Fractional Calculus: differentiation and integration of non-integer order

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Introduction: Standard calculus

- The differential calculus we all know and love was invented independently by Newton and Leibniz in the 17th century
- Newton used the notation $x, \dot{x}, \ddot{x} \ldots$
- Leibniz used the notation $y, \frac{dy}{dx}, \frac{d^2y}{dx^2}, \ldots \frac{d^ny}{dx^n}, \ldots$
- The notion of a *fractional* version of this calculus was discussed relatively soon after.

Introduction: Leibniz-L'Hôpital correspondence

- In 1695, Leibniz and L'Hôpital were discussing Leibniz's newly developed calculus when L'Hôpital asked:
- "...and what if n be $1/2$?"
- Leibniz replied:
- "It will lead to a paradox, from which one day useful consequences will be drawn."

- This was the moment the fractional calculus was born.
- **The idea:** Generalise the notion of differentiation and integration of order $n \in \mathbb{N}$ to that of order $s \in \mathbb{R}$.
- I.e. find a natural and applicable definition for $\dfrac{d^s y}{dx^s}$.

Overview

1. Work of Euler
2. Riemann-Liouville Fractional Calculus
3. Examples
4. Relationship to the Fourier Transform
5. Imbalance and Generalising to Higher Dimensions.
6. Applications: Anomalous Diffusion

Work of Euler: Gamma function

- Euler made the first step in the right direction in 1729 with the Gamma function:

$$\Gamma(s) = \int_0^{\infty} t^{s-1} e^{-t}\, dt, \tag{1}$$

which is defined for all $s \in \mathbb{C} \setminus \{0, 1, 2, 3, ...\}$.

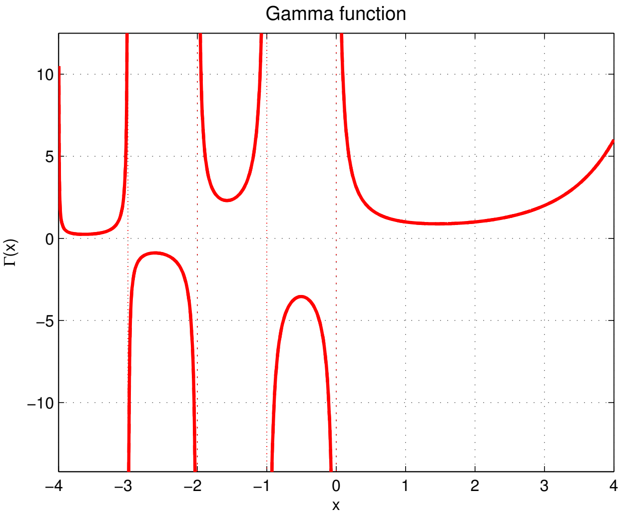
- It is easy to see that $\Gamma(1) = 1$, and integration by parts reveals the identity:

$$\Gamma(s+1) = s\Gamma(s), \quad \forall s. \tag{2}$$

- From these two facts we deduce that the Gamma function extends the factorial function:

$$\Gamma(n) = (n-1)!, \quad \forall n \in \mathbb{N}. \tag{3}$$

Euler's Gamma function



Work of Euler: fractional calculus on monomials

- A year later (1730), Euler published some ideas for fractional calculus using the Gamma function in a natural way.
- Consider the nth derivative of a monomial for an integer m:

$$y(x) = x^m. \tag{4}$$

$$\frac{d^n y}{dx^n} = \begin{cases} \frac{m!}{(m-n)!} x^{m-n} & \text{if } m \geq n, \\ 0 & \text{if } m < n. \end{cases} \tag{5}$$

- Use the Gamma function to generalise to $s, \mu \in \mathbb{R}_{\geq 0}$:

$$y(x) = x^\mu, \quad \frac{d^s y}{dx^s} = \frac{\Gamma(\mu+1)}{\Gamma(\mu - s + 1)} x^{\mu - s}. \tag{6}$$

- Notice how the poles of $\Gamma(\mu - s + 1)$ take care of the case $\mu - s \in \{-1, -2, -3, \ldots\}$, which corresponds to $m < n$ above.

Examples

- Fractional derivatives of constant functions are not necessarily zero:

$$y(x) = 1, \quad \frac{d^{\frac{1}{2}}y}{dx^{\frac{1}{2}}} = \frac{\Gamma(0+1)}{\Gamma(0-\frac{1}{2}+1)}x^{0-\frac{1}{2}} = \frac{2}{\sqrt{\pi}}x^{-\frac{1}{2}}. \qquad (7)$$

- Think about *why* the derivative of a constant function is zero.
- We can now see it as a consequence of the poles of $\Gamma(\mu - s + 1)$ when $\mu - s \in \{-1, -2, -3, ...\}$.

Work of Euler: Notes

- One can (and should) check that these fractional derivatives can be composed i.e. $\frac{d^s}{dx^s}\left(\frac{d^t y}{dx^t}\right) = \frac{d^{s+t}y}{dx^{s+t}}$.
- Assuming linearity of fractional differentiation, we can define fractional derivatives for polynomials.
- It is tempting to define fractional derivatives for all analytic functions, i.e. those that can be represented by a power series in some open set.
- However, a fair bit of nontrivial justification is required to show that this is *well*-defined. This leads to so-called Taylor-Riemann series.
- Note that by reversing the process, one can calculate some fractional-order integrals too.

Cauchy's Formula for Repeated Integration

- Now, let us consider an observation of Cauchy (1789–1857).
- Let u be a Lebesgue integrable function defined on the interval $[a, b]$ i.e. $u \in L^1(a, b)$.
- The integral operator $\mathcal{I}_a$, for each x in $[a, b]$ is defined to be:

$$\mathcal{I}_a[u](x) := \int_a^x u(t)\, dt. \tag{8}$$

- Cauchy showed that repeated application of this integral operator can be expressed with a single integral:

$$\begin{aligned} \mathcal{I}_a^n[u](x) &= \int_a^x \int_a^{t_n} \dots \int_a^{t_2} u(t_1)\, dt_1 \dots dt_2\, dt_n & (9) \\ &= \frac{1}{(n-1)!} \int_a^x (x-t)^{n-1} u(t)\, dt. & (10) \end{aligned}$$

- Integration of order $n \in \mathbb{N}$ is described by the operation:

$$\mathcal{I}_a^n[u](x) = \frac{1}{(n-1)!} \int_a^x (x-t)^{n-1} u(t)\, dt. \tag{11}$$

- The natural extension of such a definition to real order $s > 0$ is:

$$\mathcal{I}_a^s[u](x) = \frac{1}{\Gamma(s)} \int_a^x (x-t)^{s-1} u(t)\, dt. \tag{12}$$

- This is called the *Left Riemann-Liouville Fractional Integral of order s* (because we integrate to x from the left).
- We will discuss the *Right* Riemann-Liouville Fractional Integral later.

The Riemann-Liouville Fractional Integral: Notes

- This integral is very general; we can perform fractional integrals on all Lebesgue integrable u, not just monomial functions.

The Riemann-Liouville Fractional Derivative

- To define a fractional derivative we **cannot** just formally replace s by $-s$ in the Riemann-Liouville integral.
- For a given u, we do not have a finite integral for all $x \in [a, b]$ (except if u is identically zero):

$$\mathcal{D}_a^s[u](x) =^? \frac{1}{\Gamma(-s)} \int_a^x (x-t)^{-s-1} u(t)\, dt. \tag{13}$$

- There is, however a nice trick we can use to get around this.

The Riemann-Liouville Fractional Derivative

- To define a fractional derivative of order $s \in (0, 1]$ we integrate to order $1 - s$ then differentiate to order 1:

$$\mathcal{D}_a^s[u](x) = \frac{1}{\Gamma(1-s)} \frac{d}{dx} \int_a^x (x-t)^{-s} u(t)\, dt. \tag{14}$$

- More generally, to define a fractional derivative of order $s \in (k-1, k]$ for $k \in \mathbb{N}$ we integrate to order $k - s$ then differentiate to order k:

$$\mathcal{D}_a^s[u](x) = \frac{1}{\Gamma(k-s)} \frac{d^k}{dx^k} \int_a^x (x-t)^{k-1-s} u(t)\, dt, \tag{15}$$

- This is the *Left Riemann-Liouville Fractional Derivative*.

- The parameter a being involved in the fractional derivative is striking:

$$\mathcal{D}_a^s[u](x) = \frac{1}{\Gamma(k-s)} \frac{d^k}{dx^k} \int_a^x (x-t)^{k-1-s} u(t)\, dt. \qquad (16)$$

- We call this parameter the *terminal* of the derivative.
- Note that the fractional derivative evaluated at x is dependent on all the values of u between a and x.
- This is strange as classical derivatives only depend **locally** on the point of evaluation i.e. just the gradient of the graph.
- Conclusion: Riemann-Liouville fractional derivatives are **nonlocal** operators.

- Riemann and Liouville developed this calculus independently.
- Liouville published a succession of papers around 1832, and he used the terminal $a = -\infty$.
- Riemann developed the calculus in notebooks while still a student around 1848, which were published posthumously. He used the terminal $a = 0$.

Example: monomials with $a = 0$

- Let $a = 0$ and once again consider the following functions for $\mu \geq 0$:
$$u(x) = x^{\mu}. \tag{17}$$
- Then for $x, s > 0$ we have the following:
$$\mathcal{D}_a^s[u](x) = \frac{\Gamma(\mu+1)}{\Gamma(\mu-s+1)} x^{\mu-s}. \tag{18}$$
- The Riemann-Liouville fractional derivative generalises the early work of Euler!

The choice $a = -\infty$

- We will see that Liouville's choice of $a = -\infty$ can be considered the most natural.
- For example, a deep relevance of the Gamma function is revealed if we change variables $t \mapsto x - t$:

$$\begin{aligned} \mathcal{I}^s_{-\infty}[u](x) &= \frac{1}{\Gamma(s)} \int_{-\infty}^{x} (x-t)^{s-1} u(t)\, dt \qquad (19) \\ &= \frac{1}{\Gamma(s)} \int_{0}^{\infty} t^{s-1} u(x-t)\, dt \qquad (20) \end{aligned}$$

Example: The exponential function

- If we set $u(x) = e^{\gamma x}$ for $\gamma > 0$ we have:

$$\mathcal{I}^s_{-\infty}[u](x) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{\gamma(x-t)}\, dt \tag{21}$$

$$= e^{\gamma x} \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-\gamma t}\, dt \tag{22}$$

$$= \gamma^{-s} e^{\gamma x} \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t}\, dt \tag{23}$$

$$= \gamma^{-s} e^{\gamma x}. \tag{24}$$

- Similarly:

$$\mathcal{D}^s_{-\infty}[u](x) = \gamma^s e^{\gamma x}. \tag{25}$$

- Those familiar with the Fourier transform know that the Fourier transform of a derivative can be expressed by the following:

$$\mathcal{F}\left[\frac{du}{dx}\right](\xi) = (i\xi)\mathcal{F}[u], \tag{26}$$

and more generally,

$$\mathcal{F}\left[\frac{d^k u}{dx^k}\right](\xi) = (i\xi)^k\mathcal{F}[u]. \tag{27}$$

- A similar identity holds for anti-derivatives if u is compactly supported:

$$\mathcal{F}\left[\mathcal{I}^k_{-\infty}[u]\right](\xi) = (i\xi)^{-k}\mathcal{F}[u]. \tag{28}$$

Fractional Derivatives and the Fourier Transform

- With what is a surprisingly technical derivation, one can show that a similar identity holds for fractional derivatives:

$$\mathcal{F}\left[\mathcal{D}^s_{-\infty}[u]\right](\xi) = (i\xi)^s \mathcal{F}[u]. \tag{29}$$

$$\mathcal{F}\left[\mathcal{I}^s_{-\infty}[u]\right](\xi) = (i\xi)^{-s} \mathcal{F}[u]. \tag{30}$$

- This suggests that the Riemann-Liouville fractional calculus with $a = -\infty$ is very natural indeed.

- We have not been very rigorous here at all.
- The analysis involved with the fractional calculus can get very technical. The two issues we have seen so far are:
- Fractional derivatives are nonlocal.
- Fractional derivatives have an awkward definition.
- The plot thickens...

Imbalances For Fractional Derivatives

- By considering the integral operator $\mathcal{J}_b$ for $u \in L^1(a, b)$:

$$\mathcal{J}_b[u](x) := \int_x^b u(t)\, dt, \tag{31}$$

- We can derive the *Right* Riemann-Liouville Fractional Derivative:

$$\mathcal{D}^s_{,b}[u](x) = \frac{(-1)^k}{\Gamma(k-s)} \frac{d^k}{dx^k} \int_x^b (t-x)^{k-1-s} u(t)\, dt. \tag{32}$$

- Unlike in the classical derivatives, the difference between taking a fractional derivative from the left and from the right is very different.
- We see that the right fractional derivative depends on values of u between x and b, rather than a and x.

Symmetry and Higher Dimensions

- This asymmetry causes problems for generalising to higher dimensions.
- A solution is to consider the operator satisfying:

$$\mathcal{R}^s[u](x) = \mathcal{F}^{-1}\left[|\xi|^s \mathcal{F}[u]\right]. \tag{33}$$

- This operator is called the *Riesz Symmetric Fractional Derivative* or the *Fractional Laplacian*. (Note that $\mathcal{R}^2 = -\Delta$).
- In one dimension, this operator has a simple form:

$$\mathcal{R}^s = C(s)(\mathcal{D}^s_a + \mathcal{D}^s_{,b}), \tag{34}$$

for some constant $C(s)$ depending on s.

Application: Anomalous Diffusion

- In 1905, Einstein derived the diffusion equation from a Brownian motion model of particles.
- If you assume that particles diffuse by a random walk, and take the average behaviour as the number of particles tends to infinity and the time between steps tends to zero, one finds that the diffusion equation models the probability distribution u for the location of the particles:

$$u_t = \kappa \Delta u \tag{35}$$

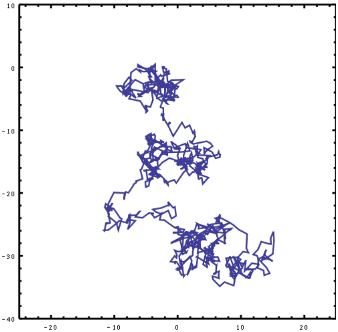
- However, a random walk is quite restrictive. The particles can only take steps at regular allotted times, and the steps can only be of a single given size. This is unrealistic, particularly if the medium is very heterogeneous.

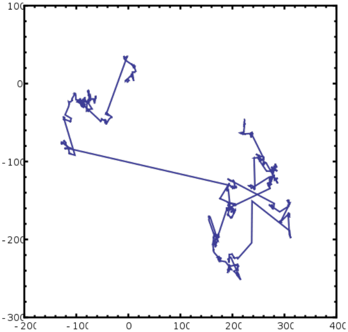
Levy Flights

- There are several alternatives to Brownian motion that can encode more properties into your diffusive process.
- We won't go into any details here, but what we are interested in is a *Levy Flight*. The particles can have different jump sizes and varying jump rates.
- A Levy flight can be parametrised by a single parameter $s \in [1, 2]$.
- $s = 2$ corresponds to Brownian motion with corresponding probability distribution the Gaussian distribution.
- $s = 1$ is an extreme Levy flight with corresponding probability distribution the Cauchy distribution.
- For other values of s we have something in between.

Levy Flights

- On the left we have a Brownian motion in two dimensions, and on the right we have an extreme Levy flight with $s = 1$.
- Note the multi-scale, or *nonlocal* nature of the Levy flight.





Anomalous Diffusion Equation

- If we take the average behaviour of the Levy flight as the step sizes shrink to zero, then we have an interesting equation modelling the probability distribution of the particles:

$$u_t = -\kappa(-\Delta)^{s/2}u, \tag{36}$$

where

$$(-\Delta)^{s/2}u = \mathcal{F}^{-1}\left[|\xi|^s \mathcal{F}[u]\right] \tag{37}$$

- This is called the *anomalous diffusion equation*.
- Skewing the Levy flight can produce various operators in the fractional calculus.

- It turns out that Leibniz's prophecy was correct!
- In the last 40 years or so, many applications of this type of theory have been found.
- Diffusive processes are ubiquitous, and more often than not they are in a heterogeneous medium:
- Cell and tissue physiology
- Contaminant transport in aquifers
- Mathematical finance
- Mathematical ecology, e.g. hunting and foraging
- Unstable magnetic fields
- The recorded phenomena in the literature is impressive, and growing