The Leja method: backward error analysis and implementation

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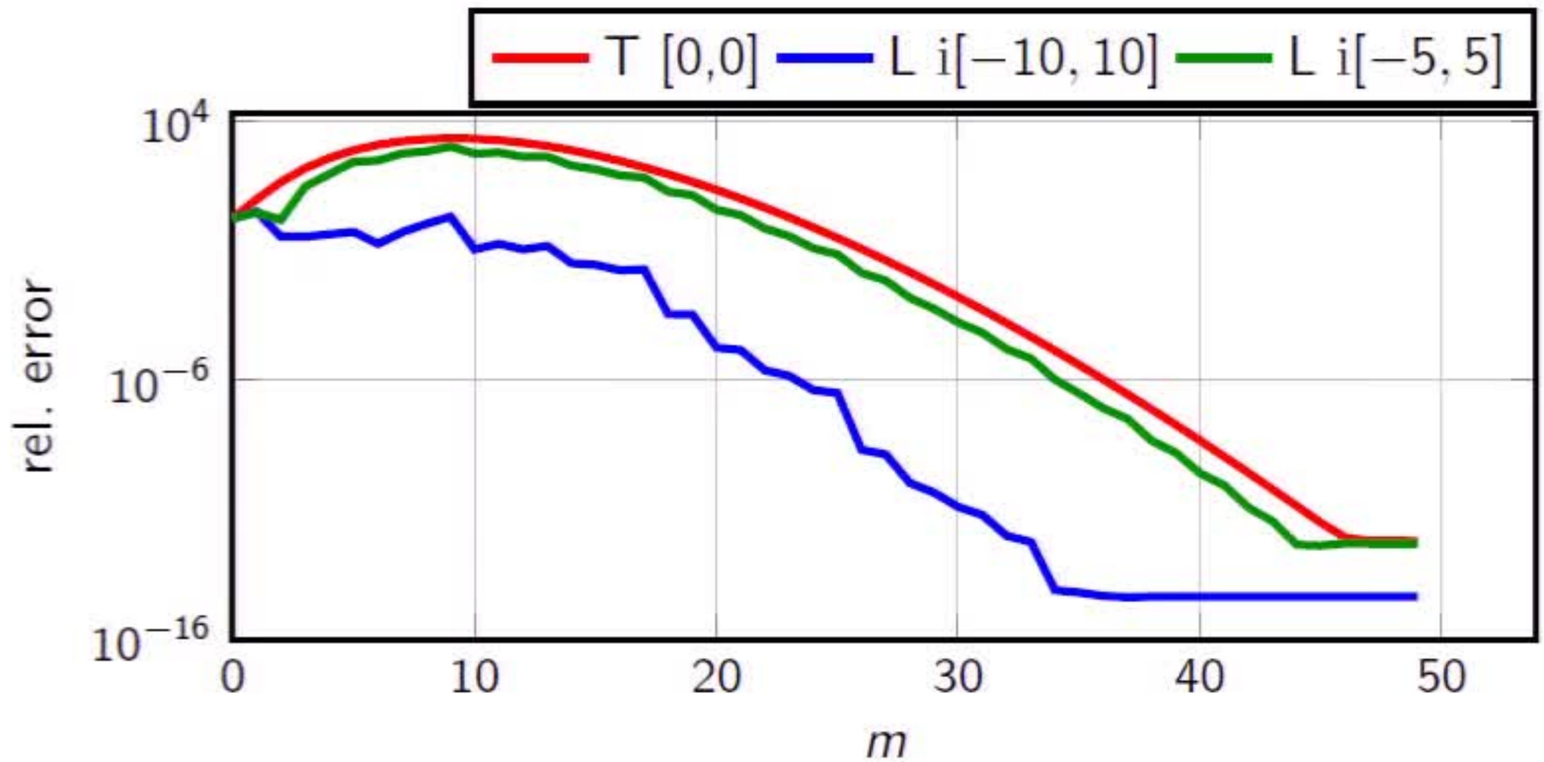
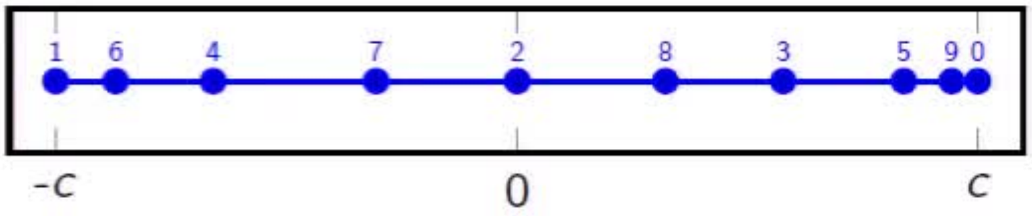
Schrödinger equation in 3D



Leja interpolation

Interpolation points



$$\xi_j \in \arg\max_{\xi \in [-c,c]} \prod_{i=0}^{j-1} |\xi - \xi_i|$$

Interpolation polynomial $L_{m,c}(x) \approx \mathrm{e}^x$ used here for

$$L_{m,c}(A)v \approx \mathrm{e}^A v,$$

costs dominated by matrix-vector products.

Theory 2

A power-series expansion of $\Delta A = h_{m+1,c}(A)$ has the bound

$$\|h_{m+1,c}(A)\| = \|\sum_{k=1}^{\infty} a_{k,c} A^k\| \leq \sum_{k=1}^{\infty} |a_{k,c}| \|A\|^k =: \tilde{h}_{m+1,c}(\|A\|).$$

We can compute

$$\theta_{m,c} := \text{unique positive root of } \frac{\tilde{h}_{m+1,c}(\theta)}{\theta} = \mathrm{tol}.$$

in high accuracy.

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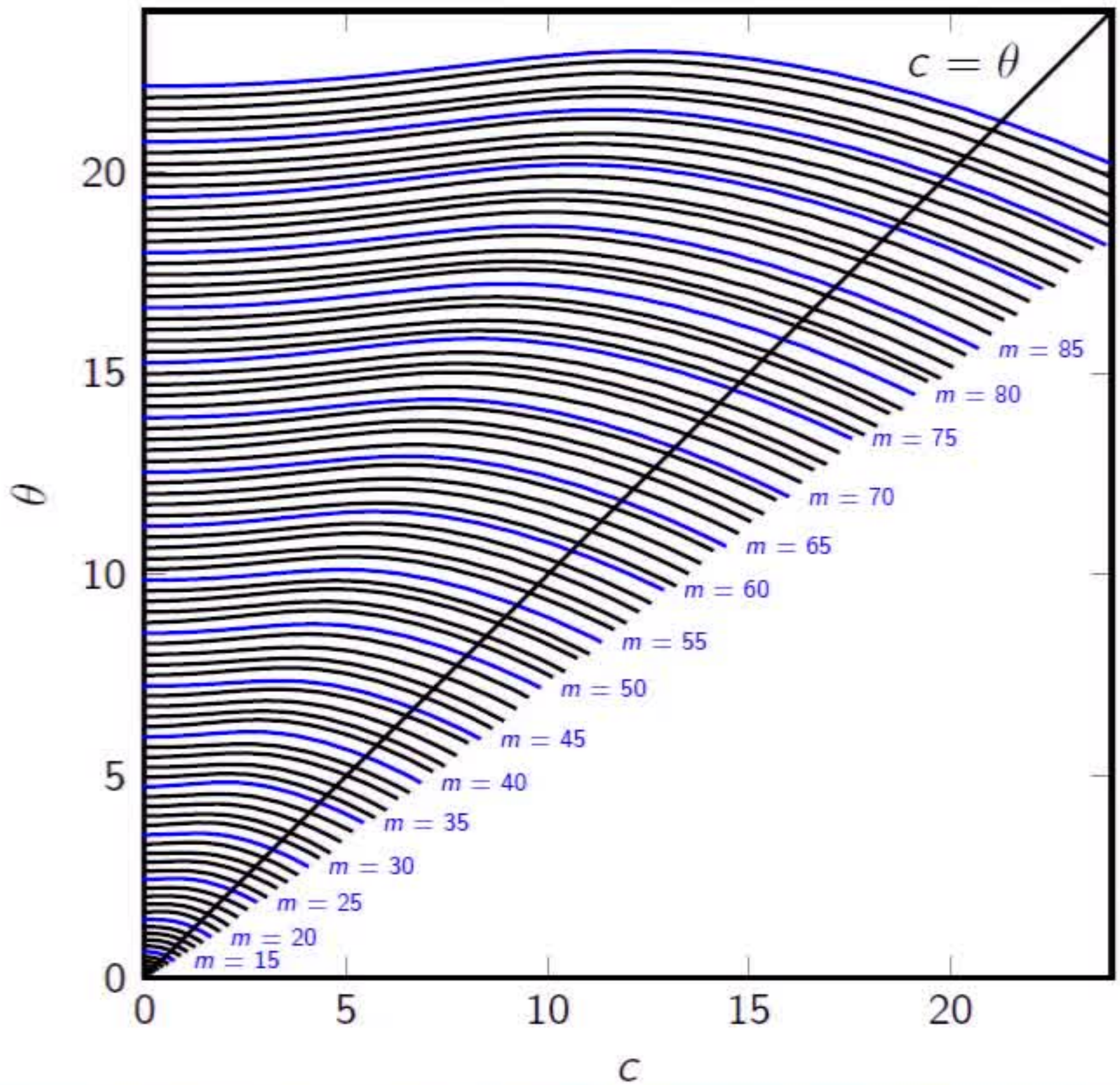
compare Al-Mohy and Higham (2011)

Theory 2



c = θ
m = 85
m = 80
m = 75
m = 70
m = 65
m = 60
m = 55
m = 50
m = 45
m = 40
m = 35
m = 30
m = 25
m = 20
m = 15
θ
c
0
5
10
15
20

Theory 3

Computation

Select m_* and s such that

$$L_{m_*}(s^{-1}A)^s = \mathrm{e}^{A+\Delta A} \quad \text{with } \|\Delta A\| \leq \mathrm{tol}\|A\|$$

is computed with the least matrix-vector products.

Total cost for interpolation polynomial of degree m

$$C_m(A) = ms = m\left\lceil \|A\|/\theta_m \right\rceil .$$

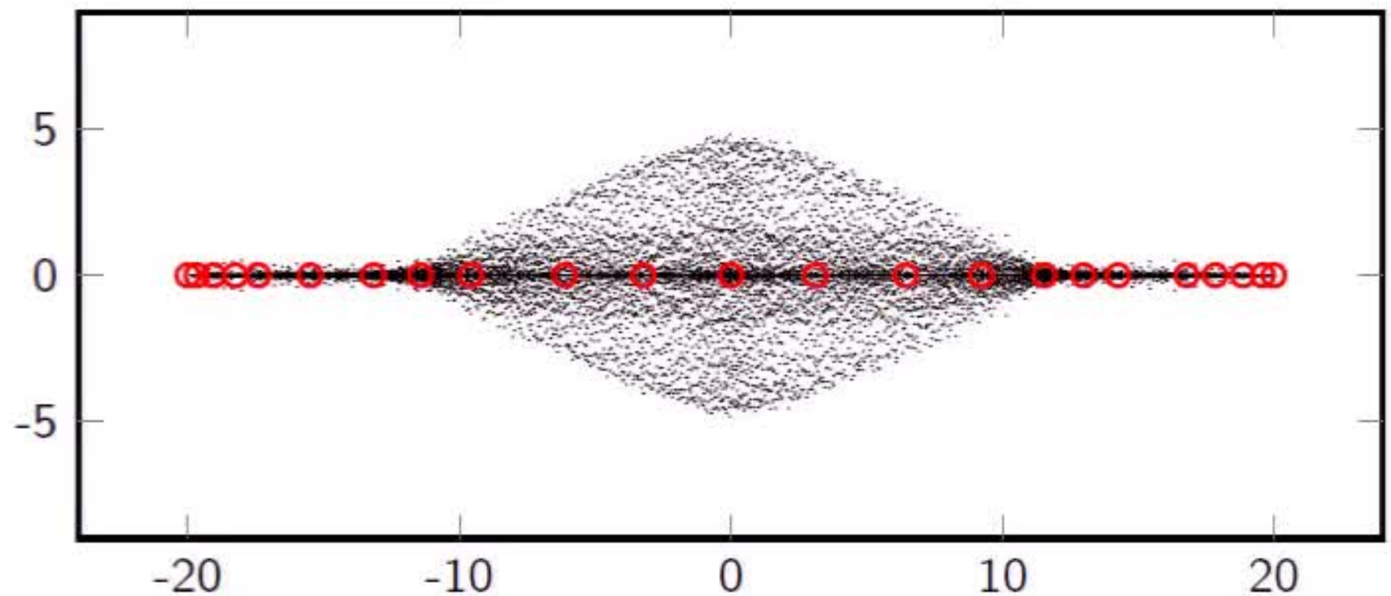
Optimal choice:

$$m_* = \underset{2\leq m \leq m_{max}}{\arg\min} \left\{ m\left\lceil \|A\|/\theta_m \right\rceil \right\} \quad s = \left\lceil \|A\|/\theta_{m_*} \right\rceil .$$

compare Al-Mohy and Higham (2011)

Algorithm - Input A, v, tol

$$\frac{1}{20}(A - \mu I)$$



Compute

$$\left[\mathrm{e}^{\mu/s} L_{98}(s^{-1}(A - \mu I))\right]^s$$

by Newton interpolation with Leja points in $[-\theta_{98}, \theta_{98}]$.