Rational Krylov for Stieltjes matrix functions: convergence and pole selection

Leonardo Robol, UniPI (joint work with S. Massei, EPFL)

13 Febbraio 2020, Montecatini, Convegno GNCS

Progetto GNCS Giovani ricercatori

- Progetto GNCS "Giovani ricercatori" 2018/2019.
- Titolo: "Metodi di proiezione per equazioni di matrici e sistemi lineari con operatori definiti tramite somme di prodotti di Kronecker, e soluzioni con struttura di rango."
- Supporto per la partecipazione alle conferenze ILAS2019 (Rio de Janeiro) e ICIAM2019 (Valencia).

Motivation: Fractional diffusion equations

We are concerned with the "fractional equivalent" of the 1D/2D Laplacian. That is, instead of considering

$$\frac{\partial^2 u}{\partial x^2} = f(x), \qquad \Delta u = f(x,y)$$

we deal with

$$\frac{\partial^\alpha u}{\partial y^\alpha} = f(x), \qquad \Delta^\alpha u = f(x,y)$$

for $1 < \alpha < 2$.

Fractional diffusion allow to model nonlocal behavior.

- Useful in describing anomalous diffusion phenomena (plasma physics, financial markets, ...)
- Several (non-equivalent) definitions in the literature: Riemann-Liouville, Caputo, Grünwald-Letkinov, Matrix Transform Method

Motivation: Matrix Transform Method

Let A be the usual discretization of the Laplacian operator.

One way to define the discrete operator M representing the derivative of order α is to impose that

$$M^{\frac{2}{\alpha}} = A \quad \iff \quad M = A^{\frac{\alpha}{2}} \quad (1 < \alpha < 2)$$

- This follows by “composition” of derivatives
- The problem is recast as computing $x := f(A)v$, with $f(z) = z^{-\frac{\alpha}{2}}$.

Evaluation of matrix functions

Let $f(z) : \Omega \to \mathbb{R}$ be an analytic function on $\Omega \subseteq \mathbb{R}^+$.

Problem 1. Given a symmetric positive definite matrix $A \in \mathbb{R}^{n \times n}$ with eigenvalues in $[\lambda_{\text{min}}, \lambda_{\text{max}}] \subset \Omega$ and $v \in \mathbb{R}^n$ compute

$$x := f(A)v.$$

Applications: system of ODEs, exponential integrators, fractional diffusion problems, network communicability measures, control theory, ...

Subspace projection methods

Let $\mathcal{U} \subset \mathbb{R}^n$ be a ℓ-dimensional subspace ($\ell \ll n$) with an orthogonal basis $U = [u_1 | \dots | u_\ell]$ and $A_\ell = U^* A U$, $v_\ell = U^* v$ be the projections of A and v on $\mathcal{U}$.

- **Linear systems**

$$x = A^{-1} v \approx x_\ell := U A_\ell^{-1} v_\ell.$$

- **Matrix functions**

$$x = f(A) v \approx x_\ell := U f(A_\ell) v_\ell.$$

Subspace projection methods

Let $\mathcal{U} \subset \mathbb{R}^n$ be a ℓ-dimensional subspace ($\ell \ll n$) with an orthogonal basis $U = [u_1|\dots|u_\ell]$ and $A_\ell = U^*AU$, $v_\ell = U^*v$ be the projections of A and v on $\mathcal{U}$.

- **Linear systems**

$$x = A^{-1}v \approx x_\ell := UA_\ell^{-1}v_\ell.$$

- **Matrix functions**

$$x = f(A)v \approx x_\ell := Uf(A_\ell)v_\ell.$$

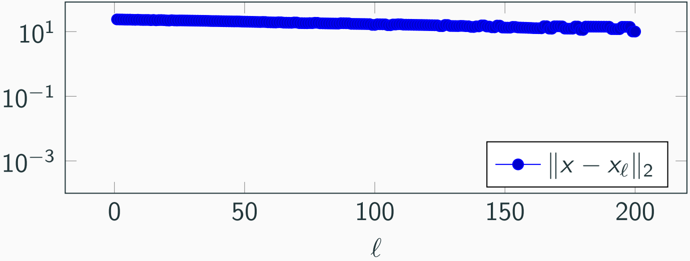
If we use the **Krylov subspace** $\mathcal{U} = \mathcal{K}_\ell(A, v) := \operatorname{span}\{v, Av, \dots, A^{\ell-1}v\}$ then,

$$\|x - x_\ell\|_2 \leq C \cdot \min_{p(z)\in\mathcal{P}_{\ell-1}} \max_{z\in[\lambda_{\min},\lambda_{\max}]} |p(z) - f(z)|,$$

where $\mathcal{P}_\ell := \{\text{poly of degree} \leq \ell\}$ and C is independent on A and f.

Polynomial approximation does not always work...

Sometimes the convergence of polynomial approximation struggles, e.g. $x = A^{-\frac{1}{2}}v$, $[\lambda_{\min}, \lambda_{\max}] \approx [10^{-5}, 4]$, $n = 1000$.



Rational Krylov method

Rational Krylov subspace. Given $\Sigma_\ell := \{\sigma_1, \dots, \sigma_\ell\} \subset \mathbb{C}$ it is defined as[1]

$$\begin{aligned}\mathcal{RK}_\ell(A, v, \Sigma_\ell) : &= q_\ell(A)^{-1}\mathcal{K}_{\ell+1}(A, v) = \left\{ \frac{p(A)}{q_\ell(A)} v : \ p(z) \in \mathcal{P}_\ell \right\} \\ &= \operatorname{span}\{v, (\sigma_1 I - A)^{-1} v, \dots, (\sigma_\ell I - A)^{-1} v\}\end{aligned}$$

where $q_\ell(z) := \prod_j (z - \sigma_j)^{-1}$.

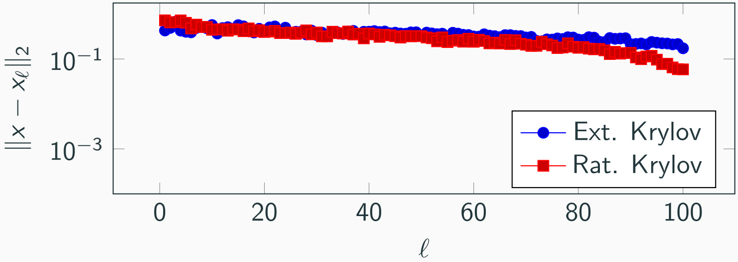
If $\mathcal{U} = \mathcal{RK}_\ell(A, v, \Sigma_\ell)$ we get a problem of rational approximation with fixed poles

$$\|x - x_\ell\|_2 \le C \cdot \min_{r(z) \in \frac{\mathcal{P}_\ell}{q_\ell(z)}} \max_{z \in [\lambda_{\min}, \lambda_{\max}]} |r(z) - f(z)|.$$

[1] last equality is valid only for distinct poles

Rational approximation does not always work...

- Uniform approximations of highly oscillatory functions on the whole positive real line are not possible for polynomials or rational functions
- In general a number of steps dependent on the norm of the operator is needed for convergence[2].
- E.g. $x = cos(A)v$, where $\|A\|_2 \approx 10^5$, $n = 1000$



[2]V. Grimm, M. Hochbruck. Rational approximation to trigonometric operators, BIT 2006.

Stieltjes functions

A favourable case is when $f(z) : \mathbb{R}^+ \to \mathbb{R}$ if defined via a Stieltjes integral:

1. $f(z) = \int_0^\infty \frac{1}{z+t} d\mu(t)$ **Cauchy-Stieltjes/Markov function**
2. $f(z) = \int_0^\infty e^{-zt} d\mu(t)$ **Laplace-Stieltjes function**

where $d\mu(t)$ is a non negative measure on $\mathbb{R}^+$.

Stieltjes functions

A favourable case is when $f(z) : \mathbb{R}^+ \to \mathbb{R}$ if defined via a Stieltjes integral:

1. $f(z) = \int_0^\infty \frac{1}{z+t} d\mu(t)$ **Cauchy-Stieltjes/Markov function**
2. $f(z) = \int_0^\infty e^{-zt} d\mu(t)$ **Laplace-Stieltjes function**

where $d\mu(t)$ is a non negative measure on $\mathbb{R}^+$.

Examples of functions in these classes are

1. $z^{-\alpha} = \frac{\sin(\alpha\pi)}{\pi} \int_0^\infty \frac{t^{-\alpha}}{z+t} dt \;\; \alpha \in (0,1), \qquad \frac{\log(1+z)}{z}, \qquad \frac{e^{-t\sqrt{z}}-1}{z}.$
2. $e^{-z}, \qquad \frac{1-e^{-z}}{z}, \qquad \varphi_j(z) := \int_0^\infty e^{-tz} \frac{[\max\{1-t,0\}]^{j-1}}{(j-1)!} dt.$

Stieltjes functions

- Laplace Stieltjes functions on $(0, \infty)$ are also known as completely monotone functions, i.e. those such that $(-1)^j f^{(j)}(z) > 0 \ \ \forall z > 0$,
- By considering $d\mu(t)$ to be a finite sum of Dirac deltas we have that rational functions of the form

$$f(z) = \sum_{j=1}^{h} \frac{\alpha_j}{z - \beta_j}, \qquad \alpha_j > 0, \quad \beta_j < 0,$$

  are Cauchy-Stieltjes.
- It holds (Bernstein's theorem[3])

$$z^{-1} \in \{Cauchy - Stieltjes\} \subset \{Laplace - Stieltjes\}.$$

[3] S. Bernstein. Sur les fonctions absolument monotones, Acta Mathematica 1929

Evaluation of Stieltjes matrix functions

Let $f(z) : \mathbb{R}^+ \to \mathbb{R}$ be ~~an analytic function~~ defined via a Stieltjes integral:

$$f(z) = \int_0^\infty g(t,z) d\mu(t) \qquad g(t,z) \in \left\{ \frac{1}{z+t}, e^{-zt} \right\}.$$

Problem 1. Given a symmetric positive definite matrix $A \in \mathbb{R}^{n\times n}$ with eigenvalues in $[\lambda_{\min}, \lambda_{\max}] \subset \Omega$ and $v \in \mathbb{R}^n$ compute

$$x := f(A)v.$$

Goal. Provide selection strategies for Σ_ℓ and estimates of the error $\|x - x_\ell\|_2$.

Outline

- **Problem 1:**

$$x = f(A)v$$

  - Cauchy-Stieltjes case
  - Laplace-Stieltjes case

- **Problem 2:**

$$x = f(I \otimes A + B \otimes I)\text{vec(low-rank matrix)}$$

  - Laplace-Stieltjes case
  - Cauchy-Stieltjes case

Cauchy-Stieltjes functions: Sketching the idea

- By writing the integral formulation of f we get:

$$f(A)v = \int_0^\infty (A + tI)^{-1} v \; d\mu(t) \approx \int_0^\infty U(A_\ell + tI)^{-1} v_\ell \; d\mu(t).$$

- So we need a space $\mathcal{RK}(A, v, \Sigma_\ell)$ that approximates simultaneously well $(A + tI)^{-1}v$ for any $t > 0$.
- **Problem:** Krylov subspaces are not shift invariant (apart from polynomial Krylov).

Cauchy-Stieltjes functions: Sketching the idea

- Approximating $(A+tI)^{-1}$ $\forall t \geq 0$, is linked to approximate $\frac{1}{\lambda+t}$ in the strip $[\lambda_{\min}, \lambda_{\max}] \times [0, \infty]$.
- We consider a Skeleton approximation of the form

$$\frac{1}{\lambda+t} \approx f_{skel}(\lambda, t) := \left[\frac{1}{\lambda+t_1}, \dots, \frac{1}{\lambda+t_\ell}\right] M^{-1} \begin{bmatrix} \frac{1}{\lambda_1+t} \\ \vdots \\ \frac{1}{\lambda_\ell+t} \end{bmatrix}, \quad M_{ij} = \left(\frac{1}{\lambda_i+t_j}\right).$$

Cauchy-Stieltjes functions: Sketching the idea

$$f_{skel}(\lambda, t) := \left[\frac{1}{\lambda + t_1}, \dots, \frac{1}{\lambda + t_\ell}\right] M^{-1} \begin{bmatrix} \frac{1}{\lambda_1 + t} \\ \vdots \\ \frac{1}{\lambda_\ell + t} \end{bmatrix}$$

Skeleton approximations have 2 crucial properties:

1 Explicit expression of the residual error[4]:

$$\frac{1}{\lambda + t} - f_{skel}(\lambda, t) = \frac{1}{\lambda + t} \cdot \frac{r(\lambda)}{r(-t)}, \qquad r(z) := \prod_j \frac{z - \lambda_j}{z + t_j}.$$

[4] Oseledets. *Lower bounds for separable approximations of the Hilbert kernel*, Sbornik 2007.

Cauchy-Stieltjes functions: Sketching the idea

$$f_{skel}(\lambda, t) := \left[\frac{1}{\lambda + t_1}, \dots, \frac{1}{\lambda + t_\ell}\right] M^{-1} \begin{bmatrix} \frac{1}{\lambda_1 + t} \\ \vdots \\ \frac{1}{\lambda_\ell + t} \end{bmatrix}$$

Skeleton approximations have 2 crucial properties:

1 Explicit expression of the residual error[4]:

$$\frac{1}{\lambda + t} - f_{skel}(\lambda, t) = \frac{1}{\lambda + t} \cdot \frac{r(\lambda)}{r(-t)}, \qquad r(z) := \prod_j \frac{z - \lambda_j}{z + t_j}.$$

2 $f_{skel}(\lambda, t)$ is a rational function in λ with poles $-t_1, \dots, -t_\ell$.
If we set $\Sigma_\ell = \{-t_1, \dots, -t_\ell\}$, then

$$f_{skel}(A, t)v \in \mathcal{RK}_\ell(A, v, \Sigma_\ell) \qquad \forall t \in [0, \infty].$$

[4] Oseledets. *Lower bounds for separable approximations of the Hilbert kernel*, Sbornik 2007.

Cauchy-Stieltjes functions: Sketching the idea

- We have the following point-wise estimate of the error [5]

$$\|(tI + A)^{-1}v - U(tI + A_\ell)^{-1}v_\ell\|_2 \leq \frac{2\|v\|_2}{\lambda_{\min} + t} \min_{r(z)\in\frac{\mathcal{P}_\ell}{\Sigma_\ell}} \frac{\max_{z\in[\lambda_{\min},\lambda_{\max}]}|r(z)|}{\min_{z\in[-\infty,0]}|r(z)|}.$$

[5] An estimate of the $\mathcal{L}^2$-norm in:
Druskin, Knizhnerman, Zaslavsky. *Solution of large scale evolutionary problems using rational Krylov subspaces with optimized shifts*, SISC 2009.

Cauchy-Stieltjes functions: Sketching the idea

- We have the following point-wise estimate of the error [5]

$$\|(tI + A)^{-1}v - U(tI + A_\ell)^{-1}v_\ell\|_2 \leq \frac{2\|v\|_2}{\lambda_{\min} + t} \min_{r(z) \in \frac{\mathcal{P}_\ell}{\Sigma_\ell}} \frac{\max_{z \in [\lambda_{\min}, \lambda_{\max}]} |r(z)|}{\min_{z \in [-\infty, 0]} |r(z)|}.$$

- Minimizing the right hand side over Σ_ℓ means solving

$$\min_{r(z) \in \mathcal{R}_{\ell,\ell}} \frac{\max_{z \in [\lambda_{\min}, \lambda_{\max}]} |r(z)|}{\min_{z \in [-\infty, 0]} |r(z)|},$$

where $\mathcal{R}_{\ell,\ell}$ is the set of (ℓ, ℓ) rational functions.

[5] An estimate of the $\mathcal{L}^2$-norm in:
Druskin, Knizhnerman, Zaslavsky. *Solution of large scale evolutionary problems using rational Krylov subspaces with optimized shifts,* SISC 2009.

Cauchy-Stieltjes functions: Sketching the idea

- This problem can be transformed via a Moebius map $T(z) = \frac{\alpha z+\beta}{\gamma z+\delta}$ into

$$\min_{r(z)\in\mathcal{R}_{\ell,\ell}} \frac{\max_{z\in[a,b]} |r(z)|}{\min_{z\in[-b,-a]} |r(z)|}. \tag{1}$$

that Zolotarev solved $\approx$ 140 years ago.

- In particular, we know explicitly the optimal poles $\widehat{\Sigma_\ell}$ of the rational function that solves (1).
So the optimal poles Σ_ℓ^* for our starting problem are given by

$$\Sigma_\ell^* := T^{-1}(\widehat{\Sigma_\ell}).$$

Theoretical result

Theorem
Let $f(z)$ be a Cauchy-Stieltjes function, U be an orthogonal basis of $\mathcal{RK}_\ell(A, v, \Sigma_\ell^*)$ and $x_\ell = Uf(A_\ell)v_\ell$. Then

$$\|f(A)v - x_\ell\|_2 \leq 8f(\lambda_{min})\|v\|_2\rho^\ell,$$

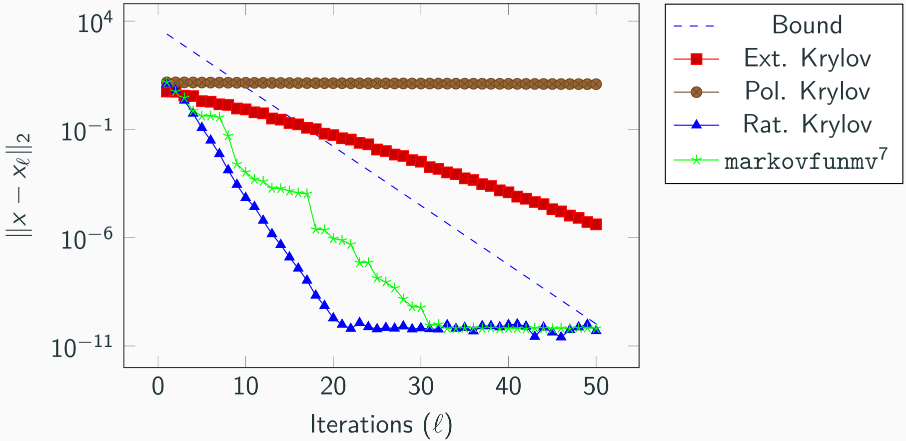
where $\rho := \exp\left(-\frac{\pi^2}{\log\left(16\frac{\lambda_{max}}{\lambda_{min}}\right)}\right)$.

Similar results by Beckermann and Reichel[6].

[6] Beckerman, Reichel. *Error estimate and evaluation of matrix functions via the Faber transform*, SINUM 2009

Numerical results

$$x = A^{-\frac{1}{2}}v, \qquad A = \mathrm{trid}(-1, 2, -1) \in \mathbb{R}^{1000\times 1000}$$



[7] Güttel, Knizhnerman. *A black-box rational Arnoldi variant for Cauchy-Stieltjes matrix functions*, BIT 2013

Laplace-Stieltjes functions

$$f(\lambda) = \int_0^\infty e^{-\lambda t} d\mu(t)$$

- The core idea is to exploit the relation:

$$e^{-\lambda t} = \frac{1}{2\pi \mathbf{i}} \int_{\mathbf{i}\mathbb{R}} \frac{e^{st}}{\lambda + s} \, ds$$

to link (parameter dependent) resolvents with exponentials.

Laplace-Stieltjes functions

$$f(\lambda) = \int_0^\infty e^{-\lambda t} d\mu(t)$$

- The core idea is to exploit the relation:

$$e^{-\lambda t} = \frac{1}{2\pi \mathbf{i}} \int_{\mathbf{i}\mathbb{R}} \frac{e^{st}}{\lambda + s}\ ds$$

  to link (parameter dependent) resolvents with exponentials.

- Then, using the approximation

$$e^{-\lambda t} \approx \int_{\mathbf{i}\mathbb{R}} f_{skel}(\lambda, s) e^{st}\ ds$$

  yields

$$\|e^{-tA}v - Ue^{-tA_\ell} v_\ell\|_2 \leq 4\gamma_\ell \max_{z\in[\lambda_{\min},\lambda_{\max}]} |r(z)|, \qquad r(z) := \prod_j \frac{z-\lambda_j}{z+\lambda_j}$$

  with U orthogonal basis of $\mathcal{RK}_\ell(A, v, \{-\lambda_1, \dots, -\lambda_\ell\})$.

Laplace-Stieltjes functions

Theorem
Let $f(z)$ be a Laplace-Stieltjes function, U be an orthogonal basis of $\mathcal{RK}_\ell(A, v, \Sigma_\ell)$ and $x_\ell = Uf(A_\ell)v_\ell$. Then there exists a choice of Σ_ℓ such that

$$\|f(A)v - x_\ell\|_2 \leq 8\gamma_\ell f(0)\|v\|_2\rho^{\frac{\ell}{2}} \qquad \rho := \exp\left(-\frac{\pi^2}{\log\left(4\frac{\lambda_{max}}{\lambda_{min}}\right)}\right),$$

where $\gamma_\ell := 2.23 + \frac{2}{\pi}\log(4\ell\frac{\lambda_{max}}{\lambda_{min}})$.

Conjecture: The result holds with $\gamma_\ell = 1$.

2D problems with tensor structure

- When considering discretization (say, finite differences) of

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y)$$

on a rectangular domain one get a linear system of the form

$$\underbrace{(A \otimes I + I \otimes A)}_{\mathcal{M}} x = v.$$

- Moreover, if $f(x, y)$ is a regular function or has a small support (e.g. a point source) then

$$v \approx \text{vec}(C)$$

where C is a low-rank matrix, i.e. $C = WZ^T$ for some tall and skinny matrices W, Z.

- Applying the matrix transform method to the fractional analogous of this problem requires to compute $f(\mathcal{M})\text{vec}(C)$.

Function evaluation and Kronecker structure

Problem 2. Given two symmetric positive definite matrices $A, B \in \mathbb{R}^{n \times n}$ with eigenvalues in $[\lambda_{\min}, \lambda_{\max}] \subset \Omega$ and $v = \mathrm{vec}(C) = \mathrm{vec}(\text{low-rank matrix}) \in \mathbb{R}^{n^2}$, compute

$$x := f(I \otimes A + B \otimes I)v, \quad \text{or equivalently} \quad X := \mathrm{vec}^{-1}(f(I \otimes A + B \otimes I)v).$$

Function evaluation and Kronecker structure

Problem 2. Given two symmetric positive definite matrices $A, B \in \mathbb{R}^{n \times n}$ with eigenvalues in $[\lambda_{\min}, \lambda_{\max}] \subset \Omega$ and $v = \text{vec}(C) = \text{vec}(\text{low-rank matrix}) \in \mathbb{R}^{n^2}$, compute

$$x := f(I \otimes A + B \otimes I)v, \quad \text{or equivalently} \quad X := \text{vec}^{-1}(f(I \otimes A + B \otimes I)v).$$

- If $f(z) = z^{-1}$, then this is equivalent to solve the Sylvester equation: we know the low-rank structure is transferred from C to X.

Problem 2. Given two symmetric positive definite matrices $A, B \in \mathbb{R}^{n \times n}$ with eigenvalues in $[\lambda_{\min}, \lambda_{\max}] \subset \Omega$ and $v = \mathrm{vec}(C) = \mathrm{vec}(\text{low-rank matrix}) \in \mathbb{R}^{n^2}$, compute

$$x := f(I \otimes A + B \otimes I)v, \quad \text{or equivalently} \quad X := \mathrm{vec}^{-1}(f(I \otimes A + B \otimes I)v).$$

- If $f(z) = z^{-1}$, then this is equivalent to solve the Sylvester equation: we know the low-rank structure is transferred from C to X.
- Does this hold in more general cases? Yes, it does.

Problem 2. Given two symmetric positive definite matrices $A, B \in \mathbb{R}^{n\times n}$ with eigenvalues in $[\lambda_{\min}, \lambda_{\max}] \subset \Omega$ and $v = \mathrm{vec}(C) = \mathrm{vec}(\text{low-rank matrix}) \in \mathbb{R}^{n^2}$, compute

$$x := f(I \otimes A + B \otimes I)v, \quad \text{or equivalently} \quad X := \mathrm{vec}^{-1}(f(I \otimes A + B \otimes I)v).$$

- If $f(z) = z^{-1}$, then this is equivalent to solve the Sylvester equation: we know the low-rank structure is transferred from C to X.
- Does this hold in more general cases? Yes, it does.
- Once again, we focus on the case where $f(z)$ is a Stieltjes function:

$$f(z) = \int_0^\infty g(t,z)d\mu(t), \qquad g(t,z) \in \left\{ \frac{1}{z+t}, e^{-zt} \right\}.$$

Galerkin projection for evaluating $f(\mathcal{M})\text{vec}(C)$

Inspired by the Galerkin projection for Sylvester equations, we may consider the following algorithm[8]:

[8] Benzi, Simoncini. *Approximation of functions of large matrices with Kronecker structure*, Numerische Mathematik, 2017.

Galerkin projection for evaluating $f(\mathcal{M})\text{vec}(C)$

Inspired by the Galerkin projection for Sylvester equations, we may consider the following algorithm[8]:

- Choose subspaces of $\mathbb{R}^n$ spanned by orthogonal matrices U, V.

[8] Benzi, Simoncini. *Approximation of functions of large matrices with Kronecker structure*, Numerische Mathematik, 2017.

Galerkin projection for evaluating $f(\mathcal{M})\text{vec}(C)$

Inspired by the Galerkin projection for Sylvester equations, we may consider the following algorithm[8]:

- Choose subspaces of $\mathbb{R}^n$ spanned by orthogonal matrices U, V.
- Evaluate the projected matrix function

$$\text{vec}(Y) = f((V \otimes U)^* \mathcal{M}(V \otimes U))\text{vec}(U^* CV) = f(\tilde{\mathcal{M}})\text{vec}(U^* CV),$$

where $\tilde{\mathcal{M}} := V^* BV \otimes I + I \otimes U^* AU$.

[8]Benzi, Simoncini. *Approximation of functions of large matrices with Kronecker structure*, Numerische Mathematik, 2017.

Galerkin projection for evaluating $f(\mathcal{M})\text{vec}(C)$

Inspired by the Galerkin projection for Sylvester equations, we may consider the following algorithm[8]:

- Choose subspaces of $\mathbb{R}^n$ spanned by orthogonal matrices U, V.
- Evaluate the projected matrix function

$$\text{vec}(Y) = f((V \otimes U)^* \mathcal{M}(V \otimes U))\text{vec}(U^* C V) = f(\tilde{\mathcal{M}})\text{vec}(U^* C V),$$

  where $\tilde{\mathcal{M}} := V^* B V \otimes I + I \otimes U^* A U$.
- Use UYV^* as approximation for X.

[8]Benzi, Simoncini. *Approximation of functions of large matrices with Kronecker structure*, Numerische Mathematik, 2017.

Evaluating the small scale matrix function

For $f(z) = z^{-1}$, evaluating $f(\mathcal{M})\text{vec}(C)$ can be done in $\mathcal{O}(n^3)$ using Bartels-Stewart.

For a more general $f(z)$ and $\mathcal{M} = I \otimes A + B \otimes I$:

- The projected matrix retains the same structure.
- $\mathcal{M}$ can be diagonalized in $\mathcal{O}(n^3)$ by diagonalizing A and B.

If $Q_A^* A Q_A = D_A$, $Q_B^* B Q_B = D_B$, then

$$\text{vec}(X) = f(\mathcal{M})\text{vec}(C) = (Q_A \otimes Q_B) f(I \otimes D_A + D_B \otimes I)\text{vec}(Q_A^* C Q_B)$$

which can be written as

$$X = Q_A(F \circ (Q_A^* C Q_B))Q_B^*, \qquad F_{ij} := f(\lambda_{A,i} + \lambda_{B,j}).$$

Again, total cost is about $\mathcal{O}(n^3)$.

Galerkin projection for evaluating $f(\mathcal{M})\mathrm{vec}(C)$

- Algorithm reduces to Galerkin for Sylvester eqs. if $f(z) = z^{-1}$.
- Proposed by Benzi & Simoncini for more general $f(z)$ using polynomial Krylov subspaces.
- Using rational Krylov subspaces yields improved convergence in ill-conditioned cases; major difficulty: how to choose the poles?

Determining the poles: Laplace-Stieltjes case

Here the situation is straightforward because $e^{-t\mathcal{M}} = e^{I\otimes(-tA)}e^{(-tB)\otimes I}$, so that

$$\begin{aligned}
\mathrm{vec}(X) &= f(\mathcal{M})\mathrm{vec}(C) \\
&= \int_0^\infty e^{-t\mathcal{M}}\mathrm{vec}(C)d\mu(t) \\
&= \mathrm{vec}\left(\int_0^\infty e^{-tA}Ce^{-tB}d\mu(t)\right) \\
&= \mathrm{vec}\left(\int_0^\infty \left(e^{-tA}W\right)\left(e^{-tB}Z\right)^T d\mu(t)\right).
\end{aligned}$$

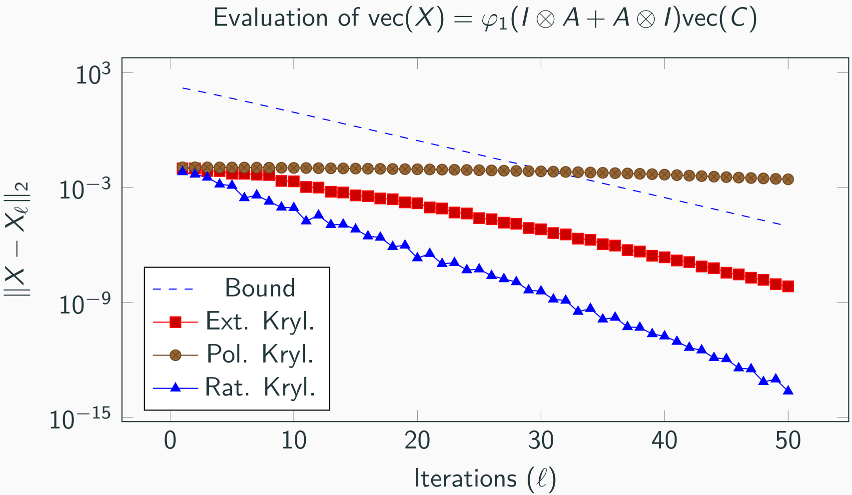
Hence we can choose the same set of poles used in 1D case, for both Krylov subspaces.

Convergence result: Laplace Stieltjes case

Theorem
There exists a choice of poles that, for any Laplace-Stieltjes function f applied to $\mathcal{M} = I \otimes A + B \otimes I$, where A, B are symmetric positive definite with spectrum contained in $[\lambda_{min}, \lambda_{max}]$, yields the convergence

$$\|X - X_\ell\|_2 \leq 16\gamma_{\ell,\kappa} f(0) \cdot \|C\|_2 \cdot \rho^{\frac{\ell}{2}}, \qquad \rho = \exp\left(\frac{\pi^2}{\log(4\frac{\lambda_{max}}{\lambda_{min}})}\right).$$

Numerical results



Determining the poles: Cauchy Stieltjes case

If $f(z) = \int_0^\infty d\mu(t)/(z+t)$ then, $f(\mathcal{M}) = \int_0^\infty d\mu(t)(tI + \mathcal{M})^{-1}$.

Since $tI + \mathcal{M} = A \otimes I + I \otimes (B + tI)$ we have

$$\mathrm{vec}(X) = f(\mathcal{M})\mathrm{vec}(C) \iff X = \int_0^\infty X_t d\mu(t), \qquad AX_t + X_t(B + tI) = C.$$

- Can we design a projection space that is good for all values of t?
- This can be related to the Zolotarev problem:

$$\frac{\max z \in [\lambda_{\min}, \lambda_{\max}] |r(z)|}{\min_{z \in (-\infty, -\lambda_{\min}]} |r(z)|}$$

- Using a Möbius transform, this can be mapped (approximately) into a Zolotarev problem on $[-2\lambda_{\max}, -\lambda_{\min}] \cup [\lambda_{\min}, 2\lambda_{\max}]$.
- We can compute optimal poles there and go back.

Convergence result: Cauchy Stieltjes case

Theorem
There exists a choice of poles that, for any Cauchy-Stieltjes function f applied to $\mathcal{M} = I \otimes A + B \otimes A$*, where* A, B *are symmetric positive definite with spectrum contained in* $[\lambda_{min}, \lambda_{max}]$*, yields the convergence*

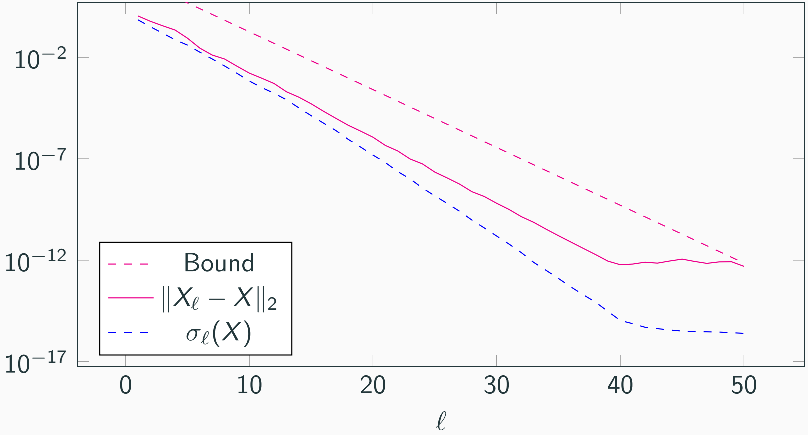
$$\|X - X_\ell\|_2 \leq 4 \cdot f(2\lambda_{min}) \cdot \left(1 + \frac{\lambda_{max}}{\lambda_{min}}\right) \cdot \|C\|_2 \cdot \rho^{-\ell}, \qquad \rho = \exp\left(\frac{\pi^2}{\log(8\frac{\lambda_{max}}{\lambda_{min}})}\right).$$

Note: the exponent for $f(z) = z^{-1}$ is $\exp\left(\frac{\pi^2}{\log(4\frac{\lambda_{\max}}{\lambda_{\min}})}\right)$.

Decaying singular values

The theory predicts the decay in the singular values as well.

Evaluation of $\mathrm{vec}(X) = (I \otimes A + A \otimes I)^{-0.7}\mathrm{vec}(C)$



Conclusions and outlook

- Practically, nested sequences of poles with the same asymptotic behavior can be used.

Possible extensions:

- Similar result for more general spectra configuration (and normal matrices) — implicitly depends on the Zolotarev rational approximation problem.
- For non-normal cases, one can resort to using the field-of-values instead of the spectrum.
- Divide and conquer methods for right hand sides obtained as vectorizations of banded or hierarchical matrices.
- Higher dimensional Laplace-like operators.

Full story:

- Rational Krylov for Stieltjes matrix functions: convergence and pole selection. S. Massei., L.R., arXiv, 2019.