



ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

ARCHIVIO ISTITUZIONALE
DELLA RICERCA

Alma Mater Studiorum Università di Bologna
Archivio istituzionale della ricerca

Inexact Arnoldi residual estimates and decay properties for functions of non-Hermitian matrices

This is the final peer-reviewed author's accepted manuscript (postprint) of the following publication:

Published Version:

Pozza S., Simoncini V. (2019). Inexact Arnoldi residual estimates and decay properties for functions of non-Hermitian matrices. BIT, 59(4), 969-986 [10.1007/s10543-019-00763-6].

Availability:

This version is available at: <https://hdl.handle.net/11585/714895> since: 2020-01-18

Published:

DOI: <http://doi.org/10.1007/s10543-019-00763-6>

Terms of use:

Some rights reserved. The terms and conditions for the reuse of this version of the manuscript are specified in the publishing policy. For all terms of use and more information see the publisher's website.

This item was downloaded from IRIS Università di Bologna (<https://cris.unibo.it/>).
When citing, please refer to the published version.

(Article begins on next page)

This is the final peer-reviewed accepted manuscript of:

Pozza, Stefano, e Valeria Simoncini. «Inexact Arnoldi residual estimates and decay properties for functions of non-Hermitian matrices». BIT Numerical Mathematics 59, n. 4 (1 dicembre 2019): 969–86.

The final published version is available online at:
<https://doi.org/10.1007/s10543-019-00763-6>

Rights / License:

The terms and conditions for the reuse of this version of the manuscript are specified in the publishing policy. For all terms of use and more information see the publisher's website.

*This item was downloaded from IRIS Università di Bologna
(<https://cris.unibo.it/>)*

When citing, please refer to the published version.

Inexact Arnoldi residual estimates and decay properties for functions of non-Hermitian matrices

Stefano Pozza^{1,2} · Valeria Simoncini^{3,4}

1 **Abstract**

2 This paper derives a priori residual-type bounds for the Arnoldi approximation of
3 a matrix function together with a strategy for setting the iteration accuracies in the
4 inexact Arnoldi approximation of matrix functions. Such results are based on the
5 decay behavior of the entries of functions of banded matrices. Specifically, a priori
6 decay bounds for the entries of functions of banded non-Hermitian matrices will be
7 exploited, using Faber polynomial approximation. Numerical experiments illustrate
8 the quality of the results.

9 **Keywords** Arnoldi algorithm · Inexact Arnoldi algorithm · Matrix functions · Faber
10 polynomials · Decay bounds · Banded matrices

11 **Mathematics Subject Classification** 65F60 · 65F10

Communicated by Daniel Kressner.

This work has been supported by the FARB12SIMO grant, Università di Bologna, by INdAM-GNCS under the 2016 Project *Equazioni e funzioni di matrici con struttura: analisi e algoritmi*, by the INdAM-GNCS “Giovani ricercatori 2016” grant, and by Charles University Research program No. UNCE/SCI/023.

✉ Stefano Pozza
pozza@karlin.mff.cuni.cz
Valeria Simoncini
valeria.simoncini@unibo.it

1 Faculty of Mathematics and Physics, Charles University, Sokolovská 83, 186 75 Praha 8, Prague, Czech Republic

2 ISTI-CNR, Pisa, Italy

3 Dipartimento di Matematica, Università di Bologna, Piazza di Porta San Donato 5, 40127 Bologna, Italy

4 IMATI-CNR, Pavia, Italy

12 **1 Introduction**

13 Matrix functions have arisen as a reliable and a computationally attractive tool for
 14 solving a large variety of application problems; we refer the reader to [27] for a
 15 thorough discussion and references. Given a complex $n \times n$ matrix A and a sufficiently
 16 regular function f , we are interested in the approximation of the matrix function $f(A)$
 17 times a vector \mathbf{v} , that is $f(A)\mathbf{v}$, where we assume that \mathbf{v} has unit Euclidean norm. To
 18 this end, we consider the orthogonal projection onto a subspace \mathcal{V}_m of dimension m
 19 much smaller than n , obtaining the approximation

20
$$f(A)\mathbf{v} \approx V_m f(H_m)\mathbf{w}, \tag{1.1}$$

21 with V_m an $n \times m$ matrix whose columns form an orthonormal basis of \mathcal{V}_m , $H_m =$
 22 $V_m^* A V_m$, and $\mathbf{w} = V_m^* \mathbf{v}$. In this paper, we will focus on the case in which \mathcal{V}_m is the
 23 *Krylov subspace*

24
$$\mathcal{K}_m(A, \mathbf{v}) = \text{span}\{\mathbf{v}, A\mathbf{v}, \dots, A^{m-1}\mathbf{v}\}$$

25 and V_m is the orthogonal basis obtained by the Arnoldi algorithm; see, e.g., [27, chapter
 26 13]. Arnoldi-type approximations for the matrix exponential have been deeply investi-
 27 gated, and estimates of the error norm $\|e^{-tA}\mathbf{v} - V_m e^{-tH_m}\mathbf{e}_1\|$ for A non-normal have
 28 been given for instance by Saad [38], by Lubich and Hochbruck in [28], and recently
 29 by Wang and Ye in [42,43]. Other methods related to the Arnoldi approximation can be
 30 found in [1,17,21,22] where *restarted* techniques are considered. Regarding rational
 31 Krylov approximations of matrix functions, we refer the reader to the review [25] and
 32 to the black-box rational Arnoldi variant given in [26].

33 When V_m is the output of the Arnoldi algorithm, H_m is an upper Hessenberg matrix;
 34 that is a banded matrix with zero elements below the second lower diagonal. It can
 35 be shown that under certain assumptions the elements of $f(H_m)$ below the main
 36 diagonal are characterized by a decay behavior. Indeed, given a square banded matrix
 37 B , the entries of the matrix function $f(B)$ for a sufficiently regular function f are
 38 characterized by a—typically exponential—decay pattern as they move away from the
 39 main diagonal. This phenomenon has been known for a long time, and it is at the basis
 40 of approximations and estimation strategies in many fields, from signal processing
 41 to quantum dynamics and multivariate statistics; for a detailed description of relevant
 42 problems and a more comprehensive list of application fields where capturing the decay
 43 is particularly important we refer the reader to [3,4,7]. The interest in *a priori* estimates
 44 that can accurately predict the decay rate of matrix functions has significantly grown
 45 in the past decades, and it has mainly focused on Hermitian matrices [5,7,9,11,12,18,
 46 35,44]; the inverse and exponential functions have been given particular attention, due
 47 to their relevance in numerical analysis and other fields. Upper bounds usually take
 48 the form

49
$$|(f(B))_{k,\ell}| \leq c\rho^{|k-\ell|}, \tag{1.2}$$

50 where $\rho \in (0, 1)$; both ρ and c depend on the spectral properties of B and on the
51 domain of f , while ρ also strongly depends on the bandwidth of B .

52 In the case of a banded Hermitian matrix B , bounds of the Arnoldi approximation
53 have been used to obtain upper estimates showing the decay phenomenon occurring
54 in the entries of $f(B)$; see for instance [7] for the exponential function. Here we will
55 exploit this connection but in the reverse direction. More precisely, we will first derive
56 decay bounds for the entries of banded non-Hermitian matrices. Then we will apply
57 such bounds to the matrix function $f(H_m)$, with H_m the upper Hessenberg matrix given
58 by the Arnoldi algorithm, obtaining a priori bounds for the quality of the approximation
59 (1.1), when a residual-based measure is used; these bounds complement available ones
60 in the already mentioned literature for the Arnoldi approximation. Furthermore, we
61 will use the described bounds in the inexact Krylov approximation of matrix functions;
62 in particular, the bounds can be used to devise a priori relaxing thresholds for the inexact
63 matrix-vector multiplications with A , whenever A is not available explicitly. These
64 last results generalize the theory developed for $f(z) = z^{-1}$ and for the eigenvalue
65 problem in [40] and [39], respectively; see also [14,31].

66 The analysis of the decay pattern for banded *non-Hermitian* matrices is significantly
67 harder than in the Hermitian case, especially for non-normal matrices. In [6] Benzi and
68 Razouk addressed this challenging case for diagonalizable matrices. They developed a
69 bound of the type (1.2), where c also contains the eigenvector matrix condition number.
70 In [33] the authors derive several qualitative bounds, mostly under the assumption
71 that A is diagonally dominant. The exponential function provides a special setting,
72 which has been explored in [29] and in [42,43]. In all these last articles, and also
73 in our approach, bounds on the decay pattern of banded non-Hermitian matrices are
74 derived that avoid the explicit reference to the possibly large condition number of
75 the eigenvector matrix. Specialized off-diagonal decay results have been obtained for
76 certain normal matrices; see, e.g., [11,20,23], and [3] for analytic functions of banded
77 matrices over C^* -algebras.

78 Starting with the pioneering work [13], most estimates for the decay behavior of the
79 entries have relied on Chebyshev and Faber polynomials as technical tool, for two main
80 reasons. Firstly, polynomials of banded matrices are again banded matrices, although
81 the bandwidth increases with the polynomial degree; see Fig. 1 below for a typical
82 example. Secondly, sufficiently regular matrix functions can be written in terms of
83 Chebyshev and Faber series, whose polynomial truncations enjoy nice approximation
84 properties for a large class of matrices, from which an accurate description of the
85 matrix function entries can be deduced. Using Faber polynomials, we will present
86 an original derivation of a family of bounds for functions of banded non-Hermitian
87 matrices. Such family can be adapted to several cases, depending on the function
88 properties and on the matrix spectral properties. Very similar bounds can be obtained
89 combining Theorem 10 in [3] with Theorem 3.7 in [6]. Another similar bound is given
90 in [33, Theorem 2.6] for the case of multi-banded matrices and in [42, Theorem 3.8] for
91 the exponential case. We also refer the reader to [36], where the bounds presented here
92 have been extended to matrices with a more general sparsity pattern. Our bounds and
93 the ones just cited make use of some approximation of the field of values (numerical
94 range) of a matrix. An accurate approximation can be computationally quite expensive
95 unless some structural properties can be exploited, as is the case for instance for

96 Toeplitz matrices ([16, Section 3]) or for network adjacency matrices ([36, Section
 97 5.3]). Fortunately, for our purposes not-too-accurate field of value approximations can
 98 suffice, limiting the computational costs.

99 The paper is organized as follows. In Sect. 2 we use Faber polynomials to give a
 100 bound that can be adapted to approximate the entries of several functions of banded
 101 matrices; as an example we consider the functions e^A and $e^{-\sqrt{A}}$. In Sect. 3 and its
 102 subsections we first show that the derived estimates can be used for a residual-type
 103 bound in the approximation of $f(A)\mathbf{v}$, for certain functions f by means of the Arnoldi
 104 algorithm. Then we describe how to employ this bound to reliably estimate the quality
 105 of the approximation when in the Arnoldi iteration the accuracy in the matrix-vector
 106 product is relaxed. Numerical experiments illustrate the quality of the bounds. We
 107 conclude with some remarks in Sect. 4 and with technical proofs in the ‘‘Appendix’’.

108 All our numerical experiments were performed using Matlab (R2013b) [34]. In all
 109 our experiments, the computation of the field of values employed the code in [10].

110 2 Decay bounds for functions of banded matrices

111 We begin recalling the definition of matrix function and some of its properties. Matrix
 112 functions can be defined in several ways (see [27, section 1]). For our presentation, it
 113 is helpful to introduce the definition that employs the Cauchy integral formula.

114 **Definition 2.1** Let $A \in \mathbb{C}^{n \times n}$ and f be an analytic function on some open $\Omega \subset \mathbb{C}$.
 115 Then

$$116 \quad f(A) = \int_{\Gamma} f(z) (zI - A)^{-1} dz,$$

117 where $\Gamma \subset \Omega$ is a Jordan curve (or a finite collection of Jordan curves) enclosing the
 118 eigenvalues of A exactly once, with mathematical positive orientation.

119 When f is analytic, Definition 2.1 is equivalent to other common definitions; see
 120 [37, section 2.3].

121 For $\mathbf{v} \in \mathbb{C}^n$, we denote with $\|\mathbf{v}\|$ the Euclidean vector norm, and for any matrix
 122 $A \in \mathbb{C}^{n \times n}$, with $\|A\|$ the induced matrix norm; that is, $\|A\| = \sup_{\|\mathbf{v}\|=1} \|A\mathbf{v}\|$. \mathbb{C}^+
 123 denotes the open right-half complex plane. Moreover, we recall that the *field of values*
 124 (or *numerical range*) of A is defined as the set $W(A) = \{\mathbf{v}^* A \mathbf{v} \mid \mathbf{v} \in \mathbb{C}^n, \|\mathbf{v}\| = 1\}$,
 125 where \mathbf{v}^* is the conjugate transpose of \mathbf{v} . We remark that the field of values of a matrix
 126 is a bounded convex subset of \mathbb{C} . Throughout the paper, \sqrt{z} stands for the principal
 127 square root of $z \in \mathbb{C}$. Analogously \sqrt{A} indicates the principal square root of the
 128 matrix A , which exists and is unique when A has no eigenvalues in \mathbb{R}^- ; see, e.g., [27,
 129 Theorem 1.29].

130 The (k, ℓ) element of a matrix A is denoted by $(A)_{k,\ell}$. The set of banded matrices
 131 is defined as follows.

132 **Definition 2.2** The notation $\mathcal{B}_n(\beta, \gamma)$ defines the set of banded matrices $A \in \mathbb{C}^{n \times n}$
 133 with upper bandwidth $\beta \geq 0$ and lower bandwidth $\gamma \geq 0$, i.e., $(A)_{k,\ell} = 0$ for $\ell - k > \beta$
 134 and $k - \ell > \gamma$.

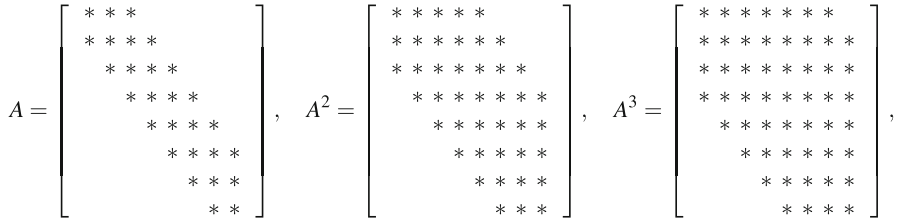


Fig. 1 Typical fill-in pattern of powers of a banded matrix $A \in \mathcal{B}_n(2, 1)$

135 We observe that if $A \in \mathcal{B}_n(\beta, \gamma)$ with $\beta, \gamma \neq 0$, for

$$136 \quad \xi := \begin{cases} \lceil (\ell - k)/\beta \rceil, & \text{if } k < \ell \\ \lceil (k - \ell)/\gamma \rceil, & \text{if } k \geq \ell \end{cases} \quad (2.1)$$

137 it holds that

$$138 \quad (A^m)_{k,\ell} = 0, \quad \text{for every } m < \xi; \quad (2.2)$$

139 see Fig. 1 for a typical fill-in pattern of A^m .

140 This characterization of banded matrices is a classical fundamental tool to prove the
 141 decay property of matrix functions, as sufficiently regular functions can be expanded
 142 in power series. Since we are interested in nontrivial banded matrices, in the following
 143 we shall assume that both β and γ are nonzero.

144 Faber polynomials extend the theory of power series to sets different from the
 145 disk, and can be effectively used to bound the entries of matrix functions. Let E
 146 be a continuum (i.e., a non-empty, compact and connected subset of \mathbb{C}) with connected
 147 complement. Then by Riemann's mapping theorem there exists a function ϕ that maps
 148 the exterior of E conformally onto $\{|z| > 1\}$ and such that

$$149 \quad \phi(\infty) = \infty, \quad \lim_{z \rightarrow \infty} \frac{\phi(z)}{z} = d > 0.$$

150 Hence, ϕ can be expressed by a Laurent expansion $\phi(z) = dz + a_0 + \frac{a_1}{z} + \frac{a_2}{z^2} + \dots$.
 151 Furthermore, for every $n > 0$ we have

$$152 \quad (\phi(z))^n = dz^n + a_{n-1}^{(n)} z^{n-1} + \dots + a_0^{(n)} + \frac{a_{-1}^{(n)}}{z} + \frac{a_{-2}^{(n)}}{z^2} + \dots .$$

153 Then the Faber polynomial for the domain E is defined by (see, e.g., [41])

$$154 \quad \Phi_n(z) = dz^n + a_{n-1}^{(n)} z^{n-1} + \dots + a_0^{(n)}, \quad \text{for } n \geq 0.$$

155 If f is analytic on E , then it can be expanded in a series of Faber polynomials for E ;
 156 that is,

$$157 \quad f(z) = \sum_{j=0}^{\infty} f_j \Phi_j(z), \quad \text{for } z \in E;$$

158 see [41, Theorem 2, p. 52]. If the spectrum of A is contained in E and f is a function
 159 analytic in E , then the matrix function $f(A)$ can be expanded as follows (see, e.g.,
 160 [41, p. 272])

$$161 \quad f(A) = \sum_{j=0}^{\infty} f_j \Phi_j(A).$$

162 If, in addition, E contains the field of values $W(A)$, then for $n \geq 1$ we get

$$163 \quad \|\Phi_n(A)\| \leq 2, \tag{2.3}$$

164 by Beckermann's Theorem 1.1 in [2].

165 By using the properties of Faber polynomials, in the following theorem we derive
 166 decay bounds for a large class of matrix functions. Notice that the estimate in [3,
 167 Theorem 10] combined with the results presented in [6, Theorem 3.7] results in similar
 168 bounds (see also [19]); moreover, in section 2 of [33], and in particular in Theorem 2.6,
 169 analogous results are discussed. Another similar bound can be found in [42, Theorem
 170 3.8] for the case $f(z) = e^z$. The derivation we describe differs from the ones listed
 171 above by using inequality (2.3).

172 **Theorem 2.3** *Let $A \in \mathcal{B}_n(\beta, \gamma)$ with field of values contained in a convex continuum*
 173 *E . Moreover, let ϕ be the conformal map sending the exterior of E onto the exterior*
 174 *of the unit disk, and let ψ be its inverse. For any $\tau > 1$ such that f is analytic on the*
 175 *level set G_τ defined as the complement of the set $\{\psi(z) : |z| > \tau\}$, it holds*

$$176 \quad |(f(A))_{k,\ell}| \leq 2 \frac{\tau}{\tau - 1} \max_{|z|=\tau} |f(\psi(z))| \left(\frac{1}{\tau}\right)^\xi,$$

177 with ξ defined by (2.1).

178 **Proof** Properties (2.2) and (2.3) imply

$$179 \quad |(f(A))_{k,\ell}| = \left| \sum_{j=0}^{\infty} f_j (\Phi_j(A))_{k,\ell} \right| = \left| \sum_{j=\xi}^{\infty} f_j (\Phi_j(A))_{k,\ell} \right| \leq 2 \sum_{j=\xi}^{\infty} |f_j|,$$

180 where the Faber coefficients f_j are given by (see, e.g., [41, chapter III, Theorem 1])

$$181 \quad f_j = \frac{1}{2\pi i} \int_{|z|=\tau} \frac{f(\psi(z))}{z^{j+1}} dz.$$

182 Noticing that $|f_j| \leq \frac{1}{(\tau)^j} \max_{|z|=\tau} |f(\psi(z))|$ gives

$$183 \quad |(f(A))_{k,\ell}| \leq 2 \max_{|z|=\tau} |f(\psi(z))| \sum_{j=\xi}^{\infty} \left(\frac{1}{\tau}\right)^j = 2 \frac{\tau}{\tau-1} \max_{|z|=\tau} |f(\psi(z))| \left(\frac{1}{\tau}\right)^{\xi}.$$

184 □

185 The choice of τ in Theorem 2.3, and thus the sharpness of the derived estimate,
 186 depends on the trade-off between the possible large size of f on the given region,
 187 and the exponential decay of $(1/\tau)^\xi$, and thus it produces an infinite family of bounds
 188 depending on the problem considered. In our examples, we apply Theorem 2.3 to the
 189 approximation of the functions $f(z) = e^z$ and $f(z) = e^{-\sqrt{z}}$, with z in a properly
 190 chosen domain.

191 **Corollary 2.4** *Let $A \in \mathcal{B}_n(\beta, \gamma)$ with field of values contained in a closed set E whose
 192 boundary is a horizontal ellipse with semi-axes $a \geq b > 0$ and center $c = c_1 + ic_2 \in$
 193 \mathbb{C} , $c_1, c_2 \in \mathbb{R}$. Then*

$$194 \quad \left| \left(e^A \right)_{k,\ell} \right| \leq 2e^{c_1} \frac{\xi + \sqrt{\xi^2 + a^2 - b^2}}{\xi + \sqrt{\xi^2 + a^2 - b^2} - (a+b)} \left(\frac{a+b}{\xi} \frac{e^{q(\xi)}}{1 + \sqrt{1 + (a^2 - b^2)/\xi^2}} \right)^{\xi},$$

195 *for $\xi > b$, with $q(\xi) = 1 + \frac{a^2 - b^2}{\xi^2 + \xi \sqrt{\xi^2 + a^2 - b^2}}$ and ξ as in (2.1).*

196 The proof is postponed to the ‘‘Appendix’’. Notice that for ξ large enough, the decay
 197 rate is of the form $((a+b)/(2\xi))^\xi$; that is, the decay is super-exponential. Moreover,
 198 in the Hermitian case, we can let $b \rightarrow 0$ in Corollary 2.4, thus obtaining a bound that
 199 is asymptotically equivalent—up to a multiplicative constant—to the one derived in
 200 [7, Theorem 4.2(ii)].

201 The function $f(z) = e^{-\sqrt{z}}$ is not analytic in the whole complex plane. This property
 202 has crucial effects on the approximation.

203 **Corollary 2.5** *Let $A \in \mathcal{B}_n(\beta, \gamma)$ with field of values contained in a closed set $E \subset \mathbb{C}^+$,
 204 whose boundary is a horizontal ellipse with semi-axes $a \geq b > 0$ and center $c \in \mathbb{C}$.
 205 Then,*

$$206 \quad \left| \left(e^{-\sqrt{A}} \right)_{k,\ell} \right| \leq 2q_2(a, b, c) \left(\frac{a+b}{|c|} \frac{1}{|1 + \sqrt{1 - (a^2 - b^2)/c^2}|} \right)^{\xi},$$

207 *with ξ defined by (2.1) and*

$$208 \quad q_2(a, b, c) = \frac{|c + \sqrt{c^2 - (a^2 - b^2)}|}{|c + \sqrt{c^2 - (a^2 - b^2)}| - (a+b)}.$$

209 The proof is given in the “Appendix”. If c is not real, then the bound in Corollary 2.5
 210 can be further improved since the ellipses considered in the proof are not the maximal
 211 one.

212 **Remark 2.6** For the sake of simplicity, in the previous corollaries horizontal ellipses
 213 were employed. However, more general convex sets E may be considered. The pre-
 214 vious bounds will change accordingly, since the optimal value for τ in Theorem 2.3
 215 does depend on the parameters associated with E . For instance, for the exponential
 216 function and a *vertical* ellipse, we can derive the same bound as in Corollary 2.4 by
 217 letting $b > a$. Notice that this is different from exchanging the role of a and b in the
 218 bound. The proof of this fact is non-trivial but technical, and it is not reported.

219 3 Residual bounds for Arnoldi and inexact Arnoldi methods

220 3.1 The Arnoldi method

221 Given a matrix $A \in \mathbb{C}^{n \times n}$ and a vector $\mathbf{v} \in \mathbb{C}^n$, for $m \geq 1$ the m th step of the
 222 Arnoldi algorithm determines an orthonormal basis $\{\mathbf{v}_1, \dots, \mathbf{v}_m\}$ for the Krylov sub-
 223 space $\mathcal{K}_m(A, \mathbf{v})$, the subsequent orthonormal basis vector \mathbf{v}_{m+1} , an $m \times m$ upper
 224 Hessenberg matrix H_m , and a nonnegative scalar $h_{m+1,m}$ such that

$$225 \quad AV_m = V_m H_m + h_{m+1,m} \mathbf{v}_{m+1} \mathbf{e}_m^T,$$

226 where $V_m = [\mathbf{v}_1, \dots, \mathbf{v}_m]$; note that $h_{m+1,m} = 0$ if and only if the algorithm stops, i.e.,
 227 $\mathcal{K}_m(A, \mathbf{v})$ is an invariant subspace of A . Due to the orthogonality of the columns of
 228 $[V_m, \mathbf{v}_{m+1}]$, the matrix H_m is the projection and restriction of A onto $\mathcal{K}_m(A, \mathbf{v})$; that
 229 is, $H_m = V_m^* A V_m$. Throughout the paper we assume exact arithmetic. As commonly
 230 performed, in our numerical computations we generated the matrix V_m by means
 231 of the *modified* Gram-Schmidt method with reorthogonalization, which ensures good
 232 orthogonality properties of the constructed basis in finite precision arithmetic; see, e.g.,
 233 [24]. Without loss of generality assume that $\|\mathbf{v}\| = 1$. Then the Arnoldi approximation
 234 to $f(A)\mathbf{v}$ is given as $V_m f(H_m) \mathbf{e}_1$; see, e.g., [27, chapter 13]. The quantity

$$235 \quad |\mathbf{e}_m^T f(H_m) \mathbf{e}_1| = |(f(H_m))_{m,1}|$$

236 – the last entry of the first column of $|f(H_m)|$ – is commonly employed to monitor the
 237 accuracy of the approximation $\|f(A)\mathbf{v} - V_m f(H_m) \mathbf{e}_1\|$; see, e.g., [38] and a related
 238 discussion in [30]. In the case of the exponential, $e^{-tA}\mathbf{v}$, the quantity

$$239 \quad r_m(t) = |h_{m+1,m} \mathbf{e}_m^T e^{-tH_m} \mathbf{e}_1|$$

240 can be interpreted as the “residual” norm of an associated differential equation; see
 241 [8] and references therein. This interpretation can be shown to be true also for other
 242 functions; see, e.g., [15, section 6]). Indeed, assume that $\mathbf{y}(t) = f(tA)\mathbf{v}$ is the solution
 243 to the differential equation $y^{(d)} = Ay$ for some d th derivative, $d \in \mathbb{N}$ and specified

244 initial conditions for $t = 0$. Let $\mathbf{y}_m(t) = V_m f(tH_m)\mathbf{e}_1 =: V_m \widehat{\mathbf{y}}_m(t)$. The vector
 245 $\widehat{\mathbf{y}}_m(t)$ is the solution to the projected differential equation $\widehat{\mathbf{y}}_m^{(d)} = H_m \widehat{\mathbf{y}}_m$ with initial
 246 condition $\widehat{\mathbf{y}}_m(0) = \mathbf{e}_1$. The differential equation residual $\mathbf{r}_m = A\mathbf{y}_m - \mathbf{y}_m^{(d)}$ can be used
 247 to monitor the accuracy of the approximate solution as follows: using the definition
 248 of \mathbf{y}_m and the Arnoldi relation, we obtain

$$\begin{aligned}
 249 \quad \mathbf{r}_m(t) &= A\mathbf{y}_m - \mathbf{y}_m^{(d)} = AV_m f(tH_m)\mathbf{e}_1 - \mathbf{y}_m^{(d)} \\
 250 &= V_m H_m f(tH_m)\mathbf{e}_1 - V_m (f(tH_m))^{(d)}\mathbf{e}_1 + \mathbf{v}_{m+1} h_{m+1,m} \mathbf{e}_m^T f(tH_m)\mathbf{e}_1 \\
 251 &= V_m (H_m \widehat{\mathbf{y}}_m - \widehat{\mathbf{y}}_m^{(d)}) + \mathbf{v}_{m+1} h_{m+1,m} \mathbf{e}_m^T f(tH_m)\mathbf{e}_1 \\
 252 &= \mathbf{v}_{m+1} h_{m+1,m} \mathbf{e}_m^T f(tH_m)\mathbf{e}_1.
 \end{aligned}$$

253 Therefore $r_m(t) = \|\mathbf{r}_m(t)\|$.

254 Without loss of generality, in the following we consider $t = 1$. Hence, for simplicity,
 255 we denote $r_m = r_m(1)$, and $\mathbf{r}_m = \mathbf{r}_m(1)$. We remark that the property $H_m = V_m^* A V_m$
 256 ensures that the field of values of H_m is contained in that of A , so that our theory can
 257 be applied using A as reference matrix to individuate the spectral region of interest.
 258 We also remark that the inclusion of $h_{m+1,m}$ in $r_m(t)$ does not influence the actual
 259 behavior of the quantity. On the one hand, it holds that $h_{m+1,m} \leq \|A\|$, so that $h_{m+1,m}$
 260 could in principle be eliminated from the bound. On the other hand, $h_{m+1,m}$ is not
 261 going to be small, unless the Krylov subspace is close to an invariant subspace of A , so
 262 that $AV_m \approx V_m H_m$. The strength of Krylov subspaces precisely relies on being able
 263 to obtain good approximations to the sought after quantities far before an invariant
 264 subspace is determined. Hence our analysis is of interest for m such that the Krylov
 265 subspace is still far from being an invariant subspace of A , for which $h_{m+1,m}$ is not
 266 small. This implies that the behavior of $h_{m+1,m} \mathbf{e}_m^T f(tH_m)\mathbf{e}_1$ is fully determined by
 267 the quantity under examination; that is, $|\mathbf{e}_m^T f(tH_m)\mathbf{e}_1|$.

268 Let a, b be the semi-axes and $c = c_1 + ic_2$ the center of an elliptical region E
 269 containing the field of values of A . For the entry $(k, \ell) \equiv (m, 1)$ of $f(tH_m)$ and
 270 lower bandwidth $\beta = 1$ of H_m , the definition in (2.1) yields $\xi = m - 1$. Hence, from
 271 Corollary 2.4 and $m > b + 1$ we deduce the inequality

$$272 \quad |r_m| \leq h_{m+1,m} 2e^{-c_1} p(m) \left(\frac{e^{q(m-1)}(a+b)}{m-1 + \sqrt{(m-1)^2 + (a^2 - b^2)}} \right)^{m-1}, \quad (3.1)$$

273 with

$$274 \quad q(m-1) = 1 + \frac{(a^2 - b^2)}{(m-1)^2 + (m-1)\sqrt{(m-1)^2 + (a^2 - b^2)}}$$

275 and

$$276 \quad p(m) = \frac{m-1 + \sqrt{(m-1)^2 + (a^2 - b^2)}}{m-1 + \sqrt{(m-1)^2 + (a^2 - b^2)} - (a+b)}.$$

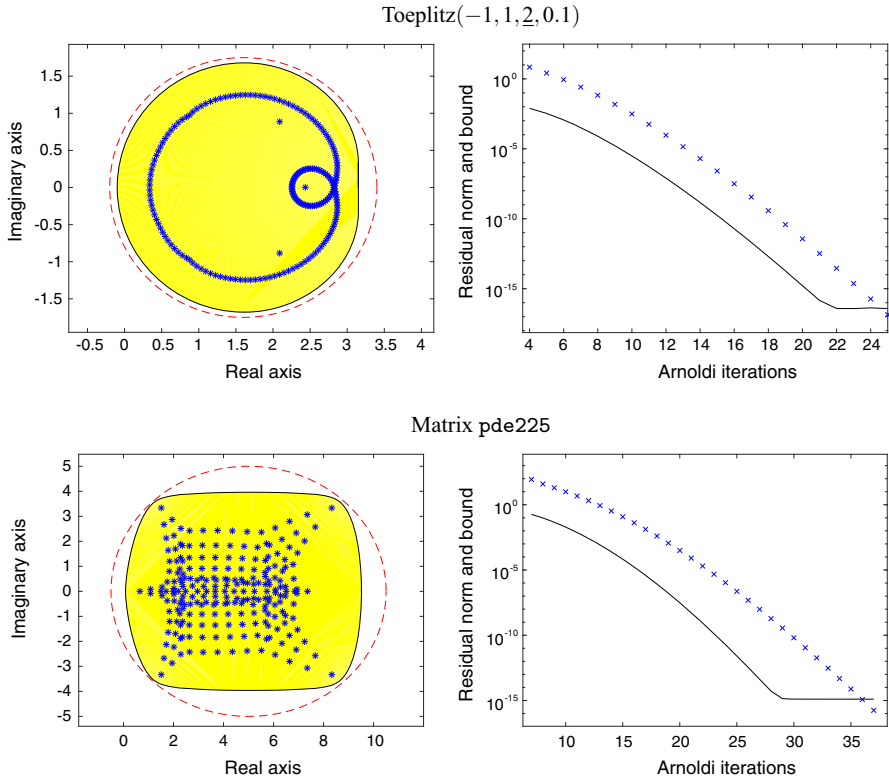


Fig. 2 Example 3.1. Approximation of $e^{-A}\mathbf{v}$, with $\mathbf{v} = (1, \dots, 1)^T/\sqrt{n}$. Top: $A = \text{Toeplitz}(-1, 1, \underline{2}, 0.1) \in \mathcal{B}_{200}(1, 2)$. Bottom: matrix pde225. Left: $W(A)$ (yellow area), eigenvalues of A (blue asterisks), and enclosing ellipse E (red dashed line). Right: residual norm as the Arnoldi iteration proceeds in the approximation (black solid line), and residual bound in (3.1) (blue \times).

277 In [42,43], a similar bound is proposed, where, however, a continuum E with rectan-
 278 gular shape is considered, instead of the elliptical one we take in Corollary 2.4.

279 **Example 3.1** Figure 2 shows the behavior of the bound in (3.1) for the residual of
 280 the Arnoldi approximation of $e^{-A}\mathbf{v}$ with $\mathbf{v} = (1, \dots, 1)^T/\sqrt{n}$. The top plots refer
 281 to $A \in \mathcal{B}_{200}(1, 2)$ with Toeplitz structure, $A = \text{Toeplitz}(-1, 1, \underline{2}, 0.1)$, where the
 282 underlined element is on the diagonal, while the previous (resp. subsequent) values
 283 denote the lower (resp. upper) diagonal entries. The bottom plots refer to the matrix
 284 pde225 of the Matrix Market repository [32]. The left figure shows the field of values
 285 of the matrix A (yellow area), its eigenvalues (blue asterisks), and the horizontal ellipse
 286 used in the bound (red dashed line). On the right, we plot the residual associated
 287 with the Arnoldi approximation as the iteration proceeds (black solid line), and the
 288 corresponding values of the bound (blue “ \times ”). Matrix exponentials were computed
 289 by the `expm` Matlab function.

290 3.2 The inexact Arnoldi method

291 In an inexact Arnoldi procedure, A is not known exactly (we consider inexactness
 292 under the assumptions and in the context of [40]). This may be due for instance to the
 293 fact that A is only implicitly available via functional operations with a vector, which
 294 can be approximated at some accuracy. To proceed with our analysis, we can formalize
 295 this inexactness at each iteration k as

$$296 \quad \tilde{\mathbf{v}}_{k+1} = A\mathbf{v}_k + \mathbf{w}_k \approx A\mathbf{v}_k. \quad (3.2)$$

297 Typically, some form of accuracy criterion is implemented, so that $\|\mathbf{w}_k\| < \epsilon$ for some
 298 ϵ . In practice, a different value of this tolerance may be used at each iteration k , i.e.,
 299 $\epsilon = \epsilon_k$; for this reason, in the following we assume that this tolerance depends on the
 300 iteration. The new vector $\tilde{\mathbf{v}}_{k+1}$ is then orthonormalized with respect to the previous
 301 basis vectors to obtain \mathbf{v}_{k+1} . In compact form, the original Arnoldi relation becomes

$$302 \quad (A + \mathcal{E}_m)V_m = V_m H_m + h_{m+1,m} \mathbf{v}_{m+1} \mathbf{e}_m^T, \quad \mathcal{E}_m = [\mathbf{w}_1, \dots, \mathbf{w}_m] V_m^*.$$

303 Here H_m is again upper Hessenberg; however, $H_m = V_m^*(A + \mathcal{E}_m)V_m$. Moreover, \mathcal{E}_m
 304 changes as m grows.

305 The quantities $\mathbf{y}_m = V_m f(H_m) \mathbf{e}_1$ and $\mathbf{r}_m = A\mathbf{y}_m - \mathbf{y}_m^{(d)}$ can still be defined as in
 306 the exact case; however the inexact Arnoldi relation should be considered to proceed
 307 further. Indeed,

$$308 \quad \mathbf{r}_m = A\mathbf{y}_m - \mathbf{y}_m^{(d)} = AV_m f(H_m) \mathbf{e}_1 - \mathbf{y}_m^{(d)} \quad (3.3)$$

$$309 \quad = -\mathcal{E}_m V_m f(H_m) \mathbf{e}_1 + V_m H_m f(H_m) \mathbf{e}_1 - \mathbf{y}_m^{(d)} + \mathbf{v}_{m+1} h_{m+1,m} \mathbf{e}_m^T f(H_m) \mathbf{e}_1$$

$$310 \quad = -[\mathbf{w}_1, \dots, \mathbf{w}_m] f(H_m) \mathbf{e}_1 + \mathbf{v}_{m+1} h_{m+1,m} \mathbf{e}_m^T f(H_m) \mathbf{e}_1. \quad (3.4)$$

311 We can still define $r_m = |h_{m+1,m} \mathbf{e}_m^T f(H_m) \mathbf{e}_1|$, but we observe that now $r_m \neq \|\mathbf{r}_m\|$.
 312 Moreover, while r_m is computable, the quantity $\|\mathbf{r}_m\|$ is not available, since A is not
 313 known exactly. With the previous notation we can write $\|\mathbf{r}_m\| \leq \|[\mathbf{w}_1, \dots, \mathbf{w}_m] f(H_m) \mathbf{e}_1\| + r_m$
 314 where

$$315 \quad \|[\mathbf{w}_1, \dots, \mathbf{w}_m] f(H_m) \mathbf{e}_1\|.$$

316 Therefore, if $\|[\mathbf{w}_1, \dots, \mathbf{w}_m] f(H_m) \mathbf{e}_1\|$ is smaller than the tolerance for the final
 317 requested accuracy, then r_m provides a good measure in a computable stopping crite-
 318 rion.

319 Following a similar discussion in [39,40], we write

$$320 \quad \|[\mathbf{w}_1, \dots, \mathbf{w}_m] f(H_m) \mathbf{e}_1\| = \left\| \sum_{j=1}^m \mathbf{w}_j \mathbf{e}_j^T f(H_m) \mathbf{e}_1 \right\| \leq \sum_{j=1}^m \|\mathbf{w}_j\| |\mathbf{e}_j^T f(H_m) \mathbf{e}_1|,$$

321 where $\|\mathbf{w}_j\| < \epsilon_j$. As a consequence, $\|[\mathbf{w}_1, \dots, \mathbf{w}_m] f(H_m) \mathbf{e}_1\|$ is small when either
 322 $\|\mathbf{w}_j\|$ or $|\mathbf{e}_j^T f(H_m) \mathbf{e}_1|$ is small, and not necessarily both. By recalling the exponential

323 decay of the entries of $f(H_m)\mathbf{e}_1$, $\|\mathbf{w}_j\|$ is in fact allowed to grow with j , in a way
 324 that is inversely proportional to the exponential decay of the corresponding entries of
 325 $f(H_m)\mathbf{e}_1$, without affecting the overall accuracy. A priori bounds on $|\mathbf{e}_j^T f(H_m)\mathbf{e}_1|$
 326 can be used to select ϵ_j when estimating $A\mathbf{v}_j$. This relaxed strategy can significantly
 327 decrease the computational cost of matrix function evaluations whenever applying A
 328 accurately is expensive. However, notice that the field of values of H_m is contained in
 329 the field of values of $A + \mathcal{E}_m$. Hence if $W(A)$ is contained in an ellipse ∂E of semi-axes
 330 a, b and center c , then $W(A + \mathcal{E}_m) \subset W(A) + W(\mathcal{E}_m)$. Since

$$331 \quad \sup_{\|z\|=1} |z^* \mathcal{E}_m z| \leq \sup_{\|z\|=1} \|\mathcal{E}_m z\| \leq \sqrt{\sum_{j=1}^m \|\mathbf{w}_j\|^2} \leq \sqrt{\sum_{j=1}^m \epsilon_j^2} =: \epsilon^{(m)},$$

332 the set $W(\mathcal{E}_m)$ is contained in the disk centered at the origin and radius $\epsilon^{(m)}$. Therefore
 333 $W(A) + W(\mathcal{E}_m)$ is contained in any set whose boundary has minimal distance from
 334 ∂E not smaller than $\epsilon^{(m)}$. One such set is contained in the ellipse ∂E_m with semi-axes
 335 $a(1 + \epsilon^{(m)}/b), b + \epsilon^{(m)}$ and center c . Indeed, $z \in \partial E_m$ can be parameterized as

$$336 \quad z = \left(1 + \frac{\epsilon^{(m)}}{b}\right) \frac{\rho}{2} \left(Re^{i\theta} + \frac{1}{Re^{i\theta}}\right) + c, \quad 0 \leq \theta \leq 2\pi,$$

337 with $\rho = \sqrt{a^2 - b^2}$, $R = (a + b)/\rho$. The distance between z and the ellipse ∂E is

$$338 \quad \left| \frac{\epsilon^{(m)}}{b} \frac{\rho}{2} \left(Re^{i\theta} + \frac{1}{Re^{i\theta}}\right) \right| \geq \left| \frac{\epsilon^{(m)}}{b} \frac{\rho}{2} \left(R - \frac{1}{R}\right) \right| = \epsilon^{(m)}.$$

339 With these definitions and notations we can introduce the following relaxation strategy
 340 for the inexactness in the Arnoldi procedure.

341 **Theorem 3.2** *Let \mathbf{r}_m be the (uncomputable) residual in (3.3) after m steps of the inexact*
 342 *Arnoldi algorithm and associated function f . Let $\epsilon^{(m)} > 0$ be the maximum allowed*
 343 *inexactness tolerance and let $\text{tol} > 0$.*

344 *If for every $j \leq m$ we have $\|\mathbf{w}_j\| \leq \bar{\epsilon}_j$ with*

$$345 \quad \bar{\epsilon}_j = \begin{cases} \frac{\text{tol}}{m} \max \left\{ 1, \frac{1}{s_j} \right\}, & \text{if } \frac{\text{tol}}{m s_j} < \frac{1}{m-j+1} \sqrt{(\epsilon^{(m)})^2 - \sum_{k=1}^{j-1} \bar{\epsilon}_k^2} \\ \frac{1}{m-j+1} \sqrt{(\epsilon^{(m)})^2 - \sum_{k=1}^{j-1} \bar{\epsilon}_k^2}, & \text{otherwise} \end{cases} \quad (3.5)$$

346 *then*

$$347 \quad \|\mathbf{r}_m\| - r_m \leq \text{tol},$$

348 *and $\left(\sum_{j=1}^m \bar{\epsilon}_j^2\right)^{\frac{1}{2}} \leq \epsilon^{(m)}$. Here s_j is the upper bound for $|\mathbf{e}_j^T f(H_m)\mathbf{e}_1|$ from Theo-*
 349 *rem 2.3 if j is such that this bound can be determined, otherwise $s_j = 1$; $W(A)$ in*

350 *Theorem 2.3 is contained in an ellipse with semiaxes $a \geq b > 0$ and center c , and E*
 351 *is the ellipse with semiaxes $a(1 + \epsilon^{(m)}/b)$, $b + \epsilon^{(m)}$ and center c .*

352 The bound of Theorem 3.2 can be specialized for the functions $f(z) = e^z$ and
 353 $f(z) = e^{-\sqrt{z}}$ using respectively Corollaries 2.4 and 2.5.

354 In the following, we report on some experiments illustrating our findings. We con-
 355 sider the norm of the differential equation residual at time $t = 1$, that is

$$356 \quad \|\mathbf{A}\mathbf{y}_m - \mathbf{y}_m^{(d)}\|, \quad (3.6)$$

357 where $\mathbf{y}_m = V_m f(H_m)\mathbf{e}_1$ is computed with an inexact Arnoldi procedure. Clearly, the
 358 matrices V_m, H_m differ as we allow ϵ_j to vary at each iteration j . Hence, we compared
 359 two different strategies for choosing ϵ_j :

- 360 (i) A fixed small tolerance $\epsilon_j \equiv \text{tol}/m$ for all j s, denoting the associated residual
 361 norm (3.6) by $\|\mathbf{r}_j\|$;
- 362 (ii) A variable accuracy $\epsilon_j := \bar{\epsilon}_j$ obtained from (3.5), denoting the associated residual
 363 norm in (3.6) by $\|\bar{\mathbf{r}}_j\|$.

364 We anticipate that our numerical experiments do not emphasize any visible degrada-
 365 tion in the differential residual norm, if we relax the accuracy in the construction of
 366 the Krylov space as it is done in (ii) above, and the two residual norms stagnate at the
 367 same level.

368 **Example 3.3** We consider the approximation of $\exp(-A)\mathbf{v}$ by the inexact Arnoldi
 369 procedure. The inexact matrix-vector product is implemented as in (3.2), with $\|\mathbf{w}_j\| =$
 370 ϵ_j . Figure 3 reports our results for $\mathbf{v} = (1, \dots, 1)^T/\sqrt{n}$ and the same matrices as in
 371 Example 3.1: $A = \text{Toeplitz}(-1, 1, 2, 0.1) \in \mathcal{B}_{200}(1, 2)$ (left), and `pd225` from
 372 the Matrix Market repository [32] (right). For this set of experiments, we considered
 373 $\text{tol} = 10^{-10}$ and $\epsilon^{(m)} = 10^{-1}$. The solid line shows the residual norm $\|\mathbf{r}_j\|$ as the
 374 iteration j proceeds for $\epsilon_j = \text{tol}/m$ (dashed line in the plot). The circles display the
 375 residual norm $\|\bar{\mathbf{r}}_j\|$ for the variable accuracy $\epsilon_j := \bar{\epsilon}_j$ (increasing asterisk curve in
 376 the plot) obtained from (3.5). The maximum number of iterations m was chosen as the
 377 smallest value for which the bound (3.1) is lower than tol , respectively $m = 20$ and
 378 $m = 31$. A larger, more conservative value could have been considered. The fields of
 379 values of the matrices can be obtained starting from those reported in the left plots
 380 of Fig. 2, where now the original semi-axes a, b of the elliptical sets considered for
 381 the computation of s_j are increased by $\epsilon^{(m)}/b$ and $\epsilon^{(m)}$ respectively. The plots show
 382 visually overlapping residual norm histories for the two choices of ϵ_j , illustrating that
 383 in practice no loss of information takes place when using the relaxation strategy.

384 Consider the second order differential equation $\mathbf{y}^{(2)} = \mathbf{A}\mathbf{y}$, with $\mathbf{y}(0) = \mathbf{v}$. Its
 385 solution can be expressed as $\mathbf{y}(t) = \exp(-t\sqrt{A})\mathbf{v}$, and our results can be applied.
 386 This time the upper bound s_j for $|\mathbf{e}_m^T f(H_m)\mathbf{e}_1|$ is obtained from Corollary 2.5.

387 **Example 3.4** For the same experimental setting as in Example 3.3, we consider approx-
 388 imating $\exp(-\sqrt{A})\mathbf{v}$, for the matrix $A = \text{Toeplitz}(-1, 1, 3, 0.1) \in \mathcal{B}_{200}(1, 2)$, the
 389 vector $\mathbf{v} = (1, \dots, 1)^T/\sqrt{200}$ and $m = 35$ iterations ($W(A)$ is given by translat-
 390 ing by 1 the field of values of the Toeplitz matrix in Example 3.1). Figure 4 reports

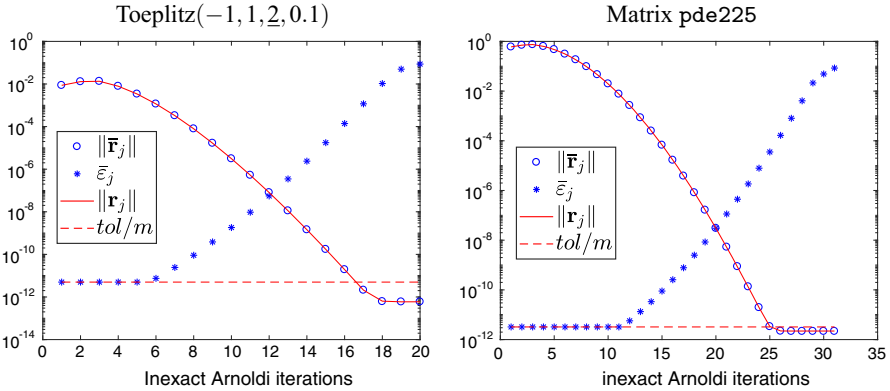


Fig. 3 Example 3.3, approximation of $e^{-A}\mathbf{v}$ with $\mathbf{v} = (1, \dots, 1)^T/\sqrt{n}$. Residual norm $\|\mathbf{r}_j\|$ with constant accuracy $\epsilon_j = \text{tol}/m$, and residual norm $\|\bar{\mathbf{r}}_j\|$ with $\epsilon_j = \bar{\epsilon}_j$ by (3.5) as the inexact Arnoldi method proceeds. Left: For $A = \text{Toeplitz}(-1, 1, \underline{2}, 0.1) \in \mathcal{B}_{200}(1, 2)$. Right: For matrix pde225 from the Matrix Market repository [32]

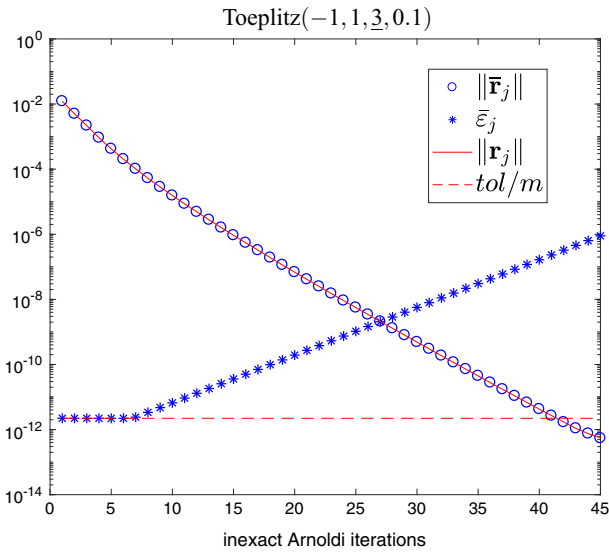


Fig. 4 Example 3.4. Approximation of $\exp(-\sqrt{A})\mathbf{v}$ with $A = \text{Toeplitz}(-1, 1, \underline{3}, 0.1) \in \mathcal{B}_{200}(1, 2)$ and $\mathbf{v} = (1, \dots, 1)^T/\sqrt{n}$. The residual norm $\|\mathbf{r}_j\|$ is obtained with constant accuracy $\epsilon_j = \text{tol}/m$; the residual norm $\|\bar{\mathbf{r}}_j\|$ is obtained with $\epsilon_j = \bar{\epsilon}_j$ given by (3.5).

391 on our findings, with the same description as for the previous example. Here s_j in
 392 (3.5) is obtained from Corollary 2.5, and it is used to relax the accuracy ϵ_j . Similar
 393 considerations apply.

394 **4 Conclusions**

395 We have considered the approximation of $f(A)\mathbf{v}$ by means of the inexact Arnoldi
 396 method, in which matrix-vector products with A cannot be computed exactly. We
 397 have first derived computable bounds for the off-diagonal decay pattern of functions
 398 of non-Hermitian banded matrices. The accuracy of the bounds depends on the quality
 399 of the set enclosing and approximating the field of values of A . Then we have used
 400 these estimates to devise a new relaxation strategy for inexact matrix-vector operations,
 401 that does not influence the convergence of the residual norm in the matrix function
 402 approximation, while decreasing the computational cost for the inexact matrix-vector
 403 product. Similar results can be obtained for other Krylov-type approximations whose
 404 projection and restriction matrix H_m has a semi-banded structure. This is the case for
 405 instance of the Extended Krylov subspace approximation; see, e.g., [30] and references
 406 therein.

407 **Acknowledgements** We are indebted with Leonid Knizhnerman for a careful reading of an earlier version
 408 of this manuscript, and for his many insightful remarks which led to great improvements of our results. We
 409 also thank Michele Benzi for several suggestions and the two referees whose remarks helped us improve
 410 the presentation.

411 **A Technical proofs**

412 **Proof of corollary 2.4**

413 Let $\rho = \sqrt{a^2 - b^2}$ be the distance between the foci and the center of the ellipse (i.e.,
 414 the boundary of E), and let $R = (a + b)/\rho$. Then a conformal map for E is

415
$$\phi(w) = \frac{w - c - \sqrt{(w - c)^2 - \rho^2}}{\rho R}, \tag{A.1}$$

416 and its inverse is

417
$$\psi(z) = \frac{\rho}{2} \left(Rz + \frac{1}{Rz} \right) + c; \tag{A.2}$$

418 see, e.g., [41, chapter II, Example 3]. Notice that

419
$$\max_{|z|=\tau} |e^{\psi(z)}| = \max_{|z|=\tau} e^{\Re(\psi(z))} = e^{\frac{\rho}{2} \left(R\tau + \frac{1}{R\tau} \right) + c_1}.$$

420 Hence by Theorem 2.3 we get

421
$$\left| \left(e^A \right)_{k,\ell} \right| \leq 2 \frac{\tau}{\tau - 1} e^{c_1} e^{\frac{\rho}{2} \left(R\tau + \frac{1}{R\tau} \right)} \left(\frac{1}{\tau} \right)^\xi.$$

422 The optimal value of $\tau > 1$ that minimizes $e^{\frac{\rho}{2}\left(R\tau + \frac{1}{R\tau}\right)} \left(\frac{1}{\tau}\right)^\xi$ is

$$423 \quad \tau = \frac{\xi + \sqrt{\xi^2 + \rho^2}}{\rho R}.$$

424 Moreover, the condition $\tau > 1$ is satisfied if and only if $\xi > \frac{\rho}{2}\left(R - \frac{1}{R}\right) = b$. Finally,
425 noticing that

$$426 \quad \psi\left(\frac{\xi + \sqrt{\xi^2 + \rho^2}}{\rho R}\right) - c_1 = \frac{1}{2}\left(\xi + \sqrt{\xi^2 + \rho^2} + \frac{\rho^2}{\xi + \sqrt{\xi^2 + \rho^2}}\right) = \xi q(\xi),$$

427 and collecting ξ the proof is completed. □

428 **Proof of corollary 2.5**

429 The function $f(z) = \exp(-\sqrt{z})$ is analytic on $\mathbb{C} \setminus (-\infty, 0)$. Since we consider the
430 principal square root, then $\Re(\sqrt{z}) \geq 0$, and

$$431 \quad |\exp(-\sqrt{z})| = \exp(-\Re(\sqrt{z})) \leq 1.$$

432 Hence, by Theorem 2.3 we can determine τ for which

$$433 \quad \left| \left(e^{-\sqrt{\lambda}} \right)_{k,\ell} \right| \leq 2 \frac{\tau}{\tau - 1} \left(\frac{1}{\tau} \right)^{\xi}.$$

434 For every $\varepsilon > 0$ close enough to zero, we set the parameter

$$435 \quad \tau_\varepsilon = |\phi(\varepsilon)| = \left| \frac{c - \varepsilon + \sqrt{(c - \varepsilon)^2 - \rho^2}}{\rho R} \right|,$$

436 with $\phi(w)$ as in (A.1) and $\psi(z)$ its inverse (A.2). Then the ellipse $\{\psi(z), |z| = \tau_\varepsilon\}$ is
437 contained in $\mathbb{C} \setminus (-\infty, 0]$. Letting $\varepsilon \rightarrow 0$ concludes the proof. □

438 **References**

- 439 1. Afanasjew, M., Eiermann, M., Ernst, O.G., Güttel, S.: Implementation of a restarted Krylov subspace
440 method for the evaluation of matrix functions. *Linear Algebra Appl.* **429**(10), 2293–2314 (2008).
441 <https://doi.org/10.1016/j.laa.2008.06.029>
- 442 2. Beckermann, B.: Image numérique, GMRES et polynômes de Faber. *C. R. Math. Acad. Sci. Paris*
443 **340**(11), 855–860 (2005)
- 444 3. Benzi, M., Boito, P.: Decay properties for functions of matrices over C^* -algebras. *Linear Algebra*
445 *Appl.* **456**, 174–198 (2014). <https://doi.org/10.1016/j.laa.2013.11.027>
- 446 4. Benzi, M., Boito, P., Razouk, N.: Decay properties of spectral projectors with applications to electronic
447 structure. *SIAM Rev.* **55**(1), 3–64 (2013). <https://doi.org/10.1137/100814019>

- 448 5. Benzi, M., Golub, G.H.: Bounds for the entries of matrix functions with applications to preconditioning.
449 BIT **39**(3), 417–438 (1999). <https://doi.org/10.1023/A:1022362401426>
- 450 6. Benzi, M., Razouk, N.: Decay bounds and $O(n)$ algorithms for approximating functions of sparse
451 matrices. Electron. Trans. Numer. Anal. **28**, 16–39 (2007)
- 452 7. Benzi, M., Simoncini, V.: Decay bounds for functions of Hermitian matrices with banded or Kronecker
453 structure. SIAM J. Matrix Anal. Appl. **36**(3), 1263–1282 (2015). <https://doi.org/10.1137/151006159>
- 454 8. Botchev, M.A., Grimm, V., Hochbruck, M.: Residual, restarting and Richardson iteration for the matrix
455 exponential. SIAM J. Sci. Comput. **35**(3), A1376–A1397 (2013)
- 456 9. Canuto, C., Simoncini, V., Verani, M.: On the decay of the inverse of matrices that are sum of Kronecker
457 products. Linear Algebra Appl. **452**, 21–39 (2014). <https://doi.org/10.1016/j.laa.2014.03.029>
- 458 10. Cowen, C.C., Harel, E.: An Effective Algorithm for Computing the Numerical Range (1995). [https://](https://www.math.iupui.edu/cowen/Downloads/33NumRange.html)
459 www.math.iupui.edu/cowen/Downloads/33NumRange.html
- 460 11. Del Buono, N., Lopez, L., Peluso, R.: Computation of the exponential of large sparse skew-symmetric
461 matrices. SIAM J. Sci. Comput. **27**(1), 278–293 (2005). <https://doi.org/10.1137/030600758>
- 462 12. Demko, S.G.: Inverses of band matrices and local convergence of spline projections. SIAM J. Numer.
463 Anal. **14**(4), 616–619 (1977). <https://doi.org/10.1137/0714041>
- 464 13. Demko, S.G., Moss, W.F., Smith, P.W.: Decay rates for inverses of band matrices. Math. Comp. **43**(168),
465 491–499 (1984). <https://doi.org/10.2307/2008290>
- 466 14. Dinh, K.N., Sidje, R.B.: Analysis of inexact Krylov subspace methods for approximating the matrix
467 exponential. Math. Comput. Simul. **138**, 1–13 (2017). <https://doi.org/10.1016/j.matcom.2017.01.002>.
468 <http://www.sciencedirect.com/science/article/pii/S0378475417300034>
- 469 15. Druskin, V., Knizhnerman, L.: Krylov subspace approximation of eigenpairs and matrix functions in
470 exact and computer arithmetic. Numer. Linear Algebra Appl. **2**(3), 205–217 (1995). [https://doi.org/](https://doi.org/10.1002/nla.1680020303)
471 [10.1002/nla.1680020303](https://doi.org/10.1002/nla.1680020303)
- 472 16. Eiermann, M.: Fields of values and iterative methods. Linear Algebra Appl. **180**, 167–197 (1993).
473 [https://doi.org/10.1016/0024-3795\(93\)90530-2](https://doi.org/10.1016/0024-3795(93)90530-2)
- 474 17. Eiermann, M., Ernst, O.G., Güttel, S.: Deflated restarting for matrix functions. SIAM J. Matrix Anal.
475 Appl. **32**(2), 621–641 (2011)
- 476 18. Eijkhout, V., Polman, B.: Decay rates of inverses of banded M-matrices that are near to Toeplitz
477 matrices. Linear Algebra Appl. **109**, 247–277 (1988). [https://doi.org/10.1016/0024-3795\(88\)90211-](https://doi.org/10.1016/0024-3795(88)90211-X)
478 [X](http://www.sciencedirect.com/science/article/pii/S0378475417300034). <http://www.sciencedirect.com/science/article/pii/S0378475417300034>
- 479 19. Ellacott, S.W.: Computation of Faber series with application to numerical polynomial approximation
480 in the complex plane. Math. Comp. **40**(162), 575–587 (1983)
- 481 20. Freund, R.: On polynomial approximations to $f_a(z) = (z-a)^{-1}$ with complex a and some applications
482 to certain non-hermitian matrices. Approx. Theory Appl. **5**, 15–31 (1989)
- 483 21. Frommer, A., Güttel, S., Schweitzer, M.: Convergence of restarted Krylov subspace methods for
484 Stieltjes functions of matrices. SIAM J. Matrix Anal. Appl. **35**(4), 1602–1624 (2014)
- 485 22. Frommer, A., Güttel, S., Schweitzer, M.: Efficient and stable Arnoldi restarts for matrix functions
486 based on quadrature. SIAM J. Matrix Anal. Appl. **35**(2), 661–683 (2014). [https://doi.org/10.1137/](https://doi.org/10.1137/13093491X)
487 [13093491X](https://doi.org/10.1137/13093491X)
- 488 23. Frommer, A., Schimmel, C., Schweitzer, M.: Bounds for the decay of the entries in inverses and
489 Cauchy-Stieltjes functions of certain sparse, normal matrices. Numer. Linear Algebra Appl. **25**(4),
490 e2131 (2018). <https://doi.org/10.1002/nla.2131>
- 491 24. Giraud, L., Langou, J., Rozložník, M., van den Eshof, J.: Rounding error analysis of the classical
492 Gram-Schmidt orthogonalization process. Numer. Math. **101**(1), 87–100 (2005)
- 493 25. Güttel, S.: Rational Krylov approximation of matrix functions: numerical methods and optimal pole
494 selection. GAMM-Mitt. **36**(1), 8–31 (2013). <https://doi.org/10.1002/gamm.201310002>
- 495 26. Güttel, S., Knizhnerman, L.: A black-box rational Arnoldi variant for Cauchy-Stieltjes matrix functions.
496 BIT **53**(3), 595–616 (2013). <https://doi.org/10.1007/s10543-013-0420-x>
- 497 27. Higham, N.J.: Functions of Matrices: Theory and Computation. Society for Industrial and Applied
498 Mathematics, Philadelphia (2008)
- 499 28. Hochbruck, M., Lubich, C.: On Krylov subspace approximations to the matrix exponential operator.
500 SIAM J. Numer. Anal. **34**, 1911–1925 (1997)
- 501 29. Iserles, A.: How large is the exponential of a banded matrix? New Zealand J. Math. **29**, 177–192 (2000)
- 502 30. Knizhnerman, L., Simoncini, V.: A new investigation of the extended Krylov subspace method for
503 matrix function evaluations. Numer. Linear Algebra Appl. **17**(4), 615–638 (2010). [https://doi.org/10.](https://doi.org/10.1002/nla.652)
504 [1002/nla.652](https://doi.org/10.1002/nla.652)

- 505 31. Kürschner, P., Freitag, M.A.: Inexact methods for the low rank solution to large scale Lyapunov
506 equations. arXiv preprint [arXiv:1809.06903](https://arxiv.org/abs/1809.06903) (2018)
- 507 32. Matrix Market: A Visual Repository of Test Data for Use in Comparative Studies of Algorithms for
508 Numerical Linear Algebra. Mathematical and Computational Sciences Division, National Institute of
509 Standards and Technology; available online at <http://math.nist.gov/MatrixMarket>
- 510 33. Mastronardi, N., Ng, M., Tyrtshnikov, E.E.: Decay in functions of multiband matrices. *SIAM J. Matrix*
511 *Anal. Appl.* **31**(5), 2721–2737 (2010). <https://doi.org/10.1137/090758374>
- 512 34. The MathWorks, Inc.: MATLAB 7, r2013b edn. (2013)
- 513 35. Meurant, G.: A review on the inverse of symmetric tridiagonal and block tridiagonal matrices. *SIAM*
514 *J. Matrix Anal. Appl.* **13**(3), 707–728 (1992). <https://doi.org/10.1137/0613045>
- 515 36. Pozza, S., Tudisco, F.: On the stability of network indices defined by means of matrix functions. *SIAM*
516 *J. Matrix Anal. Appl.* **39**(4), 1521–1546 (2018)
- 517 37. Rinehart, R.F.: The equivalence of definitions of a matrix function. *Amer. Math. Monthly* **62**(6), 395–
518 414 (1955)
- 519 38. Saad, Y.: Analysis of some Krylov subspace approximations to the matrix exponential operator. *SIAM*
520 *J. Numer. Anal.* **29**(1), 209–228 (1992). <https://doi.org/10.1137/0729014>
- 521 39. Simoncini, V.: Variable accuracy of matrix-vector products in projection methods for eigencomputation.
522 *SIAM J. Numer. Anal.* **43**(3), 1155–1174 (2005)
- 523 40. Simoncini, V., Szyld, D.B.: Theory of inexact Krylov subspace methods and applications to scientific
524 computing. *SIAM J. Sci. Comput.* **25**(2), 454–477 (2003)
- 525 41. Suetin, P.K.: Series of Faber polynomials. Gordon and Breach Science Publishers (1998). Translated
526 from the 1984 Russian original by E. V. Pankratiev [E. V. Pankrat'ev]
- 527 42. Wang, H.: The Krylov Subspace Methods for the Computation of Matrix Exponentials. Ph.D. thesis,
528 Department of Mathematics, University of Kentucky (2015)
- 529 43. Wang, H., Ye, Q.: Error bounds for the Krylov subspace methods for computations of matrix expo-
530 nentials. *SIAM J. Matrix Anal. Appl.* **38**(1), 155–187 (2017). <https://doi.org/10.1137/16M1063733>
- 531 44. Ye, Q.: Error bounds for the Lanczos methods for approximating matrix exponentials. *SIAM J. Numer.*
532 *Anal.* **51**(1), 68–87 (2013). <https://doi.org/10.1137/11085935x>