Superlinear convergence of the rational Arnoldi method for the approximation of matrix functions $f(A)b$

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Introduction

- **Given:** Large sparse matrix $A \in \mathbb{C}^{N\times N}$, vector $b \in \mathbb{C}^N$, function $f(z)$ analytic on the eigenvalues $\Lambda(A)$.
- **Task:** Compute $f(A)b$ without forming $f(A)$ explicitly.
- **Applications:**
  - $A^{-1}b$ is the solution of $Ax = b$,
  - $\exp(tA)b$ is the solution of $u'(t) = Au(t)$, $u(0) = b$,
  - $\cosh(t\sqrt{A})b$ solves $u''(t) = Au(t)$, $u(0) = b$, $u'(0) = 0$,
  - $\exp(t\sqrt{A})b$, $\mathrm{sgn}(A)b$, $\log(A)b$ (see also [9]),
  - $A^{-1/2}b$ for Neumann-to-Dirichlet maps.

The rational Arnoldi method [7, 10]

- **Principle:** Implicitly compute a low-order rational function $r_n(A)b \approx f(A)b$ with prescribed poles $\xi_1, \dots, \xi_{n-1} \in \mathbb{C}$.
- **Implementation:** Use Ruhe's rational Arnoldi process [10]:

  Set $v_1 := b/\|b\|$.

  For $j = 1, \dots, n$

  Compute $x_j := (A - \xi_j I)^{-1} v_j$.

  Orthogonalize $w_j := x_j - V_j V_j^H x_j$.

  Set $v_{j+1} := w_j/\|w_j\|$.
- **Output:** Rational Krylov basis $V_{n+1} = [v_1, \dots, v_{n+1}]$, $V_{n+1}^H V_{n+1} = I_{n+1}$, and rational Arnoldi decomposition

$$AV_{n+1}\underline{K_n} = V_{n+1}\underline{H_n}, \quad \text{with} \quad \{\underline{K_n}, \underline{H_n}\} \subset \mathbb{C}^{(n+1)\times n}.$$

- **Rational Arnoldi approximation of order n is**

$$f_n := V_n f(A_n) V_n^H b, \quad A_n := V_n^H A V_n.$$

  (Note that $f(A_n)$ is a function of a small $n \times n$ matrix.)
- **Special or limiting cases** (need to solve shifted systems)
  - polynomial Arnoldi: $\xi_1 = \xi_2 = \xi_3 = \dots = \infty$
  - shifted and inverted Arnoldi: $\xi_1 = \xi_2 = \xi_3 = \dots$
  - extended Krylov (EK): $\xi_1 = \xi_3 = \dots = 0$, $\xi_2 = \xi_4 = \dots = \infty$...

Our problem

How large is the error $\|f(A)b - f_n\|$?

- we want a priori estimates;
- a priori versus adaptive choice of poles $\xi_1, \xi_2, \dots$?
- linear versus superlinear convergence behavior?
- error should depend on f **and** A;
- in general no "residual" available.

Set $\mathcal{P}_n(\xi_1, .., \xi_{n-1})$ the set of rational functions with numerator of degree $\leq n$ and prescribed poles $\xi_1, .., \xi_{n-1}$.

Near best numerator [3]

We have exactness $f_n = f(A)b$ for all $f \in \mathcal{P}_{n-1}(\xi_1, .., \xi_{n-1})$. Thus for all $r \in \mathcal{P}_{n-1}(\xi_1, .., \xi_{n-1})$

$$(*) \quad \|f(A)b - f_n\| \leq \Big(\|(f-r)(A)\| + \|(f-r)(A_n)\|\Big)\|b\|.$$

Using the Crouzeix bound [4], we get upper bounds in terms of the best uniform approximation of f on the field of values $W(A) \supseteq W(A_n) \not\ni \xi_j$ by $\mathcal{P}_{n-1}(\xi_1, .., \xi_{n-1})$.

Expected convergence rate for Γ set of singularities of f:

- $f(z) = \exp(z)$ **entire** ($\Gamma = \{\}$): superlinear
- $f(z) = \tanh(z)$ **meromorphic** (Γ countable): superlinear
- $f(z) = \log(z)$, $f(z) = \sqrt{z}$ ($\Gamma = (-\infty, 0]$): linear.

Approach through interpolation in Ritz values [1]

There exists $r_n \in \mathcal{P}_{n-1}(\xi_1, .., \xi_{n-1})$ such that $f_n = r_n(A)b$.

- This function $r_n(z)$ is a rational interpolant for $f(z)$ with nodes $\Lambda(A_n) = \{\theta_1, \dots, \theta_n\}$, called *rational Ritz values*.
- Define the nodal function

$$s_n(z) := \frac{(z-\theta_1)\cdots(z-\theta_n)}{(z-\xi_1)\cdots(z-\xi_{n-1})}.$$

  Rational Ritz values $\{\theta_j\}$ are optimal in the sense that $\|s_n(A)b\|$ is minimal among all nodal functions.
- Interpolation error

$$\|f(A)b - f_n\| \approx \max_{x\in\Gamma} \frac{1}{|s_n(x)|} \|s_n(A)b\|,$$

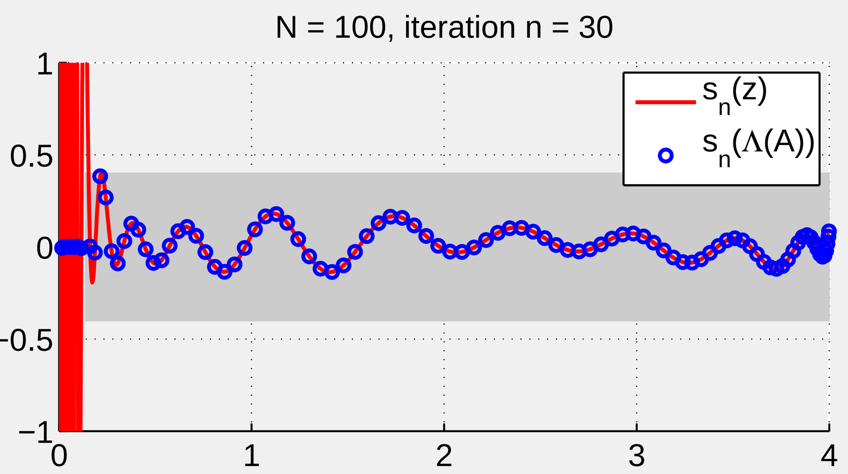
  can be derived more rigorously for Markov functions $f(z) = \int_\Gamma \frac{d\gamma(x)}{x-z}$, here $f(z) - r_n(z) = \int_\Gamma \frac{s_n(z)}{s_n(x)}\frac{d\gamma(x)}{x-z}$.

Spectral adaptivity

- Need to understand the (superlinear) decay of $\|s_n(A)b\|$.
- So far only possible for Hermitian A, in which case

$$\|s_n(A)b\| \leq \|b\| \max_{z\in\Lambda(A)} |s_n(z)|.$$

- Typical linear error bounds obtained by assuming that $s_n(z)$ is uniformly small on spectral interval $W(A) = [\lambda_{\min}, \lambda_{\max}]$.
- **This assumption ignores the fine structure of $\Lambda(A)$!**
- **Example:** $A = \mathrm{tridiag}(-1, 2, -1)$, extended Krylov.



Asymptotic distribution of Ritz values, $A = A^H$ [2]

Optimality and interlacing property of rational Ritz values allow for asymptotic description of their distribution:

- Let $\Lambda(A)$ be described by a probability measure σ, e.g.,

$$\frac{d\sigma}{dx} = \frac{1}{\pi\sqrt{x(4-x)}}, \quad x \in (0, 4).$$

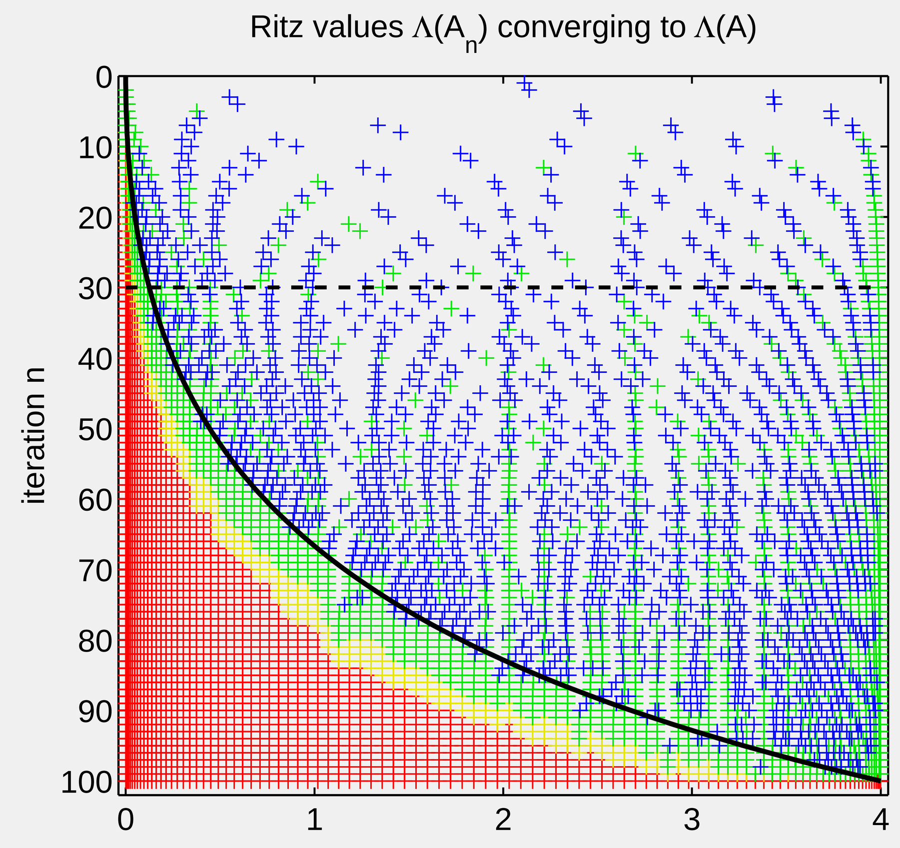
- Let the poles $\xi_1, \dots, \xi_n$ be described by a measure ν_t, $\|\nu_t\| = t = n/N$, e.g., extended Krylov

$$\nu_t = t \cdot (\delta_0 + \delta_\infty)/2.$$

- Then the distribution of Ritz values $\Lambda(A_n)$ is given as the constrained equilibrium measure $\mu_t \leq \sigma$, $\|\mu_t\| = t$, which minimizes the energy $\mu \mapsto I(\mu, \mu) - 2I(\nu_t, \mu)$,

$$I(\mu_1, \mu_2) := \iint \log \frac{1}{|x-y|} d\mu_1(x)\, d\mu_2(y).$$

  Moreover, $S(t) := \mathrm{supp}(\sigma - \mu_t) \subseteq [\lambda_{\min}, \lambda_{\max}]$.



(rigorously: weak$*$ limit of counting measures for sequences of matrices)

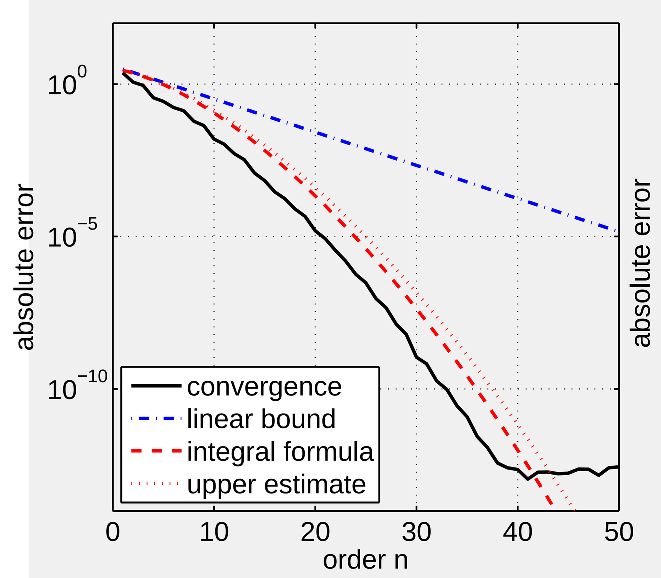
Buyarov-Rakhmanov formula [1]

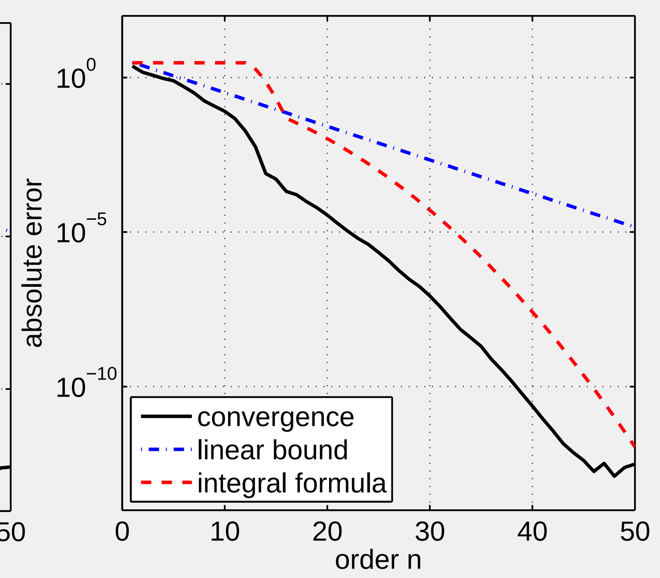
$$\|f(A)b - f_n\| \lessapprox \max_{z\in\Gamma} \exp\left(-N \int_0^t \frac{g_{S(\tau)}(z, 0) + g_{S(\tau)}(z, \infty)}{2} d\tau\right)$$

(rigorously: $\leq$ after taking Nth roots, lim sup for $n, N \to \infty, n/N \to t$)

- linear if $S(\tau) = S(0)$, superlinear if $S(\tau)$ strictly decreasing.
- similar formulas for other cyclic sequences of poles (here EK).

Typical examples: $A = \mathrm{tridiag}(-1, 2, -1)$, $f(z) = 1/\sqrt{z}$



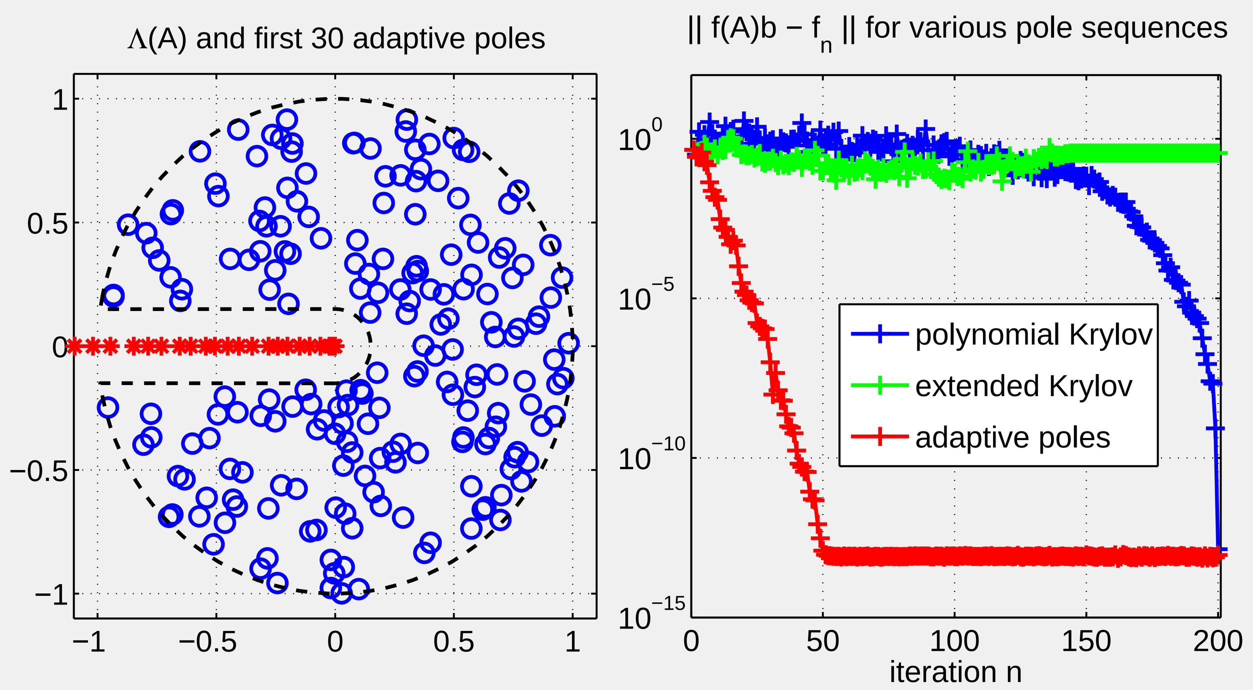


Adaptive (greedy) poles for Markov functions [5, 6, 8]

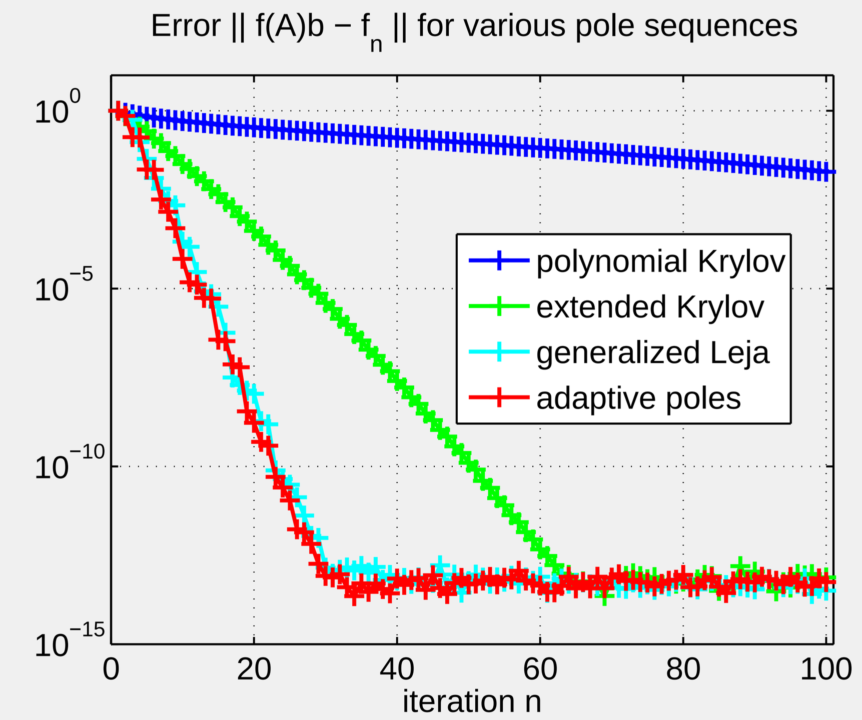
- Rational function $s_n(z)$ is explicitly known at iteration n (zeros $\{\theta_j\}$, poles $\{\xi_j\}$), can select the next pole ξ_n as

$$\xi_n = \arg\max_{x\in\Gamma} \left|\frac{1}{s_n(x)}\right|.$$

- **Feature:** So far no assumptions on the matrix A!
- **Example 1:** Compute $\log(A)b$ for highly nonnormal A.



- **Example 2:** Compute $A^{-1/2}b$ for 2D-Laplacian, $N = 10^4$.



Conjecture for adaptive (greedy) poles [1, 8]

Converged nth Ritz values are not seen by the "next" poles $\xi_n, \xi_{n+1}, \dots$, which are optimal for $(\Gamma, S(t))$! That is,

$$\mu_t = \int_0^t \widetilde{\mu}_\tau\, d\tau, \quad \nu_t = \int_0^t \widetilde{\nu}_\tau\, d\tau,$$

with probability measures $\widetilde{\mu}_\tau, \widetilde{\nu}_\tau$ equilibrium unit charges on condenser $(\Gamma, S(\tau))$.

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