Numerical methods of the fractional calculus

(continued)

Integer-order differentiation

Backward differences

Approximation of the first order derivative:

$$f'(t_k) \approx \frac{1}{h}\,\nabla f(t_k) = \frac{1}{h}\,(f_k - f_{k-1}), \quad k = 1, \ldots, N.$$

All these formulas can be written simultaneously:

$$\begin{bmatrix} h^{-1}\, f_0 \\ h^{-1}\,\nabla f(t_1) \\ h^{-1}\,\nabla f(t_2) \\ \vdots \\ h^{-1}\,\nabla f(t_{N-1}) \\ h^{-1}\,\nabla f(t_N) \end{bmatrix} = \frac{1}{h} \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & \cdots & 0 \\ \ldots & \ldots & \ldots & \ddots & \ldots & \ldots \\ 0 & \cdots & 0 & -1 & 1 & 0 \\ 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_{N-1} \\ f_N \end{bmatrix}$$

Integer-order differentiation

Backward differences

Approximation of the first order derivative:

$$B_N^1 = \frac{1}{h} \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & \cdots & 0 \\ \ldots & \ldots & \ldots & \ddots & \ldots & \ldots \\ 0 & \cdots & 0 & -1 & 1 & 0 \\ 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}$$

Generating function:

$$\beta_1(z) = h^{-1}(1-z).$$

Integer-order differentiation

Backward differences

Approximation of the second order derivative:

$$f''(t_k) \approx \frac{1}{h^2}\,\nabla^2 f(t_k) = \frac{1}{h^2}\,(f_k - 2f_{k-1} + f_{k-2}), \quad k = 2, \ldots, N$$

All these formulas can be written simultaneously, too:

$$\begin{bmatrix} h^{-2}\, f_0 \\ h^{-2}\,(-2f_0 + f_1) \\ h^{-2}\,\nabla^2 f(t_2) \\ \vdots \\ h^{-2}\,\nabla^2 f(t_{N-1}) \\ h^{-2}\,\nabla^2 f(t_N) \end{bmatrix} = \frac{1}{h^2} \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ \ldots & \ldots & \ldots & \ddots & \ldots & \ldots \\ \cdots & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & \cdots & 1 & -2 & 1 \end{bmatrix} \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_{N-1} \\ f_N \end{bmatrix}$$

Integer-order differentiation

Backward differences

Approximation of the second order derivative:

$$B_N^2 = \frac{1}{h^2} \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ \ldots & \ldots & \ldots & \ddots & \ldots & \ldots \\ \cdots & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & \cdots & 1 & -2 & 1 \end{bmatrix}$$

Generating function:

$$\beta_2(z) = h^{-2}(1 - 2z + z^2) = h^{-2}(1-z)^2$$

Integer-order differentiation

Backward differences

Approximation of the p-th order derivative:

$$B_N^p = \frac{1}{h^p} \begin{bmatrix} \omega_0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 \\ \omega_1 & \omega_0 & 0 & \ldots & 0 & 0 & 0 & 0 \\ \omega_2 & \omega_1 & \omega_0 & 0 & \ldots & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ddots & \ldots & \ldots & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ddots & \ldots & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ddots & 0 & \ldots \\ 0 & \ldots & 0 & \omega_p & \omega_{p-1} & \ldots & \omega_0 & 0 \\ 0 & 0 & \ldots & 0 & \omega_p & \omega_{p-1} & \ldots & \omega_0 \end{bmatrix} \qquad \omega_j = (-1)^j \binom{p}{j}, \qquad j = 0, 1, 2, \ldots, p$$

Generating function:

$$\beta_p(z) = h^{-p}(1-z)^p$$

Integer-order differentiation

Backward differences

For the generating functions we have:

$$\begin{aligned} \beta_2(z) &= \beta_1(z)\beta_1(z) \\ \beta_p(z) &= \underbrace{\beta_1(z)\dots\beta_1(z)}_{p} \\ \beta_{p+q}(z) &= \beta_p(z)\beta_q(z) = \beta_q(z)\beta_p(z) \end{aligned}$$

and therefore

$$\begin{aligned} B_N^2 &= B_N^1\, B_N^1, \\ B_N^p &= \underbrace{B_N^1\, B_N^1 \dots B_N^1}_{p}, \\ B_N^{p+q} &= B_N^p\, B_N^q = B_N^q\, B_N^p \end{aligned}$$

Integer-order integration

Moving upper limit

One-fold integral:

$$g_1(t) = \int_a^t f(t)dt.$$

Approximation:

$$g_1(t_k) \approx h \sum_{i=0}^{k-1} f_i, \qquad k = 1, \dots, N.$$

All these formulas can be written simultaneously:

$$\begin{bmatrix} g_1(t_1) \\ g_1(t_2) \\ g_1(t_3) \\ \vdots \\ g_1(t_N) \\ g_1(t_N+h) \end{bmatrix} = h \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 1 & 0 & \cdots & 0 \\ \dots & \dots & \dots & \ddots & \dots & \dots \\ 1 & \cdots & 1 & 1 & 1 & 0 \\ 1 & 1 & \cdots & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_{N-1} \\ f_N \end{bmatrix}$$

Left-sided fractional derivatives

$${}_aD_{t_k}^{\alpha} f(t) \approx \frac{\nabla^\alpha f(t_k)}{h^\alpha} = h^{-\alpha} \sum_{j=0}^{k} (-1)^j \binom{\alpha}{j} f_{k-j}, \qquad k = 0, 1, \dots, N.$$

$$\begin{bmatrix} h^{-\alpha}\nabla^\alpha f(t_0) \\ h^{-\alpha}\nabla^\alpha f(t_1) \\ h^{-\alpha}\nabla^\alpha f(t_2) \\ \vdots \\ h^{-\alpha}\nabla^\alpha f(t_{N-1}) \\ h^{-\alpha}\nabla^\alpha f(t_N) \end{bmatrix} = \frac{1}{h^\alpha} \begin{bmatrix} \omega_0^{(\alpha)} & 0 & 0 & 0 & \cdots & 0 \\ \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 & 0 & \cdots & 0 \\ \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \cdots & \cdots \\ \omega_{N-1}^{(\alpha)} & \ddots & \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 \\ \omega_N^{(\alpha)} & \omega_{N-1}^{(\alpha)} & \ddots & \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} \end{bmatrix} \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_{N-1} \\ f_N \end{bmatrix}$$

$$\omega_j^{(\alpha)} = (-1)^j \binom{\alpha}{j}, \qquad j = 0, 1, \dots, N.$$

Integer-order integration

Moving upper limit

Approximation of one-fold integration:

$$I_N^1 = h \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 1 & 0 & \cdots & 0 \\ \dots & \dots & \dots & \ddots & \dots & \dots \\ 1 & \cdots & 1 & 1 & 1 & 0 \\ 1 & 1 & \cdots & 1 & 1 & 1 \end{bmatrix}$$

Generating function:

$$\varphi_1(z) = h(1-z)^{-1}$$

Left-sided fractional derivatives

$$B_N^\alpha = \frac{1}{h^\alpha} \begin{bmatrix} \omega_0^{(\alpha)} & 0 & 0 & 0 & \cdots & 0 \\ \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 & 0 & \cdots & 0 \\ \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \cdots & \cdots \\ \omega_{N-1}^{(\alpha)} & \ddots & \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 \\ \omega_N^{(\alpha)} & \omega_{N-1}^{(\alpha)} & \ddots & \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} \end{bmatrix}$$

$$\beta_\alpha(z) = h^{-\alpha}(1-z)^\alpha.$$

$$B_N^\alpha B_N^\beta = B_N^\beta B_N^\alpha = B_N^{\alpha+\beta},$$

$${}_aD_t^\alpha({}_aD_t^\beta f(t)) = {}_aD_t^\beta({}_aD_t^\alpha f(t)) = {}_aD_t^{\alpha+\beta} f(t),$$

$$f^{(k)}(a) = 0, \quad k = 1, 2, \dots, r-1,$$

$$r = \max\{n, m\}$$

Integer-order integration

Moving upper limit

Notice that matrix I_N^1 is inverse to the matrix B_N^1 :

$$B_N^1 I_N^1 = I_N^1 B_N^1 \longleftrightarrow \operatorname{trunc}_N(\beta_1(z)\,\varphi_1(z)) = 1 \longleftrightarrow E.$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & \cdots & 0 \\ \dots & \dots & \dots & \ddots & \dots & \dots \\ 0 & \cdots & 0 & -1 & 1 & 0 \\ 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 1 & 0 & \cdots & 0 \\ \dots & \dots & \dots & \ddots & \dots & \dots \\ 1 & \cdots & 1 & 1 & 1 & 0 \\ 1 & 1 & \cdots & 1 & 1 & 1 \end{bmatrix} = ?$$

Integer-order integration

Moving upper limit

Two-fold integral:

$$g_2(t) = \int_a^t dt \int_a^t f(t)dt$$

Approximation:

$$\begin{aligned} g_2(t_k) &= h\sum_{i=0}^{k-1} g_1(t_i) = h\sum_{i=1}^{k-1} g_1(t_i) = h\sum_{i=1}^{k-1} h\sum_{j=0}^{i-1} f_j \\ &= h^2\sum_{i=1}^{k-1}\sum_{j=0}^{i-1} f_j = h^2\sum_{j=0}^{k-2}(k-j-1)\,f_j \\ &= h^2\Big((k-1)f_0 + (k-2)f_1 + \ldots + 2f_{k-3} + f_{k-2}\Big) \end{aligned}$$

$$k = 2, 3, \ldots, N.$$

Integer-order integration

Moving upper limit

Approximation of the two-fold integration:

$$g_2(t_k) = h^2\Big((k-1)f_0 + (k-2)f_1 + \ldots + 2f_{k-3} + f_{k-2}\Big), \quad k = 2, 3, \ldots, N.$$

All these formulas can be written simultaneously, too:

$$\begin{bmatrix} g_2(t_2) \\ g_2(t_3) \\ \vdots \\ g_2(t_N) \\ g_2(t_N+h) \\ g_2(t_N+2h) \end{bmatrix} = h^2 \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 2 & 1 & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots & \cdots & \cdots \\ \cdots & 3 & 2 & 1 & 0 & 0 \\ N & \cdots & 3 & 2 & 1 & 0 \\ N+1 & N & \cdots & 3 & 2 & 1 \end{bmatrix} \begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_{N-2} \\ f_{N-1} \\ f_N \end{bmatrix}$$

Integer-order integration

Moving upper limit

Approximation of the two-fold integration:

$$I_N^2 = h^2 \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 2 & 1 & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots & \cdots & \cdots \\ \cdots & 3 & 2 & 1 & 0 & 0 \\ N & \cdots & 3 & 2 & 1 & 0 \\ N+1 & N & \cdots & 3 & 2 & 1 \end{bmatrix}$$

Generating function:

$$\varphi_2(z) = h^2(1-z)^{-2}$$

Integer-order integration

Moving upper limit

Notice that matrix I_N^2 is inverse to the matrix B_N^2 :

$$B_N^2 I_N^2 = I_N^2 B_N^2 \longleftrightarrow \mathrm{trunc}_N\left(\beta_2(z)\,\varphi_2(z)\right) = 1 \longleftrightarrow E.$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ \cdots & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & \cdots & 1 & -2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 2 & 1 & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots & \cdots & \cdots \\ \cdots & 3 & 2 & 1 & 0 & 0 \\ N & \cdots & 3 & 2 & 1 & 0 \\ N+1 & N & \cdots & 3 & 2 & 1 \end{bmatrix} = ?$$

Integer-order integration

Moving upper limit

p-fold integration: $g_p(t) = \int_a^t d\tau_p \int_a^{\tau_p} d\tau_{p-1} \ldots \int_a^{\tau_2} f(\tau_1)d\tau_1$

Approximation:

$$I_N^p = h^p \begin{bmatrix} \gamma_0 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ \gamma_1 & \gamma_0 & 0 & 0 & \cdots & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \gamma_2 & \gamma_1 & \gamma_0 & 0 & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ \gamma_{N-1} & \cdots & \cdots & \gamma_2 & \gamma_1 & \gamma_0 & 0 \\ \gamma_N & \gamma_{N-1} & \cdots & \cdots & \gamma_2 & \gamma_1 & \gamma_0 \end{bmatrix}$$

Generating function:

$$\varphi_p(z) = h^p(1-z)^{-p}$$

Integer-order integration

Moving upper limit

Notice that matrix I_N^p is inverse to the matrix B_N^p:

$$B_N^p I_N^p = I_N^p B_N^p \longleftrightarrow \mathrm{trunc}_N\left(\beta_p(z)\,\varphi_p(z)\right) = 1 \longleftrightarrow E$$

Properties:

$$\begin{aligned} I_N^2 &= I_N^1\, I_N^1, \\ I_N^p &= \underbrace{I_N^1\, I_N^1 \ldots I_N^1}_{p}, \\ I_N^{p+q} &= I_N^p\, I_N^q = I_N^q\, I_N^p \end{aligned}$$

Matrices I_N^p commute with matrices B_N^p .

Left-sided fractional integrals

$$ {}_aD_t^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-\tau)^{\alpha-1} f(\tau)\,d\tau, \qquad (a < t < b), $$

$$ I_N^{\alpha} = (B_N^{\alpha})^{-1}. $$

$$ I_N^{\alpha} \longleftrightarrow \varphi_N(z) = \mathrm{trunc}_N\left(\beta_\alpha^{-1}(z)\right) = \mathrm{trunc}_N\left(h^{\alpha}(1-z)^{-\alpha}\right). $$

$$ I_N^{\alpha} = h^{\alpha} \begin{bmatrix} \omega_0^{(-\alpha)} & 0 & 0 & 0 & \cdots & 0 \\ \omega_1^{(-\alpha)} & \omega_0^{(-\alpha)} & 0 & 0 & \cdots & 0 \\ \omega_2^{(-\alpha)} & \omega_1^{(-\alpha)} & \omega_0^{(-\alpha)} & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \cdots & \cdots \\ \omega_{N-1}^{(-\alpha)} & \ddots & \omega_2^{(-\alpha)} & \omega_1^{(-\alpha)} & \omega_0^{(-\alpha)} & 0 \\ \omega_N^{(-\alpha)} & \omega_{N-1}^{(-\alpha)} & \ddots & \omega_2^{(-\alpha)} & \omega_1^{(-\alpha)} & \omega_0^{(-\alpha)} \end{bmatrix} $$

Initial value problems for FDEs

Discretization of an equation

Consider linear FDE with non-constant coefficients:

(R-L or Caputo)

$$ \sum_{k=1}^{m} p_k(t) D^{\alpha_k} y(t) = f(t), \qquad 0 \le \alpha_1 < \alpha_2 < \ldots < \alpha_m, \qquad n-1 < \alpha_m < n $$

Denote

$$ P_N^{(k)} = \mathrm{diag}\big(p_k(t_0), p_k(t_1), \ldots, p_k(t_N)\big) = \begin{bmatrix} p_k(t_0) & 0 & \ldots & 0 \\ 0 & p_k(t_1) & 0 & \ldots \\ 0 & \ldots & \ddots & 0 \\ 0 & \ldots & 0 & p_k(t_N) \end{bmatrix}, $$

$$ Y_N = \big(y(t_0), y(t_1), \ldots, y(t_N)\big)^T, \qquad F_N = \big(f(t_0), f(t_1), \ldots, f(t_N)\big)^T. $$

Then the discrete form of the equation is simply:

$$ \sum_{k=1}^{m} P_N^{(k)} B_N^{\alpha_k} Y_N = F_N $$

Useful matrices: Eliminators

Eliminator, $S_{r_1, r_2, \ldots, r_k}$, is obtained from the unit matrix by omitting rows with numbers $r_1, r_2, \ldots, r_k$.

How do they act:

$$ A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}; \qquad S_1 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}; $$

$$ S_1 A = \begin{bmatrix} a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}; \qquad A\, S_1^T = \begin{bmatrix} a_{12} & a_{13} \\ a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix}; \qquad S_1\, A\, S_1^T = \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix}. $$

Initial value problems for FDEs

Handling zero initial conditions

If $n-1 < \alpha_m < n$ and $y^{(k)}(t_0) = 0, \quad k = 0, 1, \ldots, n-1$, then the Riemann-Liouville and Caputo derivatives coincide.

Approximating derivatives in the above conditions by backward differences we immediately have:

$$ y(t_0) = y(t_1) = \ldots = y(t_{n-1}) = 0. $$

and the system for finding the rest is:

$$ \left\{ S_{0,1,\ldots,n-1} \left\{ \sum_{k=1}^{m} P_N^{(k)} B_N^{\alpha_k} \right\} S_{0,1,\ldots,n-1}^T \right\} \{ S_{0,1,\ldots,n-1} Y_N \} = S_{0,1,\ldots,n-1} F_N. $$

For constant coefficients it is even simpler:

$$ \sum_{k=1}^{m} p_k B_{N-n}^{\alpha_k} \{ S_{0,1,\ldots,n-1} Y_N \} = S_{0,1,\ldots,n-1} F_N. $$

Useful matrices: Eliminators

In general,

$$ S_0 \left\{ \begin{array}{c} L_N \\ U_N \end{array} \right\} S_0^T = \left\{ \begin{array}{c} L_{N-1} \\ U_{N-1} \end{array} \right\}, $$

$$ S_N \left\{ \begin{array}{c} L_N \\ U_N \end{array} \right\} S_N^T = \left\{ \begin{array}{c} L_{N-1} \\ U_{N-1} \end{array} \right\}, $$

$$ S_{0,1,\ldots,k} \left\{ \begin{array}{c} L_N \\ U_N \end{array} \right\} S_{0,1,\ldots,k}^T = \left\{ \begin{array}{c} L_{N-k-1} \\ U_{N-k-1} \end{array} \right\}, $$

$$ S_{N-k,N-k+1,\ldots,N} \left\{ \begin{array}{c} L_N \\ U_N \end{array} \right\} S_{N-k,N-k+1,\ldots,N}^T = \left\{ \begin{array}{c} L_{N-k-1} \\ U_{N-k-1} \end{array} \right\}. $$

Simultaneous multiplication of a triangular strip matrix by an eliminator $S_{0,1,\ldots,k}$ (or $S_{N-k,N-k+1,\ldots,N}$) on the left and its transpose on the right preserves the type and the structure of the triangular strip matrix, and only reduces its size by $k+1$ rows and $k+1$ columns.

Example 1: Caputo derivatives

Zero initial conditions

The problem: $y^{(\alpha)}(t) + y(t) = 1,$

$y(0) = 0, \quad y'(0) = 0$

Exact solution is: $y(t) = t^{\alpha} E_{\alpha,\alpha+1}(-t^{\alpha})$

From
$$ \sum_{k=1}^{m} p_k B_{N-n}^{\alpha_k} \{ S_{0,1,\ldots,n-1} Y_N \} = S_{0,1,\ldots,n-1} F_N. $$

$$ m = 2,\ \alpha_1 = \alpha,\ \alpha_2 = 0,\ n = 2,\ p_1 = p_2 = 1, $$

$$ B_{N-n}^{\alpha_1} = B_{N-2}^{\alpha},\ B_{N-n}^{\alpha_2} = E_{N-2},\ F_N = (\underbrace{1, 1, \ldots, 1}_{N})^T $$

the system for determining $y_k,\ k = 2, 3, \ldots, N$ is:

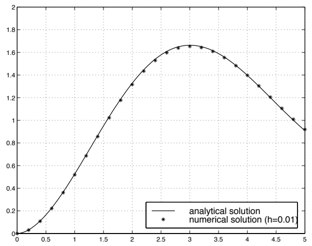
$$ \{ B_{N-2}^{\alpha} + E_{N-2} \} \{ S_{0,1} Y_N \} = S_{0,1} F_N $$

... and don’t forget to add $y_0 = y_1 = 0.$

Example 1: Caputo derivatives

Zero initial conditions

Solution of the problem $y^{(1.8)}(t) + y(t) = 1, y(0) = 0, y'(0) = 0$



Example 2: Caputo derivatives

Non-zero initial conditions: transform them to zeros.

The problem: $y^{(\alpha)}(t) + y(t) = 1,$

$$y(0) = c_0, \quad y'(0) = c_1$$

Exact solution is: $y(t) = c_0 E_{\alpha,1}(-t^\alpha) + c_1 t E_{\alpha,2}(-t^\alpha) + t^\alpha E_{\alpha,\alpha+1}(-t^\alpha)$

Introduce an auxiliary function:

$$y(t) = c_0 + c_1 t + z(t)$$

Then the problem for $z(t)$ is:

$$z^{(\alpha)}(t) + z(t) = 1 - c_0 - c_1 t,$$

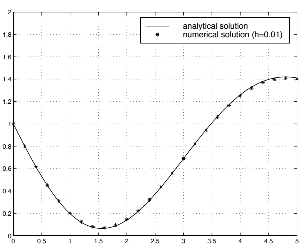
bounded RHS

$$z(0) = 0, \quad z'(0) = 0.$$

Example 2: Caputo derivatives

Non-zero initial conditions: transform them to zeros.

Solution of the problem $y^{(1.8)}(t) + y(t) = 1, y(0) = 1, y'(0) = -1$



Example 3: Riemann-Liouville derivatives

Non-zero initial conditions: transform them to zeros.

The problem: $y^{(\alpha)}(t) + y(t) = 1,$

$$y^{(\alpha-1)}(0) = c_0, \quad y^{(\alpha-2)}(0) = c_1.$$

Exact solution is:

$$y(t) = c_0 t^{\alpha-1} E_{\alpha,\alpha}(-t^\alpha) + c_1 t^{\alpha-2} E_{\alpha,\alpha-1}(-t^\alpha) + t^\alpha E_{\alpha,\alpha+1}(-t^\alpha)$$

Introduce an auxiliary function:

$$y(t) = c_0 t^{\alpha-1} + c_1 t^{\alpha-2} + z(t)$$

Then the problem for $z(t)$ is:

$$z^{(\alpha)}(t) + z(t) = 1 - c_0 t^{\alpha-1} - c_1 t^{\alpha-2}.$$

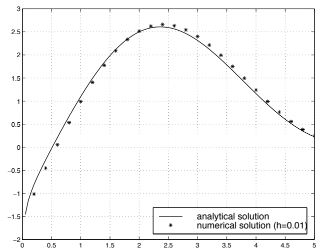
unbounded RHS

$$z(0) = 0, \quad z'(0) = 0.$$

Example 3: Riemann-Liouville derivatives

Non-zero initial conditions: transform them to zeros.

Solution of the problem $y^{(1.8)}(t) + y(t) = 1; y^{(0.8)}(0) = 1; y^{(-0.2)}(0) = -1$



Nonlinear FDEs

$y^{(\alpha_i)}(t) = {}_aD_t^{\alpha_i} y(t)$

$$y^{(\alpha_1)}(t) = f(t,\, y^{(\alpha_2)}(t),\, y^{(\alpha_3)}(t),\, \dots,\, y^{(\alpha_k)}(t)),$$

$$(0 < \alpha_1 < \alpha_2 < \ldots < \alpha_k \le n.)$$

Suppose initial conditions are already transformed to zero initial conditions. Then replacement of derivatives with their discrete analogues gives:

$$B_N^{\alpha_1} Y_N = f(Et_N,\, B_N^{\alpha_2} Y_N,\, B_N^{\alpha_3} Y_N,\, \dots,\, B_N^{\alpha_k} Y_N),$$

$$y_j = 0, \quad j = 1, 2, \dots, n-1,$$

This is a nonlinear algebraic system.

Physical interpretation of initial conditions for fractional differential equations with the Riemann-Liouville fractional derivatives

Spring-pot model

Spring-pot is a linear viscoelastic element whose behaviour is intermediate between that of elastic element (spring) and a viscous element (dashpot). The term "spring-pot" was introduced by Koeller (1984), although the concept of an element with intermediate properties had been introduced some time earlier (G. W. Scott Blair, 1930s-40s). The constitutive equation of a spring-pot is:

$$\sigma(t) = K\, {}_0D_t^{\alpha}\epsilon(t) \qquad \text{or} \qquad \epsilon(t) = \frac{1}{K}\, {}_0D_t^{-\alpha}\sigma(t)$$

We deal with the Riemann-Liouville derivatives ($n-1 \le \alpha < n$):

$${}_0D_t^{\alpha} f(t) = \frac{1}{\Gamma(n-\alpha)} \left(\frac{d}{dt}\right)^n \int_0^t \frac{f(\tau)\, d\tau}{(t-\tau)^{\alpha-n+1}}.$$

Fractional differential equations in terms of RL derivatives require initial conditions expressed in terms of initial values of fractional derivatives of the unknown function.

A typical initial value problem ($n-1 < \alpha < n$):

$${}_0D_t^{\alpha} f(t) + a f(t) = h(t); \qquad (t > 0)$$

$$\left[{}_0D_t^{\alpha-k} f(t)\right]_{t\to 0} = b_k, \qquad (k = 1, 2, \ldots, n).$$

Spring-pot model: Creep

A stress step σ_0 is applied at initial time $t = 0$. The change of $\epsilon(t)$ is described by the FDE

$${}_0D_t^{\alpha}\epsilon(t) = \frac{\sigma_0}{K}$$

An initial condition involving ${}_0D_t^{\alpha-1}\epsilon(t)$ is required. It can be found by taking the first-order integral of the constitutive equation and letting $t \to 0$

$$\left[{}_0D_t^{\alpha-1}\epsilon(t)\right]_{t\to 0} = \left[{}_0D_t^{-1}(\sigma_0/K)\right]_{t\to 0}.$$

In the considered case stress is finite at all times, therefore the required IC is

$$\left[{}_0D_t^{\alpha-1}\epsilon(t)\right]_{t\to 0} = 0.$$

K. Diethelm, N. J. Ford, A. D. Freed, and Yu. Luchko (2005):

> "A typical feature of differential equations (both classical and fractional) is the need to specify additional conditions in order to produce a unique solution. For the case of Caputo FDEs, these additional conditions are just the static initial conditions . . . , which are akin to those of classical ODEs, and are therefore familiar to us. In contrast, for Riemann-Liouville FDEs, these additional conditions constitute certain fractional derivatives (and/or integrals) of the unknown solution at the initial point $x = 0$ . . . , which are functions of x. These initial conditions are not physical; furthermore, it is not clear how such quantities are to be measured from experiment, say, so that they can be appropriately assigned in an analysis."

Spring-pot model: Impulse response

An impulse of stress defined as $B\delta(t)$ applied to the spring-pot at time $t = 0$. After that, the stress remains zero. The strain $\epsilon(t)$ for $t > 0$ is the solution of FDE

$${}_0D_t^{\alpha}\epsilon(t) = 0.$$

An initial condition involving $\left[{}_0D_t^{\alpha-1}\epsilon(t)\right]_{t\to 0}$ is required.

This can be found through integration of the constitutive equation, as

$$\left[{}_0D_t^{\alpha-1}\epsilon(t)\right]_{t\to 0} = \left[{}_0D_t^{-1}\sigma(t)/K\right]_{t\to 0},$$

which gives the following initial condition:

$$\left[{}_0D_t^{\alpha-1}\epsilon(t)\right]_{t\to 0} = B/K.$$

The key: look for inseparable twins

In a general case, when we consider some FDE for, say, $U(t)$, we have to consider also some function $V(t)$, for which some *dual relation* exists between $U(t)$ and $V(t)$. For example: stress $\sigma(t)$ and strain $\epsilon(t)$ in viscoelasticity; charge $q(t)$ and voltage $v(t)$ in electrical circuits; temperature difference $T(t)$ and the heat flux $q(t)$ in heat conduction; etc. Functions $U(t)$ and $V(t)$ are normally related by some basic physical law for the particular field of science.

In each scientific field there are such pairs of functions like the aforementioned, which are as *inseparable as Siamese twins*: the left-hand side of the initial condition involves one of them, whereas the evaluation of the right-hand side is related to the other.

Fractional Voigt model: Creep

A stress step σ_0 applied at $t = 0$. The FDE for the strain $\epsilon(t)$ is

$$E\epsilon(t) + K\,{}_0D_t^{\alpha}\epsilon(t) = \sigma_0,$$

and the IC can be found by integrating the constitutive equation and taking $t \to 0$:

$$\left[E\,{}_0D_t^{-1}\epsilon(t) + K\,{}_0D_t^{\alpha-1}\epsilon(t) = {}_0D_t^{-1}\sigma(t)\right]_{t\to 0}.$$

The limit of the right hand side is zero. A bounded stress can produce only a bounded strain, so the limit of the first-order ordinary integral of strain in the left hand side is also zero. Thus the initial condition has the form:

$$\left[{}_0D_t^{\alpha-1}\epsilon(t)\right]_{t\to 0} = 0.$$

Fractional Voigt model: Impulse response

The constitutive equation of this model is

$$\sigma(t) = E\epsilon(t) + K\,{}_0D_t^{\alpha}\epsilon(t).$$

A stress impulse $B\delta(t)$ is applied to a Voigt element at time $t = 0$. Then the FDE for $\epsilon(t)$ $(t > 0)$ is

$$E\epsilon(t) + K\,{}_0D_t^{\alpha}\epsilon(t) = 0.$$

We need an initial condition, which will involve the value of ${}_0D_t^{\alpha-1}\epsilon(t)$ for $t \to 0$. This condition can be obtained by integration of the constitutive equation as

$$\left[E\,{}_0D_t^{-1}\epsilon(t) + K\,{}_0D_t^{\alpha-1}\epsilon(t) = {}_0D_t^{-1}\sigma(t)\right]_{t\to 0}.$$

Fractional Zener model: Impulse response

$$\sigma(t) + \nu\,{}_0D_t^{\alpha}\sigma(t) = \lambda\,\epsilon(t) + \mu\,{}_0D_t^{\alpha}\epsilon(t).$$

A stress impulse $B\delta(t)$ applied at time $t = 0$. Then the FDE for $\epsilon(t)$ $(t > 0)$ is:

$$\lambda\epsilon(t) + \mu\,{}_0D_t^{\alpha}\epsilon(t) = 0.$$

We need an IC involving the initial value of ${}_0D_t^{\alpha-1}\epsilon(t)$. Integrating the constitutive equation and taking $t \to 0$, we, similarly to the Voigt model under stress impulse, obtain the initial condition in the form:

$$\left[\mu\,{}_0D_t^{\alpha-1}\epsilon(t)\right]_{t\to 0} = B$$

The limit of the right hand side is the magnitude B of the stress impulse. On physical grounds, the spring-pot cannot deform instantaneously under a finite stress, and, as is the case for a spring-pot alone, any singularity of $\epsilon(t)$ must be weaker than that of the stress impulse, thus

$$\left[{}_0D_t^{-1}\epsilon(t)\right]_{t\to 0} = 0.$$

Hence the initial condition finally takes on the form of

$$\left[K\,{}_0D_t^{\alpha-1}\epsilon(t)\right]_{t\to 0} = B.$$

Fractional Zener model: Creep

$\sigma(t) = \sigma_0$, and the FDE for $\epsilon(t)$ is:

$$\lambda\epsilon(t) + \mu\,{}_0D_t^{\alpha}\epsilon(t) = \sigma_0 + \nu\,\sigma_0\,\frac{t^{-\alpha}}{\Gamma(1-\alpha)}.$$

The initial condition to this equation,

$$\left[{}_0D_t^{\alpha-1}\epsilon(t)\right]_{t\to 0} = 0,$$

in terms of fractional derivative of $\epsilon(t)$ appeared again from consideration of its "inseparable twin" $\sigma(t)$.

Fractional Zener model: General load

$\sigma(t) = \sigma_*(t)$. The FDE for $\epsilon(t)$ is

$$\lambda \epsilon(t) + \mu \, {}_0D_t^\alpha \epsilon(t) = \sigma_*(t) + \nu \, {}_0D_t^\alpha \sigma_*(t)$$

The corresponding initial condition can be obtained as follows. Consider some small $t = a$. Starting at $t = 0$, stress $\sigma(t)$ must be recorded until $t = a$, and based on the recorded values the left hand side of the integral of the constitutive relationship must be evaluated. The obtained quantity provides an approximation of the initial value for the expression in its right hand side.

In some cases it is possible to find the limit of such approximation as $a \to 0$. For example, for a physically realisable continuous load $\sigma_*(t)$ we obtain a zero initial condition in the form:

$$\left[{}_0D_t^{\alpha-1} \epsilon(t) \right]_{t \to 0} = 0.$$