DEFLATED RESTARTING FOR MATRIX FUNCTIONS*

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Abstract. We investigate an acceleration technique for restarted Krylov subspace methods for computing the action of a function of a large sparse matrix on a vector. Its effect is to ultimately deflate a specific invariant subspace of the matrix which most impedes the convergence of the restarted approximation process. An approximation to the subspace to be deflated is successively refined in the course of the underlying restarted Arnoldi process by extracting Ritz vectors and using those closest to the spectral region of interest as exact shifts. The approximation is constructed with the help of a generalization of Krylov decompositions to linearly dependent vectors. A description of the restarted process as a successive interpolation scheme at Ritz values is given in which the exact shifts are replaced with improved approximations of eigenvalues in each restart cycle. Numerical experiments demonstrate the efficacy of the approach.

Key words. matrix function, Krylov subspace approximation, restarted Krylov subspace method, thick restarting, deflated restarting, implicitly restarted Arnoldi/Lanczos method, polynomial interpolation

1. Introduction. Numerical methods for the evaluation of $f(A)\boldsymbol{b}$, where $A \in \mathbb{C}^{N\times N}$, $\mathbf{0} \neq \boldsymbol{b} \in \mathbb{C}^N$ and f is a complex-valued function such that $f(A)$ is defined, have become an active area of research in recent years. This development is driven by certain applications but also by other numerical algorithms such as exponential integrators for ordinary differential equations, where the action of $f(A)$ on a vector $\boldsymbol{b}$ has to be computed (see the survey of Frommer and Simoncini [16] or the monograph of Higham [18, Chapter 13]). If A is large and sparse such that computing $f(A)$ is unfeasible but matrix-vector multiplications with A still practicable, then the so-called *Arnoldi approximation* to $f(A)\boldsymbol{b}$ is a popular approach (see, e.g., Ericsson [14], Knizhnerman [21] or Saad [34]). This is based on an Arnoldi decomposition‡ of A,

$$AV_m = V_m H_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^T, \tag{1.1}$$

where the columns of $V_m = [\boldsymbol{v}_1\, \boldsymbol{v}_2 \cdots \boldsymbol{v}_m] \in \mathbb{C}^{N\times m}$ form an orthonormal basis of the Krylov subspace $\mathscr{K}_m(A,\boldsymbol{b}) = \operatorname{span}\{\boldsymbol{b}, A\boldsymbol{b}, \ldots, A^{m-1}\boldsymbol{b}\}$, $\boldsymbol{b} = \|\boldsymbol{b}\|\boldsymbol{v}_1$, $\boldsymbol{v}_{m+1} \in \mathscr{K}_{m+1}(A,\boldsymbol{b})$ is orthogonal to $\mathscr{K}_m(A,\boldsymbol{b})$, $H_m = V_m^H A V_m \in \mathbb{C}^{m\times m}$ is an unreduced upper Hessenberg matrix, and $\boldsymbol{e}_m \in \mathbb{R}^m$ denotes the m-th unit coordinate vector. The Arnoldi approximation of $f(A)\boldsymbol{b}$ from $\mathscr{K}_m(A,\boldsymbol{b})$ is then defined by

$$\boldsymbol{f}_m := V_m f(V_m^H A V_m) V_m^H \boldsymbol{b} = \|\boldsymbol{b}\| V_m f(H_m)\boldsymbol{e}_1, \tag{1.2}$$

assuming that also $f(H_m)$ is defined, which in turn is implied e.g. if f is analytic on the field of values of A. Note that the approximation (1.2) requires the evaluation of f only for the $m \times m$ matrix H_m, where typically $m \ll N$.

As m becomes large (as it typically does in realistic problems), a disadvantage of the Arnoldi approximation lies in the need to store V_m, which may limit the size of the problems that can be solved due to memory constraints. In [11] we proposed

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‡When we use terminology such as *Arnoldi decomposition*, *Arnoldi approximation*, *Arnoldi algorithm*, etc. in association with a Hermitian matrix A, we tacitly assume that computations are carried out with the Hermitian Lanczos process.

a restarting technique which overcomes this deficiency. It is based on a sequence of Arnoldi decompositions

$$AV^{(j)} = V^{(j)}H^{(j)} + h^{(j)}\boldsymbol{v}^{(j)}\boldsymbol{e}_m^T, \qquad j = 1, 2, \ldots, k,$$

associated with the Krylov subspaces $\mathscr{K}_m(A, \boldsymbol{v}^{(j-1)})$, each of *fixed* dimension m and each using the last Arnoldi vector of the previous Krylov space as its initial vector, where $\boldsymbol{v}^{(0)} = \boldsymbol{b}/\|\boldsymbol{b}\|$. The mk columns of the matrices $\{V^{(j)}\}_{j=1}^k$ taken together then form a basis of $\mathscr{K}_{km}(A, \boldsymbol{b})$. In [11] and [3] it is explained how to compute an approximation $\hat{\boldsymbol{f}}_k$ to $f(A)\boldsymbol{b}$ from $\mathscr{K}_{km}(A, \boldsymbol{b})$ recursively using only $V^{(k)}$, i.e., such that updating from $\hat{\boldsymbol{f}}_{k-1}$ to $\hat{\boldsymbol{f}}_k$ requires only the storage of $V^{(k)}$. However, as is the case with restarted Krylov subspace schemes for eigenvalue problems or linear systems of equations, restarting is typically accompanied by slower convergence or even divergence of the approximation.

In this paper we show that the convergence of the restarted Arnoldi approximation can be accelerated significantly by replacing the initial vector $\boldsymbol{v}^{(j)}$ of the $(j+1)$st Krylov space by a judiciously chosen vector $\tilde{\boldsymbol{v}}^{(j)} \in \mathscr{K}_{m+1}(A, \boldsymbol{v}^{(j-1)}) \setminus \mathscr{K}_m(A, \boldsymbol{v}^{(j-1)})$. Our choice of the modified initial vectors has the effect of ultimately deflating certain spectral components from the problem. If these components are associated with eigenvalues of A close to a singularity of f, this deflation can be shown to accelerate convergence. Which eigencomponents should be deflated in case f is an entire function will be discussed below.

The deflated restarting technique for the evaluation of matrix functions is closely related to similar approaches for eigenvalue problems and the iterative solution of linear systems. The idea of restarting a Krylov subspace method dates back to the first practical Lanczos- and Arnoldi-based procedures for computing a few eigenpairs of large sparse matrices, see e.g. Saad [32, 33]. To mitigate the overwhelming storage requirements of the full algorithms, restarting with a linear combination of Ritz vectors or another suitable vector contained in the current Krylov space as the new initial vector was proposed. For a Krylov space $\mathscr{K}_m(A, \boldsymbol{b})$, such a vector has the form $p(A)\boldsymbol{b}$ for some polynomial $p \in \mathscr{P}_m$, sometimes called a *filter polynomial* since it is used to damp out undesired parts of the spectrum $\Lambda(A)$. A substantial innovation, the *implicitly restarted Arnoldi method* of Sorensen [37] enables the construction of the Arnoldi decomposition of the restarted space $\mathscr{K}_{m-k}(A, p_k(A)\boldsymbol{b})$ for a filter polynomial $p_k \in \mathscr{P}_k$, $k \le m$ from the original Arnoldi decomposition of $\mathscr{K}_m(A, \boldsymbol{b})$ given only the roots of p_k without further matrix-vector multiplications. Subsequently, a more stable variant of this procedure based on a Schur decomposition rather than a sequence of QR steps was proposed by Stewart [39]. Restarting with a Krylov space larger than the space spanned by the desired Ritz vectors was introduced by Stathopoulos, Saad and Wu in [38] as *thick restarting* and later specialized to the Hermitian Lanczos method by Wu and Simon [41]. The idea of using nearly invariant subspaces generated by a restarted Krylov method to accelerate the iterative solution process for a linear system of equations was proposed as early as 1987 by Nicolaides [27] in the context of conjugate gradient iteration, and later studied systematically for Arnoldi-based methods by Morgan [24, 25, 26]. The same basic deflation effect can also be achieved by constructing a preconditioner from the invariant subspace vectors, as proposed in [4, 13]. An analysis of these approaches can be found in [12]. In the context of approximating $f(A)\boldsymbol{b}$, Niehoff [28, Section 3.4] first pointed out how such a deflation technique could be incorporated in a restarted Krylov subspace method by applying the method for the evaluation of the exponential function, but he did not provide

further analysis.

The analysis presented here of the deflated restarting scheme is based on further generalization of decompositions of Arnoldi type as well as the characterization of Krylov subspace approximations for matrix functions as polynomial Hermite interpolation on a nested sequence of nodes, which we have found instrumental in previous work [11, 3, 2]. The former is required due to the manner in which information is transferred between successive restart cycles, in that each cycle reuses a subspace of its predecessor. As a result, this leads to linearly dependent vectors in the global representation of the restarted cycles, which is needed when approximating general matrix functions with restarted Krylov subspaces. The interpolation process of the deflated restarted method differs from that in [11, 3, 2] in that, rather than adding a fixed number of interpolation nodes with each restart cycle, we update certain nodes with steadily improving approximations of eigenvalues close to a specified target value. The interpolation view allows us to split the analysis of the convergence of the overall process into two parts: we characterize the deflated restarted Krylov subspace method as a sequence of polynomial interpolations at nodes constructed from Ritz values by the algorithm. Combining this with known results on the convergence of Ritz values associated with restarted Krylov subspaces [5], we may conclude that the updated nodes converge to the target eigenvalues of A, resulting, asymptotically, in deflation. In addition, our analysis sheds new light on the behavior of the full orthogonalization method (FOM) with deflated restarting for solving linear systems of equations, to which the deflated restarting method specializes if $f(z) = 1/z$. In contrast to our study of the interpolation node sequence, the convergence of FOM is usually analyzed geometrically by measuring the angle between an iteration space and the target eigenvector space (see, e.g., [24, Theorem 2] or [5, Theorem 3.3]).

The remainder of this paper is organized as follows. In Section 2 we introduce *Krylov-like decompositions*, providing a generalization of the Arnoldi decomposition for manipulating vectors in a Krylov space in terms of any (possibly linearly dependent) set of vectors that span such a space. In particular, we show that the application of polynomials of degree up to m in A applied to $\boldsymbol{b}$ may be evaluated using only the quantities in a Krylov-like decomposition of $\mathscr{K}_m(A, \boldsymbol{b})$, thus generalizing a well-known property of Arnoldi and Arnoldi-type decompositions (cf. [9, 34, 29, 11]) which is key to the construction of Krylov subspace approximations of $f(A)\boldsymbol{b}$. In Section 3 we describe our new algorithm for incorporating deflation into the restarted Krylov subspace approximation of $f(A)\boldsymbol{b}$. Moreover, we characterize the associated approximation as resulting from the interpolation of f at the sequence of Ritz values accumulated in the course of the restart cycles in a manner analogous the undeflated restarted method of [11]. We show that the effect of deflation on this interpolation process is that those Ritz values approximating target eigenvalues of A selected for deflation in a restart cycle are removed from the set of interpolation nodes in the following cycle and replaced by improved approximations of these eigenvalues. Since the basic mechanism at work in spectral deflation for matrix functions may not be immediately apparent through the intricacies of the algorithm, we give a simple idealized explanation of this process in Section 4. Section 5 presents several numerical experiments which serve to illustrate the properties of the deflated restarting method as well as its utility.

2. Krylov-like decompositions and approximations. We shall require somewhat more general decompositions than (1.1) of the form

$$AW_{m+\ell} = W_{m+\ell}K_{m+\ell} + \boldsymbol{w}\boldsymbol{k}_{m+\ell}^T, \tag{2.1}$$

where $K_{m+\ell} \in \mathbb{C}^{(m+\ell)\times(m+\ell)}$, $W_{m+\ell} \in \mathbb{C}^{N\times(m+\ell)}$ with $\operatorname{range}(W_{m+\ell}) = \mathscr{K}_m(A, \boldsymbol{b})$, $\boldsymbol{w} \in \mathscr{K}_{m+1}(A, \boldsymbol{b}) \setminus \mathscr{K}_m(A, \boldsymbol{b})$ and $\boldsymbol{k}_{m+\ell} \in \mathbb{C}^{m+\ell}$. Note that the columns of $W_{m+\ell}$ are linearly dependent if (and only if) $\ell > 0$.

We shall refer to (2.1) as a *Krylov-like decomposition* of A with respect to $\mathscr{K}_m(A, \boldsymbol{b})$. Under additional assumptions this simplifies to various special cases of decompositions related to Krylov spaces which have appeared in the literature: in particular, (2.1) becomes

- a *Krylov decomposition* if $\ell = 0$, in which case the columns of W_m are linearly independent and form a basis of $\mathscr{K}_m(A, \boldsymbol{b})$ (cf. Stewart [39]),
- an *Arnoldi-like decomposition* if $\ell = 0$ and the columns of W_m form an *ascending* basis* of $\mathscr{K}_m(A, \boldsymbol{b})$, in which case K_m is an unreduced upper Hessenberg matrix (cf. [11]),
- an *Arnoldi decomposition* if $\ell = 0$, the columns of W_m form an ascending basis of $\mathscr{K}_m(A, \boldsymbol{b})$ and are *orthonormal*, in which case K_m is also unreduced upper Hessenberg and which constitutes the most familiar situation (see, e.g., [9], [34]).

Let f be a function such that $f(K_{m+\ell})$ is defined. We then define the *Krylov-like approximation to* $f(A)\boldsymbol{b}$ *associated with* (2.1) as

$$\boldsymbol{f}_{m+\ell} := W_{m+\ell} f(K_{m+\ell}) \hat{\boldsymbol{b}}, \tag{2.2}$$

where $\hat{\boldsymbol{b}} \in \mathbb{C}^{m+\ell}$ is any vector such that $W_{m+\ell}\hat{\boldsymbol{b}} = \boldsymbol{b}$. Note that $\hat{\boldsymbol{b}}$ is in general not uniquely defined. However, we shall see later that the approximation $\boldsymbol{f}_{m+\ell}$ is independent of the particular choice of $\hat{\boldsymbol{b}}$ (see Remark 2.6).

To motivate the considerations that follow, we quote a well-known result about the Arnoldi approximations mentioned in the introduction.

THEOREM 2.1 (cf., e.g., [34, 19]). *The Arnoldi approximations* $\boldsymbol{f}_m$ *in* (1.2) *can be expressed as*

$$\boldsymbol{f}_m = \|\boldsymbol{b}\| V_m f(H_m) \boldsymbol{e}_1 = q_{m-1}(A)\boldsymbol{b} = \frac{1}{2\pi i} \int_\Gamma f(\lambda) \boldsymbol{x}_m(\lambda)\, \mathrm{d}\lambda.$$

Here, q_{m-1} *denotes the uniquely determined polynomial of degree* $m-1$ *which interpolates* f *in the Hermite sense at the eigenvalues of* H_m*. For the contour integral we require that* f *be analytic in and on the Jordan curve* Γ *which contains the eigenvalues of* A *and* H_m *in its interior. The vectors* $\boldsymbol{x}_m(\lambda) := \|\boldsymbol{b}\| V_m (\lambda I_m - H_m)^{-1} \boldsymbol{e}_1$ *are the approximate solutions of the linear systems* $(\lambda I_N - A)\boldsymbol{x}(\lambda) = \boldsymbol{b}$ *that are generated by* m *steps of the full orthogonalization method (FOM) with starting vectors* $\boldsymbol{x}_0(\lambda) = \boldsymbol{0}$.

We now show that analogous characterizations hold for the Krylov-like approximation $\boldsymbol{f}_{m+\ell}$ of (2.2). To this end, we require several lemmas.

LEMMA 2.2. *For any polynomial* $q(z) = \alpha_m z^m + \cdots \in \mathscr{P}_m$ *there holds*

$$q(A)\boldsymbol{b} = W_{m+\ell}\, q(K_{m+\ell})\, \hat{\boldsymbol{b}} + \alpha_m (\boldsymbol{k}_{m+\ell}^T K_{m+\ell}^{m-1} \hat{\boldsymbol{b}}) \boldsymbol{w} \tag{2.3}$$

using the notation of (2.1)*. In particular, for* $q \in \mathscr{P}_{m-1}$ *this simplifies to*

$$q(A)\boldsymbol{b} = W_{m+\ell}\, q(K_{m+\ell})\, \hat{\boldsymbol{b}}.$$

*i.e., the first j columns span $\mathscr{K}_j(A, \boldsymbol{b})$ for all $j = 1, 2, \ldots, m$

Proof: By linearity it is sufficient to verify (2.3) for the monomials $q(z) = z^j, j = 0, \ldots, m$, which follows immediately by induction: For $j = 0$ we have $A^0\boldsymbol{b} = W_{m+\ell}K_{m+\ell}^0\hat{\boldsymbol{b}} = \boldsymbol{b}$, since $\hat{\boldsymbol{b}}$ satisfies $W_{m+\ell}\hat{\boldsymbol{b}} = \boldsymbol{b}$ by assumption. Moreover, the assumption $A^{j-1}\boldsymbol{b} = W_{m+\ell}K_{m+\ell}^{j-1}\hat{\boldsymbol{b}}$ for some $j \in \{1, 2, \ldots, m\}$ yields, after multiplication by A,

$$A^j\boldsymbol{b} = A(A^{j-1}\boldsymbol{b}) = A(W_{m+\ell}K_{m+\ell}^{j-1}\hat{\boldsymbol{b}}) = W_{m+\ell}K_{m+\ell}^{j}\hat{\boldsymbol{b}} + (\boldsymbol{k}_{m+\ell}^T K_{m+\ell}^{j-1}\hat{\boldsymbol{b}})\boldsymbol{w},$$

where we have used (2.1) for the last equality. The leftmost vector in this chain of identities is contained in $\mathscr{K}_{j+1}(A, \boldsymbol{b}) \setminus \mathscr{K}_j(A, \boldsymbol{b})$ and this is only possible for the rightmost vector if $\boldsymbol{k}_{m+\ell}^T K_{m+\ell}^{j-1}\hat{\boldsymbol{b}} = 0$ for $1 \le j \le m-1$ since $\boldsymbol{w} \in \mathscr{K}_{m+1}(A, \boldsymbol{b}) \setminus \mathscr{K}_m(A, \boldsymbol{b})$. For $j = m$ we obtain the identity (2.3). □

The vector $\boldsymbol{w}$ in (2.1) lies in $\mathscr{K}_{m+1}(A, \boldsymbol{b}) \setminus \mathscr{K}_m(A, \boldsymbol{b})$ and can therefore be expressed as $\boldsymbol{w} = p_m(A)\boldsymbol{b}$ with a unique polynomial p_m of *exact* degree m. This polynomial plays a crucial role in the analysis which follows.

LEMMA 2.3. *For the polynomial p_m defined by $\boldsymbol{w} = p_m(A)\boldsymbol{b}$, there holds*

$$W_{m+\ell}\, p_m(K_{m+\ell})\hat{\boldsymbol{b}} = \boldsymbol{0}.$$

More generally, for any polynomial q there holds

$$W_{m+\ell}\, q(K_{m+\ell})\, p_m(K_{m+\ell})\hat{\boldsymbol{b}} = \boldsymbol{0}.$$

Proof: Writing $p_m(z) = \alpha_m z^m + \cdots$ and substituting $\boldsymbol{w} = p_m(A)\boldsymbol{b}$, Lemma 2.2 yields

$$p_m(A)\boldsymbol{b} = W_{m+\ell}\, p_m(K_{m+\ell})\hat{\boldsymbol{b}} + \alpha_m(\boldsymbol{k}_{m+\ell}^T K_{m+\ell}^{m-1}\hat{\boldsymbol{b}})\, p_m(A)\boldsymbol{b},$$

or, equivalently,

$$\big(1 - \alpha_m(\boldsymbol{k}_{m+\ell}^T K_{m+\ell}^{m-1}\hat{\boldsymbol{b}})\big)p_m(A)\boldsymbol{b} = W_{m+\ell}\, p_m(K_{m+\ell})\hat{\boldsymbol{b}}. \tag{2.4}$$

The vector $\boldsymbol{w} = p_m(A)\boldsymbol{b}$ is an element of $\mathscr{K}_{m+1}(A, \boldsymbol{b}) \setminus \mathscr{K}_m(A, \boldsymbol{b})$ and the right-hand side of (2.4) is an element of $\mathrm{range}(W_{m+\ell}) = \mathscr{K}_m(A, \boldsymbol{b})$. Equality in (2.4) can only hold if both sides vanish, i.e., if $W_{m+\ell}\, p_m(K_{m+\ell})\hat{\boldsymbol{b}} = \boldsymbol{0}$.

Assume next that $W_{m+\ell}K_{m+\ell}^{j-1}p_m(K_{m+\ell})\hat{\boldsymbol{b}} = \boldsymbol{0}$ for some $j \ge 1$. Then, using (2.1),

$$\begin{aligned}
W_{m+\ell}K_{m+\ell}^{j}p_m(K_{m+\ell})\hat{\boldsymbol{b}} &= (W_{m+\ell}K_{m+\ell})K_{m+\ell}^{j-1}p_m(K_{m+\ell})\hat{\boldsymbol{b}} \\
&= (AW_{m+\ell} - \boldsymbol{w}\boldsymbol{k}_{m+\ell}^T)K_{m+\ell}^{j-1}p_m(K_{m+\ell})\hat{\boldsymbol{b}} \\
&= AW_{m+\ell}K_{m+\ell}^{j-1}p_m(K_{m+\ell})\hat{\boldsymbol{b}} - (\boldsymbol{k}_{m+\ell}^T K_{m+\ell}^{j-1}p_m(K_{m+\ell})\hat{\boldsymbol{b}})\boldsymbol{w} \\
&= -(\boldsymbol{k}_{m+\ell}^T K_{m+\ell}^{j-1}p_m(K_{m+\ell})\hat{\boldsymbol{b}})\boldsymbol{w}
\end{aligned}$$

by our assumption. We now argue as in the proof of Lemma 2.2: Since $\boldsymbol{w} \in \mathscr{K}_{m+1}(A, \boldsymbol{b}) \setminus \mathscr{K}_m(A, \boldsymbol{b})$ and $W_{m+\ell}K_{m+\ell}^{j}p_m(K_{m+\ell})\hat{\boldsymbol{b}} \in \mathscr{K}_m(A, \boldsymbol{b})$ the above equation implies $W_{m+\ell}K_{m+\ell}^{j}p_m(K_{m+\ell})\hat{\boldsymbol{b}} = \boldsymbol{0}$.

We have thus inductively shown that $W_{m+\ell}K_{m+\ell}^{j}p_m(K_{m+\ell})\hat{\boldsymbol{b}} = \boldsymbol{0}$ for all j from which the assertion of the lemma follows. □

As an additional tool we state an essentially well-known property of the zeros of p_m.

LEMMA 2.4. *The zeros of p_m are contained in the spectrum of $K_{m+\ell}$. More precisely, p_m divides the characteristic polynomial of $K_{m+\ell}$.*
Proof: The j-th column of the matrix $W_{m+\ell}$ can be expressed as $p^{(j)}(A)\boldsymbol{b}$ for some polynomial $p^{(j)}$ of degree at most $m-1$. From (2.1) we conclude that these polynomials satisfy the recurrence

$$z\big[p^{(1)}(z),\dots,p^{(m+\ell)}(z)\big] = \big[p^{(1)}(z),\dots,p^{(m+\ell)}(z)\big]K_{m+\ell} + p_m(z)\boldsymbol{k}_{m+\ell}^T, \tag{2.5}$$

If z_0 is a zero of p_m, then $p_m(z_0)\boldsymbol{k}_{m+\ell}^T$ vanishes and z_0 must be an eigenvalue of $K_{m+\ell}$. Next, let z_0 be a double zero of p_m. Differentiating (2.5) gives

$$\begin{aligned} &z\left[\frac{\mathrm{d}p^{(1)}(z)}{\mathrm{d}z},\dots,\frac{\mathrm{d}p^{(m+\ell)}(z)}{\mathrm{d}z}\right] + \big[p^{(1)}(z),\dots,p^{(m+\ell)}(z)\big] \\ &= \left[\frac{\mathrm{d}p^{(1)}(z)}{\mathrm{d}z},\dots,\frac{\mathrm{d}p^{(m+\ell)}(z)}{\mathrm{d}z}\right]K_{m+\ell} + \frac{\mathrm{d}p_m(z)}{\mathrm{d}z}\boldsymbol{k}_{m+\ell}^T. \end{aligned}$$

Since $\mathrm{d}p_m(z_0)/\mathrm{d}z = 0$, we see that the eigenvalue z_0 is associated with the eigenvector $\big[p^{(1)}(z_0),\dots,p^{(m+\ell)}(z_0)\big]$ and the principal vector $\big[\mathrm{d}p^{(1)}(z_0)/\mathrm{d}z,\dots,\mathrm{d}p^{(m+\ell)}(z_0)/\mathrm{d}z\big]$. Consequently, the eigenvalue z_0 of $K_{m+\ell}$ has at least algebraic multiplicity 2. For zeros of higher order the result follows from further differentiation. □

We are now in position to prove the main theorem of this section.

THEOREM 2.5. *The Krylov-like approximation to $f(A)\boldsymbol{b}$ introduced in* (2.2) *as $\boldsymbol{f}_{m+\ell} = W_{m+\ell}f(K_{m+\ell})\hat{\boldsymbol{b}}$ can be characterized as*

$$\boldsymbol{f}_{m+\ell} = q_{m-1}(A)\boldsymbol{b},$$

where q_{m-1} interpolates f in the Hermite sense at the zeros of p_m (see Lemma 2.3), i.e., at some but, in general, not at all eigenvalues of $K_{m+\ell}$.
If Γ is a Jordan curve which contains the eigenvalues of A and $K_{m+\ell}$ in its interior and such that f is analytic in and on Γ then

$$\boldsymbol{f}_{m+\ell} = \frac{1}{2\pi i}\int_\Gamma f(\lambda)\boldsymbol{x}_{m+\ell}(\lambda)\,\mathrm{d}\lambda,$$

where $\boldsymbol{x}_{m+\ell}(\lambda) = W_{m+\ell}(\lambda I_{m+\ell} - K_{m+\ell})^{-1}\hat{\boldsymbol{b}}$ is the Krylov-like approximation to $(\lambda I_N - A)^{-1}\boldsymbol{b}$ associated with (2.1).

Proof: To show the first of the above characterizations we note that, by the definition of matrix functions, $f(K_{m+\ell}) = r(K_{m+\ell})$ with $r \in \mathscr{P}_{m+\ell-1}$ the Hermite interpolating polynomial of f at the eigenvalues of $K_{m+\ell}$. In particular, the Krylov-like approximation can be expressed as $\boldsymbol{f}_{m+\ell} = W_{m+\ell}\,r(K_{m+\ell})\hat{\boldsymbol{b}}$, and it suffices to show that

$$W_{m+\ell}\,r(K_{m+\ell})\hat{\boldsymbol{b}} = q_{m-1}(A)\boldsymbol{b}.$$

Since, by Lemma 2.4, the zeros of p_m are among the eigenvalues of $K_{m+\ell}$, the polynomial q_{m-1} also interpolates r at the zeros of p_m, and therefore $r - q_{m-1}$ must be divisible by p_m, i.e., $r = sp_m + q_{m-1}$ for some polynomial s. Thus,

$$W_{m+\ell}\,r(K_{m+\ell})\hat{\boldsymbol{b}} = W_{m+\ell}\,s(K_{m+\ell})p_m(K_{m+\ell})\hat{\boldsymbol{b}} + W_{m+\ell}q_{m-1}(K_{m+\ell})\hat{\boldsymbol{b}} = q_{m-1}(A)\boldsymbol{b}$$

since, by Lemma 2.3, $W_{m+\ell}s(K_{m+\ell})p_m(K_{m+\ell})\hat{\boldsymbol{b}} = \boldsymbol{0}$, and, by Lemma 2.2, $W_{m+\ell}q_{m-1}(K_{m+\ell})\hat{\boldsymbol{b}} = q_{m-1}(A)\boldsymbol{b}$.

The second characterization is an immediate consequence of the representation of a matrix function as a Cauchy integral. Under the given assumptions, there holds

$$f(K_{m+\ell}) = \frac{1}{2\pi i}\int_\Gamma f(\lambda)(\lambda I_{m+\ell} - K_{m+\ell})^{-1}\,\mathrm{d}\lambda.$$

□

REMARK 2.6. *As a consequence of Theorem 2.5, the approximation* $\boldsymbol{f}_{m+\ell} = W_{m+\ell} f(K_{m+\ell})\hat{\boldsymbol{b}}$ *is determined by the zeros of* p_m *but is independent of the specific choice of* $\hat{\boldsymbol{b}}$*, as long as* $W_{m+\ell}\hat{\boldsymbol{b}} = \boldsymbol{b}$.

3. The Restarted Krylov Approximation with Deflation. We briefly describe the Arnoldi method with deflated restarting which underlies our approach. We will allow m matrix-vector multiplications by A per cycle and augment the current Krylov space by ℓ approximate eigenvectors. More precisely, we identify a priori a subspace of dimension ℓ which delays convergence of the restarted Krylov subspace approximation to $f(A)\boldsymbol{b}$. As an example, if f has a finite singularity such as at the origin when solving linear systems of equations, one would choose the A-invariant subspace associated with the ℓ eigenvalues closest to this singularity. The approximation of this subspace is successively refined in the course of our algorithm with the goal of removing its influence on the convergence process. We refer to the eigenvalues associated with this subspace as *target eigenvalues*.

We note that m and ℓ need not necessarily be the same for all cycles. However we assume this here to keep the notation as simple as possible.

In the first cycle, we compute the standard Arnoldi decomposition of A with respect to $\mathscr{K}_m(A, \boldsymbol{b})$ given by $AV^{(1)} = V^{(1)}H^{(1)} + h^{(1)}\boldsymbol{v}^{(1)}\boldsymbol{e}_m^T$. We then extract ℓ eigenpairs of $H^{(1)}$. More precisely, we compute a partial Schur decomposition

$$H^{(1)}U^{(1)} = U^{(1)}T^{(1)},$$

where $T^{(1)} \in \mathbb{C}^{\ell\times\ell}$ is upper triangular and where the columns of $U^{(1)} \in \mathbb{C}^{m\times\ell}$ form an orthonormal basis of the invariant subspace associated with ℓ desired eigenvalues of $H^{(1)}$. With $Y^{(1)} := V^{(1)}U^{(1)} \in \mathbb{C}^{N\times\ell}$, there holds

$$AY^{(1)} = Y^{(1)}T^{(1)} + h^{(1)}\boldsymbol{v}^{(1)}\boldsymbol{u}^{(1)}$$

with the (generally dense) row vector $\boldsymbol{u}^{(1)} := \boldsymbol{e}_m^T U^{(1)} \in \mathbb{C}^{1\times\ell}$. We extend this factorization by m standard Arnoldi steps to obtain

$$A\,[Y^{(1)}\,V^{(2)}] = [Y^{(1)}\,V^{(2)}]\begin{bmatrix} T^{(1)} & S^{(1)} \\ h^{(1)}\boldsymbol{e}_1\boldsymbol{u}^{(1)} & H^{(2)} \end{bmatrix} + h^{(2)}\boldsymbol{v}^{(2)}\boldsymbol{e}_{\ell+m}^T. \tag{3.1}$$

Here $[Y^{(1)}\,V^{(2)}\,\boldsymbol{v}^{(2)}] \in \mathbb{C}^{n\times(\ell+m+1)}$ has orthonormal columns, $V^{(2)}\boldsymbol{e}_1 = \boldsymbol{v}^{(1)}$, $H^{(2)} \in \mathbb{C}^{m\times m}$ is an unreduced upper Hessenberg matrix, and $S^{(1)} = [Y^{(1)}]^H AV^{(2)} \in \mathbb{C}^{\ell\times m}$ is in general a dense matrix. This concludes the second cycle. For later use, we abbreviate (3.1) by

$$A\,[Y^{(1)}\,V^{(2)}] = [Y^{(1)}\,V^{(2)}]\,G^{(2)} + h^{(2)}\boldsymbol{v}^{(2)}\boldsymbol{e}_{\ell+m}^T \tag{3.1'}$$

(note that $G^{(2)}$ is not Hessenberg).

Before describing the k-th cycle ($k \geq 2$) let us summarize the situation after $k-1$ cycles:

$$\begin{aligned} AV^{(1)} &= V^{(1)}G^{(1)} + h^{(1)}\boldsymbol{v}^{(1)}\boldsymbol{e}_m^T, \\ A\,[Y^{(j-1)}\,V^{(j)}] &= [Y^{(j-1)}\,V^{(j)}]\,G^{(j)} + h^{(j)}\boldsymbol{v}^{(j)}\boldsymbol{e}_{\ell+m}^T, \qquad j = 2, 3, \ldots, k-1. \end{aligned} \tag{3.2}$$

All matrices $[Y^{(j-1)}\, V^{(j)}\, \boldsymbol{v}^{(j)}]$ have orthonormal columns. There holds $V^{(1)}\boldsymbol{e}_1 = \boldsymbol{b}/\|\boldsymbol{b}\|$ and $[Y^{(j-1)}\, V^{(j)}]\boldsymbol{e}_{\ell+1} = V^{(j)}\boldsymbol{e}_1 = \boldsymbol{v}^{(j-1)}$ $(j = 2, 3, \ldots, k-1)$. Further,

$$\begin{aligned} &G^{(1)} = H^{(1)} \in \mathbb{C}^{m\times m}, \\ &G^{(j)} = \begin{bmatrix} T^{(j-1)} & S^{(j-1)} \\ h^{(j-1)}\boldsymbol{e}_1\boldsymbol{u}^{(j-1)} & H^{(j)} \end{bmatrix} \in \mathbb{C}^{(\ell+m)\times(\ell+m)}, \qquad j = 2, 3, \ldots, k-1, \end{aligned} \tag{3.3}$$

with $H^{(j)} \in \mathbb{C}^{m\times m}$ unreduced upper Hessenberg $(j = 1, 2, \ldots, k-1)$ and $T^{(j-1)} \in \mathbb{C}^{\ell\times\ell}$ upper triangular matrices $(j = 2, 3, \ldots, k-1)$. The matrix $T^{(j-1)}$ represents the action of $G^{(j-1)}$ on the $G^{(j-1)}$-invariant subspace spanned by the (orthonormal) columns of $U^{(j-1)}$. Finally, $Y^{(j-1)} = [Y^{(j-2)}\, V^{(j-1)}]U^{(j-1)} \in \mathbb{C}^{N\times\ell}$ and $S^{(j-1)} = [Y^{(j-1)}]^H A V^{(j)}$.

In the k-th cycle we proceed analogously. We first determine a partial Schur decomposition of $G^{(k-1)}$ associated with ℓ target eigenvalues,

$$G^{(k-1)}U^{(k-1)} = U^{(k-1)}T^{(k-1)} \tag{3.4}$$

($T^{(k-1)} \in \mathbb{C}^{\ell\times\ell}$ is upper triangular, the columns of $U^{(k-1)} \in \mathbb{C}^{(\ell+m)\times\ell}$ are orthonormal) and obtain, with $Y^{(k-1)} := [Y^{(k-2)}\, V^{(k-1)}]U^{(k-1)} \in \mathbb{C}^{N\times\ell}$ and $\boldsymbol{u}^{(k-1)} := \boldsymbol{e}_{\ell+m}^T U^{(k-1)} \in \mathbb{C}^{1\times(\ell+m)}$,

$$AY^{(k-1)} = Y^{(k-1)}T^{(k-1)} + h^{(k-1)}\boldsymbol{v}^{(k-1)}\boldsymbol{u}^{(k-1)}. \tag{3.5}$$

As above, m subsequent Arnoldi steps lead to

$$A\,[Y^{(k-1)}\, V^{(k)}] = [Y^{(k-1)}\, V^{(k)}] \begin{bmatrix} T^{(k-1)} & S^{(k-1)} \\ h^{(k-1)}\boldsymbol{e}_1\boldsymbol{u}^{(k-1)} & H^{(k)} \end{bmatrix} + h^{(k)}\boldsymbol{v}^{(k)}\boldsymbol{e}_{\ell+m}^T.$$

Next we glue these decompositions together (for $j = 1, 2, \ldots, k$) to obtain

$$AW^{(k)} = W^{(k)}K^{(k)} + h^{(k)}\boldsymbol{v}^{(k)}\boldsymbol{e}_{km+(k-1)\ell}^T, \tag{3.6}$$

where $W^{(k)} = [V^{(1)}\, Y^{(1)}\, V^{(2)}\, \cdots\, Y^{(k-1)}\, V^{(k)}] \in \mathbb{C}^{N\times(km+(k-1)\ell)}$,

$$K^{(k)} := \begin{bmatrix} G^{(1)} & & & \\ F^{(1)} & G^{(2)} & & \\ & \ddots & \ddots & \\ & & F^{(k-1)} & G^{(k)} \end{bmatrix} \in \mathbb{C}^{(km+(k-1)\ell)\times(km+(k-1)\ell)},$$

$$\text{where } F^{(j)} := \begin{cases} h^{(1)}\boldsymbol{e}_{\ell+1}\boldsymbol{e}_m^T \in \mathbb{R}^{(\ell+m)\times m}, & j = 1, \\ h^{(j)}\boldsymbol{e}_{\ell+1}\boldsymbol{e}_{\ell+m}^T \in \mathbb{R}^{(\ell+m)\times(\ell+m)}, & j = 2, 3, \ldots, k-1. \end{cases}$$

Equation (3.6) represents a Krylov-like decomposition of A with respect to $\mathscr{K}_{km}(A, \boldsymbol{b})$ as introduced in Section 2 (see (2.1)).

Associated with (3.6) is the Krylov-like approximation

$$\boldsymbol{f}^{(k)} := \|\boldsymbol{b}\|W^{(k)}f(K^{(k)})\boldsymbol{e}_1 \tag{3.7}$$

(cf. (2.2) noting that $\|\boldsymbol{b}\|W^{(k)}\boldsymbol{e}_1 = \boldsymbol{b}$).

We briefly point out the simplifications which result when A is Hermitian. In this case the Arnoldi process simplifies to the Hermitian Lanczos process, and the

Hessenberg matrices $H^{(j)}$ in (3.3) are all unreduced real symmetric tridiagonal. Moreover, as can be seen from multiplying (3.2) from the left with $[Y^{(j-1)}V^{(j)}]^H$, the matrices $G^{(j)}$ are also Hermitian. In particular, $T^{(j-1)}$ is real diagonal and $S^{(j-1)} = [h^{(j-1)}\boldsymbol{e}_1\boldsymbol{u}^{(j-1)}]^H$.

By Theorem 2.5 the approximation $\boldsymbol{f}^{(k)}$ in (3.7) can be represented as $q_{km-1}(A)\boldsymbol{b}$, where the polynomial q_{km-1} Hermite-interpolates f at km of the $km + (k-1)\ell$ eigenvalues of $K^{(k)}$. We next characterize these interpolation nodes, and for this we require the following result.

LEMMA 3.1 ([24]). *Let $\theta_1^{(j)}, \ldots, \theta_\ell^{(j)}$ denote the target eigenvalues of $G^{(j)}$ in cycle j (i.e., the eigenvalues of $T^{(j)}$, counting multiplicities). Let further $\boldsymbol{v}^{(j)} \in \mathscr{K}_{jm+1}(A, \boldsymbol{b})$ have the form $p_{jm}(A)\boldsymbol{b}$. Then*

$$r_{jm-\ell}(z) = \frac{p_{jm}(z)}{\left(z - \theta_1^{(j)}\right)\cdots\left(z - \theta_\ell^{(j)}\right)}$$

is a polynomial of degree $jm - \ell$ and there holds

$$\operatorname{range}\left(\left[Y^{(j)}\, V^{(j+1)}\right]\right) = \mathscr{K}_m(A, r_{jm-\ell}(A)\boldsymbol{b}).$$

We arrive at the following theorem.

THEOREM 3.2. *The approximation to $f(A)\boldsymbol{b}$ introduced in (3.7) as $\boldsymbol{f}^{(k)} := \|\boldsymbol{b}\|W^{(k)}f(K^{(k)})\boldsymbol{e}_1$ can be characterized as*

$$\boldsymbol{f}^{(k)} = q_{km-1}(A)\boldsymbol{b},$$

where q_{km-1} interpolates f in the Hermite sense at the zeros of p_{km}. Using the notation of (3.2) and Lemma 3.1 these zeros are given by

$$\bigcup_{j=1}^{k-1}\left(\Lambda(G^{(j)}) \setminus \left\{\theta_1^{(j)}, \ldots, \theta_\ell^{(j)}\right\}\right) \cup \Lambda(G^{(k)}).$$

If Γ is a Jordan curve which contains the eigenvalues of A and $K^{(k)}$ in its interior such that f is analytic in and on Γ then

$$\boldsymbol{f}^{(k)} = \frac{1}{2\pi i}\int_\Gamma f(\lambda)\,\boldsymbol{x}^{(k)}(\lambda)\,\mathrm{d}\lambda,$$

where $\boldsymbol{x}^{(k)}(\lambda) = \|\boldsymbol{b}\|W^{(k)}\left(\lambda I - K^{(k)}\right)^{-1}\boldsymbol{e}_1$ is the approximation to the solution of $(\lambda I_N - A)\boldsymbol{x}(\lambda) = \boldsymbol{b}$ after k cycles of the restarted FOM method [24, 25, 26] with restart length m and ℓ deflated eigenvalues, beginning with $\boldsymbol{x}_0(\lambda) = \boldsymbol{0}$.

REMARK 3.3. *The standard Arnoldi approximation $\boldsymbol{f}_m$ based on the Arnoldi decomposition $AV_m = V_mH_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^T$ can be expressed as $q_{m-1}(A)\boldsymbol{b}$, where q_{m-1} Hermite-interpolates f at* all *eigenvalues of the compression H_m. Similar statements apply to approximations based on Arnoldi-like and Krylov decompositions (such as the restarted Arnoldi approximation as described in [11]). However, in the case of Krylov-like decompositions, in which the Krylov subspace is represented by possibly linearly dependent vectors, not all eigenvalues of the matrix describing the action of A on the Krylov space in terms of these generating vectors can be active as interpolation nodes.*

For the thick-restarted Arnoldi approximation $\boldsymbol{f}^{(k)}$, only the non-target eigenvalues of $\{G^{(j)}\}_{j=1}^{k-1}$ serve as interpolation points, yielding $(k-1)m-\ell$ nodes. The remaining $m+\ell$ nodes coincide with the eigenvalues of $G^{(k)}$.

Proof of Theorem 3.2: From Theorem 2.5 we know that $\boldsymbol{f}^{(k)} = q_{km-1}(A)\boldsymbol{b}$, where q_{km-1} Hermite-interpolates f at the zeros of p_{km}, which is given by $\boldsymbol{v}^{(k)} = p_{km}(A)\boldsymbol{b}$.

For cycle $j=1$ we have an Arnoldi decomposition

$$AV^{(1)} = V^{(1)}G^{(1)} + h^{(1)}\boldsymbol{v}^{(1)}\boldsymbol{e}_m^T,$$

and, by Lemma 2.3, $\boldsymbol{v}^{(1)} = p^{(1)}(A)\boldsymbol{b}$ where $p^{(1)} = p_m$ is a multiple of the characteristic polynomial of $G^{(1)}$.

In cycle $j+1$ we have a Krylov-like decomposition

$$A[Y^{(j)}\, V^{(j+1)}] = [Y^{(j)}\, V^{(j+1)}]G^{(j+1)} + h^{(j+1)}\boldsymbol{v}^{(j+1)}\boldsymbol{e}_{\ell+m}^T,$$

where $V^{(j+1)}\boldsymbol{e}_1 = p_{jm}(A)\boldsymbol{b}$. By Lemma 3.1 we know that $\operatorname{range}\left(\left[Y^{(j)}\, V^{(j+1)}\right]\right) = \mathscr{K}_m(A, r_{jm-\ell}(A)\boldsymbol{b})$, where

$$r_{jm-\ell}(z) = \frac{p_{jm}(z)}{\left(z-\theta_1^{(j)}\right)\cdots\left(z-\theta_\ell^{(j)}\right)},$$

and therefore $\boldsymbol{v}^{(j+1)} = p^{(j+1)}(A)(r_{jm-\ell}(A)\boldsymbol{b}) = (p^{(j+1)}r_{jm-\ell})(A)\boldsymbol{b} = p_{(j+1)m}(A)\boldsymbol{b}$. Since $p^{(j+1)}$ is a multiple of the characteristic polynomial of $G^{(j+1)}$, the zeros of $p_{(j+1)m}$ are the union of the eigenvalues of $G^{(j+1)}$ and the zeros of $r_{jm-\ell}$. This proves the first assertion by an obvious induction. □

Remark 3.4. *In finite-precision arithmetic the orthogonality of the approximate eigenvectors $Y^{(k-1)}$ in (3.5) is lost, but can be maintained if the block $Y^{(k-1)}$ is reorthogonalized before the Arnoldi decomposition is expanded by the vectors $V^{(k)}$. In our implementation we proceed as follows: Assume that, in the k-th cycle we have computed the partial Arnoldi decomposition*

$$A\widetilde{Y}^{(k-1)} = \widetilde{Y}^{(k-1)}T^{(k-1)} + h^{(k-1)}\boldsymbol{v}^{(k-1)}\boldsymbol{u}^{(k-1)},$$

where the columns of $\widetilde{Y}^{(k-1)}$ have lost orthogonality due to rounding errors but are still linearly independent (see (3.5)). We compute a QL-decomposition

$$[\widetilde{Y}^{(k-1)}\boldsymbol{v}^{(k-1)}] = QL =: [Y^{(k-1)}\boldsymbol{v}^{(k-1)}]\begin{bmatrix}\widehat{L} & \mathbf{0}\\ * & 1\end{bmatrix},$$

where $Q \in \mathbb{C}^{N\times(\ell+1)}$ has orthonormal columns, which in particular implies that $Y^{(k-1)}$ has orthormal columns, and where $\widehat{L} \in \mathbb{C}^{\ell\times\ell}$ is an invertible lower triangular matrix. An easy computation shows that

$$\begin{aligned} AY^{(k-1)} &= [Y^{(k-1)}\boldsymbol{v}^{(k-1)}]\begin{bmatrix}\widehat{L} & \mathbf{0}\\ * & 1\end{bmatrix}\begin{bmatrix}T^{(k-1)}\\ h^{(k-1)}\boldsymbol{u}^{(k-1)}\end{bmatrix}\widehat{L}^{-1}\\ &=: Y^{(k-1)}T_{\text{new}}^{(k-1)} + h^{(k-1)}\boldsymbol{v}^{(k-1)}\boldsymbol{u}_{\text{new}}^{(k-1)}. \end{aligned}$$

As described above this new (orthonormal) decomposition is expanded by m subsequent Arnoldi steps.

Remark 3.5. *If A and $\boldsymbol{b}$ are real, complex arithmetic can be avoided by using real Schur decompositions in (3.4).*

Finally, we describe two ways the approximants $\boldsymbol{f}^{(k)}$ of (3.7) to $f(A)\boldsymbol{b}$ can be computed from the decomposition (3.6). They correspond to Algorithms 1 and 2 in [3] (for details, see the description provided there).

Taking into account the block triangular structure of $K^{(k)}$ there holds

$$\boldsymbol{f}^{(k)} = \boldsymbol{f}^{(k-1)} + \|\boldsymbol{b}\| \begin{bmatrix} Y^{(k-1)} & V^{(k)} \end{bmatrix} \Big[f(K^{(k)}) \boldsymbol{e}_1 \Big]_{(k-1)m+(k-2)\ell+1:km+(k-1)\ell}$$

($k = 2, 3, \ldots$) with $\boldsymbol{f}^{(1)} = \|\boldsymbol{b}\| V^{(1)} f(K^{(1)}) \boldsymbol{e}_1$. Although this method (we again refer to it as Algorithm 1) has the advantage that only $Y^{(k-1)}$ and $V^{(k)}$ need to be stored to update $\boldsymbol{f}^{(k-1)}$, it requires the evaluation of $f(K^{(k)})$, i.e., the evaluation of f of a matrix whose dimension grows with the number of restarts.

Algorithm 2 avoids this drawback but it requires the knowledge of a rational approximation r to f given as a partial fraction expansion

$$f(z) \approx r(z) = \alpha_0 z + \sum_{\nu=1}^{n} \frac{\alpha_\nu}{\omega_\nu - z}.$$

Then the coefficients $\boldsymbol{h}^{(k)}$ of the update in $\boldsymbol{f}^{(k)} = \boldsymbol{f}^{(k-1)} + \|\boldsymbol{b}\| \begin{bmatrix} Y^{(k-1)} & V^{(k)} \end{bmatrix} \boldsymbol{h}^{(k)}$ can be determined by solving linear systems of fixed dimension $\ell + m$. With $\boldsymbol{f}^{(0)} = \alpha_0 \boldsymbol{b}$, we can represent $\boldsymbol{h}^{(k)}$ as $\boldsymbol{h}^{(k)} = \sum_{\nu=1}^{n} \alpha_\nu \boldsymbol{h}^{(k,\nu)}$, where

$$\begin{aligned} (\omega_\nu I_m - G^{(1)}) \boldsymbol{h}^{(1,\nu)} &= \boldsymbol{e}_1 \\ (\omega_\nu I_{\ell+m} - G^{(j)}) \boldsymbol{h}^{(j,\nu)} &= -F^{(j-1)} \boldsymbol{h}^{(j-1,\nu)} \qquad \text{for } j = 2, 3, \ldots, k \end{aligned}$$

(for $\nu = 1, 2, \ldots, n$).

To conclude this section, we summarize the algorithm by presenting a pseudocode, where the first of the update procedures is used. A Matlab code can be found online at `www.matrixfunctions.com`.

Algorithm 1: Arnoldi approximation for $f(A)\boldsymbol{b}$ with deflated restarting.

Given: A, $\boldsymbol{b}$, f, m, ℓ
Compute Arnoldi decomposition $AV^{(1)} = V^{(1)} H^{(1)} + h^{(1)} \boldsymbol{v}^{(1)} \boldsymbol{e}_m^T$
  with respect to $\mathscr{K}_m(A, \boldsymbol{b})$.
Set $F^{(1)} := h^{(1)} \boldsymbol{e}_{\ell+1} \boldsymbol{e}_m^T \in \mathbb{R}^{(\ell+m)\times m}$.
Set $\boldsymbol{f}^{(1)} := \|\boldsymbol{b}\| V^{(1)} f(H^{(1)}) \boldsymbol{e}_1$.
for $k = 2, 3, \ldots$ until convergence **do**
  Compute partial Schur decomposition $H^{(k-1)} U^{(k-1)} = U^{(k-1)} T^{(k-1)}$.
  Set $Y^{(k-1)} := V^{(k-1)} U^{(k-1)}$ and reorthogonalize (cf. Remark 3.4).
  Compute $A[Y^{(k-1)}\ V^{(k)}] = [Y^{(k-1)}\ V^{(k)}] G^{(k)} + h^{(k)} \boldsymbol{v}^{(k)} \boldsymbol{e}_{\ell+m}^T$
    by m further Arnoldi steps.
  Set $K^{(k)} := \begin{bmatrix} K^{(k-1)} & O \\ O \cdots O\ F^{(k-1)} & G^{(k)} \end{bmatrix}$.
  Set $F^{(k)} := h^{(k)} \boldsymbol{e}_{\ell+1} \boldsymbol{e}_{\ell+m}^T \in \mathbb{R}^{(\ell+m)\times(\ell+m)}$.
  Set $\boldsymbol{f}^{(k)} := \boldsymbol{f}^{(k-1)} + \|\boldsymbol{b}\| [Y^{(k-1)}\ V^{(k)}] [f(K^{(k)}]_{(k-1)m+(k-2)\ell+1:km+(k-1)\ell}$.

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4. Spectral Deflation for Matrix Functions. To motivate our deflation technique we first consider an idealized situation. Suppose we are given an A-invariant subspace with respect to which A assumes the block triangular form

$$A = \begin{bmatrix} A_1 & B \\ O & A_2 \end{bmatrix}.$$

A partial solution to the evaluation of $f(A)$ is given by a polynomial p which Hermite-interpolates f at the eigenvalues of A_1, resulting in $f(A_1) = p(A_1)$. The error of this approximation with respect to the original problem is then

$$f(A) - p(A) = \begin{bmatrix} f(A_1) & X \\ O & f(A_2) \end{bmatrix} - \begin{bmatrix} p(A_1) & Y \\ O & p(A_2) \end{bmatrix} = \begin{bmatrix} O & Z \\ O & f(A_2) - p(A_2) \end{bmatrix}$$

with a coupling matrix Z determined by the solution of the Lyapunov equation

$$A_1 Z - Z A_1 = -B[f(A_2) - p(A_2)]. \tag{4.1}$$

We further assume that the spectra of A_1 and A_2 are disjoint, in which case (4.1) has a unique solution Z which depends continuously on the right hand side, whereby convergence of $p(A_2)$ to $f(A_2)$ implies $Z \to O$. Therefore, given the eigenvalues of A_1, the original problem is reduced to the task of approximating $f(A_2)$.

Our algorithm constructs successively improved approximations of the invariant subspace associated with the target eigenvalues by steering the restarted Krylov subspaces in this direction. Despite the well-known fact that a Krylov space cannot contain an A-invariant subspace without being itself A-invariant (cf. e.g. [12]), we observe that an approximate deflation is obtained for approximately invariant subspaces.

Next, consider the situation at the beginning of the k-th restart cycle of the deflated restarting method. The update obtained in this cycle results from an interpolation at additional nodes, namely the eigenvalues of $G^{(k)}$. Assuming $\operatorname{range} Y^{(k-1)}$ has converged sufficiently close to the target space (see [5] for sufficient conditions for this to occur) implies that $h^{(k-1)}$ in (3.5) has become small and hence $G^{(k)}$ is nearly block upper triangular. The eigenvalues of $G^{(k)}$ thus consist of those of $T^{(k-1)}$ and those of $H^{(k)}$. This means that the interpolation nodes added in this cycle are $\{\theta_i^{(k-1)}\}_{i=1}^{\ell}$—these replace the target Ritz values of the preceding cycle (cf. Theorem 3.2)—in addition to the eigenvalues of $H^{(k)}$.

As a consequence of the orthogonalization in the Arnoldi process, the eigenvalues of $H^{(k)}$ can be characterized as Ritz values of a projected version of A as follows: The second block of the lower identity in (3.2) reads as

$$AV^{(k)} = Y^{(k-1)} S^{(k-1)} + V^{(k)} H^{(k)} + h^{(k)} \boldsymbol{v}^{(k)} \boldsymbol{e}_m^T.$$

Using $S^{(k-1)} = [Y^{(k-1)}]^H A V^{(k)}$ and the fact that $\operatorname{range} Y^{(k-1)} \perp \operatorname{range} V^{(k)}$, this can be rearranged to

$$(I - Y^{(k-1)}[Y^{(k-1)}]^H) A (I - Y^{(k-1)}[Y^{(k-1)}]^H) V^{(k)} = V^{(k)} H^{(k)} + h^{(k)} \boldsymbol{v}^{(k)} \boldsymbol{e}_m^T,$$

which is a standard Arnoldi decomposition of the Krylov space of the orthogonal section $A^{(k-1)}$ of A onto the orthogonal complement of $\operatorname{range} Y^{(k-1)}$ and initial vector $V^{(k)} \boldsymbol{e}_1 = \boldsymbol{v}^{(k-1)}$. Consequently, the eigenvalues of $H^{(k)}$ are the Ritz values of $A^{(k-1)}$ with respect to $\mathscr{K}_m(A^{(k-1)}, \boldsymbol{v}^{(k-1)})$. Once the target space has converged, the deflated restart algorithm behaves as the undeflated algorithm applied to A projected onto the complement of the target space. Results on the convergence properties of the restarted Arnoldi method without deflation as given in [11, 2] may thus be applied without modification to the deflated problem.

As an example, [2] treats the case of Hermitian A and restart length $m = 1$. There it was shown that, asymptotically, the Ritz values, i.e., the interpolation nodes,

alternate between two values ρ_1^* and ρ_2^* contained in the spectral interval $[\lambda_1, \lambda_N]$ of A located symmetric to its midpoint $(\lambda_1 + \lambda_N)/2$. The asymptotic convergence rate is determined by the lemniscates with foci ρ_1^* and ρ_2^* (see [2, Theorem 5.3]). Applying deflation with $\ell = 1$ and selecting, e.g., λ_1 as the target eigenvalue yields 2×2 matrices $G^{(j)}$ with eigenvalues $\theta^{(j)} \leq \rho^{(j)}$, $j \geq 2$. The approximation in the k-th cycle has the form $\boldsymbol{f}^{(k)} = q_{k-1}(A)\boldsymbol{b}$, where q_{k-1} interpolates f at the nodes $\{\rho^{(2)}, \ldots, \rho^{(k)}, \theta^{(k)}\}$, where

$$\theta_k \to \lambda_1, \quad \rho^{(2k)} \to \rho_1^*, \quad \rho^{(2k+1)} \to \rho_2^* \qquad \text{as } k \to \infty$$

but now ρ_1^* and ρ_2^* are contained in $[\lambda_2, \lambda_N]$ and lie symmetric to $(\lambda_2 + \lambda_N)/2$, where λ_2 denotes the second-smallest eigenvalue of A.

5. Numerical Examples. In this section we illustrate the behavior and the performance of our restarted Arnoldi method with and without deflation, and compare it with the unrestarted Arnoldi method. A comprehensive comparison of the deflated restarting method with other polynomial Krylov methods (see, e.g., [9, 40, 20, 8]) is beyond the scope of this paper and will be the subject of future work. Methods based on rational Krylov spaces (cf. [30, 31, 10, 23, 15, 6, 17]) may also be an attractive alternative to polynomial methods, provided that shifted linear systems $(A-\sigma I)\boldsymbol{x} = \boldsymbol{v}$ can be solved *efficiently*. However, in practical applications this is often not the case, examples being lattice QCD calculations [7]. Moreover, the linear operator A is often not accessible in explicit matrix form, but only the form of a subroutine that only returns the product $A\boldsymbol{v}$ given $\boldsymbol{v}$. We emphasize that solving the shifted systems with an inner unpreconditioned polynomial Krylov subspace iteration is not a viable approach, as the overall method is then again a polynomial Krylov subspace method.

The following computations were carried out in Matlab 2009a on an Intel Xeon 5160 at 3 GHz with 16 GB RAM. The operating system was SuSE Linux Enterprise Server (SLES) Version 10.

5.1. A Simple Example. We first illustrate several aspects of the deflated restarting Arnoldi approximation by computing $f(A)\boldsymbol{b} = A^{1/2}\boldsymbol{b}$ with

$$A = \mathrm{diag}(1, 2, \ldots, 100) \in \mathbb{R}^{100\times 100}, \qquad \boldsymbol{b} = [1, 1, \ldots, 1]^T/\sqrt{100} \in \mathbb{R}^{100}.$$

Figure 5.1 shows the errors of the unrestarted Arnoldi method and of the restarted Arnoldi method with restart length $m = 10$. As to be expected, restarting significantly slows down the speed of convergence. But we also see that this can be compensated (at least partially) by deflated restarting (again $m = 10$) with $\ell = 1, 3$ or 5 eigenvalues. On the left, the target eigenvalues were chosen as the ℓ eigenvalues of A which are closest to the singularity of f, i.e., in this case the ℓ smallest eigenvalues. The intimate connection between the Arnoldi approximation and polynomial interpolation motivates this choice. On the right, we also see that targeting the largest eigenvalues results in no improvement of the speed of convergence. Note that we have added in both figures also dotted lines depicting the convergence behavior of the restarted Arnoldi method ($m = 10$) without deflation applied to the reduced problems where the target eigenvalues have been removed, i.e., applied to $A = \mathrm{diag}(\ell+1, \ell+2, \ldots, 100)$ on the left and to $A = \mathrm{diag}(1, 2, \ldots, 100-\ell)$ on the right. These dotted lines are parallel to the corresponding solid ones, indicating that the asymptotic convergence rate of the undeflated restarting method applied to the deflated problem is equal to the asymptotic convergence rate of the deflated restarting method applied to the original problem.

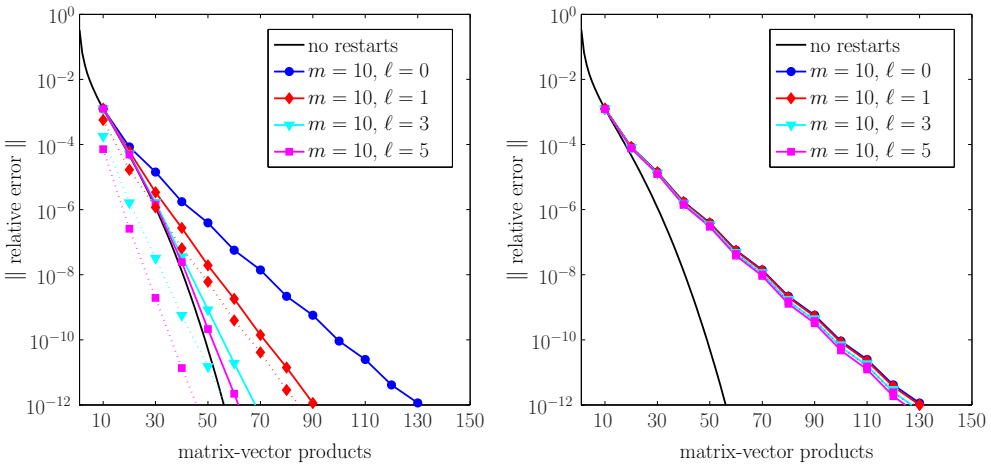

FIG. 5.1. *Approximating $A^{1/2}\boldsymbol{b}$: Convergence history of the Arnoldi method with restart length $m = 10$ and $\ell = 0, 1, 3$ and 5 target eigenvalues. The target eigenvalues are the smallest eigenvalues (left) and the largest eigenvalues (right) of A, respectively. For comparison, the dotted lines (covered by solid lines on the right) show the convergence of the restarted Arnoldi method without deflation applied to the reduced problems with the $\ell = 1, 3$ or 5 target eigenvalues removed from A.*

The appropriate choice of the target eigenvalues is not so obvious if f has more than one singularity: As an example we consider $f_1(z) = \sqrt{z - 0.95}/(101 - z)$, restart length $m = 10$ and choose the ℓ_- smallest (closest to the algebraic branch point $z = 0.95$) eigenvalues and the ℓ_+ largest (closest to the pole $z = 101$) eigenvalues of $A = \mathrm{diag}(1, 2, \ldots, 100)$ as targets, where $\ell_- + \ell_+ = \ell = 5$. Figure 5.2 shows the resulting error curves on the left, whereas the error curves on the right correspond to $f_2(z) = \sqrt{101 - z}/(z - 0.95)$, which results from exchanging the singularity types in f_1. The asymptotic convergence behavior, i.e., the linear convergence factor, of a restarted Arnoldi method depends only on the location of the singularities of f but not on their type. At first glance, the pronounced difference between both sides of Figure 5.2 seems to contradict this statement. However, the convergence curve for restarts without deflation ($\ell = 0$) for f_1 changes its slope after eight restart and shows, from then on, the same slope as the corresponding curve for f_2. Similar observations can be made for deflated restarts in the cases $\ell_- = 0$, $\ell_+ = 5$ and $\ell_- = 1$, $\ell_+ = 4$. In the remaining cases, the point of transition occurs after the relative error has been reduced to 10^{-12}.

We next consider an entire function, i.e., a function without finite singularities, such as $f(z) = \exp(-10z)$. It is clear that the eigenvectors which belong to the smallest eigenvalues of A (the largest of $-10A$) have the greatest influence on $f(A)$. Selecting ℓ of them as targets leads to a dramatic acceleration of convergence as shown in Figure 5.3. On the other hand, targeting at the ℓ largest eigenvalues of A would not lead to any improvement.

Finally, we illustrate our results on the interpolation nodes which underly the deflated restarting technique. In Theorem 3.2, these nodes are characterized as a subset of the spectrum of $K^{(k)}$ which is the union of the eigenvalues of its diagonal blocks $G^{(j)}$ $(j = 1, 2, \ldots, k)$. In Figure 5.4 these eigenvalues are plotted against j. In the terminology of Theorem 3.2 the filled (red) dots correspond to $\Lambda(G^{(j)}) \setminus \{\theta_1^{(j)}, \ldots, \theta_\ell^{(j)}\}$, whereas the crossed (blue) dots correspond to the Ritz values $\theta_1^{(j)}, \ldots, \theta_\ell^{(j)}$ which

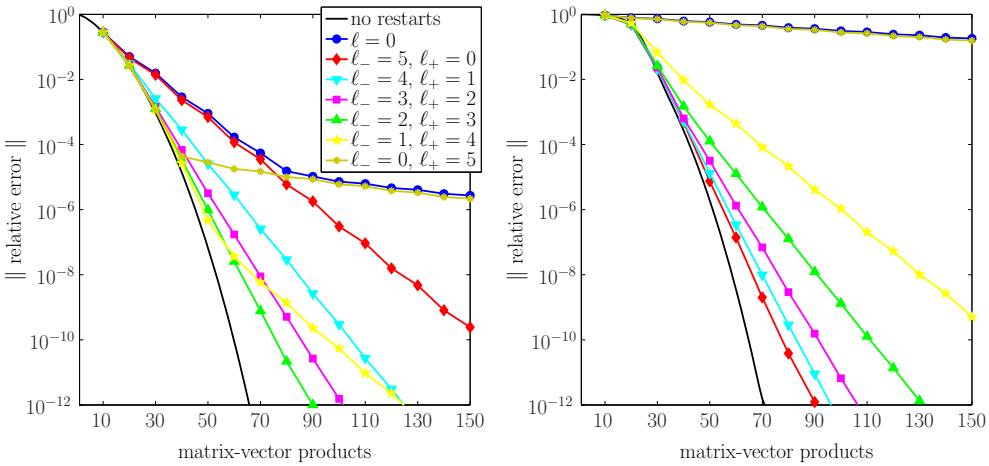

FIG. 5.2. *Approximating* $f_1(A)\boldsymbol{b} = (A - 0.95I)^{1/2}(101I - A)^{-1}\boldsymbol{b}$ *(left) and* $f_2(A)\boldsymbol{b} = (101I - A)^{1/2}(A - 0.95I)^{-1}\boldsymbol{b}$ *(right), respectively: Convergence history of the Arnoldi method with restart length* $m = 10$ *and* $\ell = 5$ *target eigenvalues* (ℓ_- *smallest and* ℓ_+ *largest). The legend on the left also applies to the plot on the right.*

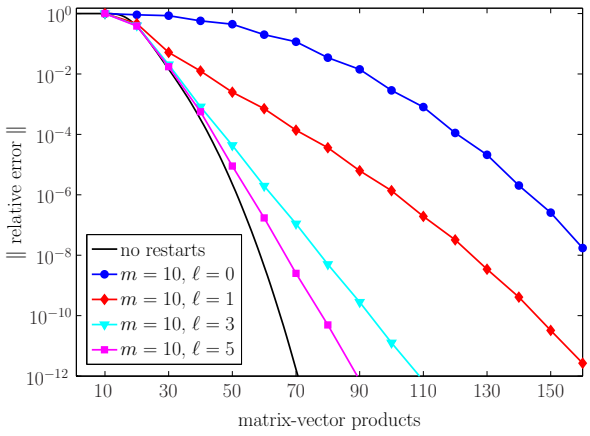

FIG. 5.3. *Approximating* $\exp(-10A)\boldsymbol{b}$*: Convergence history of the Arnoldi method with restart length* $m = 10$ *and the* $\ell = 0, 1, 3$ *and* 5 *smallest eigenvalues of* A *as targets.*

approximate the target eigenvalues. If we restart without deflation the km eigenvalues of $G^{(j)}$, $j = 1, 2, \ldots, k$, are exactly the nodes we interpolate at the k-th restart. In the case of deflation the nodes in the k-th restart are $\Lambda(G^{(j)}) \setminus \{\theta_1^{(j)}, \ldots, \theta_\ell^{(j)}\}$, $j = 1, 2, \ldots, k$, together with $\theta_1^{(k)}, \ldots, \theta_\ell^{(k)}$. The latter ones converge to the target eigenvalues of A, whereas the first ones show an asymptotically periodic behavior, i.e. they possess (at most) 2ℓ limit points in the spectral interval of A (which is observed for arbitrary restart lengths m but is proven only for $m = 1$, see [2]).

5.2. A symmetric problem: 3D-Laplacian. We approximate $f(A)\boldsymbol{b} = A^{-1/2}\boldsymbol{b}$, where $A \in \mathbb{R}^{n^3 \times n^3}$ is the matrix obtained by finite-difference discretization of the 3D-Laplace operator on the unit-cube with $n = 100$ interior grid-points in each Cartesian coordinate direction, and $\boldsymbol{b} \in \mathbb{R}^{n^3}$ is a random vector of unit length. To

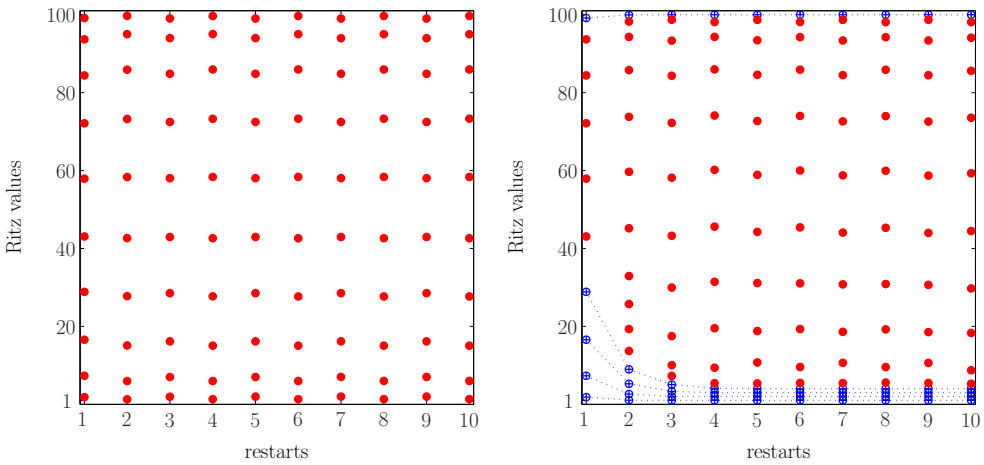

FIG. 5.4. *Interpolation points associated with restarted Arnoldi (restart length $m = 10$) without (left) and with deflation (right, with $\ell = 5$ target eigenvalues, namely the $\ell_- = 4$ smallest and the $\ell_+ = 1$ largest).*

this end we replace $f(z) = z^{-1/2}$ by its well-known Zolotarev rational approximation $r_{17}(z)$ of type $(16, 17)$ on the convex hull of $\Lambda(A)$ [1, Appendix E]. This rational approximation is sufficiently accurate to reach the absolute stopping accuracy $\varepsilon = 10^{-12}$, on which our timings of the algorithms are based. More precisely, we stopped iterating once an approximation $\boldsymbol{f}^{(k)}$ satisfied $\|f(A)\boldsymbol{b} - \boldsymbol{f}^{(k)}\| \le \varepsilon$. We considered an Arnoldi approximation of high order 1000 as "exact" solution to $f(A)\boldsymbol{b}$.

In Table 5.1 we summarize the results of our numerical tests. Since A is symmetric we have used the Lanczos three-term recurrence in both the restarted and standard (unrestarted) Krylov algorithms. The target eigenvalues are those closest to the origin. Note that the unrestarted Lanczos method requires only 395 matrix-vector products to satisfy our stopping criterion. It is known that this method yields near-optimal approximations (1.2) satisfying

$$\|f(A)\boldsymbol{b} - \boldsymbol{f}_m\| \le 2 \min_{p \in \mathscr{P}_{m-1}} \max_{z \in \Lambda(A) \cup \Lambda(H_m)} |f(z) - p(z)|$$

(cf. [14, 34]). This near-optimality is, of course, hard to beat with a restarted Lanczos method, which usually requires more matrix-vector products. However, the number of matrix-vector products of the restarted Lanczos method decreases significantly and comes closer to 395 as the number of approximate eigenvectors ℓ is increased. The number of matrix-vector products also decreases with increasing restart length m, the intuition behind this being that the restarted Lanczos method then "comes closer" to the unrestarted Lanczos method (the Krylov basis vectors become "closer" to orthogonal).

For symmetric problems the main advantage of our restarted method comes into effect when the Krylov basis vectors are sufficiently long that they can no longer be held in the main memory of the computer. If moving these vectors to secondary storage and reloading them when needed is not an attractive option, one could employ a two-pass Lanczos variant, in which the Krylov basis vectors are regenerated when they are required for assembling the approximation to $f(A)\boldsymbol{b}$. This doubles the number of matrix-vector products and is clearly not an option when matrix-vector

products are expensive, e.g., for matrices A with sufficiently many nonzero entries. In our example, where A has at most 7 nonzeros per row, the restarted method with deflation is already significantly faster than the two-pass Lanczos method, e.g., for $m = 50$ and $\ell = 5$.

A pragmatic recommendation for using a restarted Lanczos method for approximating $f(A)\boldsymbol{b}$ is to choose the restart length m as large as possible (this is dictated by the available main memory of the computer and the feasibility of evaluating $f(H^{(k)})$ efficiently). The choice of a suitable value of ℓ depends on the target eigenvalues and properties of f, but, as a rule of thumb, we found $\ell \in [0.05m, 0.1m]$ often successful. More elaborate heuristics which have been proposed in the context of restarted Krylov subspace methods for eigenvalue calculations [38, 41] could also be applied for determining ℓ.

m	ℓ	comp. time [s]	mv products	accuracy
∞ (I)	—	28.3	395	9e-13
∞ (II)	—	53.3	790	9e-13
25	0	98.7	1350	9e-13
25	1	68.5	875	9e-13
25	2	51.6	650	8e-13
25	5	**40.0**	475	9e-13
25	10	41.4	450	2e-13
50	0	61.4	850	8e-13
50	1	45.4	600	5e-13
50	2	38.1	500	4e-13
50	5	**35.4**	450	1e-13
50	10	37.3	450	1e-13

TABLE 5.1

Computation times, number of matrix-vector products and stopping accuracy for computing $A^{-1/2}\boldsymbol{b}$ with different restart lengths m and varying number of approximate eigenvectors ℓ. Here, $m = \infty$ (I) refers to the standard (unrestarted) Lanczos method, while $m = \infty$ (II) denotes the (unrestarted) two-pass Lanczos method.

5.3. A nonsymmetric problem: advection-diffusion. We consider the initial value problem (cf. [36, 3])

$$\partial_t u - \frac{1}{\mathrm{Pe}}\Delta u + \boldsymbol{a}\cdot\nabla u = 0 \qquad \text{in } \Omega = (-1,1)\times(0,1), \tag{5.1a}$$

$$u = 1 - \tanh(\mathrm{Pe}) \qquad \text{on } \Gamma_0, \tag{5.1b}$$

$$u = 1 + \tanh((2x+1)\,\mathrm{Pe}) \qquad \text{on } \Gamma_{\mathrm{in}}, \tag{5.1c}$$

$$\frac{\partial u}{\partial n} = 0 \qquad \text{on } \Gamma_{\mathrm{out}}, \tag{5.1d}$$

$$u(x,0) = u_0(x) \qquad \text{in } \Omega \tag{5.1e}$$

for the advection-diffusion equation, where the convective field is given as

$$\boldsymbol{a}(x,y) = \begin{bmatrix} 2y(1-x^2) \\ -2x(1-y^2) \end{bmatrix}, \qquad (x,y)\in\Omega,$$

and the boundary $\Gamma = \partial\Omega$ is divided into the inflow boundary $\Gamma_{\mathrm{in}} := [-1,0]\times\{0\}$, the outflow boundary $\Gamma_{\mathrm{out}} := [0,1]\times\{0\}$ and the remaining portion Γ_0. Pe denotes the Péclet number.

We discretize the advection-diffusion operator for $\mathrm{Pe} = 10$ in space using linear finite elements on a triangulation generated by the adaptive mesh generation facility in the COMSOL MULTIPHYSICS finite element software (version 3.3a). After multiplying from the left by the square root of the (lumped) mass matrix, the semi-discretized problem is a system of ODEs

$$\boldsymbol{u}'(t) = A\boldsymbol{u}(t) + \boldsymbol{g}, \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0,$$

where $A \in \mathbb{R}^{N\times N}$ with $N = 5,042, N = 12,269$ and $N = 30,341$ (after zero, one and two refinements of the mesh, respectively) and the constant inhomogeneous term $\boldsymbol{g}$ results from the inhomogeneous Dirichlet boundary condition. We then approximate the matrix exponential part of the solution

$$\boldsymbol{u}(t) = \exp(tA)(\boldsymbol{u}_0 + A^{-1}\boldsymbol{g}) - A^{-1}\boldsymbol{g} \tag{5.2}$$

at time $t = 6$, at which the flow has reached a steady state, starting from rest $\boldsymbol{u}_0 = \boldsymbol{0}$, using the unrestarted Arnoldi approximation as well as the restarted Arnoldi method with and without deflation. We note that an equivalent representation for the function $\boldsymbol{u}(t)$ in (5.2) is given by

$$\boldsymbol{u}(t) = \boldsymbol{u}_0 + t\varphi_1(tA)(A\boldsymbol{u}_0 + \boldsymbol{g}), \qquad \varphi_1(z) = \frac{\exp(z) - 1}{z}, \tag{5.3}$$

where φ_1 is known as the first so-called "phi-function" in the exponential integrator literature. The evaluation of (5.3) is slightly less expensive than that of (5.2) due to the absence of linear system solves, where it should be noted that, if solving systems with A is feasible, rational Krylov methods may be the better alternative. Moreover, (5.2) could be affected by ill-conditioning whenever eigenvalues of A approach the origin; this is not an issue in (5.3) as φ_1 is an entire function. However, we use (5.2) in our numerical computations to make the results comparable to the ones reported in [3, Section 6.3]

In [3, Section 6.3] we considered a similar advection-diffusion problem and observed a loss of about 4–6 digits of final accuracy when replacing $\exp(z)$ in (5.2) by its rational Cody–Meinardus–Varga (CMV) approximation $r_{16}(z)$ of type $(16, 16)$, compared to using the Matlab function `expm`. The reason for this loss is that the CMV approximation is only optimal on $(-\infty, 0]$ and A's field of values extends far outside this interval. We found experimentally that the restarted Arnoldi method obtains about the same final accuracy as with `expm` if we use a shifted approximation $\exp(z) \approx \exp(-\sigma)r_{16}(z+\sigma)$ with $\sigma = 15$ (similar observations were made in [22, 35]). This indicates that the loss of accuracy observed in [3] was not caused by an instability in our implementation of the restarted Arnoldi method, but can be attributed to the insufficient accuracy of the rational approximation used there.

The results of our numerical tests are given in Table 5.2, the absolute stopping accuracy being $\varepsilon = 10^{-12}$. The target eigenvalues were those closest to the origin. Besides the advantage of the fixed storage requirements of m Krylov basis vectors, the restarted Arnoldi method requires a number of inner-products which grows only linearly with the number of matrix-vector products (compared to a quadratic growth in the unrestarted case). This is the reason why the restarted Arnoldi method performs faster than the unrestarted version even for moderate problem sizes (for all three problem sizes the restarted method is about 2–4 times faster than the unrestarted, cf. Table 5.2). We again observe that deflation significantly reduces the number of matrix-vector products and thereby improves the overall performance of our restarted Arnoldi method.

N	m	ℓ	comp. time [s]	mv products	accuracy
5,042	∞	—	12.32	705	9e-13
	80	0	5.64	2800	8e-13
	80	1	3.91	1840	4e-13
	80	2	3.26	1440	7e-13
	80	5	**3.22**	1360	4e-13
	80	10	3.60	1360	2e-13
12,296	∞	—	71.1	1230	9e-13
	140	0	34.9	5040	4e-13
	140	1	24.1	3360	6e-13
	140	2	**18.7**	2520	8e-13
	140	5	19.2	2520	1e-13
	140	10	19.3	2380	4e-13
30,341	∞	—	482	2175	9e-13
	200	0	179	8200	5e-13
	200	1	152	6800	5e-13
	200	2	136	6000	1e-13
	200	5	126	5400	4e-13
	200	10	**112**	4600	5e-13

TABLE 5.2

Computation times, number of matrix-vector products and stopping accuracy for computing $\boldsymbol{u}(t) = \exp(tA)(\boldsymbol{u}_0 + A^{-1}\boldsymbol{g})$ *(cf.* (5.2)*) for* $t = 6$

with $A \in \mathbb{R}^{N\times N}$ stemming from finite-element discretizations of the same advection-diffusion problem with varying mesh-size. We compare the performance of the unrestarted Arnoldi method ($m = \infty$) with the restarted Arnoldi method with and without deflation.

6. Summary. We have shown how the spectral deflation techniques known for restarted Krylov subspace methods for computing selected eigenpairs and solving linear systems of equations can be extended to the approximation of $f(A)\boldsymbol{b}$. The associated approximation rests on an extension of the representation Lemma 2.2 to Krylov-like decompositions, which in turn represents a generalization of the Krylov decompositions of Stewart to accommodate linearly dependent vectors. The resulting deflated restarting scheme was characterized as an interpolation process, in which a number of interpolation nodes close to the target are replaced by improved eigenvalue approximations in each cycle. Numerical examples indicate that this technique can substantially accelerate restarted Arnoldi approximations to $f(A)\boldsymbol{b}$ by deflating eigenvalues close to singularities or dominant values of f. To our best knowledge, this deflated restarting technique is the only available Krylov method for approximating $f(A)\boldsymbol{b}$ with short recurrences *and* spectral adaptation, even in the absence of a-priori information on the spectrum of A.

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