Exponential Integrators for Fractional Partial Differential Equations

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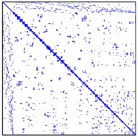
Outline

Exponential integrators for ODEs

$$U'(t) = AU(t) + F(t, U(t)), \qquad U(0) = U_0$$

- the size of the system is very large ($10^3 \sim 10^6$)
- A is a sparse matrix
- A stiff but $F(t, U(t))$ non stiff: implicit or explicit methods ?

Non zero entries of A



Problems from spatial discretization of PDEs

Main idea of Exponential integrators

$$U(t) = e^{tA}U_0 + \int_0^t e^{(t-\tau)A}F(\tau, U(\tau))d\tau$$

Device numerical schemes that use the evaluation of e^{tA}

Advantages: stability (stiff term evaluated exactly) with explicit schemes
Disadvantages: computation of e^{tA}

Exponential integrators for ODEs

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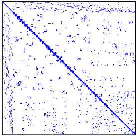

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Exponential integrators for ODEs: examples

$$U(t) = e^{tA}U_0 + \int_0^t e^{(t-\tau)A}F(\tau, U(\tau))d\tau$$

Integration on a grid $t_n = nh$

- $F(\tau, U(\tau))$ approximated by $F_n = F(t_n, U_n)$ on $[t_n, t_{n+1}]$

  Exponential Euler : $U_{n+1} = e^{hA}U_n + h\varphi_1(hA)F_n$

- $F(\tau, U(\tau))$ approximated by linear interpolation $F_n + \frac{t_n-\tau}{t_n-t_{n-1}}\big(F_n - F_{n-1}\big)$

  Second order E.I. : $U_{n+1} = e^{hA}U_n + h\varphi_1(hA)F_n + h\varphi_2(hA)\big(F_n - F_{n-1}\big)$

- Other approaches: Exponential Runge–Kutta, Exponential Adams methods, Exponential Rosenbrock-type methods, and so on ...

$$\varphi_1(z) = \frac{e^z - 1}{z}, \quad \varphi_2(z) = \frac{e^z - z - 1}{z^2}$$

Review papers and software package

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Exponential integrators

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Acta Numerica 2010

NORGES TEKNISK-NATURVITENSKAPELIGE UNIVERSITET

A review of exponential integrators for first order semi-linear problems

by

Borislav V. Minchev and Will M. Wright

PREPRINT
NUMERICS NO. 2/2005

`http://www.math.ntnu.no/preprint/numerics/`

EXPINT : A MATLAB package for exponential integrators[1].

available at `http://www.math.ntnu.no/num/expint/matlab.php`

[1] Håvard Berland, Bård Skaflestad, and Will M. Wright. "EXPINT—A MATLAB package for exponential integrators". In: *ACM Trans. Math. Softw.* 33.1 (2007).

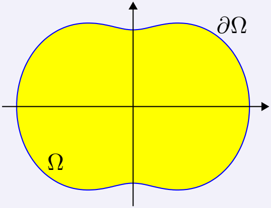
Fractional partial differential equation

Time–fractional diffusion

$$\frac{\partial^{\alpha}}{\partial t^{\alpha}} u(t,x) = \nu \nabla^2 u(t,x) + f(t,x)$$

I.C. : $u(0,x) = u_0(x)$

B.C. : $u(t,x) = g(t,x), t > 0, x \in \partial\Omega$



$0 < \alpha < 1$: fractional diffusion equation

$1 < \alpha < 2$: fractional wave equation

Papers of Schneider and Wyss (1989)[2] and Mainardi (1996)[3]

[2] W. R. Schneider and W. Wyss. "Fractional diffusion and wave equations". In: *J. Math. Phys.* 30.1 (1989), pp. 134–144.

[3] F. Mainardi. "The fundamental solutions for the fractional diffusion-wave equation". In: *Appl. Math. Lett.* 9.6 (1996), pp. 23–28.

From a FPDE to a system of FDEs: the linear case

$$\frac{\partial^{\alpha}}{\partial t^{\alpha}} u(t,x) = \nu \nabla^2 u(t,x) + f(t,x)$$

$$\frac{d^{\alpha}}{dt^{\alpha}} U(t) = AU(t) + F(t), \quad U(0) = U_0$$

$A \longleftrightarrow \nu\nabla^2$ $\qquad$ $F(t) \longleftrightarrow$ Linear source term and B.C. $\qquad$ $U_0 \longleftrightarrow$ I.C.

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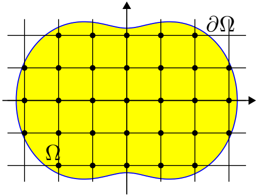
Finite difference methods



$$\nabla^2 u_{i,j}(t) \approx \frac{u_{i-1,j}(t) - 2u_{i,j}(t) + u_{i+1,j}(t)}{(\Delta x_1)^2} + \frac{u_{i,j-1}(t) - 2u_{i,j}(t) + u_{i,j+1}(t)}{(\Delta x_2)^2}$$

$$u_{i,j}(t) = u(t, x_{1_i}, x_{2_j})$$

$$U(t) = \Big(u_{1,1}(t), u_{2,1}(t), \dots, u_{N_1,1}(t), \dots, u_{1,N_2}(t), \dots, u_{N_1,N_2}(t) \Big)^T$$

From a FPDE to a system of FDEs: the linear case

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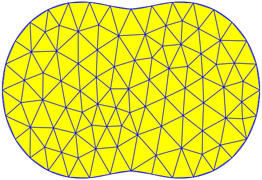
Finite elements methods



$$u(t,x) \approx u_h(t,x) = \sum_{j=1}^{N_h} U_j(t)\Phi_j(x)$$

$$\sum_{j=1}^{N_h} \frac{d^\alpha}{dt^\alpha} U_j(t)(\Phi_j, \Phi_k) + \sum_{j=1}^{N_h} U_j(t)(\nabla^2\Phi_j, \nabla^2\Phi_k) = (f, \Phi_k)$$

$k = 1, \ldots, N_h$

From a FPDE to a system of FDEs: non linear case

$$\frac{\partial^{\alpha}}{\partial t^{\alpha}} u(t,x) = \nu \nabla^2 u(t,x) + f(t, u(t,x))$$

$$\frac{d^{\alpha}}{dt^{\alpha}} U(t) = AU(t) + F(t, U(t)), \quad U(0) = U_0$$

Examples of non linear time–fractional PDEs:

- Bonhoeffer–van der Pol and Brusselator[4]
- other problems[5]

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[4] V. Gafiychuk and B. Datsko. "Mathematical modeling of different types of instabilities in time fractional reaction-diffusion systems". In: *Comput. Math. Appl.* 59.3 (2010), pp. 1101–1107.

[5] V. Gafiychuk, B. Datsko, and V. Meleshko. "Mathematical modeling of time fractional reaction–diffusion systems". In: *J. Comput. Appl. Math.* 220.1-2 (2008), pp. 215–225.

Generalization of Exponential Integrators to FDEs

$$\frac{d^{\alpha}}{dt^{\alpha}}U(t) = A \cdot U(t) + F(t)$$

$$\frac{d^{\alpha}}{dt^{\alpha}}U(t) = A \cdot U(t) + F(t, U(t))$$

Linear term:
$A \cdot U(t)$ stiff
A large and sparse

Source term:
$F(t)$ linear
$F(t, U(t))$ non linear but non–stiff

Main steps:

1. Derivation of a Variation–of–constant formula for FDEs
2. Application of a discretization scheme
3. Evaluation of a counterpart of the exponential function

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The variation–of–constant formula for FDEs

$$\frac{d^{\alpha}}{dt^{\alpha}} U(t) = AU(t) + F(t)$$

$\Downarrow$ *in the Laplace transform domain*

$$s^{\alpha} \hat{U}(s) - s^{\alpha-1} U_0 = A\hat{U}(s) + \hat{F}(s)$$

$\Downarrow$ *solve w.r.t.* $\hat{U}(s)$

$$\hat{U}(s) = s^{\alpha-1}\left(s^{\alpha} I - A\right)^{-1} U_0 + \left(s^{\alpha} I - A\right)^{-1} \hat{F}(s)$$

$\Downarrow$ *in the time domain*

$$\text{V.o.C. :} \quad U(t) = e_{\alpha,1}(t; -A) U_0 + \int_0^t e_{\alpha,\alpha}(t-s; -A) F(s) ds$$

The kernel $e_{\alpha,\beta}(t; A)$ and the Mittag–Leffler (ML) function

$$e_{\alpha,\beta}(t; A) = \mathcal{L}^{-1}\left(s^{\alpha-\beta}\left(s^{\alpha} I + A\right)^{-1}\right) = t^{\beta-1} E_{\alpha,\beta}\left(-t^{\alpha} A\right)$$

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

The variation–of–constant formula for FDEs

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

Fractional exponential Euler method

1. Write the Variation–of–Constants (VoC) formula in a piecewise form

$$U(t_n) = e_{\alpha,1}(t_n; -A)U_0 + \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} e_{\alpha,\alpha}(t_n - s; -A)F(s)ds$$

2. Approximate $F(s)$ by a constant value

$$F(s) \approx F_j = F(t_j), \quad s \in [t_j, t_{j+1}]$$

3. Exactly integrate

$$U(t_n) = e_{\alpha,1}(t_n; -A)U_0 + h^\alpha \sum_{j=0}^{n-1} W_{n-j} F_j$$

$$W_n = e_{\alpha,\alpha+1}(n; -h^\alpha A) - e_{\alpha,\alpha+1}(n-1; -h^\alpha A)$$

Adams Exponential Integrators for FDEs

1. Write the Variation–of–Constants (VoC) formula in a piecewise form

$$U(t_n) = e_{\alpha,1}(t_n; -A)U_0 + \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} e_{\alpha,\alpha}(t_n - s; -A)F(s)ds$$

2. Approximate $F(s)$ by a L-degree polynomial in each interval $[t_j, t_{j+1}]$

$$F(s) = F(t_j + \theta h) \approx \sum_{\ell=0}^{L} (-1)^\ell \binom{-\theta+1}{\ell} \nabla^\ell F_{j+1}$$

   - $F_n = F(t_n)$
   - $\nabla^\ell F_n$: backward differences of order ℓ
   - $\binom{-\theta+1}{\ell}$: binomial coefficients

3. Exactly integrate

Adams Exponential Integrators for FDEs

$$U_n = S.T. + h^\alpha \sum_{j=L}^{n-1} \sum_{\ell=0}^{L} \varphi_{\alpha,\ell}(n-j; -h^\alpha A) \nabla^\ell F_{j+1}$$

$$\begin{aligned}\varphi_{\alpha,\ell}(n;z) &= (-1)^\ell \int_0^1 \binom{-\theta+1}{\ell} e_{\alpha,\alpha}(n-\theta;z)\,d\theta \\ &= \sum_{k=0}^{\ell} \big(p_{\ell,k} e_{\alpha,\alpha+k+1}(n;z) - q_{\ell,k} e_{\alpha,\alpha+k+1}(n-1;z) \big)\end{aligned}$$

	$p_{\ell,0}$	$p_{\ell,1}$	$p_{\ell,2}$	$p_{\ell,3}$	$p_{\ell,4}$	$q_{\ell,0}$	$q_{\ell,1}$	$q_{\ell,2}$	$q_{\ell,3}$	$q_{\ell,4}$
$\ell = 0$	1					1				
$\ell = 1$	-1	1				0	1			
$\ell = 2$	0	$-\frac{1}{2}$	1			0	$\frac{1}{2}$	1		
$\ell = 3$	0	$-\frac{1}{6}$	0	1		1	0	$\frac{1}{3}$	1	
$\ell = 4$	0	$-\frac{1}{12}$	$-\frac{1}{12}$	$\frac{1}{2}$	1	0	$\frac{1}{4}$	$\frac{11}{12}$	$\frac{3}{2}$	1

Adams Exponential Integrators for FDEs

$$U_n = S.T. + h^\alpha \sum_{j=L}^{n-1} \sum_{\ell=0}^{L} \varphi_{\alpha,\ell}(n-j; -h^\alpha A) \nabla^\ell F_{j+1}$$

Main advantages: accuracy and stability[6]

- Order depends on the smoothness of the linear source term and not of the true solution

$$F(t) \in \mathcal{C}^{L+1} \implies \mathrm{Error} = \mathcal{O}\big(h^{L+1}\big)$$

- Stiffness due to large values in $\sigma(A)$ does not affect the stability

Some problems to solve:

- evaluation of $\varphi_{\alpha,\ell}(n; -h^\alpha A)$ (and hence the ML functions)

[6] R. Garrappa. "A family of Adams exponential integrators for fractional linear systems". In: *Comput. Math. Appl.* (2013), in print.

Application in control theory problems

Linear time–invariant system of FDEs

$$\begin{cases} D_0^{\alpha} x(t) = Ax(t) + Bu(t) \\ y(t) = C^T x(t), \quad x(0) = x_0 \end{cases} \qquad A \in \mathbb{R}^{N\times N},\ B \in \mathbb{R}^{N\times m},\ C \in \mathbb{R}^{N\times p}$$

No need for direct evaluation of the state $x(t)$:

$$\text{V.o.C. :} \quad y(t) = C^T e_{\alpha,1}(t;-A)x_0 + \int_0^t C^T e_{\alpha,\alpha}(t-s;-A)Bu(s)ds$$

$$\text{Fractional Exp. Adams:} \ y_n = S.T. + h^{\alpha} \sum_{j=L}^{n-1} \sum_{\ell=0}^{L} \varphi_{\alpha,\ell}(n-j;-h^{\alpha}A)\nabla^{\ell} u_{j+1}$$

$$\varphi_{\alpha,\ell}(n-j;Z) = C^T \sum_{k=0}^{\ell} \big(p_{\ell,k} e_{\alpha,\alpha+k+1}(n;Z) - q_{\ell,k} e_{\alpha,\alpha+k+1}(n-1;Z) \big) B$$

MIMO : external dimensions m and p smaller than the internal dimension N

SISO : scalar weights

From a FPDE to a system of FDEs: the non linear case

$$\frac{\partial^{\alpha}}{\partial t^{\alpha}} u(t,x) = \nu \nabla^2 u(t,x) + f(t, u(t,x))$$

$$\frac{d^{\alpha}}{dt^{\alpha}} U(t) = AU(t) + F(t, U(t)), \quad U(0) = U_0$$

Fractional exponential Euler scheme:

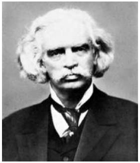
$$U_n = e_{\alpha,1}(t_n; -A)U_0 + h^{\alpha} \sum_{j=0}^{n-1} W^{(1)}_{n-j} F_j$$

Fractional exponential trapezoidal scheme:

$$U_n = e_{\alpha,1}(t_n; -A)U_0 + h^{\alpha} \tilde{W}_n F_0 + h^{\alpha} \left(\sum_{j=1}^{n-1} W^{(2)}_{n-j} F_j - W^{(2)}_0 F_{n-2} + 2W^{(2)}_0 F_{n-1} \right)$$

$$W^{(1)}_n = e_{\alpha,\alpha+1}(n; -h^{\alpha}A) - e_{\alpha,\alpha+1}(n-1; -h^{\alpha}A)$$
$$W^{(2)}_0 = e_{\alpha,\alpha+2}(1; -h^{\alpha}A)$$
$$W^{(2)}_n = e_{\alpha,\alpha+2}(n-1; -h^{\alpha}A) - 2e_{\alpha,\alpha+2}(n; -h^{\alpha}A) + e_{\alpha,\alpha+2}(n+1; -h^{\alpha}A)$$
$$\tilde{W}_n = e_{\alpha,\alpha+2}(n-1; -h^{\alpha}A) + e_{\alpha,\alpha+1}(n; -h^{\alpha}A) - e_{\alpha,\alpha+2}(n; -h^{\alpha}A)$$

The Mittag–Leffler function



Introduced in 1903 by Magnus Gösta Mittag–Leffler

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

The generalization with two parameters

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

A generalized Mittag–Leffler function

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

t is the independent variable $\quad$ λ is a real/complex scalar/matrix argument

We will focus on $\alpha, \beta \in \mathbb{R}$ and $\beta = \alpha + k$, $k = 0, 1, \ldots$

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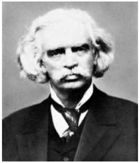

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The ML function and FDEs

$$e_{\alpha,\beta}(t;\lambda) = t^{\beta-1}E_{\alpha,\beta}(-t^{\alpha}\lambda) \qquad E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}$$

The ML function plays for FDEs the same role of the exp function for ODEs

ODE : $\begin{cases} Dy(t) + \lambda y(t) = 0 \\ y(0) = y_0 \end{cases}$ True solution $y(t) = e^{-t\lambda} y_0$

FDE : $0 < \alpha < 1$ $\begin{cases} {}^{C}_{0}D^{\alpha} y(t) + \lambda y(t) = 0 \\ y(0) = y_0 \end{cases}$ True solution $y(t) = e_{\alpha,1}(t;\lambda) y_0$

ML function generalizes the exp function $e_{1,1}(t;\lambda) = e^{-t\lambda}$

- Books of Podlubny (1999) and Mainardi (2011)
- Code `mlf.m` available in the File Exchange service of MATLAB CENTRAL

Numerical evaluation of the ML function

Some challenging problems: fast evaluation of $e_{\alpha,\beta}(t;\lambda)$
extension to matrix arguments

$$e_{\alpha,\beta}(t;\lambda) = t^{\beta-1}E_{\alpha,\beta}(-t^{\alpha}\lambda), \quad E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}$$

Convergence of the series can be extremely slow

The Laplace transform

$$\mathcal{L}\Big(e_{\alpha,\beta}(t;\lambda)\,;\,s\Big) = \frac{s^{\alpha-\beta}}{s^{\alpha}+\lambda}$$

Numerical quadrature in the inversion formula

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

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$$e_{\alpha,\beta}(t;\lambda) = t^{\beta-1}E_{\alpha,\beta}(-t^{\alpha}\lambda), \quad E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}$$

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Numerical quadrature in the inversion formula

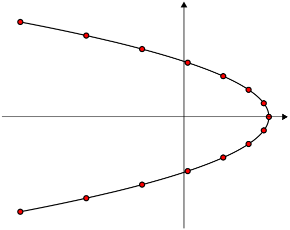
$$e_{\alpha,\beta}(t,\lambda) = \frac{1}{2\pi i}\int_{\mathcal{C}} e^{st}\frac{s^{\alpha-\beta}}{s^{\alpha}+\lambda}ds,$$

Numerical inversion of the LT: choice of the contour

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

Parabolic contour:

- simplicity of the contour
  $\mathcal{C} : z(u) = \mu(iu+1)^2$
- extension to matrices with real spectrum
- good accuracy with fast computation
- availability of error estimates for exp[7]
- extension to the Mittag–Leffler function[8]



[7] J. A. C. Weideman and L. N. Trefethen. "Parabolic and hyperbolic contours for computing the Bromwich integral". In: *Math. Comp.* 76.259 (2007), pp. 1341–1356.

[8] R. Garrappa and M. Popolizio. "Evaluation of generalized Mittag–Leffler functions on the real line". In: *Adv. Comput. Math.* (2012), in print.

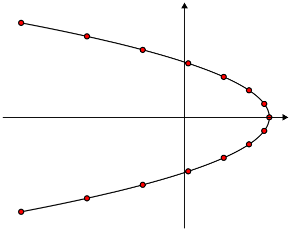
Numerical inversion of the LT on parabolic contours

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

Main steps in numerical inversion of LT on parabolic contours:

Determination of:

- Geometry parameter μ for $\mathcal{C} : z(u) = \mu(iu+1)^2$
- Number N of quadrature nodes $z_k = \mu(ikh+1)^2$, $k = -N, \dots, N$
- Step–size h



$$e^{[h,N]}_{\alpha,\beta}(t,\lambda) = \frac{h}{2\pi i}\sum_{k=-N}^{N} e^{tz_k} z_k' z_k^{\alpha-\beta}\big(z_k^\alpha+\lambda\big)^{-1}$$

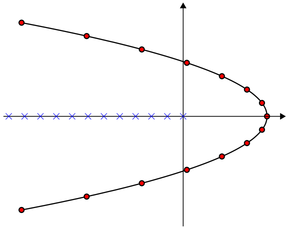
Numerical inversion of the LT on parabolic contours

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

Main steps in numerical inversion of LT on parabolic contours:

Determination of:

- Geometry parameter μ for $\mathcal{C} : z(u) = \mu(iu+1)^2$
- Number N of quadrature nodes $z_k = \mu(ikh+1)^2$, $k = -N, \dots, N$
- Step–size h



$$e_{\alpha,\beta}^{[h,N]}(t, A) = \frac{h}{2\pi i}\sum_{k=-N}^{N} e^{tz_k} z_k' z_k^{\alpha-\beta}\left(z_k^{\alpha} I + A\right)^{-1}$$

Numerical inversion of the LT on parabolic contours

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

Main steps in numerical inversion of LT on parabolic contours:

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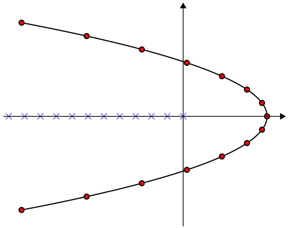


$$e^{[h,N]}_{\alpha,\beta}(t, A)\cdot F_j = \frac{h}{2\pi i}\sum_{k=-N}^{N} e^{tz_k} z'_k z_k^{\alpha-\beta}\big(z_k^{\alpha} I + A\big)^{-1}\cdot F_j$$

Solve $\big(z_k^{\alpha} I + A\big) y = F_j$

Numerical inversion of the LT on parabolic contours

Selection of contour and quadrature parameters. Main goal:

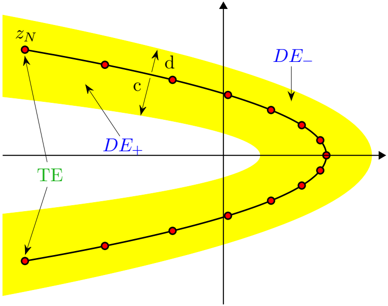
$$Error = e_{\alpha,\beta}(t,\lambda) - e_{\alpha,\beta}^{[h,n]}(t,\lambda) = DE + TE \approx \epsilon$$

Discretization error :

- $DE = DE_{+} + DE_{-}$
  - $DE_{+} = \dfrac{M_{+}(c)}{e^{2\pi c/h} - 1} \quad 0 < c \leq 1$
  - $DE_{-} = \dfrac{M_{-}(d)}{e^{2\pi d/h} - 1} \quad d > 0$

Truncation error :

- $TE = \mathcal{O}\big(|\mathcal{E}_{\alpha,\beta}(z_N)|\big)$

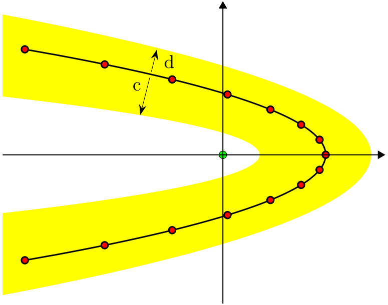


$$M_{+}(c) = \max_{0<r\leq c} \int_{-\infty}^{\infty} \big|\mathcal{E}_{\alpha,\beta}(z(u+ir))\big| du \qquad M_{-}(d) = \max_{0<s\leq d} \int_{-\infty}^{\infty} \big|\mathcal{E}_{\alpha,\beta}(z(u-is))\big| du$$

Singularities of the LT of the ML

$$\mathcal{E}_{\alpha,\beta}(s) = \mathcal{L}\Big(e_{\alpha,\beta}(t;\lambda)\,;\,s\Big) = \frac{s^{\alpha-\beta}}{s^{\alpha}+\lambda}$$

$0 < \alpha < 1 \qquad \beta > \alpha$



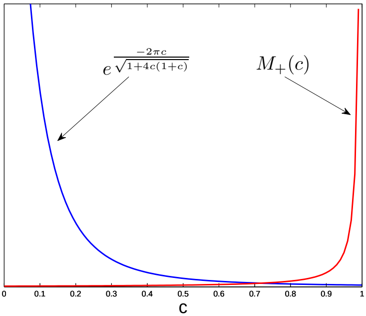
$$DE_{+} = \frac{M_{+}(c)}{e^{2\pi c/h}-1} \quad \text{but} \quad M_{+}(c) \to \infty \quad \text{when} \quad c \to 1$$

Error analysis for the ML function

$$DE_{+} \approx DE_{-} \approx TE \approx \varepsilon$$

$$Error = M_{+}(c)e^{-2\pi c/h}$$

$$h = \frac{\sqrt{1+4c(1+c)}}{N}$$



Balance $e^{-2\pi c/\sqrt{1+4c(1+c)}}$ and $M_{+}(c)$ to keep N at a low value[9]

[9] R. Garrappa and M. Popolizio. "Evaluation of generalized Mittag–Leffler functions on the real line". In: *Adv. Comput. Math.* (2012), in print.

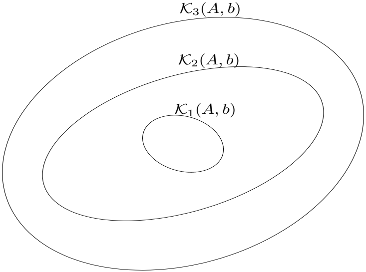
Krylov subspace methods

Originally devised to find the solution of

$$Ax = b$$

- Iterative methods
- Look for approximation $x_m \approx A^{-1}b$ in

$$\mathcal{K}_m(A, b) = span\{b,\ Ab,\ A^2b,\ \ldots,\ A^{m-1}b\}$$



Krylov subspace methods

Main steps in Krylov subspace methods

① Construction of $\mathcal{K}_m(A, b) = span\{b, Ab, \ldots, A^{m-1}b\}$

② Choice of $x_m \in \mathcal{K}_m(A, b)$

Krylov subspace methods

Main steps in Krylov subspace methods

① Construction of $\mathcal{K}_m(A,b) = span\{b,\ Ab,\ \ldots,\ A^{m-1}b\}$

② Choice of $x_m \in \mathcal{K}_m(A,b)$

① Construction of $\mathcal{K}_m(A,b)$

- Numerical instability with the basis $\{b,\ Ab,\ A^2b,\ \ldots,\ A^{m-1}b\}$
- Need of orthogonal basis $v_i^T v_j = 0,\ i \neq j$

Arnoldi or Lanczos algorithm

$$\{v_1, v_2, \ldots, v_m\} = \mathcal{K}_m(A,b)$$

$$
\begin{array}{l}
v_1 = b/\|b\|_2 \\
\text{for} k = 1, 2, \ldots \\
\quad H_{i,k} = v_k^T A^T v_i, \quad i = 1, \ldots, k \\
\quad \hat{v}_{k+1} = Av_k - \sum_{i=1}^{k} H_{i,k} v_i \\
\quad H_{k+1,k} = \|\hat{v}_{k+1}\|_2 \\
\quad v_{k+1} = \hat{v}_{k+1}/H_{k+1,k} \\
\text{end}
\end{array}
$$

Krylov subspace methods

Main steps in Krylov subspace methods

① Construction of $\mathcal{K}_m(A, b) = span\{b, Ab, \ldots, A^{m-1}b\}$

② Choice of $x_m \in \mathcal{K}_m(A, b)$

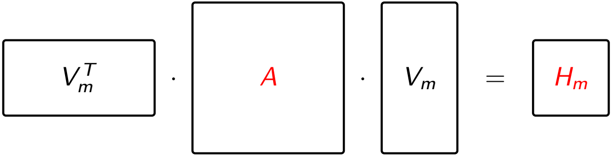
② Choice of $x_m \in \mathcal{K}_m(A, b)$

- Minimize the residual $r_m = \|b - Ax_m\|$
- Different norms
- GMRES, MINRES, FOM, CG, ...

Projections on Krylov subspaces

$$V_m^T A V_m = H_m \in \mathbb{R}^{m \times m}$$

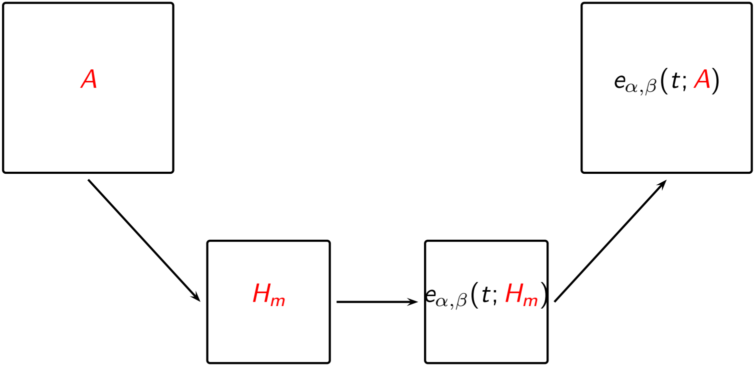
- $V_m = \left[v_1, v_2, \dots, v_m \right] \in \mathbb{R}^{N \times m}$ vectors of the basis $\mathcal{K}_m(A, b)$
- $V_m^T V_m = I \in \mathbb{R}^{m \times m}$
- H_m is upper Hessenberg



Projections on Krylov subspaces

$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T$$

$$e_{\alpha,\beta}(t; A) b \approx V_m e_{\alpha,\beta}(t; H_m) V_m^T b = \|b\|_2 V_m e_{\alpha,\beta}(t; H_m) e_1$$



Krylov subspaces methods

Main features:

- ✓ Only matrix–vector products
- ✓ Exploit the sparsity of A
- ✓ Convergence in a finite number of steps
- ✓ Recent applications to the Mittag–Leffler function[10] [11] [12] [13]

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[10] R. Garrappa and M. Popolizio. "On the use of matrix functions for fractional partial differential equations". In: *Math. Comput. Simulation* 81.5 (2011).
[11] I. Moret and P. Novati. "On the convergence of Krylov subspace methods for matrix Mittag-Leffler functions". In: *SIAM J. Numer. Anal.* 49.5 (2011).
[12] I. Moret and M. Popolizio. "The restarted shift-and-invert Krylov method for matrix functions". In: *Numer Lin. Algebr.* (2012). in print.
[13] I. Moret. "A note on Krylov methods for fractional evolution problems". In: *Numer. Func. Anal. Opt.* 34.5 (2013), pp. 539–556.

Numerical test: 2D diffusion time–fractional equation

$$\frac{\partial^\alpha}{\partial t^\alpha} u(t,x,y) = \nu \left(\frac{\partial^2}{\partial x^2} u(t,x,y) + \frac{\partial^2}{\partial y^2} u(t,x,y) \right)$$

- $\hookrightarrow$ 2D square domain : $\Omega = [0,1] \times [0,1]$
- $\hookrightarrow$ Initial conditions : $u(0,x,y) = x(1-x)y(1-y)$
- $\hookrightarrow$ Homogeneous boundary conditions : $u(t,x,y) = 0, \quad (x,y) \in \partial\Omega$

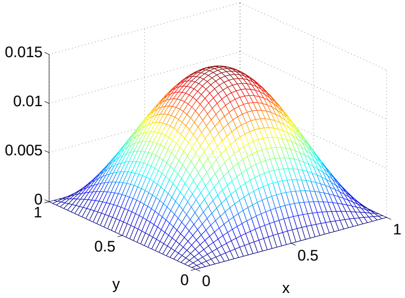
Spatial discretization - Equispaced grid on Ω:

$$\frac{d^\alpha}{dt^\alpha} U(t) = AU(t), \quad U(0) = U_0 \qquad \Longrightarrow \qquad U(t) = e_{\alpha,1}(t; -A) U_0$$

Numerical test: 2D diffusion time–fractional equation

Time simulation at $t = 1$ for $\alpha = 0.7$ and $\nu = 0.1$

Numerical Solution



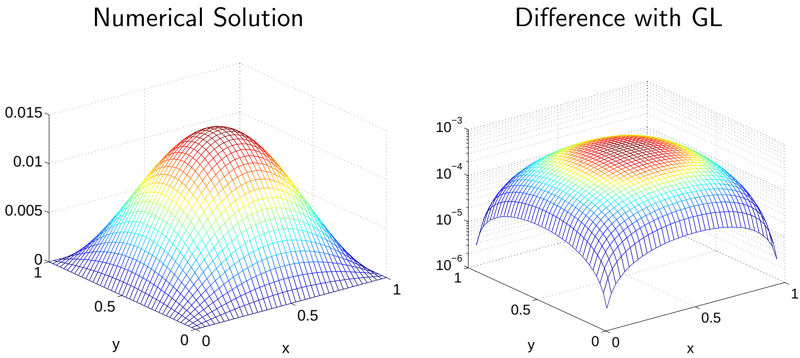
Difference with GL

Spatial mesh–grid $N_x = N_y = 40$ - Step–size $h = 2^{-4} = 0.625 \times 10^{-1}$

Comparison with the implicit Grünwald–Letnikov scheme (first order)

Numerical test: 2D diffusion time–fractional equation

Time simulation at $t = 1$ for $\alpha = 0.7$ and $\nu = 0.1$

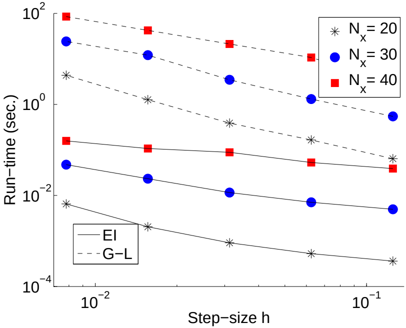


Spatial mesh–grid $N_x = N_y = 40$ - Step–size $h = 2^{-4} = 0.625 \times 10^{-1}$

Comparison with the implicit Grünwald–Letnikov scheme (first order)

Numerical test: 2D diffusion time–fractional equation

Time of execution for $t \in [0, 1]$



EI = Exponential integrator
G-L = Grünwald–Letnikov

Numerical test: 1D time–fractional ADR equation

$$\frac{\partial^\alpha}{\partial t^\alpha} u + \varepsilon \frac{\partial}{\partial x} u = \nu \frac{\partial^2}{\partial x^2} u + \frac{1}{2} u(u - \frac{1}{2})(u - 1)$$

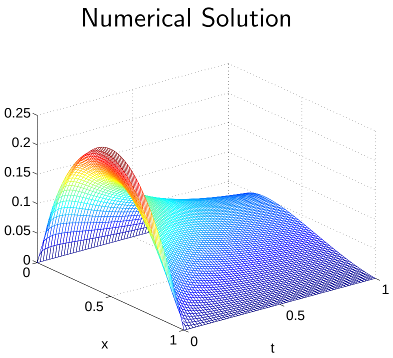
- ↪ 1D domain : $\Omega = [0, 1]$
- ↪ Initial conditions : $u(0, x) = x(1 - x)$
- ↪ Boundary conditions : $u(t, 0) = 0$, $u(t, 1) = 0$

Spatial mesh–grid $N_x = 80$

$$\frac{d^\alpha}{dt^\alpha} U(t) = AU(t) + F(t, U(t)), \quad U(0) = U_0$$

Numerical test: 1D time–fractional ADR equation

Time simulation at $t = 1$ for $\alpha = 0.7$ and $\nu = 0.1$

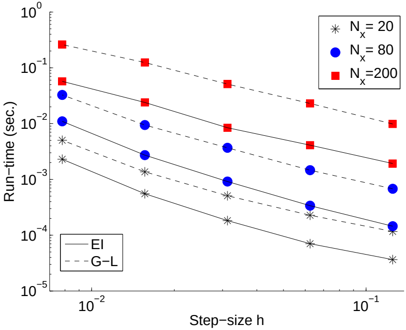


Spatial mesh–grid $N_x = 80$ - Step–size $h = 2^{-6} = 0.156 \times 10^{-1}$

Comparison with the implicit Grünwald–Letnikov scheme (first order)

Numerical test: 1D time–fractional ADR equation

Time of execution for $t \in [0, 1]$



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Concluding remarks

- Exponential integrators seem to be promising for FPDEs
  - Good stability properties
  - Explicit schemes
  - Competitive computation with respect to classical methods
  - Higher accuracy for linear problems
- Open problems
  - Enhance the computation of the generalized ML functions
  - Efficient algorithms for the ML function with matrix arguments

Some references

[1] R. Garrappa. "A family of Adams exponential integrators for fractional linear systems". In: *Comput. Math. Appl.* (2013), in print.

[2] R. Garrappa. "Exponential integrators for time–fractional partial differential equations". In: *European Physical Journal* (2013), to appear.

[3] R. Garrappa and M. Popolizio. "Evaluation of generalized Mittag–Leffler functions on the real line". In: *Adv. Comput. Math.* (2012), in print.

[4] R. Garrappa and M. Popolizio. "Generalized exponential time differencing methods for fractional order problems". In: *Comput. Math. Appl.* 62.3 (2011), pp. 876–890.

[5] R. Garrappa and M. Popolizio. "On accurate product integration rules for linear fractional differential equations". In: *J. Comput. Appl. Math.* 235.5 (2011), pp. 1085–1097.

[6] R. Garrappa and M. Popolizio. "On the use of matrix functions for fractional partial differential equations". In: *Math. Comput. Simulation* 81.5 (2011).