Automated parameter selection for rational Arnoldi approximation of Markov functions

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Rational Arnoldi is a powerful method for approximating functions of large sparse matrices times a vector. The selection of asymptotically optimal parameters for this method is crucial for its fast convergence. We present a heuristic for the automated pole selection when the function to be approximated is of Markov type, such as the matrix square root. The performance of this approach is demonstrated at several numerical examples.

1 Introduction

We are interested in the efficient approximation of a matrix function $f(A)\boldsymbol{v}$, where $A \in \mathbb{C}^{N\times N}$, $\boldsymbol{v} \in \mathbb{C}^N \setminus \{\boldsymbol{0}\}$, and the function is of Markov (or Cauchy–Stieltjes) type

$$f(z) = \int_\Gamma \frac{\mathrm{d}\gamma(x)}{z-x} \tag{1}$$

with some (complex) measure γ supported on a closed set $\Gamma \in \mathbb{C}$. A particularly important example of such a function is

$$f(z) = z^{-1/2} = \int_{-\infty}^{0} \frac{1}{z-x}\,\frac{\mathrm{d}x}{\pi\sqrt{-x}}.$$

The problem of approximating $f(A)\boldsymbol{v}$ is of considerable interest in many areas of scientific computing. For instance, some interesting solutions of the equation

$$A\boldsymbol{u}(t) - \frac{\mathrm{d}^2\boldsymbol{u}}{\mathrm{d}t^2}(t) = g(t)\boldsymbol{v}$$

can be represented as $\boldsymbol{u}(t) = f(A)\boldsymbol{v}$, $f(z)$ being a rational function of $\sqrt{z}$ and $e^{-t\sqrt{z}}$ (cf. [4, 6]). Other examples are the computation of Neumann-to-Dirichlet and Dirichlet-to-Neumann maps [1, 5].

In most applications, A is very large and sparse (e.g., as a finite-element discretization of a differential operator) so that explicitly computing and storing the dense matrix $f(A)$ is infeasible. A popular method that circumvents this problem is known as *rational Arnoldi*. It is based on the extraction of an approximation $\boldsymbol{f}_n$ from a rational Krylov space [12, 13]

$$\begin{aligned} \mathcal{Q}_n(A,\boldsymbol{v}) &:= \operatorname{span}\left\{ \frac{p_{n-1}}{q_{n-1}}(A)\boldsymbol{v} \;:\; p_{n-1} \text{ polynomial of degree} \le n-1 \right\}, \\ q_{n-1}(z) &:= \prod_{\substack{j=1\\ \xi_j\neq\infty}}^{n-1} (z-\xi_j), \end{aligned} \tag{2}$$

where the parameters $\xi_j \in \overline{\mathbb{C}}$ are different from the eigenvalues $\Lambda(A)$. Note that fractions in (2) run over the linear space of rational functions of type $(n-1, n-1)$ with a prescribed denominator q_{n-1}, and that $\mathcal{Q}_n(A,\boldsymbol{v})$ reduces to a polynomial Krylov space if we set all poles $\xi_j = \infty$. If the dimension of $\mathcal{Q}_n(A,\boldsymbol{v})$ is n, as we assume in the following, we can compute an orthonormal basis $V_n = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n]$. The rational Arnoldi approximation is then defined as

$$\boldsymbol{f}_n := V_n f(A_n) V_n^H \boldsymbol{v}, \quad A_n := V_n^H A V_n. \tag{3}$$

If n is relatively small, then $f(A_n)$ can be evaluated using algorithms for dense matrix functions (see [10]). It is well known that $\boldsymbol{f}_n$ is a near-optimal approximation for $f(A)\boldsymbol{v}$ from $\mathcal{Q}_n(A,\boldsymbol{v})$ (see, e.g., [3,4,9]), that is, $\boldsymbol{f}_n$ is very close to the orthogonal projection $V_n V_n^H f(A)\boldsymbol{v}$. Therefore the poles ξ_j need to be chosen such that $\mathcal{Q}_n(A,\boldsymbol{v})$ contains a good approximation for

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$f(A)\boldsymbol{v}$, and of course, such a choice depends both on the spectral properties of A and the function $f(z)$. This necessity for choosing optimal parameters is a serious problem that prevents rational Arnoldi from being used in practice more widely. Recently, interesting strategies for the adaptive selection of the poles ξ_j have been proposed for the exponential function [7] and the transfer function [8]. We shall build on these ideas for proposing an adaptive pole selection strategies for functions of type (1).

This paper is structured as follows: In Section 2 we review the rational Arnoldi method and some of its important properties. In Section 3 we present our adaptive version of rational Arnoldi for functions of type (1). Finally, in Section 4, we demonstrate the performance of our parameter-free (free of mathematically essential parameters) algorithm at some numerical examples. Throughout $\|\cdot\|$ denotes the Euclidian norm and I is the identity matrix of size $N \times N$. Vectors are printed in bold face.

2 Rational Arnoldi method

A stable iterative procedure for computing an orthonormal basis $V_n = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n]$ of the rational Krylov space $\mathcal{Q}_n(A, \boldsymbol{v})$ with poles ξ_j is the rational Arnoldi algorithm by A. Ruhe [13]. Let σ be a finite number different from all ξ_j, and define $\widetilde{A} := A - \sigma I$ and $\tilde{\xi}_j := \xi_j - \sigma$. Note that the rational Krylov space $\widetilde{\mathcal{Q}}_n(\widetilde{A}, \boldsymbol{v})$ build with the poles $\tilde{\xi}_j$ coincides with $\mathcal{Q}_n(A, \boldsymbol{v})$. We may therefore as well construct an orthonormal basis for $\widetilde{\mathcal{Q}}_n(\widetilde{A}, \boldsymbol{v})$ in the following.

Starting with $\boldsymbol{v}_1 = \boldsymbol{v}/\|\boldsymbol{v}\|$, in each iteration $j = 1, \ldots, n$ one utilizes a modified Gram–Schmidt procedure to orthogonalize

$$\boldsymbol{w}_{j+1} = \big(I - \widetilde{A}/\tilde{\xi}_j\big)^{-1} \widetilde{A}\boldsymbol{v}_j \tag{4}$$

against $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_j\}$ as to obtain the vector $\boldsymbol{v}_{j+1}$, $\|\boldsymbol{v}_{j+1}\| = 1$, satisfying the relation

$$\boldsymbol{v}_{j+1} h_{j+1,j} = \boldsymbol{w}_{j+1} - \sum_{i=1}^{j} \boldsymbol{v}_i h_{i,j}, \quad h_{i,j} = \boldsymbol{v}_i^H \boldsymbol{w}_{j+1}. \tag{5}$$

Equating (4) and (5), and collecting the Fourier coefficients in $H_n = [h_{i,j}] \in \mathbb{C}^{n\times n}$, we obtain in the n-th iteration of the rational Arnoldi algorithm a decomposition

$$\widetilde{A}V_n\big(I_n + H_n \mathrm{diag}(\tilde{\xi}_1^{-1}, \ldots, \tilde{\xi}_n^{-1})\big) + \boldsymbol{v}_{n+1} h_{n+1,n} \tilde{\xi}_n^{-1} \boldsymbol{e}_n^T = V_n H_n + \boldsymbol{v}_{n+1} h_{n+1,n} \boldsymbol{e}_n^T, \tag{6}$$

where I_n denotes the $n \times n$ identity matrix and $\boldsymbol{e}_n$ its last column. Note that the second summand on the left-hand side of (6) vanishes when setting $\tilde{\xi}_n = \infty$ (i.e., $\xi_n = \infty$, which corresponds to a polynomial Krylov step, cf. [3, 9]). In this case we find that the matrix A_n required for computing the rational Arnoldi approximation (3) can be calculated from (6) without explicit projection as

$$\begin{aligned} A_n &= V_n^H A V_n = V_n^H \widetilde{A} V_n + \sigma I_n \\ &= H_n\big(I_n + H_n \mathrm{diag}(\tilde{\xi}_1^{-1}, \ldots, \tilde{\xi}_n^{-1})\big)^{-1} + \sigma I_n. \end{aligned} \tag{7}$$

Remark 2.1 In exact arithmetic the rational Arnoldi approximation (3) is independent of the choice of σ. However, for numerical stability of the rational Arnoldi algorithm, σ should have a large enough distance to the poles ξ_j, because otherwise the pole and the zero in the fraction of (4) may "almost cancel out", causing accuracy loss in the rational Krylov basis [11].

We now list some well-known properties of the rational Arnoldi approximation (3) which are relevant for our further ongoing. The interested reader may be referred to [3, 9] for more details.

1. By the definition of $\mathcal{Q}_n(A, \boldsymbol{v})$ there exists a rational function $r_n(z)$ of type $(n-1, n-1)$ such that

   $$\boldsymbol{f}_n = r_n(A)\boldsymbol{v} = \frac{p_{n-1}}{q_{n-1}}(A)\boldsymbol{v}.$$

2. This function $r_n(z)$ is actually a rational interpolant for $f(z)$ with prescribed denominator and interpolation nodes $\Lambda(A_n) = \{\theta_1, \ldots, \theta_n\}$, the so-called rational Ritz values. Defining the *rational nodal function* of type $(n, n-1)$,

   $$s_n(z) := \frac{\prod_{k=1}^{n}(z - \theta_k)}{q_{n-1}(z)}, \tag{8}$$

   by the Hermite–Walsh formula for rational interpolants (see, e.g., [14, Theorem VIII.2] or [2]) we have

   $$\|f(A)\boldsymbol{v} - r_n(A)\boldsymbol{v}\| \le \|s_n(A)\boldsymbol{v}\| \cdot \left\| \int_\Gamma \frac{(xI - A)^{-1}}{s_n(x)} \, \mathrm{d}\gamma(x) \right\|. \tag{9}$$

3. The term $\|s_n(A)\boldsymbol{v}\|$ is minimal among all rational functions of the form $\tilde{s}_n(z) = (z^n + \alpha_{n-1}z^{n-1} + \cdots + \alpha_0)/q_{n-1}(z)$ (see, e.g., [9, Lemma 4.5]).

3 Adaptive pole selection

Note that the rational nodal function $s_n(z)$ of (8) is explicitly known in the n-th iteration of the rational Arnoldi method: It has poles $\xi_1, \ldots, \xi_{n-1}$ and its zeros are the rational Ritz values $\Lambda(A_n)$. The aim of an adaptive pole selection strategy is, of course, to make (a bound for) the approximation error (9) smallest possible in every iteration of the rational Arnoldi method. In view of (9) we will therefore try to make $|s_n(x)|$ uniformly large on Γ by choosing the next pole ξ_n as

$$|s_n(\xi_n)| = \min_{x\in\Gamma} |s_n(x)|.$$

This choice is a straightforward adaption of a pole selection heuristic proposed in [7, 8], where the nodal function has to be large on a negative real interval Γ and small on $-\Gamma$. In our case we do not have such a symmetry, but still we hope that our nodal rational function s_n is large on Γ and small on some "relevant subset" of the numerical range of A (recall from above that $\|s_n(A)\boldsymbol{v}\|$ is minimal!). In Algorithm 1 we summarize our rational Arnoldi method with adaptive pole selection.

Algorithm 1. Rational Arnoldi method for $f(A)\boldsymbol{v}$ with adaptive poles.

Input: Function $f(z)$ of type (1), matrix $A \in \mathbb{C}^{N\times N}$, vector $\boldsymbol{v} \in \mathbb{C}^N \setminus \{\boldsymbol{0}\}$.

Output: Rational Arnoldi approximations $\boldsymbol{f}_j$ and pole sequence $\xi_1, \xi_2, \ldots$

1. Set $\boldsymbol{v}_1 := \boldsymbol{v}/\|\boldsymbol{v}\|$.
2. For $j = 1, \ldots, n$
3. Temporarily set $\xi_j = \infty$, perform polynomial Krylov step for $\boldsymbol{w}_{j+1}$ and orthogonalize (eqns. (4) and (5)).
4. Compute projection $A_j = V_j^H A V_j$ using eqn. (7).
5. If required, compute j-th order Arnoldi approximation $\boldsymbol{f}_j = V_j f(A_j) V_j^H \boldsymbol{v}$.
6. Compute $\Lambda(A_j) = \{\theta_1, \ldots, \theta_j\}$ and find minimum $\xi_j \in \Gamma$ of $|s_j(z)| = \left|\prod_{k=1}^{j}(z-\theta_k)\Big/ q_{j-1}(z)\right|$.
7. Perform rational Krylov step for $\boldsymbol{w}_{j+1}$ and orthonormalize for $\boldsymbol{v}_{j+1}$ (eqns. (4) and (5)).

In a practical implementation of Algorithm 1 one would use an a-posteriori error estimator in Step 5 to stop the iteration if $\|f(A)\boldsymbol{v} - \boldsymbol{f}_j\|$ is below some tolerance. Note that, in contrast to the algorithms presented in [7, 8], we do not require any estimation for the spectral interval of A; in fact, we will demonstrate in the following section that our algorithm performs well also for highly nonsymmetric and nonnormal matrices. A detailed analysis of this algorithm will be subject of future work.

4 Numerical experiments

To test the performance of our method, we first consider the computation of $A^{-1/2}\boldsymbol{v}$ with $\boldsymbol{v} = [1, \ldots, 1]^T$ and the matrices

$$A_1 = \mathrm{diag}(1, 1.01, \ldots, 1000) \quad \text{and} \quad A_2 = \mathrm{diag}(1, 1.01, \ldots, 1.1, 500, 500.01, \ldots, 1000).$$

Note that both matrices have the same spectral interval, but A_2 has a large gap in its spectrum. For Hermitian A we have

$$\|f(A)\boldsymbol{v} - \boldsymbol{f}_n\| \le \|\boldsymbol{v}\| \max_{z\in\Lambda(A)} |f(z) - r_n(z)| \le \|\boldsymbol{v}\| \max_{z\in[\lambda_{\min},\lambda_{\max}]} |f(z) - r_n(z)|.$$

It is well-known that, knowing $[\lambda_{\min}, \lambda_{\max}]$, one can explicitly construct a sequence of rational interpolants $\{r_n\}$ for $f(z)$ which reduces the uniform approximation error for $f(z)$ on $[\lambda_{\min}, \lambda_{\max}]$ linearly with an optimal rate given by capacity of the underlying condenser $\mathrm{cap}([\lambda_{\min}, \lambda_{\max}], \Gamma)$, in our case with $\Gamma = (-\infty, 0]$. Using the near-optimality property of rational Arnoldi it was shown in [3] that there exists a pole sequence $\xi_1, \xi_2, \ldots$ and a constant $C > 0$ independent of n such that the error reduction is at least linear

$$\|f(A)\boldsymbol{v} - \boldsymbol{f}_n\| \le C \cdot \mathrm{cap}([\lambda_{\min}, \lambda_{\max}], \Gamma)^{-n} \lesssim C \cdot \exp(\pi^2/\log(16\lambda_{\max}/\lambda_{\min}))^{-n}. \tag{10}$$

In Figure 1 (left) we show the convergence of Algorithm 1 for the two matrices A_1, A_2 and also the convergence rate (10) with $\lambda_{\min} = 1$ and $\lambda_{\min} = 500$ respectively. Notice that, although $\lambda_{\min}(A_2) = 1$, the method converges as if $\lambda_{\min} = 500$ because the few smallest eigenvalues are "deflated" in early iterations of the method.

We now consider 1000×1000 matrices A_3 and A_4 being the finite-difference discretization of the 1D- and 3D-Laplacian with homogeneous Dirichlet boundary, respectively, and random $\boldsymbol{v} \in \mathbb{R}^{1000}$. In Figure 1 (right) we show the convergence of Algorithm 1. Note that the convergence seems slightly faster than the linear rate of (10), particularly in later iterations, as superlinear convergence effects take place due to spectral adaption of the rational Arnoldi method [2].

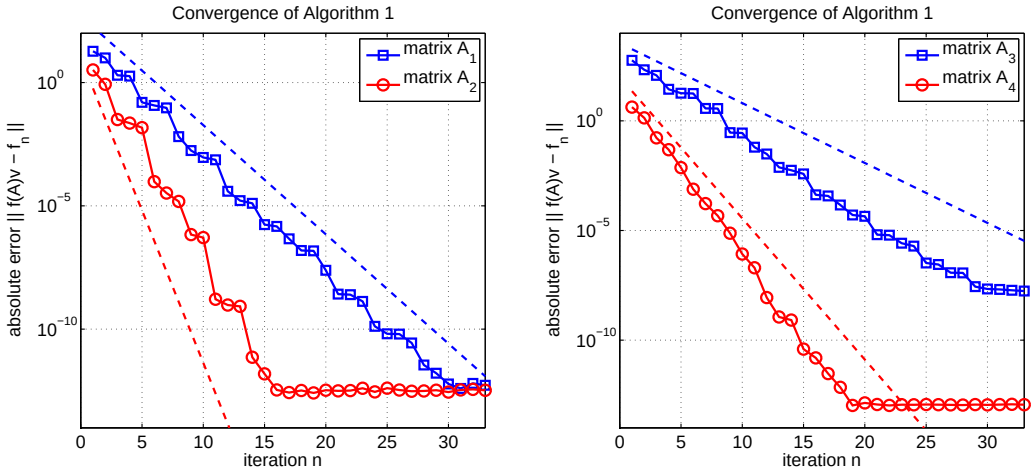

Fig. 1 Convergence of rational Arnoldi for $f(A)\boldsymbol{v} = A^{-1/2}\boldsymbol{v}$, for various symmetric matrices $A_1, \ldots, A_4$ (described in the text), where the poles are chosen adaptively on $\Gamma = (-\infty, 0]$. The dashed lines indicate the linear convergence rate of (10).

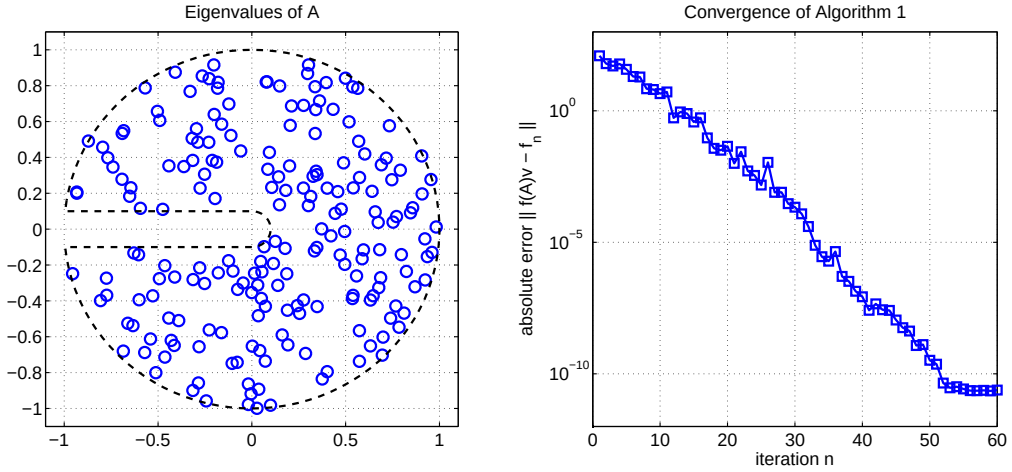

Fig. 2 Left: Eigenvalues of a highly nonnormal random matrix $A \in \mathbb{C}^{200\times 200}$. Right: Convergence of rational Arnoldi for $f(A)\boldsymbol{v} = A^{-1/2}\boldsymbol{v}$, random vector $\boldsymbol{v}$, with adaptive poles on $\Gamma = (-\infty, 0]$.

The last example is more challenging: Consider a random diagonalizable matrix $A \in \mathbb{C}^{200\times 200}$ having eigenvalues in the unit disk under the constraint that the distance of each eigenvalue to Γ is at least 0.1. The eigenvalues of this matrix are shown in Figure 2 (left). We remark that A is highly nonnormal: Although the moduli of its eigenvalues are nicely bounded above and below, it has a condition number of $\approx 2.5 \times 10^4$. To our best knowledge, no existing convergence theory is able to explain why Algorithm 1 converges so robustly even for this matrix (see Figure 2, right). Note that the usual arguments involving the numerical range of A fail here, as this set is not even disjoint from Γ.

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