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#2 Numerical fractional differentiation

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How do we do steps forward?

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G. W. Leibniz (1695–1697)

In the letters to J. Wallis and J. Bernulli (in 1697) Leibniz mentioned the possible approach to fractional-order differentiation in that sense, that for non-integer values of n the definition could be the following:



L. Euler (1730)

$$\begin{split} \frac{d^n x^m}{dx^n} &= m(m-1)\,\dots\,(m-n+1)x^{m-n}\\ \Gamma(m+1) &= m(m-1)\,\dots\,(m-n+1)\,\Gamma(m-n+1)\\ \frac{d^n x^m}{dx^n} &= \frac{\Gamma(m+1)}{\Gamma(m-n+1)}x^{m-n}. \end{split}$$
 Euler suggested to use this relationship also for negative or non-integer (rational) values of *n*. Taking m=1 and $n=\frac{1}{2}$, Euler obtained:

 $rac{d^{1/2}x}{dx^{1/2}} = \sqrt{rac{4x}{\pi}} \qquad \left(=rac{2}{\sqrt{\pi}}x^{1/2}
ight)$

S. F. Lacroix adopted Euler's derivation for his successful textbook (*Traité du Calcul Différentiel et du Calcul Intégral*, Courcier, Paris, t. 3, 1819; pp. 409–410).

TRAITÉ ÉLÉMENTAIRE

CALCUL DIFFÉRENTIEL

CALCUL INTÉGRAL,

PAR S.-F. LACROIX.

SEPTIÈME ÉDITION,

BEVUE ET AUGMENTÉE DE NOTES Par MM. HERMITE et J.-A. SERRET, HERMIN DE L'OUTURT.

J. B. J. Fourier (1820-1822)

The first step to generalization of the notion of differentiation for **arbitrary functions** was done by J. B. J. Fourier (*Théorie Analytique de la Chaleur*, Didot, Paris, 1822; pp. 499–508).

After introducing his famous formula

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(z) dz \int_{-\infty}^{\infty} \cos{(px - pz)} dp,$$

Fourier made a remark that

and this relationship could serve as a definition of the n-th order derivative for non-integer n.

N. H. Abel (1823–1826)

N. H. Abel: Solution de quelques problèmes à l'aide d'intégrales définies (1823). *Œuvres complètes de Niels Henrik Abel*, vol. 1, Grondahl, Christiania, 1881, pp. 11–18.

In fact, Abel solved the equation

$$\int\limits_{0}^{x}rac{s'(\eta)d\eta}{(x-\eta)^{lpha}}=\psi(x)$$

Simply a Caputo derivative
$$d^lpha$$

x),
$$\Gamma(1-\alpha) \frac{d}{dx^{\alpha}} s(x) = \psi(x)$$

for an arbitrary α (and not just for $\alpha = \frac{1}{2}$):

$$s(x)=rac{\sin{(\pilpha)}}{\pi}x^{lpha}\int\limits_{0}^{1}rac{\psi(xt)dt}{(1-t)^{1-lpha}}.$$

After that, Abel expressed the obtained solution with the help of an integral of order $\alpha :$

$$s(x) = rac{1}{\Gamma(1-lpha)} rac{d^{-lpha}\psi(x)}{dx^{-lpha}}$$

J. Liouville (1832–1855)

Three approaches: I. Following Leibniz: $\frac{d^m e^{ax}}{dx^n} = a^m e^{ax},$ $f(x) = \sum_{n=0}^{\infty} c_n e^{a_n x},$ $\frac{d^{\nu} f(x)}{dx^{\nu}} = \sum_{n=0}^{\infty} c_n a_n^{\nu} e^{a_n x}$

J. Liouville (1832–1855)

Three approaches: II. *Integrals* of non-integer order:

$$\int^{\mu} \Phi(x) dx^{\mu} = \frac{1}{(-1)^{\mu} \Gamma(\mu)} \int_{0}^{\infty} \Phi(x+\alpha) \alpha^{\mu-1} d\alpha$$
$$\int^{\mu} \Phi(x) dx^{\mu} = \frac{1}{\Gamma(\mu)} \int_{0}^{\infty} \Phi(x-\alpha) \alpha^{\mu-1} d\alpha$$
or (after the substitution $\tau = x + \alpha, \tau = x - \alpha$)
$$\int^{\mu} \Phi(x) dx^{\mu} = \frac{1}{(-1)^{\mu} \Gamma(\mu)} \int_{x}^{\infty} (\tau - x)^{\mu-1} \Phi(\tau) d\tau$$
$$\int^{\mu} \Phi(x) dx^{\mu} = \frac{1}{\Gamma(\mu)} \int_{-\infty}^{x} (x-\tau)^{\mu-1} \Phi(\tau) d\tau.$$

J. Liouville (1832–1855)

Three approaches: III. Derivatives of non-integer order:

$$\begin{split} \frac{d^{\mu}F(x)}{dx^{\mu}} &= \frac{(-1)^{\mu}}{h^{\mu}}(F(x) - \frac{\mu}{1}F(x+h) + \\ &+ \frac{\mu(\mu-1)}{1\cdot 2}F(x+2h) - \dots) \\ \frac{d^{\mu}F(x)}{dx^{\mu}} &= \frac{1}{h^{\mu}}(F(x) - \frac{\mu}{1}F(x-h) + \\ &+ \frac{\mu(\mu-1)}{1\cdot 2}F(x-2h) - \dots). \end{split}$$

(Equality is in the sense $\lim_{h \to 0}$).

Liouville was the first, who realized the possibility of considereation of *left-sided* and *right-sided* fractional integrals and derivatives.

G. F. B. Riemann (1847; 1876)

Riemann used a generalization of the Taylor series for obtaining a formula for fractional-order integration, which is given below in contemporary notation:

$$D^{-
u}f(x)=rac{1}{\Gamma(
u)}\int\limits_{c}^{x}(x-t)^{
u-1}f(t)dt+\psi(t)$$

Riemann introduced an arbitrary (complementary) function $\psi(x)$ because he did not fixed the lower bound of integration c– a disadvantage, which cannot be removed in the framework of his approach.

Cauchy's formula:

$$f^{(n)}(z) = rac{n!}{2\pi i} \int\limits_{C} rac{f(t)}{(t-z)^{n+1}} dt$$

For non-integer $n=\nu$ a branch point of the function $(t-z)^{-\nu-1}$ appears instead of a pole:

$$D^{\nu}f(z) = rac{\Gamma(
u+1)}{2\pi i} \int\limits_{c}^{x^{*}} rac{f(t)}{(t-z)^{
u+1}} dt$$





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The GI algorithm

Recall the Grunwald-Letnikov definition:

$${}_{a}D_{t}^{\alpha}f(t) = \lim_{h \to 0} \frac{a\Delta_{h}^{\alpha}f(t)}{h^{\alpha}}, \qquad {}_{a}\Delta_{h}^{\alpha}f(t) = \sum_{j=0}^{\left\lfloor\frac{t-\alpha}{h}\right\rfloor} (-1)^{j} \binom{\alpha}{j} f(t-jh).$$

Omitting the limit gives the simplest approximation:

$$_{a}D_{t}^{\alpha}f(t) \approx _{a}\Delta_{h}^{\alpha}f(t)$$

The GI algorithm

Omitting the limit in the Grunwald-Letnikov definition gives the simplest formula for approximate calculations:

$$_{a}D_{t}^{\alpha}f(x) \approx \left(\frac{\left[\frac{\mathbf{x}-a}{N}\right]^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f\left(\mathbf{x}-j\left[\frac{\mathbf{x}-a}{N}\right]\right) \right)$$

For a = 0 we have:

$$_{0}D_{t}^{\alpha}f(x) \approx \frac{x^{-q}N^{q}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)}f_{j}$$

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Computation of binomial coefficients Using recurrence relationships

For the implementation we need to compute

$$w_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}, \qquad k = 0, 1, 2, ...$$

The recurrence relationships can be used:

$$w_0^{(\alpha)} = 1; \quad w_k^{(\alpha)} = \left(1 - \frac{\alpha + 1}{k}\right) w_{k-1}^{(\alpha)}, \quad k = 1, 2, 3, \dots$$

Computation of binomial coefficients Using FFT (fast Fourier transform)

The binomial coefficients can be considered as the coefficients of the power series expansion

$$(1-z)^{\alpha} = \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} z^k = \sum_{k=0}^{\infty} w_k^{(\alpha)} z^k$$

Taking $z = e^{-i\varphi}$ we obtain

$$(1 - e^{-i\varphi})^{\alpha} = \sum_{k=0}^{\infty} w_k^{(\alpha)} e^{-ik\varphi}$$

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The fast Fourier transform (FFT) can be used here!





Higher-order approximations

We have seen the first-order approximation:

$${}_{0}D_{t}^{\alpha}f(x) \approx h^{-\alpha}\sum_{k=0}^{[t/h]} w_{k}^{(\alpha)}f(t-kh)$$

The weights $w_k^{(\alpha)}$, $(k = 0, 1, 2, ..., n, n = \begin{bmatrix} t \\ h \end{bmatrix}$) assigned to the values f(t-jh) are the first n+l coefficients of the Taylor series expansion of the function

$$\omega_1^{(\alpha)}(z) = (1-z)^{\alpha} = \left(\omega_1(z)\right)^{\alpha}$$

Higher-order approximations Christian Lubich's formulas: $\omega_2^{(\alpha)}(z) = (\frac{3}{2} - 2z + \frac{1}{2}z^2)^{\alpha}$,

$$\begin{split} \omega_3^{(\alpha)}(z) &= (\frac{11}{6} - 3z + \frac{3}{2}z^2 - \frac{1}{3}z^2)^{\alpha},\\ \omega_4^{(\alpha)}(z) &= (\frac{25}{12} - 4z + 3z^2 - \frac{4}{3}z^3 + \frac{1}{4}z^4)^{\alpha},\\ \omega_6^{(\alpha)}(z) &= (\frac{137}{60} - 5z + 5z^2 - \frac{10}{3}z^3 + \frac{5}{4}z^4 - \frac{1}{5}z^5)^{\alpha},\\ \omega_6^{(\alpha)}(z) &= (\frac{147}{60} - 6z + \frac{15}{2}z^2 - \frac{20}{3}z^3 + \frac{15}{4}z^4 - \frac{6}{5}z^5 + \frac{1}{6}) \end{split}$$

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Expand these functions in Taylor series and use the coefficients as weights in the formula

$${}_0D_t^{\alpha}f(t)\approx \ h^{-\alpha}\sum_{k=0}^{[t/h]}w_k \ f(t-kh)$$

The G2 algorithm

Oldham and Spanier (1974) observed that the approximations

$${}_{a}D_{t}^{-1}f(x) = \lim_{N \to \infty} \left\{ \frac{x-a}{N} \sum_{j=0}^{N-1} f\left(x - [j+\frac{1}{2}] \left[\frac{x-a}{N} \right] \right) \right\}$$
$${}_{a}D_{t}^{1}f(x) = \lim_{N \to \infty} \left\{ \left[\frac{x-a}{N} \right]^{-1} \sum_{j=0}^{1} [-]^{j} f\left(x - [j-\frac{1}{2}] \left[\frac{x-a}{N} \right] \right) \right\}$$

give faster convergence, and suggested "fractional central differences"

$${}_{a}D_{t}^{q}f(x) = \lim_{N \to \infty} \left\{ \frac{\left[\frac{x-a}{N}\right]^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f\left(x - \left[j - \frac{1}{2}q\right] \left[\frac{x-a}{N}\right]\right) \right\}$$

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The G2 algorithm

Taking lower terminal a = 0 we have

$${}_0D_t^q f(x) = \lim_{N \to \infty} \left\{ \frac{x^{-q} N^q}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f\left(x + \frac{qx}{2N} - \frac{jx}{N}\right) \right\}$$

This formula uses the function values other than at nodes, so we have to interpolate (Langrange three point interpolation):

$$f\left(x + \frac{qx}{2N} - \frac{jx}{N}\right) \approx \left[\frac{q}{4} + \frac{q^2}{8}\right] f\left(x + \frac{x}{N} - \frac{jx}{N}\right) + \left[1 - \frac{q^2}{4}\right] f\left(x - \frac{jx}{N}\right) + \left[\frac{q^2}{8} - \frac{q}{4}\right] f\left(x - \frac{x}{N} - \frac{jx}{N}\right)$$

This gives the G2 algorithm:

$${}_{0}D_{t}^{q}f(x) = \frac{x^{-q}N^{q}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)}\{f_{j} + \frac{1}{4}q[f_{j-1} - f_{j+1}] + \frac{1}{8}q^{2}[f_{j-1} - 2f_{j} + f_{j+1}]\}$$

The RI algorithm

GI and G2 are based on fractional differences. RI and R2 are based on approximation of integration.

Take q < 0 (fractional integration):

$${}_{0}D_{t}^{q}f(x) = \frac{1}{\Gamma(-q)} \int_{0}^{x} \frac{f(y) \, dy}{[x-y]^{q+1}} = \frac{1}{\Gamma(-q)} \int_{0}^{x} \frac{f(x-y) \, dy}{y^{q+1}}$$

$$= \frac{1}{\Gamma(-q)} \sum_{j=0}^{N-1} \int_{jx/N}^{[jx+x]/N} \frac{f(x-y) \, dy}{y^{q+1}}$$





$$\begin{aligned} & \text{Det RI and R2 are restricted to negatives orders (integration only). How to extend beyond this "wall": \\ & \text{Let us take } 0 \leq q < 1. \text{Then} \\ & \sigma D_t^q f(x) = \frac{x^{-q}f(0)}{\Gamma(1-q)} + \frac{1}{\Gamma(1-q)} \int_0^x \left[\frac{df}{dy}(y) \right] \frac{dy}{[x-y]^q} \\ & = \frac{1}{\Gamma(1-q)} \left\{ \frac{f(0)}{x^q} + \sum_{j=0}^{n-1} \int_{j_{x/N}}^{(j_{x+x})/N} \left[\frac{dy}{dy}(x-y) \right] \frac{dy}{y^q} \right\} \end{aligned}$$

$$\text{This leads to the Ll algorithm:} \\ & \sigma D_t^q f(x) = \frac{x^{-q}N}{\Gamma(2-q)} \left\{ \frac{[1-q]f_N}{N^q} + \sum_{j=0}^{n-1} [f_j - f_{j+1}][(j+1)^{1-q} - j^{1-q}] \right\} \\ & = \frac{1}{\Gamma(1-q)} \left\{ \frac{f(0)}{x^q} + \sum_{j=0}^{n-1} \int_{j_{x/N}}^{(j_{x+x})/N} \left[\frac{dy}{dy}(x-y) \right] \frac{dy}{y^q} \right\} \end{aligned}$$

The L2 algorithm

Similarly, taking $1 \leq q < 2$ we can write

 ${}_{0}D_{t}^{q}f(x) = \frac{x^{-q}f(0)}{\Gamma(1-q)} + \frac{x^{1-q}f^{(1)}(0)}{\Gamma(2-q)} + \frac{1}{\Gamma(2-q)} \int_{0}^{x} \frac{f^{(2)}(y) \, dy}{[x-y]^{q-1}}$ $= \frac{1}{\Gamma(2-q)} \left[\frac{[1-q]f(0)}{x^{q}} + \frac{f^{(1)}(0)}{x^{q-1}} + \sum_{j=0}^{N-1} \int_{jx/N}^{[jx+x]/N} \frac{f^{(2)}(x-y) \, dy}{y^{q-1}} \right]$

We need some approximations for the first and second order derivatives here.

The L2 algorithm

Using the approximations

$$\begin{split} f^{(1)}(0) &\approx \frac{f\left(\frac{x}{N}\right) - f(0)}{x/N} = \frac{N}{x} \left[f_{N-1} - f_N \right] \\ \int_{j_{X/N}}^{(j_{X}+x)/N} f^{(2)}(x-y) \frac{dy}{y^{q-1}} &\approx \frac{f\left(x + \frac{x}{N} - \frac{jx}{N}\right) - 2f\left(x - \frac{jx}{N}\right) + f\left(x - \frac{x}{N} - \frac{jx}{N}\right)}{[x/N]^2} \int_{j_{X/N}}^{(j_{X}+x)/N} \frac{dy}{y^{q-1}} \\ &= \frac{x^{-q}N^q}{2-q} \left[f_{j-1} - 2f_j + f_{j+1} \right] [(j+1)^{2-q} - j^{2-q}] \end{split}$$

we obtain the L2 algorithm

$${}_{0}D_{t}^{q}f(x) = \frac{x^{-q}N^{q}}{\Gamma(3-q)} \left[\frac{[1-q][2-q]f_{N}}{N^{q}} + \frac{[2-q][f_{N-1}-f_{N}]}{N^{q-1}} + \sum_{j=0}^{N-1} [f_{j-1}-2f_{j}+f_{j+1}][(j+1)^{2-q}-j^{2-q}] \right]$$



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