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On the computation of the scalar and the matrix Mittag-Leffler functions

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Numerical Linear Algebra Group Meeting
Manchester, 14 November 2019

The (scalar) Mittag-Leffler function (1)

The Mittag-Leffer (ML) function is a complex function that is defined by the convergent series

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad \Re(\alpha) > 0 \tag{1}$$

where $z \in \mathbb{C}$ and $\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} \mathrm{d}t$ is the Euler gamma function.

• Solution of linear fractional differential equations - generalization of the exponential function

• Practical interest - $\alpha,\ \beta \in \mathbb{R}$ with $\alpha > 0$, particularly $0 < \alpha < 1$ and $\beta > 0$

The (scalar) Mittag-Leffler function (2)

- Recurrence relations between the ML functions with different parameters:

$$E_{\alpha,\beta}(z) = \frac{1}{m}\sum_{k=0}^{m-1} E_{\alpha/m,\beta}\left(e^{2\pi ki/m} z^{1/m}\right), \quad m \geq 1, m \in \mathbb{N},$$

$$E_{\alpha,\beta}(z) = \frac{1}{\Gamma(\beta)} + zE_{\alpha,\beta+\alpha}(z),$$

- Different behaviours in the complex plane with varying parameters:

$$E_{1,1}(z) = e^z, \quad E_{1,2}(z) = \frac{e^z - 1}{z}, \quad E_{\frac{1}{2},1}(z) = e^{z^2}\operatorname{erfc}(-z)$$

$$E_{2,1}(-z^2) = \cos(z), \quad E_{2,2}(z) = \frac{\sinh\sqrt{z}}{\sqrt{z}}, \quad E_{2,1}(z^2) = \cosh(z)$$

Computing the scalar ML function

1. Region-dependent methods:

• Truncate the series $E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k+\beta)}$ directly for small $|z|$

• Approximate the asymptotic expansions of the ML function for large $|z|$

• Evaluate the integral representations of the ML function for intermediate $|z|$

2. Numerical inversion of the Laplace transform on parabolic contours.

Truncating the (Taylor) series (1)

For $|z| < r$ for some $r > 0$, one can use finitely many terms of the series (1) to achieve a prescribed accuracy

$$R_N(z) = \left| E_{\alpha,\beta}(z) - \sum_{k=0}^{N} \frac{z^k}{\Gamma(\alpha k + \beta)} \right| \leq \epsilon.$$

For $|z| < 1$ the maximum number of terms $N(z)$ is given by [1, Thm. 4.1]

$$N(z) \geq \max\left\{ \lceil (2-\beta)/\alpha \rceil + 1, \left\lceil \frac{\ln(\epsilon(1-|z|))}{\ln(|z|)} \right\rceil + 1 \right\}, \quad |z| < 1.$$

- $N(z)$ increases rapidly as $z \to 1$; for example if $\epsilon =$1e-15, $N(0.9) \geq 351$ and $N(0.95) \geq 733$

Truncating the (Taylor) series (2)

- Potential overflow problems by the Gamma function: $\Gamma(171.624) = \infty$ in floating-point arithmetic,

$$N_{\mathtt{max}} := \lfloor \frac{171.624 - \beta}{\alpha} \rfloor .$$

- Avoid the overflow problems by using

$$z^k / \Gamma(\alpha k + \beta) = \exp(k \ln(z) - \ln \Gamma(\alpha k + \beta)). \qquad (2)$$

- For very small $|z|$, say, $|z| < 0.5$, directly compute each term in the standard definition (1).

For $0.5 \le |z| \le 0.95$ [1], use the exponential-logarithmic identity (2) in computation.

Evaluating the integral representations (1)

- The ML function can be represented as an improper integral along the Hankel loop:

$$E_{\alpha,\beta}(z) = \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{\lambda^{\alpha-\beta}e^{\lambda}}{\lambda^{\alpha}-z}d\lambda,$$

where $\mathcal{C}$ is a Hankel contour that starts and ends at $-\infty$ and encloses the circular disc $|\lambda| \leq |z|^{1/\alpha}$.

- Deforming the contour and applying the Cauchy's residue theorem, we can obtain [2] for $0 < \alpha < 1$:

$$E_{\alpha,\beta}(z) = \frac{1}{\alpha}z^{(1-\beta)/\alpha}e^{z^{1/\alpha}} + \frac{1}{2\pi i\alpha}\int_{\gamma(\epsilon;\delta)} \frac{e^{\zeta^{1/\alpha}}\zeta^{(1-\beta)/\alpha}}{\zeta - z}d\zeta, z \in G_1(\epsilon;\delta),$$

$$E_{\alpha,\beta}(z) = \frac{1}{2\pi i\alpha}\int_{\gamma(\epsilon;\delta)} \frac{e^{\zeta^{1/\alpha}}\zeta^{(1-\beta)/\alpha}}{\zeta - z}d\zeta, z \in G_2(\epsilon;\delta),\ \delta \in (\frac{\pi\alpha}{2}, \pi\alpha].$$

Evaluating the integral representations (2)

- Here the complex plane is divided by $\gamma(\epsilon;\delta)$ into two distinct regions $G_1(\epsilon;\delta)$ and $G_2(\epsilon;\delta)$.
- Different techniques are required in $G_1(\epsilon;\delta)$ and $G_2(\epsilon;\delta)$.
- To compute the integral we need to distinguish different cases for $\arg(z)$, for example [3],

$$|\arg(z)| > \pi\alpha, \quad |\arg(z)| = \pi\alpha, \quad |\arg(z)| < \pi\alpha.$$

- For the integral representations, the partitions of the complex plane and $\arg(z)$ can be more complicated [1]!

Approximating the asymptotic expansions (1)

The Poincaré asymptotic expansions for the ML functions in the complex plane as $|z| \to \infty$. For $0 < \alpha < 1$

$$E_{\alpha,\beta}(z) = \frac{1}{\alpha} z^{(1-\beta)/\alpha} e^{z^{1/\alpha}} - \sum_{k=1}^{N} \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + \mathcal{O}(|z|^{-1-N}), |\arg(z)| < \pi\alpha,$$

$$E_{\alpha,\beta}(z) = -\sum_{k=1}^{N} \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + \mathcal{O}(|z|^{-1-N}), |\arg(z)| > \pi\alpha.$$

To find the truncation point N for a prescribed accuracy

$$R_N(z) = \left| E_{\alpha,\beta}(z) - \Big(-\sum_{k=1}^{N} \frac{z^{-k}}{\Gamma(\beta - \alpha k)} \Big) \right| \le \epsilon, |\arg(z)| > \pi\alpha.$$

Approximating the asymptotic expansions (2)

$$R_N(z) = \left| E_{\alpha,\beta}(z) - \left(\frac{1}{\alpha} z^{(1-\beta)/\alpha} e^{z^{1/\alpha}} - \sum_{k=1}^{N} \frac{z^{-k}}{\Gamma(\beta - \alpha k)}\right) \right| \leq \epsilon,$$

$$|\arg(z)| < \pi\alpha.$$

It requires that [1, Thm. 4.2]

$$N \approx \frac{1}{\alpha} |z|^{1/\alpha}, \quad |z| \geq (-2 \log \frac{\epsilon}{C})^{\alpha},$$

where C is a constant dependent on α and β. In practice, it is approximated by $C \approx 1/(\pi \sin \pi\alpha)$.

Inverting the Laplace transform (1)

The generalised Mittag-Leffler function is defined as

$$e_{\alpha,\beta}(t;\lambda) = t^{\beta-1}E_{\alpha,\beta}(t^{\alpha}\lambda), \quad t \in \mathbb{R}^{+}, \lambda \in \mathbb{C}.$$

- $E_{\alpha,\beta}(\lambda) = e_{\alpha,\beta}(1;\lambda)$.

$$\mathcal{L}(e_{\alpha,\beta}(t;\lambda)) = \frac{s^{\alpha-\beta}}{s^{\alpha}-\lambda} =: \mathcal{E}_{\alpha,\beta}(s;\lambda), \quad \Re(s) > 0.$$

We can obtain the integral representation of the generalized ML function

$$e_{\alpha,\beta}(t;\lambda) = \frac{1}{2\pi i}\int_{L} e^{st}\mathcal{E}_{\alpha,\beta}(s;\lambda)ds, \tag{3}$$

where L is the Bromwich line $\gamma + iy, -\infty < y < +\infty$ such that γ is greater than the real part of all singularities of $\mathcal{E}_{\alpha,\beta}(s;\lambda)$.

Inverting the Laplace transform (2)

Deformation of L into parabolas:

$$\mathcal{C} : z(u) = \mu(iu + 1)^2, \quad -\infty < u < \infty.$$

• Fast decay of the exponential factor
Approximating (3) by the trapezoidal rule, with uniform step size h:

$$e_{\alpha,\beta}^{[h,N]}(t;\lambda) = \frac{h}{2\pi i} \sum_{k=-N}^{N} e^{z(u_k)t} \frac{z(u_k)^{\alpha-\beta}}{z(u_k)^{\alpha} - \lambda} z'(u_k), \quad u_k := kh.$$

• How to choose the three free parameters μ, h, N?

• Control the numerical error $e_{\alpha,\beta}(t;\lambda) - e_{\alpha,\beta}^{[h,N]}(t;\lambda)$?

General framework for the trapezoidal rule

Consider the absolutely convergent integral on the real line

$$I = \int_{-\infty}^{\infty} g(u)du,$$

whose infinite and finite trapezoidal approximations are

$$I_h = h \sum_{k=-\infty}^{\infty} g(kh), \quad I_{h;N} = h \sum_{k=-N}^{N} g(kh).$$

- the truncation error $|I_h - I_{h;N}| = TE(\mu, h, N)$ [4, Thm. 2.1]
- the discretization error $|I - I_h| = DE(\mu, h) \leq DE_+ + DE_-$
- For a chosen N, asymptotically balance the errors DE_+, DE_- and TE!

Inverting the Laplace transform (3)

• $\mathcal{C}$ encloses the singularities of $\mathcal{E}_{\alpha,\beta}(s;\lambda)$ on the left?
The singularities of $\mathcal{E}_{\alpha,\beta}(s;\lambda)$:

$$s^k_{\alpha,\lambda} = \lambda^{\frac{1}{\alpha}} e^{\frac{2k\pi}{\alpha} i}, \quad k \in \mathbb{Z}.$$

If we write λ in the exponential form $\lambda = re^{\theta i}, r \geq 0$, then

$$s^k_{\alpha,\lambda} = r^{\frac{1}{\alpha}} e^{\frac{\theta + 2k\pi}{\alpha} i}, \quad k \in \mathbb{Z}.$$

• Branch-cut along the negative real axis, in the main Riemann sheet

$$-\pi < \frac{\theta + 2k\pi}{\alpha} \leq \pi \quad \Rightarrow \quad -\frac{\alpha}{2} - \frac{\theta}{2\pi} < k < \frac{\alpha}{2} - \frac{\theta}{2\pi}, \; k \in \mathbb{Z}.$$

$\Rightarrow$ For $\alpha > 0$ singularities can appear at any region in the complex plane!

Inverting the Laplace transform (4)

The state-of-the-art algorithm [5] uses the Cauchy's residue theorem, to remove some of the singularities by

$$e_{\alpha,\beta}(t;\lambda) = \frac{1}{\alpha}\sum_{s\in S} s^{1-\beta}e^{st} + \frac{1}{2\pi i}\int_{\mathcal{C}} e^{st}\mathcal{E}_{\alpha,\beta}(s;\lambda)ds,$$

and determine the poles to be removed and the optimal parabolic contour $\mathcal{C}$.

• The chosen optimal parabolic contour is dependent on the input argument λ!

The matrix Mittag-Leffler function

We are interested in is the ML function with a matrix argument, that is,

$$E_{\alpha,\beta}(A) = \sum_{k=0}^{\infty} \frac{A^k}{\Gamma(\alpha k + \beta)},$$

where $A \in \mathbb{C}^{n\times n}$.

- $E_{1,1}(A) = e^A$.
- Represent solutions of linear fractional differential equation systems.
- $\alpha,\ \beta \in \mathbb{R}$ with $\alpha > 0$, particularly $0 < \alpha < 1$ and $\beta > 0$

Computing the matrix ML function

Consider the generalizability of the methods for the scalar function.

• Truncate the series $E_{\alpha,\beta}(A) = \sum_{k=0}^{\infty} \frac{A^k}{\Gamma(\alpha k+\beta)}$ directly for small $\|A\|$

For $\|A\| < r$ for some $r > 0$ (practically $r = 0.95$) in order to achieve a prescribed accuracy ϵ

$$R_N(A) = \left\| E_{\alpha,\beta}(A) - \sum_{k=0}^{N} \frac{A^k}{\Gamma(\alpha k + \beta)} \right\| \leq \epsilon,$$

the maximum number of terms $N(A)$ in the Taylor series for $r = 1$ is given by

$$N(A) \geq \max\left\{ \lceil (2-\beta)/\alpha \rceil + 1, \left\lceil \frac{\ln(\epsilon(1-\|A\|))}{\ln(\|A\|)} \right\rceil + 1 \right\}.$$

Computing the matrix ML function

- The asymptotic expansions of $E_{\alpha,\beta}(z)$ as $|z| \to \infty$:

$$E_{\alpha,\beta}(z) = \frac{1}{\alpha} z^{(1-\beta)/\alpha} e^{z^{1/\alpha}} - \sum_{k=1}^{N} \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + \mathcal{O}(|z|^{-1-N}), |\arg(z)| < \pi\alpha,$$

$$E_{\alpha,\beta}(z) = - \sum_{k=1}^{N} \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + \mathcal{O}(|z|^{-1-N}), |\arg(z)| > \pi\alpha.$$

- The integral representations of the ML function:

$$E_{\alpha,\beta}(z) = \frac{1}{\alpha} z^{(1-\beta)/\alpha} e^{z^{1/\alpha}} + \frac{1}{2\pi i \alpha} \int_{\gamma(\epsilon;\delta)} \frac{e^{\zeta^{1/\alpha}} \zeta^{(1-\beta)/\alpha}}{\zeta - z} d\zeta, z \in G_1(\epsilon;\delta),$$

$$E_{\alpha,\beta}(z) = \frac{1}{2\pi i \alpha} \int_{\gamma(\epsilon;\delta)} \frac{e^{\zeta^{1/\alpha}} \zeta^{(1-\beta)/\alpha}}{\zeta - z} d\zeta, z \in G_2(\epsilon;\delta), \ \delta \in (\frac{\pi\alpha}{2}, \pi\alpha].$$

Computing the matrix ML function

- Padé approximation

The Padé approximants r_{kk} uniformly approximate $E_{\alpha,\beta}$ as $k \to \infty$ in the unit circle $D = \{z : |z| \le 1\}$ [6].
The scaling and squaring method for the matrix exponential:

$$e^A = \left(e^{A/2^s}\right)^{2^s} \approx r(A/2^s)^{2^s}.$$

For arbitrary α, β, $E_{\alpha,\beta}(A_1 + A_2) \ne E_{\alpha,\beta}(A_1)E_{\alpha,\beta}(A_2)$.
For any $z \in \mathbb{C}$, $\lim_{m\to\infty} z^{1/m} = 1$, and

$$E_{\alpha,\beta}(A) = \frac{1}{2}\left(E_{\alpha/2,\beta}(A^{1/2}) + E_{\alpha/2,\beta}(-A^{1/2})\right)$$

Compute $E_{\alpha,\beta}(A) \Rightarrow$ compute $E_{\alpha/2^s,\beta}(B)$, $\Lambda(B)$ close to 1.

Computing the matrix ML function

- Numerically inverting the Laplace transform on parabolic contours $\mathcal{C} : z(u) = \mu(iu+1)^2, \quad -\infty < u < \infty.$

The generalised matrix Mittag-Leffler function

$$e_{\alpha,\beta}(t;A) = t^{\beta-1}E_{\alpha,\beta}(t^\alpha A), \quad t \in \mathbb{R}^+, A \in \mathbb{C}^{n\times n}.$$

$$\Rightarrow e_{\alpha,\beta}(t;A) = \frac{1}{2\pi i}\int_{\mathcal{C}} e^{st}s^{\alpha-\beta}(s^\alpha I - A)^{-1}ds.$$

$$= \frac{1}{2\pi i}\int_{-\infty}^{\infty} e^{z(u)t}z(u)^{\alpha-\beta}z'(u)(z(u)^\alpha I - A)^{-1}du$$

$$e_{\alpha,\beta}^{[h,N]}(t;A) = \frac{h}{2\pi i}\sum_{k=-N}^{N} e^{z(u_k)t}z(u_k)^{\alpha-\beta}z'(u_k)(z(u_k)^\alpha I - A)^{-1}, u_k := kh.$$

Choose the free parameters μ, h, N to control the numerical error $\|e_{\alpha,\beta}(t;A) - e_{\alpha,\beta}^{[h,N]}(t;A)\|$?

Computing the matrix ML function

- $\mathcal{C}$ encloses the singularities of $\mathcal{E}_{\alpha,\beta}(s; A)$ on the left?

The singularities of the scalar function $\mathcal{E}_{\alpha,\beta}(s; \lambda)$:

$$s_{\alpha,\lambda}^{k} = r^{\frac{1}{\alpha}} e^{\frac{\theta+2k\pi}{\alpha} i}, \quad k \in \mathbb{Z}.$$

- Branch-cut along the negative real axis, in the main Riemann sheet

$$-\pi < \frac{\theta + 2k\pi}{\alpha} \leq \pi \quad \Rightarrow \quad -\frac{\alpha}{2} - \frac{\theta}{2\pi} < k < \frac{\alpha}{2} - \frac{\theta}{2\pi}, \; k \in \mathbb{Z}. \tag{4}$$

- The contour $\mathcal{C}$ depends on the input argument λ.

Cauchy's residue theorem?

If $\lambda \in \mathbb{R}$ with $\lambda \leq 0$, then $\theta = \pi$ and (4) implies such $k \in \mathbb{Z}$ does not exist when $0 < \alpha < 1$.

- For $\lambda \leq 0$, the origin is the only singularity $\Rightarrow \mu > 0$.

Computing the matrix ML function

Similarly to the scalar case, asymptotically balancing the discretization error and the truncation error gives
when $\beta < \alpha + 1$,

$$c = 1,\ N = \left\lceil -\frac{\sqrt{1+4c(1+c)}}{2\pi c}\log\epsilon \right\rceil,\ h = \frac{3}{N},\ \mu = \frac{\pi N}{12t};$$

when $\beta = \alpha + 1$,

$$c = 0.92,\ N = \left\lceil -\frac{\sqrt{1+4c(1+c)}}{2\pi c}\log\epsilon \right\rceil,\ h = \frac{3}{N},\ \mu = \frac{\pi N}{12t};$$

when $\beta > \alpha + 1$,

$$c = 1 - \epsilon^{\frac{\gamma-2}{2(\alpha-\beta+1)\gamma}},\ N = \left\lceil -\frac{\sqrt{1+\gamma c(2+\gamma c)}}{\gamma\pi c}\log\epsilon \right\rceil,$$

$$h = -\frac{\gamma\pi c}{\log\epsilon},\ \mu = \frac{-\log\epsilon}{\gamma c(2+\gamma c)t},$$

where $\gamma \in (0,2)$ is a free parameter, ϵ is the tolerance.

Numerical experiments (1)

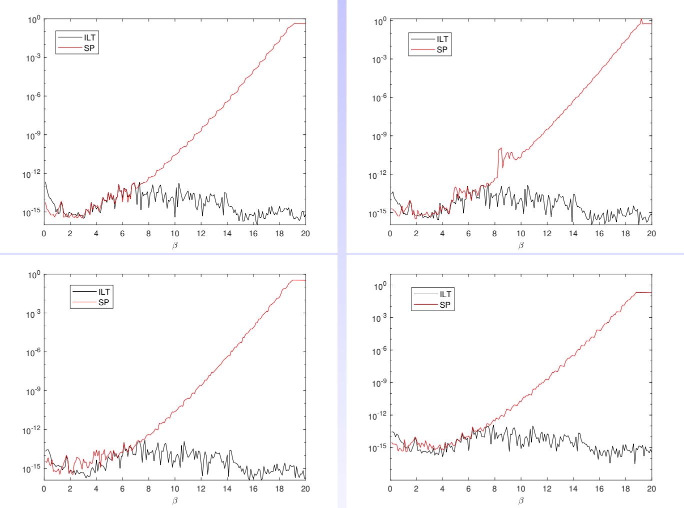

Figure: Top left: $\alpha = 0.2$; top right: $\alpha = 0.4$; bottom left: $\alpha = 0.6$; bottom right: $\alpha = 0.8$. $\epsilon =$ 5e-16. *A* symmetric negative definite.

Numerical experiments (2)

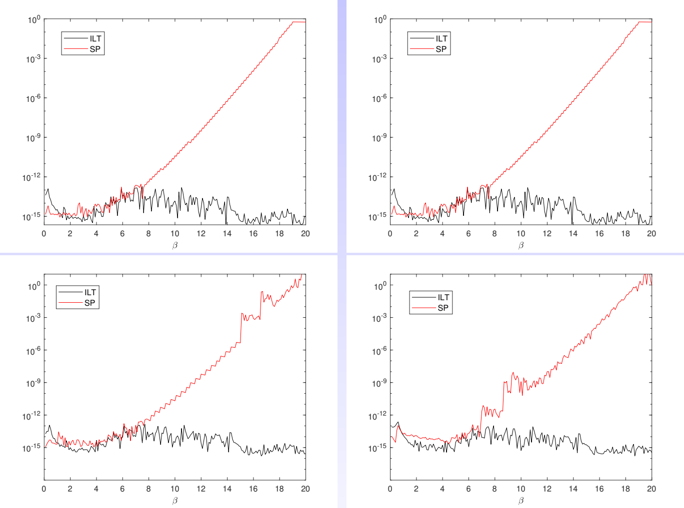

Figure: Top left: $\alpha = 0.2$; top right: $\alpha = 0.4$; bottom left: $\alpha = 0.6$; bottom right: $\alpha = 0.8$. $\epsilon = 5\text{e-}16$. A random with $-20 < \lambda < 0$.

Numerical experiments (3)

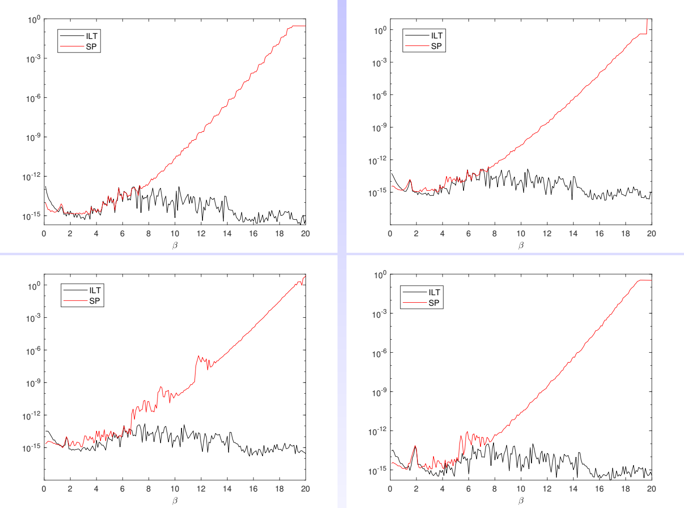

Figure: Top left: $\alpha = 0.2$; top right: $\alpha = 0.4$; bottom left: $\alpha = 0.6$; bottom right: $\alpha = 0.8$. $\epsilon =$ 5e-16. A symmetric Toeplitz.

An aside

Consider again the argument of the singularities in the main Riemann sheet

$$-\pi < \frac{\theta + 2k\pi}{\alpha} \leq \pi \quad \Rightarrow \quad -\frac{\alpha}{2} - \frac{\theta}{2\pi} < k < \frac{\alpha}{2} - \frac{\theta}{2\pi}, \; k \in \mathbb{Z}.$$

If we make an assumption that $\lambda = re^{\theta i}$ lies on the left half-plane, then $\theta \in [-\pi, -\pi/2] \cup [\pi/2, \pi]$.

• $k \in \mathbb{Z}$ does not exist when $0 < \alpha < 1/2$.

• Use the same scheme to evaluate the matrix ML function with $0 < \alpha < 1/2$ for any matrix with spectrum on the left half-plane.

Current and future work

- 1.Compute the Schur decomposition of $A \Rightarrow f(A) = Qf(T)Q^*$.
- 2.Use the Parlett recurrence

$$f_{ij} = t_{ij}\frac{f_{ii}-f_{jj}}{t_{ii}-t_{jj}} + \sum_{k=i+1}^{j-1}\frac{f_{ik}t_{kj}-t_{ik}f_{kj}}{t_{ii}-t_{jj}}, \quad i<j, \quad t_{ii}\neq t_{jj}$$

in block level with reordering [7] to compute the off-diagonal blocks.

How to compute $f(T_{ii})$?

- $\min|\lambda_1-\lambda_2|\leq\delta$.
- $f(T_{ii}) = \sum_{k=0}^{\infty}\frac{f^{(k)}(\sigma)}{k!}(T_{ii}-\sigma I)^k$ and truncate the series?
- Approximate diagonalization [8] for computing $E_{\alpha,\beta}(A)$ or $E_{\alpha,\beta}(T_{ii})$ in higher precision?

Thank you for your attention.

Any questions?

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