The global extended-rational Arnoldi method for matrix function approximation

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Received: date / Accepted: date

Abstract The numerical computation of matrix functions such as $f(A)V$, where $A$ is an $n \times n$ large and sparse square matrix, $V$ is an $n \times p$ block with $p \ll n$ and $f$ is a nonlinear matrix function, arises in various applications such as network analysis ($f(t) = \exp(t)$ or $f(t) = t^3$), machine learning ($f(t) = \log(t)$), theory of quantum chromodynamics ($f(t) = t^{1/2}$), electronic structure computation, and others. In this work, we propose the use of global extended-rational Arnoldi method for computing approximations of such expressions. The derived method projects the initial problem onto an global extended-rational Krylov subspace $\mathcal{K}_m(A, V) = \text{span}\{\prod_{i=1}^{m} (A - s_i I_n)^{-1}1, V, A V, \ldots, A^{m-1}V\}$ of a low dimension. An adaptive procedure for the selection of shift parameters $\{s_1, \ldots, s_m\}$ is given. The proposed method is also applied to solve parameter dependent systems. Numerical examples are presented to show the performance of the global extended-rational Arnoldi for these problems.

Keywords Extended-rational Krylov subspace, matrix function, parameter dependent systems, global Arnoldi method, exponential function, skeleton approximation.

1 Introduction

Let $A \in \mathbb{R}^{n \times n}$ be a large and sparse matrix, and let $V \in \mathbb{R}^{n \times p}$ with $1 \leq p \ll n$. We are interested in approximating numerically expressions of the form

$$\mathcal{F}(f) := f(A)V$$

(1)
where \( f \) is a function that is defined on the convex hull of the spectrum of \( A \). The superscript \( T \) denotes transposition. The need to evaluate matrix functions of the forms (1) arises in various applications such as in network analysis [16], machine learning [29], electronic structure computation [4, 32] and the solution of ill-posed problems [17, 21]. When the matrix \( A \) is a small to medium size, the matrix function \( f(A) \) can be determined by the spectral factorization of \( A \); see [23, 21], for discussions on several possible definitions of matrix functions. In many applications, the matrix \( A \) is large that it is impractical to evaluate its spectral factorization. For this case, several projection methods have been developed. These methods consist of projecting the problem (1) onto a Krylov subspace with a small dimension. The projected part \( H \) of \( A \) is then used to evaluate \( f(H) \) by determining the spectral factorization of \( H \) and then get an approximation of \( f(A)V \). In the context of approximating the action of a matrix function \( f(A) \) on a some vector \( v \in \mathbb{R}^n \), several polynomial methods [5, 15, 33, 24] based on the standard Arnoldi and Lanczos Krylov methods have been proposed. Druskin and Knizhnerman [11], have shown that when \( f \) cannot be approximated accurately by polynomials on the spectrum of \( A \), then \( f(A)v \) cannot be approximated accurately by classical methods. They proposed the extended Krylov method for the symmetric case and the process was generalized to the nonsymmetric matrices by Simoncini in [35]. This method was applied to approximate the solution of the Sylvester, Riccati and Lyapunov equations [3, 22, 35].

Another technique for the evaluation of matrix functions is the rational Arnoldi method. This process was first proposed by Ruhe [31] in the context of computing the eigenvalues and have been used during the last years for the approximation of matrix functions, see [20, 30, 12, 13, 14, 28]. In this paper, we present the global extended-rational Arnoldi method to approximate the matrix function (1). The extended-rational Arnoldi method was proposed and applied to model reduction by [2]. As mentioned in [4], the extended-rational Krylov subspace (5) is richer than the rational Krylov subspace and represents a generalization of the extended Krylov subspace. We propose an adaptive computation of the shifts \((s_i)\) to generate an \(F\)-orthonormal basis for (5) in the case where \( f(A) = \{e^{-tA}, (A - \sigma I_n)^{-1}\} \) for definite matrix \( A \). This procedure is based on a generalization of the procedure used in [12]. In addition, we apply the proposed method to solve parameter dependent systems [29] with multiple right hand sides [19, 34]. These parameter systems have numerous applications in control theory, structural dynamics and time-dependent PDEs; see [18].

This paper is organized as follows. In Section 2, we give some preliminaries and then we introduce the global extended-rational Arnoldi process with some properties. Section 3 describes the application of this process to the approximation of the matrix function given in (1) and solving the parameter systems. We also propose an adaptive computation of the shifts \((s_i)\). Finally, some numerical experiments that illustrate the quality of the computed approximations are presented in Section 5.

2 The global extended-rational Arnoldi method

2.1 Preliminaries and notations

We begin by recalling some notations and definitions that will be used throughout this paper. The Kronecker product satisfies the following properties

1. \((A \otimes B)(C \otimes D) = AC \otimes BD\).
2. \((A \otimes B)^T = A^T \otimes B^T\).
Based on the Gram-Schmidt orthogonalization process, the first two blocks computed via the formulas

\[ R \]  

the subspace of \( \mathbb{R}^{n \times p} \) into block columns \( M_i, N_j \in \mathbb{R}^{n \times p} \), and define the \( \circ \)-product of the matrices \( M \) and \( N \) as

\[ M^T \circ N = [(N_j, M_i)]_{i=1}^{j=p} \in \mathbb{R}^{n \times l}. \]  

The following proposition gives some properties satisfied by the above product.

**Proposition 1** \((6, 7)\) Let \( A, B, C \in \mathbb{R}^{n \times p} \), \( D \in \mathbb{R}^{n \times n} \), \( L \in \mathbb{R}^{l \times p} \), and \( \alpha \in \mathbb{R} \). Then we have,

1. \( (A + B)^T \circ C = A^T \circ C + B^T \circ C \).
2. \( A^T \circ (B + C) = A^T \circ B + A^T \circ C \).
3. \( (\alpha A)^T \circ C = \alpha (A^T \circ C) \).
4. \( (A^T \circ B)^T = B^T \circ A \).
5. \( (DA)^T \circ B = A^T \circ (D^T B) \).
6. \( A^T \circ (B(L \otimes I_p)) = (A^T \circ B)L \).

2.2 Description of the process

Global Krylov subspace techniques were first proposed in \((26)\) for solving linear systems of equations with multiple right hand sides and also for large-scale Lyapunov matrix equations. The global extended-rational Krylov subspace was first introduced in \((2)\) and it is defined as the subspace of \( \mathbb{R}^{n \times p} \) spanned by the vectors (blocks)

\[ V, A^1V, A^2V, \ldots, A^{m-1}V, (A - s_1I_n)^{-1}V, (A - s_1I_n)^{-1}(A - s_2I_n)^{-1}V, \ldots, \prod_{i=1}^{m}(A - s_iI_n)^{-1}V. \]

This subspace is denoted by

\[ X^n_m(A, V) = \text{span}\left\{ V, (A - s_1I_n)^{-1}V, \ldots, A^{m-1}V, \prod_{i=1}^{m}(A - s_iI_n)^{-1}V \right\} \subset \mathbb{R}^{n \times p} \]  

where \( \{s_1, s_2, \ldots, s_m\} \) are some selected complex parameters all distinct from the eigenvalues of \( A \). We notice here that the subspace \( X^n_m(A, V) \) is a subspace of \( \mathbb{R}^{n \times p} \) so the vectors are blocks of size \( n \times p \). We assume that all the vectors (blocks) in \((3)\) are linearly independent. Now, we describe the global extended-rational Arnoldi process to generate an \( F \)-orthonormal basis \( X^{2m+2}_{2m+1}(A, V) = \{V_1, V_2, \ldots, V_{2m+2}\} \) with \( V_i \in \mathbb{R}^{n \times p} \) for the global extended-rational Krylov subspace \( X^{2m+1}_{2m+1}(A, V) \), and we derive some algebraic relations related to this process. The block vector \( V_i \)'s are said to be \( F \)-orthonormal, (with respect to the Frobenius inner product), if

\[ \langle V_i, V_k \rangle_F := \text{trace}(V_i^T V_k) = \begin{cases} 1 & j = k, \\ 0 & j \neq k. \end{cases} \]

Based on the Gram-Schmidt orthogonalization process, the first two blocks \( V_1 \) and \( V_2 \) are computed via the formulas

\[ V_1 = \frac{V}{\alpha_{1,1}}, \]

\[ V_2 = \frac{V}{\alpha_{2,2}}, \quad V_2 = (A - s_1I_n)^{-1}V - \alpha_{2,1}V_1, \]  

(4)
where \( \alpha_{1i} = \| V \|_F, \alpha_{12} = \langle (A - s_i I_n)^{-1} V, V \rangle_F \) and \( \alpha_{22} = \| \tilde{V}_2 \|_F \). To compute the block vectors \( V_{2j+1} \) and \( V_{2j+2} \), for \( j = 1, \ldots, m - 1 \), we use the following formulas

\[
\begin{align*}
    h_{2j+1,2j+1} V_{2j+1} &= A V_{2j+1} - \sum_{i=1}^{2j} h_{2j,2j} V_i = \tilde{V}_{2j+1} \\
    h_{2j+2,2j+2} V_{2j+2} &= (A - s_j I_n)^{-1} V_{2j} - \sum_{i=1}^{2j+1} h_{2j,2j} V_i = \tilde{V}_{2j+2}
\end{align*}
\]

(5)

where the coefficients \( h_{1,2j-1}, \ldots, h_{2j,2j-1} \) and \( h_{1,2j}, \ldots, h_{2j+1,2j} \) are determined so that the vectors satisfy the \( F \)-orthogonality condition

\[
V_{2j+1} \perp_F V_1, \ldots, V_{2j} \quad \text{and} \quad V_{2j+2} \perp_F V_1, \ldots, V_{2j+1}.
\]

Thus, the coefficients \( h_{1,2j-1}, \ldots, h_{2j,2j-1} \) and \( h_{1,2j}, \ldots, h_{2j+1,2j} \) are written as

\[
h_{2j,2j-1} = \langle A V_{2j-1}, V_j \rangle_F \quad \text{and} \quad h_{2j,2j} = \langle (A - s_j I_n)^{-1} V_{2j}, V_j \rangle_F
\]

(6)

The coefficients \( h_{2j+1,2j-1} \) and \( h_{2j+2,2j} \) are such that \( \| V_{2j+1} \|_F = 1 \) and \( \| V_{2j+2} \|_F = 1 \) respectively. Hence,

\[
h_{2j+1,2j-1} = \| \tilde{V}_{2j+1} \|_F \quad \text{and} \quad h_{2j+2,2j} = \| \tilde{V}_{2j+2} \|_F
\]

(7)

The global extended-rational Arnoldi algorithm is summarized in the following algorithm (Algorithm 1).

**Algorithm 1 The global extended-rational Arnoldi algorithm (GERA)**

Inputs: Matrix \( A \), initial block \( V \), and the shifts \( \{ s_1, \ldots, s_m \} \).

1. \( \alpha_{11} = \| V \|_F; V_1 = V / \alpha_{11} \);
2. \( \alpha_{12} = \langle (A - s_1 I_n)^{-1} V, V \rangle_F; \tilde{V}_2 = (A - s_1 I_n)^{-1} V - \alpha_{12} V_1 \);
3. \( \alpha_{22} = \| \tilde{V}_2 \|_F; V_2 = \tilde{V}_2 / \alpha_{22} \);
4. For \( j = 1, m \)
   
   a. \( V_{2j+1} = A V_{2j-1} \)
   b. For \( i = 1:2j \)
      
      - \( h_{2j,2j-1} = \langle V_{2j+1}, V_j \rangle_F \);
      - \( \tilde{V}_{2j+1} = V_{2j+1} - h_{2j,2j-1} V_j \);
      - endfor
   c. \( h_{2j+1,2j} = \| \tilde{V}_{2j+1} \|_F \);
   d. \( V_{2j+1} = V_{2j+1}/h_{2j+1,2j-1} \);
   e. \( V_{2j+2} = (A - s_j I_n)^{-1} V_{2j} \);
   f. For \( i = 1:2j+1 \)
      
      - \( h_{2j,2j} = \langle V_{2j+2}, V_j \rangle_F \);
      - \( \tilde{V}_{2j+2} = V_{2j+2} - h_{2j,2j} V_j \);
      - endfor
   g. \( h_{2j+2,2j} = \| \tilde{V}_{2j+2} \|_F \);
   h. \( V_{2j+2} = V_{2j+2}/h_{2j+2,2j} \);
   i. endfor

Output: \( F \)-Orthonormal basis \( V_{2m+2} = \{ V_1, \ldots, V_{2m+2} \} \).

The set of shifts \( \{ s_1, \ldots, s_m \} \) is chosen a priori or adaptively during the algorithm. The selection of shifts will be explained later. If all \( h_{2j+1,2j-1} \) and \( h_{2j+2,2j} \) are numerically nonzero, then Algorithm 1 determines an \( F \)-orthonormal basis \( V_1, \ldots, V_{2m+2} (V_j \in \mathbb{R}^{n \times p}) \) of the global
Using properties of the Tsenberg matrices where \( h \) and \( t \). The next proposition gives the entries of \( \mathcal{F}_{2m} = [h_{i,j}] \in \mathbb{R}^{2(m+1) \times 2m} \). We now introduce the \( 2m \times 2m \) matrix given by

\[
\mathcal{F}_{2m} = \mathcal{F}_{2m}^T \circ A \mathcal{F}_{2m} = [t_{i,j}],
\]

(8)

where \( t_{ij} = \langle Av_i, V_j \rangle_F, i, j = 1, \ldots, 2m \). \( \mathcal{F}_{2m} \) is the restriction of the matrix \( A \) to the extended-rational Krylov subspace \( \mathcal{K}^e_m(A, V) \).

**Proposition 2** Let the matrix \( A \in \mathbb{R}^{n \times n} \), and let \( V \in \mathbb{R}^{n \times p} \). The F-orthonormal basis \( V_1, \ldots, V_{2m+2} \) determined by the recursion formulas (6) satisfies, for \( j = 1, \ldots, m \)

\[
AV_{2j-1} \text{ and } AV_{2j} \in \text{span}\{V_1, \ldots, V_{2j+1}\}
\]

(9)

We notice that in the formulas given by (9), \( \mathcal{P}_{2m} \) is a block upper Hessenberg matrix with \( 2 \times 2 \) blocks, since \( \langle AV_{2j-1}, V_i \rangle_F = 0 \) and \( \langle AV_{2j}, V_i \rangle_F = 0 \) (for \( j = 1, \ldots, m, i \geq 2j+2 \)).

**Proposition 3** Assume that \( m \) steps of Algorithm (7) have been run and let \( \mathcal{F}_{2m} = \mathcal{F}_{2m+2}^T \circ A \mathcal{F}_{2m} \), then we have the following relations

\[
AY_{2m} = Y_{2m+2}^T (Y_{2m} \odot I_p)
\]

\[
= Y_{2m} (Y_{2m} \odot I_p) + V_{2m+1} \left[ [t_{2m+1,2m-1}, t_{2m+1,2m}] E_{2m}^T \otimes I_p \right],
\]

(10)

where the matrix \( E_{2m} = [e_{2m-1}, e_{2m}] \in \mathbb{R}^{2m \times 2} \) corresponds to the last two columns of the identity matrix \( I_{2m} \).

**Proof** According to (9), we obtain \( AY_{2m} \in \mathcal{K}^e_{m+1}(A, V) \), then there exists a matrix \( T \in \mathbb{R}^{(2m+2) \times 2m} \) such that

\[
AY_{2m} = Y_{2m+2} (T \odot I_p).
\]

Using properties of the \( \odot \)-product, we obtain

\[
Y_{2m+2}^T \circ AY_{2m} = Y_{2m+2}^T \circ \left[ Y_{2m+2} (T \odot I_p) \right]
\]

\[
= (Y_{2m+2} \odot Y_{2m+2})^T \circ T = T
\]

It follows that \( T = \mathcal{F}_{2m} \). Since \( \mathcal{F}_{2m} \) is an upper block Hessenberg matrix with \( 2 \times 2 \) blocks and \( t_{2j+1,2j} = \langle Av_{2j}, v_{2j+2} \rangle_F = 0 \) then \( Y_{2m+2} (T \odot I_p) \) can be decomposed as follows

\[
Y_{2m+2} (T \odot I_p) = Y_{2m} \mathcal{F}_{2m} + V_{2m+1} \left[ [t_{2m+1,2m-1}, t_{2m+1,2m}] E_{2m}^T \right]
\]

Which completes the proof.

The next proposition gives the entries of \( \mathcal{F}_{2m} \) in terms of the recursion coefficients. This will allow us to compute the entries quite efficiently.

**Proposition 4** Let \( \mathcal{F}_{2m} = [t_{1,1}, \ldots, t_{2m}] \) and \( \mathcal{H}_{2m} = [h_{1,1}, \ldots, h_{2m}] \) be the upper block Hessenberg matrices where \( h \) and \( t \) are the \( j \)-th column of \( \mathcal{H}_{2m} \) and \( \mathcal{F}_{2m} \), respectively. Then the odd columns are such that

\[
t_{2j-1} = h_{2j-1} \quad \text{for } j = 1, \ldots, m.
\]

(11)
The even columns satisfy the following relations
\[ t_{2j} = \frac{(\alpha_{1j} + s_j \alpha_{12})e_1 + s_1 \alpha_{2j}e_2 - \alpha_{1j} h_{1j}}{\alpha_{2j}} \]  
(12)
and for \( j = 1 \ldots m - 1 \)
\[ t_{2j+2} = \frac{1}{h_{2j+2j}} \left[ s_j h_{2j+2j} e_{2j+2} + e_{2j} - \sum_{i=1}^{2j+1} h_{1j} (t_{i} - s_j e_{i}) \right], \]  
(13)
where \( e_i \) corresponds to the \( i \)-th column vector of the canonical basis \( \mathbb{R}^{2m+2} \) and \( \alpha_{1j}, \alpha_{12} \) and \( \alpha_{2j} \) are defined from (4).

**Proof** We have \( t_{2j-1} = \gamma_{2m+2}' \circ A V_{2j-1} \). Therefore, (11) follows from the expression of \( h_{2j-1} \) in (5). Using (4), we obtain
\[ \alpha_{1j} V_1 + \alpha_{2j} V_2 = \alpha_{1j} (A - s_j I_n)^{-1} V_1. \]

Multiplying this last equality by \( (A - s_j I_n) \) from the left gives
\[ \alpha_{1j} (A - s_j I_n) V_1 + \alpha_{2j} (A - s_j I_n) V_2 = \alpha_{1j} V_1. \]
Then the vector \( AV_2 \) is written as follows
\[ AV_2 = \frac{1}{\alpha_{2j}} \left[ (\alpha_{1j} + s_j \alpha_{12}) V_1 + s_1 \alpha_{2j} V_2 - \alpha_{1j} A V_1 \right]. \]

The relation (12) is obtained by multiplying \( AV_2 \) by \( \gamma_{2m+2}' \) with the \( \circ \)-product from the left since \( t_{2j} = \gamma_{2m+2}' \circ A V_{2j} \). The formula (13) is obtained from the expression of \( AV_{2j+2} \) for \( j = 1, \ldots, m - 1 \). Thus, multiplying the second equality in (5) by \( (A - s_j I_n) \) from the left gives
\[ h_{2j+2j} (A - s_j I_n) V_{2j+2} = V_{2j} - \sum_{i=1}^{2j+1} h_{1j} (A - s_j I_n) V_i. \]
Then,
\[ AV_{2j+2} = \frac{1}{h_{2j+2j}} \left[ h_{2j+2j} s_j V_{2j+2} + V_{2j} - \sum_{i=1}^{2j+1} h_{1j} (AV_i - s_j V_i) \right]. \]

The expression (13) is easily obtained by multiplying \( AV_{2j+2} \) by \( \gamma_{2m+2}' \) with the \( \circ \)-product from the left. This concludes the proof of the proposition.

We notice that if \( A \) is a symmetric matrix, then the restriction matrix \( \mathcal{J}_{2m} \) in (5) reduces to a symmetric and pentadiagonal matrix with the following nontrivial entries,
\[ t_{i,j-1} = h_{i,j-1} \] for \( i \in \{ 2j - 3, \ldots, 2j + 1 \} \),
\[ t_{1j} = [\alpha_{1j} - (t_{1j} - s_j) \alpha_{12}] / \alpha_{2j}, \]
\[ t_{2j} = s_1 - t_{2j} \alpha_{1j} / \alpha_{2j}, \]
\[ t_{3j} = -t_{3j} \alpha_{12} / \alpha_{2j}. \]
And for \( j = 1, \ldots, m - 1 \)
\[ t_{2j+1,2j+2} = (s_j h_{2j+1,2j} - \sum_{i=2j-1}^{2j+1} t_{2j+1,i} h_{i,2j}) / h_{2j+2,2j}, \]
\[ t_{2j+2,2j+2} = s_j - t_{2j+2,2j+1} h_{2j+1,2j} / h_{2j+2,2j}, \]
and
\[ t_{2j+3,2j+2} = -t_{2j+3,2j+1} h_{2j+1,2j} / h_{2j+2,2j}. \]
3 Application to the approximation of matrix functions

In this section, we will show how to use the global extended-rational Arnoldi algorithm to approximate expression of the form \( f(A)V \). As in [20], the global extended-rational Krylov subspace \( \mathcal{K}_m(A, V) \) defined in [3] can be written as

\[
\mathcal{K}_m(A, V) = \{ X_{2m} \in \mathbb{R}^{n \times p} / X_{2m} = f_2m(\mathcal{K}_{2m} \otimes I_p) \text{ where } \mathcal{K}_{2m} \in \mathbb{R}^{2m} \}. \tag{14}
\]

Then the expression \( f(A)V \) can be approximated by

\[
f_{2m} := \mathcal{P}_{2m}(f(A)V) = \| V \|_F f_2m(f(\mathcal{P}_{2m})e_1 \otimes I_p), \tag{15}
\]

where \( \mathcal{P}_{2m}(X) = f_{2m}(f(\mathcal{P}_{2m})e_1 \otimes I_p) \in \mathcal{K}_m(A, V) \) for some \( X \in \mathbb{R}^{n \times p} \).

The \( n \times mp \) matrix \( f_{2m} = [V_1, V_2, \ldots, V_{2m}] \) is the matrix corresponding to the \( F \)-orthonormal basis for \( \mathcal{K}_m(A, V) \) constructed by applying \( m \) steps of Algorithm [3] to the pair \((A, V)\). \( \mathcal{K}_{2m} \) is the projection matrix defined by [3] and \( e_1 \) corresponds to the first column of the identity matrix \( I_{2m} \).

Lemma 1 (Exactness) Let \( \mathcal{P}_{2m} \in \mathbb{R}^{n \times 2mp} \) be the matrix generated by Algorithm [3] and let \( \mathcal{P}_{2m} \) the matrix as defined by [3]. Then for any rational function \( r_{2m} \in \Pi_{2m}/q_{2m} \) we have

\[
r_{2m}(A)V = \| V \|_F f_{2m}[(r_{2m}(\mathcal{P}_{2m})e_1) \otimes I_p] \tag{16}
\]

In particular, if \( r_{2m} \in \Pi_{2m-1}/q_{2m} \) then the global extended-rational Arnoldi approximation is exact, i.e., we have

\[
r_{2m}(A)V = \| V \|_F f_{2m}[(r_{2m}(\mathcal{P}_{2m})e_1) \otimes I_p] \tag{17}
\]

where \( \Pi_{2m} \) denotes the set of polynomials of degree at most \( 2m \) and \( q_{2m} \) is the polynomial of degree \( m \), i.e., \( q_m(z) = (z-s_1) \ldots (z-s_m) \).

Proof Following the idea in [20] Lemma 3.1], we consider \( q = q_m(A)^{-1}V \) and we first show by induction that

\[
\mathcal{P}_{2m}(A^j q) = f_{2m}(f_{2m}(\mathcal{P}_{2m} X_{2m} ^T \otimes q) \otimes I_p) \quad \text{for } j = 0, \ldots, 2m. \tag{18}
\]

Assertion [13] is obviously true for \( j = 0 \). Assume that it is true for some \( j < m \). Then by the definition of a extended-rational Krylov space we have \( \mathcal{P}_{2m}(A^j q) = A^j q \), and therefore

\[
\mathcal{P}_{2m}(A^{j+1} q) = \mathcal{P}_{2m}(A \mathcal{P}_{2m}(A^j q)) = \mathcal{P}_{2m}(A \mathcal{P}_{2m}(f_{2m}(f_{2m}(\mathcal{P}_{2m} X_{2m}^T \otimes q) \otimes I_p)))
\]

\[
= f_{2m}(f_{2m}(f_{2m}(f_{2m}(\mathcal{P}_{2m}(X_{2m}^T \otimes q)) \otimes I_p)) \otimes I_p)
\]

Using the properties of the \( \circ \) product, we obtain

\[
= f_{2m}(f_{2m}(f_{2m}(f_{2m}(\mathcal{P}_{2m}(X_{2m}^T \otimes q)) \otimes I_p)) \otimes I_p) = f_{2m}(f_{2m}(f_{2m}(f_{2m}(\mathcal{P}_{2m}(X_{2m}^T \otimes q)) \otimes I_p)) \otimes I_p),
\]

which establishes [13]. By linearity, we obtain

\[
V = q_m(A)q = f_{2m}(q_m(\mathcal{P}_{2m})(f_{2m}(X_{2m}^T \otimes q)) \otimes I_p).
\]

Using the properties of the \( \circ \) product, we obtain

\[
f_{2m}^T q = \| V \|_F q_m^{-1} (\mathcal{P}_{2m})e_1
\]

Replacing \( f_{2m}^T \circ q \) in [13] completes the proof.
We consider a convex compact set $\Lambda \subseteq \mathbb{R}$ and we define $\mathcal{A}(\Lambda)$ as the set of analytic functions in a neighborhood of $\Lambda$ equipped with the uniform norm $\| \cdot \|_{L^\infty(\Lambda)} \cdot \mathcal{W}(\Lambda) := \{ x^T A x : x \in \mathbb{R}^n, \| x \| = 1 \}$ will denote the convex hull. In [8], it was shown that there exists a universal constant $C = 1 + \sqrt{2}$ such that

$$\| f(B) \| \leq C \| f \|_{L^\infty(\Lambda)}, \quad \forall f \in \mathcal{A}(\Lambda),$$

where $B \in \mathbb{R}^{n \times n}$, with $\mathcal{W}(B) \subseteq \Lambda$. Based on this inequality, the following result gives an upper bound for the norm of the error $f(A)V - \hat{f}^{est}_{2m}(A)V$, where $\hat{f}^{est}_{2m}$ is the approximation given by (15).

**Corollary 1** We assume that $\mathcal{W}(A) \cup \mathcal{W}(\mathcal{F}_{2m}) \subseteq \Lambda$, and let $f \in \mathcal{A}(\Lambda)$. Then the global extended-rational Arnoldi approximation $\hat{f}^{est}_{2m}$ defined by (15) satisfies

$$\| f(A)V - \hat{f}^{est}_{2m}(A)V \|_F \leq 2C \| V \|_F \min_{r_{2m} \in \Pi_{2m-1/4m}} \| f - r_{2m} \|_{L^\infty(\Lambda)}$$

**Proof** According to [17], we have $r_{2m}(A)V = \| V \|_F \mathcal{F}_{2m}(r_{2m}(\mathcal{F}_{2m})e_1 \otimes I_p)$ for every rational function $r_{2m} \in \Pi_{2m-1/4m}$. Thus,

$$\| f(A)V - \hat{f}^{est}_{2m}(A)V \|_F \leq \| f(A)V - \| V \|_F \mathcal{F}_{2m}(f(\mathcal{F}_{2m})e_1 \otimes I_p) - r_{2m}(A)V \|_F + \| V \|_F \mathcal{F}_{2m}(r_{2m}(\mathcal{F}_{2m})e_1 \otimes I_p)\|_F \leq \| V \|_F \| f(A) - r_{2m}(A) \|_F + \| V \|_F \mathcal{F}_{2m}(f(\mathcal{F}_{2m} - r_{2m}(\mathcal{F}_{2m}))e_1 \otimes I_p)\|_F \leq 2C \| V \|_F \| f - r_{2m} \|_{L^\infty(\Lambda)}.$$ 

Which completes the proof.

### 3.1 Shifted linear systems

We consider the solution of the parameterized nonsingular linear systems with multiple right hand sides

$$(A - \sigma I_n)X = B,$$  \hspace{1cm} (19)

which needs to be solved for many values of $\sigma$, where $B \in \mathbb{R}^{n \times p}$. The solution $X = X(\sigma)$ may be written as $X = (A - \sigma I)^{-1}B \equiv f(A)B$, with $f(z) = (z - \sigma)^{-1}$ is the resolvent function. Then the approximate solutions $X_{2m} = X_{2m}(\sigma) \in \mathbb{R}^{n \times p}$ generated by the global extended-rational algorithm to the pair $(A, R_0)$ are obtained as follows

$$Z_{2m}(\sigma) = X_{2m}(\sigma) - X_0(\sigma) \in \mathcal{R}.\mathcal{H}_{2m}(A, R_0)$$

where $R_0 = R_0(\sigma) = B - (A - \sigma I)^{-1}X_0(\sigma)$ are the residual block vectors associated to initial guess $X_0(\sigma)$. By (13) $Z_{2m}(\sigma) = \mathcal{Y}_{2m}(Y_{2m}(\sigma) \otimes I_p)$ where $Y_{2m}(\sigma) \in \mathbb{R}^{2m}$ is determined such that the new residual $R_{2m}(\sigma) = B - (A - \sigma I_n)X_{2m}$ associated to $X_{2m}$ is $F$-orthogonal to $\mathcal{R}.\mathcal{H}_{2m}(A, R_0)$. This yields

$$X_{2m}(\sigma) = X_0 + \mathcal{Y}_{2m}(Y_{2m}(\sigma) \otimes I_p) \quad \text{and} \quad \mathcal{Y}_{2m}^T R_{2m}(\sigma) = 0$$  \hspace{1cm} (20)

Using (20) relations and the following decomposition

$$(A - \sigma I_n) \mathcal{Y}_{2m} = \mathcal{Y}_{2m}[(\mathcal{F}_{2m} - \sigma I_{2m}) \otimes I_p] + V_{2m+1} \left( I_{2m+1,2m} \mathcal{E}_m^T \otimes I_p \right),$$  \hspace{1cm} (21)
the reduced linear system can be written as
\[
(\mathcal{F}_{2m} - \sigma I_{2m})Y_{2m}(\sigma) = \|R_0\|_F e_1,
\]
then the approximate solution will be
\[
X_{2m} = \|R_0\|_F Y_{2m}(\mathcal{F}_{2m} - \sigma I_{2m})^{-1} e_1 \otimes I_p.
\]
This equality is equivalent to (15) when \(f(A) = (A - \sigma I_n)^{-1}\) corresponds to the resolvent function. In order to find a good choice of shift parameters \(\{s_1, \ldots, s_m\}\) in the Algorithm [1] we consider the following function
\[
f_{2m,m}(\lambda, s) = f_{\lambda_1, \ldots, \lambda_{2m}, s_1, \ldots, s_m}(\lambda, s) = f_{m,m}(\lambda, s) - \frac{1}{\lambda - s} \begin{bmatrix}
ge_{2m}(\lambda) \\
g_{m}(s) \\
\end{bmatrix}
\]
where \(f_{m,m} = f_{\lambda_1, \ldots, \lambda_{2m}, s_1, \ldots, s_m}\) corresponds to the so-called skeleton approximation introduced in the study of Tyryshnikov [36], i.e.,
\[
f_{m,m}(\lambda, s) := \begin{bmatrix}
\frac{1}{\lambda - s_1} & \cdots & \frac{1}{\lambda - s_m}
\end{bmatrix} M^{-1} \begin{bmatrix}
\frac{1}{\lambda_1 - s} \\
\vdots \\
\frac{1}{\lambda_m - s}
\end{bmatrix}, \quad M_{ij} = \frac{1}{\lambda_i - s_j}
\]
\(\lambda_1, \ldots, \lambda_{2m}\) are the eigenvalues of \(\mathcal{F}_{2m}\), and
\[
ge_m(z) = \frac{(z - \lambda_1) \cdots (z - \lambda_m)}{(z - s_1) \cdots (z - s_m)} \quad g_{2m}(z) = \frac{(z - \lambda_1) \cdots (z - \lambda_{2m})}{(z - s_1) \cdots (z - s_m)}
\]

**Proposition 5** The function \(f_{2m,m}\) defined in (23) is an \([2m-1]m\) rational function of the first variable \(\lambda\), and an \([(2m-1)]2m\) rational function of the second variable \(s\) interpolating \((\lambda - s)^{-1}\) at \(\lambda = \lambda_1, \ldots, \lambda_{2m}\) and \(s = s_1, \ldots, s_m\). Moreover, the relative error of this interpolation is
\[
\epsilon(\lambda, s) = 1 - (\lambda - s) f_{2m,m}(\lambda, s) = \frac{g_{2m}(\lambda)}{g_{m}(s)}
\]
**Proof** The rational function \(f_{2m,m}\) can be expressed as
\[
f_{2m,m}(\lambda, s) = f_{m,m}(\lambda, s) - \frac{\psi(\lambda, s)}{\lambda - s (\lambda - s_1) \cdots (\lambda - s_m)(s - \lambda_1) \cdots (s - \lambda_{2m})}
\]
where
\[
\psi(\lambda, s) = (\lambda - \lambda_1) \cdots (\lambda - \lambda_m)(s - s_1) \cdots (s - s_m)[(\lambda - \lambda_{m+1}) \cdots (\lambda - \lambda_{2m}) - (s - \lambda_{m+1}) \cdots (s - \lambda_{2m})]
\]
Observe that \(\psi(\lambda, s)\) is divisible by \((\lambda - s)\), then there exists a function \(\phi\) such that \(\psi(\lambda, s) = (\lambda - s) \phi(\lambda, s)\). Moreover, \(\phi\) is a polynomial function of degree \(2m - 1\) of each variable. Then \(f_{2m,m}\) simplifies to
\[
f_{2m,m}(\lambda, s) = f_{m,m}(\lambda, s) - \frac{\phi(\lambda, s)}{(\lambda - s_1) \cdots (\lambda - s_m)(s - \lambda_1) \cdots (s - \lambda_{2m}) - (\lambda - s_1) \cdots (\lambda - s_m)(s - \lambda_1) \cdots (s - \lambda_{2m})}
\]
\[
= \frac{f_{m,m}(\lambda, s)(\lambda - s_1) \cdots (\lambda - s_m)(s - \lambda_1) \cdots (s - \lambda_{2m}) - \phi(\lambda, s)}{(\lambda - s_1) \cdots (\lambda - s_m)(s - \lambda_1) \cdots (s - \lambda_{2m})}
\]
Using the relation error equation (24), we get

\[\frac{1}{\lambda_i - s} \left[ 1 - \frac{g_m(\lambda)}{g_m(s)} \right] + \frac{1}{\lambda_i - s} \frac{g_m(\lambda)}{g_m(s)} = \frac{1}{\lambda_i - s}.\]

Which means that \( f_{2m,m}(\lambda_i, s) \) interpolates \((\lambda - s)^{-1}\) at \(\lambda = \lambda_1, \ldots, \lambda_m\) and \(s = s_1, \ldots, s_m\). The relative error is

\[1 - (\lambda - s)f_{2m,m}(\lambda, s) = 1 - (\lambda - s) \left[ f_{m,m}(\lambda, s) - \frac{1}{\lambda_i - s} \left( \frac{g_{2m}(\lambda)}{g_{2m}(s)} - \frac{g_m(\lambda_i)}{g_m(s)} \right) \right].\]

Using the relation error equation (24), we conclude that

\[1 - (\lambda - s)f_{2m,m}(\lambda, s) = \frac{g_{2m}(\lambda)}{g_{2m}(s)}.\]

Using the same techniques as in [28], we can show that

\[Z_{2m}(\sigma) = f_{2m,m}(A, \sigma)R_0.\]

By this equality, the residual \(R_{2m}(\sigma)\) can be expressed as

\[R_{2m}(\sigma) = R_0 - (A - \sigma I_s)f_{2m,m}(A, \sigma)R_0 = \frac{g_{2m}(A)R_0}{g_{2m}(\sigma)},\] (25)
From [9, Proposition 2], the characteristic polynomial of $\mathcal{P}_{2m}$ minimizes $\|p(A)R_0\|_F$ over all monic polynomial of degree 2, so that the numerator in (25) satisfies

$$\|s_{2m}(A)R_0\|_F = \min_{\lambda_1, \ldots, \lambda_{2m}} \|(A - \lambda_1 I_n) \cdots (A - \lambda_{2m} I_n)(A - s_1 I_n)^{-1} \cdots (A - s_m I_n)^{-1} R_0\|_F$$

With this result, and (25) equation, the next shift parameter $s_{m+1}$ is selected as

$$s_{m+1} = \arg\max_{\sigma \in \Sigma} \frac{1}{|s_{2m}(\sigma)|}$$

where $\Sigma$ is the set of the shifts associated to the parameterized linear systems [19]. The following result on the norm of the residual $R_{2m}(\sigma)$ allows us to stop the iterations without having to compute matrix products with the large matrix $A$.

**Theorem 1** Let $V_{2m}(\sigma)$ be the exact solution of the reduced linear system (22) and let $X_{2m}(\sigma)$ be the approximate solution of linear system (19) after $m$ iterations of the extended rational global Arnoldi algorithm. Then the residual $R_{2m}(\sigma)$ satisfies

$$\|R_{2m}(\sigma)\|_F = \|R_0(\sigma)\|_F \|\tau_{2m}E_m^{T}(\mathcal{P}_{2m} - \sigma I_{2m})^{-1}e_1\|_F$$

where $\tau_{2m} = [t_{2m+1,2m-1}, t_{2m+1,2m}]$

**Proof**

$$R_{2m}(\sigma) = B - (A - \sigma_i I_n)X_{2m} = B - (A - \sigma_i I_n)(X_0 + \gamma_{2m}(V_{2m} \otimes I_p)).$$

Using (21) decomposition, we obtain

$$= R_0 - \gamma_{2m}(\mathcal{P}_{2m} - \sigma I_{2m}) \otimes I_p + V_{2m+1}(\tau_{2m}E_m^{T} \otimes I_p)(V_{2m} \otimes I_p).$$

$$= R_0 - \gamma_{2m}(\|R_0(\sigma)\|_F e_1 \otimes I_p) - V_{2m+1}(\tau_{2m}E_m^{T} \otimes I_p).$$

$$= V_{2m+1}(\tau_{2m}E_m^{T} \otimes I_p).$$

As $m$ increases, the column of block vectors that must be stored increases. As in (22) [34], we can restart the algorithm every some fixed $m$ steps. According to (27), we observe that the residuals $R_{2m}(\sigma)$ are colinear to the block vector $V_{2m+1}$. Then it is possible to restart with $V_{2m+1}$ and $\beta_{m}(\sigma) = \text{trace}(V_{2m+1}^{T}R_{2m}(\sigma))$ see, Algorithm 2 [line 8].

**Algorithm 2** Restarted shifted linear system algorithm

*Input: Matrix $A$, block vector $B$, $\Sigma$ the set of shifts, $\varepsilon$ a desired tolerance.*

1. Set $\beta_0(\sigma) = \|B\|_F$, $V_1 = B/\beta_0(\sigma)$ and $\Sigma = \emptyset$.
2. Compute $\gamma_{2m}$ and $\mathcal{P}_{2m}$ using the global extended-rational Arnoldi algorithm.
3. Solve the reduced shifted linear system $(\mathcal{P}_{2m} - \sigma_i I_{2m})V_{2m} = \beta_i(\sigma)e_1$, for $\sigma \in \Sigma \setminus \Sigma_e$.
4. Compute $\|R_{2m}(\sigma)\|_F$ using (25), for $\sigma \in \Sigma \setminus \Sigma_e$.
5. Compute $X_{2m}(\sigma) = V_{2m}(\sigma) + V_{2m}(V_{2m}(\sigma) \otimes I_p)$, for $\sigma \in \Sigma \setminus \Sigma_e$.
6. Select the new $\sigma \in \Sigma \setminus \Sigma_e$ such that $\|R_{2m}(\sigma)\|_F < \varepsilon$. Update set $\Sigma$ of converged shifted systems.
7. if $\Sigma \setminus \Sigma_e = \emptyset$ Stop
8. else Set $V_1 = V_{2m+1}$ and $\beta_{m}(\sigma) = \text{trace}(V_{2m+1}^{T}R_{2m}(\sigma))$, for $\sigma \in \Sigma \setminus \Sigma_e$. 
3.2 Application to the approximation of $e^{-tA}V$, $t > 0$

In this subsection, we consider the computation of $U(t) = e^{-tA}V$ where $t > 0$, for a given large and sparse matrix $A$ and a given block vector $V$ of size $n \times p$. Based on the $F$-orthonormal basis defining the matrix $\mathcal{F}_{2m}$ generated by the global extended-rational algorithm, the expression of $U(t)$ can be approximated as

$$U_{2m}(t) = \|V\|_F \mathcal{F}_{2m}((-e^{-t\mathcal{F}_{2m}}e_1) \otimes I_p).$$

(28)

Indeed, the inverse Laplace representation of the resolvent function is written as follows

$$e^{-tA}V = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{s}(A+sI_n)^{-1}V ds.$$

We have seen that the approximation of $(A+sI)^{-1}V$ is

$$\mathcal{P}_{2m}((A+sI)^{-1}V) = \|V\|_F \mathcal{F}_{2m}((-\mathcal{F}_{2m}+sI)\mathcal{F}_{2m}^{-1}e_1 \otimes I_p).$$

Then,

$$\mathcal{P}_{2m}(e^{-tA}V) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{st}[\mathcal{P}_{2m}((A+sI)^{-1}V)] ds.$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{st}[\|V\|_F \mathcal{F}_{2m}((-\mathcal{F}_{2m}+sI)\mathcal{F}_{2m}^{-1}e_1 \otimes I_p)] ds.$$

$$= \|V\|_F \mathcal{F}_{2m} \left( \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{st}((-\mathcal{F}_{2m}+sI)\mathcal{F}_{2m}^{-1}e_1) ds \otimes I_p \right).$$

$$= \|V\|_F \mathcal{F}_{2m}(e^{-t\mathcal{F}_{2m}}e_1 \otimes I_p).$$

We recall that $U(t) = e^{-tA}V$ is the solution of the differential problem

$$U'(t) = -AU(t), \quad t > 0$$

$$U(0) = V, \quad U(\infty) = 0. \quad (29)$$

The residual with respect to this ODE is given by

$$R_{2m}(t) = U_{2m}'(t) + AU_{2m}(t).$$

Following the idea in [33], and by the first equation in (10), the residual is given by the quantity

$$R_{2m}(t) = \mathcal{F}_{2m}(\tau_m E_{2m}^T e^{-t\mathcal{F}_{2m}}e_1 \otimes I_p).$$

Applying the first result of [27] Lemma 1) to $R_{2m}(t)$, we obtain the following stopping criterion

$$\|R_{2m}(t)\|_F = \|\tau_m E_{2m}^T e^{-t\mathcal{F}_{2m}}e_1\|_F$$

(30)

where $\tau_m = \{t_{2m+1.2m+1}\}$ and $E_{2m}$ are defined in [10].

The following result which concerns the approximation of the exponential will be the key to find a good choice of the shift parameters independently on the parameter $t$. This result is obtained by following some ideas in [14].
Theorem 2 We assume that \( A \) is a positive matrix with spectrum contained on \([0, \infty)\). Then we have the following error bound

\[
\sup_{t \in [0, \infty)} \| e^{-tA} V - U_{2m}(t) \|_F \leq \frac{1}{\| g_{2m}(A) \|_F} \max_{s \in \mathbb{R}} \frac{1}{|g_{2m}(-s)|} \]  \tag{31}

Proof

\[
e^{-tA} V - U_{2m}(t) = e^{-tA} V - \| V \|_F \mathcal{Y}_{2m}(sI) e_1 \otimes I_p
\]

\[
= \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{t(A + sI_n)} V - \| V \|_F (A + sI_n) \mathcal{Y}_{2m}((A + sI_n)^{-1} e_1 \otimes I_p) ds
\]

We have \( \| V \| \mathcal{Y}_{2m}((A + sI_n)^{-1} e_1 \otimes I_p) = f_{2m,m}(A, -s) \), then

\[
= \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{t(A + sI_n)} V - (A + sI_n) f_{2m,m}(A, -s)V ds
\]

\[
= \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{t(A + sI_n)} \frac{g_{2m}(A)V}{g_{2m}(-s)} ds
\]

then

\[
\| e^{-tA} V - U_{2m}(t) \|_F \leq \frac{\| g_{2m}(A) \|_F}{\min_{s \in \mathbb{R}} |g_{2m}(-s)|} \sup_{\lambda \in [0, \infty)} |h(\lambda, t)|
\]

where \( h(\lambda, t) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{t(\lambda + s)^{-1}} ds \). We observe that \( h(\lambda, t) \) corresponds to the inverse Laplace transform of \( 1/(\lambda + s) \), then \( h(\lambda, t) = e^{-\lambda t} \). Which leads to obtain

\[
\| e^{-tA} V - U_{2m}(t) \|_F \leq \frac{\| g_{2m}(A) \|_F}{\min_{s \in \mathbb{R}} |g_{2m}(-s)|}
\]

This shows (31) since \( \max_{s \in \mathbb{R}} \{1/|g_{2m}(-s)|\} = 1/\min_{s \in \mathbb{R}} \{ |g_{2m}(-s)| \} \).

As for rational Arnoldi approximation, and when working with bounded positive definite matrix \( A \), Druskin et al. [12] showed that real shifts on the spectrum of \( A \) can also reach the minimum in (31) inequality. We observe that the function \( g_{2m}^{-1}(-s) \) has poles at \( s = -\lambda_i \in [-\lambda_{\max}, -\lambda_{\min}], i = 1, \ldots, 2m \). Following the same techniques in [12 Proposition 2.3], we can show that all the extrema of \( |g_{2m}^{-1}(-s)| \) are ripples (local maxima of \( |g_{2m}^{-1}(-s)| \)) located only between the interpolation points \( \{\lambda_i\}_{i=1}^{2m} \), such that there is one and only one ripple between two adjacent interpolation points. With the result, the next shift parameter \( s_{m+1} \) is selected as the corresponding argument of the maximum of \( |g_{2m}^{-1}(-\lambda_{\max})|, |g_{2m}^{-1}(-\lambda_{\min})| \) and the \( 2m - 1 \) local maxima between the interpolation points. The algorithm for constructing the next shift parameter is given in Algorithm 3. Algorithm 3 describes how approximations of \( e^{-tA} V \) are computed by the adaptive global extended-rational method.
Algorithm 3 The procedure for selecting the shift parameters of exponential function

Inputs: \( \{ \lambda_i \}_{i=1}^{2m} \), the set of interpolation points (the eigenvalues of \( T_{2m} \)).

1. Estimate \( \lambda_{\min} \) and \( \lambda_{\max} \).
2. For \( j = 1 : 2m - 1 \)
   a. \( \mu_j = \arg \max_{s \in [\lambda_j, \lambda_{j+1}]} \left\{ \frac{1}{|g_{2m}(-s)|}, \frac{1}{|g_{2m}(-\lambda_{\min})|}, \frac{1}{|g_{2m}(-\lambda_{\max})|} \right\} \)
   b. endfor
3. \( s_{m+1} = \arg \max_{\mu_1, \ldots, \mu_{2m-1}, \lambda_{\min}, \lambda_{\max}} \left\{ \frac{1}{|g_{2m}(-\mu_1)|}, \frac{1}{|g_{2m}(-\lambda_{\min})|}, \frac{1}{|g_{2m}(-\lambda_{\max})|} \right\} \)

Algorithm 4 Approximation of \( e^{-tA}V \) by the adaptive global extended-rational method (AGER)

Inputs: Matrix \( A \), initial block \( V \).

1. Choose a tolerance \( tol > 0 \), a maximum number of \( \text{itermax} \) iterations.
2. Estimate \( \lambda_{\min} \) and set \( s_1 = \lambda_{\min} \).
3. For \( m = 1 : \text{itermax} \)
   a. Compute \( \gamma_{2m} \) and \( \tilde{T}_{2m} \) using the global extended-rational Arnoldi algorithm \[8\]
   b. Compute \( \gamma_{2m} = e^{\tilde{T}_{2m}}e_1 \), and compute \( \|R_{2m}\| \) given by \[30\].
   c. if \( \|R_{2m}\|_F \leq tol \), stop,
   d. else Find \( s_{m+1} \) by using Algorithm \[3\]
   e. endfor The approximate solution \( U_{2m} \) given by \[28\].

4 Numerical experiments

In this section, we give some numerical results to show the performance of the global extended-rational Arnoldi method. All experiments were carried out with MATLAB R2015a on a computer with an Intel Core i-3 processor and 3.89 GBytes of RAM. The computations were done with about 15 significant decimal digits. The proposed method is applied to the approximation of \( f(A)V \) given in \[1\], and to solve the shifted linear systems \[19\] with multiple right hand sides for many values of \( \sigma \).

4.1 Examples for the shifted linear systems

In this subsection, we present some results of solving shifted linear systems of the form \[19\]. We compare the results obtained by the restarted global extended-rational Arnoldi (resGERA), the restarted global extended Arnoldi (resGEA) and the restarted global FOM (resGFOM) methods. The right hand side \( B \) was chosen randomly with entries uniformly distributed on \([0,1]\). The shifts \( \sigma \) are taken to be values uniformly distributed in the interval \([-5,0]\). In Example 1 and Example 2, the stopping criterion used for Algorithm 2 was \( \|R_{2m}(\sigma)\|_F \leq 2 \cdot 10^{-12} \) and the initial guess was zero. The dimension of the subspaces was chosen to be \( m = 10, 20 \).

Example 1 In this experiment, we consider the nonsymmetric matrices \( A_1 \) and \( A_2 \) given in \[34\] and \[11\], respectively. These matrices were obtained from the centered finite difference discretization (CFDD) of the elliptic operators \( L_1(u) \) and \( L_2(u) \), respectively,

\[
L_1(u) = -\Delta u + 50(x+y)u_x + 50(x+y)u_y,
L_2(u) = -\Delta u + \sin(xy)u_x + e^u u_y + (x+y)u.
\]

(32)
on the unit square \([0, 1] \times [0, 1]\) with Dirichlet homogeneous boundary conditions. The number of inner grid points in both directions was \(n_0\) and the dimension of matrices is \(n = n_0^2\).

In Table 1 we reported results for \(\text{resGERA}, \text{resGEA}\) and \(\text{resGFOM}\). We used different values of the dimension \(n\) \((\{2500, 10000\) and \(22500\})\) and two different block sizes \(p = 5, 10\). The dimension of the subspace is chosen to be \(m = 10\) and \(m = 20\). As shown from this table, the \(\text{resGFOM}\) requires a higher number of restarts and cpu-time to reach convergence. Although the \(\text{resGEA}\) is able to reduce the number of restarts, \(\text{resGERA}\) is much better in terms of number of restarts and cpu-time.

| Matrices | \(n\) | subspace dimension | GERAM | GEAM | GFOM |
|---------|-------|-------------------|-------|------|------|
|         |       |                   | Time(s)/(#Cycles) | Time(s)/(#Cycles) | Time(s)/(#Cycles) |
| \(A_1\) | 2500  | 10                | 5.12 (2)         | 9.65 (6)         | 17.56 (47)        |
|         | 2500  | 20                | 2.81 (1)         | 7.90 (4)         | 38.75 (28)        |
|         | 10000 | 10                | 8.17 (2)         | 17.23 (8)        | 156.67 (57)       |
|         | 10000 | 20                | 7.35 (1)         | 27.47 (5)        | 171.39 (32)       |
|         | 22500 | 10                | 10.43 (2)        | 27.36 (9)        | 558.76 (94)       |
|         | 22500 | 20                | 18.76 (1)        | 20.86 (6)        | 555.96 (45)       |
| \(A_2\) | 2500  | 10                | 17.78 (2)        | 10.57 (11)       | 367.14 (91)       |
|         | 2500  | 20                | 17.18 (1)        | 20.37 (4)        | 538.48 (45)       |
|         | 10000 | 10                | 16.69 (2)        | 27.11 (6)        | -                 |
|         | 10000 | 20                | 14.45 (1)        | 20.61 (4)        | -                 |
|         | 22500 | 10                | 35.10 (2)        | 50.12 (5)        | -                 |
|         | 22500 | 20                | 34.09 (1)        | 42.51 (3)        | -                 |

Example 2 In this example, we used the nonsymmetric matrices \(\text{pde}2961, \text{ebp1}, \text{add}32\) and the symmetric matrix \(\text{mhd}3200b\) from the Suite Sparse Matrix Collection [10]. Some details on these matrices are given in Table 2. Results for several choices of the block size \(p\) are reported in Table 3. The results show that the \(\text{GERAM}\) and \(\text{GEAM}\) yield significantly smaller cycles than \(\text{GFOM}\). Moreover, the \(\text{GERAM}\) is faster than \(\text{GEAM}\) for all matrices.

| Matrices | Original Problem | size \(n\) | \(\lambda_{\min}\) | \(\lambda_{\max}\) | \(\text{cond}(A)\) | \(\text{nnz}\) |
|----------|-----------------|------------|-------------------|-------------------|------------------|-------------|
| \(\text{pde}2961\) | economic problem | 2961       | 0.04              | 12.12             | 6.42 \cdot 10^2  | 14585       |
| \(\text{ebp1}\)    | thermal problem  | 14734      | 4.85 \cdot 10^{-5} | 15.66             | 5940.66         | 95053       |
| \(\text{mhd}3200b\) | electromagnetics Problem | 3200 | 1.36 \cdot 10^{-13} | 2.19              | 1.60 \cdot 10^{13} | 18316     |
| \(\text{add}32\)   | circuit simulation problem | 4960 | 4.21 \cdot 10^{-4} | 0.06              | 1.36 \cdot 10^2  | 19848       |
We used the nonsymmetric matrices \( A \) in this example, we consider a semi discretization of the partial differential equation

\[
\frac{\partial U}{\partial t} - \Delta U + (x+y)\frac{\partial U}{\partial x} + (x-y)\frac{\partial U}{\partial y} = 0 \quad \text{on } (0,1)^2 \times (0,1)
\]

\[
U(x,y,0) = 0 \quad \text{on } \partial(0,1)^2, \forall t \in [0,1]
\]

\[
U(x,y,t) = U_0(x,y) \forall x,y \in [0,1]^2.
\]

where

\[
U_0(x,y) = \left\{ u_0^{(1)}(x,y), u_0^{(2)}(x,y), u_0^{(3)}(x,y) \right\}
\]

\[
= \left\{ \sin(\pi x) \sin(\pi y), \sin(2\pi x) \sin(\pi y), \sin(2\pi x) \sin(2\pi y) \right\},
\]

We used the nonsymmetric matrices \( A_{100} \) and \( A_{150} \) coming from CFDD of the operator

\[
\mathcal{L}_0(u) = -\Delta u + (x+y)u_x + (x-y)u_y,
\]

on the \([0,1] \times [0,1]\). The size of \( A_{100} \) is \( 100 \times 100 \) and the size of \( A_{150} \) is \( 150 \times 150 \). The subscript 100 and 150 denotes the number of inner grid points in both directions. The block \( V \) is set to the values of the initial functions \( U_0(x,y) \) on the finite-difference mesh \( (x_i,y_j) \), with \( x_i = (i-1)/(n_0 - 1) \) and \( y_j = (j-1)/(n_0 - 1) \), for \( i,j = 1, \ldots, n_0 \), i.e., \( V(n_0\times i + j, k) = u_0^{(k)}(x_i, y_j), k = 1, 2, 3 \). In this case, the block size is \( p = 3 \). We computed approximations of \( U(t) = e^{-tA}V \) correspond to the solution of partial differential equation. These approximations are given by the AGER method; see, Algorithm 4 and the adaptive rational Arnoldi method (ARA) described in 12. We used different values of time parameters \( t = \{1/10, 1/3, 2/3, 1\} \). The algorithms were stopped when residual norm \( \|R_{2n}(t)\| \) is less than \( 5 \times 10^{-9} \).

In Table 4, we present results of this experiment. As shown in this table, the AGER method requires fewer iterations and CPU-time than ARA method.

In the following examples, we compare the performance of GERA method with the performance of the rational Arnoldi (RA) method and the standard global Arnoldi (SGA) method. In all examples, \( A \in \mathbb{R}^{1000 \times 1000} \), and the block \( V \in \mathbb{R}^{n \times n} \) was generated randomly with entries uniformly distributed on \([0,1]\). The dimension of the Krylov subspace is chosen

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**Table 3** Example 1: Shifted solvers for some matrices from the Suite Sparse Matrix Collection matrices

| Test problem | subspace dimension | GERAM Time(s)(#Cycles) | GEAM Time(s)(#Cycles) | GFOM Time(s)(#Cycles) |
|--------------|--------------------|------------------------|-----------------------|-----------------------|
| \( A_1 = pde2961 \) \( n = 2961 \) \( s = 5 \) | 10 | 9.07 (8) | 10.57 (11) | 20.72 (91) |
| \( A_2 = cpb1 \) \( n = 14734 \) \( s = 10 \) | 20 | 8.10 (2) | 9.90 (5) | 23.03 (25) |
| \( A_3 = mhd32000b \) \( n = 3200 \) \( s = 10 \) | 10 | 10.28 (9) | 52.03 (82) | 321 (583) |
| \( A_4 = add32 \) \( n = 4960 \) \( s = 5 \) | 20 | 5.34 (3) | 7.14 (5) | 9.21 (24) |

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4.2 Examples for the approximation of \( f(A)V \)

**Example 3** In this example, we consider a semi discretization of the partial differential equation

\[
\frac{\partial U}{\partial t} - \Delta U + (x+y)\frac{\partial U}{\partial x} + (x-y)\frac{\partial U}{\partial y} = 0 \quad \text{on } (0,1)^2 \times (0,1)
\]

\[
U(x,y,0) = 0 \quad \text{on } \partial(0,1)^2, \forall t \in [0,1]
\]

\[
U(x,y,t) = U_0(x,y) \forall x,y \in [0,1]^2.
\]

where

\[
U_0(x,y) = \left\{ u_0^{(1)}(x,y), u_0^{(2)}(x,y), u_0^{(3)}(x,y) \right\}
\]

\[
= \left\{ \sin(\pi x) \sin(\pi y), \sin(2\pi x) \sin(\pi y), \sin(2\pi x) \sin(2\pi y) \right\},
\]

We used the nonsymmetric matrices \( A_{100} \) and \( A_{150} \) coming from CFDD of the operator

\[
\mathcal{L}_0(u) = -\Delta u + (x+y)u_x + (x-y)u_y,
\]

on the \([0,1] \times [0,1]\). The size of \( A_{100} \) is \( 100 \times 100 \) and the size of \( A_{150} \) is \( 150 \times 150 \). The subscript 100 and 150 denotes the number of inner grid points in both directions. The block \( V \) is set to the values of the initial functions \( U_0(x,y) \) on the finite-difference mesh \( (x_i,y_j) \), with \( x_i = (i-1)/(n_0 - 1) \) and \( y_j = (j-1)/(n_0 - 1) \), for \( i,j = 1, \ldots, n_0 \), i.e., \( V(n_0\times i + j, k) = u_0^{(k)}(x_i, y_j), k = 1, 2, 3 \). In this case, the block size is \( p = 3 \). We computed approximations of \( U(t) = e^{-tA}V \) correspond to the solution of partial differential equation. These approximations are given by the AGER method; see, Algorithm 4 and the adaptive rational Arnoldi method (ARA) described in 12. We used different values of time parameters \( t = \{1/10, 1/3, 2/3, 1\} \). The algorithms were stopped when residual norm \( \|R_{2n}(t)\| \) is less than \( 5 \times 10^{-9} \).

In table 4, we present results of this experiment. As shown in this table, the AGER method requires fewer iterations and CPU-time than ARA method.

In the following examples, we compare the performance of GERA method with the performance of the rational Arnoldi (RA) method and the standard global Arnoldi (SGA) method. In all examples, \( A \in \mathbb{R}^{1000 \times 1000} \), and the block \( V \in \mathbb{R}^{n \times n} \) was generated randomly with entries uniformly distributed on \([0,1]\). The dimension of the Krylov subspace is chosen
Table 4 Example 3: Approximation of $e^{-iA}V$ for two matrix dimensions for the operator given by (19).

| Test problem | Adaptive global extended-rational Arnoldi method | Adaptive rational Arnoldi method |
|--------------|--------------------------------------------------|----------------------------------|
|              | Sp. dimen. | Res. norm | Time(s) | Sp. dimen. | Res. norm | Time(s) |
| $A_{100}$    |            |           |         |            |           |         |
| $t = 1/10$   | 50         | $2.15 \times 10^{-9}$ | 5.77    | 100        | $1.06 \times 10^{-9}$ | 108.09  |
| $t = 1/3$    | 40         | $5.85 \times 10^{-9}$ | 4.72    | 95         | $1.14 \times 10^{-9}$ | 83.20   |
| $t = 2/3$    | 28         | $1.19 \times 10^{-9}$ | 2.98    | 60         | $1.98 \times 10^{-9}$ | 24.53   |
| $t = 1$      | 16         | $1.94 \times 10^{-9}$ | 2.13    | 32         | $2.22 \times 10^{-9}$ | 10.06   |
| $A_{150}$    |            |           |         |            |           |         |
| $t = 1/10$   | 54         | $3.26 \times 10^{-9}$ | 13.48   | 100        | $7.00 \times 10^{-7}$ | 275.16  |
| $t = 1/3$    | 46         | $3.77 \times 10^{-9}$ | 11.37   | 100        | $2.06 \times 10^{-6}$ | 274.45  |
| $t = 2/3$    | 30         | $1.87 \times 10^{-9}$ | 7.72    | 96         | $5.82 \times 10^{-9}$ | 260.12  |
| $t = 1$      | 30         | $1.29 \times 10^{-9}$ | 6.02    | 50         | $3.73 \times 10^{-9}$ | 56.71   |

$m = 20$. We determine the actual value $f$ given by (1) using funm function in MATLAB. In the tables, we display the errors $Er(f_{m}^{SA}) = \| f - f_{m}^{SA} \|$, for the SA method $Er(f_{m/2}^{ER}) = \| f - f_{m/2}^{ER} \|$ for the GERA method and $Er(f_{m}^{RA}) = \| f - f_{m}^{RA} \|$ for the RA method. In the extended-rational method, the poles are chosen as $s_{j} = 0.1i$ for $i = 1, \ldots, 10$, while in the rational method the poles are chosen as $s_{j} = 0.05i$ for $i = 1, \ldots, 20$.

Example 4 Let $A = [a_{i,j}]$ be the symmetric positive definite Toeplitz matrix with entries $a_{i,j} = 1/(1 + i + j)$ (23). Results for several functions are reported in Table 5. As shown, the approximations computed with the GERA method are more accurate than approximations determined by the RA and SGA methods.

| $f(x)$  | $Er(f_{m}^{SA})$ | $Er(f_{m}^{RA})$ | $Er(f_{m}^{RA})$ |
|---------|------------------|------------------|------------------|
| $\sqrt{x}$ | $1.47 \times 10^{-12}$ | $3.69 \times 10^{-7}$ | $2.44 \times 10^{-5}$ |
| $\ln x$   | $3.38 \times 10^{-12}$ | $1.13 \times 10^{-7}$ | $2.84 \times 10^{-4}$ |
| $\exp(-\sqrt{x})$ | $1.79 \times 10^{-11}$ | $2.12 \times 10^{-8}$ | $2.38 \times 10^{-4}$ |

Example 5 The matrix used in this example is a block diagonal with $2 \times 2$ blocks of the form

$$
\begin{bmatrix}
a_{i} & c \\
-c & a_{i}
\end{bmatrix}
$$

where $c = 1/2$ and $a_{i} = (2i - 1)/(n + 1)$ for $i = 1, \ldots, n/2$ (33). Table 5 displays computed results, and shows that approximations computed with the GERA method have higher accuracy than approximations obtained by the RA and SGA methods.

Table 6 Example 5: $A \in \mathbb{R}^{n \times n}$ is a block diagonal matrix with $2 \times 2$ blocks. $n = 1000$ and block size $p = 5$.

| $f(x)$  | $Er(f_{m/2}^{RA})$ | $Er(f_{m}^{RA})$ | $Er(f_{m}^{RA})$ |
|---------|------------------|------------------|------------------|
| $\sqrt{x}$ | $2.99 \times 10^{-10}$ | $1.26 \times 10^{-9}$ | $5.84 \times 10^{-4}$ |
| $\ln x$   | $7.04 \times 10^{-10}$ | $4.54 \times 10^{-9}$ | $8.2 \times 10^{-3}$ |
| $\exp(-\sqrt{x})$ | $5.38 \times 10^{-10}$ | $4.53 \times 10^{-9}$ | $5.56 \times 10^{-4}$ |
5 Conclusion

This paper describes the global extended-rational Arnoldi method for the approximation of $f(A)V$ and for solving parameter dependent systems \cite{19}. We proposed an adaptive procedure to compute the shifts when $f(A) = e^{-tA}$ or $f(A) = (A - \sigma I)^{-1}$. The numerical results show that the proposed algorithms AGER (resGERA) require fewer iterations (number of restarts) and cpu-time as compared to other projection-type methods when approximating $f(A)V$ and when solving parameter dependent systems.

References

1. O. Abidi, M. Hached, and K. Jbilou, A global rational Arnoldi method for model reduction, J. Comput. Appl. Math., 325(2017) 175–187.
2. O. Abidi, Méthodes de sous-espaces de Krylov rationnelles pour le contrôle et la réduction de modèles, PhD thesis, Université du Littoral Côte d’Opale, 2016.
3. S. Agoujil, A. Bentbib, K. Jbilou, and M. Sadek, A minimization method for large Sylvester matrix problems, Elect. Trans. Numer. Anal., 43(2014) 45–59.
4. S. Baroni, R. Gebauer, O. B. Malcioglu, Y. Saad, P. Umari, and J. Xian, Harnessing molecular excited states with Lanczos chains, J. Phys. Condens. Mat., 22(2010), Art. Id. 074204, 8 pages.
5. B. Beckermann, and L. Reichel, Error estimation and evaluation of matrix functions via the Faber transform, SIAM J. Numer. Anal., 47(2009) 3849–3883.
6. M. Bellalij, K. Jbilou, and H. Sadok, New convergence results on the global GMRES method for diagonalizable matrices, J. Comput. Appl. Math., 219(2008) 350–358.
7. R. Bouyouli, K. Jbilou, R. Sadaka, and H. Sadok, Convergence properties of some block Krylov subspace methods for multiple linear systems, J. Comput. Appl. Math., 196(2006) 498–511.
8. M. Crouzeix, and C. Palencia, The numerical range is a $1+\sqrt{2}$-spectral set., SIAM J. Matrix Anal. Appl., 38(2017) 649–655.
9. B. Datta, M. Heyouni, and K. Jbilou, The global Arnoldi process for solving the Sylvester-Observer equation, J. Comput. Appl. Math., 29(2010) 527–544.
10. T. Davis, and Y. HU, The SuiteSparse Matrix Collection, https://sparse.tamu.edu.
11. V. Druskin, and L. Knizhnerman, Extended Krylov subspace approximations of the matrix square root and related functions. SIAM J. Matrix Anal. Appl., 19(1998) 755–771.
12. V. Druskin, C. E. Lieberman, and M. Zaslavsky, On Adaptive Choice of Shifts in Rational Krylov Subspace Reduction of Evolutionary Problems, SIAM J. Sci. Comput., 32(2010) 2485–2496.
13. V. Druskin, and V. Simoncini, Adaptive rational Krylov subspaces for large-scale dynamical systems, J. Sysconle, 60(2011) 546–560.
14. V. Druskin, L. Knizhnerman, and M. Zaslavsky, Solution of large scale evolutionary problems using rational Krylov subspaces with optimized shifts, SIAM J. Sci. Comput., 31(2009) 3760–3780.
15. V. Druskin, and L. Knizhnerman, Two polynomial methods of calculating functions of symmetric matrices. U.S.S.R. Comput. Math. Math. Phys., 29(1989) 112–121.
16. E. Estrada, The Structure of Complex Networks, Oxford University Press, Oxford, 2012.
17. C. Fenu, L. Reichel, G. Rodriguez, and H. Sadok, GCV for Tikhonov regularization by partial SVD, BIT, 57(2017) 1019–1039.
18. A. Ferrini, F. Perotti, and V. Simoncini, Iterative system solvers for the frequency analysis of linear mechanical systems, Comp. Meth. in App. Mech. and Engin., 190(2000) 1719–1739.
19. G. Gu, and V. Simoncini, Numerical solution of parameter-dependent linear systems. J. Numer. Linear Algebra w/App., 12(2005) 923–940.
20. S. Güttel, Rational Krylov approximation of matrix functions: Numerical methods and optimal pole selection, GAMM-Mitteilungen 36(2013) 8–31.
21. P. C. Hansen, Rank-Deficient and Discrete Ill-Posed Problems, SIAM, Philadelphia, 1998.
22. M. Heyouni, and K. Jbilou, An extended block Arnoldi algorithm for large-scale solutions of the continuous-time algebraic Riccati equation, Elect. Trans. Numer. Anal., 33(2009) 53–62.
23. N. J. Higham, Functions of matrices: theory and computation. SIAM, Philadelphia, (2008).
24. M. Hochbruck, and C. Lubich, On Krylov subspace approximations to the matrix exponential operator, SIAM J. Numer. Anal., 34(1997) 1911–1925.
25. C. Jagels, and L. Reichel, The extended Krylov subspace method and orthogonal Laurent polynomials, Linear Algebra Appl. 431(2009) 441–458.
26. K. Jbilou, A. Messaoudi, and H. Sadok, Global FOM and GMRES algorithms for matrix equations, Appl. Numer. Math., 31(1999) 49–63.
27. K. Jbilou, Low rank approximate solutions to large Sylvester matrix equations, Appl. Math. Comp., 177(2006) 365–376.
28. L. Knizhnerman, V. Druskin, and M. Zaslavsky, On optimal convergence rate of the rational Krylov subspace reduction for electromagnetic problems in unbounded domains, SIAM J Numer Anal., 47(2009) 953–971.
29. T. T. Ngo, M. Bellalij, and Y. Saad, The trace ratio optimization problem, SIAM Rev., 54(2012) 545–569.
30. S. Pranic, L. Reichel, G. Rodriguez, Z. Wang, and X. Yu, A rational Arnoldi process with applications, Numer. Linear Algebra Appl., 23(2016) 1007–1022.
31. A. Ruhe, Rational Krylov sequence methods for eigenvalue computation, Lin. Alg. Appl., 58(1984) 391–405.
32. Y. Saad, J. Chelikowsky, and S. Shontz, Numerical methods for electronic structure calculations of materials, SIAM Rev., 52(2010) 3–54.
33. Y. Saad, Analysis of some Krylov subspace approximations to the matrix exponential operator, SIAM J. Numer. Anal., 29(1992) 209–228.
34. V. Simoncini, Extended Krylov subspace for parameter dependent systems, Appl. Numer. Math., 60(2010) 550–560.
35. V. Simoncini, A new iterative method for solving large-scale Lyapunov matrix equations, SIAM J. Sci. Comput., 29(2007) 1268–1288.
36. E. Tyrtyshnikov, Mosaic-skeleton approximations, Calcolo, 33(1996) 47–57.