcal{W}_m}^{\mathcal{T}_m}\right)\boldsymbol{r}_0,$$

where $P_{\mathcal{W}_m}^{\mathcal{T}_m}$ denotes the oblique projection onto $\mathcal{W}_m$ orthogonal to $\mathcal{T}_m$.

We know from Remark 4.2 that H_m being nonsingular is equivalent to $\mathcal{W}_m \oplus \mathcal{V}_m^{\perp_V} = \mathcal{H}$. But since, for every $\boldsymbol{h} \in \mathcal{H}$, $\boldsymbol{h} \perp_V \mathcal{V}_m$ if and only if $\boldsymbol{h} \perp \mathcal{T}_m$, the oblique projection $P_{\mathcal{W}_m}^{\mathcal{T}_m}$ exists if H_m is nonsingular.

The simple observation that the QMR and QOR approximations are the MR and OR approximations, respectively, obtained when replacing the original inner product $(\cdot,\cdot)$ with the basis-dependent inner product $(\cdot,\cdot)_V$ implies that the assertions of the preceding sections, particularly those of Theorem 3.4 and Propositions 3.8 and 4.7, are valid for any pair of QMR/QOR methods. Note, however, that when formulating these results for QMR/QOR methods each occurrence of the original norm must be replaced by the $\|\cdot\|_V$-norm and that angles are understood to be defined with respect to $(\cdot,\cdot)_V$.

As an example, we mention that

$$\boldsymbol{w}_m^{\mathrm{QMR}} = \hat{s}_m^2 \boldsymbol{w}_{m-1}^{\mathrm{QMR}} + \hat{c}_m^2 \boldsymbol{w}_m^{\mathrm{QMR}},$$

where

$$\hat{s}_m := \sin \measuredangle_V(\boldsymbol{r}_{m-1}^{\mathrm{QMR}}, \mathcal{W}_m), \quad \hat{c}_m := \cos \measuredangle_V(\boldsymbol{r}_{m-1}^{\mathrm{QMR}}, \mathcal{W}_m)$$

and $\measuredangle_V(\boldsymbol{r}_{m-1}^{\mathrm{QMR}}, \mathcal{W}_m)$ denotes the angle between $\boldsymbol{r}_{m-1}^{\mathrm{QMR}}$ and $\mathcal{W}_m$ with respect to the inner product $(\cdot,\cdot)_V$.

We conclude our discussion of abstract QMR and QOR approximations with a comment on the effect of applying the smoothing procedures introduced in Section 3, namely minimal and quasi-minimal residual smoothing, to the QOR approximations. We first note that the two are no longer equivalent. Specifically, if we define

$$\alpha_m^{\mathrm{MR}} := \frac{(\boldsymbol{d}_{m-1}^{\mathrm{QMR}}, \boldsymbol{d}_{m-1}^{\mathrm{QMR}} - \boldsymbol{d}_m^{\mathrm{QOR}})}{\|\boldsymbol{d}_{m-1}^{\mathrm{QMR}} - \boldsymbol{d}_m^{\mathrm{QOR}}\|^2} \tag{4.26}$$

then, in general, $\boldsymbol{w}_m^{\mathrm{QMR}} \neq (1-\alpha_m^{\mathrm{MR}})\boldsymbol{w}_{m-1}^{\mathrm{QMR}} + \alpha_m^{\mathrm{MR}} \boldsymbol{w}_m^{\mathrm{QOR}}$ because the formula (4.26) for the smoothing parameter α_m^{MR} was derived in order that the errors of the smoothed approximations solve a local approximation problem with respect to the inner product $(\cdot,\cdot)$, which is different from the inner product $(\cdot,\cdot)_V$ which characterizes the QMR and QOR approximations. Minimal residual smoothing therefore does not lead from QOR to QMR.

It is an easy consequence of Remark 4.3 that the situation is different if we apply QMR smoothing. If we set

$$\alpha_m^{\mathrm{QMR}} = \frac{1/\|\boldsymbol{r}_m^{\mathrm{QOR}}\|_V^2}{\sum_{j=0}^m 1/\|\boldsymbol{r}_j^{\mathrm{QOR}}\|_V^2},$$

then $\boldsymbol{w}_m^{\mathrm{QMR}} = (1 - \alpha_m^{\mathrm{QMR}})\boldsymbol{w}_{m-1}^{\mathrm{QMR}} + \alpha_m^{\mathrm{QMR}} \boldsymbol{w}_m^{\mathrm{QOR}}$ does indeed hold (*cf.* Pro-

position 3.8). But since $\boldsymbol{r}_m^{\mathrm{QOR}} = \gamma \boldsymbol{v}_{m+1}$ for some $\gamma \in \mathbb{C}$, we have

$$\|\boldsymbol{r}_m^{\mathrm{QOR}}\|_V = |\gamma| = \|\boldsymbol{r}_m^{\mathrm{QOR}}\|/\|\boldsymbol{v}_{m+1}\|$$

and consequently

$$\alpha_m^{\mathrm{QMR}} = \frac{\|\boldsymbol{v}_{m+1}\|^2/\|\boldsymbol{r}_m^{\mathrm{QOR}}\|^2}{\sum_{j=0}^m \|\boldsymbol{v}_{j+1}\|^2/\|\boldsymbol{r}_j^{\mathrm{QOR}}\|^2}.$$

If we make the usual assumption that the basis vectors $\boldsymbol{v}_j$ have unit length ($\|\boldsymbol{v}_j\| = 1$ for all j), then

$$\alpha_m^{\mathrm{QMR}} = \frac{1/\|\boldsymbol{r}_m^{\mathrm{QOR}}\|^2}{\sum_{j=0}^m 1/\|\boldsymbol{r}_j^{\mathrm{QOR}}\|^2},$$

and the QMR and QOR approximants are related by exactly the formulas which hold for a proper MR/OR pair, namely,

$$\boldsymbol{w}_m^{\mathrm{QMR}} = \frac{\sum_{j=0}^m \boldsymbol{w}_j^{\mathrm{QOR}}/\|\boldsymbol{r}_j^{\mathrm{QOR}}\|^2}{\sum_{j=0}^m 1/\|\boldsymbol{r}_j^{\mathrm{QOR}}\|^2} \quad \text{and} \quad \boldsymbol{r}_m^{\mathrm{QMR}} = \frac{\sum_{j=0}^m \boldsymbol{r}_j^{\mathrm{QOR}}/\|\boldsymbol{r}_j^{\mathrm{QOR}}\|^2}{\sum_{j=0}^m 1/\|\boldsymbol{r}_j^{\mathrm{QOR}}\|^2}.$$

QMR smoothing applied to CGS and Bi-CGSTAB is discussed in Walker (1995). For smoothing techniques applied to the general class of Lanczos-type product methods, see Ressel and Gutknecht (1998).

The above analysis might lead one to believe that the QMR approximations will move steadily further away from the MR approximation at each step. The following observation due to Stewart (1998) shows that this is not necessarily the case, but that the QMR approximation may under certain conditions recover, regardless of how far it may have deviated from the (optimal) MR approximation in earlier steps.

Proposition 4.11. We have $\boldsymbol{w}_m^{\mathrm{QMR}} = \boldsymbol{w}_m^{\mathrm{MR}}$ if and only if $\tilde{\boldsymbol{v}}_{m+1} \perp \mathcal{W}_m$, and $\boldsymbol{w}_m^{\mathrm{QOR}} = \boldsymbol{w}_m^{\mathrm{OR}}$ if and only if $\boldsymbol{v}_{m+1} \perp \mathcal{V}_m$.

Proof. By Proposition 4.6, we have both $\mathcal{W}_m = \operatorname{span}\{\hat{\boldsymbol{v}}_1, \ldots, \hat{\boldsymbol{v}}_m\}$ and $\boldsymbol{r}_m^{\mathrm{QMR}} \in \operatorname{span}\{\tilde{\boldsymbol{v}}_{m+1}\}$. Since $\boldsymbol{r}_m^{\mathrm{QMR}} = \boldsymbol{r}_m^{\mathrm{MR}}$ if and only if $\boldsymbol{r}_m^{\mathrm{QMR}} \perp \mathcal{W}_m$, the first assertion is proved. The analogous assertion for the QOR approximation follows from $\boldsymbol{r}_m^{\mathrm{QOR}} \in \operatorname{span}\{\boldsymbol{v}_{m+1}\}$; hence $\boldsymbol{r}_m^{\mathrm{QOR}} \perp \mathcal{V}_m$ if and only if $\boldsymbol{v}_{m+1} \perp \mathcal{V}_m$. □

4.4. Every method is an MR and an OR method

In Section 4.3 we saw how the QMR and QOR approximations can be reinterpreted as MR and OR approximations with respect to the basis-dependent inner product $(\cdot,\cdot)_V$. It turns out that an analogous interpretation is possible for *any* reasonable sequence of approximations $\{\boldsymbol{w}_m\}$ to

a given $\boldsymbol{r}_0 \in \mathcal{H}$, in fact, as we will show, both as an MR *and* as an OR approximation.

In the remainder of this section $\{\mathcal{W}_m\}_{m=0}^{L}$ denotes any sequence of nested spaces with $\dim \mathcal{W}_m = m$ (in particular, $\mathcal{W}_0 = \{\boldsymbol{0}\}$), and $\{\mathcal{V}_m\}_{m=1}^{L}$ denotes the associated sequence of error spaces $\mathcal{V}_m = \operatorname{span}\{\boldsymbol{r}_0\} + \mathcal{W}_{m-1}$ relative to $\boldsymbol{r}_0 \in \mathcal{H}$.

Theorem 4.12. Assume $\{\boldsymbol{h}_m\}_{m=0}^{L}$ is a sequence of approximations to $\boldsymbol{r}_0 \in \mathcal{H}$ such that $\boldsymbol{h}_m \in \mathcal{W}_m$ and $\boldsymbol{h}_L = \boldsymbol{r}$. Then an inner product $(\cdot,\cdot)_V$ on $\mathcal{V}_L = \mathcal{W}_L$ such that

$$\|\boldsymbol{r}_0 - \boldsymbol{h}_m\|_V = \min_{\boldsymbol{w}\in\mathcal{W}_m} \|\boldsymbol{r} - \boldsymbol{w}\|_V, \qquad m = 1, 2, \ldots, L-1,$$

exists if and only if $\boldsymbol{h}_m \in \mathcal{W}_{m-1}$ implies $\boldsymbol{h}_m = \boldsymbol{h}_{m-1}$ for $m = 1, 2, \ldots, L-1$ or, in other words, if and only if

$$\text{either} \quad \boldsymbol{h}_m \in \mathcal{W}_m \setminus \mathcal{W}_{m-1} \quad \text{or} \quad \boldsymbol{h}_m = \boldsymbol{h}_{m-1}, \qquad m = 1, 2, \ldots, L-1. \tag{4.27}$$

Proof. If the vectors $\{\boldsymbol{h}_m\}_{m=1}^{L-1}$ are the best approximations to $\boldsymbol{r}_0$ from $\mathcal{W}_m$ with respect to some inner product $(\cdot,\cdot)_V$, then, whenever $\boldsymbol{h}_m$ happens to lie also in $\mathcal{W}_{m-1}$, $\boldsymbol{h}_m$ must also be the best approximation to $\boldsymbol{r}_0$ from $\mathcal{W}_{m-1}$, whereby $\boldsymbol{h}_m = \boldsymbol{h}_{m-1}$, which proves the necessity of (4.27).

Conversely, assuming that (4.27) is satisfied, we write

$$\boldsymbol{r}_0 = (\boldsymbol{h}_1 - \boldsymbol{h}_0) + (\boldsymbol{h}_2 - \boldsymbol{h}_1) + \cdots + (\boldsymbol{h}_L - \boldsymbol{h}_{L-1})$$

and construct a basis $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_L\}$ of $\mathcal{W}_L$ by setting

$$\boldsymbol{w}_m := \begin{cases} \boldsymbol{h}_m - \boldsymbol{h}_{m-1}, & \text{if } \boldsymbol{h}_m \in \mathcal{W}_m \setminus \mathcal{W}_{m-1}, \\ \text{an arbitrary vector from } \mathcal{W}_m \setminus \mathcal{W}_{m-1}, & \text{if } \boldsymbol{h}_m = \boldsymbol{h}_{m-1}. \end{cases}$$

Note that, for each m, $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$ is a basis of $\mathcal{W}_m$. We further define the 'Fourier coefficients' α_m by

$$\alpha_m := \begin{cases} 1, & \text{if } \boldsymbol{h}_m \in \mathcal{W}_m \setminus \mathcal{W}_{m-1}, \\ 0, & \text{if } \boldsymbol{h}_m = \boldsymbol{h}_{m-1}, \end{cases} \qquad m = 1, \ldots, L,$$

so that $\boldsymbol{r}_0 = \alpha_1 \boldsymbol{w}_1 + \alpha_2 \boldsymbol{w}_2 + \cdots + \alpha_L \boldsymbol{w}_L$ and

$$\boldsymbol{h}_m = \alpha_1 \boldsymbol{w}_1 + \alpha_2 \boldsymbol{w}_2 + \cdots \alpha_m \boldsymbol{w}_m, \qquad m = 1, \ldots, L,$$

that is, $\boldsymbol{h}_m$ is simply the truncated 'Fourier expansion' of $\boldsymbol{r}_0$. Defining the inner product $(\cdot,\cdot)_V$ such that $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_L\}$ are orthonormal then leads to the desired conclusion. □

The next theorem establishes the analogous result for the OR (or, more precisely, the QOR) approximation.

Theorem 4.13. If $\{\boldsymbol{h}_m\}_{m=1}^{L}$ is a sequence of approximations to $\boldsymbol{r}_0 \in \mathcal{H}$ such that $\boldsymbol{h}_m \in \mathcal{W}_m$ and $\boldsymbol{h}_L = \boldsymbol{r}_0$, then an inner product $(\cdot,\cdot)_{\tilde{V}}$ on $\mathcal{V}_L = \mathcal{W}_L$ such that

$$\boldsymbol{r}_0 - \boldsymbol{h}_m \perp_{\tilde{V}} \mathcal{V}_m, \qquad m = 1, 2, \ldots, L-1,$$

exists if and only if $\boldsymbol{h}_m \in \mathcal{W}_m \setminus \mathcal{W}_{m-1}$ for $m = 1, 2, \ldots, L-1$.

Proof. Assume that, for all $m = 1, 2, \ldots, L-1$, the vectors $\boldsymbol{h}_m$ are the OR approximations to $\boldsymbol{r}_0$ from $\mathcal{W}_m$ with respect to some inner product $(\cdot,\cdot)_{\tilde{V}}$. If now, for some m, $\boldsymbol{h}_m \in \mathcal{W}_{m-1}$, then $\boldsymbol{r}_m := \boldsymbol{r}_0 - \boldsymbol{h}_m \in \operatorname{span}\{\boldsymbol{r}_0\} + \mathcal{W}_{m-1} = \mathcal{V}_m$, that is, $\boldsymbol{r}_m \in \mathcal{V}_m \cap \mathcal{V}_m^{\perp} = \{\boldsymbol{0}\}$, which implies $\boldsymbol{h}_m = \boldsymbol{r}_0$. But this is impossible unless $\boldsymbol{r}_0 \in \mathcal{W}_m$, that is, $m = L$, and we have thus established that $\boldsymbol{h}_m \in \mathcal{W}_m \setminus \mathcal{W}_{m-1}$ for $m = 1, \ldots, L-1$.

Conversely, since $\boldsymbol{h}_m \in \mathcal{W}_m \setminus \mathcal{W}_{m-1}$ implies $\boldsymbol{r}_m \in \mathcal{V}_{m+1} \setminus \mathcal{V}_m$ for $m = 1, \ldots, L-1$, we see that $\{\boldsymbol{r}_0, \boldsymbol{r}_1, \ldots, \boldsymbol{r}_{L-1}\}$ ($\boldsymbol{h}_0 = \boldsymbol{r}_0$) is a basis of $\mathcal{V}_L$ such that, for every $m = 1, \ldots, L-1$, $\{\boldsymbol{r}_0, \boldsymbol{r}_1, \ldots, \boldsymbol{r}_{m-1}\}$ is a basis of $\mathcal{V}_m$. Defining the inner product $(\cdot,\cdot)_{\tilde{V}}$ such that $\{\boldsymbol{r}_0, \ldots, \boldsymbol{r}_{L-1}\}$ is an orthogonal basis of $\mathcal{V}_L$ leads to the desired conclusion. □

We have formulated these two theorems for the case of a sequence terminating with $\boldsymbol{h}_L = \boldsymbol{r}_0$, as this is the situation when solving linear equations in finite dimensions by MR and OR approximations, at least in the absence of rounding error. When the sequence of approximations does not terminate, we may proceed analogously to Theorem 4.12 with the difference that the inner product is then defined on the union of all error spaces $\mathcal{V}_m$ and we need not have convergence of the approximation to $\boldsymbol{r}_0$ in the associated norm. Similar considerations apply for a formulation of Theorem 4.13 for a nonterminating approximation sequence.

In summary, we conclude that, by allowing the inner product to vary, the concept of MR and OR approximations becomes sufficiently general to include any reasonable sequence of approximations. Of course, this result is of a rather academic nature since an application in which such approximation problems arise often comes with a natural norm to be minimized. In view of this one might say that methods should not be compared on the grounds of whether they minimize a norm, but whether the norm being minimized is appropriate for the problem at hand. However, it does show that the given MR/OR framework includes all reasonable approximation schemes.

5. Krylov subspace methods and related algorithms

We now return to our original problem of approximating the solution of an operator equation (1.1) using MR and OR approximations. As mentioned in the introduction, this amounts to approximating the residual $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$ of a given initial approximation $\boldsymbol{x}_0$ in the sequence of nested approximation

spaces $\mathcal{W}_m = A\mathcal{C}_m$, which are the images under A of a sequence of m-dimensional nested correction spaces $\mathcal{C}_m \subset \mathcal{H}$. In accordance with (3.10), the resulting residual spaces are $\mathcal{V}_m = \operatorname{span}\{\boldsymbol{r}_0\} + A\mathcal{C}_{m-1}$, and thus both the approximation and residual spaces are determined by the sequence of correction spaces. In this equation-solving setting the termination index L defined in (4.4) becomes

$$\begin{aligned} L &= \min\{m : \boldsymbol{r}_0 \in A\mathcal{C}_m\} = \min\{m : \boldsymbol{b} = A(\boldsymbol{x}_0 + \boldsymbol{c}), \boldsymbol{c} \in \mathcal{C}_m\} \\ &= \min\{m : A^{-1}\boldsymbol{b} \in \boldsymbol{x}_0 + \mathcal{C}_m\}, \end{aligned} \tag{5.1}$$

that is, the MR and OR methods terminate when the exact solution is found, at least in exact arithmetic. In general one has $\boldsymbol{r}_0 \in \mathcal{C}_m$, so that a sufficient condition for termination is the A-invariance of the correction space. The angles which determine the rate of convergence (*cf.* (3.5), (3.11)) are now

$$\measuredangle(\boldsymbol{r}_m^{\mathrm{MR}}, A\mathcal{C}_m) = \measuredangle(\mathcal{V}_m, A\mathcal{C}_m) = \measuredangle(\operatorname{span}\{\boldsymbol{r}_0\} + A\mathcal{C}_{m-1}, A\mathcal{C}_m).$$

We note that all statements about MR and OR approximations made in the previous sections immediately carry over to the associated equation-solving methods, in particular those of Theorems 3.4 and 3.5 as well as the results of Proposition 3.8 on minimal and quasi-minimal residual smoothing. Note also that, by the injectivity of A, relation (3.20) among the MR and OR approximations of $\boldsymbol{r}_0$ implies

$$\boldsymbol{c}_m^{\mathrm{MR}} = s_m^2\, \boldsymbol{c}_{m-1}^{\mathrm{MR}} + c_m^2\, \boldsymbol{c}_m^{\mathrm{OR}}$$

for the associated correction vectors $\boldsymbol{c}^{\mathrm{MR}}$ and $\boldsymbol{c}^{\mathrm{OR}}$, and hence, by the identity $s_m^2 + c_m^2 = 1$, we obtain the analogous relation

$$\boldsymbol{x}_m^{\mathrm{MR}} = s_m^2\, \boldsymbol{x}_{m-1}^{\mathrm{MR}} + c_m^2\, \boldsymbol{x}_m^{\mathrm{OR}} \tag{5.2}$$

for the approximations of $A^{-1}\boldsymbol{b}$.

Although in principle any nested sequence of correction spaces leads to the MR/OR methods discussed so far for solving (1.1), by far the most popular of such subspace correction methods employ *Krylov subspaces* as correction spaces, that is,

$$\mathcal{C}_m = \mathcal{K}_m := \mathcal{K}_m(A, \boldsymbol{r}_0) := \operatorname{span}\{\boldsymbol{r}_0, A\boldsymbol{r}_0, \ldots, A^{m-1}\boldsymbol{r}_0\}, \qquad m = 0, 1, \ldots.$$

The name refers to a method introduced by Krylov (1931) for determining divisors of the minimal polynomial of an operator for the purpose of computing eigenvalues, in which such spaces were used (see also Householder (1964, Section 6.1)). In this case the residual spaces

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

coincide with the correction spaces, so that Krylov subspace MR and OR methods are special cases of the abstract MR and OR methods described in

Section 3 with

$$\mathcal{C}_m = \mathcal{V}_m = \mathcal{K}_m(A, \boldsymbol{r}_0), \qquad \mathcal{W}_m = A\mathcal{K}_m(A, \boldsymbol{r}_0) = \mathcal{K}_m(A, A\boldsymbol{r}_0). \tag{5.3}$$

The associated angles governing convergence in this case are thus

$$\measuredangle(\boldsymbol{r}_m^{\mathrm{MR}}, A\mathcal{K}_m) = \measuredangle(\mathcal{K}_m, A\mathcal{K}_m), \tag{5.4}$$

and the termination index L may now be characterized by

$$\begin{aligned} L &= \min\{m : A^{-1}\boldsymbol{b} \in \boldsymbol{x}_0 + \mathcal{K}_m(A, \boldsymbol{r}_0)\} \\ &= \min\{m : A^{-1}\boldsymbol{r}_0 \in \mathcal{K}_m(A, \boldsymbol{r}_0)\} \\ &= \min\{m : \mathcal{K}_m(A, \boldsymbol{r}_0) = \mathcal{K}_{m+1}(A, \boldsymbol{r}_0)\}. \end{aligned} \tag{5.5}$$

In the remainder of this section, we discuss some of the advantages of Krylov subspaces as correction spaces, review the most important examples of Krylov subspace algorithms, and recover some well-known results on Krylov subspace methods by specializing the abstract results of Sections 3 and 4.

Before turning to Krylov subspace methods, however, we point out that MR and OR methods which use non-Krylov correction spaces have received increasing attention recently. Methods of this type are the EN-method of Eirola and Nevanlinna (1989), the FGMRES method of Saad (1993), the GMRESR algorithm of van der Vorst and Vuik (1994), the augmented GMRES methods of Morgan (2000) and the GCROT method of de Sturler (1999). We refer to Eiermann, Ernst and Schneider (2000) for an overview and an analysis of these approaches.

5.1. Why Krylov subspaces?

The use of (shifted) Krylov spaces to construct approximate solutions to linear equations, at least implicitly, is as old as classical stationary iteration methods (see, *e.g.*, Varga (1999)): given a splitting $A = M - N$ with M nonsingular, the induced stationary iteration

$$\boldsymbol{x}_m = T\boldsymbol{x}_{m-1} + \boldsymbol{c}, \qquad m = 1, 2, \ldots \tag{5.6}$$

with $T = M^{-1}N$ and $\boldsymbol{c} = M^{-1}\boldsymbol{b}$ generates the approximations

$$\boldsymbol{x}_m = \boldsymbol{x}_0 + (I + T + \cdots + T^{m-1})\boldsymbol{r}_0 \in \boldsymbol{x}_0 + \mathcal{K}_m(T, \boldsymbol{r}_0).$$

From this perspective, one can view Krylov subspace MR and OR methods as a cleverer strategy for choosing the approximations in $\boldsymbol{x}_0 + \mathcal{K}_m$ or, equivalently, as techniques which accelerate the convergence of the stationary iterative method (5.6). This was the motivation in Varga (1999), where the term *semi-iterative methods* is used for this approach. In view of (5.5), a subtle difference between such stationary iterations and Krylov subspace MR and OR methods is that the latter terminate with the exact solution

whenever the Krylov space becomes A-invariant, which is not the case for stationary methods or those based on Chebyshev recursions (Varga 1999).

The main reason for the prevalence of Krylov subspaces as correction spaces for MR/OR methods is the ease by which these can be generated, namely by multiplication of a vector by A in each step, an inexpensive operation whenever A is represented by a sparse or structured matrix or when the action of A can be implemented efficiently without reference to a matrix representation. Moreover, the fact that the correction and residual spaces coincide for Krylov subspace methods allows the same basis to be used for both in computations, which further reduces computing and storage requirements.

Whether or not Krylov spaces are well suited as correction spaces will, in view of (5.4) and the results of Section 3, depend on the behaviour of the sequence of angles $\measuredangle(\mathcal{K}_m, A\mathcal{K}_m)$. There are classes of problems for which this behaviour is very favourable. An example where the angles actually tend to zero, which, in view of (3.15), implies superlinear convergence of the MR and OR approximants, is given by second-kind Fredholm equations (see Section 6.4). On the other hand, there are matrix problems of dimension n for which $\measuredangle(\mathcal{K}_m, A\mathcal{K}_m) = \pi/2$ for $m = 1, 2, \ldots, n-1$, that is, no Krylov subspace method is able to improve the initial residual until the very last step. The convergence properties of Krylov subspace methods will be discussed in more detail in Section 6.

A great simplification in the analysis of Krylov subspace methods arises from the representation

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

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

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

is thus always surjective but fails to be an isomorphism if and only if there exists a nonzero polynomial $q \in \mathcal{P}_{m-1}$ 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 with $c(A)\boldsymbol{r}_0 = \boldsymbol{0}$ 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 such that $\mathcal{K}_m = \mathcal{K}_{m+1}$ and thus coincides with the index L introduced in (4.4) (*cf.* also (5.1) and (5.5)),

$$L = \min\{m : \mathcal{K}_m = \mathcal{K}_{m+1}\} = \min\{\deg q \,:\, q \text{ monic and } q(A)\boldsymbol{r}_0 = \boldsymbol{0}\}. \tag{5.7}$$

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

Since every vector $\boldsymbol{x} \in \boldsymbol{x}_0 + \mathcal{K}_m$ is of the form $\boldsymbol{x} = \boldsymbol{x}_0 + q_{m-1}(A)\boldsymbol{r}_0$ for

some $q_{m-1} \in \mathcal{P}_{m-1}$, the corresponding residual $\boldsymbol{r} = \boldsymbol{b} - A\boldsymbol{x}$ can be written as

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

Note that the *residual polynomial* p_m satisfies the normalization condition $p_m(0) = 1$. Characterizations of the residual polynomials which belong to the MR and OR iterates as well as their zeros were first given by Stiefel (1958) in the Hermitian case and by Freund (1992) in the non-Hermitian case; a concise presentation can be found in Eiermann *et al.* (2000).

Finally, we note that the MR and OR approximations of an arbitrary vector $\boldsymbol{r} \in \mathcal{H}$ from a given sequence of nested spaces $\{\mathcal{W}_m\}_{m=0}^{L}$, $\dim \mathcal{W}_m = m$, can always be interpreted as Krylov subspace MR and OR approximations of the solution of a linear operator equation: indeed, relation (4.3) uniquely determines a linear operator A on the spaces $\{\mathcal{V}_m\}_{m=0}^{L}$, and A has $\mathcal{V}_L$ as an invariant subspace. If A is then extended to an invertible operator on the entire space $\mathcal{H}$, then the MR and OR approximation sequences for $\boldsymbol{r}$ coincide with the corresponding Krylov subspace approximations for solving the equation $A\boldsymbol{e} = \boldsymbol{r}$ with initial guess $\boldsymbol{e}_0 = \boldsymbol{0}$.

As already mentioned at the beginning of this section, the results of Sections 2, 3 and 4 also hold for the equation-solving MR and OR methods. For the particular class of Krylov subspace methods many of these identities, in particular (3.21) and (5.2), have been derived separately for each method, for example in the papers of Brown (1991), Freund (1992), Gutknecht (1993*a*), and Cullum and Greenbaum (1996). In these works, however, the sines and cosines result from the Givens rotations needed to construct a QR decomposition of the Hessenberg matrix analogous to (4.3) in the course of a specific algorithm for computing the MR and OR approximations. Section 4, specifically Theorem 4.5, reveals the more fundamental significance of these rotation angles, namely as the angles between the subspaces $\mathcal{K}_m(A, \boldsymbol{r}_0)$ and $A\mathcal{K}_m(A, \boldsymbol{r}_0)$. Moreover, all these relations have been derived in the previous sections as properties of the abstract MR and OR approximation schemes on nested subspaces, of which equation solving based on Krylov subspaces is just one particular instance.

5.2. Algorithms based on orthonormal bases

The algorithms which have been proposed in the literature for calculating MR and OR approximations for solving linear equations are based on one of the coordinate representations introduced in Section 4. The novelty, in the context of equation-solving, is that one requires the coordinates of the correction vector in $\mathcal{C}_m$ as well as those of the residual approximation in $\mathcal{W}_m$.

Using an orthonormal basis of $\mathcal{W}_m$

The trivial construction of the MR/OR approximations in terms of an orthonormal basis of $\mathcal{W}_m$ described in Section 4.1 becomes a little more interesting

when solving equations. Given an ascending basis $C_m = [\boldsymbol{c}_1, \ldots, \boldsymbol{c}_m]$ of $\mathcal{C}_m$, the most direct approach is to orthonormalize the image sequence $\{A\boldsymbol{c}_j\}$ and then proceed as in Section 4.1. Because the spaces are nested, the orthonormalization results in a QR decomposition

$$AC_m = W_m R_m \tag{5.8}$$

with an upper triangular matrix $R_m \in \mathbb{C}^{m\times m}$ and a set of orthonormal basis vectors $W_m = [\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m]$ of $\mathcal{W}_m$. The MR approximation $\boldsymbol{x}_m^{\mathrm{MR}}$ of the solution of (1.1) with respect to $\mathcal{C}_m$ is given by $\boldsymbol{x}_m^{\mathrm{MR}} = \boldsymbol{x}_0 + C_m \boldsymbol{y}_m^{\mathrm{MR}}$ with a coefficient vector $\boldsymbol{y}_m^{\mathrm{MR}} \in \mathbb{C}^m$. By (4.1) the coefficient vector of $P_{\mathcal{W}_m}\boldsymbol{r}_0$ with respect to W_m is $W_m^*\boldsymbol{r}_0$, hence we must have $AC_m\boldsymbol{y}_m^{\mathrm{MR}} = W_m W_m^*\boldsymbol{r}_0$, which, in view of (5.8), leads to $\boldsymbol{y}_m^{\mathrm{MR}} = R_m^{-1}W_m^*\boldsymbol{r}_0$. If no Galerkin breakdown occurs at this step, that is, if $(\boldsymbol{r}_0, \boldsymbol{w}_m) \neq 0$, then the OR approximation $\boldsymbol{x}_m^{\mathrm{OR}} = \boldsymbol{x}_0 + C_m\boldsymbol{y}_m^{\mathrm{OR}}$ is defined and may be computed following (4.2) by solving

$$R_m \boldsymbol{y}_m^{\mathrm{OR}} = \begin{bmatrix} (\boldsymbol{r}_0, \boldsymbol{w}_1) \\ \vdots \\ (\boldsymbol{r}_0, \boldsymbol{w}_{m-1}) \\ \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2/(\boldsymbol{w}_m, \boldsymbol{r}_0) \end{bmatrix}, \tag{5.9}$$

or by using (5.2) and noting $c_m = |(\boldsymbol{w}_m, \boldsymbol{r}_0)|/\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|$, $s_m = \sqrt{1-c_m^2}$. The main computational expense of this algorithm lies in the orthogonalization process and the solution of a triangular system whenever the approximations are desired. In the Krylov subspace case (5.3), the correction spaces are $\mathcal{C}_1 = \mathrm{span}\{\boldsymbol{r}_0\}$ and $\mathcal{C}_{m+1} = \mathrm{span}\{\boldsymbol{r}_0\} + \mathcal{W}_m, m = 1, \ldots, L$. An obvious candidate for the new vector in the ascending basis of $\mathcal{C}_{m+1}$ is $\boldsymbol{c}_{m+1} := \boldsymbol{w}_m$, a vector which is constructed in the previous step by orthonormalizing $A\boldsymbol{w}_{m-1}$ against the orthonormal basis of $\mathcal{W}_{m-1}$. This choice results in $C_{m+1} = [\boldsymbol{r}_0, \boldsymbol{w}_1, \ldots, \boldsymbol{w}_m]$, so that no separate basis for the correction spaces is necessary. Although it appears to be the most straightforward implementation, this method was only recently proposed for computing MR approximations by Walker and Zhou (1994).

The more well-known *generalized conjugate residual* (GCR) algorithm, introduced by Eisenstat, Elman and Schultz (1983), can be derived from the fact that the image under A of the MR correction $\boldsymbol{c}_m^{\mathrm{MR}}$ is the best approximation $W_m W_m^*\boldsymbol{r}_0$ of $\boldsymbol{r}_0$ from $\mathcal{W}_m$: if the basis C_m is taken to consist of the pre-images under A of a set of orthonormal basis vectors W_m of $\mathcal{W}_m$, then we obtain

$$\boldsymbol{c}_m^{\mathrm{MR}} = A^{-1}W_m W_m^*\boldsymbol{r}_0 = C_m W_m^*\boldsymbol{r}_0.$$

In this case the coefficient vector $\boldsymbol{y}_m^{\mathrm{MR}}$ of the MR correction with respect to C_m consists simply of the Fourier coefficients $W_m^*\boldsymbol{r}_0$, that is, no triangular system needs to be solved. The corresponding OR coefficient vector is

obtained, again in view of (4.2), by

$$\boldsymbol{y}_m^{\mathrm{OR}} = [(\boldsymbol{r}_0, \boldsymbol{w}_1), \ldots, (\boldsymbol{r}_0, \boldsymbol{w}_{m-1}), \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|^2/(\boldsymbol{w}_m, \boldsymbol{r}_0)]^\top. \tag{5.10}$$

The associated residual vectors may be formed by using the same coefficient vectors, but with respect to the orthonormal basis W_m.

For the Krylov subspace GCR algorithm different ways of extending the bases C_m and W_m have been proposed in the literature. The older variant, introduced in Eisenstat *et al.* (1983), generates in step m the new basis vector $\boldsymbol{w}_m$ by orthonormalizing $A\boldsymbol{r}_{m-1}$ against the previously generated orthonormal basis of $\mathcal{W}_{m-1}$, while simultaneously updating $\boldsymbol{r}_{m-1}$ to obtain $\boldsymbol{c}_m = A^{-1}\boldsymbol{w}_m$. This approach has the drawback that it fails to extend the Krylov space whenever two consecutive MR approximations coincide, that is, when a Galerkin breakdown occurs. For this reason, Eisenstat *et al.* (1983) state that the algorithm should only be used for linear systems where A is *positive real*, which means that its Hermitian part $(A + A^*)/2$ is positive definite. As will be explained in Section 6.1, the algorithm may in fact be used provided $0 \notin W(A)$, a slightly more general criterion. An easy remedy for this deficiency is to extend the basis W_{m-1} by instead orthogonalizing $A\boldsymbol{w}_{m-1}$ against W_{m-1}, which results in the Arnoldi process for $\mathcal{W}_m = K_m(A, A\boldsymbol{r}_0)$ for generating the $\boldsymbol{w}_m$-sequence, while the $\boldsymbol{c}_m$-sequence is again maintained such that $A\boldsymbol{c}_m = \boldsymbol{w}_m$. This observation is pointed out in Rozložník and Strakoš (1996), where many equivalent MR implementations are also compared with regard to their numerical stability.

The GCR algorithm belongs to the vast lineage of generalizations of the *conjugate gradient* and *conjugate residual methods* of Hestenes and Stiefel (1952), and we refer to Ernst (2000) and the monograph of Greenbaum (1997) for systematic surveys of this family of Krylov subspace methods.

Using an orthonormal basis of $\mathcal{V}_m$

The equation-solving Krylov subspace MR/OR algorithms based on the abstract scheme of Section 4.2 are the *generalized minimum residual method* (GMRES) of Saad and Schultz (1986) and the *full orthogonalization method* (FOM) introduced by Saad (1981). These algorithms proceed by successively constructing an orthonormal basis $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m\}$ of $\mathcal{V}_m = \mathcal{K}_m(A, \boldsymbol{r}_0)$ beginning with $\mathcal{V}_1 = \mathrm{span}\{\boldsymbol{r}_0\}$. We observe that this is exactly the Gram–Schmidt procedure introduced in (4.5) with $\boldsymbol{w}_m = A\boldsymbol{v}_m$, $m = 1, \ldots, L$, which in this setting is known as the *Arnoldi process*. In this case equation (4.3) reads

$$AV_m = V_{m+1}\tilde{H}_m = V_m H_m + [\boldsymbol{0}, \ldots, \boldsymbol{0}, \eta_{m+1,m}\boldsymbol{v}_{m+1}] \tag{5.11}$$

and the upper Hessenberg matrix $\tilde{H}_m$ is given by

$$\tilde{H}_m = [(A\boldsymbol{v}_k, \boldsymbol{v}_j)] \in \mathbb{C}^{(m+1)\times m}, \qquad j = 1, \ldots, k+1, \quad k = 1, \ldots, m. \tag{5.12}$$

Equation (5.12) reveals that, in the Krylov subspace case, the Hessenberg matrix H_m has a closer connection to the operator A than merely expressing the basis W_m in terms of V_{m+1} as in equation (4.3): here it is also the *orthogonal section* of A onto $\mathcal{K}_m$, that is, it represents the linear map $P_{\mathcal{K}_m} A|_{\mathcal{K}_m} : \mathcal{K}_m \to \mathcal{K}_m$ with respect to the basis V_m. To compute the coordinate vector $\boldsymbol{y}_m^{\mathrm{MR}}$ of the MR approximation $\boldsymbol{x}_m^{\mathrm{MR}} = \boldsymbol{x}_0 + V_m \boldsymbol{y}_m^{\mathrm{MR}}$, we note that, in view of (5.11), the corresponding residual has the form $\boldsymbol{r}_m^{\mathrm{MR}} = \boldsymbol{r}_0 - V_{m+1}\tilde{H}_m \boldsymbol{y}_m^{\mathrm{MR}} = V_{m+1}(\beta \boldsymbol{u}_1 - \tilde{H}_m \boldsymbol{y}_m^{\mathrm{MR}})$, and hence the minimum residual condition again determines $\boldsymbol{y}_m^{\mathrm{MR}}$ as the solution of the least-squares problem (4.7). Just as in Section 4.2, the GMRES algorithm uses a QR factorization of $\tilde{H}_m$ constructed from Givens rotations to solve this least-squares problem and thus, by Theorem 4.5, the rotation angles of these Givens rotations coincide with the angles (5.4) between the subspaces $\mathcal{K}_m(A, \boldsymbol{r}_0)$ and $A\mathcal{K}_m(A, \boldsymbol{r}_0)$.

The FOM implementation of the OR approach, which is also based on the Arnoldi process (*cf.* (5.11)), computes the coordinate vector $\boldsymbol{y}_m^{\mathrm{OR}} \in \mathbb{C}^m$ of the OR approximation $\boldsymbol{x}_m^{\mathrm{OR}} = \boldsymbol{x}_0 + V_m \boldsymbol{y}_m^{\mathrm{OR}}$ just as in Lemma 4.1 as the solution of the linear system (4.8), which requires H_m that be nonsingular. We recall from Remark 4.2 that this condition is consistent with our previous result, namely that $\measuredangle(\mathcal{K}_m, A\mathcal{K}_m) \neq \pi/2$.

The GMRES and FOM algorithms and the variants mentioned above implement the MR and OR approach for solving (1.1) in the case of general injective A. The method of choice for constructing an orthonormal basis of $\mathcal{V}_m = \mathcal{K}_m(A, \boldsymbol{r}_0)$ is the Arnoldi process, of which there exist several modifications with varying degrees of stability in the presence of round-off error (see, *e.g.*, the discussions in Rozložník, Strakoš and Tůma (1996) and Greenbaum, Rozložník and Strakoš (1997)). Whenever A is self-adjoint, the Arnoldi process simplifies to the Hermitian Lanczos process (Lanczos 1950), with the result that the Hessenberg matrix in the fundamental relation (5.11) is tridiagonal, with all the computational benefits mentioned at the beginning of Section 4.3. In particular, the short recurrences for the basis vectors allow the approximations and residuals to be inexpensively obtained by clever update formulas. Well-known algorithms that follow this approach to implement the MR and OR approximations in the self-adjoint and positive definite case are the CR/CG algorithms of Hestenes and Stiefel (1952), and an MR/OR pair of algorithms for the self-adjoint but possibly indefinite case is MINRES/CG due to Paige and Saunders (1975).

5.3. Using a non-orthogonal basis

In this section we continue our discussion of Krylov subspace MR and OR algorithms for the iterative solution of (1.1) with MR/OR pairs such as QMR/BCG and TFQMR/CGS, which work with a non-orthogonal basis of

the Krylov space. These represent examples of the MR/OR approximations discussed in Section 4.3 for solving equations using Krylov spaces.

To this end, let $\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_L \in \mathcal{H}$ be *any* set of ascending basis vectors, *i.e.*, linearly independent vectors such that $\{\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m\}$ forms a basis of $\mathcal{V}_m = \mathcal{K}_m(A, \boldsymbol{r}_0)$ for $m = 1, \ldots, L$ (in particular, $\boldsymbol{r}_0 = \beta \boldsymbol{v}_1$ for some $0 \neq \beta \in \mathbb{C}$). Such a basis leads naturally to a (quasi-)minimal residual as well as to a (quasi-)orthogonal residual method. Since, for every $1 \leq m \leq L$, $A\boldsymbol{v}_m \in \operatorname{span}\{\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_{m+1}\}$, where we set $\boldsymbol{v}_{L+1} = \boldsymbol{0}$, there exists an upper Hessenberg matrix $\tilde{H}_m \in \mathbb{C}^{(m+1)\times m}$ such that (*cf.* (4.3) and (5.11))

$$AV_m = V_m H_m + [\boldsymbol{0}, \ldots, \boldsymbol{0}, \eta_{m+1,m}\boldsymbol{v}_{m+1}] = V_{m+1}\tilde{H}_m. \tag{5.13}$$

As in (5.12), the mth column of $\tilde{H}_m$ contains the coefficients of $A\boldsymbol{v}_m \in \mathcal{K}_{m+1}(A, \boldsymbol{r}_0)$ with respect to the basis vectors $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}$. We are thus in the situation of Section 4.3 with $\mathcal{V}_m = \mathcal{K}_m(A, \boldsymbol{r}_0)$ and $\mathcal{W}_m = A\mathcal{K}_m(A, \boldsymbol{r}_0)$. Defining the auxiliary inner products $(\cdot,\cdot)_V$ on $\mathcal{V}_L$ and $(\cdot,\cdot)_{\boldsymbol{v}}$ on the coordinate space $\mathbb{C}^L$ as in (4.22) and (4.21), respectively, we obtain the QMR approximation

$$\boldsymbol{x}_m^{\mathrm{QMR}} := \boldsymbol{x}_0 + V_m \boldsymbol{y}_m^{\mathrm{QMR}} = \boldsymbol{x}_0 + \boldsymbol{c}_m^{\mathrm{QMR}}$$

of the solution $A^{-1}\boldsymbol{b}$ by requiring that $A\boldsymbol{c}_m^{\mathrm{QMR}}$ be the MR approximation to $\boldsymbol{r}_0$ with respect to the inner product $(\cdot,\cdot)_V$. Just as in Section 4.3, the coefficient vector $\boldsymbol{y}_m^{\mathrm{QMR}} \in \mathbb{C}^m$ is characterized as the unique solution of the least-squares problem (4.7). Analogously, the associated QOR approximation

$$\boldsymbol{x}_m^{\mathrm{QOR}} := \boldsymbol{x}_0 + V_m \boldsymbol{y}_m^{\mathrm{QOR}} = \boldsymbol{x}_0 + \boldsymbol{c}_m^{\mathrm{QOR}}$$

is obtained if $A\boldsymbol{c}_m^{\mathrm{OR}}$ is the OR approximation of $\boldsymbol{r}_0$ with respect to the inner product $(\cdot,\cdot)_V$, that is, if the coordinate vector $\boldsymbol{y}_m^{\mathrm{QOR}} \in \mathbb{C}^m$ satisfies the linear system of equations (4.25).

As stated in Section 4, the residuals of the QMR and QOR iterates are the errors of the MR and OR approximations of $\boldsymbol{r}_0$ with respect to the inner product $(\cdot,\cdot)_V$, and therefore the results of Theorem 3.4 on the residual norms hold for the QMR and QOR residuals $\boldsymbol{r}_m^{\mathrm{QMR}} = \boldsymbol{b} - A\boldsymbol{x}_m^{\mathrm{QMR}}$ and $\boldsymbol{r}_m^{\mathrm{QOR}} = \boldsymbol{b} - A\boldsymbol{x}_m^{\mathrm{QOR}}$, albeit with respect to the norm $\|\cdot\|_V$. The same applies to the statements of Theorem 3.5 and Corollary 3.6 for the QMR and QOR approximations $\boldsymbol{w}_m^{\mathrm{QMR}} = A\boldsymbol{c}_m^{\mathrm{QMR}}$ and $\boldsymbol{w}_m^{\mathrm{QOR}} = A\boldsymbol{c}_m^{\mathrm{QOR}}$, where the angles are understood with respect to the inner product $(\cdot,\cdot)_V$. Finally, the bounds in Theorem 4.8 relating the two different norms as well as the assertions of Propositions 4.9, 4.10 and 4.11 all hold for the QMR and QOR residuals, respectively.

The motivation for using non-orthogonal bases in Krylov subspace MR and OR methods comes from the potential savings in storage and computation when using algorithms for generating a basis of $\mathcal{K}_m(A, \boldsymbol{r}_0)$ which lead

to a Hessenberg matrix in relation (5.13) with only a small number of non-zero bands. A tridiagonal Hessenberg matrix can be achieved using the non-Hermitian Lanczos process. The non-Hermitian variant of the Lanczos process is generally less expensive than the Arnoldi process, requiring in addition the generation of a basis of a Krylov space with respect to the adjoint A^* and thus storage for several additional vectors and, which can be expensive, multiplication by A^* at each step. The result are two bi-orthogonal, in general non-orthogonal, bases. The non-Hermitian Lanczos process may break down before the Krylov space becomes stationary, and in finite arithmetic this leads to numerical instabilities in the case of near-breakdowns. This problem is addressed by so-called look-ahead techniques for the non-Hermitian Lanczos process (*cf.* Freund, Gutknecht and Nachtigal (1993), Gutknecht (1997) and the references therein), which result in a pair of block-biorthogonal bases and a Hessenberg matrix which is as close to tridiagonal form as possible while maintaining stability.

Remark 5.1. We have mentioned that Krylov subspace QMR/QOR methods have the advantage of being able to work with an arbitrary basis of the Krylov space, in particular also with a non-orthogonal basis. As the bounds (4.24) show, how close the QMR iterates come to minimizing the residual in the original norm depends on the Euclidean condition number of the Gram matrices M_m, that is, on the largest and smallest singular value of $V_m = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m]$ (interpreted as an operator from $\mathbb{C}^m$ to $\mathcal{K}_m(A, \boldsymbol{r}_0)$). The largest singular value of V_m is bounded by $\sqrt{m+1}$ if the basis vectors are normalized with respect to the original norm. When the look-ahead Lanczos algorithm is used to generate the basis, bounds on the smallest singular value may be obtained depending on the look-ahead strategy being followed (Freund *et al.* 1993).

Examples: QMR/BCG and TFQMR/CGS

We now consider two specific examples of Krylov subspace QMR/QOR algorithms, the QMR method of Freund and Nachtigal (1991) and the BCG method due to Lanczos (1952) as well as the TFQMR and CGS methods due to Freund (1993) and Sonneveld (1989), respectively. As another QMR/QOR pair, we mention the QMRCGSTAB method of Chan, Gallopoulos, Simoncini, Szeto and Tong (1994) and BICGSTAB developed by van der Vorst (1992) and Gutknecht (1993*b*).

The QMR algorithm of Freund and Nachtigal proceeds exactly as described above, with the basis of the Krylov space generated by the look-ahead Lanczos algorithm. The QOR counterpart of Freund and Nachtigal's QMR is the BCG algorithm, the iterates of which are characterized by

$$\boldsymbol{x}_m^{\mathrm{BCG}} \in \boldsymbol{x}_0 + \mathcal{K}_m(A, \boldsymbol{r}_0), \qquad \boldsymbol{r}_m^{\mathrm{BCG}} \perp \mathcal{K}_m(A^*, \tilde{\boldsymbol{r}}_0).$$

The algorithm proceeds by generating a basis of the Krylov space $\mathcal{K}_m(A^*, \tilde{\boldsymbol{r}}_0)$, where $\tilde{\boldsymbol{r}}_0$ is an arbitrary starting vector, simultaneously with a basis V_m of $\mathcal{K}_m(A, \boldsymbol{r}_0)$ in such a way that these two bases are biorthogonal. If $\boldsymbol{y} \in \mathbb{C}^m$ denotes the coefficient vector of the BCG approximation with respect to V_m, then the biorthogonality requirement

$$\boldsymbol{r}_m^{\mathrm{BCG}} = V_{m+1}(\beta \boldsymbol{u}_1 - \tilde{H}_m \boldsymbol{y}) \perp \mathcal{K}_m(A^*, \tilde{\boldsymbol{r}}_0),$$

implies $\boldsymbol{r}_m^{\mathrm{BCG}} \perp_V \mathcal{V}_m$, which is equivalent to $H_m \boldsymbol{y} = \beta \boldsymbol{u}_1$. The last equality identifies $\boldsymbol{x}_m^{\mathrm{BCG}}$ as the mth QOR iterate.

To treat the TFQMR/CGS pair, recall that the residual of any Krylov subspace approximation can be expressed as $\boldsymbol{r}_m = p_m(A)\boldsymbol{r}_0$ in terms of a polynomial p_m of degree m satisfying $p_m(0) = 1$. Sonneveld (1989) defined the CGS iterate $\boldsymbol{x}_m^{\mathrm{CGS}} \in \boldsymbol{x}_0 + \mathcal{K}_{2m}(A, \boldsymbol{r}_0)$ such that

$$\boldsymbol{r}_m^{\mathrm{CGS}} = [p_m(A)]^2 \boldsymbol{r}_0, \quad \text{where} \quad \boldsymbol{r}_m^{\mathrm{BCG}} = p_m(A)\boldsymbol{r}_0.$$

It is shown by Freund (1993) that $\boldsymbol{x}_m^{\mathrm{CGS}} = \boldsymbol{x}_0 + Y_{2m}\boldsymbol{z}_{2m}$ for a coefficient vector $\boldsymbol{z}_{2m} \in \mathbb{C}^{2m}$, where $\mathcal{K}_{2m}(A, \boldsymbol{r}_0) = \operatorname{span}\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_{2m}\}$. Moreover, there exists a sequence $\{\boldsymbol{w}_n\}$ such that $\boldsymbol{r}_0 = \beta \boldsymbol{w}_1$ and

$$AY_n = W_{n+1}\tilde{H}_n, \qquad n = 1, \ldots, 2L.$$

In terms of this sequence, we find

$$\boldsymbol{r}_m^{\mathrm{CGS}} = W_{2m+1}\big(\beta \boldsymbol{u}_1 - \tilde{H}_{2m}\boldsymbol{z}_{2m}\big),$$

where $H_{2m}\boldsymbol{z}_{2m} = \beta \boldsymbol{u}_1$, that is,

$$\boldsymbol{r}_m^{\mathrm{CGS}} \perp_W \operatorname{span}\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_{2m}\} = \mathcal{K}_{2m}(A, \boldsymbol{r}_0),$$

which identifies CGS as an OR method. The corresponding MR method is Freund's transpose-free QMR method TFQMR (*cf.* (Freund 1993, Freund 1994)), the iterates of which are defined as

$$\boldsymbol{x}_n^{\mathrm{TFQMR}} = \boldsymbol{x}_0 + Y_n \boldsymbol{z}_n, \quad n = 1, \ldots, 2L,$$

where the coefficient vector $\boldsymbol{z}_n \in \mathbb{C}^n$ solves the least-squares problem

$$\|\beta \boldsymbol{u}_1 - \tilde{H}_n \boldsymbol{z}_n\|_2 \to \min_{\boldsymbol{z} \in \mathbb{C}^n}.$$

In other words,

$$\|\boldsymbol{r}_n^{\mathrm{TFQMR}}\|_W = \min_{\boldsymbol{x} \in \boldsymbol{x}_0 + \mathcal{K}_n(A, \boldsymbol{r}_0)} \|\boldsymbol{b} - A\boldsymbol{x}\|_W.$$

Comparison of residuals

The availability of a sequence of vectors $\{\tilde{\boldsymbol{v}}_j\}_{j \geq 1}$ which is biorthogonal to the Krylov basis $\{\boldsymbol{v}_j\}$ permits a convenient representation of the QOR residual via (4.11). If

$$(\boldsymbol{v}_j, \tilde{\boldsymbol{v}}_k) = \delta_{jk} d_j, \qquad j, k = 1, \ldots, L,$$

and if both sequences are normalized to one, then, since the MR-residual at step $m-1$ lies in $\mathcal{W}_{m-1} \subset \mathcal{V}_m$, we have $\boldsymbol{r}_{m-1}^{\mathrm{MR}} = \sum_{j=1}^{m} (\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \tilde{\boldsymbol{v}}_j/d_j)\boldsymbol{v}_j$. Inserting $\boldsymbol{r} - \boldsymbol{w} = \boldsymbol{r}_{m-1}^{\mathrm{MR}}$ in (4.11) then yields

$$\boldsymbol{r}_m^{\mathrm{QOR}} = (\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \hat{\boldsymbol{w}}_{m+1})_V \, \boldsymbol{v}_{m+1} = \boldsymbol{v}_{m+1} \sum_{j=1}^{m} \frac{\overline{g}_j}{\overline{d}_j} (\boldsymbol{r}_{m-1}^{\mathrm{MR}}, \tilde{\boldsymbol{v}}_j)\boldsymbol{v}_j,$$

which, after taking norms and applying the Cauchy–Schwarz inequality, becomes

$$\|\boldsymbol{r}_m^{\mathrm{QOR}}\| \leq \|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\| \sum_{j=1}^{m} \frac{|g_j|}{|d_j|}.$$

This bound is a slightly improved version of a bound by Hochbruck and Lubich (1998).

6. Residual and error bounds

The usual residual and error bounds for Krylov subspace MR methods follow directly from the defining equation (1.2a),

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = \min_{\boldsymbol{c} \in \mathcal{K}_m(A, \boldsymbol{r}_0)} \|\boldsymbol{b} - A(\boldsymbol{x}_0 + \boldsymbol{c})\| = \min_{\boldsymbol{c} \in \mathcal{K}_m(A, \boldsymbol{r}_0)} \|\boldsymbol{r}_0 - A\boldsymbol{c}\|,$$

and the close connection between Krylov subspaces and polynomials (see Section 5.1) which immediately leads to

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = \min_{q \in \mathcal{P}_{m-1}} \|\boldsymbol{r}_0 - Aq(A)\boldsymbol{r}_0\| = \min_{\substack{p \in \mathcal{P}_m \\ p(0)=1}} \|p(A)\boldsymbol{r}_0\|,$$

that is, to

$$\frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_0\|} \leq \min_{\substack{p \in \mathcal{P}_m \\ p(0)=1}} \|p(A)\|.$$

If A is normal, the right-hand side represents a standard polynomial approximation problem,

$$\min_{\substack{p \in \mathcal{P}_m \\ p(0)=1}} \|p(A)\| = \sup_{\substack{p \in \mathcal{P}_m \\ p(0)=1}} \max_{\lambda \in \Lambda(A)} |p(\lambda)| \leq \min_{\substack{p \in \mathcal{P}_m \\ p(0)=1}} \max_{\lambda \in \Omega} |p(\lambda)|, \tag{6.1}$$

where $\Omega \subset \mathbb{C}$ is an arbitrary compact set which contains $\Lambda(A)$, the spectrum of A (of course, a useful bound will only be obtained when $0 \notin \Omega$). Most bounds, for instance, the standard bound for the conjugate gradient method, are derived in this way.

If A is not normal, then it is no longer true that its spectrum determines the convergence behaviour of a Krylov MR method (see Section 6.3).

Subsequent investigations into whether larger sets in the complex plane associated with A such as its field of values (Eiermann 1993) or pseudospectrum (Trefethen 1992) can predict convergence behaviour have to date failed to produce an analogous theoretical tool in the non-normal case. We refer to Embree (1999) for a detailed discussion of these issues.

In this section we will concentrate on bounds for the residual and error norms of Krylov subspace methods which are obtained by specializing Theorem 3.4. A similar approach in this direction has been taken by Saad (2000). Our goal is to relate properties of the operator A to the decay of the numbers s_m.

6.1. Residual bounds

Estimates based on the angles between $\mathcal{K}_m := \mathcal{K}_m(A, \boldsymbol{r}_0)$ and $A\mathcal{K}_m$ naturally involve the field of values of A, which is defined by

$$W(A) := \left\{ \frac{(A\boldsymbol{v}, \boldsymbol{v})}{(\boldsymbol{v}, \boldsymbol{v})} : \mathbf{0} \neq \boldsymbol{v} \in \mathcal{H} \right\}.$$

Theorem 6.1. The residual with index m of a Krylov MR method satisfies

$$\frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_0\|} \leq \prod_{j=1}^{m} \sqrt{1 - \nu_j(A)\tilde{\nu}_j(A^{-1})}, \tag{6.2}$$

where the quantities $\nu_j(A)$ and $\tilde{\nu}_j(A^{-1})$ are defined as

$$\nu_j(A) := \inf\{|z| : z \in W(A|_{\mathcal{S}_j}\},$$
$$\tilde{\nu}_j(A^{-1}) := \inf\{|z| : z \in W(A^{-1}|_{A\mathcal{S}_j}\}$$

and $\mathcal{S}_j \subseteq \mathcal{H}$ denotes a subspace which contains $\operatorname{span}\{\boldsymbol{r}_{j-1}^{\mathrm{MR}}\} = \mathcal{K}_j \cap (A\mathcal{K}_{j-1})^{\perp}$.

Proof. From (3.15), the fact that $s_j = \sin \measuredangle(\boldsymbol{r}_{j-1}^{\mathrm{MR}}, A\mathcal{K}_j)$ as well as $\boldsymbol{r}_{j-1}^{\mathrm{MR}} \in \mathcal{K}_j \cap (A\mathcal{K}_{j-1})^{\perp}$, we conclude

$$\begin{aligned}
\frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_0\|} &= \prod_{j=1}^{m} s_j = \prod_{j=1}^{m} \sin \measuredangle(\boldsymbol{r}_{j-1}^{\mathrm{MR}}, A\mathcal{K}_j) \\
&= \prod_{j=1}^{m} \left(1 - \sup_{\boldsymbol{v} \in \mathcal{K}_j} \frac{|(\boldsymbol{r}_{j-1}^{\mathrm{MR}}, A\boldsymbol{v})|^2}{\|\boldsymbol{r}_{j-1}^{\mathrm{MR}}\|^2 \, \|A\boldsymbol{v}\|^2} \right)^{1/2} \\
&\leq \prod_{j=1}^{m} \left(1 - \frac{|(\boldsymbol{r}_{j-1}^{\mathrm{MR}}, A\boldsymbol{r}_{j-1}^{\mathrm{MR}})|^2}{\|\boldsymbol{r}_{j-1}^{\mathrm{MR}}\|^2 \, \|A\boldsymbol{r}_{j-1}^{\mathrm{MR}}\|^2} \right)^{1/2} \\
&= \prod_{j=1}^{m} \left(1 - \left| \frac{(A\boldsymbol{r}_{j-1}^{\mathrm{MR}}, \boldsymbol{r}_{j-1}^{\mathrm{MR}})}{(\boldsymbol{r}_{j-1}^{\mathrm{MR}}, \boldsymbol{r}_{j-1}^{\mathrm{MR}})} \right| \left| \frac{(\boldsymbol{r}_{j-1}^{\mathrm{MR}}, A\boldsymbol{r}_{j-1}^{\mathrm{MR}})}{(A\boldsymbol{r}_{j-1}^{\mathrm{MR}}, A\boldsymbol{r}_{j-1}^{\mathrm{MR}})} \right| \right)^{1/2}
\end{aligned}$$

$$= \prod_{j=1}^{m} \left(1 - \left| \frac{(A\boldsymbol{r}_{j-1}^{\mathrm{MR}}, \boldsymbol{r}_{j-1}^{\mathrm{MR}})}{(\boldsymbol{r}_{j-1}^{\mathrm{MR}}, \boldsymbol{r}_{j-1}^{\mathrm{MR}})} \right| \left| \frac{(A^{-1}A\boldsymbol{r}_{j-1}^{\mathrm{MR}}, A\boldsymbol{r}_{j-1}^{\mathrm{MR}})}{(A\boldsymbol{r}_{j-1}^{\mathrm{MR}}, A\boldsymbol{r}_{j-1}^{\mathrm{MR}})} \right| \right)^{1/2}$$

$$\leq \prod_{j=1}^{m} \left(1 - \inf_{\boldsymbol{s} \in \mathcal{S}_j} \left| \frac{(A\boldsymbol{s}, \boldsymbol{s})}{(\boldsymbol{s}, \boldsymbol{s})} \right| \inf_{\boldsymbol{t} \in A\mathcal{S}_j} \left| \frac{(A^{-1}\boldsymbol{t}, \boldsymbol{t})}{(\boldsymbol{t}, \boldsymbol{t})} \right| \right)^{1/2}$$

$$= \prod_{j=1}^{m} \left(1 - \nu_j(A)\tilde{\nu}_j(A^{-1}) \right)^{1/2}. \qquad \square$$

For the choice $\mathcal{S}_j = \mathcal{H}$, we obtain the following simpler bound.

Corollary 6.2. The MR residual with index m satisfies

$$\frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_0\|} \leq \left(1 - \nu(A)\nu(A^{-1}) \right)^{m/2}, \tag{6.3}$$

where $\nu(A) := \inf\{|z| : z \in W(A)\}$.

Of course, the bound of Corollary 6.2 only yields a reduction provided $0 \notin W(A)$, which also implies $0 \notin W(A^{-1})$; see Horn and Johnson (1991, p. 66).

If A is a positive real matrix, that is, if its Hermitian part $H := (A+A^*)/2$ is positive definite, then $\nu(A) = \lambda_{\min}(H) > 0$ and

$$\nu(A^{-1}) = \min_{\boldsymbol{v} \in \mathcal{H}} \frac{(A^{-1}\boldsymbol{v}, \boldsymbol{v})}{(\boldsymbol{v}, \boldsymbol{v})} = \min_{\boldsymbol{w} \in \mathcal{H}} \frac{(\boldsymbol{w}, A\boldsymbol{w})}{(\boldsymbol{w}, \boldsymbol{w})} \frac{(\boldsymbol{w}, \boldsymbol{w})}{(A\boldsymbol{w}, A\boldsymbol{w})} \geq \frac{\lambda_{\min}(H)}{\|A\|^2},$$

in view of which Corollary 6.2 yields a bound first given by Elman (1982):

$$\frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_0\|} \leq \left(1 - \frac{\lambda_{\min}(H)^2}{\lambda_{\max}(A^T A)} \right)^{m/2} \tag{6.4}$$

(for a collection of similar bounds, see Joubert (1994)). Since (see the proof of Theorem 6.1)

$$\frac{\|\boldsymbol{r}_m^{\mathrm{MR}}\|}{\|\boldsymbol{r}_{m-1}^{\mathrm{MR}}\|} = s_m \leq 1 - \nu(A)\nu(A^{-1}) < 1,$$

the residual norms of a Krylov MR method decrease strictly monotonically if A is positive real or, slightly more generally, if $W(A)$ is contained in any half-plane $\{z : \mathrm{Re}\,(e^{i\alpha}z) > 0\}$ with $\alpha \in \mathbb{R}$. Note that, in view of Corollary 3.2, this implies that Galerkin breakdowns can be excluded for OR methods applied to such systems.

Remark 6.3. If, in the derivation of the residual bound (6.2), one makes the cruder estimate

$$\frac{\|\boldsymbol{r}_j^{\mathrm{MR}}\|^2}{\|\boldsymbol{r}_{j-1}^{\mathrm{MR}}\|^2} \leq 1 - \frac{|(\boldsymbol{r}_{j-1}^{\mathrm{MR}}, A\boldsymbol{r}_{j-1}^{\mathrm{MR}})|^2}{\|\boldsymbol{r}_{j-1}^{\mathrm{MR}}\|^2 \, \|A\boldsymbol{r}_{j-1}^{\mathrm{MR}}\|^2} \leq 1 - \inf_{\boldsymbol{v} \in \mathcal{H}} \frac{|(\boldsymbol{v}, A\boldsymbol{v})|^2}{\|\boldsymbol{v}\|^2 \, \|A\boldsymbol{v}\|^2} =: \sin^2(\gamma(A)),$$

where $\gamma(A)$ is the largest angle between a nonzero vector $\boldsymbol{v} \in \mathcal{H}$ and its image $A\boldsymbol{v}$, one thus obtains the bound $\sin^m \gamma(A)$ on the residual reduction after m steps. The angle $\gamma(A)$ was introduced by Wielandt (1996) (see also Gustafson and Rao (1996)).

6.2. Error bounds

When solving a linear system (1.1) approximately using successive iterates $\boldsymbol{x}_m$, the residual $\boldsymbol{r}_m = \boldsymbol{b} - A\boldsymbol{x}_m$ may be the only computable indication of the progress of the solution process. The quantity of primary interest, however, is the error $\boldsymbol{e}_m = \boldsymbol{x} - \boldsymbol{x}_m = A^{-1}\boldsymbol{r}_m$.

For Krylov subspace methods, we have $\boldsymbol{x}_m \in \boldsymbol{x}_0 + \mathcal{K}_m$, so that $\boldsymbol{e}_m = \boldsymbol{e}_0 - \boldsymbol{v}$ for some $\boldsymbol{v} \in \mathcal{K}_m$. Of course, the best one could do is to select this $\boldsymbol{v} \in \mathcal{K}_m$ as the best approximation to $\boldsymbol{e}_0$ from $\mathcal{K}_m(A, \boldsymbol{r}_0) = A\mathcal{K}_m(A, \boldsymbol{e}_0)$. This would correspond to computing the MR approximation of $\boldsymbol{e}_0$ with respect to the sequence of spaces $\mathcal{W}_m = A\mathcal{K}_m(A, \boldsymbol{e}_0)$, a process which would require knowledge of the initial error and hence the solution $\boldsymbol{x}$. The relation between residuals and errors, however, allows us to bound the error of the MR approximation with respect to this best possible approximation.

Lemma 6.4. The error $\boldsymbol{e}_m^{\mathrm{MR}}$ of the MR approximation satisfies

$$\|\boldsymbol{e}_m^{\mathrm{MR}}\| \le \kappa(A) \inf_{\boldsymbol{v} \in \mathcal{K}_m} \|\boldsymbol{e}_0 - \boldsymbol{v}\|, \tag{6.5}$$

where $\kappa(A) = \|A\|\,\|A^{-1}\|$ denotes the condition number of A.

Proof. We have

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| = \min_{\boldsymbol{w} \in A\mathcal{K}_m} \|\boldsymbol{r}_0 - \boldsymbol{w}\| = \min_{\boldsymbol{v} \in \mathcal{K}_m} \|A(\boldsymbol{e}_0 - \boldsymbol{v})\| \le \|A\| \min_{\boldsymbol{v} \in \mathcal{K}_m} \|\boldsymbol{e}_0 - \boldsymbol{v}\|,$$

and thus the assertion follows from $\|\boldsymbol{e}_m^{\mathrm{MR}}\| = \|A^{-1}\boldsymbol{r}_m^{\mathrm{MR}}\| \le \|A^{-1}\|\,\|\boldsymbol{r}_m^{\mathrm{MR}}\|$. □

Thus, the error of the MR approximation is within the condition number of A of the error of the best approximation to $\boldsymbol{e}_0$ from the Krylov space. In view of the relation (3.16), this translates to the following bound for the OR error:

$$\|\boldsymbol{e}_m^{\mathrm{OR}}\| \le \frac{\kappa(A)}{c_m} \inf_{\boldsymbol{v} \in \mathcal{K}_m} \|\boldsymbol{e}_0 - \boldsymbol{v}\|. \tag{6.6}$$

However, a stronger bound can be obtained if the field of values of A is bounded away from the origin.

Theorem 6.5. If $\nu(A) = \inf\{|z| : z \in W(A)\} > 0$, then the Krylov OR error satisfies

$$\frac{\|\boldsymbol{e}_m^{\mathrm{OR}}\|}{\|\boldsymbol{e}_0\|} \le \frac{\|A\|}{\nu(A)} \inf_{\boldsymbol{v} \in \mathcal{K}_m} \|\boldsymbol{e}_0 - \boldsymbol{v}\|.$$

Proof. From the characterization of the OR approximation we have $\boldsymbol{e}_m^{\mathrm{OR}} = \boldsymbol{e}_0 - \boldsymbol{v}$ for some $\boldsymbol{v} \in \mathcal{K}_m(A, \boldsymbol{r}_0)$ subject to

$$\boldsymbol{r}_m^{\mathrm{OR}} = A\boldsymbol{e}^{\mathrm{OR}} \perp \mathcal{K}_m(A, \boldsymbol{r}_0) \quad \Leftrightarrow \quad \boldsymbol{e}_m^{\mathrm{OR}} \perp A^*\mathcal{K}_m(A, \boldsymbol{r}_0).$$

This means that the OR error is obtained as the error of an OR approximation of $\boldsymbol{e}_0$ from the space $\mathcal{K}_m(A, \boldsymbol{r}_0)$ orthogonal to $A^*\mathcal{K}_m(A, \boldsymbol{r}_0)$. Thus, $\boldsymbol{e}_m^{\mathrm{OR}} = (I - P_{\mathcal{K}_m}^{A^*\mathcal{K}_m})\boldsymbol{e}_0$ and Theorem 2.9 implies

$$\frac{\|\boldsymbol{e}_m^{\mathrm{OR}}\|}{\|\boldsymbol{e}_0\|} \le \|I - P_{\mathcal{K}_m}^{A^*\mathcal{K}_m}\| = \frac{1}{\cos \measuredangle(\mathcal{K}_m, A^*\mathcal{K}_m)}.$$

We bound the cosine of the largest canonical angle between $\mathcal{K}_m$ and $A^*\mathcal{K}_m$ by

$$\begin{aligned}
\cos^2 \measuredangle(\mathcal{K}_m, A^*\mathcal{K}_m) &= \sup_{\boldsymbol{u}\in\mathcal{K}_m} \sup_{\boldsymbol{v}\in\mathcal{K}_m} \frac{|(\boldsymbol{u}, A^*\boldsymbol{v})|^2}{\|\boldsymbol{u}\|^2 \, \|A^*\boldsymbol{v}\|^2} \\
&\ge \sup_{\boldsymbol{v}\in\mathcal{K}_m} \frac{|(\boldsymbol{v}, A^*\boldsymbol{v})|^2}{\|\boldsymbol{v}\|^2 \, \|A^*\boldsymbol{v}\|^2} = \sup_{\boldsymbol{v}\in\mathcal{K}_m} \frac{(A\boldsymbol{v}, \boldsymbol{v})}{(\boldsymbol{v}, \boldsymbol{v})} \frac{(A^*\boldsymbol{v}, \boldsymbol{v})}{(A^*\boldsymbol{v}, A^*\boldsymbol{v})} \\
&\ge \inf_{\boldsymbol{v}\in\mathcal{K}_m} \left| \frac{(A\boldsymbol{v}, \boldsymbol{v})}{(\boldsymbol{v}, \boldsymbol{v})} \right| \inf_{\boldsymbol{v}\in\mathcal{K}_m} \left| \frac{(A^*\boldsymbol{v}, \boldsymbol{v})}{(A^*\boldsymbol{v}, A^*\boldsymbol{v})} \right| \ge \nu(A)\nu\big((A^*)^{-1}\big) \\
&= \nu(A)\nu(A^{-1}) \ge \frac{\nu(A)^2}{\|A\|^2},
\end{aligned}$$

where the last inequality has already been used to prove (6.4). □

If the Hermitian part $H := (A + A^*)/2$ of A is positive definite, that is, if A is positive real, then $(H\cdot, \cdot)$ is an inner product and thus defines a norm $\|\cdot\|_H$ on $\mathcal{H}$. The next theorem, which is due to Starke (1994), shows that the OR error measured in this norm is optimal up to a factor which depends on the skew-Hermitian part $S := (A - A^*)/2$ of A.

Theorem 6.6. If A is positive real with Hermitian and skew-Hermitian parts H and S, then the Krylov OR error satisfies

$$\|\boldsymbol{e}_m^{\mathrm{OR}}\|_H \le \big(1 + \rho(H^{-1}S)\big) \inf_{\boldsymbol{v}\in\mathcal{K}_m} \|\boldsymbol{e}_0 - \boldsymbol{v}\|_H,$$

where $\rho(H^{-1}S)$ denotes the spectral radius of $H^{-1}S$.

Proof. Since $\boldsymbol{r}_m^{\mathrm{OR}} = A\boldsymbol{e}_m^{\mathrm{OR}} \perp \mathcal{K}_m$, noting that $(H\boldsymbol{v}, \boldsymbol{v}) = \mathrm{Re}\,(A\boldsymbol{v}, \boldsymbol{v})$, $(S\boldsymbol{v}, \boldsymbol{v}) = i\mathrm{Im}\,(A\boldsymbol{v}, \boldsymbol{v})$ and $\boldsymbol{e}_m^{\mathrm{OR}} - \boldsymbol{e}_0 \in \mathcal{K}_m$, we have

$$\begin{aligned}
\|\boldsymbol{e}_m^{\mathrm{OR}}\|_H^2 &= (H\boldsymbol{e}_m^{\mathrm{OR}}, \boldsymbol{e}_m^{\mathrm{OR}}) \\
&\le |(A\boldsymbol{e}_m^{\mathrm{OR}}, \boldsymbol{e}_m^{\mathrm{OR}})| = |(A\boldsymbol{e}_m^{\mathrm{OR}}, \boldsymbol{e}_0)| = |(A\boldsymbol{e}_m^{\mathrm{OR}}, \boldsymbol{e}_0 - \boldsymbol{v})|
\end{aligned}$$

for arbitrary $\boldsymbol{v} \in \mathcal{K}_m$, and therefore

$$\|\boldsymbol{e}_m^{\mathrm{OR}}\|_H^2 \leq |(H\boldsymbol{e}_m^{\mathrm{OR}}, \boldsymbol{e}_0 - \boldsymbol{v}) + (S\boldsymbol{e}_m^{\mathrm{OR}}, \boldsymbol{e}_0 - \boldsymbol{v})|.$$

The first term is bounded by $\|\boldsymbol{e}_0 - \boldsymbol{v}\|_H \|\boldsymbol{e}_m^{\mathrm{OR}}\|_H$, and for the second term we obtain

$$\begin{aligned}
|(S\boldsymbol{e}_m^{\mathrm{OR}}, \boldsymbol{e}_0 - \boldsymbol{v})| &= |(H^{1/2}H^{-1/2}SH^{-1/2}H^{1/2}\boldsymbol{e}_m^{\mathrm{OR}}, \boldsymbol{e}_0 - \boldsymbol{v})| \\
&\leq \|H^{-1/2}SH^{-1/2}H^{1/2}\boldsymbol{e}_m^{\mathrm{OR}}\| \|\boldsymbol{e}_0 - \boldsymbol{v}\|_H \\
&\leq \|H^{-1/2}SH^{-1/2}\| \|\boldsymbol{e}_m^{\mathrm{OR}}\|_H \|\boldsymbol{e}_0 - \boldsymbol{v}\|_H \\
&= \rho(H^{-1}S) \|\boldsymbol{e}_m^{\mathrm{OR}}\|_H \|\boldsymbol{e}_0 - \boldsymbol{v}\|_H,
\end{aligned}$$

which, together with the bound for the first term, yields the assertion. □

An immediate consequence of Theorem 6.6 is that, for a Hermitian positive definite operator A, the OR method, which simplifies to the well-known conjugate gradient method in this case, yields the smallest possible error in the A-norm.

Remark 6.7. In view of the remark preceding Lemma 6.4 that the best approximation of the initial error $\boldsymbol{e}_0$ from the Krylov space $\mathcal{K}_m(A, \boldsymbol{r}_0) = A\mathcal{K}_m(A, \boldsymbol{e}_0)$ has the same structure as the best approximation of $\boldsymbol{r}_0$ from $A\mathcal{K}(A, \boldsymbol{r}_0)$ with $\boldsymbol{r}_0$ replaced by $\boldsymbol{e}_0$, the infimum in (6.5) and (6.6) may be bounded in an analogous manner to the MR residual in Theorem 6.1, Corollary 6.2 and Remark 6.3.

6.3. Quantities that determine the rate of convergence

We begin by recalling that, as a result of Theorem 3.4, the residual norm history of the MR and OR methods is completely determined by the sequence of angles between the spaces $\mathcal{V}_m$ and $\mathcal{W}_m$, which specialize to $\mathcal{K}_m(A, \boldsymbol{r}_0)$ and $A\mathcal{K}_m(A, \boldsymbol{r}_0)$, respectively, for Krylov subspace methods. In other words, convergence depends only on the sequence of these spaces and their relative position. Furthermore, Theorem 4.5 and the ensuing discussion revealed that the sines and cosines of these angles appear as the parameters of the Givens rotations in the recursive construction of the QR-factorizations (4.12) of the Hessenberg matrices $\tilde{H}_m$, $m = 1, \ldots, L$. As a consequence, we note that all the information regarding the progress of the solution algorithm is contained in the Q-factors. In particular, the residual norm history of the MR/OR approximations associated with the Arnoldi relations

$$AV_m = V_{m+1}\tilde{H}_m = V_{m+1}Q_m \begin{bmatrix} R_m \\ \mathbf{0} \end{bmatrix}, \qquad m = 1, \ldots, L,$$

is independent of the matrices R_m. For later reference, we state this observation as follows.

Lemma 6.8. Let L denote the termination index (5.7), and

$$AV_L = V_L H_L = V_L Q_{L-1}^H R_L = \hat{V}_L R_L$$

the Arnoldi decomposition (5.11). Further, let $\tilde{R}_L$ be any nonsingular upper triangular matrix and define $\tilde{A}$ by

$$\tilde{A}V_L = V_L Q_{L-1}^H \tilde{R}_L = \hat{V}_L \tilde{R}_L.$$

Then A and $\tilde{A}$ are *MR-equivalent* in the sense that the Krylov MR method produces identical residual vectors $\boldsymbol{r}_m^{\mathrm{MR}}$ for both systems $A\boldsymbol{x} = \boldsymbol{b}$ and $\tilde{A}\boldsymbol{x} = \tilde{\boldsymbol{b}}$ provided the starting vectors $\boldsymbol{x}_0$ and $\tilde{\boldsymbol{x}}_0$ are chosen such that $\boldsymbol{b} - A\boldsymbol{x}_0 = \tilde{\boldsymbol{b}} - \tilde{A}\tilde{\boldsymbol{x}}_0$.

Furthermore, Lemma 6.8 reveals that there is a particularly simple matrix $\tilde{A}$ which, for the same initial residual $\boldsymbol{r}_0$, displays the identical MR/OR residual norm history, namely the unitary matrix obtained by setting R_L (and thus all $\{R_j\}_{j=1}^L$) equal to the identity. If $\mathcal{V}_L$ is a proper subspace of $\mathcal{H}$, $\tilde{A}$ may be made unique by extending it to be the identity on the complementary space. This observation, that for each linear system of equations there exists a linear system of equations with a unitary matrix for which MR/OR display the identical convergence behaviour, was first pointed out by Greenbaum and Strakoš (1994).

Lemma 6.8 is the point of departure for an approach for computing convergence bounds for GMRES given in Liesen (2000). This is obtained by applying the standard convergence bound (6.1) to the MR-equivalent matrix Q_{L-1}, which yields

$$\|\boldsymbol{r}_m^{\mathrm{MR}}\| \leq \min_{\substack{p \in \mathcal{P}_m \\ p(0)=1}} \max_{\lambda \in \Lambda(Q_{L-1})} |p(\lambda)|.$$

(We note that Liesen used somewhat more complicated MR-equivalent systems.) Since such a bound involves quantities not available until step L, which generally far exceeds the feasible number of iteration steps, Liesen suggests approximating the quantities in the above bound by those available at iteration step $m \ll L$. It is, however, clear that this works only under additional assumptions since, in general, Q_m need not contain any information about the progress of the MR iteration beyond step m. It is not difficult to show that any given sequence of residual norms $\|\boldsymbol{r}_0\| \geq \|\boldsymbol{r}_1^{\mathrm{MR}}\| \geq \cdots \geq \|\boldsymbol{r}_m^{\mathrm{MR}}\|$ can be complemented in such a way that the iteration stagnates from step $m+1$ until step $L-1$, that is, $\|\boldsymbol{r}_m^{\mathrm{MR}}\| = \cdots = \|\boldsymbol{r}_{L-1}^{\mathrm{MR}}\|$.

As another consequence of Lemma 6.8, quantities such as the singular values of $\tilde{H}_m$, which coincide with those of R_m, can play no role in the rate of convergence.

Lemma 6.9. For any given linear system of equations (1.1), there is a linear system with coefficient matrix $\tilde{A}$ for which GMRES exhibits the identical convergence history, and for which $\tilde{A}$ has arbitrarily prescribed nonzero singular values.

Proof. Let L denote the termination index of A with respect to the given system as defined in (5.7). For any Krylov subspace method applied to this system, only the L singular values of $A|_{\mathcal{K}_L}$ are noticeable, hence A can be defined arbitrarily on $\mathcal{K}_L^{\perp}$. To prescribe the singular values of $A|_{\mathcal{K}_L}$, let $\tilde{R}_L$ denote an upper triangular $L \times L$ matrix possessing L arbitrary nonzero singular values. With $\hat{V}_L$ denoting the Paige–Saunders basis (4.17), the matrix $\tilde{A}$ by $\tilde{A}\hat{V}_L = \hat{V}_L\tilde{R}_L$ clearly possesses the same set of singular values and, by Proposition 6.8, $\tilde{A}$ is MR-equivalent to A. □

By the same technique, we can prescribe, for fixed m, the singular values of $\tilde{H}_m$ since, in view of (4.12), these coincide with those of R_m.

For the singular values of the square Hessenberg matrices H_m there is a slight complication. From (4.19) we recall that a QR-factorization of H_m is given by

$$H_m = Q_{m-1}^H \begin{bmatrix} R_{m-1} & \boldsymbol{r} \\ \mathbf{0} & \tau \end{bmatrix}.$$

The mth plane rotation is determined so that the vector $[\tau \ \eta_{m+1,m}]^\top$ is rotated to the vector $[r_{m,m} \ 0]^\top$, where $r_{m,m}$ is the entry in the (m,m)-position of R_m (*cf.* (4.15)). This implies that $\tau = c_m r_{m,m}$. Thus, if we prescribe R_m to be a diagonal matrix, then the singular values of H_m are given by $|r_{1,1}|, \ldots, |r_{m-1,m-1}|, c_m|r_{m,m}|$ and thus can be selected arbitrarily. The only exception occurs when $c_m = 0$, that is, H_m is singular and clearly only $m-1$ singular values can be chosen freely.

We remark that the same proof shows that, also in the case of an OR method, neither the singular values of A nor those of $\tilde{H}_m$ or H_m determine the convergence behaviour.

We conclude this subsection with a brief discussion of the role eigenvalues play for the convergence of MR methods. The bound (6.1) shows that the spectrum controls the convergence behaviour if A is normal. There are, however, examples of non-normal matrices which show that, in general, $\Lambda(A)$ may have no influence: Greenbaum, Strakoš and Ptak (1996) demonstrate that, for *any* nonincreasing finite sequence of positive real numbers $\rho_0 \geq \rho_1 \geq \cdots \geq \rho_{n-1}$ and *any* choice of (not necessarily distinct) nonzero complex numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$, one can construct a matrix $A \in \mathbb{C}^{n\times n}$ and an initial residual $\boldsymbol{r}_0$ with $\Lambda(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ and $\|\boldsymbol{r}_m^{\mathrm{MR}}\| = \rho_m$ $(m = 0, 1, \ldots, n-1)$. We illustrate this result by one of their striking examples. Any matrix

A in Frobenius form,

$$A = \begin{bmatrix} 0 & 0 & \cdots & 0 & -\alpha_0 \\ 1 & 0 & \cdots & 0 & -\alpha_1 \\ 0 & 1 & \cdots & 0 & -\alpha_2 \\ \vdots & & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -\alpha_{n-1} \end{bmatrix} \in \mathbb{C}^{n\times n},$$

has $\zeta^n + \alpha_{n-1}\zeta^{n-1} + \cdots + \alpha_1\zeta + \alpha_0$ as its characteristic polynomial, so its eigenvalues can be arbitrarily prescribed. If we choose $\boldsymbol{b}$ and $\boldsymbol{r}_0$ such that $\boldsymbol{r}_0 = \boldsymbol{u}_1$ is the first unit vector, then, for $m = 1, 2, \ldots, n-1$, the approximation space $A\mathcal{K}_m(A, \boldsymbol{r}_0)$ is the span of the unit vectors $\boldsymbol{u}_2, \boldsymbol{u}_3, \ldots, \boldsymbol{u}_m$. The best approximation to $\boldsymbol{r}_0$ from this space is obviously the null vector leading to $\|\boldsymbol{r}_0\| = \|\boldsymbol{r}_1^{\mathrm{MR}}\| = \cdots = \|\boldsymbol{r}_{n-1}^{\mathrm{MR}}\| = 1$ independently of the chosen spectrum. In general it is therefore impossible to predict the convergence behaviour of an MR method such as GMRES (and of any other Krylov subspace method) on the basis of the eigenvalue distribution of A alone. Although this fact has been emphasized in several recent papers, it is still a widespread but nonetheless incorrect belief that spectral properties of the coefficient matrix (*i.e.*, without any additional assumptions on its departure from normality) determine the speed of convergence of GMRES.

6.4. An application: compact operators

Many applications such as the solution of elliptic boundary value problems by the integral equation method require the solution of second-kind Fredholm equations, that is, operator equations (1.1) in which A has the form $A = \lambda I + K$ with $\lambda \neq 0$ and $K : \mathcal{H} \to \mathcal{H}$ is a compact operator. The development of fast multiplication algorithms (*cf.* Greengard and Rokhlin (1987), Hackbusch and Nowak (1989)) has made Krylov subspace methods attractive as solution algorithms for discretizations of these problems, since they require only applications of the (discrete) operator to vectors. Moreover, as shown by Moret (1997) for GMRES and by Winther (1980) for CG, Krylov subspace methods converge q-superlinearly for operator equations involving compact perturbations of (multiples of) the identity.

The reason for this is that, for these operators, the sines s_m of the canonical angles between the Krylov space $\mathcal{K}_m$ and $A\mathcal{K}_m$ converge to zero. To show this, we recall a basic result on compact operators and orthonormal systems.

Theorem 6.10. Let $K : \mathcal{H} \to \mathcal{H}$ be a compact linear operator and $\{\boldsymbol{v}_m\}_{m\geq 1} \subset \mathcal{H}$ be an orthonormal system. Then

$$\lim_{m\to\infty} (K\boldsymbol{v}_m, \boldsymbol{v}_{m+1}) = 0.$$

Proof. See, for example, Ringrose (1971). □

The next lemma, which is due to Moret (1997), gives a bound on the quantity $s_m = \sin \measuredangle(\mathcal{K}_m, A\mathcal{K}_m)$.

Lemma 6.11. Let $\{\boldsymbol{v}_j\}_{j\geq 1}$ be the Arnoldi basis defined in (5.11) of $\mathcal{K}_m$, where $A : \mathcal{H} \to \mathcal{H}$ possesses a bounded inverse. Then

$$s_m \leq \|A^{-1}\| \, (\boldsymbol{v}_{m+1}, A\boldsymbol{v}_m).$$

Proof. Let $\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m\}$ denote an ascending orthonormal basis of $A\mathcal{K}_m$. Since $A^{-1}\boldsymbol{w}_m \in \mathcal{K}_m$, we can write $(\boldsymbol{v}_{m+1}, \boldsymbol{w}_m) = (\boldsymbol{v}_{m+1}, AP_{\mathcal{K}_m}A^{-1}\boldsymbol{w}_m)$. Moreover, since $A\boldsymbol{v}_j \in \mathcal{K}_m \perp \boldsymbol{v}_{m+1}$ for $1 \leq j \leq m-1$, we have

$$\begin{aligned}
|(\boldsymbol{v}_{m+1}, AP_{\mathcal{K}_m}A^{-1}\boldsymbol{w}_m)| &= |(\boldsymbol{v}_{m+1}, \sum_{j=1}^{m}(A^{-1}\boldsymbol{w}_m, \boldsymbol{v}_j)A\boldsymbol{v}_j)| \\
&= |(\boldsymbol{v}_{m+1}, (A^{-1}\boldsymbol{w}_m, \boldsymbol{v}_m)A\boldsymbol{v}_m)| \\
&= |(A^{-1}\boldsymbol{w}_m, \boldsymbol{v}_m)(\boldsymbol{v}_{m+1}, A\boldsymbol{v}_m)| \\
&\leq \|A^{-1}\| \, (A\boldsymbol{v}_m, \boldsymbol{v}_{m+1}).
\end{aligned}$$

Note that the modulus in $|(A\boldsymbol{v}_m, \boldsymbol{v}_{m+1})|$ can be omitted since $(A\boldsymbol{v}_m, \boldsymbol{v}_{m+1}) = \|(I - P_{\mathcal{V}_m})A\boldsymbol{v}_m\| \geq 0$. The assertion now follows from Lemma 3.3. □

Corollary 6.12. Let $A = \lambda I + K$ with $\lambda \neq 0$ and $K : \mathcal{H} \to \mathcal{H}$ compact, let $\{\boldsymbol{v}_j\}_{j\geq 1}$ denote the Arnoldi basis of $\mathcal{K}_m$. Then the sines s_m of largest canonical angle between $\mathcal{K}_m$ and $A\mathcal{K}_m$ form a null sequence.

Proof. Lemma 6.11 and Theorem 6.10 yield

$$s_m \leq (\boldsymbol{v}_{m+1}, A\boldsymbol{v}_m) \, \|A^{-1}\| = (\boldsymbol{v}_{m+1}, K\boldsymbol{v}_m) \, \|A^{-1}\| \to 0,$$

since A^{-1} is bounded whenever $\lambda \neq 0$. □

In particular, since $s_m \to 0$ implies that $s_m < 1$ for m sufficiently large, this means that the OR approximation is always defined except for possibly a finite number of indices. Moreover, as s_m is bounded away from one, c_m is accordingly bounded away from zero, hence the relation (3.16) also implies the q-superlinear convergence of the OR approximation. We summarize this result in the following theorem.

Theorem 6.13. Given $K : \mathcal{H} \to \mathcal{H}$ compact, $0 \neq \lambda \in \mathbb{C}$ and $\boldsymbol{b} \in \mathcal{H}$, let $\boldsymbol{x}_0 \in \mathcal{H}$ be an initial guess at the solution of (1.1) with $A = \lambda I + K$. Then the OR approximation with respect to the space $\mathcal{K}_m$ exists for all sufficiently large m. Moreover, the sequence of MR and OR approximations converge q-superlinearly.

We remark that the rate of superlinear convergence may be quantified in terms of the rate of decay of the singular values of K (see Moret (1997)). We also note, in view of (4.24), that this result applies to all MR/OR pairs of Krylov subspace methods including QMR/BCG, given a bound on the conditioning of the basis of the Krylov space being used. For bases generated by the look-ahead Lanczos method such bounds are guaranteed, for instance, by the implementation given in Freund (1993).

7. Conclusions and final remarks

We have presented a unifying framework for describing and analysing Krylov subspace methods by first introducing the abstract MR and OR approximation methods on nested sequences of subspaces, applying these to solving equations and then specializing further to the Krylov subspace setting. All known relations between MR/OR-type Krylov methods were shown to hold in the abstract formulation. In particular, the angles appearing in the Givens QR factorization of the Hessenberg matrix used in many Krylov subspace algorithms were identified as angles between the Krylov spaces and their images under A. Moreover, depending on whether orthogonal or non-orthogonal bases are employed, both MR/OR and QMR/QOR methods can be described and analysed in the same manner. Furthermore, we have shown that essentially all nested approximation schemes – and therefore also essentially all Krylov subspace methods – can be interpreted as QMR/QOR methods. The description of the algorithms in terms of angles was subsequently used to derive some of the previously known error and residual bounds.

Another benefit of the analysis in this paper is that, at least conceptually, it separates the issue of generating bases from the method for computing the approximations. Indeed, other algorithms besides Lanczos or Arnoldi could be used to generate the bases required for the MR and OR methods, but this is seldom done for lack of promising alternatives: Le Calvez and Saad (1999) introduce a nonstandard inner product and develop a QMR-like algorithm not based on the Lanczos algorithm.

Besides the basis-dependent inner product of QMR/QOR approximations, it can also be advantageous to use other fixed inner products other than the Euclidean inner product on the coordinate space. For an example of a nonstandard inner product used in conjunction with GMRES see Starke (1997).

We have made no mention in this paper of preconditioning, which is indispensable for most problems of practical relevance; when preconditioning is accounted for, our results apply to the preconditioned system.

We believe that our approach provides a simple and intuitive way of describing Krylov subspace algorithms which simplifies many of the standard

proofs and brings out the connections among the many algorithms in the literature.

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