Rational Krylov methods for the approximation of matrix functions

Bernhard Beckermann, Michael Eiermann, Oliver G. Ernst,
Stefan Güttel and Raf Vandebril

Praha–Freiberg Joint Seminar III
15 May 2009

Outline

Motivation

We consider the initial-boundary value problem

$$\begin{aligned} \partial_t u - \Delta u &= 0 && \text{in } \Omega = (0,1)^3, \quad t > 0, \\ u(x,t) &= 0 && \text{on } \Gamma = \partial\Omega, \quad t > 0, \\ u(x,0) &= u_0(x) && \text{in } \Omega. \end{aligned}$$

Seven-point stencil on a uniform grid involving n interior grid points in each Cartesian direction yields IVP

$$\begin{aligned} \boldsymbol{u}'(t) &= A\boldsymbol{u}(t), \quad t > 0, \\ \boldsymbol{u}(0) &= \boldsymbol{u}_0, \end{aligned}$$

with $N \times N$ matrix A ($N = n^3$) and an initial vector $\boldsymbol{u}_0$ consisting of the values $u_0(x)$ at the grid points x, the solution of which is given by

$$\boldsymbol{u}(t) = f_t(A)\boldsymbol{u}_0, \quad f_t(z) = \exp(t\,z).$$

Approximation methods for $f(A)\boldsymbol{b}$ can be characterized by

- the m-dimensional approximation space $\mathscr{V}_m$,
- the extraction method (here: Rayleigh-Ritz, shift-invert).

Define Krylov space of order m

$$\mathscr{K}_m(A,\boldsymbol{b}) = \mathsf{span}\{\boldsymbol{b}, A\boldsymbol{b}, \ldots, A^{m-1}\boldsymbol{b}\}.$$

- There exists an invariance index L such that $\mathscr{K}_{L-1} \subset \mathscr{K}_L = \mathscr{K}_{L+1}$.
- $\mathscr{K}_m \cong \mathscr{P}_{m-1}$ for $m \leq L$.
- The exact solution $f(A)\boldsymbol{b}$ is contained in $\mathscr{K}_L$.

Polynomial vs. rational Krylov

Method 1 (Lanczos)

Space: Approximate $f(A)\boldsymbol{b}$ in $\mathscr{V}_m = \mathscr{K}_m(A, \boldsymbol{b})$.

Extraction: Compute ONB V_m of $\mathscr{V}_m$ and set

$$\boldsymbol{f}_m = V_m f(V_m^* A V_m) V_m^* \boldsymbol{b}.$$

We refer to this as *Rayleigh-Ritz extraction*.

Note: $V_m^* A V_m$ is a *Rayleigh-quotient* of A.

Method 2 (shift-invert Lanczos)

Space: Approximate $f(A)\boldsymbol{b}$ in $\mathscr{V}_m = \mathscr{K}_m((A-\xi I)^{-1}, \boldsymbol{b})$.

Extraction: Compute ONB V_m of $\mathscr{V}_m$ satisfying

$$(A-\xi I)^{-1} V_m = V_m T_m + \boldsymbol{v}_{m+1} t_{m+1,m} \boldsymbol{e}_m^T,$$

and back-transform T_m:

$$\boldsymbol{f}_m = V_m f([T_m^{-1} + \xi I]) V_m^* \boldsymbol{b}.$$

[Moret & Novati, 2004], [van den Eshof & Hochbruck, 2005]

Note: The Rayleigh-quotient of A would be

$$V_m^* A V_m = [T_m^{-1} + \xi I] - V_m^* A \boldsymbol{v}_{m+1} t_{m+1,m} \boldsymbol{e}_m^T T_m^{-1}.$$

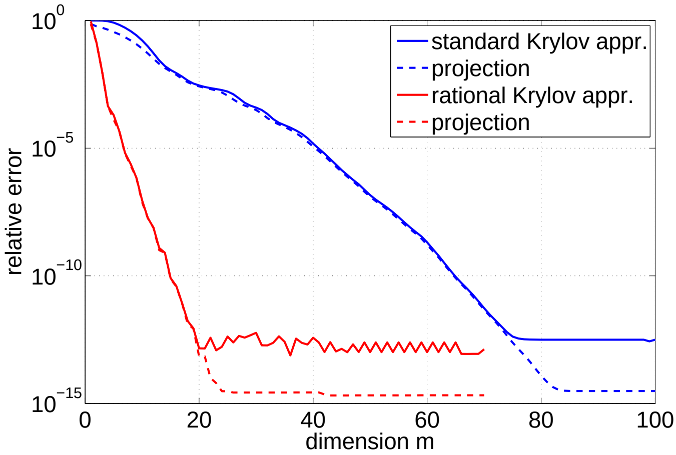


Figure: Heat equation $N = 15^3 = 3,375,\ t = 0.1,\ \xi = 1.$

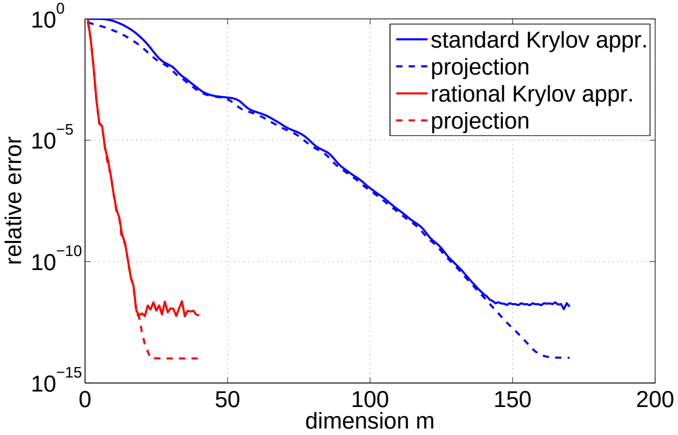


Figure: Heat equation $N = 31^3 = 29,791$, $t = 0.1$, $\xi = 1$.

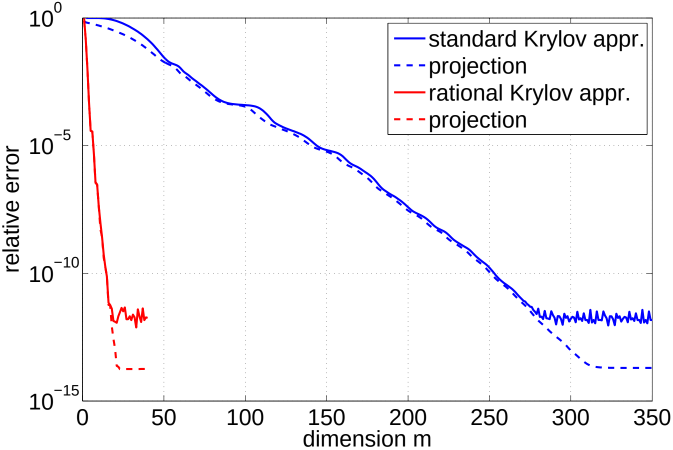


Figure: Heat equation $N = 63^3 = 250,047$, $t = 0.1$, $\xi = 1$.

Operation count

Recall: $N = n^3$

	Lanczos	**SI-Lanczos**
Iterations	$m \sim \sqrt{\|tA\|} = O(n)$ *	$m = \text{const.}$
Operator/It.	$O(N)$	$O(N)$ **
Orthogonalize/It.	$O(N)$	$O(N)$
Total	$O(nN)$	$O(N)$

Additionally, one evaluation of $f(T_m)$ typically involves $O(m^2)$ operations.

*) see [Hochbruck & Lubich, 1997]

**) for an ideal multigrid method

Discussion

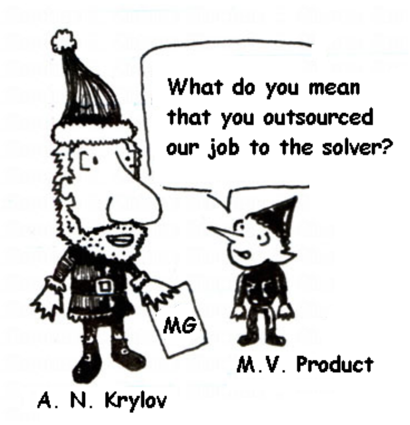
In polynomial Krylov methods the matrix A is only incorporated through matrix-vector products $A\boldsymbol{v}$.

In rational Krylov methods we need to solve linear systems $(A - \xi I)^{-1}\boldsymbol{v}$.

But: Rational functions have much better approximation properties than polynomials (if "good" poles available).

And: Rational functions allow for straightforward parallelization by partial fraction expansion.

$\Rightarrow$ Maybe we could benefit from progress made for the solution of linear systems by displacing iteration work to the linear system solver.


What do you mean that you outsourced our job to the solver?
MG
M.V. Product
A. N. Krylov

Rational Krylov spaces

Definition

Let q_{m-1} be a polynomial of degree $\leq m-1$ which is nonzero at all eigenvalues of A. Then

$$\mathscr{V}_m = q_{m-1}(A)^{-1}\mathscr{K}_m(A, \boldsymbol{b})$$

is the *rational Krylov space of order m associated with A, $\boldsymbol{b}$, and q_{m-1}.*

Basic facts:

- $\mathscr{V}_m = \mathscr{K}_m(A, q_{m-1}(A)^{-1}\boldsymbol{b})$,
- $\mathscr{V}_m \cong \mathscr{P}_{m-1}/q_{m-1}$ for $m \leq L$,
- $\dim \mathscr{V}_m = \min\{m, L\}$,
- $\mathscr{V}_m \subseteq \mathscr{V}_L = \mathscr{K}_L$,
- $f(A)\boldsymbol{b} \in \mathscr{V}_L$.

Computationally more practical are nested spaces, which result when

$$q_{m-1}(z) := \prod_{\substack{j=1 \\ \xi_j \neq \infty}}^{m-1} (z - \xi_j)$$

for a given fixed pole sequence $(\xi_1, \xi_2, \ldots) \subset \overline{\mathbb{C}}$.

We then have

- $\mathscr{V}_1 \subset \mathscr{V}_2 \subset \cdots \subset \mathscr{V}_L = \mathscr{K}_L$.

Note: If all $\xi_j = \infty$, then $\mathscr{V}_m = q_{m-1}(A)^{-1}\mathscr{K}_m = \mathscr{K}_m$.

Algorithm 1: Rational Arnoldi algorithm [Ruhe, 1984]

Given: $A, \boldsymbol{b}, (\xi_1, \xi_2, \ldots)$

$\boldsymbol{v}_1 := \boldsymbol{b}/\|\boldsymbol{b}\|$

for $j = 1, 2, \ldots, m$ **do**

  $\boldsymbol{w} := (I - A/\xi_j)^{-1} A \boldsymbol{v}_j$

  for $i = 1, 2, \ldots, j$ **do**

    $h_{i,j} := \langle \boldsymbol{w}, \boldsymbol{v}_i \rangle$

    $\boldsymbol{w} := \boldsymbol{w} - \boldsymbol{v}_i h_{i,j}$

  end

  $h_{j+1,j} := \|\boldsymbol{w}\|$

  $\boldsymbol{v}_{j+1} := \boldsymbol{w}/h_{j+1,j}$

end

(Problems with $\xi_j = 0$ and breakdown can be fixed.)

Rational Arnoldi decompositions

With $D_m = \mathrm{diag}(\xi_1^{-1}, \ldots, \xi_m^{-1})$ there holds

$$AV_m(H_m D_m + I_m) + A\boldsymbol{v}_{m+1} h_{m+1,m}\xi_m^{-1}\boldsymbol{e}_m^T = V_m H_m + \boldsymbol{v}_{m+1} h_{m+1,m}\boldsymbol{e}_m^T.$$

More shortly,

$$\boxed{AV_{m+1}\underline{K_m} = V_{m+1}\underline{H_m}}$$

where $\underline{K_m}$ and $\underline{H_m}$ are upper Hessenberg matrices of size $(m+1)\times m$.

Note: If $\xi_m = \infty$, then $V_m^* A V_m = H_m(H_m D_m + I_m)^{-1}$
[Deckers & Bultheel, 2008], [Beckermann & Reichel, 2008].

Remarks:

- $V_m^* A V_m$ can also be computed recursively from $V_{m-1}^* A V_{m-1}$ without the artificial pole $\xi_m = \infty$.
- In SI-Lanczos the compression $H_m (H_m D_m + I_m)^{-1}$ is used without setting $\xi_m = \infty$.
- Generalizing the polynomial case, the RADs satisfy

$$(\tau A - \sigma I)\, V_{m+1} \underline{K_m} = V_{m+1} (\tau \underline{H_m} - \sigma \underline{K_m}).$$

This makes the RKM suitable for functions $f^{\tau,\sigma}(z) = g(\tau z - \sigma)$.

Rayleigh-Ritz extraction

Lemma (Exactness)

Let $q_{m-1}(A)^{-1}\mathscr{K}_m(A,\boldsymbol{b})$ *be a rational Krylov space of dimension* m *with ONB* V_m*. Then for* $R_m := V_m^* A V_m$ *and every rational function* r *of the form* $r = p/q_{m-1}$ *(*$p \in \mathscr{P}_{m-1}$*) there holds*

$$r(A)\boldsymbol{b} = V_m r(R_m) V_m^* \boldsymbol{b}.$$

Proof: Use $q_{m-1}(A)^{-1}\mathscr{K}_m(A,\boldsymbol{b}) = \mathscr{K}_m(A, q_{m-1}(A)^{-1}\boldsymbol{b})$ and apply arguments of polynomial Krylov spaces.

Lemma (Interpolation)

Let $\boldsymbol{c} := q_{m-1}(A)^{-1}\boldsymbol{b}$ *and* V_m *be an ONB basis of* $q_{m-1}(A)^{-1}\mathscr{K}_m(A,\boldsymbol{b}) = \mathscr{K}_m(A,\boldsymbol{c})$, $R_m := V_m^* A V_m$. *Then*

$$V_m f(R_m)\, V_m^* \boldsymbol{b} = V_m \widetilde{f}(R_m)\, V_m^* \boldsymbol{c} = \widetilde{p}_{m-1}(A)\boldsymbol{c},$$

where $\widetilde{f} := q_{m-1} \cdot f$ *and* $\widetilde{p}_{m-1}$ *is a polynomial of degree* $m-1$ *that Hermite-interpolates* $\widetilde{f}$ *at* $\Lambda(R_m)$.

Proof: To prove the first equality, note that $\deg(q_{m-1}) \leq m-1$ and $q_{m-1}(A)\boldsymbol{c} = \boldsymbol{b}$. By Lemma (Exactness) there holds $\boldsymbol{b} = V_m q_{m-1}(R_m)\, V_m^* \boldsymbol{c}$. The second equality results from interpolation properties of polynomial Krylov methods.

Let w_m denote the characteristic polynomial of R_m and let Γ be a contour containing $\Lambda(R_m)$ in $\mathrm{int}(\Gamma)$. Furthermore f is assumed to be analytic in $\mathrm{int}(\Gamma)$ (then so is $\widetilde{f}$). The polynomial $\widetilde{p}_{m-1}$ can be expressed using Hermite's formula

$$\widetilde{p}_{m-1}(z) = \frac{1}{2\pi i} \int_\Gamma \frac{w_m(\zeta) - w_m(z)}{w_m(\zeta)(\zeta - z)} \widetilde{f}(\zeta)\, d\zeta,$$

and for the interpolation error

$$\widetilde{f}(z) - \widetilde{p}_{m-1}(z) = \frac{1}{2\pi i} \int_\Gamma \frac{w_m(z)}{w_m(\zeta)(\zeta - z)} \widetilde{f}(\zeta)\, d\zeta.$$

Dividing this equation by $q_{m-1}(z)$ and setting $r_m(z) := w_m(z)/q_{m-1}(z)$ we obtain

$$f(z) - \widetilde{p}_{m-1}(z)/q_{m-1}(z) = \frac{1}{2\pi i}\int_\Gamma \frac{r_m(z)}{r_m(\zeta)(\zeta - z)} f(\zeta)\, d\zeta.$$

Using Lemma (Interpolation) we have the following representation for the error of a Rayleigh-Ritz approximation

$$f(A)\boldsymbol{b} - V_m f(R_m)\, V_m^* \boldsymbol{b} = \left(\frac{1}{2\pi i}\int_\Gamma (\zeta I - A)^{-1} f(\zeta)/r_m(\zeta)\, d\zeta\right) r_m(A)\boldsymbol{b}$$

Example: Choose Γ to wind around $\Sigma = F(A)$. Then choose q_{m-1} such that $r_m = w_m/q_{m-1}$ is small on Σ and large on Γ.

A related problem is

Theorem

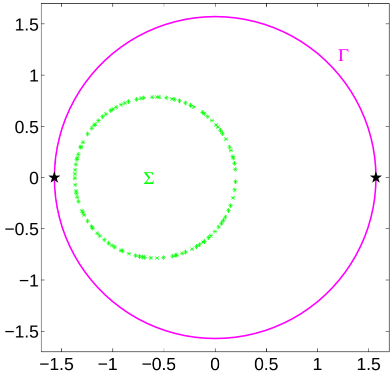
Given two compact disjoint sets Σ and Γ. Denote by $\mathscr{R}_{m-1}^{m}$ the set of rational functions of type $(m, m-1)$ with zeros in Σ and poles in Γ. There holds

$$\min_{\left(r_m \in \mathscr{R}_{m-1}^{m}\right)_{m\geq 1}} \limsup_{m\to\infty} \left(\frac{\max_{z\in\Sigma} r_m(z)}{\min_{z\in\Gamma} r_m(z)} \right)^{1/m} = c(\Sigma, \Gamma) < 1,$$

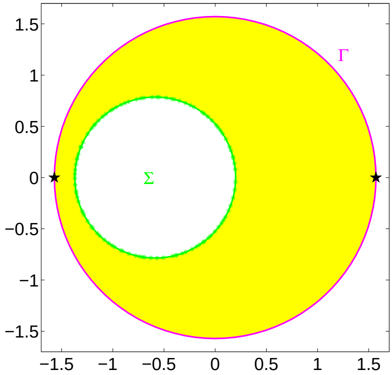
where $c(\Sigma, \Gamma)$ is the capacity of the plane condenser with plates Σ and Γ.

Idea: Use the poles of optimal rational functions r_m^* as poles for a rational Krylov space.

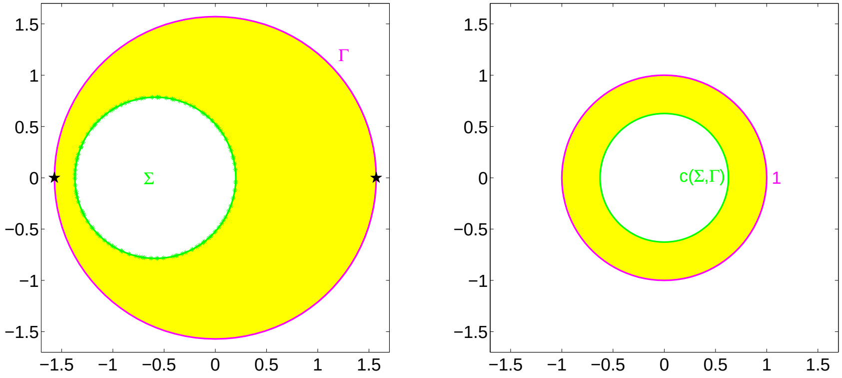
Example: (inspired by C. Beattie) We approximate $\tan(A)\boldsymbol{b}$ for $A = 0.2I - \frac{\pi}{4}U$, where U is a unitary random matrix.
We choose $\Gamma = \{z : |z| = \frac{\pi}{2}\}$.



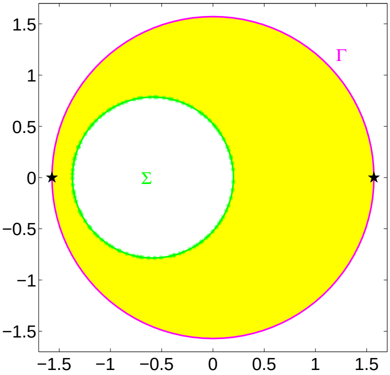
Example: (inspired by C. Beattie) We approximate $\tan(A)\boldsymbol{b}$ for $A = 0.2I - \frac{\pi}{4}U$, where U is a unitary random matrix.
We choose $\Gamma = \{z : |z| = \frac{\pi}{2}\}$.

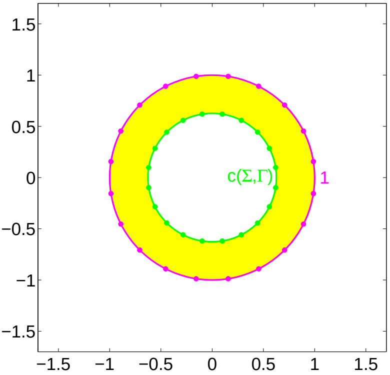


Example: (inspired by C. Beattie) We approximate $\tan(A)\boldsymbol{b}$ for $A = 0.2I - \frac{\pi}{4}U$, where U is a unitary random matrix.
We choose $\Gamma = \{z : |z| = \frac{\pi}{2}\}$.

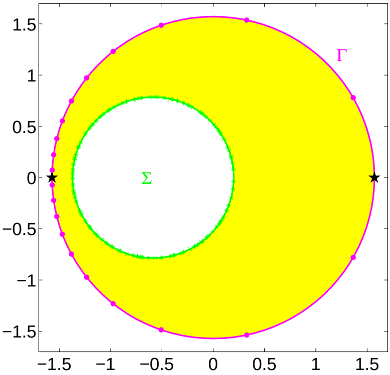


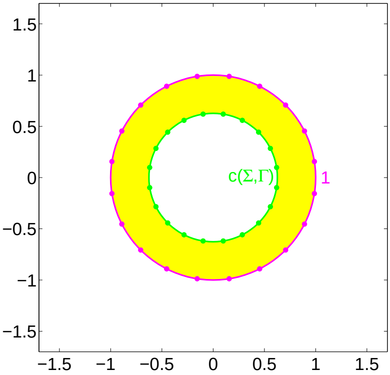
Example: (inspired by C. Beattie) We approximate $\tan(A)\boldsymbol{b}$ for $A = 0.2I - \frac{\pi}{4}U$, where U is a unitary random matrix.
We choose $\Gamma = \{z : |z| = \frac{\pi}{2}\}$.





Example: (inspired by C. Beattie) We approximate $\tan(A)\boldsymbol{b}$ for $A = 0.2I - \frac{\pi}{4}U$, where U is a unitary random matrix.
We choose $\Gamma = \{z : |z| = \frac{\pi}{2}\}$.





Example: (inspired by C. Beattie) We approximate $\tan(A)\boldsymbol{b}$ for $A = 0.2I - \frac{\pi}{4}U$, where U is a unitary random matrix.
We choose $\Gamma = \{z : |z| = \frac{\pi}{2}\}$.

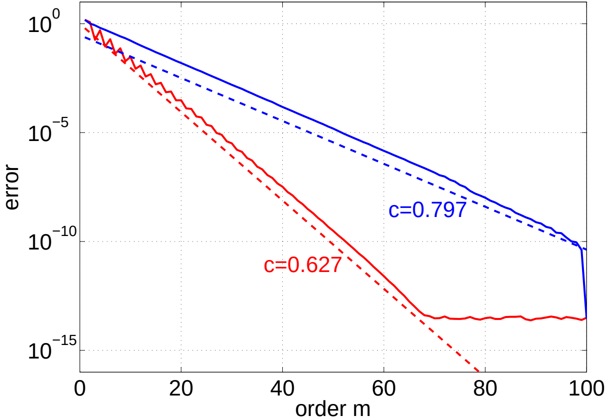


Figure: Rational (red) vs. polynomial (blue) Krylov approximation

Note: We have not chosen the σ_j given in the last theorem. These interpolation points are chosen implicitly by Rayleigh-Ritz extraction.

However, we observe that supplying optimal poles to the rational Krylov method yields an optimal error reduction in the sense, that the error is reduced with the optimal convergence rate $c(\Sigma, \Gamma)$ from the rational approximation problem.

Hence, the Rayleigh-Ritz extraction has implicitly chosen near-optimal interpolation points.

Lemma (Optimality)

Let $q_{m-1}(A)^{-1}\mathscr{K}_m(A,\boldsymbol{b})$ be a rational Krylov space of dimension m with ONB V_m. Let $R_m := V_m^* A V_m$ and $\Sigma = F(A)$. Then

$$\|f(A)\boldsymbol{b} - V_m f(R_m) V_m^* \boldsymbol{b}\| \leq 2C \, \|\boldsymbol{b}\| \min_{p \in \mathscr{P}_{m-1}} \|f - p/q_{m-1}\|_\Sigma$$

with a constant $C \leq 11.08$ [Crouzeix, 2007].
If A is self-adjoint the result holds for $C = 1$.

Aim: Choose poles q_{m-1} such that there exists a rational function p/q_{m-1} which is close to f on Σ.

- Lemma (Optimality) implies: It makes no sense to solve the linear systems in the RKM with an unpreconditioned polynomial Krylov method.
- More elaborate a-priori estimates are available, e.g., for Markov functions by using the Faber transform to consider approximation problems on the unit disk instead of Σ (see, e.g., [Druskin & Knizhnerman, 1989], [Knizhnerman, 1991], [Beckermann & Reichel, 2008]).
- It can be shown that SI-Lanczos extraction is also quasi-optimal. In some cases the optimal pole can be found by Remez' algorithm [Hochbruck & Lubich 1997].

Orthogonal rational functions

Given ONB $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m$ of $q_{m-1}(A)^{-1}\mathscr{K}_m(A, \boldsymbol{b})$.

There exist polynomials $p_1, \ldots, p_m$ of (not nec. ascending) degree $m-1$ such that

$$\boldsymbol{v}_j = p_j(A)\, q_{m-1}(A)^{-1}\boldsymbol{b} =: r_j(A)\boldsymbol{b}.$$

Let $A = U\Lambda U^*$ be normal, $U^*U = I$. Then

$$\delta_{j,k} = \langle r_j(A)\boldsymbol{b}, r_k(A)\boldsymbol{b}\rangle_2 = \langle r_j(\Lambda)\, U^*\boldsymbol{b}, r_k(\Lambda)\, U^*\boldsymbol{b}\rangle_2 = \langle r_j(z), r_k(z)\rangle_\mu$$

where

$$\langle r_j(z), r_k(z)\rangle_\mu := \sum_{i=1}^{n} r_j(\lambda_i)\overline{r_k(\lambda_i)}\, w(\lambda_i)^2,$$

$w(\lambda_i) = |\boldsymbol{e}_i^T U^*\boldsymbol{b}|$. Hence, the r_j are orthonormal rational functions with respect to the inner product $\langle\,\cdot\,,\,\cdot\,\rangle_\mu$.

- It is well known that orthogonal rational functions satisfy short recurrences if A is self-adjoint. One can modify the rational Arnoldi algorithm to make it "Lanczos-like" (at the cost of 2 additional MVP per iteration). [Bultheel et al, 1999].

The following interpretation is also possible

$$\begin{aligned} \delta_{j,k} &= \langle r_j(A)\boldsymbol{b}, r_k(A)\boldsymbol{b}\rangle_2 = \left\langle (p_j/q_{m-1})(\Lambda)\, U^*\boldsymbol{b}, (p_k/q_{m-1})(\Lambda)\, U^*\boldsymbol{b}\right\rangle_2 \\ &= \langle p_j, p_k\rangle_{\mu_m}, \end{aligned}$$

where

$$\langle p_j(z), p_k(z)\rangle_{\mu_m} := \sum_{i=1}^{n} p_j(\lambda_i)\overline{p_k(\lambda_i)}\, w(\lambda_i)^2\, |q_{m-1}(\lambda_i)|^{-2}.$$

Immediate connection to orthogonal polynomials (with varying weight function), Gaussian quadrature, continued fractions, ... (see, e.g., [Strakos, 1993], [Golub & Meurant, 1994]).

Rational Ritz values

Let A be self-adjoint with distinct eigenvalues $\Lambda(A) = \{\lambda_1 < \cdots < \lambda_N\}$.

Definition

Given an ONB V_m of $q_{m-1}(A)^{-1}\mathscr{K}_m(A, \boldsymbol{b})$, the eigenvalues θ_j of $V_m^* A V_m$ are called *rational Ritz values of order* m. We set

$$\Theta = \{\theta_1 < \cdots < \theta_m\}.$$

As we have seen, these rational Ritz values are nodes of rational interpolants and therefore of special interest.

From $q_{m-1}(A)^{-1}\mathscr{K}_m(A,\boldsymbol{b}) = \mathscr{K}_m(A, q_{m-1}(A)^{-1}\boldsymbol{b})$ we conclude:

1. $\Theta \subset F(A) = [\lambda_1, \lambda_N]$.
2. Interlacing: there is always an eigenvalue λ_k in $(\theta_{\kappa-1}, \theta_\kappa)$.
3. The Θ are the zeros of the monic minimizer

$$p^* = \arg \min_{p \in \mathscr{P}_m^\infty} \|p(A) q_{m-1}(A)^{-1}\boldsymbol{b}\|.$$

Questions:

- Do the rational Ritz values "converge" to eigenvalues?
- If yes, how large is $\mathrm{dist}(\lambda_k, \Theta)$ as a function of m?

In the polynomial case there is a rule of thumb [Trefethen & Bau, 1997]: The Lanczos iteration tends to converge to eigenvalues in regions of "too little charge" for an equilibrium distribution.

This rule has been quantified using potential theoretic tools by [Kuijlaars, 2000], [Beckermann, 2000] and used to explain superlinear CG convergence [Beckermann & Kuijlaars, 2001].

This theory has been extended to the rational Krylov case [Beckermann, G. & Vandebril, 2009].

Strictly speaking, "convergence" of Ritz values makes sense only in an asymptotic setting:

Consider a sequence of self-adjoint matrices $A_N \in \mathbb{C}^{N \times N}$ with eigenvalues

$$\Lambda_N = \Lambda(A_N) = \{\lambda_{1,N} < \cdots < \lambda_{N,N}\},$$

and the associated normalized counting measures

$$\chi_N(\Lambda_N) = \frac{1}{N} \sum_{x \in \Lambda_N} \delta_x.$$

Accordingly, we will also consider sequences of vectors $\boldsymbol{b}_N$ and sets Θ_N and Ξ_N (set of Ritz values and poles with $m(N)$ elements).

Notational conventions:

We add an index N to all quantities. More precisely, we consider

- Hermitian matrices $A_N \in \mathbb{C}^{N \times N}$ with distinct eigenvalues $\lambda_{1,N} < \cdots < \lambda_{N,N}$, spectra $\Lambda_N = \Lambda(A_N)$,
- starting vectors $\boldsymbol{b}_N \in \mathbb{C}^N$ with eigencomponents $w_N(\lambda_{j,N}) \in [0,1]$,
- a multiset $\Xi_N \subset \mathbb{R} \setminus \Lambda_N$ of the $m-1$ poles $\xi_{1,N}, \ldots, \xi_{m-1,N}$, and
- a set Θ_N of mth rational Ritz values $\theta_{1,N} < \cdots < \theta_{m,N}$ for $(A_N, \boldsymbol{b}_N)$ and the poles Ξ_N.

Here $m = m(N)$ will always be chosen such that $m(N)/N \to t \in (0, \|\sigma\|)$ as $N \to \infty$, where $\|\sigma\| = \sigma(\mathbb{C})$.

(H1) The spectra and pole sets are uniformly bounded: there exist compact sets Λ and Ξ such that for all N there holds $\Lambda_N \subset \Lambda$ and $\Xi_N \subset \Xi$.

(H2) The matrices A_N have an asymptotic eigenvalue distribution described by some measure σ: we have $\chi_N(\Lambda_N) \to \sigma$ for $N \to \infty$.

(H3) We have a weak separation of eigenvalues: for any sequence $\Lambda_N \ni \lambda_{k(N),N} \to \lambda$ for $N \to \infty$ there holds

$$\limsup_{\delta \to 0+} \limsup_{N \to \infty} \frac{1}{N} \sum_{0<|\lambda_{j,N}-\lambda_{k(N),N}|\leq\delta} \log \frac{1}{|\lambda_{j,N} - \lambda_{k(N),N}|} = 0.$$

It follows that $z \mapsto U^\sigma(z)$ is continuous.

(H4) The multisets of poles Ξ_N counting multiplicities have an asymptotic behavior described by some measure ν: we have $\chi_N(\Xi_N) \to \nu$ for $N \to \infty$.

(H5) The eigencomponents $w_N(\lambda_{k,N}) \in [0,1]$ are sufficiently large

$$\liminf_{N\to\infty} \min_k w_N(\lambda_{k,N})^{1/N} = 1.$$

(H6) We have a strict separation of poles from eigenvalues: $\Lambda \cap \Xi$ is empty. It follows from assumptions **(H1)** and **(H4)** that U^ν is continuous on Λ.

Example: Consider N equi-spaced eigenvalues on $[-1, 1]$. In this case

$$d\sigma = \frac{1}{2}\, dx|_{[-1,1]}.$$

Let $t = 0.7$ be fixed. For $N = 100$ we place 69 poles at the point $x = 1$, i.e.,

$$\Xi_{100} = \{1, 1, \ldots, 1\}, \quad \#\Xi_{100} = 69.$$

Then Θ_{100} is the set of $tN = 70$ rational Ritz values.

For $N = 1000$ we place 699 poles at the point $x = 1$. Then Θ_{1000} is the set of $tN = 700$ rational Ritz values.

We have $\chi_N(\Xi_N) \to \nu = t \cdot \delta_1$.

Tools from Potential Theory

Given a (signed) Borel measure μ, its logarithmic potential is defined as

$$U^{\mu}(z) = \int \log \frac{1}{|x-z|} \, \mathrm{d}\mu(x).$$

The mutual logarithmic energy of measures μ_1 and μ_2 is defined as

$$I(\mu_1, \mu_2) = \int U^{\mu_1}(y) \, \mathrm{d}\mu_2(y).$$

We set $I(\mu) = I(\mu, \mu)$.

Informally spoken, the rational Ritz values will distribute according to a measure μ which describes a minimal energy state under the attraction of an external field generated by the poles. We look for a minimizer of

$$\mu \mapsto I(\mu - \nu) = I(\mu) - 2I(\mu, \nu) + I(\nu) \geq 0,$$

where

$$\mu \in \mathscr{M}_t^\sigma := \{\mu \text{ Borel measure} : \mu \geq 0, \mu \leq \sigma, \|\mu\| = t\}.$$

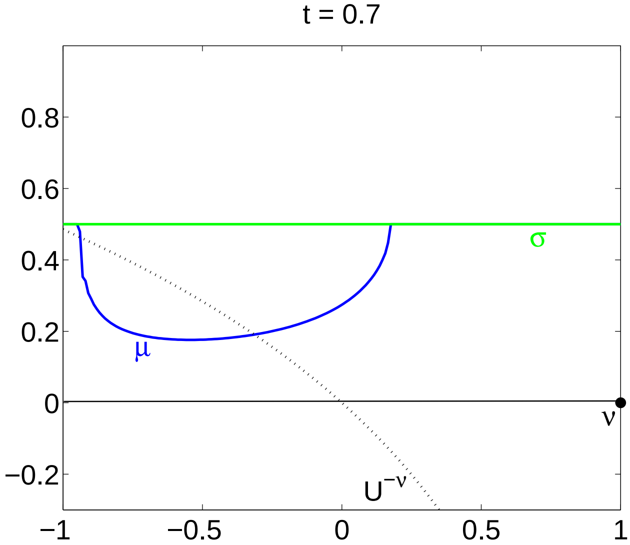
However, this requires $I(\nu) < \infty$. We instead minimize

$$\mu \mapsto I(\mu) - 2I(\mu, \nu)$$

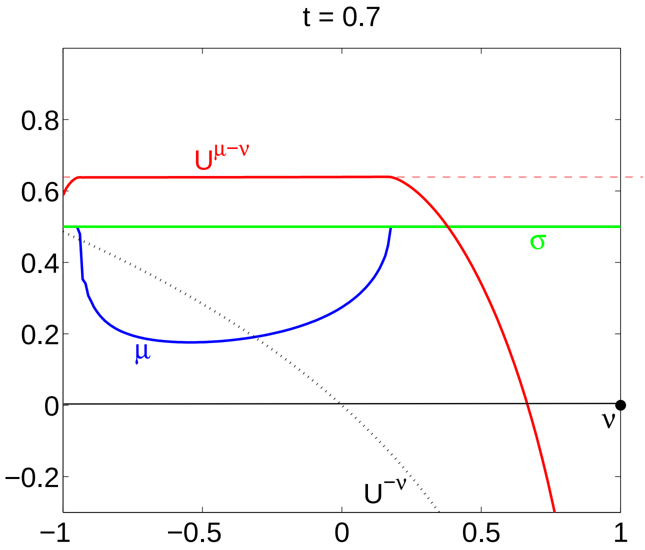
(a strictly convex function over the convex and closed set $\mathscr{M}_t^\sigma$).

$\Rightarrow$ **Constrained energy problem with external field** $Q(z) = U^{-\nu}(z)$.

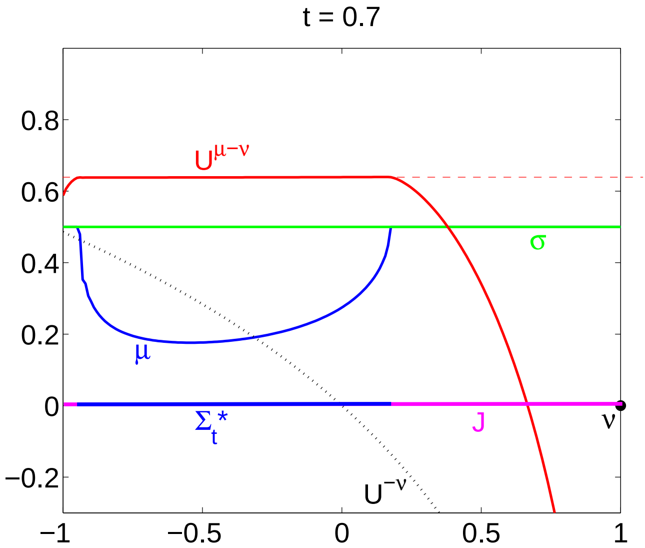
Example: Equi-spaced eigenvalues on $[-1, 1]$, $\mathrm{d}\sigma/\mathrm{d}x = 1/2$.



Example: Equi-spaced eigenvalues on $[-1,1]$, $\mathrm{d}\sigma/\mathrm{d}x = 1/2$.



Example: Equi-spaced eigenvalues on $[-1, 1]$, $\mathrm{d}\sigma/\mathrm{d}x = 1/2$.



Theorem (Beckermann, G. & Vandebril, 2009)

*Under assumptions **(H1)–(H6)** there holds*

$$\chi_N(\Theta_N) \to \mu,$$

with the positive finite Borel measure μ *being the unique minimizer of* $\mu \mapsto I(\mu) - 2I(\nu, \mu)$ *within* $\mathscr{M}_t^\sigma$.

Define F *as the maximum of* $U^{\mu-\nu}$ *in the whole complex plane, and* $\Sigma_t^* = \{z \in \mathbb{C} : U^{\mu-\nu}(z) = F\}$. *In a closed interval* $J \subset \mathbb{R} \setminus \Sigma_t^* \subset \mathbb{R} \setminus \operatorname{supp}(\sigma - \mu)$, *all sequences* $J \ni \lambda_{k(N),N} \to \lambda$ *for* $N \to \infty$ *satisfy*

$$\lim_{N\to\infty} \operatorname{dist}(\lambda_{k(N),N}, \Theta_N)^{1/N} = \exp(2(U^{\mu-\nu}(\lambda) - F)),$$

with the possible exclusion of at most one unique "exceptional index" $k^*(N)$.

The proof of this theorem uses basic results about the asymptotics of discrete polynomials due to Rakhmanov, Dragnev & Saff, Van Assche & Kuijlaars, Beckermann, and others.

However, more work has to be done to bring it to a satisfactory form for applications:

1. For the convergence of $\mathrm{dist}(\lambda_{k(N),N}, \Theta_N)^{1/N}$ we should just insure that the eigencomponent $w_N(\lambda_{k(N),N})^{1/N} \to 1$, but **(H5)** requires all eigencomponents to be large.
2. In **(H6)** we ask for strict separation of spectra and poles. Actually, we expect a very fast convergence of Ritz values if there are poles very close to eigenvalues, which is forbidden by **(H6)**. The theorem is not applicable to our example with the equi-spaced eigenvalues.

Theorem

*Assume that **(H1)–(H4)** hold, and let the minimizing measure* $\mu \in \mathscr{M}_t^\sigma$ *and* $F \in \mathbb{R}$ *be as before. Replace **(H6)** by*

(H6') *Consider the Jordan decomposition of the signed measure* $\nu - \sigma = \nu_0 - \sigma_0$. *Both* $\operatorname{supp}(\sigma)$ *and* $\operatorname{supp}(\nu_0)$ *are finite unions of closed intervals, and* U^ν *is cont. at each* $x \in \Lambda$ *with* $U^\nu(x) < \infty$.

Then we have for any sequence $\Lambda_N \ni \lambda_{k(N),N} \to \lambda$

$$\limsup_{N\to\infty} \operatorname{dist}(\lambda_{k(N),N}, \Theta_N)^{1/N} \leq e^{U^{\mu-\nu}(\lambda)-F} \limsup_{N\to\infty} \; w_N(\lambda_{k(N),N})^{-1/N}.$$

*If in addition **(H5)** holds, then*

$$\limsup_{N\to\infty} \operatorname{dist}(\lambda_{k(N),N}, \Theta_N)^{1/N} \leq e^{2(U^{\mu-\nu}(\lambda)-F)},$$

with $J \ni \lambda_{k(N),N} \neq \lambda_{k^*(N),N}$ *as before.*

Note that **(H1)** requires the spectra and poles to be uniformly bounded for all N. This does not allow for poles at infinity and excludes the case of polynomial Ritz values.

It is possible to apply a fractional transformation to A_N and Ξ_N, i.e., to consider transformed eigenvalues and *finite* poles

$$\underline{\lambda}_{j,N} = \frac{1}{\lambda_{j,N} - \tau}, \quad \underline{\xi}_{j,N} = \frac{1}{\xi_{j,N} - \tau},$$

for a suitable $\tau \in \mathbb{R}$ and to measure all distances in the chordal metric (instead of the Euclidian).

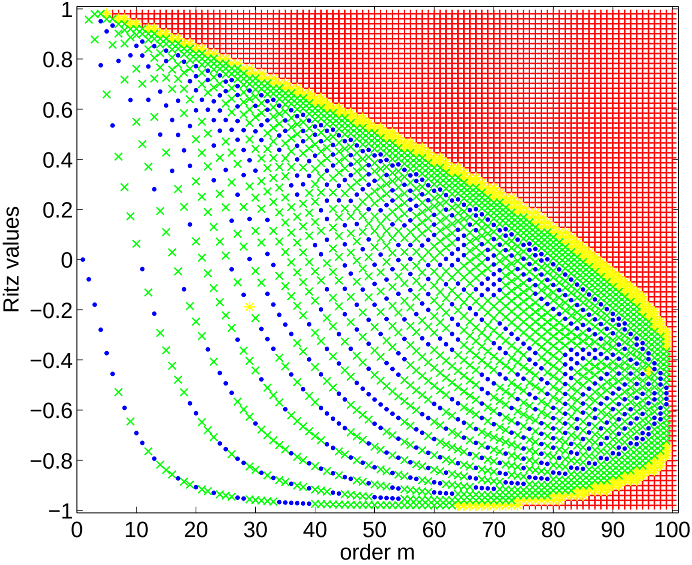
Hence **(H1)** is not an essential requirement.

Examples

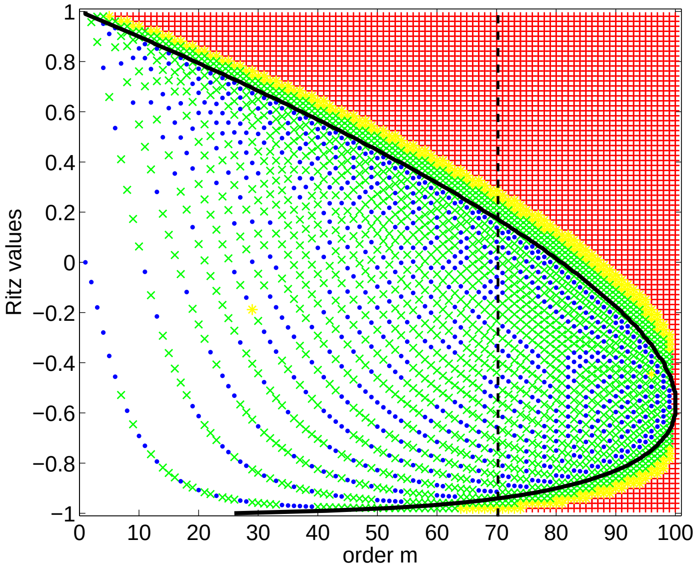
To visualize the distance of a Ritz value θ to the spectrum, we use the following color code:

Symbol	Color	Relative distance of a Ritz value θ to the spectrum
$+$	Red	$\mathrm{dist}(\theta, \Lambda(A_N)) < 10^{-7.5}$
$*$	Yellow	$10^{-7.5} \leq \mathrm{dist}(\theta, \Lambda(A_N)) < 10^{-5}$
$\times$	Green	$10^{-5} \leq \mathrm{dist}(\theta, \Lambda(A_N)) < 10^{-2.5}$
$\cdot$	Blue	$10^{-2.5} \leq \mathrm{dist}(\theta, \Lambda(A_N))$

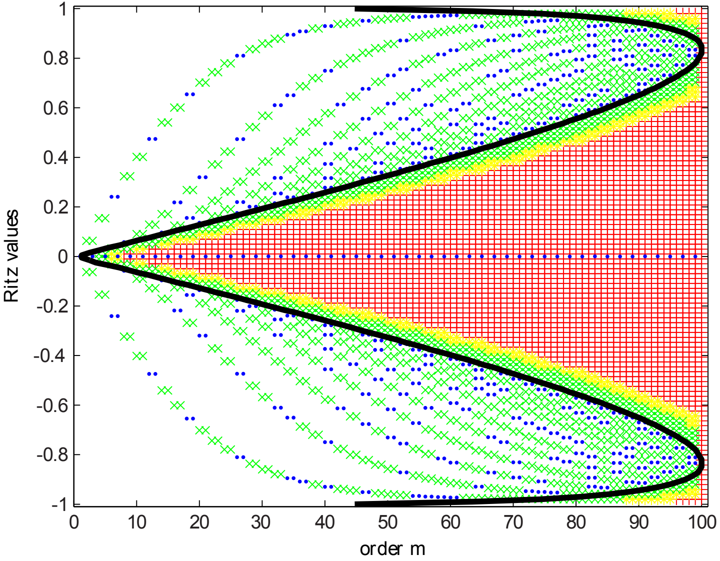
Equi-spaced eigenvalues in $[-1, 1]$, all poles at $x = 1$, $\nu_t = t \cdot \delta_1$



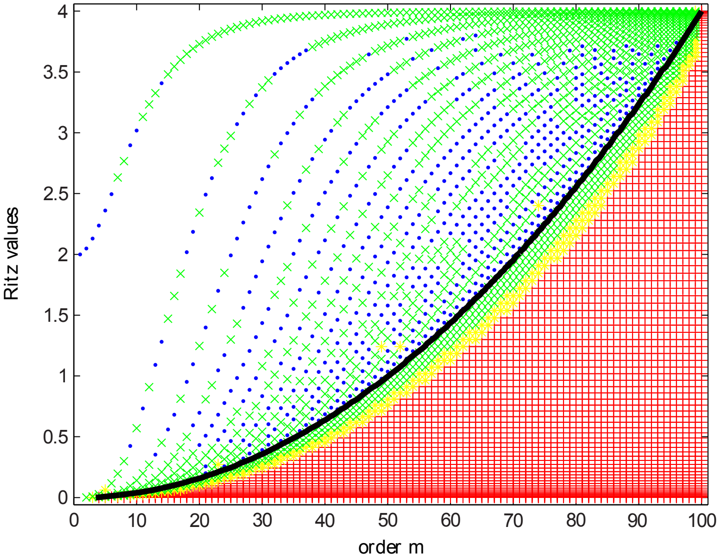
Equi-spaced eigenvalues in $[-1, 1]$, all poles at $x = 1$, $\nu_t = t \cdot \delta_1$



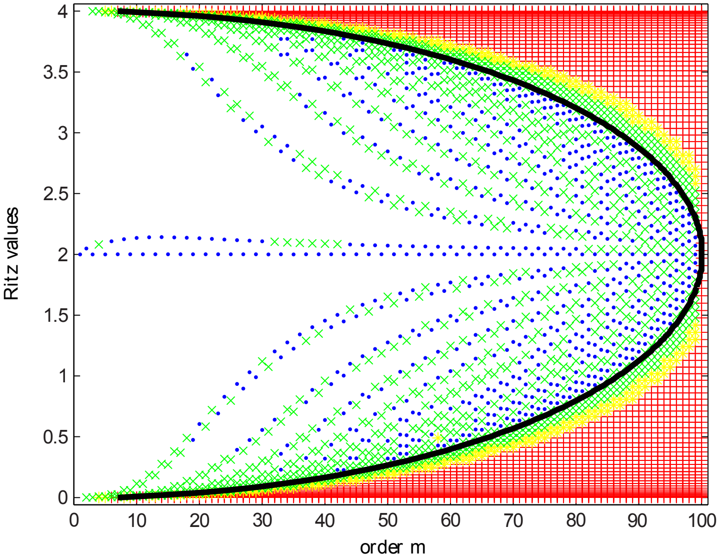
Equi-spaced eigenvalues in $[-1, 1]$, all poles at $x = 0$, $\nu_t = t \cdot \delta_0$



1D-Laplacian on $[0,4]$, $\nu_t = t/2 \cdot \delta_0$



1D-Laplacian on $[0, 4]$, $\nu_t = t/2 \cdot \delta_0 + t/2 \cdot \delta_4$



Analytic example: Consider

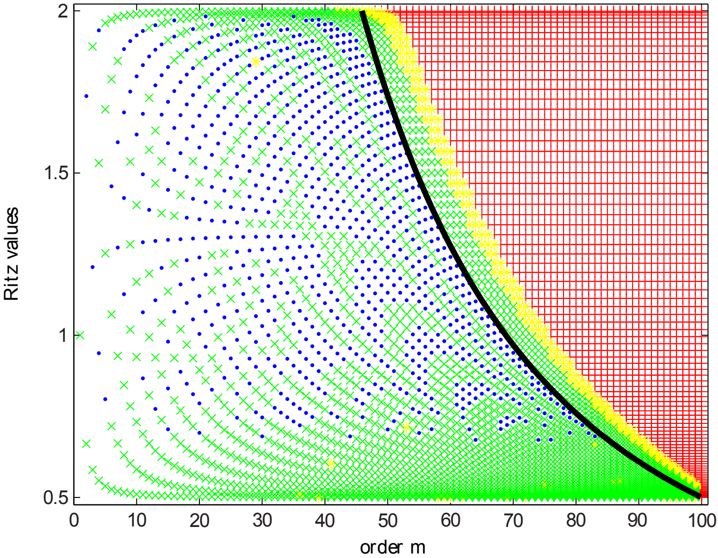
$$A_N = \begin{pmatrix} q^0 & q^1 & q^2 & \\ q^1 & q^0 & q^1 & \ddots \\ q^2 & q^1 & q^0 & \ddots \\ & \ddots & \ddots & \ddots \end{pmatrix} \in \mathbb{R}^{N\times N}$$

for $q \in (0,1)$.

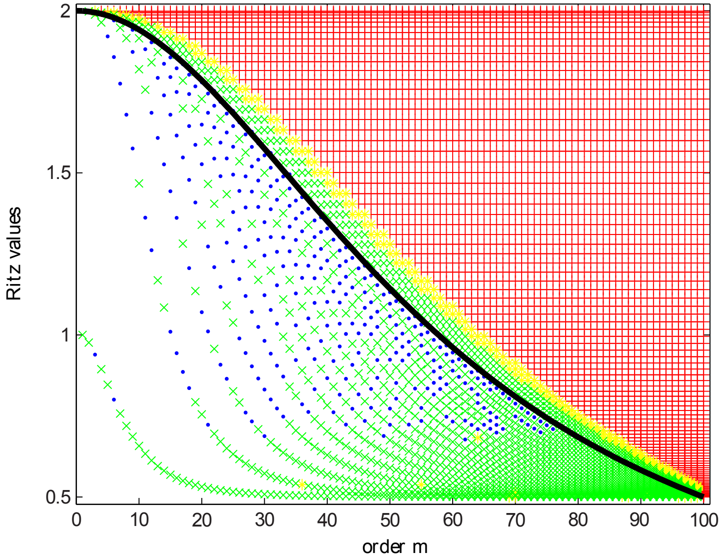
It is known [Kac, Murdock & Szegő, 1953] that $\chi_N(A_N) \to \sigma$, $\mathrm{supp}(\sigma) = [\alpha, \beta]$, with density

$$\frac{\mathrm{d}\sigma}{\mathrm{d}x}(x) = \frac{1}{\pi x \sqrt{(x-\alpha)(\beta-x)}}, \qquad \alpha = \frac{1-q}{1+q}, \qquad \beta = \frac{1+q}{1-q}.$$

Kac example, $q = 1/3$, $\nu = t \cdot \delta_{10}$



Kac example, $q = 1/3$, $\nu = t \cdot \delta_2$



Outlook

- Explain superlinear convergence of RKMs for $f(A)\boldsymbol{b}$,
- Possible spectral adaption of optimal poles,
- Develop (general) a-posteriori bounds for the error,
- Efficient implementation, parallelization,
- Inexact solves of the linear systems,
- Multigrid methods for shifted operators,
- Application to real-world problems (e.g., from geophysical prospecting).