MANCHESTER 1824

The University of Manchester

M\crNA
Manchester Numerical Analysis

Computing the Matrix Mittag-Leffler Function

Xiaobo Liu
School of Mathematics
The University of Manchester

Numerical Linear Algebra Group Meeting
Manchester, 27 March 2019

The (scalar) Mittag-Leffler Function

The Mittag-Leffer (ML) function is a complex function that depends on two parameters α and β, with $\Re(\alpha) > 0$:

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

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

- Generalization of the exponential function
- Solution of linear fractional differential equations

Define $f(A)$ via the Jordan Canonical Form

$$A = ZJZ^{-1} = Z\,\mathrm{diag}(J_1, \dots, J_p)Z^{-1}, J_k = \begin{bmatrix} \lambda_k & 1 & & \\ & \lambda_k & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_k \end{bmatrix}_{m_k \times m_k}$$

$$\Rightarrow f(A) := Zf(J)Z^{-1} = Z\,\mathrm{diag}(f(J_1), \dots, f(J_p))Z^{-1}$$

$$f(J_k) := \begin{bmatrix} f(\lambda_k) & f'(\lambda_k) & \dots & \frac{f^{(m_k-1)}(\lambda_k)}{(m_k-1)!} \\ & f(\lambda_k) & \ddots & \vdots \\ & & \ddots & f'(\lambda_k) \\ & & & f(\lambda_k) \end{bmatrix}$$

The Matrix Mittag-Leffler Function

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

- Practical interest of values of α, β
- Practical interest of matrix A

Schur-Parlett Algorithm

1. $A = UTU^{-1} \Rightarrow f(A) = f(UTU^{-1}) = Uf(T)U^{-1}$
2. The diagonal elements of $F := f(T) \Rightarrow f_{ii} = f(t_{ii})$
3. $TF = FT \Rightarrow$ the Parlett's recurrence:

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

4. Compute the off-diagonal elements of $F = f(T)$
   for example: a superdiagobal at a time
   $f_{12} = t_{12}(f_{11} - f_{22})/(t_{11} - t_{22}), f_{23} = t_{23}(f_{22} - f_{33})/(t_{22} - t_{33}), \dots,$
   $f_{13} = t_{13}(f_{11} - f_{33})/(t_{11} - t_{33}) + (t_{23}f_{12} - t_{12}f_{23})/(t_{11} - t_{33}), \dots$
5. $f(A) = Uf(T)U^{-1}$

Schur-Parlett Algorithm with Reordering

The block Parlett recurrence:

$$T_{ii}F_{ij} - F_{ij}T_{jj} = F_{ii}T_{ij} - T_{ij}F_{jj} + \sum_{k=i+1}^{j-1} (F_{ik}T_{kj} - T_{ik}F_{kj}), \quad i < j. \quad (1)$$

1. $A = UTU^*$
2. Reorder T to block triangular form $\widetilde{T}$, eigenvalues of $\widetilde{T} = Q^*TQ$: same diagonal block $\Rightarrow$ close different diagonal blocks $\Rightarrow$ sufficiently well separated
3. Evaluate the diagonal blocks $F_{ii} = f(\widetilde{T}_{ii})$ from a Taylor series $f(\widetilde{T}_{ii}) = \sum_{k=0}^{\infty} \frac{f^{(k)}(\sigma)}{k!}(\widetilde{T}_{ii} - \sigma I)^k, \sigma = \mathrm{trace}(\widetilde{T}_{ii})/n$
4. Solve the Sylvester equations (1) for $F_{ij} \Rightarrow f(\widetilde{T}) = F$
5. $f(A) = UQF(UQ)^*$

Computing Derivatives of the ML Function

Computing matrix ML function $\Rightarrow$ Schur-Parlett algorithm
$\Rightarrow$ computing the derivatives of the scalar ML function:

$$\frac{\mathrm{d}^k}{\mathrm{d}z^k} E_{\alpha,\beta}(z) = \sum_{j=k}^{\infty} \frac{(j)_k}{\Gamma(\alpha j + \beta)} z^{j-k}, \quad k \in \mathbb{N},$$

with $(j)_k$ representing the falling factorial

$$(j)_k = j(j-1)\cdots(j-k+1).$$

- We briefly introduce three methods

1. Truncating the Series
2. Numerical Inversion of the Laplace Transform
3. Summation Formula

1.Truncating the Series (1)

$$\frac{\mathrm{d}^k}{\mathrm{d}z^k} E_{\alpha,\beta}(z) \approx \sum_{j=k}^{J} \frac{(j)_k}{\Gamma(\alpha j + \beta)} z^{j-k} \quad ?$$

$\Gamma(172) = \inf, j_{\max} \approx \lfloor \frac{171.624-\beta}{\alpha} \rfloor$. For a target accuracy τ,

$$\frac{(j_{\max})_k}{\Gamma(\alpha j_{\max} + \beta)} |z|^{j_{\max}-k} \leq \tau,$$

and this inequality imposes an upper bound on the modulus of z:

$$|z| \leq \left(\tau \frac{\Gamma(\alpha j_{\max} + \beta)}{(j_{\max})_k}\right)^{\frac{1}{j_{\max}-k}}.$$

Table: Upper bound on $|z|$ to 2 digits with different α and k.

Value of α	Value of k	Upper bound on $|z|$
$\alpha = 0.5$	2	7.07
$\alpha = 0.5$	10	6.44
$\alpha = 1.0$	2	51.37
$\alpha = 1.0$	10	48.47

Here $\beta = 1$ is fixed and the tolerance τ is set to be 10^{-15}.

The range of z will reduce when α becomes smaller.

1. Truncating the Series (3)

We compute the ratio $r(z, k, \alpha, \beta, j)$ between two successive terms in $\frac{\mathrm{d}^k}{\mathrm{d}z^k} E_{\alpha,\beta}(z)$:

$$r(z, k, \alpha, \beta, j) = \frac{z(j+1)\Gamma(\alpha j + \beta)}{(j+1-k)\Gamma(\alpha j + \alpha + \beta)} > 1?$$

$\Rightarrow$ The modulus of the terms in the series can rapidly grow before decreasing for some choices of (z, k, α, β)

$\Rightarrow$ Significant numerical cancellation in fixed precision arithmetic!

Comments on Truncating the Series

- It is confined to small arguments
- Significant numerical cancellation can happen in the summation
- Its convergence can be extremely slow

2. Numerical Inversion of the Laplace Transform (LT) (1)

The LT of a function $f(t)$ is defined by

$$\mathcal{L}\{f(t)\} := \int_0^{\infty} f(t)e^{-st}\mathrm{d}t = F(s), \quad s \in \mathbb{C}.$$

The inverse Laplace transform (ILT) is given by

$$\mathcal{L}^{-1}\{F\}(t) := \frac{1}{2\pi i}\int_L e^{st}F(s)\mathrm{d}s = \frac{1}{2\pi i}\lim_{y\to\infty}\int_{\gamma-iy}^{\gamma+iy} e^{st}F(s)\mathrm{d}s,$$

where L is a vertical line $\gamma + iy, -\infty < y < +\infty$ in the complex plane such that γ is greater than the real part of all singularities of $F(s)$.

2. Numerical Inversion of LT (2)

Choose $C = L + C_R$ encloses all poles z_i of $e^{st}F(s)$,

$$\frac{1}{2\pi i}\int_L e^{st}F(s)\mathrm{d}s = \sum \mathrm{Res}(e^{st}F(s), z_i) - \frac{1}{2\pi i}\int_{C_R} e^{st}F(s)\mathrm{d}s,$$

where $L = \gamma + iy,\ |y| < M$ for some $M > 0$.
Using the *Jordan's lemma*, for a semicircular contour C_R

$$\lim_{y\to\infty}\int_{C_R} e^{st}F(s)\mathrm{d}s = 0, \quad t > 0.$$

Here the condition $F(s) \to 0$ as $|s| \to \infty$ is required.

$$\mathcal{L}^{-1}\{F\}(t) = \sum \mathrm{Res}(e^{st}F(s), z_i) = \frac{1}{2\pi i}\int_{\mathcal{C}} e^{st}F(s)\mathrm{d}s, \quad t > 0,$$

where $\mathcal{C}$ is a contour that encloses all the poles z_i of $F(s)$, and $F(s) \to 0$ as $|s| \to \infty$.

2. Numerical Inversion of LT (3)

For any $t > 0$, the LT of the function $f(t) := t^{\beta-1}E^{\gamma}_{\alpha,\beta}(t^{\alpha}z)$ that based on the Prabhakar function

$$E^{\gamma}_{\alpha,\beta}(z) := \frac{1}{\Gamma(\gamma)}\sum_{k=0}^{\infty}\frac{\Gamma(k+\gamma)z^k}{k!\Gamma(\alpha k+\beta)}$$

is given by

$$\mathcal{L}\{f(t)\} = \mathcal{L}\{t^{\beta-1}E^{\gamma}_{\alpha,\beta}(t^{\alpha}z); s\} = \frac{s^{\alpha\gamma-\beta}}{(s^{\alpha}-z)^{\gamma}},$$

where $\Re(s) > 0$, and $|zs^{-\alpha}| < 1$.

$$\Rightarrow \quad \mathcal{L}\{E^{\gamma}_{\alpha,\beta}(z); s\} = \frac{s^{\alpha\gamma-\beta}}{(s^{\alpha}-z)^{\gamma}}, \quad \Re(s) > 0, \; |zs^{-\alpha}| < 1.$$

2. Numerical Inversion of LT (4)

$$\frac{\mathrm{d}^k}{\mathrm{d}z^k} E_{\alpha,\beta}(z) = \sum_{j=0}^{\infty} \frac{(j+k)_k}{\Gamma(\alpha j + \alpha k + \beta)} z^j = k! E_{\alpha,\alpha k+\beta}^{k+1}(z).$$

Setting $\gamma \leftarrow k+1$, and $\beta \leftarrow \alpha k + \beta \quad \Rightarrow$

$$\mathcal{L}\{\frac{\mathrm{d}^k}{\mathrm{d}z^k} E_{\alpha,\beta}(z); s\} = k!\mathcal{L}\{E_{\alpha,\alpha k+\beta}^{k+1}(z); s\} =: k! H_k(s; z),$$

where

$$H_k(s; z) = \frac{s^{\alpha(k+1)-(\alpha k+\beta)}}{(s^\alpha - z)^{k+1}} = \frac{s^{\alpha-\beta}}{(s^\alpha - z)^{k+1}}.$$

2. Numerical Inversion of LT (5)

The derivatives of the ML function can be evaluated in the form of the integral

$$\frac{\mathrm{d}^k}{\mathrm{d}z^k}E_{\alpha,\beta}(z) = \mathcal{L}^{-1}\{k!H_k(s;z)\}(t=1) = \frac{k!}{2\pi i}\int_{\mathcal{C}} e^s H_k(s;z)\mathrm{d}s$$

over any contour $\mathcal{C}$ that encloses all the poles of $H_k(s;z)$ in the complex plane.

Now the task is to numerically evaluate

$$\frac{k!}{2\pi i}\int_{\mathcal{C}} e^s \frac{s^{\alpha-\beta}}{(s^\alpha - z)^{k+1}}\mathrm{d}s$$

over a suitably chosen contour $\mathcal{C}$.

2. Numerical Inversion of LT (6)

- Generally, the accuracy of Numerical Inversion of LT will decrease as k increases

- This method works for parameters $\alpha, \beta > 0$ since we require the $H_k(s; z) = \mathcal{O}(s^{-(\alpha k+\beta)}) \to 0$ as $|s| \to \infty$

3. Summation Formula

(Summation formula of Prabhakar type). Let $\alpha > 0$ and $\beta \in \mathbb{R}$. For any $k \in \mathbb{N}$,

$$\frac{\mathrm{d}^k}{\mathrm{d}z^k} E_{\alpha,\beta}(z) = \frac{1}{\alpha^k} \sum_{j=0}^{k} c_j^{(k)} E_{\alpha,\alpha k+\beta-j}(z),$$

where constants $c_j^{(k)}, j = 0, 1, \ldots, k$ can be calculated recursively.

- $k + 1$ coefficients to compute
- $k + 1$ different ML functions to be summed

$\Rightarrow$ As k increases, $c_j^{(k)}$ becomes hard to obtain, numerical errors accumulate either from computing $c_j^{(k)}$ or from summing the ML functions.

Balance of Derivatives

Let $\alpha > 0$ and $\beta \in \mathbb{R}$. For any $k \in \mathbb{N}$ and $p \le k$,

$$\frac{\mathrm{d}^k}{\mathrm{d}z^k} E_{\alpha,\beta}(z) = \frac{1}{\alpha^{k-p}} \sum_{j=0}^{k-p} c_j^{(k-p)} \frac{\mathrm{d}^p}{\mathrm{d}z^p} E_{\alpha,(k-p)\alpha k+\beta-j}(z),$$

where $c_j^{(k)}, j = 0, 1, \ldots, k$ are the same as before.

• Represents the kth order derivatives of the ML function in terms of lower order derivatives.

Strategy for the *k*th Derivative of ML function

- For ‘small arguments’, compute by truncating the series.

- Otherwise, switch to the summation formula or the numerical inversion of the LT.

- Derivative balancing formula is used to avoid evaluating high order derivatives.

Comments

- Computing the derivatives of the scalar ML function
- The descriptions of the method are not satisfactory
- Computational cost
- Currently no specialized algorithm for matrix ML

Thank you for your attention.

Any questions?

References I

- P. I. Davies and N. J. Higham.
  A Schur–Parlett Algorithm for Computing Matrix Functions.
  SIAM J. Matrix Anal. Appl., 25(2):464–485, 2003.

- R. Garrappa and M. Popolizio.
  Computing the Matrix Mittag-Leffler Function with Applications to Fractional Calculus.
  Journal of Scientific Computing, 77:129–153, 2018.

- R. Garrappa.
  Numerical evaluation of two and three parameter Mittag-Leffler functions.
  SIAM Journal on Numerical Analysis, 53(3):1350–1369, 2015.

References II

N. J. Higham.
Functions of Matrices: Theory and Computation.
Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2008.

B. N. Parlett.
A Recurrence among the Elements of Functions of Triangular Matrices.
Linear Algebra and its Applications, 14(2):117–121, 1976.

T. R. Prabhakar.
A Singular Integral Equation with A Generalized Mittag-Leffler Function in the Kernel.
Yokohama Math Journal, 19(1):7-15, 1971.