Identification of the derivative order in fractional differential equations

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Algorithmes Stochastiques et Applications – LMA Poitiers

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Probabilistic arguments $\Longrightarrow$ The master Equation (Montroll & Weiss, 1965)

$$p(x,t) = \delta(x)\,\varphi(t) + \int_0^t \psi(t-\tau)\left(\int_{-\infty}^{+\infty} w(x-\xi)p(\xi,\tau)\,d\xi\right)d\tau, \qquad (1)$$

where

- $\delta(x)$ is the Dirac measure.
- $\varphi(t) := 1 - \int_0^t \psi(\tau)\,d\tau$ (Survival probability at the origin).
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From Master Equation to Fractional Differential Equations

Theorem 1 (R. Gorenflo & F. Mainardi)

Assume that :

- $w(x) \sim c_1 \, |x|^{-(\alpha+1)}$ *as* $|x| \longrightarrow +\infty$, *with* $\alpha \in]0,2[$.
- $\psi(t) \sim c_2 \, t^{-(\beta+1)}$ *as* $t \longrightarrow +\infty$, *with* $\beta \in]0,1[$.

Then, up to scaling the variables :

- $x \longleftarrow (\Delta x) \times x$,
- $t \longleftarrow (\Delta t) \times t$,
- *with* $(\Delta x)^\alpha = c_3 \, (\Delta t)^\beta$,

the master equation (1) goes over to the space-time fractional diffusion equation :

$$\begin{cases} \mathscr{D}_t^\beta \, p(x,t) \; - \; {}_0D_1^\alpha \, p(x,t) = 0, \quad 0 < \alpha < 2, \quad 0 < \beta < 1, \\ u(x, 0^+) = \delta(x), \quad x \in \mathbb{R}, \quad t > 0, \end{cases}$$

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Definitions and notations

Let $u : [a,b] \to \mathbb{R}$, an integrable function, $\alpha > 0$.

Definition 2 (Riemann-Liouville's fractional integral and derivative)

1. The left and right sided Riemann-Liouville fractional integrals of order α :

$$\begin{cases} {}_aI^{\alpha}\, u(x) &= \dfrac{1}{\Gamma(\alpha)} \displaystyle\int_a^x \dfrac{u(t)}{(x-t)^{1-\alpha}} dt, \\ I_b^{\alpha}\, u(x) &= \dfrac{1}{\Gamma(\alpha)} \displaystyle\int_x^b \dfrac{u(t)}{(t-x)^{1-\alpha}} dt. \end{cases}$$

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For $0 < \alpha < 1$, we get :

- $_aD^\alpha\, u(x) = \dfrac{1}{\Gamma(1-\alpha)} \dfrac{d}{dx} \left(\displaystyle\int_a^x \dfrac{u(t)}{(x-t)^\alpha} dt \right).$
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By permuting the operators $\dfrac{d^n}{dx^n}$ and $I^{n-\alpha}$, we obtain :

Definition 3 (Caputo's fractional derivative)

- Left-sided Caputo fractional derivative : $_a\mathscr{D}^\alpha\, u(x) =_a I^{n-\alpha} u^{(n)}(x)$,
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Identification of the derivative order in fractional differential equations

Consider the boundary value problem :

$$\begin{cases} -\dfrac{d}{dx}\left[k(x)D_x^{\alpha,\theta}u(x)\right] = f(x), \ x \in \Omega =]a, b[, \\ \\ u(a) = u(b) = 0, \end{cases} \qquad (2)$$

- $0 < \alpha < 1$, $0 \leq \theta \leq 1$.
- The source term $f \in L^2(\Omega)$.
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The cost function

To this end, we introduce the quadratic cost function :

$$J(\alpha) := \frac{1}{2}\int_{\Omega}\left[u_{\alpha}(x) - z(x)\right]^2 \, dx, \quad (3)$$

where :

- u_{α} : the solution of the BVP ((2)).
- z : an experimental measure of the the exact solution.

To perform a descent method, we have to compute

- $\dfrac{d\,u_{\alpha}}{d\alpha}$
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Theorem 4

Let u_α *be the solution of* (2)*. Then* $\dfrac{d\,u_\alpha}{d\,\alpha}$ *is the solution to the following BVP*

$$\begin{cases} -\dfrac{d}{dx}\left[k(x)D_x^{\alpha,\theta}\,w\right] = \dfrac{d}{dx}\left[k(x)\widehat{D}_x^{\alpha,\theta}u_\alpha\right],\ x\in\Omega=(a,b),\\ w(a) = w(b) = 0, \end{cases} \tag{4}$$

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Proof

Let u_α be the solution of (2), then

$$-\frac{d}{dx}\left[k(x)D_x^{\alpha,\theta}u_\alpha(x)\right] = f(x),\ x \in \Omega = (a,b). \tag{5}$$

We will detail the derivative of the equation (5) with respect to α:

$$-\frac{d}{d\alpha}\left(\frac{d}{dx}\left[k(x)D_x^{\alpha,\theta}u_\alpha(x)\right]\right) = -\frac{d}{dx}\left(k(x)\frac{d}{d\alpha}\left[D_x^{\alpha,\theta}u_\alpha(x)\right]\right) = 0,\ x \in \Omega = (a,b). \tag{6}$$

It is clear that

$$\frac{d}{d\alpha}\left[D_x^{\alpha,\theta}u_\alpha(x)\right] = \theta\frac{d}{d\alpha}\left[{}_aD_x^{\alpha}u_\alpha(x)\right] + (1-\theta)\frac{d}{d\alpha}\left[{}_xD_b^{\alpha}u_\alpha(x)\right].$$

Let us start by the first derivative $\frac{d}{d\alpha}\left[{}_aD_x^{\alpha}u_\alpha(x)\right]$. A direct computation gives

$$\begin{aligned}\frac{d}{d\alpha}\left[{}_aD_x^{\alpha}u_\alpha(x)\right] &= \frac{d}{d\alpha}\left[\frac{d}{dx}\left(\int_a^x \frac{(x-t)^{-\alpha}}{\Gamma(1-\alpha)}u_\alpha(t)dt\right)\right] \\ &= \frac{d}{dx}\left(\int_a^x \frac{(x-t)^{-\alpha}}{\Gamma(1-\alpha)}\ln\left(\frac{1}{x-t}\right)u_\alpha(t)dt\right) + \\ &+ \frac{\Gamma'(1-\alpha)}{\Gamma(1-\alpha)}\,{}_aD_x^{\alpha}u_\alpha(x) + {}_aD_x^{\alpha}\frac{du_\alpha}{d\alpha}(x),\end{aligned}$$

Proof $\cdots$

We mention here that the first integral

$$\int_a^x (x-t)^{-\alpha} \ln\left(\frac{1}{x-t}\right) u(t)dt$$

is of Bertrand type and is consequently convergent if u is continuous on $[a,b]$. That is,

$$\frac{d}{d\alpha}\left[{}_aD_x^\alpha u_\alpha(x)\right] = {}_a\widehat{D}_x^\alpha u_\alpha(x) + {}_aD_x^\alpha \frac{du_\alpha}{d\alpha}(x), \qquad (7)$$

The same computations with ${}_xD_b^\alpha$ lead to

$$\frac{d}{d\alpha}\left[D_x^{\alpha,\theta} u_\alpha(x)\right] = \widehat{D}_x^{\alpha,\theta} u_\alpha(x) + {}_aD_x^{\alpha,\theta} \frac{du_\alpha}{d\alpha}(x). \qquad (8)$$

Using the fact that

$$\frac{d}{d\alpha}\left[D_x^{\alpha,\theta} u_\alpha(x)\right] = \frac{d}{d\alpha} f(x) = 0 \text{ and } \frac{d}{d\alpha} u_\alpha(a) = \frac{d}{d\alpha} u_\alpha(b) = 0$$

we obtain the result.

Steepest Descent Method

Steepest Descent algorithm

1. Initialization : Choose $\alpha_0 \in]0,1[$.
2. Solve Problems (2) and (4) with α_n to obtain u_{α_n} and w_{α_n}.
3. Descent direction : $-J'(\alpha_n) = -\int_\Omega w_{\alpha_n}(x)[u_{\alpha_n}(x) - z(x)]\,dx$.
4. Update : $\alpha_{n+1} = \alpha_n - \rho J'(\alpha_n)$, with $\rho > 0$ sufficiently small.

A finite difference numerical method

- Uniform discretization $(x_n)_{0\leq n\leq N}$ of (a,b), with $x_0 = a$ and $x_N = b$.
- $I_n := [x_{n-1}, x_n]$, for every $n \in \{1, 2, \cdots, N\}$.
- The step size $h = x_n - x_{n-1} = (b-a)/N$.
- $x_{n+\frac{1}{2}} = (x_n + x_{n+1})/2$ is the center of I_{n+1}.
- Notation : $v^n = v(x_n)$.
- Given v defined on $[a,b]$, for every $n \in \{1, 2, \cdots, N\}$ and $x \in I_n$, we define the backward difference at x by:

$$\delta v(x) = \delta v^n := v^n - v^{n-1}.$$

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A finite difference numerical method

- Uniform discretization $(x_n)_{0 \le n \le N}$ of (a,b), with $x_0 = a$ and $x_N = b$.
- $I_n := [x_{n-1}, x_n]$, for every $n \in \{1, 2, \cdots, N\}$.
- The step size $h = x_n - x_{n-1} = (b-a)/N$.
- $x_{n+\frac{1}{2}} = (x_n + x_{n+1})/2$ is the center of I_{n+1}.
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Left-sided fractional derivative

We set $\theta = 1$, then (2) reduces to :

$$-\frac{d}{dx}\left[k(x)\,{}_aD_x^{\alpha}u\right](x) = f(x).$$

The finite difference scheme is expressed as :

$$\frac{\omega(h)}{h^2}\left(\sum_{j=1}^{n-1}\left(k^{n-\frac{1}{2}}\left[w_{n,j}-w_{n,j+1}\right]-k^{n+\frac{1}{2}}\left[w_{n+1,j}-w_{n+1,j+1}\right]\right)U^j + \left(k^{n-\frac{1}{2}}-k^{n+\frac{1}{2}}\left(2^{1-\alpha}-2\right)\right)U^n - k^{n+1}U^{n+1}\right) = f^n,$$

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Matrix formulation

$$B_L = \frac{\omega(h)}{h^2} \begin{pmatrix} c_{1,1} & -k^{3/2} & 0 & \cdots & \cdots & 0 \\ c_{2,1} & c_{2,2} & -k^{5/2} & 0 & \cdots & 0 \\ \vdots & \vdots & & & & \vdots \\ & & & & & 0 \\ c_{N-2,1} & c_{N-2,2} & \cdots & \cdots & c_{N-2,N-2} & -k^{N-3/2} \\ c_{N-1,1} & c_{N-1,2} & \cdots & \cdots & c_{N-1,N-2} & c_{N-1,N-1} \end{pmatrix}$$

$${}_{n,j} = \begin{cases} k^{n-\frac{1}{2}} - k^{n+\frac{1}{2}}\left[2^{1-\alpha} - 2\right] & j = n, \\ a_{n,j} - a_{n+1,j} & j < n, \end{cases}$$

$$a_{n,j} = \begin{cases} k^{n-\frac{1}{2}} & j = n, \\ k^{n-\frac{1}{2}}\left[w_{n,j} - w_{n-1,j}\right] & j < n. \end{cases}$$

Finite difference solution

Solve the linear system $B_L U = F$,

- $U = [U^1, U^2, \cdots, U^{N-1}]^T$
- $F = [f^1, f^2, \cdots, f^{N-1}]^T$.

Right-sided fractional derivative

We set $\theta = 0$, then (2) reduces to :

$$-\frac{d}{dx}\left[k(x)\ D_b^{\alpha} u\right](x) = f(x).$$

The matrix of right-sided fractional derivative is

$$B_R = \frac{\omega(h)}{h^2}\begin{pmatrix} d_{1,1} & d_{1,2} & d_{1,3} & d_{1,4} & d_{1,5} & \cdots & d_{1,N-1} \\ -k^{3/2} & d_{2,2} & d_{2,3} & d_{2,4} & d_{2,5} & \cdots & d_{2,N-1} \\ 0 & -k^{5/2} & d_{3,3} & d_{3,4} & d_{3,5} & \cdots & d_{3,N-1} \\ 0 & 0 & -k^{7/2} & d_{4,4} & d_{4,5} & \cdots & d_{4,N-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -k^{N-3/2} & d_{N-1,N-1} \end{pmatrix}$$

$$d_{n,j} = \begin{cases} k^{n-\frac{1}{2}}(w_{j,n} - w_{j,n-1}) - k^{n+\frac{1}{2}}(w_{j,n+1} - w_{j,n}) & j > n, \\ k^{n+\frac{1}{2}} - k^{n-\frac{1}{2}}[2^{1-\alpha} - 2], & j = n. \end{cases}$$

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Finite difference solution: Solving the linear system $B_R\, U = F$.

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Two-sided fractional derivative

Return to problem (2). To get a finite difference approximation, we combine the difference schemes. The finite difference solution $(U^n)_n \simeq (u^n)_n$ of the fractional problem is given by

$$\begin{array}{l} k^{n-\frac{1}{2}} [\theta \;_a I^{1-\alpha} \delta U(x_n) + (1-\theta) \; I_b^{1-\alpha} \delta U(x_{n-1})] \\ -k^{n+\frac{1}{2}} [\theta \;_a I^{1-\alpha} \delta U(x_{n+1}) + (1-\theta) \; I_b^{1-\alpha} \delta U(x_n)] = h^2 f^n, \end{array}$$

for $n = 1, \cdots, N-1$, and $U^0 = U^N = 0$.

Finite difference solution

The finite difference solution is obtained by solving the linear system $B\,U = F$, where $B = \theta B_L + (1-\theta) B_R$.

Finite difference scheme for (4)

The same arguments are performed for the the BVP (4).

- The same matrices B_L, B_R and B.
- Preparation of the RHS, with slight modifications (to handle with the Logarithm terms).
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Numerical Results

We choose :

- $\theta = 1/2$.
- $\widehat{\alpha} = 0.6$.
- The measure z of $u_{\widehat{\alpha}}$ in $\Omega =]0, 1[$ defined by $z(x) = 10^4 x^{3.8}(1-x)^{3.8}$,
- The source term f defined by $f(x) = D_x^{\widehat{\alpha},\theta} z(x)$,

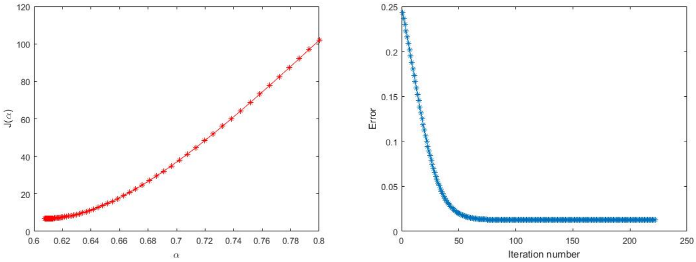

Figure 1: Left: The cost function $J(\alpha)$, with initialization $\alpha_0 = 0.8$. Right: Relative error for α in the steepest descent scheme.

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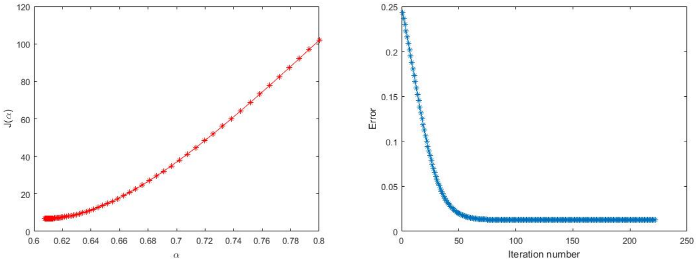
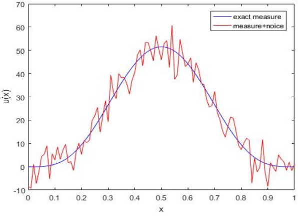
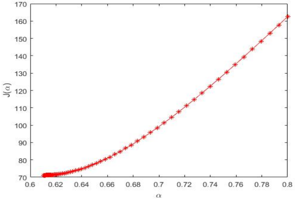


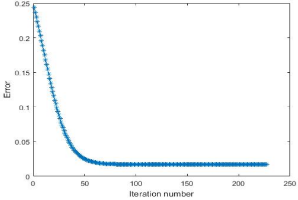
Figure 1: Left: The cost function $J(\alpha)$, with initialization $\alpha_0 = 0.8$. Right: Relative error for α in the steepest descent scheme.



(a) The exact observation (blue) and a noisy observation (red) with an additive white gaussian noise of SNR $= 20$.



(b) Relative error for α in the steepest descent scheme.



(c) Relative error for α in the steepest descent scheme.

Application to the Taylor-Couette flow

We consider an application to coaxial annular flow in which a fluid is confined between two cylinders of radii R_{in} and R_{out}. A fractional order model governing the fluid velocity $u_\theta(r,t)$:

$$\begin{cases} \frac{\rho}{\mathbb{V}}\frac{\partial u_\theta}{\partial t} + \frac{\rho}{\mathbb{G}}\mathscr{D}_t^{2-\beta}u_\theta = \frac{\partial^2 u_\theta}{\partial r^2} + \frac{1}{r}\frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r^2}, \quad R_{in} < r < R_{out},\ 0 < t \leq T \\ u_\theta(R_{in},t) = \phi_i(t),\ u_\theta(R_{out},t) = \phi_o(t), \quad 0 \leq t \leq T, \\ u_\theta(r,0) = \frac{\partial u_\theta(r,0)}{\partial t} = 0, \quad R_{in} < r < R_{out}, \end{cases}$$

with $\beta \in]0,1[$. The constants ρ, $\mathbb{V}$ and $\mathbb{G}$ are given positive physical parameters.

$$\frac{\rho}{\mathbb{V}}\delta_t u_i^{s-1/2} + \frac{\rho}{\Gamma(\beta)(G)}\frac{1}{\Delta t}\left[a_0\delta_t u_i^{s-1/2} - \sum_{j=1}^{s-1}(a_{n-j-1} - a_{n-j})\delta_t u_i^{j-1/2}\right] = \delta_r^2 u_i^{s-1/2} + \frac{1}{2r_i}\left(\frac{\delta_r u_i^s + \delta_r u_i^{s-1}}{2}\right) - \frac{u_i^{s-1/2}}{r_i^2}, \tag{9}$$

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Matrix form:

$$AU = B \tag{10}$$

where

$$U = \begin{bmatrix} u_1^s \\ u_2^s \\ \vdots \\ u_{N-1}^s \end{bmatrix} \tag{11}$$

and

$$A = \begin{pmatrix} d_1 & \frac{-1}{4r_1\Delta r} - \frac{1}{2(\delta r)^2} & & \\ \frac{1}{4r_2\Delta r} - \frac{1}{2(\delta r)^2} & d_2 & \frac{-1}{4r_2\Delta r} - \frac{1}{2(\delta r)^2} & \\ \ddots & \ddots & \ddots & \\ & & \frac{1}{4r_{N-1}\Delta r} - \frac{1}{2(\delta r)^2} & d_{N-1} \end{pmatrix}$$

with $d_i = \left(\frac{\rho}{\mathbb{V}} \frac{1}{\Delta t} + \frac{\rho}{\Gamma(\beta)\mathbb{G}} \frac{a_0}{(\Delta t)^2} + \frac{1}{2(r_i)^2} + \frac{1}{(\Delta r)^2} \right)$ for $1 \leq i \leq N-1$ and B is the column vector containing all the terms coming from the previous time iteration.

Taylor-Couette numerical simulations

We choose $\widehat{\beta} = 0.7$ which will be supposed to be unknown. We are interested to find $\widehat{\beta}$ by considering a measure z of the solution $u_\theta(\widehat{\beta})$ on $]R_{in}, R_{out}[\times]0, T[$.

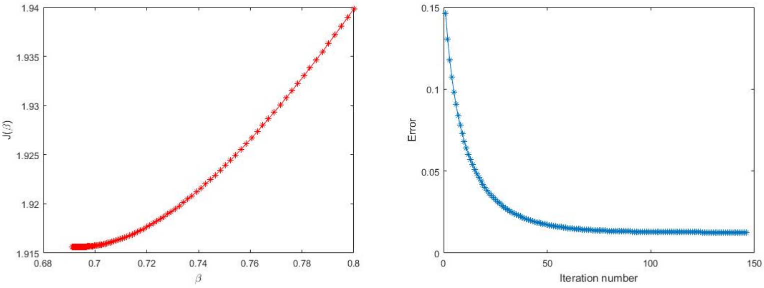

Figure 3: Left: The cost function $J(\beta)$, with initialization $\beta_0 = 0.8$. Right: Relative error for β in the steepest descent scheme.

Thank you for your attention !