Leja interpolation for matrix functions

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Innovative Time Integrators

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Aim

Problem

Exponential integrator schemes require the evaluation or approximation of a matrix function acting on vectors. We denote this action by

$$\phi(A)v, \quad A \in \mathbb{R}^{d\times d}, \quad v \in \mathbb{R}^{d},$$

for some analytic function ϕ.

Ansatz

Polynomial interpolation with Leja points.

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Overview

1. Polynomial interpolation with Newton's scheme
2. Introduction to Leja points
3. Extension to the matrix case
4. Computation
5. Future work

Newton interpolation

Ansatz

Let f be a function, analytic in an open set $K \subset \mathbb{C}$ and $\{\xi_i\}_{i=0}^n$ points in K. The Newton interpolation uses the ansatz

$$p(x) = a_0 + a_1(x - \xi_0) + a_2(x - \xi_0)(x - \xi_1) + \dots \\ \dots + a_n(x - \xi_0) \cdots (x - \xi_n).$$

Divided differences

We define the divided differences $f[\xi_j, \dots, \xi_k]$ of f at the points $\{\xi_i\}_{i=0}^n$ as

$$f[\xi_j, \dots, \xi_k] := \frac{f[\xi_{j+1}, \dots, \xi_k] - f[\xi_j, \dots, \xi_{k-1}]}{\xi_k - \xi_j}, \quad f[\xi_i] = f(\xi_i).$$

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Newton interpolation 2

Rewritten

With the divided differences the scheme can be written in a more stable and compact from (reduction of round-off errors)

$$p_n(x) = f[\xi_0] + \sum_{j=1}^{n} f[\xi_0, \ldots, \xi_j] \prod_{k=0}^{j-1} (x - \xi_k).$$

Remark

- *It is easy to compute p_{n+1} from p_n.*
- *Optimally conditioned interpolation for Chebyshev points.*

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Definition of Leja points

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Define a sequence of points with same convergence properties as Chebyshev points, but computational advantages

Definition (Leja points)

Let $K \subset \mathbb{C}$ be a compact set then the sequence of Leja points $\{\xi_i\}_{i=0}^{\infty}$ for K is defined recursively as:

- ξ_0 *can be chosen arbitrary, normally* $|\xi_0| = \max_{z \in K} |z|$
- ξ_m *is then defined as*

$$\xi_m \in \arg\max_{z \in K} \prod_{i=0}^{m-1} |z - \xi_i|, \quad m > 0.$$

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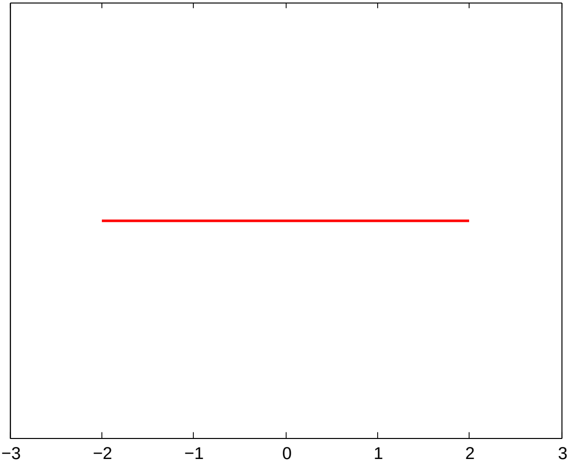

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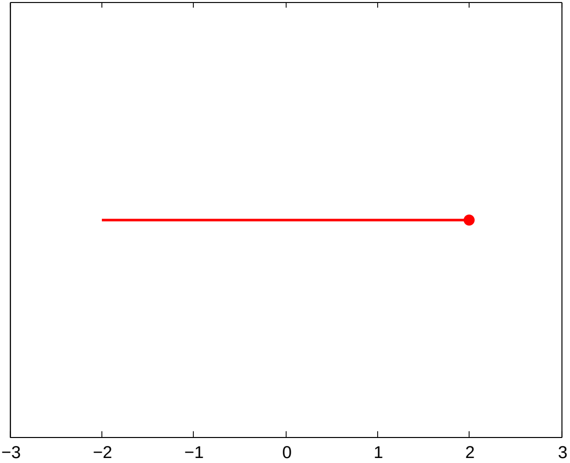

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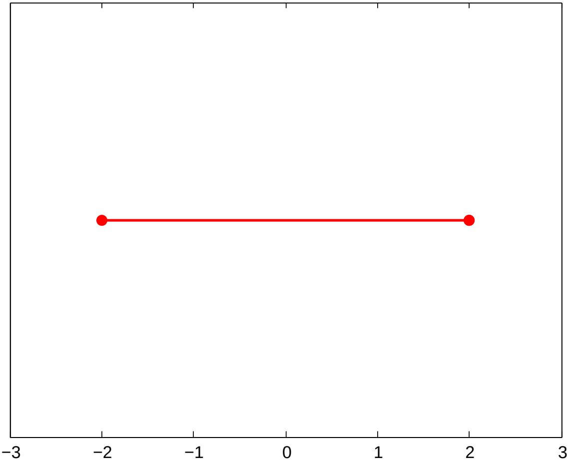

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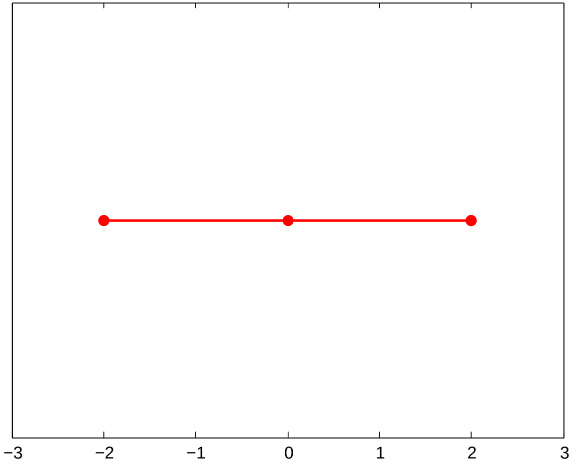

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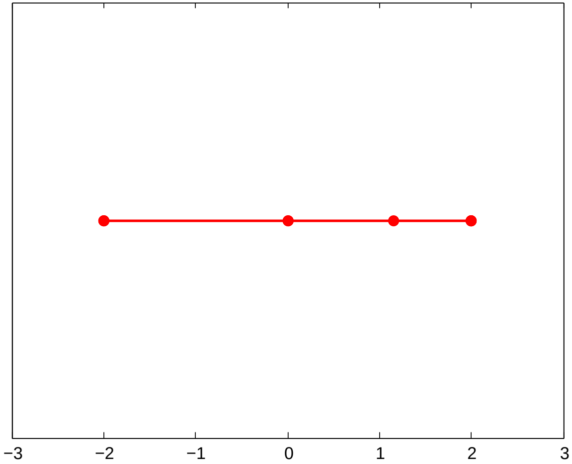

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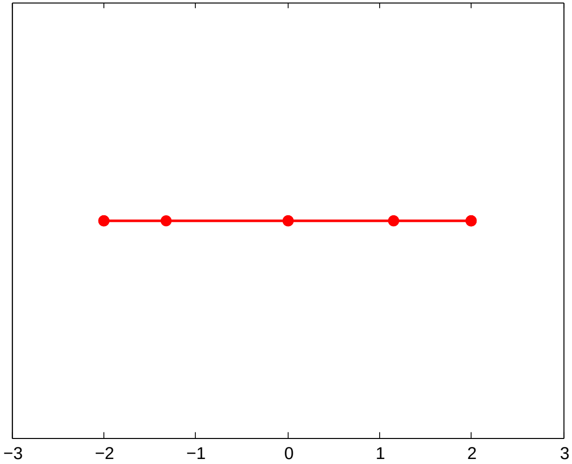

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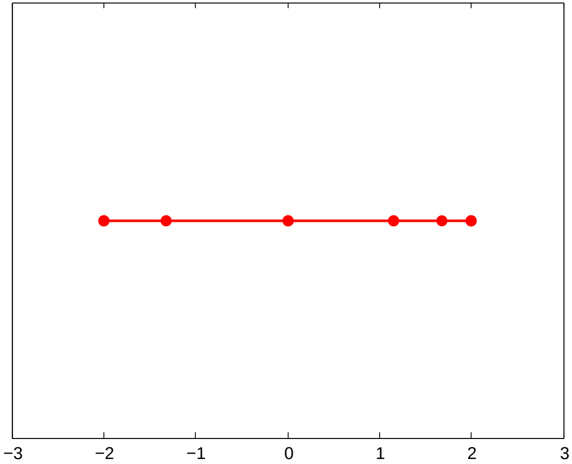

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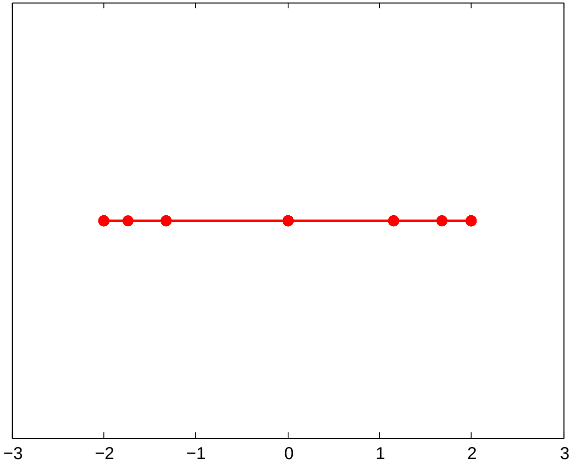

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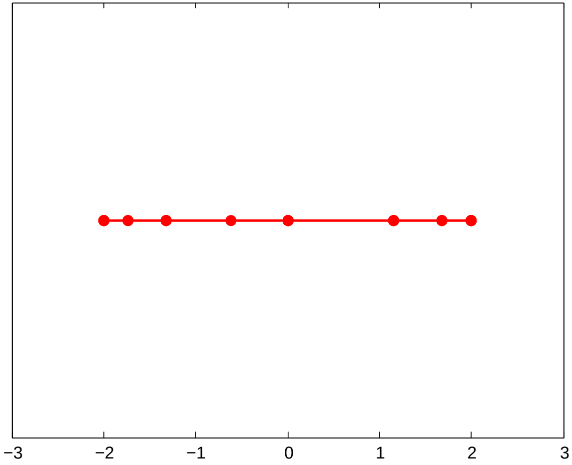

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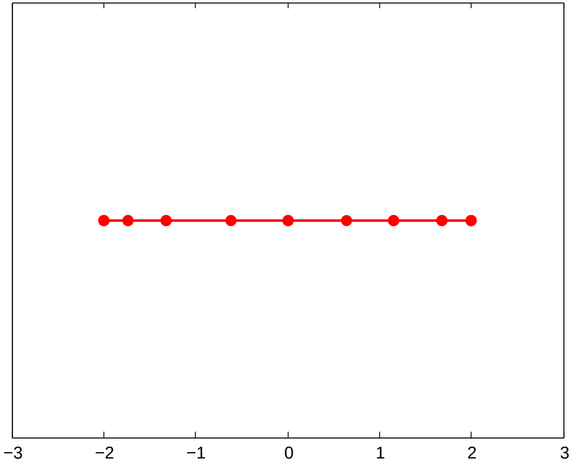

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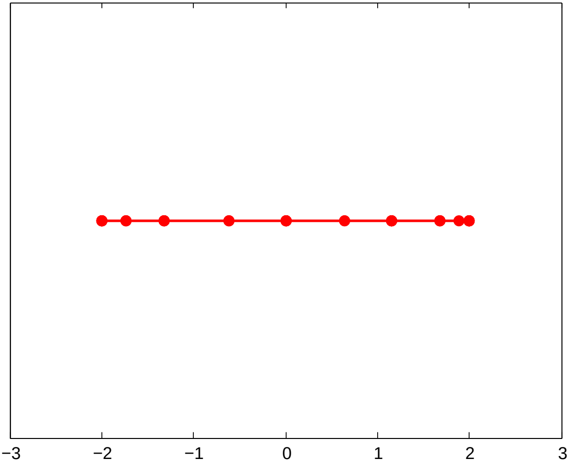

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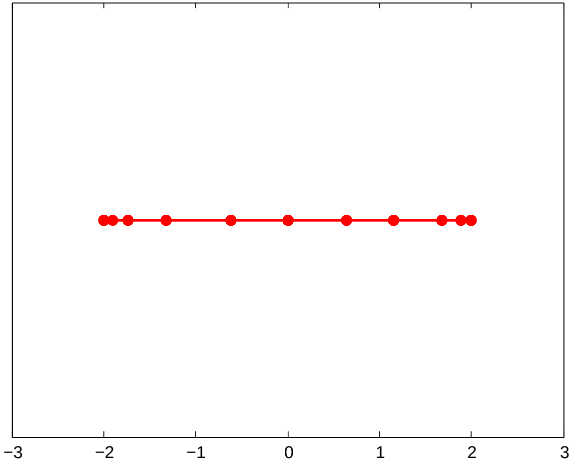

Computation

Computation of Leja points

- For $K \subset \mathbb{C}$ compact, $\{\xi_i\} \in \partial K$.
- Replace K by discrete $S_M \subset \partial K$ with $|S_M| = M$.

Remark

- *For our purposes m Leja points in* $[-2, 2]$.

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Convergence and stability

Convergence

For entire functions super-linear convergence can be shown.

Stability

Let $T : \mathbb{C}^{m+1} \to \mathbb{P}_m$ map a sequence of points $\{\xi_i\}$ to the interpolation polynomial in Newton form.

- $\mathrm{cond}(T)$ grows exponentially for arbitrary points.
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Nodes	equidistant	rand. chosen	Chebyshev	Leja
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Convergence for matrix functions

Preliminaries

- Let f be analytic in $K = B(0, R_{max}) \subset \mathbb{C}$
- Let $\{p_m\} \in \mathbb{P}_m$ be the polynomial interpolation to f in the Leja points of K

The sequence $\{p_m\}$ converges asymptotically like the best uniform approximation polynomial to f in K.

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Let $A \in \mathbb{R}^{n\times n}$, $v \in \mathbb{R}^n$ and $\sigma(A) \subset B(0, R)$ for some $0 < R < R_{max}$. Then $\{p_m(A)v\}$ converges to $f(A)v$.

Corollary

For an entire functions f this means that

$$\limsup_{m\to\infty} \|f(A)v - p_m(A)v\|_2^{1/m} = 0$$

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Computation of φ-functions

Problem

We want to compute $\varphi_k(hA)v$ for the entire functions

$$\varphi_k(\tau z) = \tau^{-k} \int_0^{\tau} e^{(\tau - s)z} \frac{s^{k-1}}{(k-1)!}\, ds, \quad k \geq 1.$$

up to a specified tolerance.

Algorithm

Leja interpolation of φ-functions

Input: A, v, h, tol, k

Compute rough estimate of spectrum $h\sigma(A)$:

$$(-a, -\mathrm{i}b), (0, -\mathrm{i}b), (0, \mathrm{i}b), (a, \mathrm{i}b) \quad a, b \geq 0$$

If: $a \geq b$ Newton interpolation on real Leja points in $[-a, 0]$

$a < b$ Newton interpolation on conjugate pairs of Leja points in $D = \{z \in D : \Re z = -a/2, \Im z \in [-b, b]\}$ (real arithmetic).

Output: approximation of $\varphi_k(hA)v$ with accuracy tol

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Computation of divided differences d_i at shifted $\varphi_k(h(c-\gamma\xi_i))$.

Initialise: $q_0 = v$, $p_0(hA)v = d_0 q_0$

while: $\|e_m\| \leq tol$

$$q_m = (hA - \xi_{m-1})q_{m-1},$$
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return: $p_m(hA)v$, $\|e_m\|$

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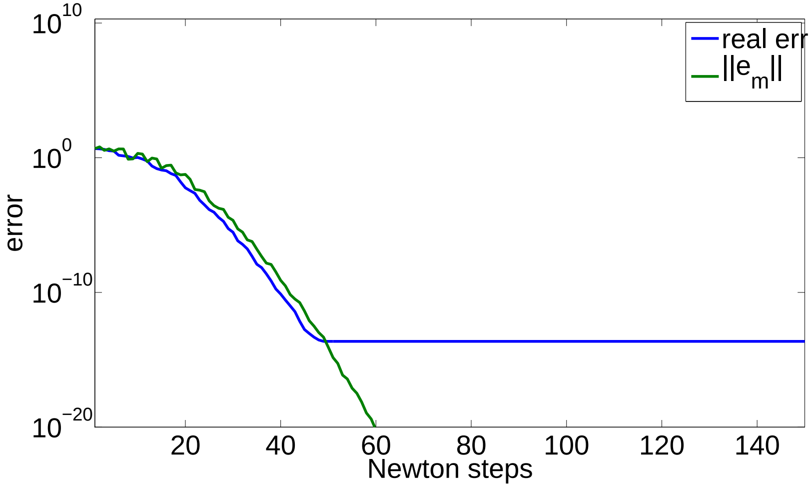
Example

Example (2D advection-diffusion)

Computation of $\mathrm{e}^{hA}v$ *with polynomial interpolation in Leja points for:*

- *dimension of A:* 10.000×10.000,
- *Peclet number* 0.303,
- $v = [1, \ldots, 1]^{\mathsf{T}}$,
- $h = 5e\text{-}4$,
- *tolerance* $1e\text{-}12$.

Example - 2D advection-diffusion, h =5e-4



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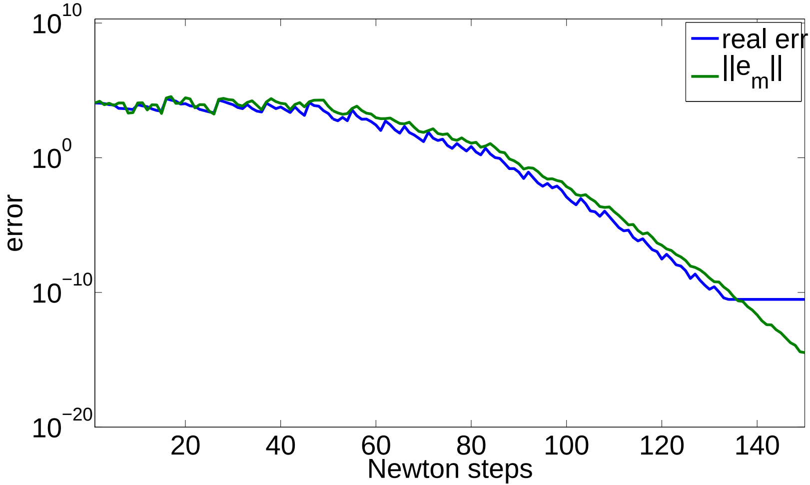

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$y = v$
for $j = 1 : L$
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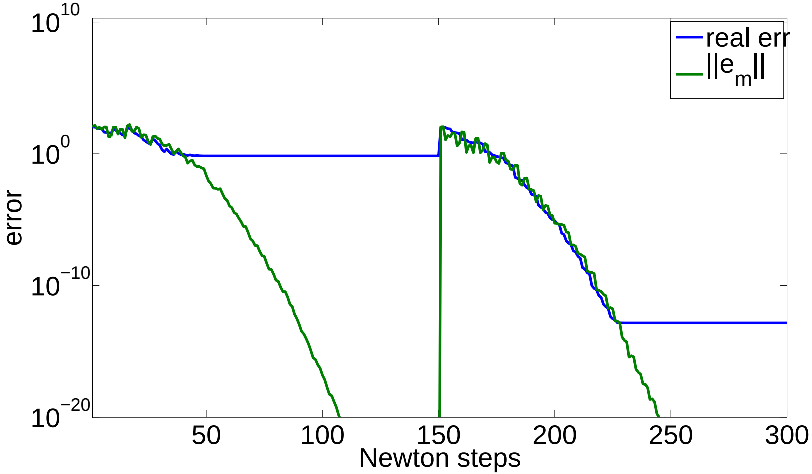

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- multiply-accumulate functionality
- parallel data access
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Parallelisation on GPU:

- primary matrix-vector multiplications
- multiply-accumulate functionality
- parallel data access
- data transfer
- data types

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Computation of divided differences

Standard computation

$$f[\xi_j, \ldots, \xi_k] := \frac{f[\xi_{j+1}, \ldots, \xi_k] - f[\xi_j, \ldots, \xi_{k-1}]}{\xi_k - \xi_j}, \quad f[\xi_i] = f(\xi_i).$$

- easy to implement with low storage demands
- vulnerable to round-off errors
- stable computation via matrix function

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Stable dd via matrix function [M. Caliari 2007]

Matrix computation

Divided differences $\{d_i\}$ of $f(h(c+\gamma\xi_i))$ at $\xi_i \in [-2,2]$ are the first column of the matrix function $f(H_m)$ for

$$H_m = h(cI_{m+1} + \gamma T_m), \quad T_m = \begin{bmatrix} \xi_0 & & & & \\ 1 & \xi_2 & & & \\ & 1 & \ddots & & \\ & & \ddots & \ddots & \\ & & & 1 & \xi_m \end{bmatrix}.$$

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Computation of $\varphi(H_m)$

- scale H_m by $\tau = 1/L$ s.t. $\max_i |\tau x_i| < 1.59$ for $x_i = h(c + \gamma\xi_i)$,
- compute $\varphi(\tau H_m)$ by Taylor expansion,
- recover, in L steps, $\varphi(H_m)e_1$ via recurrence relation.

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Thank you for your attention. Enjoy the wine!

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