BLOCK KRYLOV SUBSPACE METHODS FOR FUNCTIONS OF MATRICES II: MODIFIED BLOCK FOM*

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Abstract. We analyze an expansion of the generalized block Krylov subspace framework of [Electron. Trans. Numer. Anal., 47 (2017), pp. 100-126]. This expansion allows the use of low-rank modifications of the matrix projected onto the block Krylov subspace and contains, as special cases, the block GMRES method and the new block Radau-Arnoldi method. Within this general setting, we present results that extend the interpolation property from the non-block case to a matrix polynomial interpolation property for the block case, and we relate the eigenvalues of the projected matrix to the latent roots of these matrix polynomials. Some convergence results for these modified block FOM methods for solving linear system are presented. We then show how *cospatial* residuals can be preserved in the case of families of shifted linear block systems. This result is used to derive computationally practical restarted algorithms for block Krylov approximations that compute the action of a matrix function on a set of several vectors simultaneously. We prove some convergence results and present numerical results showing that two modifications of FOM, the block harmonic and the block Radau-Arnoldi methods for matrix functions, can significantly improve the convergence behavior.

Key words. generalized block Krylov methods, block FOM, block GMRES, restarts, families of shifted linear systems, multiple right-hand sides, matrix polynomials, matrix functions

AMS subject classifications. 65F60, 65F50, 65F10, 65F30

1. Introduction and motivation.

Block Krylov subspace methods for solving s simultaneous linear systems

$$A\boldsymbol{X} = \boldsymbol{B}, \quad \text{where } A \in \mathbb{C}^{n\times n}, \quad \boldsymbol{B} = [\boldsymbol{b}_1|\cdots|\boldsymbol{b}_s] \in \mathbb{C}^{n\times s}$$

bear the potential to be faster than methods that treat individually the systems $A\boldsymbol{x}_i = \boldsymbol{b}_i$, $i = 1, \ldots, s$, for two reasons. One is that a block Krylov subspace contains more information than the individual subspaces, so that one can extract more accurate approximations for the same total investment of matrix-vector multiplications. Furthermore, the multiplication of A with a block vector $\boldsymbol{B}$ can be implemented more efficiently than s individual matrix-vector multiplications, requiring less memory access and, in a parallel environment, allowing for batch communication.

In this work, we present and analyze a general framework for block Krylov subspace methods. We build on the approach introduced in [22], which allows for the treatment of various variants of block Krylov subspaces via corresponding block inner products and the related block Arnoldi process to generate a block orthogonal basis. We extend the block FOM method considered in [22] to a general framework for extracting approximations from the block Krylov subspace. These approximations can all be expressed via a matrix polynomial, and we completely characterize the situations in which a block Krylov subspace approximation satisfies an important matrix polynomial exactness property, thus generalizing [21, Lemmas 1.3 and 1.4] for the

*This version dated 10/04/19.

Funding: This work was supported in part by the U.S. National Science Foundation under grant DMS-1418882, the U.S. Department of Energy under grant DE-SC 0016578, Deutsche Forschungsgemeinschaft through the collaborative research centre SFB-TRR55, and the Swiss National Science Foundation under grant 200020 178806.

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single right-hand side case. For the "classical" block inner product, our analysis includes the block FOM method [40], a special case of which is block CG [36], the block GMRES method, and the block Radau-Arnoldi method which arises from the corresponding method for the single right-hand side case for Hermitian matrices from [21]. For a different block inner product, our analysis also comprises the respective so-called *global* methods; see, e.g., [1, 6, 9, 28, 31, 34, 38, 50].

We then turn to methods for families of shifted linear systems with multiple right-hand sides, i.e.,

$$(A + tI)\boldsymbol{X}(t) = \boldsymbol{B}. \tag{1.1}$$

Such problems arise, e.g., in lattice quantum chromodynamics [18, 48], hydraulic tomography [3, 42], the PageRank problem [49], and in the evaluation of matrix functions when approximated via a rational function– for example, the matrix exponential for time-dependent differential equations [2, 5, 26, 30]. An important requirement in this context is that the block Krylov subspaces be independent of t and thus have to be built only once for all t. A prominent challenge is to preserve this fact when having to perform restarts, meaning that we must require that the column spans of the block residuals do not depend on the shift t. We present a complete analysis of how to obtain this kind of "shift invariance" and discuss to what extent known results on convergence in the presence of restarts for the non-block case ($s = 1$) carry over to $s > 1$.

The analysis and implementation of approximations to (1.1) are crucial in developing block Krylov methods for matrix functions, which is the last topic we address: the approximation of $f(A)\boldsymbol{B}$, where $f : D \subseteq \mathbb{C} \to \mathbb{C}$ is a function defined on the spectrum of A in the sense of [29]. When f can be expressed in integral form as $f(z) = \int_\Gamma \frac{g(t)}{z-t}\, \mathrm{d}t$, we use the results for shifted linear systems to derive a representation of the error which is mandatory to efficiently perform restarts. Our analysis allows for different block Krylov subspace extraction approaches corresponding to block FOM, block GMRES, block Radau-Arnoldi, etc. We consider in some detail the special case where f is a Stieltjes function, i.e., $f(z) = \int_0^\infty (z-t)^{-1}\, \mathrm{d}\mu(t)$.

The paper is organized as follows. In Section 2, we summarize the generalized block Krylov framework, consider how block iterates and residuals can be expressed using matrix polynomials, and develop the polynomial exactness result, which is important for the subsequent sections. We also prove a result on the latent roots of the residual matrix polynomial, generalizing results from [16, 44]. Section 3 summarizes how known and new block Krylov subspace methods fit into our general framework, with a particular emphasis on block GMRES and the new block Radau-Arnoldi method. In Section 4 we treat restarts for families of shifted linear systems and matrix functions. Illustrative numerical experiments are presented in Section 5 before we finish with our conclusions.

2. The block Krylov framework.

In this section we recall the concept of a general block inner product introduced in [22] and its relation to block Krylov subspaces and matrix polynomials. New results include the polynomial exactness property, Theorem 2.7, and a result on the latent roots of the matrix polynomial expressing the block residual, Theorem 2.9.

2.1. General block Krylov subspaces and the block Arnoldi process.

To clarify our notation, let I_m denote the $m \times m$ identity matrix. Then the kth canonical unit vector $\widehat{\boldsymbol{e}}_k^m \in \mathbb{C}^m$ is the kth column of I_m, and the kth canonical block unit vector is

$$\widehat{\boldsymbol{E}}_k^{ms\times s} := \widehat{\boldsymbol{e}}_k^m \otimes I_s = \underset{\uparrow k}{[0\cdots 0\ I_s\ 0\cdots 0]^T} \in \mathbb{C}^{ms\times s},$$

where $\otimes$ denotes the Kronecker product. We drop the superscripts for $\widehat{\boldsymbol{E}}_k^{ms\times s}$ when the dimensions are clear from context, and likewise for the identity, in which case we may drop the subscript.

Let $\mathbb{S}$ be a *-subalgebra of $\mathbb{C}^{s\times s}$ with identity; that is, with $S, T \in \mathbb{S}$, $\alpha \in \mathbb{C}$, we have $\alpha S + T, ST, S^* \in \mathbb{S}$, along with $I \in \mathbb{S}$. General block inner products as introduced in [22] take their values in $\mathbb{S}$.

Definition 2.1. *A mapping $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$ from $\mathbb{C}^{n\times s} \times \mathbb{C}^{n\times s}$ to $\mathbb{S}$ is called a* block inner product onto $\mathbb{S}$ *if it satisfies the following conditions for all $\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{Z} \in \mathbb{C}^{n\times s}$ and $C \in \mathbb{S}$:*

(i) $\mathbb{S}$*-linearity:* $\langle\!\langle \boldsymbol{X}+\boldsymbol{Y}, \boldsymbol{Z}C \rangle\!\rangle_{\mathbb{S}} = \langle\!\langle \boldsymbol{X}, \boldsymbol{Z} \rangle\!\rangle_{\mathbb{S}} C + \langle\!\langle \boldsymbol{Y}, \boldsymbol{Z} \rangle\!\rangle_{\mathbb{S}} C$*;*
(ii) symmetry: $\langle\!\langle \boldsymbol{X}, \boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}} = \langle\!\langle \boldsymbol{Y}, \boldsymbol{X} \rangle\!\rangle_{\mathbb{S}}^*$*;*
(iii) definiteness: $\langle\!\langle \boldsymbol{X}, \boldsymbol{X} \rangle\!\rangle_{\mathbb{S}}$ *is positive definite if $\boldsymbol{X}$ has full rank, and* $\langle\!\langle \boldsymbol{X}, \boldsymbol{X} \rangle\!\rangle_{\mathbb{S}} = 0$ *if and only if $\boldsymbol{X} = 0$.*

Note that since $\alpha I \in \mathbb{S}$ for all $\alpha \in \mathbb{C}$, (i) implies in particular that

$$\langle\!\langle \boldsymbol{X}, \alpha\boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}} = \alpha \langle\!\langle \boldsymbol{X}, \boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}}, \ \ \langle\!\langle \alpha\boldsymbol{X}, \boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}} = \overline{\alpha} \langle\!\langle \boldsymbol{X}, \boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}}.$$

Definition 2.2. *A mapping N which maps all $\boldsymbol{X} \in \mathbb{C}^{n\times s}$ with full rank on a matrix $N(\boldsymbol{X}) \in \mathbb{S}$ is called a* scaling quotient *if for all such $\boldsymbol{X}$, there exists $\boldsymbol{Y} \in \mathbb{C}^{n\times s}$ such that $\boldsymbol{X} = \boldsymbol{Y}N(\boldsymbol{X})$ and $\langle\!\langle \boldsymbol{Y}, \boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}} = I_s$.*

Let us mention that since $\langle\!\langle \boldsymbol{X}, \boldsymbol{X} \rangle\!\rangle_{\mathbb{S}} = N(\boldsymbol{X})^* N(\boldsymbol{X})$ is positive definite, and if $\boldsymbol{X}$ has full rank, then the scaling quotient $N(\boldsymbol{X})$ is nonsingular.

These definitions give rise to block-based notions of orthogonality and normalization.

Definition 2.3. *(i)* $\boldsymbol{X}, \boldsymbol{Y} \in \mathbb{C}^{n\times s}$ *are* block orthogonal*, if* $\langle\!\langle \boldsymbol{X}, \boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}} = 0_s$*.*
(ii) $\boldsymbol{X} \in \mathbb{C}^{n\times s}$ *is* block normalized *if* $N(\boldsymbol{X}) = I_s$*.*
(iii) $\{\boldsymbol{X}_j\}_{j=1}^m \subset \mathbb{C}^{n\times s}$ *is* block orthonormal *if* $\langle\!\langle \boldsymbol{X}_i, \boldsymbol{X}_j \rangle\!\rangle_{\mathbb{S}} = \delta_{ij} I_s$*.*

We say that a set of vectors $\{\boldsymbol{X}_j\}_{j=1}^m \subset \mathbb{C}^{n\times s}$ $\mathbb{S}$*-spans* a space $\mathscr{K} \subseteq \mathbb{C}^{n\times s}$ and write $\mathscr{K} = \operatorname{span}^{\mathbb{S}}\{\boldsymbol{X}_j\}_{j=1}^m$, if $\mathscr{K}$ is given as

$$\operatorname{span}^{\mathbb{S}}\{\boldsymbol{X}_j\}_{j=1}^m := \Big\{ \sum_{j=1}^m \boldsymbol{X}_j \Gamma_j : \Gamma_j \in \mathbb{S} \text{ for } j = 1, \ldots, m \Big\}.$$

The set $\{\boldsymbol{X}_j\}_{j=1}^m$ constitutes a block orthonormal basis for $\mathscr{K} = \operatorname{span}^{\mathbb{S}}\{\boldsymbol{X}_j\}_{j=1}^m$ if it is block orthonormal. Clearly, $\mathbb{S}$-spans are vector subspaces of $\mathbb{C}^{n\times s}$, and we define the *mth block Krylov subspace for A and $\boldsymbol{B}$ (with respect to $\mathbb{S}$)* as

$$\mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B}) := \operatorname{span}^{\mathbb{S}}\{\boldsymbol{B}, A\boldsymbol{B}, \ldots, A^{m-1}\boldsymbol{B}\}.$$

Table 2.1 summarizes combinations of $\mathbb{S}$, $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$, and N that lead to established block Krylov subspaces. Note that $\{\alpha I_s : \alpha \in \mathbb{C}\}$ and $\mathbb{C}^{s\times s}$ are the smallest and largest possible *-subalgebras with identity, respectively. It then holds, with obvious notation, that for any *-algebra $\mathbb{S}$ with identity

$$\mathbb{S}^{\mathrm{Gl}} \subseteq \mathbb{S},\ \mathbb{S}^{\mathrm{Li}} \subseteq \mathbb{S}^{\mathrm{Cl}} \text{ and } \mathscr{K}_m^{\mathrm{Gl}}(A, \boldsymbol{B}) \subseteq \mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B}),\ \mathscr{K}_m^{\mathrm{Li}}(A, \boldsymbol{B}) \subseteq \mathscr{K}_m^{\mathrm{Cl}}(A, \boldsymbol{B}), \quad (2.1)$$

	$\mathbb{S}$	$\langle\!\langle \boldsymbol{X}, \boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}}$	$N(\boldsymbol{X})$
classical (Cl)	$\mathbb{C}^{s \times s}$	$\boldsymbol{X}^* \boldsymbol{Y}$	R, where $\boldsymbol{X} = \boldsymbol{Q}R$, and $\boldsymbol{Q} \in \mathbb{C}^{n \times s}, \boldsymbol{Q}^*\boldsymbol{Q} = I_s$
global (Gl)	$\mathbb{C}I_s$	$\frac{1}{s}\,\mathrm{trace}\,(\boldsymbol{X}^*\boldsymbol{Y})I_s$	$\frac{1}{\sqrt{s}} \left\lVert \boldsymbol{X} \right\rVert_{\mathrm{F}} I_s$
loop-interchange (Li)	$I_s \otimes \mathbb{C}$	$\mathrm{diag}(\boldsymbol{X}^*\boldsymbol{Y})$	$\mathrm{diag}([\lVert \boldsymbol{x}_1 \rVert_2, \ldots, \lVert \boldsymbol{x}_s \rVert_2])$

Table 2.1: Choices of $\mathbb{S}$, $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$, and N in common block paradigms. Here the diag operator works in two ways: when the argument is a matrix, it returns a diagonal matrix taken from the diagonal of the input; when the argument is a vector, it builds a diagonal matrix whose diagonal entries are those of the vector.

Algorithm 2.1 Block Arnoldi process

If A is block self-adjoint, the process simplifies to block Lanczos, since in line 6 we would then have that $H_{j,k} = 0$ for $j < k-1$ and $H_{k-1,k} = H_{k,k-1}^*$.

1: **Given:** A, $\boldsymbol{B}$, $\mathbb{S}$, $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$, N, m
2: Compute $B = N(\boldsymbol{B})$ and $\boldsymbol{V}_1 = \boldsymbol{B}B^{-1}$
3: **for** $k = 1, \ldots, m$ **do**
4:     Compute $\boldsymbol{W} = A\boldsymbol{V}_k$
5:     **for** $j = 1, \ldots, k$ **do**
6:         $H_{j,k} = \langle\!\langle \boldsymbol{V}_j, \boldsymbol{W} \rangle\!\rangle_{\mathbb{S}}$
7:         $\boldsymbol{W} = \boldsymbol{W} - \boldsymbol{V}_j H_{j,k}$
8:     **end for**
9:     Compute $H_{k+1,k} = N(\boldsymbol{W})$ and $\boldsymbol{V}_{k+1} = \boldsymbol{W}H_{k+1,k}^{-1}$
10: **end for**
11: **return** B, $\boldsymbol{\mathcal{V}}_m = [\boldsymbol{V}_1|\ldots|\boldsymbol{V}_m]$, $\mathcal{H}_m = (H_{j,k})_{j,k=1}^m$, $\boldsymbol{V}_{m+1}$, and $H_{m+1,m}$

a fact which will be useful later when establishing comparison results.

Algorithm 2.1 formulates the block generalization of the Arnold process. It computes a block orthonormal basis $\{\boldsymbol{V}_j\}_{j=1}^m \subset \mathbb{C}^{n \times s}$ of the block Krylov subspace $\mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B})$. It simplifies to the block Lanczos processs if A is block self-adjoint with respect to $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$ according to the following definition; see also [22].

Definition 2.4. *$A \in \mathbb{C}^{n \times n}$ is* block self-adjoint *if for all $\boldsymbol{X}, \boldsymbol{Y} \in \mathbb{C}^{n \times s}$,*

$$\langle\!\langle A\boldsymbol{X}, \boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}} = \langle\!\langle \boldsymbol{X}, A\boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}}.$$

Note that if $A = A^*$, then A is block self-adjoint for the three block inner products shown in Table 2.1.

We always assume that Algorithm 2.1 runs to completion without breaking down, i.e., that we obtain

(i) a block orthonormal basis $\{\boldsymbol{V}_k\}_{k=1}^{m+1} \subset \mathbb{C}^{n \times s}$, such that each $\boldsymbol{V}_k$ has full rank and $\mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B}) = \mathrm{span}^{\mathbb{S}}\{\boldsymbol{V}_k\}_{k=1}^m$, and

(ii) a block upper Hessenberg matrix $\mathcal{H}_m \in \mathbb{S}^{m \times m}$ and $H_{m+1,m} \in \mathbb{S}$,

all satisfying the *block Arnoldi relation*

$$A\boldsymbol{\mathcal{V}}_m = \boldsymbol{\mathcal{V}}_m \mathcal{H}_m + \boldsymbol{V}_{m+1} H_{m+1,m} \widehat{\boldsymbol{E}}_m^* = \boldsymbol{\mathcal{V}}_{m+1} \underline{\mathcal{H}}_m, \tag{2.2}$$

where $\boldsymbol{\mathcal{V}}_m = [\boldsymbol{V}_1|\dots|\boldsymbol{V}_m] \in \mathbb{C}^{n\times ms}$, and

$$\mathcal{H}_m = \begin{bmatrix} H_{1,1} & H_{1,2} & \dots & H_{1,m} \\ H_{2,1} & H_{2,2} & \dots & H_{2,m} \\ & \ddots & \ddots & \vdots \\ & & H_{m,m-1} & H_{m,m} \end{bmatrix}, \ \underline{\mathcal{H}}_m := \begin{bmatrix} \mathcal{H}_m \\ H_{m+1,m}\widehat{\boldsymbol{E}}_{m+1}^* \end{bmatrix}.$$

By construction, the block Arnoldi vectors $\boldsymbol{V}_i$ $\mathbb{S}$-span the block Krylov subspace $\mathscr{K}_m^{\mathbb{S}}(A,\boldsymbol{B})$. As in the scalar case, any element $\boldsymbol{X} \in \mathscr{K}_m^{\mathbb{S}}(A,\boldsymbol{B})$ has a unique representation in terms of these block Arnoldi vectors in the sense that in the representation

$$\boldsymbol{X} = \sum_{i=1}^{m} \boldsymbol{V}_i \Gamma_i, \ \ \Gamma_i \in \mathbb{S}, \tag{2.3}$$

the "block coefficients" Γ_i are unique.

PROPOSITION 2.5. *The representation* (2.3) *is unique.*

Proof. Taking block inner products with the basis vectors $\boldsymbol{V}_j$ gives $\langle\!\langle \boldsymbol{V}_j, \boldsymbol{X}\rangle\!\rangle_{\mathbb{S}} = \Gamma_j$, $j = 1,\dots,m$. ∎

2.2. Matrix polynomials over $\mathbb{S}$. We denote as $\mathbb{P}_m(\mathbb{S})$ the space of all polyomials P of degree at most m and with coefficients $\Gamma_k \in \mathbb{S}$, $P : \mathbb{C} \to \mathbb{S}$, $P(z) = \sum_{k=0}^{m} z^k \Gamma_k$, and use the notation $P(A) \circ \boldsymbol{B}$ introduced in [32] to denote

$$P(A) \circ \boldsymbol{B} := \sum_{k=0}^{m} A^k \boldsymbol{B} \Gamma_k. \tag{2.4}$$

When regarded as a mapping from $\mathbb{C}$ to $\mathbb{S}$, P is often termed a λ-*matrix* [11, 12, 13, 24, 33]. In (2.4), P is considered a mapping from $\mathbb{C}^{n\times n} \times \mathbb{C}^{n\times s}$ to $\mathbb{C}^{n\times s}$. This interpretation allows for the characterization of block Krylov subspaces using matrix polynomials as

$$\mathscr{K}_m^{\mathbb{S}}(A,\boldsymbol{B}) = \{Q(A) \circ \boldsymbol{B} : Q \in \mathbb{P}_{m-1}(\mathbb{S})\}.$$

As a consequence, we have the following characterization of the block residual, which will be used later.

Remark 2.6. For any block vector $\boldsymbol{X} = Q(A) \circ \boldsymbol{B} \in \mathscr{K}_m^{\mathbb{S}}(A,\boldsymbol{B})$, the corresponding residual $\boldsymbol{R} = \boldsymbol{B} - A\boldsymbol{X}$ can be written as $\boldsymbol{R} = P_m(A) \circ \boldsymbol{B}$, with $P_m \in \mathbb{P}_m(\mathbb{S})$ and $P_m(0) = I$. Indeed, $P_m(z) = I = zQ(z)$, for some $Q \in \mathbb{P}_{m-1}(\mathbb{S})$.

For a given element $\boldsymbol{X}_m = Q(A) \circ \boldsymbol{B}$ of $\mathscr{K}_m^{\mathbb{S}}(A,\boldsymbol{B})$, $Q \in \mathbb{P}_{m-1}(\mathbb{S})$, a natural question is how this element is represented in terms of the block Arnoldi basis $\boldsymbol{\mathcal{V}}_m$, i.e., as $\boldsymbol{X}_m = \boldsymbol{\mathcal{V}}_m \boldsymbol{\Xi}_m$, for block coefficients $\boldsymbol{\Xi}_m$. The polynomial exactness property formulated in the following theorem shows that $\boldsymbol{\Xi}_m$ arises from evaluating Q on the block Hessenberg matrix $\mathcal{H}_m$ or a modification thereof that changes only the last block column. The theorem will be useful in the context of restarts for families of shifted linear systems and for matrix functions in Section 4. We use the notation introduced with the block Arnoldi process, Algorithm 2.1.

THEOREM 2.7.

(i) For any matrix of the form $\mathcal{H}_m + \mathcal{M}$, where $\mathcal{M} = \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*$, $\boldsymbol{M} \in \mathbb{S}^m$, we have

$$Q(A) \circ \boldsymbol{B} = \boldsymbol{\mathcal{V}}_m Q(\mathcal{H}_m + \mathcal{M}) \circ \widehat{\boldsymbol{E}}_1 B \textit{ for all } Q \in \mathbb{P}_{m-1}(\mathbb{S}). \tag{2.5}$$

(ii) If (2.5) *holds for some matrix* $\mathcal{M} \in \mathbb{S}^{m \times m}$*, then* $\mathcal{M} = \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*$ *with* $\boldsymbol{M} \in \mathbb{S}^m$*.*

Proof. To prove (i), observe first that $\mathcal{H}_m + \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*$ is still block upper Hessenberg. So in its j-th power all block subdiagonals beyond the j-th are zero. In particular, for the bottom left block,

$$\widehat{\boldsymbol{E}}_m^*(\mathcal{H}_m + \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*)^j \widehat{\boldsymbol{E}}_1 = 0, \;\; j = 1, \dots, m-2. \tag{2.6}$$

To obtain (2.5) it is sufficient to show that

$$A^j \boldsymbol{B} = \boldsymbol{\mathcal{V}}_m (\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B, \;\; j = 0, \dots, m-1. \tag{2.7}$$

This certainly holds for $j = 0$, since $A^0 \boldsymbol{B} = \boldsymbol{B} = \boldsymbol{V}_1 B = \boldsymbol{\mathcal{V}}_m \widehat{\boldsymbol{E}}_1 B$. If (2.7) holds for some $j \in \{0, \dots, m-2\}$, then $A^{j+1}\boldsymbol{B} = AA^j\boldsymbol{B} = A\boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B$. Using the block Arnoldi relation (2.2) we then obtain that

$$\begin{aligned} A^{j+1}\boldsymbol{B} &= (\boldsymbol{\mathcal{V}}_m \mathcal{H}_m + \boldsymbol{V}_{m+1} H_{m+1,m} \widehat{\boldsymbol{E}}_m^*)(\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B \\ &= \boldsymbol{\mathcal{V}}_m \mathcal{H}_m (\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B + \boldsymbol{V}_{m+1} H_{m+1,m} \widehat{\boldsymbol{E}}_m^* (\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B. \end{aligned} \tag{2.8}$$

Herein, the second term vanishes due to (2.6) and, again due to (2.6), $\mathcal{M}(\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B = \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*(\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B = 0$ for $j = 1, \dots, m-2$. Thus, equation (2.8) becomes

$$\begin{aligned} A^{j+1}\boldsymbol{B} &= \boldsymbol{\mathcal{V}}_m \mathcal{H}_m (\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B \\ &= \boldsymbol{\mathcal{V}}_m \mathcal{H}_m (\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B + \boldsymbol{\mathcal{V}}_m \mathcal{M} (\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B \\ &= \boldsymbol{\mathcal{V}}_m (\mathcal{H}_m + \mathcal{M})^{j+1} \widehat{\boldsymbol{E}}_1 B, \end{aligned}$$

completing the proof for (i). Note that by taking $\mathcal{M} = 0$, (i) gives that

$$A^j \boldsymbol{B} = \boldsymbol{\mathcal{V}}_m \mathcal{H}_m^j \widehat{\boldsymbol{E}}_1 B, \;\; j = 0, \dots, m-1. \tag{2.9}$$

To prove (ii), by assumption we now have that in particular

$$A^j \boldsymbol{B} = \boldsymbol{\mathcal{V}}_m (\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B, \;\; j = 0, \dots, m-1,$$

as well as, by (2.9),

$$A^j \boldsymbol{B} = \boldsymbol{\mathcal{V}}_m \mathcal{H}_m^j \widehat{\boldsymbol{E}}_1 B, \;\; j = 0, \dots, m-1,$$

giving

$$\boldsymbol{\mathcal{V}}_m \mathcal{H}_m^j \widehat{\boldsymbol{E}}_1 B = \boldsymbol{\mathcal{V}}_m (\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1 B, \;\; j = 0, \dots, m-1.$$

Since $\boldsymbol{\mathcal{V}}_m$ has full rank and B is nonsingular, all this implies that $\mathcal{H}_m^j \widehat{\boldsymbol{E}}_1 = (\mathcal{H}_m + \mathcal{M})^j \widehat{\boldsymbol{E}}_1$ for $j = 0, \dots, m-1$, yielding

$$\mathcal{H}_m^j \widehat{\boldsymbol{E}}_1 = (\mathcal{H}_m + \mathcal{M}) \mathcal{H}_m^{j-1} \widehat{\boldsymbol{E}}_1, \quad \text{for } j = 1, \dots, m-1.$$

We thus have

$$\mathcal{M} \mathcal{H}_m^{j-1} \widehat{\boldsymbol{E}}_1 = 0 \quad \text{for } j = 1, \dots, m-1. \tag{2.10}$$

For $j = 1$ (2.10) directly gives that $\mathcal{M}\widehat{\boldsymbol{E}}_1 = 0$. Inductively now, assume that $\mathcal{M}\widehat{\boldsymbol{E}}_\ell = 0$ for $\ell = 0, \dots, j$ for some $j \geq 0$, $j < m-1$. The relation (2.10), with $j-1$ replaced by j, can be written as

$$0 = \mathcal{M}\mathcal{H}_m^j \widehat{\boldsymbol{E}}_1 = \mathcal{M} \sum_{\ell=1}^{m} \widehat{\boldsymbol{E}}_\ell \widehat{\boldsymbol{E}}_\ell^* \mathcal{H}_m^j \widehat{\boldsymbol{E}}_1 = \mathcal{M} \sum_{\ell=1}^{j+1} \widehat{\boldsymbol{E}}_\ell \widehat{\boldsymbol{E}}_\ell^* \mathcal{H}_m^j \widehat{\boldsymbol{E}}_1,$$

with the last equality holding since all block subdiagonals beyond the $j+1$-st are zero in $\mathcal{H}_m^j$. With the inductive assumption we thus obtain $\mathcal{M}\widehat{\boldsymbol{E}}_{j+1}\widehat{\boldsymbol{E}}_{j+1}^*\mathcal{H}_m^j\widehat{\boldsymbol{E}}_1 = 0$. We now note that

$$\widehat{\boldsymbol{E}}_{j+1}^*\mathcal{H}_m^j\widehat{\boldsymbol{E}}_1 = H_{j+1,j}H_{j,j-1}\cdots H_{2,1},$$

and herein all factors $H_{\ell+1,\ell}$ are nonsingular, since they arise as scaling quotients in the block Arnoldi process, Algorithm 2.1. This relation implies that $\mathcal{M}\widehat{\boldsymbol{E}}_{j+1} = 0$, thus completing the inductive proof of (ii). ◻

Theorem 2.7 generalizes to blocks what is known in the case $s = 1$; see, e.g., [21, Lemmas 1.3 and 1.4], as well as [4, 14, 19, 37, 39, 48].

The block FOM approximation $\boldsymbol{X}_m$ for a block linear system $A\boldsymbol{X} = \boldsymbol{B}$ is given as (see [40])

$$\boldsymbol{X}_m^{\text{fom}} := \boldsymbol{\mathcal{V}}_m\mathcal{H}_m^{-1}\boldsymbol{\mathcal{V}}_m^*\boldsymbol{B} = \boldsymbol{\mathcal{V}}_m\mathcal{H}_m^{-1}\widehat{\boldsymbol{E}}_1 B.$$

Note that $\boldsymbol{X}_m^{\text{fom}}$ is indeed in $\mathscr{K}_{m-1}^{\mathbb{S}}(A,\boldsymbol{B})$, because $\mathcal{H}_m^{-1}$ can be expressed as a polynomial in $\mathcal{H}_m$ and is thus in $\mathbb{S}^{m\times m}$.

More generally, we can consider a whole family of approximations from $\mathscr{K}_{m-1}^{\mathbb{S}}(A,\boldsymbol{B})$ of the form

$$\boldsymbol{X}_m = \boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + \mathcal{M})^{-1}\widehat{\boldsymbol{E}}_1 B, \quad \text{where } \mathcal{M} = \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*.$$

We will see in Section 3 that, for example, block GMRES approximations are contained in this family. In light of Theorem 2.7, such types of $\boldsymbol{X}_m$ satisfy

$$\boldsymbol{X}_m = \boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + \mathcal{M})^{-1}\widehat{\boldsymbol{E}}_1 B = Q_{m-1}(A)\circ\boldsymbol{B} = \boldsymbol{\mathcal{V}}_m Q_{m-1}(\mathcal{H}_m + \mathcal{M})\circ\widehat{\boldsymbol{E}}_1 B \quad (2.11)$$

for some $Q_{m-1} \in \mathbb{P}_{m-1}(\mathbb{S})$. This observation motivates the following definition.

Definition 2.8. *Given $\mathcal{H} \in \mathbb{S}^{m\times m}$, $\boldsymbol{\Xi} \in \mathbb{S}^m$, and $f : D \subset \mathbb{C} \to \mathbb{C}$ such that $f(\mathcal{H}) \in \mathbb{S}^{m\times m}$ is defined, we say that $Q \in \mathbb{P}_{m-1}(\mathbb{S})$* interpolates f on the pair $(\mathcal{H},\boldsymbol{\Xi})$ *if*

$$Q(\mathcal{H})\circ\boldsymbol{\Xi} = f(\mathcal{H})\boldsymbol{\Xi}.$$

With the block Vandermonde matrix

$$\boldsymbol{\mathcal{W}} := [\boldsymbol{\Xi} \mid \mathcal{H}\boldsymbol{\Xi} \mid \cdots \mid \mathcal{H}^{m-1}\boldsymbol{\Xi}] \in \mathbb{S}^{m\times m}, \quad (2.12)$$

we see that $Q(z) = \sum_{j=0}^{m-1} z\Gamma_j$ interpolates f on the pair $(\mathcal{H},\boldsymbol{\Xi})$ if and only if $\boldsymbol{\Gamma} = [\Gamma_0|\cdots|\Gamma_{m-1}]^T \in \mathbb{S}^m$ solves

$$\boldsymbol{\mathcal{W}}\boldsymbol{\Gamma} = f(\mathcal{H})\boldsymbol{\Xi}. \quad (2.13)$$

Consequently, an interpolating polynomial exists if $\boldsymbol{\mathcal{W}}$ is nonsingular.

The matrix polynmial Q_{m-1} from (2.11) interpolates the function $f : z \to z^{-1}$ on the pair $(\mathcal{H}_m + \mathcal{M}, \widehat{\boldsymbol{E}}_1 B)$ since $\boldsymbol{\mathcal{V}}_m$ has full rank. Our last contribution in this section relates the eigenvalues of $\mathcal{H}_m + \mathcal{M}$ to the latent roots of the "residual matrix polynomial" $P_m(z) = I - zQ_{m-1}(z) \in \mathbb{P}_m(\mathbb{S})$. Recall that the *latent roots* of a matrix polynomial P are the zeros of the function $\det(P(z)) : z \in \mathbb{C} \to \mathbb{C}$; see, e.g., [13, 24, 33].

Theorem 2.9. *Let $\mathcal{H} \in \mathbb{S}^{m\times m}$ be nonsingular and let $\boldsymbol{\Xi} \in \mathbb{S}^m$ be such that the block Vandermonde matrix (2.12) is nonsingular. Let $Q_{m-1} \in \mathbb{P}_{m-1}(\mathbb{S})$ be the matrix polynomial interpolating $f(z) = z^{-1}$ on the pair $(\mathcal{H},\boldsymbol{\Xi})$ and let $\chi(z)$ be the characteristic polynomial of $\mathcal{H}$. Then the residual matrix polynomial $P_m(z) = I - zQ_{m-1}(z) = \sum_{i=0}^m z^i\Upsilon_i$ satisfies*

$$\det(P_m(z)) = \chi(z)/\chi(0). \quad (2.14)$$

In particular, the latent roots of P_m coincide with the eigenvalues of $\mathcal{H}$ including (algebraic) multiplicity.

Proof. We first prove the result under the following additional assumptions:
(i) $\mathcal{H}$ is diagonizable and all its eigenvalues are distinct, i.e., we have

$$\mathcal{H} = \mathcal{X}\Lambda\mathcal{X}^{-1},$$

where $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_{ms}), \lambda_i \neq \lambda_j$ for $i \neq j$, $\mathcal{X} \in \mathbb{C}^{ms\times ms}$ nonsingular.
(ii) All rows in $\mathcal{X}^{-1}\boldsymbol{\Xi}$ are non-zero.
With these assumptions, let $x_j^* \neq 0$ denote row j of $\mathcal{X}^{-1}$; i.e., x_j^* is a left eigenvector for the eigenvalue λ_j of $\mathcal{H}$:

$$x_j^*\mathcal{H} = \lambda_j x_j^*.$$

From $0 = P_m(\mathcal{H}) \circ \boldsymbol{\Xi} = \sum_{i=0}^m \mathcal{H}^i \boldsymbol{\Xi}\Upsilon_i$, we obtain, multiplying with x_j^* from the left, that

$$0 = \sum_{i=0}^m \lambda_j^i x_j^* \boldsymbol{\Xi}\Upsilon_i = x_j^*\boldsymbol{\Xi}\sum_{i=0}^m \lambda_j^i \Upsilon_i = (x_j^*\boldsymbol{\Xi}) \cdot P_m(\lambda_j).$$

By assumption (ii), $x_j^*\boldsymbol{\Xi} \neq 0$, so it is a left eigenvector to the eigenvalue 0 of $P_m(\lambda_j)$; i.e., $\det(P_m(\lambda_j)) = 0$. Since this holds for all j and $\det(P(z))$ is a polynomial of degree ms, we have $\det(P(z)) = c\prod_{j=1}^{ms}(z-\lambda_j)$, and since $\det(P(0)) = \det(I) = 1$ we have $c = \prod_{j=1}^{ms}(-\lambda_j)^{-1} = \frac{1}{\chi(0)}$.

We now turn to the situation where (i) and (ii) do not necessarily hold and use an argument based on continuity. Let $\mathcal{H} = \mathcal{T}\mathcal{J}\mathcal{T}^{-1}$ with $\mathcal{J}$ being the Jordan canonical form of $\mathcal{H}$. Then $\mathcal{J}$ is a bidiagonal matrix with the eigenvalues λ_i of $\mathcal{H}$ on the diagonal according to their algebraic multiplicity. Let $\epsilon_0 > 0$ denote the minimal distance between the distinct eigenvalues

$$\epsilon_0 := \min\{|\lambda_i - \lambda_j| : \lambda_i \neq \lambda_j\},$$

and let

$$\mathcal{J}_\epsilon = \mathcal{J} + \frac{\epsilon}{2}\operatorname{diag}\left(\left[\frac{1}{1}, \frac{1}{2}, \ldots, \frac{1}{ms}\right]\right).$$

Then for $0 < \epsilon \leq \epsilon_0$ the diagonal elements of $\mathcal{J}_\epsilon$, which are the eigenvalues $\lambda_i^{(\epsilon)}$ of $\mathcal{J}_\epsilon$, are all different. For all such ϵ we therefore have that $\mathcal{H}_\epsilon = \mathcal{T}\mathcal{J}_\epsilon\mathcal{T}^{-1}$ is diagonizable with ms pairwise different eigenvalues,

$$\mathcal{H}_\epsilon = \mathcal{X}_\epsilon\Lambda_\epsilon\mathcal{X}_\epsilon^{-1}, \;\; \Lambda_\epsilon = \operatorname{diag}(\lambda_i^{(\epsilon)}),$$

and that $\|\mathcal{H}_\epsilon - \mathcal{H}\|_2 \leq \frac{\epsilon}{2}\|\mathcal{T}\|_2\|\mathcal{T}^{-1}\|_2$. For $\delta > 0$ consider now $\mathcal{X}_{\epsilon,\delta} = \mathcal{X}_\epsilon + \delta[\, I_s | \ldots | \, I_s]^*\boldsymbol{\Xi}^*$. Then

$$\mathcal{X}_{\epsilon,\delta}\boldsymbol{\Xi} = \mathcal{X}_\epsilon\boldsymbol{\Xi} + \delta[\, I_s | \ldots | \, I_s]^*\boldsymbol{\Xi}^*\boldsymbol{\Xi}.$$

The block vector $\boldsymbol{\Xi}$ has full rank since the Vandermonde matrix $\boldsymbol{\mathcal{W}}$ from (2.12) is nonsingular. So for all i the i-th row $e_i^*\boldsymbol{\Xi}^*\boldsymbol{\Xi}$ of $\boldsymbol{\Xi}^*\boldsymbol{\Xi}$ is non-zero. Therefore, for

$$0 \leq \delta < \delta_1(\epsilon) := \min_i\{\|e_i^*\mathcal{X}_\epsilon\boldsymbol{\Xi}\|_2 : e_i^*\mathcal{X}_\epsilon\boldsymbol{\Xi} \neq 0\} / \max_i\{\|e_i^*\boldsymbol{\Xi}^*\boldsymbol{\Xi}\|_2\},$$

we have that all rows in $\mathcal{X}_{\epsilon,\delta}\boldsymbol{\Xi}$ are non-zero. Choose $\delta > 0$ small enough such that, in addition,

$$\mathcal{H}_{\epsilon,\delta} := \mathcal{X}_{\epsilon,\delta}\Lambda_\epsilon\mathcal{X}_{\epsilon,\delta}^{-1}$$

satisfies $\|\mathcal{H}_{\epsilon,\delta} - \mathcal{H}_\epsilon\|_2 \leq \epsilon$. Then, since $\|\mathcal{H}_{\epsilon,\delta} - \mathcal{H}\|_2 \leq \frac{\epsilon}{2}\|\mathcal{T}\|_2\|\mathcal{T}^{-1}\|_2 + \epsilon$, the Vandermonde matrix

$$[\Xi|\mathcal{H}_{\epsilon,\delta}\Xi| \dots \mathcal{H}_{\epsilon,\delta}^{m-1}\Xi]$$

is nonsingular if ϵ is small enough. For such ϵ, let $Q_{m-1}^{\epsilon,\delta}$ be the polynomial interpolating $f(z) = z^{-1}$ on the pair $(\mathcal{H}_{\epsilon,\delta}, \Xi)$. By part (i), the corresponding residual matrix polynomial $P_m^{\epsilon,\delta}(z) = I - zQ_{m-1}^{\epsilon,\delta}(z)$ satisfies

$$\det(P_m^{\epsilon,\delta}(z)) = \chi^{\epsilon,\delta}(z)/\chi^{\epsilon,\delta}(0), \tag{2.15}$$

where $\chi^{\epsilon,\delta}(z)$ is the characteristic polynomial of $\mathcal{H}^{\epsilon,\delta}$. As solutions of the system (2.13), the matrix coefficients of $Q_{m-1}^{\epsilon,\delta}(z)$ and thus the coefficients of the polynomial $\det(P_m^{\epsilon,\delta}(z))$ depend continuously on the entries of $\mathcal{H}^{\epsilon,\delta}$, as well as the coefficients of the characteristic polynomial $\chi^{\epsilon,\delta}(z)$. By continuity then, and since $\|\mathcal{H} - \mathcal{H}^{\epsilon,\delta}\|_2 \leq \frac{\epsilon}{2}\|\mathcal{T}\|_2\|\mathcal{T}^{-1}\|_2 + \epsilon$, taking the limit $\epsilon \to 0$ in (2.15) gives (2.14). ◻

If $\mathcal{H} = \mathcal{H}_m + \mathcal{M}$ with $\mathcal{M} = \boldsymbol{M}\widehat{\boldsymbol{E}}_1^*, \boldsymbol{M} \in \mathbb{S}^m$, where $\mathcal{H}_m$ arises from the Arnoldi process with starting block vector $\boldsymbol{B}$, the block Vandermonde matrix (2.12) is

$$[\widehat{\boldsymbol{E}}_1 B \,|\, (\mathcal{H}_m + \mathcal{M})\widehat{\boldsymbol{E}}_1 B \,|\, \cdots \,|\, (\mathcal{H}_m + \mathcal{M})^{m-1}\widehat{\boldsymbol{E}}_1 B].$$

This matrix is block upper triangular, with $\prod_{j=1}^{i-1} H_{i-j+1,i-j} B$ as its i-th diagonal block. Since we assume the Arnoldi process runs without breakdown until step m, all matrices $H_{j+1,j}$ exist and are nonsingular, since they are the scaling quotients from the block Arnoldi process. Therefore, the block Vandermonde matrix is nonsingular, and we obtain the following corollary to Theorem 2.9.

Corollary 2.10. *Let $\mathcal{H} = \mathcal{H}_m + \mathcal{M} \in \mathbb{S}^{m\times m}$, $\mathcal{M} = \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*$ with $\boldsymbol{M} \in \mathbb{S}^m$ be nonsingular. Let $Q_{m-1} \in \mathbb{P}_{m-1}(\mathbb{S})$ interpolate $f(z) = z^{-1}$ on the pair $(\mathcal{H}_m + \mathcal{M}, \widehat{\boldsymbol{E}}_1 B)$ and let $\chi(z)$ be the characteristic polynomial of $\mathcal{H}_m + \mathcal{M}$. Then the residual matrix polynomial $P_m(z) = I - zQ_{m-1}(z)$ satisfies* $\det(P_m(z)) = \chi(z)/\chi(0)$.

Parts of this corollary have been observed in various constellations in the literature before. For example, for block GMRES–where the assumptions on $\mathcal{H}$ are fulfilled, as we will see in section 3.2–it was shown in [44, Theorem 3.3] that for the classical block inner product, the latent roots are exactly the roots of the characteristic polynomial; see also [43]. This result does not, however, contain the result on the algebraic multiplicities. The same result for the global inner product was formulated in [16, Theorem 3.1].

3. Block FOM and its low-rank modifications.

Given a block inner product $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$ and the output of the corresponding block Arnoldi process, the common property of the block Krylov subspace methods to be discussed in this section is that they take their m-th iterate, approximating the solution of the block linear system $A\boldsymbol{X} = \boldsymbol{B}$, as

$$\boldsymbol{X}_m = \boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*)^{-1}\widehat{\boldsymbol{E}}_1 B \text{ with } \boldsymbol{M} \in \mathbb{S}^m. \tag{3.1}$$

Theorem 2.7 shows that these are iterates for which the defining polynomial $\boldsymbol{X}_m = Q_{m-1}(A) \circ \boldsymbol{B}$ is the one interpolating $(\mathcal{H}_m + \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*)^{-1}$ on the pair $(\mathcal{H}_m + \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*, \widehat{\boldsymbol{E}}_1 B)$.

3.1. Block FOM.

The m-th block FOM approximation $\boldsymbol{X}_m^{\text{fom}}$ is variationally characterized by the Galerkin condition

$$\langle\!\langle \boldsymbol{B} - A\boldsymbol{X}_m^{\text{fom}}, \boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}} = 0 \text{ for all } \boldsymbol{Y} \in \mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B}). \tag{3.2}$$

As was shown in [22], (3.2) is satisfied if we take $\boldsymbol{M} = 0$ in (3.1),

$$\boldsymbol{X}_m^{\text{fom}} = \boldsymbol{\mathcal{V}}_m \mathcal{H}_m^{-1} \widehat{\boldsymbol{E}}_1 B,$$

and the residual $\boldsymbol{R}_m^{\text{fom}} = \boldsymbol{B} - A\boldsymbol{X}_m^{\text{fom}}$ is *cospatial* to the next block Arnoldi vector,

$$\boldsymbol{R}_m^{\text{fom}} = \boldsymbol{V}_{m+1} C_m \text{ with } C_m \in \mathbb{S}; \tag{3.3}$$

see also Theorem 4.1 below. If $\mathcal{H}_m$ is singular, the block FOM approximation does not exist. To state results on convergence, we introduce the scalar inner product $\langle \cdot, \cdot \rangle_{\mathbb{S}}$

$$\langle \boldsymbol{X}, \boldsymbol{Y} \rangle_{\mathbb{S}} := \operatorname{trace} \langle\!\langle \boldsymbol{Y}, \boldsymbol{X} \rangle\!\rangle_{\mathbb{S}}. \tag{3.4}$$

The properties of $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$ from Definition 2.1 guarantee that (3.4) is a true inner product on $\mathbb{C}^{n \times s}$. Naturally, it induces the norm

$$\|\boldsymbol{X}\|_{\mathbb{S}} := \langle \boldsymbol{X}, \boldsymbol{X} \rangle_{\mathbb{S}}^{1/2}.$$

For the classical, global, and loop-interchange paradigms from Table 2.1, $\|\cdot\|_{\mathbb{S}}$ is the familiar Frobenius norm in all three cases.

As a complement to the notion of block self-adjointness, we use the following notion of positive definiteness.

Definition 3.1. *$A \in \mathbb{C}^{n \times n}$ is* block positive definite *with respect to the block inner product $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$ if $\langle\!\langle A\boldsymbol{X}, \boldsymbol{X} \rangle\!\rangle_{\mathbb{S}}$ is Hermitian and positive definite for all full rank $\boldsymbol{X} \in \mathbb{C}^{n \times s}$ and positive semidefinite and non-zero for all rank-deficient $\boldsymbol{X} \neq 0$.*

We immediately obtain the following: if A is block self-adjoint with respect to $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$ according to Definition 2.4, then A is also self-adjoint with respect to $\langle \cdot, \cdot \rangle_{\mathbb{S}}$. If, in addition, A is block positive definite according to Definition 3.1, then A is also positive definite with respect to $\langle \cdot, \cdot \rangle_{\mathbb{S}}$.

If A is block self-adjoint and block positive definite with respect to $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$, the block FOM iterates can be computed efficiently using short recurrences. The resulting *block CG* method was first described and analyzed in [36] for the classical paradigm. Several authors have considered various aspects of numerical stability and strategies for "deflation" corresponding to the case that a block Lanczos vector becomes numerically rank-deficient; for a thorough discussion of the literature, see [7]. The following convergence result for a general block inner product $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$ was basically proven in [22, Theorem 3.7]. It uses the scalar A inner product $\langle \boldsymbol{X}, \boldsymbol{Y} \rangle_{A\text{-}\mathbb{S}} := \langle A\boldsymbol{X}, \boldsymbol{Y} \rangle_{\mathbb{S}}$ and transports the standard CG convergence result to the general block case.

Theorem 3.2. *Let $A \in \mathbb{C}^{n \times n}$ be self-adjoint and positive definite with respect to $\langle \cdot, \cdot \rangle_{\mathbb{S}}$. Then the error $\boldsymbol{E}_m^{\text{fom}} := \boldsymbol{X}_m^{\text{fom}} - \boldsymbol{X}_*$, where $\boldsymbol{X}_* = A^{-1}\boldsymbol{B}$, satisfies*

$$\left\|\boldsymbol{E}_m^{\text{fom}}\right\|_{A\text{-}\mathbb{S}} = \min_{\boldsymbol{X} \in \mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B})} \|\boldsymbol{X}_* - \boldsymbol{X}\|_{A\text{-}\mathbb{S}} \leq \xi_m \|\boldsymbol{B}\|_{A\text{-}\mathbb{S}}, \tag{3.5}$$

with

$$\xi_m := \frac{2}{c^m + c^{-m}}, \; c := \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}, \; \kappa := \frac{\lambda_{\max}}{\lambda_{\min}}, \tag{3.6}$$

and $\lambda_{\min}$ and $\lambda_{\max}$ denoting the smallest and largest eigenvalues of A, respectively.

We note that the theorem applies in particular for a matrix A which is block self-adjoint and block positive definite with respect to the block inner product $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$.

If A is Hermitian and positive definite with respect to the standard inner product, it is also block self-adjoint and block positive definite with respect to the block inner products corresponding to the classical, the global and the loop-interchanged paradigm from Table 2.1. Moreover, all three paradigms yield the same induced scalar inner product $\langle \boldsymbol{V}, \boldsymbol{W} \rangle_{\mathbb{S}} = \operatorname{trace} \boldsymbol{V}^* \boldsymbol{W}$, termed the *Frobenius inner product*. The corresponding common A-norm $\langle \cdot, \cdot \rangle_{A\text{-}\mathbb{S}}$ is $\|\boldsymbol{X}\|_{A\text{-F}} := \operatorname{trace} \boldsymbol{X}^* A \boldsymbol{X}$. Given the nestedness of the block Krylov subspaces (2.1), the optimality property of Theorem 3.2 yields the following additional result.

THEOREM 3.3. *Let $\boldsymbol{E}_m^{\text{Gl}}$, $\boldsymbol{E}_m^{\text{Li}}$ and $\boldsymbol{E}_m^{\text{Cl}}$ denote the errors of the m-th block FOM approximations corresponding to the global, loop-interchange, and classical paradigms, respectively. Moreover, let $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$ be a block inner product for which the corresponding scalar inner product satisfies $\langle \boldsymbol{V}, \boldsymbol{W} \rangle_{\mathbb{S}} = \operatorname{trace} \boldsymbol{V}^* \boldsymbol{W}$ and denote $\boldsymbol{E}_m^{\mathbb{S}}$ the error of the corresponding block FOM iterate. Then*

$$\left\|\boldsymbol{E}_m^{\text{Cl}}\right\|_{A\text{-}F} \leq \left\|\boldsymbol{E}_m^{\text{Li}}\right\|_{A\text{-}F}, \left\|\boldsymbol{E}_m^{\mathbb{S}}\right\|_{A\text{-}F} \leq \left\|\boldsymbol{E}_m^{\text{Gl}}\right\|_{A\text{-}F}.$$

3.2. Block GMRES. The m-th block GMRES iterate from $\mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B})$ is defined via the Petrov-Galerkin condition

$$\langle\!\langle \boldsymbol{B} - A\boldsymbol{X}_m^{\text{gmr}}, A\boldsymbol{Y} \rangle\!\rangle_{\mathbb{S}} = 0 \text{ for all } \boldsymbol{Y} \in \mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B}). \tag{3.7}$$

This is equivalent to requiring

$$\langle \boldsymbol{B} - A\boldsymbol{X}_m^{\text{gmr}}, A\boldsymbol{Y} \rangle_{\mathbb{S}} = 0 \text{ for all } \boldsymbol{Y} \in \mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B})$$

for the derived scalar inner product $\langle \cdot, \cdot \rangle_{\mathbb{S}}$. Since for any $\boldsymbol{Y} \in \mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B})$ we have that

$$\begin{aligned}
&\langle \boldsymbol{B} - A(\boldsymbol{X}_m^{\text{gmr}} - \boldsymbol{Y}), \boldsymbol{B} - A(\boldsymbol{X}_m^{\text{gmr}} - \boldsymbol{Y}) \rangle_{\mathbb{S}} \\
&\qquad = \langle \boldsymbol{B} - A\boldsymbol{X}_m^{\text{gmr}}, \boldsymbol{B} - A\boldsymbol{X}_m^{\text{gmr}} \rangle_{\mathbb{S}} - \langle \boldsymbol{B} - A\boldsymbol{X}_m^{\text{gmr}}, A\boldsymbol{Y} \rangle_{\mathbb{S}} \\
&\qquad\quad - \langle A\boldsymbol{Y}, \boldsymbol{B} - A\boldsymbol{X}_m^{\text{gmr}} \rangle_{\mathbb{S}} + \langle A\boldsymbol{Y}, A\boldsymbol{Y} \rangle_{\mathbb{S}} \\
&\qquad = \langle \boldsymbol{B} - A\boldsymbol{X}_m^{\text{gmr}}, \boldsymbol{B} - A\boldsymbol{X}_m^{\text{gmr}} \rangle_{\mathbb{S}} + \langle A\boldsymbol{Y}, A\boldsymbol{Y} \rangle_{\mathbb{S}},
\end{aligned}$$

we then see that the Petrov-Galerkin condition (3.7) is equivalent to the block GMRES iterate minimizing the $\mathbb{S}$-norm of the block residual. That is,

$$\boldsymbol{X}_m^{\text{gmr}} = \operatorname{argmin}_{\boldsymbol{X} \in \mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B})} \|\boldsymbol{B} - A\boldsymbol{X}\|_{\mathbb{S}}. \tag{3.8}$$

For the classical paradigm, this equivalence has been observed in [44, Section 1], and for the global paradigm in [28, Section 3.2] and [16, Section 2.2].

Representing $\boldsymbol{X}_m^{\text{gmr}} = \boldsymbol{\mathcal{V}}_m \boldsymbol{\Xi}^{\text{gmr}}$ with the coefficient block vector $\boldsymbol{\Xi}_m^{\text{gmr}} \in \mathbb{S}^m$, the block Arnoldi relation (2.2) and the $\langle \cdot, \cdot \rangle_{\mathbb{S}}$-orthogonality of the block Arnoldi basis show that the minimizing property (3.8) turns into a least squares problem for $\boldsymbol{\Xi}_m^{\text{gmr}}$, expressed via the Frobenius norm $\|\cdot\|_{\text{F}}$:

$$\boldsymbol{\Xi}^{\text{gmr}} = \operatorname{argmin}_{\boldsymbol{\Xi} \in \mathbb{S}^m} \|\widehat{\boldsymbol{E}}_1 B - \underline{\mathcal{H}}_m \boldsymbol{\Xi}\|_F.$$

This is the approach of choice for obtaining $\boldsymbol{X}_m^{\text{gmr}}$ computationally. On the more theoretical side, it is of interest to see that the block GMRES iterates can be regarded as modified block FOM iterates in the sense of (3.1).

THEOREM 3.4. *Assume that $\mathcal{H}_m$ is nonsingular. Then the m-th block GMRES iterate $\boldsymbol{X}_m^{\text{gmr}}$ is given as $\boldsymbol{X}_m^{\text{gmr}} = \boldsymbol{\mathcal{V}}_m \boldsymbol{\Xi}^{\text{gmr}}$, where*

$$\boldsymbol{\Xi}^{\text{gmr}} = (\mathcal{H}_m + \mathcal{M}^{\text{gmr}})^{-1} \widehat{\boldsymbol{E}}_1 B \textit{ with } \mathcal{M}^{\text{gmr}} = \mathcal{H}_m^{-*} \widehat{\boldsymbol{E}}_m H_{m+1,m}^* H_{m+1,m} \widehat{\boldsymbol{E}}_m^*. \tag{3.9}$$

Proof. We have to show that the Petrov-Galerkin condition (3.7) is satisfied, i.e.

$$\langle\!\langle A\boldsymbol{\mathcal{V}}_m\boldsymbol{\Theta}, \boldsymbol{B} - A\boldsymbol{\mathcal{V}}_m\boldsymbol{\Xi}^{\mathrm{gmr}}\rangle\!\rangle_{\mathbb{S}} = 0 \text{ for all } \boldsymbol{\Theta} \in \mathbb{S}^m.$$

From the block Arnoldi relation (2.2), we have for any $\boldsymbol{\Theta} \in \mathbb{S}^m$

$$\langle\!\langle A\boldsymbol{\mathcal{V}}_m\boldsymbol{\Theta}, \boldsymbol{B} - A\boldsymbol{\mathcal{V}}_m\boldsymbol{\Xi}^{\mathrm{gmr}}\rangle\!\rangle_{\mathbb{S}} = \langle\!\langle \boldsymbol{\mathcal{V}}_{m+1}\underline{\mathcal{H}}_m\boldsymbol{\Theta}, \boldsymbol{\mathcal{V}}_{m+1}(\widehat{\boldsymbol{E}}_1 B - \underline{\mathcal{H}}_m\boldsymbol{\Xi}^{\mathrm{gmr}})\rangle\!\rangle_{\mathbb{S}}.$$

Using square brackets $[\cdot]_i$ to denote the i-th block component $\widehat{\boldsymbol{E}}_i^*\boldsymbol{V} \in \mathbb{S}$ of a block vector $\boldsymbol{V} \in \mathbb{S}^m$, the basic properties of $\langle\!\langle\cdot,\cdot\rangle\!\rangle_{\mathbb{S}}$ from Definition 2.1 and the block orthonormality of the block Arnoldi vectors $\boldsymbol{V}_i$ give

$$\begin{aligned}
&\langle\!\langle \boldsymbol{\mathcal{V}}_{m+1}\underline{\mathcal{H}}_m\boldsymbol{\Theta}, \boldsymbol{\mathcal{V}}_{m+1}(\widehat{\boldsymbol{E}}_1 B - \underline{\mathcal{H}}_m\boldsymbol{\Xi}^{\mathrm{gmr}})\rangle\!\rangle_{\mathbb{S}} \\
&\quad = \langle\!\langle \textstyle\sum_{i=1}^{m+1} \boldsymbol{V}_i[\underline{\mathcal{H}}_m\boldsymbol{\Theta}]_i, \sum_{i=1}^{m+1} \boldsymbol{V}_i[\widehat{\boldsymbol{E}}_1 B - \underline{\mathcal{H}}_m\boldsymbol{\Xi}^{\mathrm{gmr}}]_i\rangle\!\rangle_{\mathbb{S}} \\
&\quad = \textstyle\sum_{i=1}^{m+1}[\underline{\mathcal{H}}_m\boldsymbol{\Theta}]_i^*[\widehat{\boldsymbol{E}}_1 B - \underline{\mathcal{H}}_m\boldsymbol{\Xi}^{\mathrm{gmr}}]_i \\
&\quad = \boldsymbol{\Theta}^*\underline{\mathcal{H}}_m^*(\widehat{\boldsymbol{E}}_1 B - \underline{\mathcal{H}}_m\boldsymbol{\Xi}_m^{\mathrm{gmr}}) \\
&\quad = \boldsymbol{\Theta}^*(\underline{\mathcal{H}}_m^*\widehat{\boldsymbol{E}}_1 B - \underline{\mathcal{H}}_m^*\underline{\mathcal{H}}_m\boldsymbol{\Xi}_m^{\mathrm{gmr}}).
\end{aligned}$$

So the proof is accomplished once we have shown that $\underline{\mathcal{H}}_m^*\underline{\mathcal{H}}_m\boldsymbol{\Xi}_m^{\mathrm{gmr}} = \underline{\mathcal{H}}_m^*\widehat{\boldsymbol{E}}_1 B$. To this end, note that

$$\underline{\mathcal{H}}_m^* = [\mathcal{H}_m^* \,|\, \widehat{\boldsymbol{E}}_m H_{m+1,m}^*], \tag{3.10}$$

which gives $\underline{\mathcal{H}}_m^*\underline{\mathcal{H}}_m = \mathcal{H}_m^*\mathcal{H}_m + \widehat{\boldsymbol{E}}_m H_{m+1,m}^* H_{m+1,m}\widehat{\boldsymbol{E}}_m^*$. Together with (3.9) this shows

$$\begin{aligned}
\underline{\mathcal{H}}_m^*\underline{\mathcal{H}}_m\boldsymbol{\Xi}_m^{\mathrm{gmr}} &= (\mathcal{H}_m^*\mathcal{H}_m + \widehat{\boldsymbol{E}}_m H_{m+1,m}^* H_{m+1,m}\widehat{\boldsymbol{E}}_m^*)\boldsymbol{\Xi}_m^{\mathrm{gmr}} = \mathcal{H}_m^*\widehat{\boldsymbol{E}}_1^{(m)} B \\
&= \underline{\mathcal{H}}_m^*\widehat{\boldsymbol{E}}_1^{(m+1)} B, \qquad \text{(superscripts in } \widehat{\boldsymbol{E}}_1 \text{ indicate the dimension)}
\end{aligned}$$

where the last equality follows from (3.10). ∎

Recall that a matrix $A \in \mathbb{C}^{n\times n}$ is termed *positive real*, if $\mathrm{Re}(x^*Ax) \in \mathbb{C}^+$, the open right half plane, for all $x \neq 0$, and that this concept trivially extends to other inner products than the standard one. A positive real matrix has all of its, possibly non-real, eigenvalues in $\mathbb{C}^+$. For the non-block case ($s = 1$), an important result from [15] (see also [41] and the improvement in [46]), states that if A is positive real, the norm of the m-th GMRES residual is reduced by at least a constant factor independent of m. Our next theorem shows that this extends to the general block case. It uses the following quantities which are well defined and positive if A is positive real with respect to $\langle\cdot,\cdot\rangle_{\mathbb{S}}$:

$$\gamma := \min\left\{\frac{\mathrm{Re}(\langle\boldsymbol{V}, A\boldsymbol{V}\rangle_{\mathbb{S}})}{\langle\boldsymbol{V},\boldsymbol{V}\rangle_{\mathbb{S}}} : \boldsymbol{V} \in \mathbb{C}^{n\times s}, \boldsymbol{V} \neq 0\right\},$$

$$\nu_{\max} := \max\left\{\frac{\langle A\boldsymbol{V}, A\boldsymbol{V}\rangle_{\mathbb{S}}}{\langle\boldsymbol{V},\boldsymbol{V}\rangle_{\mathbb{S}}} : \boldsymbol{V} \in \mathbb{C}^{n\times s}, \boldsymbol{V} \neq 0\right\}.$$

THEOREM 3.5. *Assume that A is positive real with respect to the inner product $\langle\cdot,\cdot\rangle_{\mathbb{S}}$. Then for $m = 1, 2, \ldots$ the block GMRES residuals $\boldsymbol{R}_m^{\mathrm{gmr}} = \boldsymbol{B} - A\boldsymbol{X}_m^{\mathrm{gmr}}$ satisfy*

$$\|\boldsymbol{R}_m^{\mathrm{gmr}}\|_{\mathbb{S}} \leq \left(1 - \frac{\gamma^2}{\nu_{\max}}\right)^{1/2} \left\|\boldsymbol{R}_{m-1}^{\mathrm{gmr}}\right\|_{\mathbb{S}}. \tag{3.11}$$

Proof. Let $P_{m-1} \in \mathbb{P}_{m-1}(\mathbb{S})$ be the residual matrix polynomial for $\boldsymbol{R}_{m-1}^{\text{gmr}}$, i.e., $\boldsymbol{R}_{m-1}^{\text{gmr}} = P_{m-1}(A) \circ \boldsymbol{B}$, and let R be the matrix polynomial $R(z) = I - z(\alpha I)$, where $\alpha \in \mathbb{R}$ is yet to be determined. Because the matrix coefficients in R are scalar multiplies of the identity, we have $(RQ)(A) \circ \boldsymbol{V} = R(A) \cdot (Q(A) \circ \boldsymbol{V})$ for all matrix polynomials Q and all $\boldsymbol{V} \in \mathbb{S}^m$. Since by (3.8) the $\mathbb{S}$-norm of $\boldsymbol{R}_m = P_m(A) \circ \boldsymbol{B}$ is minimal over all polynomials P in $\mathbb{P}_m(\mathbb{S})$ with $P(0) = I$, we have that

$$\|\boldsymbol{R}_m^{\text{gmr}}\|_{\mathbb{S}} \leq \|(RP_{m-1})(A) \circ \boldsymbol{B}\|_{\mathbb{S}} = \|R(A) \cdot (P_{m-1}(A) \circ \boldsymbol{B})\|_{\mathbb{S}} \leq \|R(A)\|_{\mathbb{S}} \left\|\boldsymbol{R}_{m-1}^{\text{gmr}}\right\|_{\mathbb{S}}.$$

Morover, for all $\boldsymbol{V} \in \mathbb{C}^{n \times s}$

$$\begin{aligned}\langle R(A)\boldsymbol{V}, R(A)\boldsymbol{V}\rangle_{\mathbb{S}} &= \langle \boldsymbol{V} - \alpha A\boldsymbol{V}, \boldsymbol{V} - \alpha A\boldsymbol{V}\rangle_{\mathbb{S}} \\ &= \langle \boldsymbol{V}, \boldsymbol{V}\rangle_{\mathbb{S}} - 2\alpha \text{Re}(\langle \boldsymbol{V}, A\boldsymbol{V}\rangle_{\mathbb{S}}) + \alpha^2 \langle A\boldsymbol{V}, A\boldsymbol{V}\rangle_{\mathbb{S}},\end{aligned}$$

which gives

$$\|R(A)\|_{\mathbb{S}}^2 \leq 1 - 2\alpha\gamma + \alpha^2 \nu_{\max}.$$

With $\alpha = \gamma/\nu_{\max}$ minimizing the right-hand side, the inequality (3.11) follows. ∎

As a side remark, let us note that A is positive real with respect to $\langle \cdot, \cdot \rangle_{\mathbb{S}}$ if it is block positive real according to the following definition.

DEFINITION 3.6. *$A \in \mathbb{C}^{n \times n}$ is called* block positive real *if $\langle\langle A\boldsymbol{V}, \boldsymbol{V}\rangle\rangle_{\mathbb{S}} \in \mathbb{S}$ is positive real with respect to the standard inner product for all full rank block vectors $\boldsymbol{V}$ and has at least one eigenvalue with positive real part for all $\boldsymbol{X} \neq 0$.*

If A is positive real with respect to the standard inner product, then it is also positive real for the block inner products corresponding to the global, loop-interchange, and classical paradigms and, more generally, to any derived scalar inner product $\langle \cdot, \cdot \rangle_{\mathbb{S}}$ for which $\langle \boldsymbol{V}, \boldsymbol{W}\rangle_{\mathbb{S}} = \text{trace}\, \boldsymbol{V}^*\boldsymbol{W}$. Thus, Theorem 3.5 applies particularly to that case. Since $\|\cdot\|_{\mathbb{S}}$ then reduces to the Frobenius norm in all these cases, the minimization property (3.8) together with the nestedness of the respective Krylov subspaces gives the following analogue to what was formulated in Theorem 3.3 for block FOM. See also [16, Theorem 2.4].

THEOREM 3.7. *Let $\boldsymbol{R}_m^{\text{Gl}}$, $\boldsymbol{R}_m^{\text{Li}}$, and $\boldsymbol{R}_m^{\text{Cl}}$ denote the residuals of the m-th block GMRES approximations corresponding to the global, loop-interchange, and classical paradigms, respectively. Moreover, let $\langle\langle \cdot, \cdot \rangle\rangle_{\mathbb{S}}$ be a further block inner product for which the corresponding scalar inner product satisfies $\langle \boldsymbol{V}, \boldsymbol{W}\rangle_{\mathbb{S}} = \text{trace}\, \boldsymbol{V}^*\boldsymbol{W}$, and let $\boldsymbol{R}_m^{\mathbb{S}}$ denote the corresponding block GMRES residual. Then*

$$\left\|\boldsymbol{R}_m^{\text{Cl}}\right\|_F \leq \left\|\boldsymbol{R}_m^{\text{Li}}\right\|_F, \left\|\boldsymbol{R}_m^{\mathbb{S}}\right\|_F \leq \left\|\boldsymbol{R}_m^{\text{Gl}}\right\|_F.$$

3.3. Block Radau-Arnoldi. The idea of the Radau-Arnoldi approach is to modify the FOM approach by imposing an additional constraint on the residual that is also independent of $\boldsymbol{B}$. This can be useful, for instance, as a means to use previously built-up information such as in the case of restarts and thus in particular when dealing with matrix functions; see Section 4. Here, we describe the method for linear systems.[1]

[1] The method was introduced for the non-block case in [21] as the Radau-Lanczos method, wherein the name reflects the relationship between Gauß-Radau quadrature and the Lanczos procedure; see [25]. We use "Radau-Arnoldi" here, since we do not require A to be Hermitian positive definite and rely on the (block) Arnoldi process.

We need the polynomials $\widehat{P}_{j-1} \in \mathbb{P}_{j-1}(\mathbb{S})$, $j = 1, \ldots m$, which describe the block Arnoldi vectors $\boldsymbol{V}_j$, $j = 1, \ldots, m$, as

$$\boldsymbol{V}_j = \widehat{P}_{j-1}(A) \circ \boldsymbol{B}, \quad j = 1, \ldots, m.$$

The block Arnoldi relation (2.2), $A\boldsymbol{\mathcal{V}}_m = \boldsymbol{\mathcal{V}}_{m+1}\underline{\mathcal{H}}_m$, directly turns into a corresponding relation for these matrix polynomials

$$z \cdot \left[\widehat{P}_0(z) \mid \cdots \mid \widehat{P}_{m-1}(z)\right] = \left[\widehat{P}_0(z) \mid \cdots \mid \widehat{P}_m(z)\right] \cdot \underline{\mathcal{H}}_m, \tag{3.12}$$

with $\widehat{P}_0 = B^{-1}$.

We now fix an $S \in \mathbb{S}$, and require the residual $\boldsymbol{R}_m^{\mathrm{ra}}$ of the m-th block Radau-Arnoldi approximation $\boldsymbol{X}_m^{\mathrm{ra}} \in \mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B})$ to be $\langle\langle\cdot,\cdot\rangle\rangle_{\mathbb{S}}$-orthogonal to $\mathscr{K}_{m-1}^{\mathbb{S}}(A, \boldsymbol{B})$ (rather than to $\mathscr{K}_m^{\mathbb{S}}(A, \boldsymbol{B})$ as in block FOM),

$$\boldsymbol{R}_m^{\mathrm{ra}} = P_m^{\mathrm{ra}}(A) \circ \boldsymbol{B} \perp_{\langle\langle\cdot,\cdot\rangle\rangle_{\mathbb{S}}} \mathscr{K}_{m-1}^{\mathbb{S}}(A, \boldsymbol{B}), \tag{3.13}$$

and ask $P_m^{\mathrm{ra}}(z) \in \mathbb{P}_m(\mathbb{S})$ to satisfy the additional constraints

$$P_m^{\mathrm{ra}}(S) = 0_s \text{ and } P_m^{\mathrm{ra}}(0) = I_s. \tag{3.14}$$

A matrix polynomial P is *regular* if there exists some $z \in \mathbb{C}$ such that $\det(P(z)) \neq 0$. Residual polynomials are always regular, since they are the identity at 0. A matrix $\widetilde{S} \in \mathbb{C}^{s\times s}$ is called a *solvent* for $P_m \in \mathbb{P}_m(\mathbb{C}^{s\times s})$ if $P_m(\widetilde{S}) = 0$. It is known for regular matrix polynomials that then P_m can be factored as $P_m(z) = (zI - \widetilde{S})P_{m-1}^{\widetilde{S}}(z)$ with $P_{m-1}^{\widetilde{S}} \in \mathbb{P}_{m-1}(\mathbb{C}^{s\times s})$; see [33, Theorem 3.3] and its corollary, as well as [35, Theorem 2.17]. The constraints (3.14) can thus equivalently be formulated as

$$P_m^{\mathrm{ra}} \in \overline{\mathbb{P}}_m^S(\mathbb{S}), \tag{3.15}$$

where

$$\overline{\mathbb{P}}_m^S(\mathbb{S}) := \{P \in \mathbb{P}_m(\mathbb{S}) : P(z) = (zI - S)P_{m-1}^S(z),\ P_{m-1}^S \in \mathbb{P}_{m-1}(\mathbb{S}) \text{ and } P(0) = I_s\}.$$

The following theorem shows that, just as for block GMRES, the block Radau-Arnoldi iterates are modified block FOM iterates in the sense of (3.1).

Theorem 3.8. *Assume that $\widehat{P}_{m-1}(S)$ is nonsingular and define*

$$\widetilde{P}_m = \widehat{P}_m - \widehat{P}_{m-1}\Gamma, \quad \textit{where } \Gamma = \widehat{P}_{m-1}(S)^{-1}\widehat{P}_m(S) \in \mathbb{S}. \tag{3.16}$$

Moreover, assume that $\mathcal{H}_m + \mathcal{M}^{\mathrm{ra}}$ is nonsingular, where $\mathcal{M}^{\mathrm{ra}} = \widehat{\boldsymbol{E}}_m(\Gamma H_{m+1,m})\widehat{\boldsymbol{E}}_m^*$. Then we have

$$\boldsymbol{X}_m^{\mathrm{ra}} = \boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + \mathcal{M}^{\mathrm{ra}})^{-1}\widehat{\boldsymbol{E}}_1 B \tag{3.17}$$

and

$$\boldsymbol{R}_m^{\mathrm{ra}} = \boldsymbol{B} - A\boldsymbol{X}_m^{\mathrm{ra}} = P_m^{\mathrm{ra}}(A) \circ \boldsymbol{B} \textit{ with } P_m^{\mathrm{ra}} = \widetilde{P}_m \cdot \widetilde{P}_m(0)^{-1}, \tag{3.18}$$

where $\widetilde{P}_m(0)$ is nonsingular.

Proof. If we use $\widetilde{P}_m$ instead of $\widehat{P}_m$, an analogue of the block Arnoldi relation (3.12) holds if we add $\Gamma H_{m+1,m}$ to the (m, m) block entry of $\mathcal{H}_m$,

$$z \cdot \left[\widehat{P}_0 \mid \cdots \mid \widehat{P}_{m-1}\right] = \left[\widehat{P}_0 \mid \cdots \mid \widehat{P}_{m-1} \mid \widetilde{P}_m\right] \cdot \underline{\widetilde{\mathcal{H}}}_m,$$

with

$$\underline{\widetilde{\mathcal{H}}}_m = \begin{bmatrix} \widetilde{\mathcal{H}}_m \\ H_{m+1,m}\widehat{\boldsymbol{E}}_m^* \end{bmatrix}, \quad \widetilde{\mathcal{H}}_m = \mathcal{H}_m + \mathcal{M}^{\mathrm{ra}}.$$

Evaluating all matrix polynomials on $(A, \boldsymbol{B})$ with the $\circ$ operator induces a block Arnoldi-type relation for the block vectors $\boldsymbol{V}_{j+1} = \widehat{P}_j(A) \circ \boldsymbol{B}$, $j = 0, \dots, m-1$, and the block vector $\widetilde{\boldsymbol{V}}_{m+1} = \widetilde{P}_m(A) \circ \boldsymbol{B}$:

$$A\left[\boldsymbol{V}_1 \mid \cdots \mid \boldsymbol{V}_m\right] = \left[\boldsymbol{V}_1 \mid \cdots \mid \boldsymbol{V}_m \mid \widetilde{\boldsymbol{V}}_{m+1}\right] \underline{\widetilde{\mathcal{H}}}_m.$$

With this we see that for $\boldsymbol{X}_m^{\mathrm{ra}}$ defined in (3.17) we have

$$\begin{aligned} \boldsymbol{B} - A\boldsymbol{X}_m^{\mathrm{ra}} &= \boldsymbol{B} - A\boldsymbol{\mathcal{V}}_m \widetilde{\mathcal{H}}_m^{-1} \widehat{\boldsymbol{E}}_1 B \\ &= \boldsymbol{B} - [\boldsymbol{\mathcal{V}}_m \mid \widetilde{\boldsymbol{V}}_{m+1}] \begin{bmatrix} \widetilde{\mathcal{H}}_m \\ H_{m+1,m}\widehat{\boldsymbol{E}}_m^* \end{bmatrix} \widetilde{\mathcal{H}}_m^{-1} \widehat{\boldsymbol{E}}_1 B \\ &= \boldsymbol{B} - \boldsymbol{\mathcal{V}}_m \widehat{\boldsymbol{E}}_1 B - \widetilde{\boldsymbol{V}}_{m+1}(H_{m+1,m}\widehat{\boldsymbol{E}}_m^* \widetilde{\mathcal{H}}_m^{-1} \widehat{\boldsymbol{E}}_1 B) \\ &= -\widetilde{\boldsymbol{V}}_{m+1}(H_{m+1,m}\widehat{\boldsymbol{E}}_m^* \widetilde{\mathcal{H}}_m^{-1} \widehat{\boldsymbol{E}}_1 B), \end{aligned}$$

showing that $\boldsymbol{R}_m^{\mathrm{ra}} = P_m^{\mathrm{ra}}(A) \circ \boldsymbol{B}$ with $P_m^{\mathrm{ra}} = \widetilde{P}_m \cdot \widetilde{C}_m$ and $\widetilde{C}_m = -H_{m+1,m}\widehat{\boldsymbol{E}}_m^* \widetilde{\mathcal{H}}_m^{-1} \widehat{\boldsymbol{E}}_1 B$.

To see that $\widetilde{C}_m = \widetilde{P}_m(0)^{-1}$, or, equivalently, that $P_m^{\mathrm{ra}}(0) = I$, we first note that by Remark 2.6, there exists $P_m \in \mathbb{P}_m(\mathbb{S})$, with $P_m(0) = I$ such that $\boldsymbol{R}_m^{\mathrm{ra}} = P_m(A) \circ \boldsymbol{B}$. Now, the uniqueness property stated in Proposition 2.5, reformulated in terms of matrix polynomials, shows that when expressed as $\sum_{i=0}^m \widehat{P}_i \Gamma_i$, the two polynomials P_m^{ra} and P_m have identical coefficients Γ_i. In particular, their values at 0 coincide, thus $P_m^{\mathrm{ra}}(0) = P_m(0) = I$.

By the block Arnoldi process, the block vectors $\boldsymbol{V}_{m+1}$ and $\boldsymbol{V}_m$ are $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$-orthogonal to $\mathscr{K}_{m-1}^{\mathbb{S}}(A, \boldsymbol{B})$ and so is $\widetilde{P}_m(A) \circ \boldsymbol{B} = \widehat{P}_m(A) \circ \boldsymbol{B} + (\widehat{P}_{m-1}(A) \circ \boldsymbol{B})\Gamma = \boldsymbol{V}_{m+1} + \boldsymbol{V}_m \Gamma$. Moreover, $\widetilde{P}_m(S) = 0$. The scaled version $P_m^{\mathrm{ra}} = \widetilde{P}_m \cdot \widetilde{P}_m(0)^{-1}$ of $\widetilde{P}_m$ then satisfies (3.13) as well as (3.14). ∎

Remark 3.9. Since $P_m^{\mathrm{ra}}(z) = (zI - S)P_{m-1}^S(z)$, see (3.15), every eigenvalue of S is a latent root of P_m^{ra}, and thus, by Theorem 2.9, is also an eigenvalue of $\mathcal{H}_m + \mathcal{M}^{\mathrm{ra}}$, including algebraic multiplicity. The block Radau-Arnoldi method can thus be regarded as a modified block FOM method which prescribes the eigenvalues of S as eigenvalues for the modified matrix $\mathcal{H}_m + \mathcal{M}^{\mathrm{ra}}$.

It is always possible to compute $\mathcal{M}^{\mathrm{ra}}$ by evaluating $\widehat{P}_{m-1}(S)$ and $\widehat{P}_m(S)$ using the recurrences (3.12). In the non-block case $s = 1$, there is a more elegant and stable way to obtain $\mathcal{M}^{\mathrm{ra}}$, as is described in [25, 21], for the case that A is self-adjoint. An analogue for the block case holds if S commutes with $\widehat{P}_i(S)$ for $i = 1, \dots, m-1$, which is the case, e.g., if S is a multiple of the identity. Indeed, then, the polynomial block Arnoldi relation (3.12), evaluated at S,

$$S \cdot \left[\widehat{P}_0(S) \mid \cdots \mid \widehat{P}_{m-1}(S)\right] = \left[\widehat{P}_0(S) \mid \cdots \mid \widehat{P}_m(S)\right] \cdot \underline{\mathcal{H}}_m, \tag{3.19}$$

can be rewritten as

$$\left[\widehat{P}_0(S) \mid \cdots \mid \widehat{P}_{m-1}(S)\right](I_m \otimes S) = \left[\widehat{P}_0(S) \mid \cdots \mid \widehat{P}_m(S)\right] \cdot \underline{\mathcal{H}}_m.$$

This gives

$$\left[\widehat{P}_0(S) \mid \cdots \mid \widehat{P}_{m-1}(S)\right](\mathcal{H}_m - I_m \otimes S) = -\widehat{P}_m(S) H_{m+1,m} \widehat{\boldsymbol{E}}_m^*, \tag{3.20}$$

showing that $\Gamma^{-1} = \widehat{P}_m(S)^{-1}\widehat{P}_{m-1}(S)$ is the last block entry of the solution $\boldsymbol{X}$ of the linear system. Written in transposed form, $\boldsymbol{X}(\mathcal{H}_m - I_m \otimes S) = H_{m+1,m}\widehat{\boldsymbol{E}}_m^*$, i.e.,

$$\widehat{P}_m(S)^{-1}\widehat{P}_{m-1}(S) = H_{m+1,m}\widehat{\boldsymbol{E}}_m^*(\mathcal{H}_m - I_m \otimes S)^{-1}\widehat{\boldsymbol{E}}_m.$$

Note that if S does not commute with all the $\widehat{P}_i(S)$, it is not possible to cast (3.12) into a block system with a matrix from $\mathbb{S}^{m\times m}$ and a block right-hand side from $\mathbb{S}^m$.

If A is block self-adjoint with respect to $\langle\!\langle\cdot,\cdot\rangle\!\rangle_{\mathbb{S}}$, the block Radau-Arnoldi method simplifies to the block Radau-Lanczos method. Theorems 2.2 and 2.3 in [21] for the non-block case induce the following convergence result for block Radau-Lanczos. It is formulated using the errors $\boldsymbol{E}_m^{\text{ra}} = A^{-1}\boldsymbol{B} - \boldsymbol{X}_m^{\text{ra}} = A^{-1}\boldsymbol{R}_m^{\text{ra}} = P_m^{\text{ra}}(A) \circ \boldsymbol{X}_*$ where $\boldsymbol{X}_* = A^{-1}\boldsymbol{B}$.

THEOREM 3.10. *Assume that A is block self-adjoint with respect to $\langle\!\langle\cdot,\cdot\rangle\!\rangle_{\mathbb{S}}$ and positive definite with respect to $\langle\cdot,\cdot\rangle_{\mathbb{S}}$. Let $0 < \lambda_{\min} \leq \lambda_{\max}$ denote the smallest and largest eigenvalues of A, respectively, and let $S = \sigma I_s$ with $\sigma > \lambda_{\max}$. Finally, let $A_\sigma = A(\sigma I - A)^{-1}$ and let $\langle\cdot,\cdot\rangle_{A_\sigma\text{-}\mathbb{S}}$ denote the inner product $\langle \boldsymbol{X}, \boldsymbol{Y}\rangle_{A_\sigma\text{-}\mathbb{S}} = \langle A_\sigma \boldsymbol{X}, \boldsymbol{Y}\rangle_{\mathbb{S}}$ with associated norm $\|\cdot\|_{A_\sigma\text{-}\mathbb{S}}$. Then*

$$\|\boldsymbol{E}_m^{\text{ra}}\|_{A_\sigma\text{-}\mathbb{S}} = \min\{\|P_m(A)\circ \boldsymbol{X}_*\|_{A_\sigma\text{-}\mathbb{S}} : P_m \in \overline{\mathbb{P}}_m^S(\mathbb{S})\} \tag{3.21}$$

and

$$\|\boldsymbol{E}_m^{\text{ra}}\|_{A_\sigma\text{-}\mathbb{S}} \leq \left(1 - \frac{\lambda_{\min}}{\sigma}\right)\xi_{m-1}\,\|\boldsymbol{X}_*\|_{A_\sigma\text{-}\mathbb{S}} \quad \text{with } \xi_{m-1} \text{ as in (3.6).} \tag{3.22}$$

Proof. Since for any $P \in \mathbb{P}_m(\mathbb{S})$ and $\boldsymbol{X} \in \mathbb{C}^{n\times s}$ we have $A(P(A)\circ\boldsymbol{X}) = P(A)\circ(A\boldsymbol{X})$, we obtain

$$\begin{aligned}
\|P_m(A)\circ\boldsymbol{X}_*\|_{A_\sigma\text{-}\mathbb{S}}^2 &= \langle A(\sigma I - A)^{-1}P_m(A)\circ\boldsymbol{X}_*, P_m(A)\circ\boldsymbol{X}_*\rangle_{\mathbb{S}} \\
&= \langle AP_m(A)\circ\boldsymbol{X}_*, (\sigma I - A)^{-1}A^{-1}AP_m(A)\circ\boldsymbol{X}_*\rangle_{\mathbb{S}} \\
&= \langle P_m(A)\circ A\boldsymbol{X}_*, (\sigma I - A)^{-1}A^{-1}P_m(A)\circ A\boldsymbol{X}_*\rangle_{\mathbb{S}} \\
&= \langle P_m(A)\circ\boldsymbol{B}, (\sigma I - A)^{-1}A^{-1}P_m(A)\circ\boldsymbol{B}\rangle_{\mathbb{S}}.
\end{aligned}$$

Now observe that $P_m \in \overline{\mathbb{P}}_m^S(\mathbb{S})$ can be written as $P_m = P_m^{\text{ra}} + T_m$ where $T_m = P_m - P_m^{\text{ra}}$ satisfies $T_m(S) = 0$ and $T_m(0) = 0$, implying $T_m(z) = (zI - S)zT_{m-2}^S(z)$ with $T_{m-2}^S \in \mathbb{P}_{m-2}(\mathbb{S})$. Also note that for any $Q \in \mathbb{P}_m(\mathbb{S})$ and $P(z) = (zI_s - \sigma I)Q(z)$ we have that $P(A)\circ\boldsymbol{B} = (\sigma I_n - A)\cdot(Q(A)\circ\boldsymbol{B})$, an equality which has no counterpart if S is not of the form σI. Given this, for any $P_m(z) = P_m^{\text{ra}}(z) + (zI - \sigma I)zT_{m-2}^S$, we obtain that

$$\begin{aligned}
&\langle P_m(A)\circ\boldsymbol{B}, (\sigma I - A)^{-1}A^{-1}(P_m(A)\circ\boldsymbol{B})\rangle_{\mathbb{S}} \\
&\quad= \langle P_m^{\text{ra}}(A)\circ\boldsymbol{B}, (\sigma I - A)^{-1}A^{-1}(P_m^{\text{ra}}(A)\circ\boldsymbol{B})\rangle_{\mathbb{S}} \\
&\qquad+ \langle P_m^{\text{ra}}(A)\circ\boldsymbol{B}, (\sigma I - A)^{-1}A^{-1}(\sigma I - A)A(T_{m-2}^S(A)\circ\boldsymbol{B})\rangle_{\mathbb{S}} \\
&\qquad+ \langle(\sigma I - A)A(T_{m-2}^S(A)\circ\boldsymbol{B}), (\sigma I - A)^{-1}A^{-1}[P_m^{\text{ra}}(A)\circ\boldsymbol{B}]\rangle_{\mathbb{S}} \\
&\qquad+ \langle(\sigma I - A)A(T_{m-2}^S(A)\circ\boldsymbol{B}), (\sigma I - A)^{-1}A^{-1}(\sigma I - A)A(T_{m-2}^S(A)\circ\boldsymbol{B})\rangle_{\mathbb{S}}.
\end{aligned}$$

Herein, the second summand $\langle P_m^{\mathrm{ra}}(A) \circ \boldsymbol{B}, T_{m-2}^S(A) \circ \boldsymbol{B}\rangle_{\mathbb{S}}$ vanishes due to the variational characterization (3.13) of the block Radau-Arnoldi method, and so does the third summand, which is equal to $\langle T_{m-2}^S(A) \circ \boldsymbol{B}, P_m^{\mathrm{ra}}(A) \circ \boldsymbol{B}\rangle_{\mathbb{S}}$. Finally, the fourth summand equals $\langle (\sigma I - A)A(T_{m-2}^S(A) \circ \boldsymbol{B}), T_{m-2}^S(A) \circ \boldsymbol{B}\rangle_{\mathbb{S}}$ and is thus non-negative, since $(\sigma I - A)A$ is self-adjoint and positive definite with respect to $\langle \cdot, \cdot \rangle_{\mathbb{S}}$. This proves (3.21).

The estimate (3.22) follows from results in [21] and [22]. The proof of Theorem 2.3 in [21] constructs a scalar polynomial $p_m(z)$ of degree m with $p_m(\sigma) = 0$ and $p_m(0) = 1$ for which $\max_{\lambda \in \mathrm{spec}(A)} |p_m(\lambda)| \leq \left(1 - \frac{\lambda_{\min}}{\sigma}\right) \xi_{m-1}$. Associating with $p_m(z) = \sum_{i=0}^m c_i z^i$ the matrix polynomial

$$P_m(z) = \sum_{i=0}^{m} z^i \cdot (c_i I_s) \in \overline{\mathbb{P}}_m^S(\mathbb{S}),$$

we have that $P_m(A) \circ \boldsymbol{X}_* = p_m(A)\boldsymbol{X}_*$, and Lemma 3.6 in [22] shows that the operator norm $\|p_m(A)\|_{A_\sigma\text{-}\mathbb{S}}$ is given as $\|p_m(A)\|_{A_\sigma\text{-}\mathbb{S}} = \max_{\lambda \in \mathrm{spec}(A)} |p_m(\lambda)|$. Putting things together gives (3.22). ∎

The variational characterization (3.21), together with the nestedness of the respective block Krylov subspaces, gives the following comparison result in analogy to Theorems 3.3 and 3.7.

THEOREM 3.11. *Under the assumptions of Theorem 3.10, let* $\boldsymbol{E}_m^{\mathrm{Gl}}$, $\boldsymbol{E}_m^{\mathrm{Li}}$ *and* $\boldsymbol{E}_m^{\mathrm{Cl}}$ *denote the errors of the m-th block Radau-Arnoldi approximations corresponding to the global, loop-interchange, and classical paradigms, respectively. Moreover, let* $\langle\langle \cdot, \cdot \rangle\rangle_{\mathbb{S}}$ *be a block inner product for which the corresponding scalar inner product satisfies* $\langle \boldsymbol{V}, \boldsymbol{W} \rangle_{\mathbb{S}} = \mathrm{trace}\, \boldsymbol{V}^* \boldsymbol{W}$ *and denote* $\boldsymbol{E}_m^{\mathbb{S}}$ *the error of the corresponding block Radau-Arnoldi iterate. Then*

$$\left\|\boldsymbol{E}_m^{\mathrm{Cl}}\right\|_{A_\sigma\text{-}\mathbb{S}} \leq \left\|\boldsymbol{E}_m^{\mathrm{Li}}\right\|_{A_\sigma\text{-}\mathbb{S}}, \left\|\boldsymbol{E}_m^{\mathbb{S}}\right\|_{A_\sigma\text{-}\mathbb{S}} \leq \left\|\boldsymbol{E}_m^{\mathrm{Gl}}\right\|_{A_\sigma\text{-}\mathbb{S}}.$$

As a last remark we note that a result similar to Theorem 3.10 holds if we take $0 < \sigma < \lambda_{\min}$, where $A(\sigma I - A)^{-1}$ is replaced by $A(A - \sigma I)^{-1}$, and the factor $(1 - \lambda_{\min}/\sigma)$ in (3.22) by $|1 - \lambda_{\max}/\sigma|$ (which is larger than 1).

4. Shifted systems and matrix functions. We now turn to the task of computing solutions for a family of shifted block linear systems

$$(A + tI)\boldsymbol{X}(t) = \boldsymbol{B}, \quad t \text{ from some finite subset of } \mathbb{C}, \tag{4.1}$$

and the evaluation of a matrix function acting on a block vector

$$\boldsymbol{F} = f(A)\boldsymbol{B}.$$

The introductions in [45, 47] offer a thorough discussion of the literature pertaining to (4.1). We refer to the book [29] for a general treatment of matrix functions and just note that for $f : D \subset \mathbb{C} \to \mathbb{C}$ and $A \in \mathbb{C}^{n \times n}$, the matrix function $f(A) \in \mathbb{C}^{n \times n}$ is defined if D contains the spectrum of A and f is $\ell - 1$ times differentiable at every eigenvalue with multiplicity ℓ in the minimal polynomial of A. Often $f(A)$ can be expressed as an integral, and we here concentrate on the case of a Stieltjes function, meaning that f that can be written as a Riemann-Stieltjes integral

$$f : \mathbb{C} \setminus (-\infty, 0] \to \mathbb{C}, \quad f(z) = \int_0^\infty \frac{1}{z + t} \, \mathrm{d}\mu(t), \tag{4.2}$$

where μ is monotonically increasing and nonnegative on $[0,\infty)$ and $\int_0^\infty \frac{1}{t+1}\,\mathrm{d}\mu(t) < \infty$. Note in particular that $f(z) = z^{-\alpha}$ is a Stieltjes function for $\alpha \in (0,1)$[27], and that $f(A)$ is defined if A has no eigenvalue in $(-\infty, 0]$; see, e.g.,[19]. Given a Stieltjes function f, we have that

$$f(A)\boldsymbol{B} = \int_0^\infty (A + tI)^{-1}\boldsymbol{B}\,\mathrm{d}\mu(t),$$

thus establishing the close connection with (4.1). This connection is also present if f is holomorphic on a domain D containing the spectrum of A, since by Cauchy's integral theorem we then have for a contour Γ in D enclosing the spectrum of A that

$$f(z) = \frac{1}{2\pi i}\int_\Gamma \frac{f(t)}{z-t}\,\mathrm{d}t \;\Rightarrow\; f(A)\boldsymbol{B} = \frac{1}{2\pi i}\int_\Gamma f(t)(A - tI)^{-1}\boldsymbol{B}\,\mathrm{d}t.$$

4.1. Block Krylov subspace approximations. The block Arnoldi process Algorithm 2.1 is shift-invariant in the sense that if we start with the same block vector $\boldsymbol{B}$ but with matrix $A + tI$ instead of A we retrieve exactly the same block Arnoldi vectors $\boldsymbol{V}_k, k = 1, \ldots, m$, with the block upper Hessenberg matrix changing from $\mathcal{H}_m$ to $\mathcal{H}_m + tI$. For a family of shifted linear systems (4.1) we can thus perform the block Arnoldi process only once (for A and $\boldsymbol{B}$) and then compute the block Krylov subspace approximations for the various t simultaneously. Within our general framework from Section 3, the respective iterates $\boldsymbol{X}_m(t)$ are then given as

$$\boldsymbol{X}_m(t) = \boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + tI + \mathcal{M}_t)^{-1}\widehat{\boldsymbol{E}}_1 B, \quad \text{where } \mathcal{M}_t = \boldsymbol{M}_t\widehat{\boldsymbol{E}}_m^*,\ \boldsymbol{M}_t \in \mathbb{S}^m. \qquad (4.3)$$

If $\mathcal{M}_t$ does not depend on t, $\mathcal{M}_t = \mathcal{M}$, we can use this in the integral representation for the matrix function case to obtain the block Krylov subspace approximation $\boldsymbol{F}_m$ for $f(A)\boldsymbol{B}$, namely,

$$\boldsymbol{F}_m := \int_0^\infty \boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + tI + \mathcal{M})^{-1}\widehat{\boldsymbol{E}}_1 B\,\mathrm{d}\mu(t)$$

$$= \boldsymbol{\mathcal{V}}_m \int_0^\infty (\mathcal{H}_m + tI + \mathcal{M})^{-1}\,\mathrm{d}\mu(t)\,\widehat{\boldsymbol{E}}_1 B \;=\; \boldsymbol{\mathcal{V}}_m f(\mathcal{H}_m + \mathcal{M})\widehat{\boldsymbol{E}}_1 B.$$

For $\mathcal{M} = 0$ this reduces to the standard block Arnoldi approximation $\boldsymbol{\mathcal{V}}_m f(\mathcal{H}_m)\widehat{\boldsymbol{E}}_1 B$, termed $\mathrm{B(FOM)}^2$ (block FOM for functions of matrices) in [22].

4.2. Restarts and cospatiality. A crucial question now is whether we can perform restarts efficiently for shifted systems as well as for matrix functions. If convergence is not very fast, restarts become mandatory in the matrix function case, since there the entire block Krylov basis $\boldsymbol{\mathcal{V}}_m$ is always needed to obtain $\boldsymbol{F}_m$. A similar situation holds for the shifted system case, except when A is block self-adjoint and positive definite. In such a case, we can arrange a block CG method in a manner which uses short recurrences in both, the block Lanczos process as well as the update of the iterates.

To take advantage of the shifted nature of our systems for a restart after m iterations, we here aim for *cospatial* block residuals in the sense that

$$\boldsymbol{R}_m(t) = \boldsymbol{B} - (A + tI)\boldsymbol{X}_m(t) = \boldsymbol{R}_m(0)C_m(t), \text{ where } C_m(t) \in \mathbb{S}, \qquad (4.4)$$

Then, after a restart, the block Arnoldi process for the new cycle needs again to be computed only once for all t, now starting with the vector $\boldsymbol{R}_m(0)$ (or any other block vector which is cospatial to $\boldsymbol{R}_m(0)$). In the shifted system case, the computed approximations for $(A+tI)^{-1}\boldsymbol{R}_m(t)$ are to be multiplied with the cospatiality factor $C_m(t)$ from the right to obtain the correction to be added to $\boldsymbol{X}_m(t)$ from the first cycle, and we can proceed similarly for all further cycles, updating the products of the cospatiality factors. This approach was also pursued in [47] for block GMRES; more involved approaches which side-step the need for cospatial residuals include [45].

In the matrix function case, having cospatial residuals allows us to find an expression for the error of the block Krylov subspace approximation as

$$\begin{aligned}\boldsymbol{F}-\boldsymbol{F}_m &= \int_0^\infty (A+tI)^{-1}\boldsymbol{B} - \boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + tI + \mathcal{M})^{-1}\widehat{\boldsymbol{E}}_1 B \,\mathrm{d}\mu(t)\\ &= \int_0^\infty (A+tI)^{-1}\boldsymbol{R}_m(t)\,\mathrm{d}\mu(t) \qquad (4.5)\\ &= \int_0^\infty (A+tI)^{-1}\boldsymbol{R}_m(0)C_m(t)\,\mathrm{d}\mu(t).\end{aligned}$$

Interestingly, the latter expression does not represent a standard matrix function applied to a block vector. Rather, the situation is analogous to the matrix polynomial case: using the *matrix integral* $J(z) : \mathbb{C}\setminus(-\infty,0] \to \mathbb{S}$, $J(z) = \int_0^\infty \frac{1}{z+t} C_m(t)\,\mathrm{d}\mu(t)$ we can express $\boldsymbol{F}-\boldsymbol{F}_m$ above as

$$\boldsymbol{F}-\boldsymbol{F}_m = J(A)\circ \boldsymbol{R}_m(0) := \int_0^\infty (A+tI)^{-1}\boldsymbol{R}_m(0)C_m(t)\,\mathrm{d}\mu(t).$$

The following theorem shows that we indeed have cospatial residuals if $\mathcal{M}_t$ in (4.3) does not depend on t. It also shows that the shifted residuals are cospatial to the block vector

$$\boldsymbol{U}_m := \boldsymbol{\mathcal{V}}_{m+1}\begin{bmatrix}\boldsymbol{M}\\ -H_{m+1,m}\end{bmatrix}, \qquad (4.6)$$

with cospatiality factors that are easily available. The theorem thus also suggests that algorithmically one should build restarts upon $\boldsymbol{U}_m$ rather than $\boldsymbol{R}_m(0)$, since the former is easily computed. We again use square brackets to denote block components, specifically $[\boldsymbol{\Xi}]_m := \widehat{\boldsymbol{E}}_m^*\boldsymbol{\Xi}$ for $\boldsymbol{\Xi} \in \mathbb{S}^m$.

THEOREM 4.1. *Let* $\mathcal{M} = \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*$ *with* $\boldsymbol{M} \in \mathbb{S}^m$ *and let*

$$\boldsymbol{\Xi}_m(t) = (\mathcal{H}_m + \mathcal{M} + tI)^{-1}\widehat{\boldsymbol{E}}_1 B$$

be the block coefficient vector for the block Krylov subspace approximation $\boldsymbol{X}_m(t) = \boldsymbol{\mathcal{V}}_m\boldsymbol{\Xi}_m(t)$ *of the linear system* (4.1). *Then with* $\boldsymbol{U}_m$ *as in* (4.6) *it holds that*

$$\boldsymbol{R}_m(t) = \boldsymbol{U}_m[\boldsymbol{\Xi}_m(t)]_m. \qquad (4.7)$$

Proof. The block Arnoldi relation (2.2) gives

$$\begin{aligned}\boldsymbol{R}_m(t) &= \boldsymbol{B} - \boldsymbol{\mathcal{V}}_{m+1}\left(\underline{\mathcal{H}}_{m+1} + t\begin{bmatrix} I\\0\end{bmatrix}\right)\boldsymbol{\Xi}_m(t)\\ &= \boldsymbol{\mathcal{V}}_{m+1}\left(\begin{bmatrix}\widehat{\boldsymbol{E}}_1 B\\ 0\end{bmatrix} - \left(\underline{\mathcal{H}}_{m+1} + t\begin{bmatrix} I\\0\end{bmatrix}\right)\boldsymbol{\Xi}_m(t)\right)\\ &= \boldsymbol{\mathcal{V}}_{m+1}\begin{bmatrix}\widehat{\boldsymbol{E}}_1 B - (\mathcal{H}_m + tI)\boldsymbol{\Xi}_m(t)\\ -H_{m+1,m}[\boldsymbol{\Xi}_m(t)]_m\end{bmatrix}.\end{aligned}$$

Herein, $\widehat{\boldsymbol{E}}_1 B - (\mathcal{H}_m + tI)\Xi_m(t) = \boldsymbol{M}[\Xi_m(t)]_m$, since by the definition of $\Xi_m(t)$

$$\widehat{\boldsymbol{E}}_1 B - (\mathcal{H}_m + tI)\Xi_m(t) - \boldsymbol{M}[\Xi_m(t)]_m = \widehat{\boldsymbol{E}}_1 B - (\mathcal{H}_m + tI + \boldsymbol{M}\widehat{\boldsymbol{E}}_m^*)\Xi_m(t) = 0.$$

This shows (4.7). ∎

A consequence of this theorem is that the cospatiality factors $C_m(t)$ for the residuals from (4.4) are given as $C_m(t) = [\Xi_m(0)]_m^{-1}[\Xi_m(t)]_m$.

Assume now that we solve the block linear system $A\boldsymbol{X} = \boldsymbol{B}$ with a restarted modified block FOM method, performing cycles of length m. We use an upper index (k) to denote quantities belonging to cycle k. At the end of cycle $k+1$ we update the iterate $\boldsymbol{X}_m^{(k)}(0)$ by an approximate solution $\boldsymbol{Z}_m^{(k)}(0)$ of the residual equation $A\boldsymbol{Z}^{(k)}(0) = \boldsymbol{R}_m^{(k)}(0) := \boldsymbol{B} - A\boldsymbol{X}_m^{(k)}(0)$ which, given (4.7), we obtain as $\widetilde{\boldsymbol{Z}}_m^{(k)}(0)[\Xi_m^{(k)}(0)]_m$ with $\widetilde{\boldsymbol{Z}}_m^{(k)}(0)$ being the modified block FOM approximation for the solution of $A\widetilde{\boldsymbol{Z}}^{(k)}(0) = \boldsymbol{U}_m^{(k)}$,

$$\boldsymbol{X}_m^{(k+1)}(0) = \boldsymbol{X}_m^{(k)}(0) + \widetilde{\boldsymbol{Z}}_m^{(k)}(0)[\Xi_m^{(k)}(0)]_m.$$

Likewise, the iterates for the restarted method for the shifted linear system $(A + tI)\boldsymbol{X} = \boldsymbol{B}$ are obtained as

$$\boldsymbol{X}_m^{(k+1)}(t) = \boldsymbol{X}_m^{(k)}(t) + \widetilde{\boldsymbol{Z}}_m^{(k)}[\Xi_m^{(k)}(t)]_m,$$

and the block residuals $\boldsymbol{R}_m^{(k)}(t) = \boldsymbol{B} - A\boldsymbol{X}_m^{(k)}(t)$ are given as

$$\boldsymbol{R}_m^{(k)}(t) = \boldsymbol{U}_m^{(k)} G_m^{(k)}(t) \text{ with } G_m^{(k)}(t) = [\Xi_m^{(k)}(t)]_m \cdot [\Xi_m^{(k-1)}(t)]_m \cdots [\Xi_m^{(1)}(t)]_m. \quad (4.8)$$

Taking integrals over t, we define

$$\boldsymbol{F}_m^{(k)} := \int_0^\infty \boldsymbol{X}_m^{(k)}(t)\,\mathrm{d}\mu(t)$$

as the restarted modified block FOM approximation for the matrix Stieltjes function $f(A)\boldsymbol{B}$. The above results directly give

$$\begin{aligned} f(A)\boldsymbol{B} - \boldsymbol{F}_m^{(k)} &= \int_0^\infty (A+tI)^{-1}\boldsymbol{B} - \boldsymbol{X}_m^{(k)}(t)\,\mathrm{d}\mu(t) \quad (4.9)\\ &= \int_0^\infty (A+tI)^{-1}\left(\boldsymbol{B} - (A+tI)\boldsymbol{X}_m^{(k)}(t)\right)\mathrm{d}\mu(t)\\ &= \int_0^\infty (A+tI)^{-1}\boldsymbol{U}_m^{(k)} G_m^{(k)}(t)\,\mathrm{d}\mu(t) \end{aligned}$$

as a representation for the error. We summarize all this in the following theorem, where we use the matrix integrals

$$J_m^{(0)}(z) := \int_0^\infty (z+t)^{-1} I_s\,\mathrm{d}\mu(t), \;\; J_m^{(k)}(z) := \int_0^\infty (z+t)^{-1} G_m^{(k)}(t)\,\mathrm{d}\mu(t),\; k = 1, 2, \ldots,$$

with $G_m^{(k)}(t) \in \mathbb{S}$ from (4.8).

THEOREM 4.2. *Let f be a Stieltjes function, $f(z) = \int_0^\infty (z+t)^{-1}\,\mathrm{d}\mu$ and put $\boldsymbol{F}_m^{(0)} = 0$. For $k = 0, 1, \ldots$, set the k-th modified block FOM correction to be*

$$\boldsymbol{D}_m^{(k)} := \boldsymbol{\mathcal{V}}_m^{(k+1)} J_m^{(k)}\big(\mathcal{H}_m^{(k+1)} + \mathcal{M}^{(k+1)}\big) \circ \widehat{\boldsymbol{E}}_1 B^{(k+1)}, \quad (4.10)$$

such that $\boldsymbol{F}_m^{(k+1)} = \boldsymbol{F}_m^{(k)} + \boldsymbol{D}_m^{(k)}$. *Then for* $k = 0, 1, \ldots,$ *the* $k+1$*-st modified block FOM error* $\boldsymbol{D}^{(k+1)} := f(A)\boldsymbol{B} - \boldsymbol{F}_m^{(k+1)}$ *is given as*

$$\boldsymbol{D}^{(k+1)} = J_m^{(k+1)}(A) \circ \boldsymbol{U}_m^{(k+1)}. \tag{4.11}$$

Algorithm 4.1 summarizes how to implement a modified block FOM method for functions of matrices, from now on termed *modified B(FOM)*^{2}. It encounters the same preallocation issues as [22, Algorithm 2] in the case that the nodes of the quadrature are not fixed a priori.

Algorithm 4.1 Modified B(FOM)^2 for functions of matrices with restarts

1: Given f, A, $\boldsymbol{B} = \boldsymbol{U}_m^{(0)}$, $\mathbb{S}$, $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$, N, m, `tol`
2: **for** $k = 0, 1, \ldots,$ until convergence **do** {cycle $k+1$}
3: Run Algorithm 2.1 with inputs A, $\boldsymbol{U}_m^{(k)}$, $\mathbb{S}$, $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$, N, and m, store $\boldsymbol{\mathcal{V}}_{m+1}^{(k+1)}$ in place of the previous basis $\boldsymbol{\mathcal{V}}_{m+1}^{(k)}$, store $B^{(k+1)}$
4: Compute $\widetilde{\boldsymbol{D}}_m^{(k)} := \boldsymbol{\mathcal{V}}_m^{(k+1)} J_m^{(k)}\big(\mathcal{H}_m^{(k+1)} + \mathcal{M}^{(k+1)}\big) \circ \widehat{\boldsymbol{E}}_1$, where $J_m^{(k)}$ is evaluated via quadrature. This requires the computation of the cospatial factors $G_m^{(k)}(t) = [\boldsymbol{\Xi}_m^{(k)}(t)]_m [\boldsymbol{\Xi}_m^{(k-1)}(t)]_m \cdots [\boldsymbol{\Xi}_m^{(1)}(t)]_m$ (see (4.8)) at a set of quadrature nodes, which could be variable
5: Update $\boldsymbol{F}_m^{(k+1)} = \boldsymbol{F}_m^{(k)} + \widetilde{\boldsymbol{D}}_m^{(k)}$
6: Store $H_{m+1,m}^{(k+1)}$, $\mathcal{M}^{(k+1)}$
7: Compute $\boldsymbol{U}_m^{(k+1)} = \boldsymbol{\mathcal{V}}_M^{(k+1)} \begin{bmatrix} \mathcal{M}^{(k+1)} \\ -H_{m+1,m}^{(k+1)} \end{bmatrix}$
8: **end for**
9: **return** $\boldsymbol{F}_m^{(k+1)}$

In the following sections, we discuss special instances of Algorithm 4.1 for the different modifications analyzed in Section 3.

4.3. Shifted block FOM and B(FOM)^2. For any t, the block FOM iterates that approximate the solution of (4.1) are given by $\boldsymbol{X}_m^{\text{fom}}(t) = \boldsymbol{\mathcal{V}}_m \boldsymbol{\Xi}_m^{\text{fom}}(t)$ with $\boldsymbol{\Xi}_m^{\text{fom}}(t) = (\mathcal{H}_m + tI)^{-1} \widehat{\boldsymbol{E}}_1 B$, so we have that $\boldsymbol{M} = 0$ for all t. Theorem 4.1 shows that the residuals $\boldsymbol{R}_m^{\text{fom}}(t)$ are all cospatial to $\boldsymbol{U}_m^{\text{fom}} = -\boldsymbol{V}_{m+1} H_{m+1,m}$, i.e., to $\boldsymbol{V}_{m+1}$. If A is self-adjoint and positive definite with respect to $\langle \cdot, \cdot \rangle_{\mathbb{S}}$, [22] uses the bound (3.5) for every shift $t \geq 0$ to obtain a convergence result for restarted block FOM for families of shifted linear systems as well as for unmodified B(FOM)^2 for Stieltjes functions of matrices; see [22, Theorem 4.5]. (Note that unmodified B(FOM)^2 is equivalent to Algorithm 4.1 with $\boldsymbol{M} = 0$; cf. [22, Algorithm 2].)

4.4. Shifted block GMRES and harmonic block Arnoldi for matrix functions. The situation is different for block GMRES: From (3.9) we have $\boldsymbol{X}_m^{\text{gmr}}(t) = \boldsymbol{\mathcal{V}}_m \boldsymbol{\Xi}_m^{\text{gmr}}(t)$ with

$$\boldsymbol{\Xi}^{\text{gmr}}(t) = (\mathcal{H}_m + tI + \mathcal{M}^{\text{gmr}}(t))^{-1} \widehat{\boldsymbol{E}}_1 B,$$

where

$$\mathcal{M}^{\text{gmr}}(t) = \boldsymbol{M}^{\text{gmr}}(t) \widehat{\boldsymbol{E}}_m^*, \text{ and } \boldsymbol{M}^{\text{gmr}}(t) = (\mathcal{H}_m + tI)^{-*} \widehat{\boldsymbol{E}}_m H_{m+1,m}^* H_{m+1,m},$$

showing that $\boldsymbol{M}^{\text{gmr}}(t)$ indeed depends on t. In order to maintain cospatial residuals for shifted linear systems, one thus has to pick one value for t, typically $t = 0$, for which "true" block GMRES is performed, giving the block vector $\boldsymbol{M}$. This same block vector is then used for all the other shifts to obtain the block iterates according to (3.1). These block iterates are *not* the block GMRES iterates for the shifted system, so their block residuals do not satisfy the minimization property (3.8). They are, however, all cospatial to $\boldsymbol{U}_m$ from (4.6) with $\boldsymbol{M} = \boldsymbol{M}^{\text{gmr}}(0)$.

In this manner we can efficiently perform restarts for families of shifted linear systems as well as for Stieltjes functions of matrices. In the non-block case, this approach goes back to [17] for families of shifted systems and to [19] for Stieltjes functions of matrices. In accordance with [19], the resulting method for matrix functions is referred to as the *harmonic block Arnoldi* method.

If we were to transfer the convergence analysis from [22] to the shifted block GMRES case, we would need a result analogous to Theorem 3.5 for the iterates of the shifted systems, which are not "true" block GMRES iterates. It seems hard to find the right analogue, and we could obtain only partial results based on the following theorem which is also of interest on its own. The theorem uses shifted matrix polynomials, where for $P(z) = \sum_{i=0}^m z^i \Gamma_i$ its shifted counterpart $P^{(t)}(z)$ is defined as

$$P^{(t)}(z) := P(z+t) = \sum_{i=0}^{m} z^i \Gamma_i^{(t)} \text{ with } \Gamma_i^{(t)} = \sum_{j=i}^{m} \tbinom{j}{i} t^{j-i} \Gamma_j. \tag{4.12}$$

Note that for $\boldsymbol{V} \in \mathbb{C}^{n \times s}$ we have

$$P^{(-t)}(A+tI) \circ \boldsymbol{V} = P(A) \circ \boldsymbol{V}.$$

The following theorem gives an alternative representation of the cospatiality factors $C_m(t)$ in terms of the residual matrix polynomial.

THEOREM 4.3. *Let $P(z) \in \mathbb{P}_m(\mathbb{S})$ be the matrix polynomial expressing the residual $\boldsymbol{R}_m(0) = \boldsymbol{B} - A\boldsymbol{X}_m(0)$ with $\boldsymbol{X}_m(0) = \boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + \mathcal{M})^{-1}\widehat{\boldsymbol{E}}_1 B$ as $\boldsymbol{R}_m(0) = P(A) \circ \boldsymbol{B}$ and assume that for some $t \in \mathbb{C}$ the matrix $P(-t) \in \mathbb{S}$ is nonsingular. Then $\mathcal{H}_m + \mathcal{M} + tI$ is nonsingular, and the block residual $\boldsymbol{R}_m(t) = \boldsymbol{B} - (A+tI)\boldsymbol{X}_m(t)$ with $\boldsymbol{X}_m(t) = \boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + \mathcal{M} + tI)^{-1}\widehat{\boldsymbol{E}}_1 B$ satisfies*

(i) $\boldsymbol{R}_m(t) = P_t(A+tI) \circ \boldsymbol{B}$ with $P_t(z) := P^{(-t)}(z) \cdot P(-t)^{-1}$.

(ii) $\boldsymbol{R}_m(t) = \boldsymbol{R}_m(0) C_m(t)$ with $C_m(t) = P(-t)^{-1}$.

Proof. We first note that (ii) follows immediately once (i) is established, since

$$\begin{aligned} P_t(A+tI) \circ \boldsymbol{B} &= \left(P^{(-t)}(A+tI) \cdot P(-t)^{-1}\right) \circ \boldsymbol{B} \\ &= \left(P(A) \cdot P(-t)^{-1}\right) \circ \boldsymbol{B} \,=\, (P(A) \circ \boldsymbol{B}) \cdot P(-t)^{-1}. \end{aligned}$$

To prove (i), we systematically use the polynomial exactness property formulated in Theorem 2.7. We have $\boldsymbol{X}_m(0) = Q(A)\boldsymbol{B}$, where the matrix polynomial $Q \in \mathbb{P}_{m-1}(\mathbb{S})$ interpolates $f(z) = z^{-1}$ on the pair $(\mathcal{H}_m + \mathcal{M}, \widehat{\boldsymbol{E}}_1 B)$. The matrix residual polynomial $P(z)$ is thus given as $P(z) = I - zQ(z)$ and we have that

$$P(\mathcal{H}_m + \mathcal{M}) \circ (\widehat{\boldsymbol{E}}_1 B) = 0.$$

Now, the matrix polynomial $P_t(z)$ defined in (i) satisfies

$$\begin{aligned} P_t(\mathcal{H}_m + \mathcal{M} + tI) \circ (\widehat{\boldsymbol{E}}_1 B) &= \left(P(\mathcal{H}_m + \mathcal{M}) \cdot P(-t)^{-1}\right) \circ (\widehat{\boldsymbol{E}}_1 B) \\ &= \Big(P(\mathcal{H}_m + \mathcal{M}) \circ (\widehat{\boldsymbol{E}}_1 B)\Big) \cdot P(-t)^{-1} \,=\, 0, \end{aligned} \tag{4.13}$$

and since $P_t \in \mathbb{P}_m(\mathbb{S})$ with $P_t(0) = I$, we can represent it as $P_t(z) = I - zQ_t(z)$ with $Q_t \in \mathbb{P}_{m-1}(\mathbb{S})$. Equation (4.13) then shows that Q_t interpolates $f(z) = z^{-1}$ on the pair $(\mathcal{H}_m + \mathcal{M} + tI, \widehat{\boldsymbol{E}}_1 B)$, which means that $\boldsymbol{X}_m(t) = \boldsymbol{\mathcal{V}}_m(\mathcal{H}_m + \mathcal{M} + tI)^{-1}\widehat{\boldsymbol{E}}_1 B$ is given as $\boldsymbol{X}_m(t) = Q_t(A) \circ \boldsymbol{B}$ and thus $\boldsymbol{R}_m(t) = P_t(A) \circ \boldsymbol{B}$. ∎

COROLLARY 4.4. *Assume that $\mathcal{H}_m + \mathcal{M}$ has all its eigenvalues in $\mathbb{C}^+$ and let $t \geq 0$. Then the cospatiality factors $C_m(t) \in \mathbb{S}$ from Theorem 4.3 satisfy*

$$|\det(C_m(t))| \leq 1.$$

Irrespective of the block inner product $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$, this holds in particular if A is positive real with respect to the standard inner product and $\mathcal{M} = 0$ (block FOM) or $\mathcal{M} = \mathcal{M}^{\mathrm{gmr}} = \mathcal{H}_m^{-*}(\widehat{\boldsymbol{E}}_m H_{m+1,m}^* H_{m+1,m} \widehat{\boldsymbol{E}}_m^*)$ (block GMRES).

Proof. Let $\lambda_i \in \mathbb{C}^+, i = 1, \ldots, ms$, denote the eigenvalues of $\mathcal{H}_m + \mathcal{M}$. By the result on the latent roots from Theorem 2.9 we have $\det(P(z)) = \prod_{i=1}^{ms}(1 - \frac{z}{\lambda_i})$, which gives that

$$|\det(P(-t))| = \prod_{i=1}^{ms} |1 + \tfrac{t}{\lambda_i}|.$$

For $t > 0$, since $\mathrm{Re}(\lambda_i) > 0$, we have $\mathrm{Re}(\frac{t}{\lambda_i}) > 0$ and thus $|1 + \frac{t}{\lambda_i}| > 1$ for all i. This gives $|\det(P(-t)| > 1$ and thus $|\det(C_m(t))| = |\det(P(-t)^{-1})| < 1$.

To prove the remaining part of the corollary, assume that A is positive real. By the block Arnoldi relation (2.2) we have for $x \in \mathbb{C}^{ms}$

$$x^* \mathcal{H}_m x = x^* \boldsymbol{\mathcal{V}}_m^* A \boldsymbol{\mathcal{V}}_m x = (\boldsymbol{\mathcal{V}}_m x)^* A (\boldsymbol{\mathcal{V}}_m x).$$

Since $\boldsymbol{\mathcal{V}}_m$ has full rank and thus $\boldsymbol{\mathcal{V}}_m x \neq 0$ for $x \neq 0$, this shows that $\mathcal{H}_m$ is positive real. An eigenpair (x, λ) of $\mathcal{H}_m$ therefore satisfies $\lambda = \frac{x^* \mathcal{H}_m x}{x^* x} \in \mathbb{C}^+$, which is the assertion for $\mathcal{M} = 0$ (block FOM). For block GMRES, where $\mathcal{M} = \mathcal{M}^{\mathrm{gmr}} = \mathcal{H}_m^{-*}(\widehat{\boldsymbol{E}}_m H_{m+1,m}^* H_{m+1,m} \widehat{\boldsymbol{E}}_m^*)$, let $(\mathcal{H}_m + \mathcal{M}^{\mathrm{gmr}})x = \lambda x$ for some $x \in \mathbb{C}^{ms}, x \neq 0$. Then $(\mathcal{H}_m^* \mathcal{H}_m + \mathcal{H}_m^* \mathcal{M}^{\mathrm{gmr}})x = \lambda \mathcal{H}_m^* x$ and thus

$$\underbrace{x^* \mathcal{H}_m^* \mathcal{H}_m x}_{>0} + \underbrace{x^* (\widehat{\boldsymbol{E}}_m H_{m+1,m}^* H_{m+1,m} \widehat{\boldsymbol{E}}_m^*) x}_{\geq 0} = \lambda \underbrace{x^* \mathcal{H}_m x}_{\in \mathbb{C}^+},$$

which gives $\lambda \in \mathbb{C}^+$. ∎

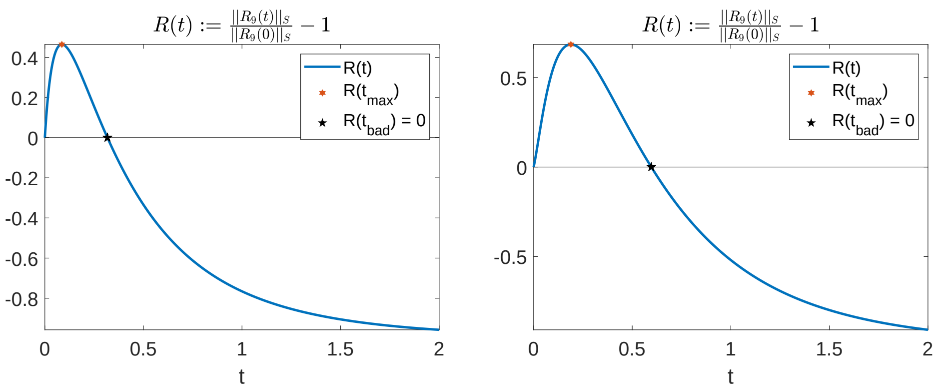
Theorem 4.3 covers block FOM and block GMRES for the global, loop-interchange, and classical paradigms if A is positive real with respect to the standard inner product. In particular, it also applies for global, loop-interchange, and classical block CG if A is Hermitian and positive definite real with respect to the standard inner product.

Corollary 4.4 has a geometric interpretation: the volume of the parallelepiped spanned by the columns of $\boldsymbol{R}_m(0)$ is $\det(D)$ for any $D \in \mathbb{C}^{s \times s}$ in a representation $\boldsymbol{R}_m(0) = \boldsymbol{Q} D$ with $\boldsymbol{Q} \in \mathbb{C}^{n \times s}$ having orthonormal columns. The volume of the parallelepiped spanned by $\boldsymbol{R}_m(t)$ is $\det(D)\det(C_m(-t))$, and thus smaller than that for $\boldsymbol{R}_m(0)$. Note that this does not exclude that some columns of $\boldsymbol{R}_m(t)$ can have arbitrarily larger length than those of $\boldsymbol{R}_m(0)$, provided angles between the columns of $\boldsymbol{R}_m(t)$ are sufficiently acute.

When specialized to the non-block case, Corollary 4.4 delivers a strong result: $C_m(-t)$ is now a scalar, which is less than 1 in modulus by the corollary, implying that for positive shifts the norms of the shifted residuals are all smaller than the norms of the non-shifted residuals. For the CG method this observation relies on [37], and for shifted GMRES for positive real matrices it can be found in [17]. That this also holds for FOM for positive real matrices seems to not have been observed before.

	ρ	$\|\cdot\|_{\mathrm{F}}$	$\|\cdot\|_{2\,\max}$	$\|\cdot\|_2$
block FOM	16,841	117	121	123
block GMRES	10,092	98	93	105

(a) Number of instances (out of 10^4 samples, each for $m = 1, \ldots, 9$) refuting monotonicity conjectures. ρ: spectral radius of $C_m(t)$ larger than 1; $\|\cdot\|_{\mathrm{F}}, \|\cdot\|_{2\,\max}, \|\cdot\|_2$: $\|\boldsymbol{R}_m(t)\| > \|\boldsymbol{R}_m(0)\|$ for the respective norm, all for $t = 0.1$.



(b) Relative difference of the residual Frobenius norms as a function of t for selected samples

Fig. 4.1: Results of experiments on residuals of shifted systems

For the block case, rather than having a result just on the determinant, we would prefer a result which shows $\|C_m(t)\| < 1$ for an appropriate norm. After several unfruitful attempts in this direction, we performed some numerical experiments to find counterexamples. We generated self-adjoint block tridiagonal 20×20 matrices $\mathcal{H}$ where each diagonal and off-diagonal block is a randomly generated Hermitian and a positive definite 2×2 matrix. These matrices $\mathcal{H}$ are then scaled and shifted so that their spectral interval is exactly $[0.1, 10]$. For these matrices $\mathcal{H}$, the block Lanczos process for the classical block inner product and with $\widehat{\boldsymbol{E}}_1$ as a starting block vector just reproduces $\mathcal{H}$ as the block upper Hessenberg matrix. We take $t = 0.1$ as our shift parameter. Within $10,000$ samples and the values $m = 1, \ldots, 9$, we found a significant number of instances for which $C_m(t)$ has an eigenvalue larger than 1 in modulus. So $\|C_m(t)\| < 1$ cannot hold for whatever norm we choose. Moreover, we also found instances for which $\|\boldsymbol{R}_m(t)\| > \|\boldsymbol{R}_m(0)\|$ for the $\mathbb{S}$-norm (which is the Frobenius norm in this case), the 2-norm, and the norm $\|\cdot\|_{2\,\max}$ given by the maximum of the 2-norms of individual columns. Similar observations hold for block GMRES. Detailed numbers are given in Figure 4.1(a). To illustrate this further, for block FOM as well as for block GMRES, we picked one of the samples for which $\|\boldsymbol{R}_m(0.1)\|_{\mathrm{F}} > \|\boldsymbol{R}_m(0)\|_{\mathrm{F}}$ and computed $\boldsymbol{R}_m(t)$ for many values of t, so as to be able to plot the relative difference $1 - \|\boldsymbol{R}_m(t)\|_{\mathrm{F}} \,/\, \|\boldsymbol{R}_m(0)\|_{\mathrm{F}}$ as a function of t. These graphs are given in Figure 4.1(b).

4.5. Block Radau-Arnoldi for shifted systems and matrix functions. For block Radau-Arnoldi, fix a step m and denote by P the m-th residual polynomial of the non-shifted system, $\boldsymbol{R}_m^{\mathrm{ra}} = P(A) \circ \boldsymbol{B}$. By Theorem 4.3, the residuals $\boldsymbol{R}_m^{\mathrm{ra}}(t)$ of the shifted block Radau-Arnoldi iterates $\boldsymbol{X}_m^{\mathrm{ra}}(t) = \boldsymbol{\mathcal{V}}_m \boldsymbol{\Xi}_m^{\mathrm{ra}}$, with $\boldsymbol{\Xi}_m^{\mathrm{ra}} = (\mathcal{H}_m + tI + \mathcal{M}^{\mathrm{ra}})^{-1} \widehat{\boldsymbol{E}}_1 B$, satisfy

$$\boldsymbol{R}_m^{\mathrm{ra}}(t) = P_t(A + tI) \circ \boldsymbol{B},$$

where $P_t(z) = P^{(-t)}(z) P(-t)^{-1}$ and $P^{(-t)}$ is defined in (4.12). Thus, $P(S) = 0$ implies $P_t(S + tI) = 0$, and we see that the shifted block Radau-Arnoldi iterates are precisely the iterates of the block Radau-Arnoldi method for the shifted system prescribing $S + tI$ as a solvent for the residual polynomial. It is this property that allows us to prove a convergence result for Stieltjes functions of matrices in the same spirit as that of the non-block result in [21].

THEOREM 4.5. *Assume that A is block self-adjoint with respect to $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathbb{S}}$ and positive definite with respect to $\langle \cdot, \cdot \rangle_{\mathbb{S}}$. Let $0 < \lambda_{\min} \leq \lambda_{\max}$ denote the smallest and largest eigenvalue of A, respectively, and let $S = \sigma I_s$ with $\sigma > \lambda_{\max}$. Finally, let $A_{\sigma,t} = (A + tI)(\sigma I - A)^{-1}$ and let $\langle \cdot, \cdot \rangle_{A_{\sigma,t}\text{-}\mathbb{S}}$ denote the inner product $\langle \boldsymbol{X}, \boldsymbol{Y} \rangle_{A_{\sigma,t}\text{-}\mathbb{S}} = \langle A_{\sigma,t} \boldsymbol{X}, \boldsymbol{Y} \rangle_{\mathbb{S}}$ with associated norm $\|\cdot\|_{A_{\sigma,t}\text{-}\mathbb{S}}$. Assume that we perform a restart after every cycle of length m, and denote $\boldsymbol{E}_m^{(k)}(t)$ the error of the Radau-Arnoldi iterate $\boldsymbol{X}_m^{(k)}(t)$ for shift t after k such cycles. Then*

(i) With $\xi_m(t) := \frac{2}{c(t)^m + c(t)^{-m}}$, $c(t) := \frac{\sqrt{\kappa(t)} - 1}{\sqrt{\kappa(t)} + 1}$, $\kappa(t) := \frac{\lambda_{\max} + t}{\lambda_{\min} + t}$ we have

$$\left\| \boldsymbol{E}_m^{(k)}(t) \right\|_{A_{\sigma,t}\text{-}\mathbb{S}} \leq \left(1 - \tfrac{\lambda_{\min} + t}{\sigma + t}\right)^k \cdot \xi_{m-1}(t)^k \cdot \left\| (A + tI)^{-1} \boldsymbol{B} \right\|_{A_{\sigma,t}\text{-}\mathbb{S}}.$$

(ii) For a Stieltjes function $f = \int_{t=0}^{\infty} (z + t)^{-1} \,\mathrm{d}\mu(t)$, the error $f(A)\boldsymbol{B} - \boldsymbol{F}_m^{(k)}$ of the block Arnoldi-Radau method, where $\boldsymbol{F}_m^{(k)} = \int_{t=0}^{\infty} \boldsymbol{X}_m^{(k)}(t) \,\mathrm{d}\mu(t)$, satisfies

$$\left\| f(A)\boldsymbol{B} - \boldsymbol{F}_m^{(k)} \right\|_{A_\sigma\text{-}\mathbb{S}} \leq C \cdot \xi_{m-1}(0)^k \cdot \|\boldsymbol{B}\|_{A_\sigma\text{-}\mathbb{S}},$$

with $C = \frac{\lambda_{\max}(\sigma - \lambda_{\min})^2}{\lambda_{\min}(\sigma - \lambda_{\max})} f(\sigma)$.

Proof. Part (i) is just Theorem 3.10 for the matrices $A + tI$, extended to restarts. To prove (ii) we use the norm comparison result formulated in [22, Lemma 4.4], which states that for every rational function g that is positive on $\mathbb{R}^+$ and the associated norm $\|\boldsymbol{X}\|_{g(A)\text{-}\mathbb{S}} := \langle g(A)\boldsymbol{X}, \boldsymbol{X} \rangle_{\mathbb{S}}^{1/2}$, we have

$$\sqrt{g_{\min}}\, \|\boldsymbol{X}\|_{\mathbb{S}} \leq \|\boldsymbol{X}\|_{g(A)\text{-}\mathbb{S}} \leq \sqrt{g_{\max}}\, \|\boldsymbol{X}\|_{\mathbb{S}},$$

where $g_{\min}$ and $g_{\max}$ are the minimum and maximum, respectively, of g on $\mathrm{spec}(A)$. Applying this result twice we obtain

$$\|\boldsymbol{X}\|_{A_\sigma\text{-}\mathbb{S}} \leq \sqrt{\frac{\max\{\lambda/(\sigma-\lambda) : \lambda \in \mathrm{spec}(A)\}}{\min\{(\lambda+t)/(\sigma-\lambda) : \lambda \in \mathrm{spec}(A)\}}} \cdot \|\boldsymbol{X}\|_{A_{\sigma,t}\text{-}\mathbb{S}} \leq \sqrt{\frac{\lambda_{\max}/(\sigma - \lambda_{\max})}{(\lambda_{\min}+t)/(\sigma-\lambda_{\min})}}\, \|\boldsymbol{X}\|_{A_{\sigma,t}\text{-}\mathbb{S}}, \tag{4.14}$$

and, similarly,

$$\|\boldsymbol{X}\|_{A_{\sigma,t}\text{-}\mathbb{S}} \leq \sqrt{\frac{\max\{(\lambda+t)/(\sigma-\lambda) : \lambda \in \mathrm{spec}(A)\}}{\min\{\lambda/(\sigma-\lambda) : \lambda \in \mathrm{spec}(A)\}}} \cdot \|\boldsymbol{X}\|_{A_\sigma\text{-}\mathbb{S}} \leq \sqrt{\frac{(\lambda_{\max}+t)/(\sigma - \lambda_{\max})}{\lambda_{\min}/(\sigma-\lambda_{\min})}}\, \|\boldsymbol{X}\|_{A_\sigma\text{-}\mathbb{S}}. \tag{4.15}$$

From (4.9), and using (4.14), we obtain

$$\begin{aligned}\left\|f(A)\boldsymbol{B}-\boldsymbol{F}_m^{(k)}\right\|_{A_\sigma\text{-}\mathbb{S}} &= \left\|\int_0^\infty \boldsymbol{E}_m^{(k)}(t)\,\mathrm{d}\mu(t)\right\|_{A_\sigma\text{-}\mathbb{S}}\\ &\le \int_0^\infty \left\|\boldsymbol{E}_m^{(k)}(t)\right\|_{A_\sigma\text{-}\mathbb{S}}\,\mathrm{d}\mu(t)\\ &\le \int_0^\infty \sqrt{\tfrac{\lambda_{\max}(\sigma-\lambda_{\min})}{(\lambda_{\min}+t)(\sigma-\lambda_{\max})}}\cdot\left\|\boldsymbol{E}_m^{(k)}(t)\right\|_{A_{\sigma,t}\text{-}\mathbb{S}}\,\mathrm{d}\mu(t).\end{aligned}$$

Using (i), the fact that $\xi_m(t)\le\xi_m(0)=:\xi_m$ for $t\ge 0$, and (4.15), we have

$$\begin{aligned}&\left\|f(A)\boldsymbol{B}-\boldsymbol{F}_m^{(k)}\right\|_{A_\sigma\text{-}\mathbb{S}}\\ &\le \int_0^\infty \sqrt{\tfrac{\lambda_{\max}(\sigma-\lambda_{\min})}{(\lambda_{\min}+t)(\sigma-\lambda_{\max})}}\left(1-\tfrac{\lambda_{\min}+t}{\sigma+t}\right)^k\xi_{m-1}^k\,\|\boldsymbol{B}\|_{A_{\sigma,t}\text{-}\mathbb{S}}\,\mathrm{d}\mu(t)\\ &\le \int_0^\infty \sqrt{\tfrac{\lambda_{\max}(\sigma-\lambda_{\min})}{(\lambda_{\min}+t)(\sigma-\lambda_{\max})}}\cdot\left(1-\tfrac{\lambda_{\min}+t}{\sigma+t}\right)^k\xi_{m-1}^k\sqrt{\tfrac{(\lambda_{\max}+t)/(\sigma-\lambda_{\max})}{\lambda_{\min}/(\sigma-\lambda_{\min})}}\,\|\boldsymbol{B}\|_{A_\sigma\text{-}\mathbb{S}}\,\mathrm{d}\mu(t)\\ &= \int_0^\infty \sqrt{\tfrac{\lambda_{\max}+t}{\lambda_{\min}+t}}\cdot\sqrt{\tfrac{\lambda_{\max}}{\lambda_{\min}}}\cdot\tfrac{\sigma-\lambda_{\min}}{\sigma-\lambda_{\max}}\cdot\left(\tfrac{\sigma-\lambda_{\min}}{\sigma+t}\right)^k\xi_{m-1}^k\,\|\boldsymbol{B}\|_{A_\sigma\text{-}\mathbb{S}}\,\mathrm{d}\mu(t).\end{aligned}$$

Since $(\lambda_{\max}+t)/(\lambda_{\min}+t)\le\lambda_{\max}/\lambda_{\min}$ for all $t\ge 0$ and $0\le\left(\frac{\sigma-\lambda_{\min}}{\sigma+t}\right)^k\le\frac{\sigma-\lambda_{\min}}{\sigma+t}$, this finally gives

$$\begin{aligned}\left\|f(A)\boldsymbol{B}-\boldsymbol{F}_m^{(k)}\right\|_{A_\sigma\text{-}\mathbb{S}} &\le \tfrac{\lambda_{\max}(\sigma-\lambda_{\min})^2}{\lambda_{\min}(\sigma-\lambda_{\max})}\xi_{m-1}^k\cdot\int_0^\infty\frac{1}{\sigma+t}\,\mathrm{d}\mu(t)\cdot\|\boldsymbol{B}\|_{A_\sigma\text{-}\mathbb{S}}\\ &= \tfrac{\lambda_{\max}(\sigma-\lambda_{\min})^2}{\lambda_{\min}(\sigma-\lambda_{\max})}f(\sigma)\cdot\xi_{m-1}^k\cdot\|\boldsymbol{B}\|_{A_\sigma\text{-}\mathbb{S}}\,.\end{aligned}$$

∎

Note that this proof makes no effort to keep the constant C small.

5. Numerical experiments.

We report numerical results obtained with a MATLAB 2019a implementation run on a Thinkpad X1 Carbon with Windows 10 64-bit, an Intel Core i7 processor, and 16GB of RAM; more difficult tests were run in MATLAB 2018a on the Fidis cluster at EPFL.[2] All code is publicly available at https://gitlab.com/katlund/bfomfom-main/.

We start with an academic example that illustrates the theoretical results for linear systems from the previous sections.

Example 5.1. A is a diagonal matrix of dimension $n = 5000$, the $s = 10$ right-hand sides are generated randomly using MATLAB's `rand` command and normalized with `qr`, and the initial block vector X_0 is zero.

a) The diagonal entries of A are linearly spaced in the interval $[10^{-2}, 10^2]$, i.e., $a_{ii} = 10^{-2} + (i-1)d$ where $d = (10^2 - 10^{-2})/(n-1)$.
b) The diagonal entries of A are logarithmically spaced in the interval $[10^{-2}, 10^2]$, i.e., $a_{ii} = 10^{e_i}$, where $e_i = -2 + 4(i-1)/(n-1)$.
c) The diagonal elements of A come in complex conjugate pairs. Their $n/2$ different real parts are linearly spaced in $[10^{-2}, 10^2]$, their imaginary parts are taken randomly with uniform distribution in $[0, 1]$.

[2] https://scitas.epfl.ch/hardware/fidis/

The matrices A from Example 5.1a and b are Hermitian and positive definite, and thus the comparison results for the methods based on the classical, loop-interchange, and global block inner products hold for block FOM (Theorem 3.3), block GMRES (Theorem 3.7) and block Radau-Arnoldi (Theorem 3.11). This is illustrated in Figure 5.1 where we plot the respective norms of the error for the first 50 inner iterations (i.e., the first cycle, without restarts). We observe that for both matrices, the methods relying on the loop-interchange or global block inner product perform almost indistinguishably, whereas the classical approach yields faster convergence for Example 5.1a, but only marginal improvement for classical GMRES in the same example and in Example 5.1b.

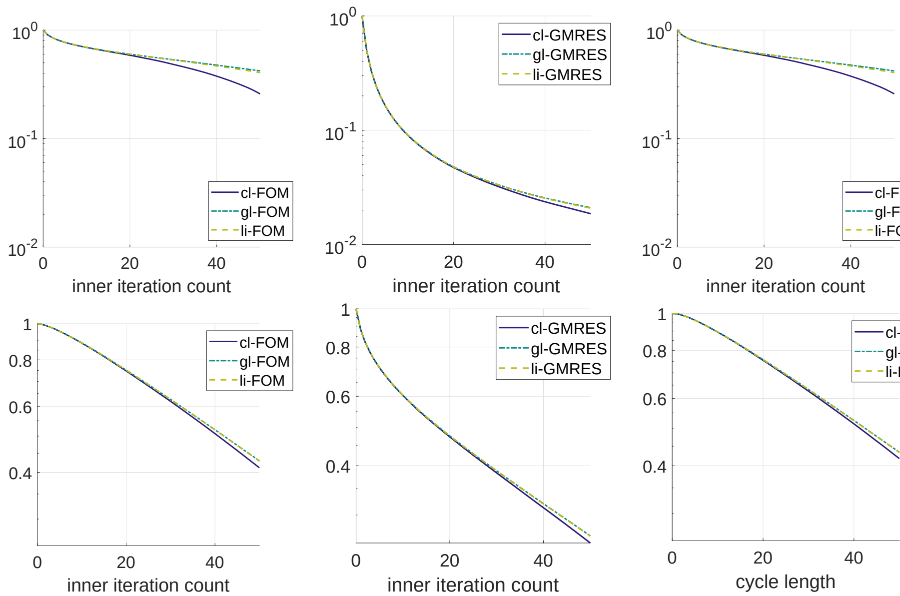


Fig. 5.1: Error norms for 50 inner iterations of the first cycle for Example 5.1a (top row) and b (bottom row), with cycle length $m = 25$. FOM error is measured in $\|\cdot\|_{A\text{-F}}$, GMRES in $\|\cdot\|_{A^*A}$, and RA in $\|\cdot\|_{A(\sigma I-A)^{-1}-\text{F}}$. The RA solvent is chosen as $1.01\lambda_{\max} \cdot I_s$.

Figure 5.2 gives further results for Example 5.1a. Its top row shows convergence plots for a cycle length of $m = 25$ displaying the Frobenius norm of the block residual for all methods. The bottom row presents a study for different cycle lengths m, giving the number of cycles necessary to decrease the initial Frobenius norm of the residual by a factor of 10^{-10}. The top row shows that block FOM, block GMRES and block Radau-Arnoldi converge for all block inner products considered here, that the convergence speed is quite similar between FOM, GMRES and Radau-Arnoldi, that the loop-interchange and global inner product give almost identical results, and that the classical block inner product methods converge the faster the larger m. One should be aware, though, that the arithmetic work that comes in addition to the matrix-vector multiplications is substantially larger for the classical block inner product than for the others: each block inner product has cost $\mathcal{O}(ns^2)$ whereas this cost is only $\mathcal{O}(sn)$ for the loop-interchange and global block inner products. Moreover, as opposed to the other two block inner products, there is no additional sparsity structure other than block upper Hessenberg that one can take advantage of when working with $\mathcal{H}_m$. So, the accelerated convergence comes at the price of extra arithmetic work.

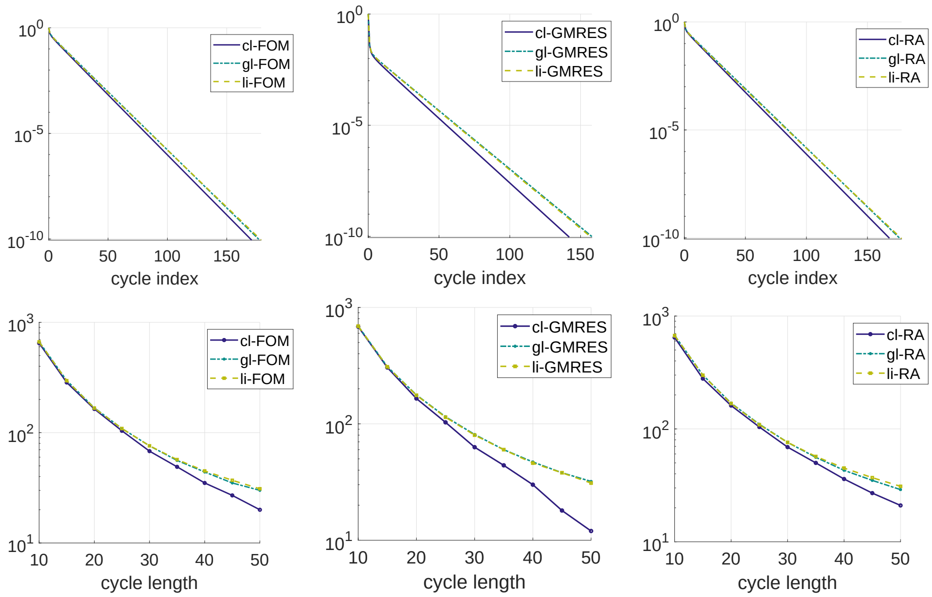


Fig. 5.2: Top row: error norm versus cycle index for Example 5.1a, $m = 25$. Bottom row: number of cycles needed to converge versus cycle length for Example 5.1a. FOM error is measured in $\|\cdot\|_{A\text{-F}}$, GMRES in $\|\cdot\|_{A^*A}$, and RA in $\|\cdot\|_{A(\sigma I-A)^{-1}-\text{F}}$. The RA solvent is chosen as $1.01\lambda_{\max} \cdot I_s$.

Figure 5.3 deals with Example 5.1c. The matrix A is not Hermitian but positive real. The convergence plots in the top row show that now restarted block FOM diverges, that convergence is restored when using the block Radau-Arnoldi approach and that, in accordance with Theorem 3.5, the block GMRES methods all converge.

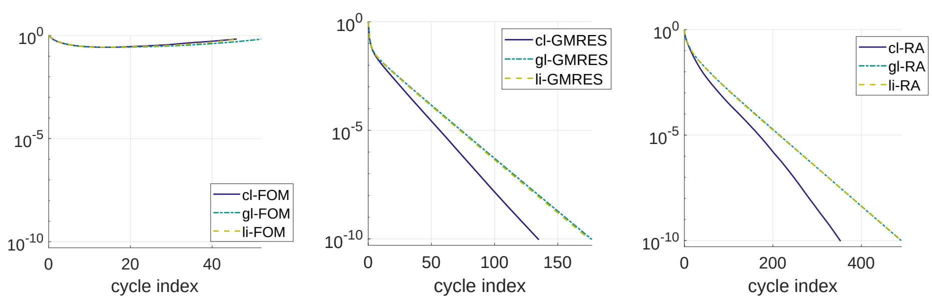


Fig. 5.3: Error norm versus cycle index for Example 5.1c, $m = 25$, $s = 10$. All errors are measured in the Frobenius norm.

We now turn to matrix functions and first consider the inverse square root $z^{-1/2}$, which is a Stieltjes function, since $z^{-1/2} = \frac{1}{\pi}\int_0^\infty \frac{t^{-1/2}}{z+t}\,\mathrm{d}t$. In order to evaluate the matrix function and the subsequent error representations (4.11) we proceed as in [20] and [22], using the Cayley transform $t = -\beta\frac{1-x}{1+x}$ with $\beta = \operatorname{trace}(A)$ to map the infinite integration interval $[0, \infty)$ onto $(-1, 1]$, where we then use Gauß-Legendre quadrature with an adaptive strategy to determine the number of quadrature nodes.

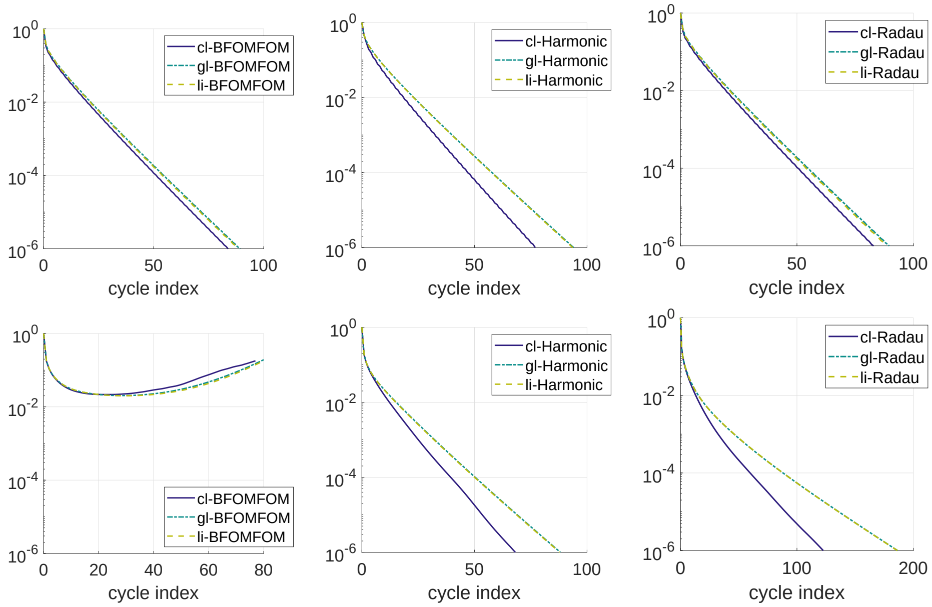


Fig. 5.4: Error norm versus cycle index for the inverse square root of Example 5.1a (top row) and c (bottom row). All errors are measured in the Frobenius norm. $m = 25$, $s = 10$.

Figure 5.4 shows convergence plots for the matrices from Example 5.1a and c and a random right-hand side that now has imaginary components. We observe that the various methods perform similarly as in the linear system case. In particular, the classical inner product yields faster convergence than loop-interchange and global, which are again nearly indistinguishable. However, in terms of wall-clock times, the global methods converged much more quickly than the other methods– 30 minutes versus hours– and the quadrature tolerance had to be set two orders of magnitude lower than the desired error tolerance for convergence to be achieved at all. For the non-Hermitian matrix, the block FOM methods do not converge while the block GMRES and the block Radau-Arnoldi methods do. Note that since A is diagonal, we can compute $A^{-1/2}\boldsymbol{B}$ directly which allows us to easily compute the error of the various approximations.

We consider another Stieltjes function as well, $\frac{\log(z+1)}{z} = \int_0^\infty \frac{1}{z+t} \, \mathrm{d}\mu(t)$, where $\mathrm{d}\mu(t) = t^{-1}H(t+1)$ and $H(t)$ is the Heaviside function. The matrix logarithm arises, for example, in Markov models and the solution of linear dynamical systems; see, e.g., [29, Chapter 2]. Figure 5.5 shows convergence curves for $\frac{\log(z+1)}{z}$ on Example 5.1c; since the matrix is positive real, the principal logarithm is defined. We see that only the classical and loop-interchange harmonic and Radau methods converge, with the Radau methods converging with the fewest cycles. The largest real part of the spectrum times $1.01 \cdot I_s$ is chosen as the prescribed solvent. For $m = 25$, all methods converge in roughly 28 cycles, except the modified global methods, which stagnate. We also considered the logarithmic function on Example 5.1a and b. All methods converge in just 5 cycles, except for the modified global methods, which again stagnate. We do not show the convergence curves for these additional tests.

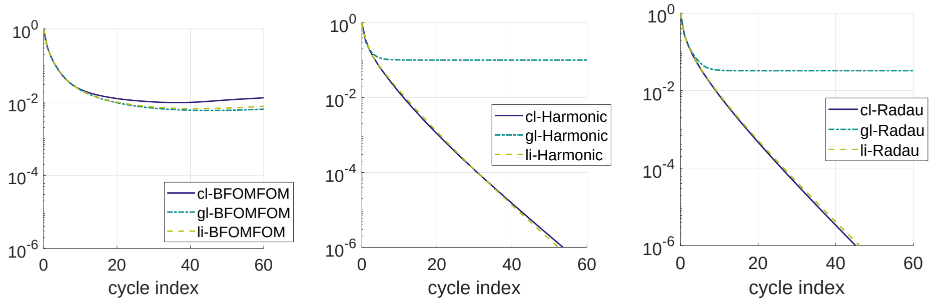


Fig. 5.5: Error norm versus cycle index for $\frac{\log(z+1)}{z}$ of Example 5.1 c. All errors are measured in the Frobenius norm. $m = 15$, $s = 10$.

Example 5.2. We take $A = Q^2$ and compute $A^{-1/2}$, where Q is the kernel matrix for the overlap operator arising in simulations from lattice QCD, see [23]. Lattice QCD is the most widely used discretization of quantum chromodynamics (QCD) which is the fundamental physical theory of the quarks as the constituents of matter. Here, Q is the "symmetrized" Wilson-Dirac matrix, a discretization of the Dirac operator on a 4-dimensional equispaced space-time lattice in presence of a stochastic "gauge" background field. As opposed to other discretizations, the overlap operator preserves the important property of chiral symmetry on the lattice at the price of requiring the action of the sign function $\text{sign}(Q)$ on vectors to be evaluated. We compute $\text{sign}(Q)$ as $Q \cdot (Q^2)^{-1/2}$. At zero chemical potential, $\mu = 0$, the matrix Q is Hermitian, but for $\mu > 0$ the matrix Q starts to deviate from hermiticity; see [8] for details. We used the matrix `conf6_0-8x8-30`, available at the SuiteSparse Matrix Collection [10], and took the right-hand side $\boldsymbol{B}$ as the first 12 canonical unit vectors. This corresponds to a typical situation when computing quark propagators, where one has to take all combinations of the four spin and three color quantum numbers into account. The dimension of the resulting matrix is $n = 12 \cdot 8^4 = 49,152$.

Table 5.1 shows results for $\mu = 0.3$. The reference value for an "exact" evaluation of $(Q^2)^{-1}\boldsymbol{B}$ was determined beforehand using the harmonic method and stopping when the Frobenius norm of the correction computed in one cycle was less than 10^{-12}. The table reports the number of iterations required to reduce the initial error by a factor of $\epsilon = 10^{-6}$ for different cycle lengths $m = 2, 5, 10$. We see that for all values of m the harmonic method with the classical block inner product needs the fewest iterations. For $m = 2$ the advantages of the harmonic method are substantial, and as m increases, they become less pronounced. For $m = 10$ all (modified) FOM methods for all block inner products need almost the same number of cycles. We note also that for these methods to converge, the quadrature tolerance was set to $10^{-3}\epsilon$ for $m = 2$ and $10^{-2}\epsilon$ for $m = 5, 10$.

6. Conclusions. In this paper we have contributed several results to the theory of block Krylov subspace methods for linear systems and for matrix functions. These results hold for general block inner products, and thus in particular for the classical block methods and the so-called global methods. We have completely characterized those modifications of the basic block FOM approach for which the polynomial exactness property–which is the natural extension of the polynomial interpolation property

	$m=2$			$m=5$			$m=10$		
	Cl	Li	Gl	Cl	Li	Gl	Cl	Li	Gl
B(FOM)^2	613	627	628	103	106	107	29	31	31
harmonic	453	577	504	89	103	105	29	31	31
Radau-Arnoldi	731	733	734	106	110	110	30	31	31

Table 5.1: Inverse square root for QCD matrix (Example 5.2 with chemical potential $\mu = 0.3$): number of iterations required to reduce the initial error by a factor of 10^{-6}. $s = 12$.

from the non-block case–holds. This result is crucial to obtaining restart procedures for computing the action of a matrix function on a block vector, just as is the possibility for keeping block residuals for shifted linear systems cospatial.

We have shown how cospatiality can be maintained algorithmically and contributed theoretical results on the convergence of these shifted system methods. The situation turns out to be more complex than in the non-block case. Our main result shows that the modulus of the determinant of the cospatiality matrix factor for the shifted residual matrix polynomials is smaller than one. This result uses a further result on the connection between latent roots of residual polynomials and the (modified) block upper Hessenberg matrix, for which we have completed partial characterizations known from the literature.

We have presented a series of numerical experiments, which tend to indicate that, in the presence of restarts, the benefits of using a block Krylov subspace are mostly visible only when using the classical inner product; even then, a reduction in wall-clock time still depends on how far the decrease in cycles is outweighed by the larger arithmetic costs per cycle. The numerical experiments also show several situations in which the new harmonic block FOM approach performs better than the standard block FOM approach and where fixing a solvent in the new Radau-Arnoldi methods can restore convergence in cases where standard block FOM diverges.

Acknowledgments. We would like to thank Kirk Soodhalter for many useful discussions, and Teodor Nikolov for helping run numerical tests on the cluster.

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