PDEs, Matrix Functions and Krylov Subspace Methods

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Outline

Outline

Initial Value Problems

By the variation-of-constants formula the solution of the IVP

$$\dot{\boldsymbol{u}} = \boldsymbol{A}\boldsymbol{u} + \boldsymbol{g}, \quad \boldsymbol{u}(t_0) = \boldsymbol{u}_0, \qquad \boldsymbol{A} \in \mathbb{C}^{N\times N}; \boldsymbol{g}, \boldsymbol{u}_0 \in \mathbb{C}^N,$$

is given by

$$\boldsymbol{u}(t) = e^{(t-t_0)\boldsymbol{A}}\boldsymbol{u}_0 + (t-t_0)\,\varphi_1\big((t-t_0)\boldsymbol{A}\big)\boldsymbol{g}, \qquad t > t_0,$$

with the "Phi-function"

$$\varphi_1(z) = \frac{e^z - 1}{z}.$$

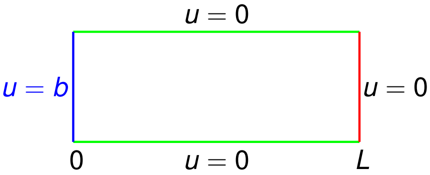
Such relations are the basis of exponential integrators, which address stiffness in ODE systems (in particular MOL semi-discretizations) by explicitly evaluating the action of $e^{\boldsymbol{A}}$ or $\varphi_1(\boldsymbol{A})$ on a vector.

[Hocbruck et al. (1998)], [Minchev & Wright (2005)], [Schmelzer (2007)].

Outline

Dirichlet-Neumann Maps (1)

$$
\begin{aligned}
Au(x) - u_{xx} &= 0, \quad x \in (0, L), \qquad L > 0\\
-u_x(0) &= b,\\
u(L) &= 0.
\end{aligned}
$$

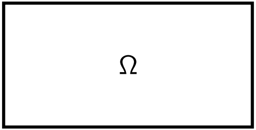


Mapping which assigns $b \mapsto u(0)$ (Neumann-Dirichlet map, impedance function) given by

$$
u(0) = f(A)b, \quad f(z) = \begin{cases} \frac{1}{\sqrt{z}}, & L = \infty, \\ \frac{\tanh(L\sqrt{z})}{\sqrt{z}}, & L < \infty. \end{cases}
$$

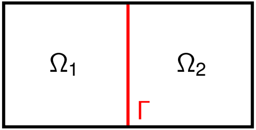
[Druskin & Knizhnerman (1999)]

Model problem



$$\begin{aligned} -\Delta u = f \quad &\text{on} \quad \Omega, \\ u = 0 \quad &\text{on } \partial\Omega \end{aligned}$$

may be reformulated as ($i = 1, 2$)



$$\begin{aligned} -\Delta u_i = f \quad &\text{on} \quad \Omega_i, \\ u_i = 0 \quad &\text{on } \partial\Omega_i \setminus \Gamma \\ \partial_n u_i = S u_i \quad &\text{on } \Gamma \end{aligned}$$

in terms of Dirichlet-Neumann mapping (Steklov-Poincaré operator) $S : H_{00}^{1/2}(\Gamma) \to H_{00}^{-1/2}(\Gamma)$. A spectrally equivalent preconditioner to S is given by $\boldsymbol{M}(\boldsymbol{M}^{-1}\boldsymbol{L})^{1/2}$, where $\boldsymbol{M}$ and $\boldsymbol{L}$ are Galerkin mass and stiffness matrices for basis functions restricted to Γ. [Arioli & Loghin (2008)].

Outline

Stochastic Differential Equations

Certain problems in population dynamics and neutron transport lead to Itô differential equations

$$d\boldsymbol{y}(t) = \boldsymbol{f}(t, \boldsymbol{y}(t))\, dt + \boldsymbol{A}^{1/2}(t, \boldsymbol{y}(t))\, d\boldsymbol{W}(t), \qquad \boldsymbol{y}(t_0) = \boldsymbol{y}_0,$$

with $\boldsymbol{f}$ and $\boldsymbol{A}$ known vector and matrix-valued functions and $\boldsymbol{W}(t)$ a (vector) Wiener process.
Approximation using the Euler-Maruyama method results in the iteration

$$\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + \Delta t\, \boldsymbol{f}(t_n, \boldsymbol{y}_n) + \sqrt{\Delta t}\boldsymbol{A}^{1/2}(t_n, \boldsymbol{y}_n)\omega_n$$

with ω_n sampled from a multivariate normal distribution.
[Allen, Baglama & Boyd (2000)]

Outline

1. Matrix Functions and Differential Equations
   - Initial Value Problems
   - Dirichlet-Neumann Maps
   - Stochastic Differential Equations
   - Frequency Domain Model Reduction

2. Krylov Subspace Approximation
   - Algorithm
   - Restarting
   - Convergence
   - A Posteriori Error Estimation

Frequency Domain Model Reduction

Time-dependent Maxwell's equations on a bounded domain Ω

$$\partial_t(\sigma \boldsymbol{E}) + \nabla\times(\mu\,\nabla\times \boldsymbol{E}) = -\partial_t \boldsymbol{J}^{(i)}, \quad \boldsymbol{n}\times\boldsymbol{E} = \boldsymbol{0} \text{ on } \partial\Omega, \quad \boldsymbol{E}(t_0) = \boldsymbol{E}_0.$$

Instead of MOL-discretization, switch to frequency domain

$$\nabla\times(\mu\,\nabla\times \boldsymbol{E}) + i\omega\sigma\boldsymbol{E} = \boldsymbol{q}, \qquad \boldsymbol{n}\times\boldsymbol{E} = 0 \text{ on } \partial\Omega$$

for $\omega \in [\omega_{\min}, \omega_{\max}]$. FE discretization in space gives

$$(\boldsymbol{K} + i\omega\boldsymbol{M})\boldsymbol{u} = \boldsymbol{q}, \qquad \omega \in [\omega_{\min}, \omega_{\max}].$$

If solution of interest only at p locations (receiver locations), introduce restriction matrix $\boldsymbol{R}$ and evaluate

$$\boldsymbol{f}(\omega) = \boldsymbol{R}^\top(\boldsymbol{K} + i\omega\boldsymbol{M})^{-1}\boldsymbol{q}, \qquad \omega \in [\omega_{\min}, \omega_{\max}].$$

[Börner, E. & Spitzer (2008)].

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Krylov Subspace Approximation of $f(\boldsymbol{A})\boldsymbol{b}$

Given	$\boldsymbol{A} \in \mathbb{C}^{n \times n}$,
	$f : D \to \mathbb{C}$ analytic, $W(\boldsymbol{A}) \subset D$,
	$\boldsymbol{b} \in \mathbb{C}^n$, $\|\boldsymbol{b}\| = 1$,
compute	$f(\boldsymbol{A})\boldsymbol{b}$.

Approximate in Kylov subspace

$$f(\boldsymbol{A})\boldsymbol{b} \approx \boldsymbol{f}_m \in \mathscr{K}_m(\boldsymbol{A}, \boldsymbol{b}) = \{\boldsymbol{v} = p(\boldsymbol{A})\boldsymbol{b} : p \in \mathscr{P}_{m-1}\}, \qquad m = 1, 2, \dots$$

Basic Algorithm

Arnoldi-like decomposition

$$\begin{aligned}\boldsymbol{A}\boldsymbol{V}_m = \boldsymbol{V}_m\boldsymbol{H}_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^\top \\ \operatorname{ran}(\boldsymbol{V}_m) = \mathscr{K}_m(\boldsymbol{A},\boldsymbol{b}),\ \ \boldsymbol{V}_m^H\boldsymbol{V}_m = \boldsymbol{I} \\ \boldsymbol{b} = \boldsymbol{V}_m\boldsymbol{e}_1, \\ \boldsymbol{H}_m \text{ unreduced upper Hessenberg}\end{aligned}$$

Approximant

$$\boldsymbol{f}_m := \boldsymbol{V}_m f(\boldsymbol{H}_m)\boldsymbol{e}_1 = \boldsymbol{V}_m f(\boldsymbol{H}_m)\boldsymbol{V}_m^H\boldsymbol{b}.$$

- Requires evaluation of (first column of) $f(\boldsymbol{H}_m)$ for small dense matrix $\boldsymbol{H}_m$.
- Simplification: $\boldsymbol{H}_m$ Hermitian tridiagonal for $\boldsymbol{A}$ Hermitian (Hermitian Lanczos process).

Three Interpretations

- **Subspace approximation.** $\boldsymbol{H}_m = \boldsymbol{V}_m^H \boldsymbol{A} \boldsymbol{V}_m$ represents $\boldsymbol{A}$ on $\mathscr{K}_m(\boldsymbol{A}, \boldsymbol{b})$ w.r.t. $\boldsymbol{V}_m$. Approximate $f(\boldsymbol{A})$ with $f(\boldsymbol{H}_m)$ there.

- **Cauchy integral.** For a contour Γ with $W(\boldsymbol{A}) \subset \operatorname{int} \Gamma$,

$$f(\boldsymbol{A})\boldsymbol{b} = \frac{1}{2\pi i} \int_\Gamma f(\lambda)(\lambda \boldsymbol{I} - \boldsymbol{A})^{-1} \boldsymbol{b} \, d\lambda$$
$$\approx \frac{1}{2\pi i} \int_\Gamma f(\lambda) \underbrace{\boldsymbol{V}_m(\lambda \boldsymbol{I} - \boldsymbol{H}_m)^{-1} \boldsymbol{V}_m^H \boldsymbol{b}}_{=:\boldsymbol{x}_m(\lambda)} \, d\lambda = \boldsymbol{V}_m f(\boldsymbol{H}_m) \boldsymbol{e}_1.$$

$\boldsymbol{x}_m(\lambda)$: Galerkin approx. of $\boldsymbol{x}(\lambda) := (\lambda \boldsymbol{I} - \boldsymbol{A})^{-1} \boldsymbol{b}$ w.r.t. $\mathscr{K}_m(\boldsymbol{A}, \boldsymbol{b})$.

- **Interpolation.** If $p \in \mathscr{P}_{m-1}$ Hermite-interpolates f at nodes $\Lambda(\boldsymbol{H}_m)$, then

$$f(\boldsymbol{A})\boldsymbol{b} \approx p(\boldsymbol{A})\boldsymbol{b} = \boldsymbol{V}_m p(\boldsymbol{H}_m) \boldsymbol{e}_1 = \boldsymbol{V}_m f(\boldsymbol{H}_m) \boldsymbol{e}_1.$$

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$$

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$$

A Key Relation

For Arnoldi(-like) decomposition of $\mathscr{K}_m(\boldsymbol{A}, \boldsymbol{b})$

$$\boldsymbol{A}\boldsymbol{V}_m = \boldsymbol{V}_m\boldsymbol{H}_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^\top,$$

denote $\gamma_m := \prod_{j=1}^m h_{j+1,j}$.

For any polynomial $p \in \mathscr{P}_{m-1}$ there holds

$$p(\boldsymbol{A})\boldsymbol{b} = \boldsymbol{V}_m\, p(\boldsymbol{H}_m)\boldsymbol{e}_1$$

and, for $p \in \mathscr{P}_m$ with leading coefficient α_m,

$$p(\boldsymbol{A})\boldsymbol{b} = \boldsymbol{V}_m\, p(\boldsymbol{H}_m)\boldsymbol{e}_1 + \alpha_m\gamma_m\boldsymbol{v}_{m+1}.$$

[Druskin & Knizhnerman (1989)], [Saad (1992)], [Paige & al. (1995)].

Outline

Restarting

- For large Krylov spaces storage and computation for Arnoldi process too expensive.
- Remedy: periodically restart Arnoldi process with new initial vector.
- Short recurrences for Arnoldi/Lanczos don't carry over to approximation; two-pass algorithm another option.
- Difficulties: no residual vector, recursive update of approximation.
- Restarting method based on divided differences.

Divided Differences

For function f, nodes $\vartheta_1, \dots, \vartheta_m \in \mathbb{C}$, denote by

$$w_m(z) := \prod_{j=1}^{m} (z - \vartheta_j) \quad \text{nodal polynomial,}$$

$$I_{w_m} f \in \mathscr{P}_{m-1} \quad \text{Hermite interpolant to } f \text{ at } \{\vartheta_j\}_{j=1}^m,$$

$$\Delta_{w_m} f := \frac{f - I_{w_m} f}{w_m} \quad m\text{-th order divided difference of } f \text{ w.r.t. } w_m.$$

Then $f = I_{w_m} f + \Delta_{w_m} f \cdot w_m,$

$$\begin{aligned} f(\boldsymbol{A})\boldsymbol{b} &= [I_{w_m} f](\boldsymbol{A})\boldsymbol{b} + [\Delta_{w_m} f](\boldsymbol{A})\, w_m(\boldsymbol{A})\boldsymbol{b} \\ &= \boldsymbol{V}_m [I_{w_m} f](\boldsymbol{H}_m)\boldsymbol{e}_1 + [\Delta_{w_m} f](\boldsymbol{A})(\boldsymbol{V}_m \underbrace{w_m(\boldsymbol{H}_m)}_{=O} \boldsymbol{e}_1 + \gamma_m \boldsymbol{v}_{m+1}) \\ &= \boldsymbol{f}_m + \gamma_m [\Delta_{w_m} f](\boldsymbol{A}) \boldsymbol{v}_{m+1}. \end{aligned}$$

General Error Representation

Theorem (Eiermann & E., 2006)

Given a function f, matrix $\boldsymbol{A} \in \mathbb{C}^{n \times n}$, vector $\boldsymbol{b} \in \mathbb{C}^n$, and the Arnoldi decomposition $\boldsymbol{A}\boldsymbol{V}_m = \boldsymbol{V}_m\boldsymbol{H}_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^\top$, then the error of the Krylov subspace approximation $\boldsymbol{f}_m$ of $f(\boldsymbol{A})\boldsymbol{b}$ is given by

$$f(\boldsymbol{A})\boldsymbol{b} - \boldsymbol{f}_m = g(\boldsymbol{A})\boldsymbol{v}_{m+1}, \tag{1}$$

where $g(z) = \gamma_m[\Delta_{w_m} f](z)$ and $w_m \in \mathscr{P}_m$ denotes the (monic) nodal polynomial associated with $\Lambda(\boldsymbol{H}_m)$.

Naive approach: update $\boldsymbol{f}_m$ by explicit evaluation of divided differences (block Newton interpolation).

This is (severely) unstable.

Restart Algorithm 1 [Eiermann & E. (2006)]

k standard Arnoldi decompositions of $\boldsymbol{A}$

$$\boldsymbol{A}\boldsymbol{V}_j = \boldsymbol{V}_j\boldsymbol{H}_j + h_{j+1}\boldsymbol{v}_{jm+1}\boldsymbol{e}_m^T, \quad j = 1, 2, \dots, k,$$

of the m-dim. Krylov spaces $\mathscr{K}_m(\boldsymbol{A}, \boldsymbol{v}_{(j-1)m+1})$, glued together,

$$\boldsymbol{A}\hat{\boldsymbol{V}}_k = \hat{\boldsymbol{V}}_k\hat{\boldsymbol{H}}_k + h_{k+1}\boldsymbol{v}_{km+1}\boldsymbol{e}_{km}^T, \tag{2}$$

where $\hat{\boldsymbol{V}}_k := [\boldsymbol{V}_1 \ \boldsymbol{V}_2 \ \cdots \ \boldsymbol{V}_k] \in \mathbb{C}^{n\times km}$,

$$\hat{\boldsymbol{H}}_k := \begin{bmatrix} \boldsymbol{H}_1 & & & \\ \boldsymbol{E}_2 & \boldsymbol{H}_2 & & \\ & \ddots & \ddots & \\ & & \boldsymbol{E}_k & \boldsymbol{H}_k \end{bmatrix} \in \mathbb{C}^{km\times km}, \qquad \boldsymbol{E}_j := h_j\boldsymbol{e}_1\boldsymbol{e}_m^T \in \mathbb{R}^{m\times m}.$$

(2) is an Arnoldi-like decomposition of $\mathscr{K}_{km}(\boldsymbol{A}, \boldsymbol{b})$. Compute

$$\hat{\boldsymbol{f}}_k := \hat{\boldsymbol{V}}_k f(\hat{\boldsymbol{H}}_k)\boldsymbol{e}_1 = \hat{\boldsymbol{f}}_{k-1} + \boldsymbol{V}_k[f(\hat{\boldsymbol{H}}_k)\boldsymbol{e}_1]_{(k-1)m+1:km}.$$

Restart Algorithm 2 [Afanasjew, Eiermann, E. & Güttel (2008)]

Instead of $f(\boldsymbol{A})\boldsymbol{b}$, evaluate $r(\boldsymbol{A})\boldsymbol{b}$ where $f(\lambda) \approx r(\lambda) = \sum_{\ell=1}^{n_p} \frac{\alpha_\ell}{\omega_\ell - \lambda}$ is a suitably accurate rational approximation of f. Now

$$r(\hat{\boldsymbol{H}}_k)\boldsymbol{e}_1 = \sum_{\ell=1}^{n_p} \alpha_\ell(\omega_\ell \boldsymbol{I} - \boldsymbol{A})^{-1}\boldsymbol{e}_1 =: \sum_{\ell=1}^{n_p} \alpha_\ell \hat{\boldsymbol{r}}_\ell.$$

Due to block bidiagonal structure of $\hat{\boldsymbol{H}}_k$, each of the n_p systems $(\omega_\ell \boldsymbol{I} - \boldsymbol{A})\hat{\boldsymbol{r}}_\ell = \boldsymbol{e}_1$ can be solved recursively:

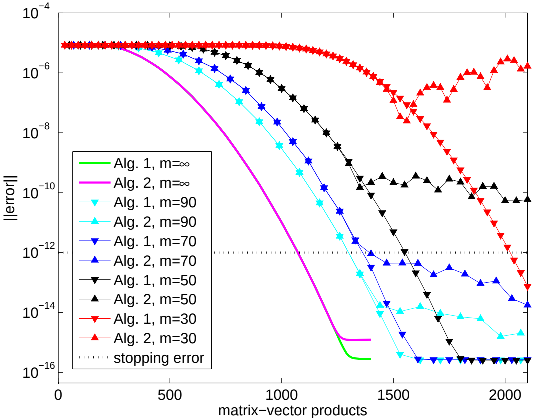
$$(\omega_\ell \boldsymbol{I} - \boldsymbol{H}_1)\boldsymbol{r}_{\ell,1} = \boldsymbol{e}_1, \qquad (\omega_\ell \boldsymbol{I} - \boldsymbol{H}_j)\boldsymbol{r}_{\ell,j} = \boldsymbol{E}_j \boldsymbol{r}_{\ell,j-1}, \quad j = 2, \ldots, k,$$

where $\hat{\boldsymbol{r}}_\ell = [\boldsymbol{r}_{\ell,1}^T, \boldsymbol{r}_{\ell,2}^T, \ldots, \boldsymbol{r}_{\ell,k}^T]^T$. Last block of $r(\hat{\boldsymbol{H}}_k)\boldsymbol{e}_1$ now obtained as

$$[O, \ldots, O, \boldsymbol{I}]\, r(\hat{\boldsymbol{H}}_k)\boldsymbol{e}_1 = \sum_{\ell=1}^{n_p} \alpha_\ell \boldsymbol{r}_{\ell,k}.$$

Numerical Example

$$\boldsymbol{f} = e^{t\boldsymbol{A}}\boldsymbol{b}$$
$$t = 10^{-3},$$
$$\boldsymbol{A} = [\nabla\times(\mu^{-1}\,\nabla\times\,\cdot)]_h$$
$$\dim \boldsymbol{A} = 565\,326$$
$$\Lambda(\boldsymbol{A}) \subset [-10^8, 0]$$



Deflated Restarting

- Compensate for deterioration of convergence due to restarting by augmenting the Krylov subspace with nearly invariant subspaces.
- Identify a subspace which slows convergence, approximate this space and eliminate its influence from the iteration process.
- In practice: Approximate eigenspaces associated with eigenvalues close to singularities of f (for $f = \exp$, approximate eigenspaces which belong to "large" eigenvalues).
- Well known for eigenproblems [Wu & Simon (2000)], [Stewart (2001)] and linear systems [Morgan (2002)].
  For matrix functions, first proposed by [Niehoff (2006)].

Numerical Example

$$\boldsymbol{f} = e^{t\boldsymbol{A}}\boldsymbol{b}$$

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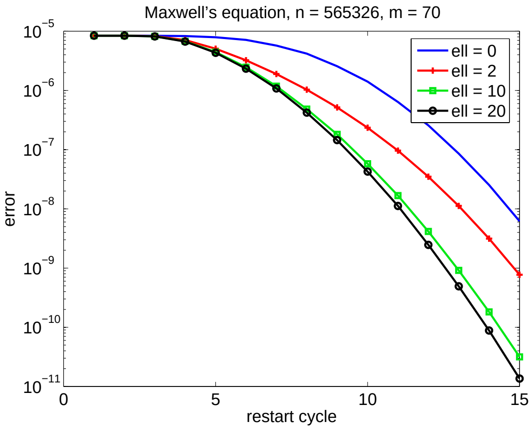
$$\dim \boldsymbol{A} = 565\,326$$

$$\Lambda(\boldsymbol{A}) \subset [-10^8, 0]$$

target: eigenvalues closest to origin.



Outline

Basic Error Bounds

For m-th (unrestarted) Krylov subspace approximation $\boldsymbol{f}_m \approx f(\boldsymbol{A})\boldsymbol{b}$ and any $p \in \mathscr{P}_{m-1}$, there holds

$$\begin{aligned} \|f(\boldsymbol{A})\boldsymbol{b} - \boldsymbol{f}_m\| &\leq \|f(\boldsymbol{A})\boldsymbol{b} - p(\boldsymbol{A})\boldsymbol{b}\| + \|\boldsymbol{f}_m - p(\boldsymbol{A})\boldsymbol{b}\| \\ &= \|(f-p)(\boldsymbol{A})\boldsymbol{b}\| + \|\boldsymbol{V}_m(f-p)(\boldsymbol{H}_m)\boldsymbol{e}_1\|. \end{aligned}$$

For $\boldsymbol{A} = \boldsymbol{A}^H$ we conclude

$$\|f(\boldsymbol{A})\boldsymbol{b} - \boldsymbol{f}_m\| \leq 2 \inf_{p \in \mathscr{P}_{m-1}} \|f - p\|_{\infty,[\lambda_{\min}(\boldsymbol{A}),\lambda_{\max}(\boldsymbol{A})]}.$$

For general $\boldsymbol{A}$:

$$\|f(\boldsymbol{A})\boldsymbol{b} - \boldsymbol{f}_m\| \leq C \inf_{p \in \mathscr{P}_{m-1}} \|f - p\|_{\infty,W(\boldsymbol{A})},$$

where $C \approx 13$ is Crouziex's universal constant.

Sequence of Krylov subspace approximations $\boldsymbol{f}_m \approx f(A)\boldsymbol{b}$ uniquely determined by (any) triangular scheme of interpolation nodes $\vartheta_j^{(m)} \in \mathbb{C}$ or their associated nodal polynomials $w_m \in \mathscr{P}_m$ ($w_0(z) \equiv 1$)

$$\begin{array}{llll} \vartheta_1^{(1)} & & & \\ \vartheta_1^{(2)} & \vartheta_2^{(2)} & & \\ \vartheta_1^{(3)} & \vartheta_2^{(3)} & \vartheta_3^{(3)} & \\ \vdots & \vdots & & \ddots \end{array} \qquad \begin{aligned} v_1(z) &= z - \vartheta_1^{(1)}, \\ v_2(z) &= (z - \vartheta_1^{(2)})(z - \vartheta_2^{(2)}), \\ v_3(z) &= (z - \vartheta_1^{(3)})(z - \vartheta_2^{(3)})(z - \vartheta_3^{(3)}), \\ &\vdots \end{aligned}$$

making up the vectors in associated Arnoldi-like decomposition, i.e., $\boldsymbol{v}_m = v_{m-1}(\boldsymbol{A})\boldsymbol{b}, m = 1, 2, \dots$.

Question: How quickly does $\boldsymbol{f}_m$ converge to $f(\boldsymbol{A})\boldsymbol{b}$ and how does this depend on $\boldsymbol{A}$, $\boldsymbol{b}$, f and $\{\vartheta_j^{(m)}\}$?

More Refined Bounds

Interpolation Theory: prescribed nodes

Under the assumption that the interpolation nodes are

- contained in a fixed compact set $\Omega \subset \mathbb{C}$,
- distributed asymptotically according to measure μ supported on Ω,

one can show

$$\begin{cases} \|f(\boldsymbol{A})\boldsymbol{b} - \boldsymbol{f}_m\|^{1/m} \leq C, & \text{if } f \text{ has finite singularities,} \\ (m\|f(\boldsymbol{A})\boldsymbol{b} - \boldsymbol{f}_m\|)^{1/m} \leq C, & \text{if } f \text{ is entire of order 1,} \end{cases}$$

where the constant C depends on

- the domain of analyticity and type of f,
- $\Lambda(A)$
- relative to the level curves of the logarithmic potential associated with μ.

Basic Quantities

Counting measure μ_m associated with m-th interpolation nodes:

$$\mu_m = \frac{1}{m}\sum_{j=1}^{m} \delta_{\vartheta_j^{(m)}} \qquad \text{where, for any } M \subset \mathbb{C},\ \delta_\vartheta(M) = \begin{cases} 1, & \vartheta \in M, \\ 0, & \text{otherwise.} \end{cases}$$

For every measure μ supported on the compact set $\Omega \subset \mathbb{C}$ we define the logarithmic potential $U^\mu : \mathbb{C} \to \mathbb{R}_0^+$ of μ by

$$U^\mu(z) = \int_\Omega \log \frac{1}{|z-t|}\, d\mu(t) = -\int_\Omega \log|z-t|\, d\mu(t).$$

For the counting measure we have

$$U^{\mu_m}(z) = -\frac{1}{m}\sum_{j=1}^{m} \log|z-\vartheta_j^{(m)}|,$$

and therefore, since $|v_m(z)|^{1/m}| = \left(\prod_{j=1}^{m} |z-\vartheta_j^{(m)}|\right)^{1/m}$,

$$\log|v_m(z)|^{1/m} = \frac{1}{m}\sum_{j=1}^{m} \log|z-\vartheta_j^{(m)}| = -U^{\mu_m}(z).$$

Example

Two well-known node sequences

Equidistant: $$\vartheta_j^{(m)} = -1 + 2\frac{j-1}{m-1}$$

$$\mu_m \xrightarrow{*} \mu, \; d\mu(t) = \tfrac{1}{2}\, dt$$

$$U^{\mu}(z) = 1 - \mathrm{Re}[(1-z)\log(1-z) + (1+z)\log(1+z)]$$

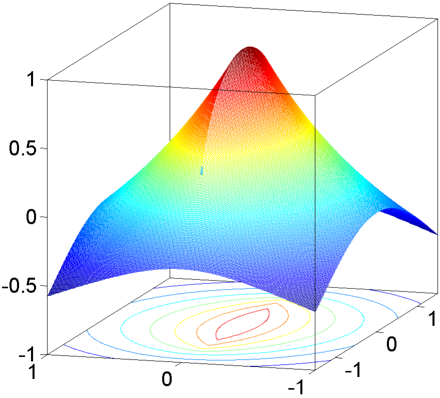
Chebyshev: $$\vartheta_j^{(m)} = \cos\frac{(j-1)\pi}{m-1}$$

$$\mu_m \xrightarrow{*} \mu, \; d\mu(t) = \frac{1}{\pi}\frac{dt}{\sqrt{1-t^2}}$$

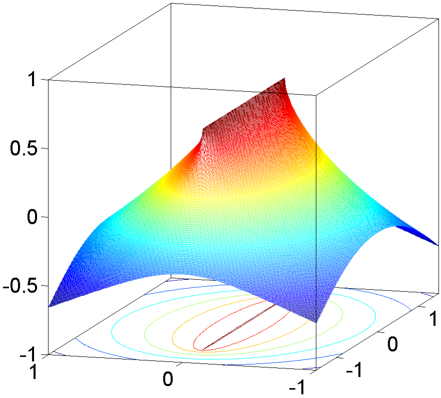
$$U^{\mu}(z) = e^{-1/2} - \log\left|z - \sqrt{z^2-1}\right|$$

Example

Their logarithmic potentials



Equidistant

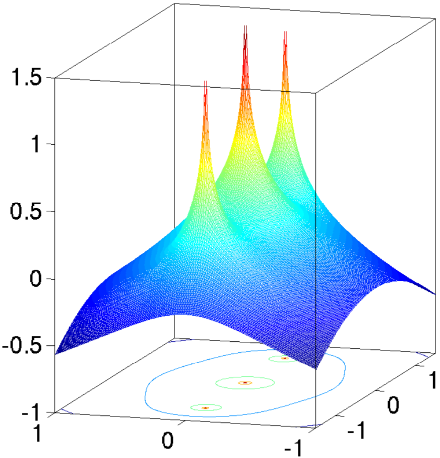


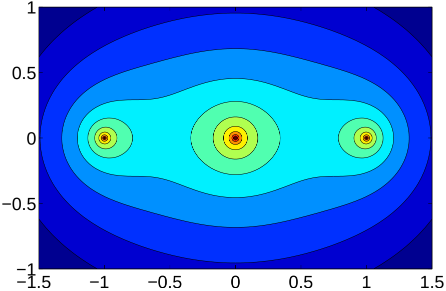
Chebyshev

Another Example

Typical for restarting

Repeat nodes $\vartheta = -1, 0, 1$ cyclically, $\mu_m \xrightarrow{*} \mu = \frac{1}{3}(\delta_{-1} + \delta_0 + \delta_1)$

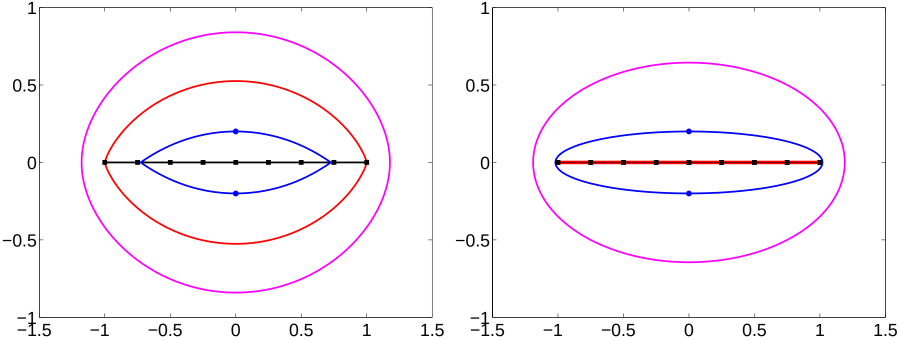




Potential Level Sets

For $\rho \geq 0$ define the level sets $\quad \Omega_\mu(\rho) := \{z : U^\mu(z) \geq -\log(\rho)\}$
and set

$$\rho_\mu(A) := \inf\{\rho : \Lambda(A) \subset \Omega_\mu(\rho)\},$$
$$\rho_\mu(f) := \inf\{\rho : f \text{ analytic in } \Omega_\mu(\rho)\}$$



$[\lambda_{\min}(A), \lambda_{\max}(A)] = [-1, 1], \qquad f(z) = 1/(1 + 25z^2)$

Can extend from linear systems to matrix functions the techniques of Kuijlaars and Beckermann to quantify the effect of interpolating at successively better approximations of parts of $\Lambda(\boldsymbol{A})$.

The asymptotic convergence factor of the Arnoldi approximation can be described using potentials of constrained equilibrium measures. The error is given by

- c_m^m if f has finite singularities, where $c_m < 1$ is a non-increasing function of m which depends on the eigenvalue distribution of A.
- $(c_m/m)^m$ if f is entire of order 1, where c_m is a non-increasing function of m.

Outline

1. Matrix Functions and Differential Equations
   - Initial Value Problems
   - Dirichlet-Neumann Maps
   - Stochastic Differential Equations
   - Frequency Domain Model Reduction

2. Krylov Subspace Approximation
   - Algorithm
   - Restarting
   - Convergence
   - A Posteriori Error Estimation

- For f rational, $\boldsymbol{A}$ Hermitian
  - Derive upper and lower bounds by exploiting collinearity of Galerkin residuals for shifted linear systems [Frommer & Simoncini (2008)]
  - Use CG-lower bounds of [Strakos & Tichy (2002)] for shifted systems and sum. [Frommer & Simoncini (2008)]
- For general f, Hermitian $\boldsymbol{A}$
  - Can derive upper and lower bounds based on error representation formula (divided differences) [Eiermann, E. & Güttel (2008)]
- For general f, general $\boldsymbol{A}$
  - Can use auxuliary nodes in error representation formula to obtain estimates, upper or lower bounds [Saad (1992)], [Philippe & Sidje (1993)], [Eiermann, E. & Güttel (2008)]

Summary

- Evaluation of $f(\boldsymbol{A})\boldsymbol{b}$ required for many PDE applications.
- (Restarted) Krylov subspace methods effective for large problems.
- Asymptotic convergence behavior well understood, at least in Hermitian case.
- Several estimators available for error of Krylov subspace approximation to $f(\boldsymbol{A})\boldsymbol{b}$.

Further Reading

Martin Afanasjew, Michael Eiermann, Oliver G. Ernst, and Stefan Güttel.
On a generalization of the steepest descent method for matrix functions.
Electron. Trans. Numer. Anal., 2008.
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Linear Algebra and its Applications, 2008 (to appear).

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Fast 3D simulation of transient electromagnetic fields by model reduction in the frequency domain using Krylov subspace projection.
Geophysical Journal International, 73(3):766–780, 2008.

Michael Eiermann and Oliver G. Ernst.
A restarted Krylov subspace method for the evaluation of matrix functions.
SIAM Journal on Numerical Analysis, 44:2481–2504, 2006.

Michael Eiermann, Oliver G. Ernst, and Stefan Güttel.
Asymptotic convergence analysis of Krylov subspace approximations to matrix funcions using potential theory.
(in preparation).

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A posteriori error estimation for Krylov subspace approximation of matrix functions.
(in preparation).