New trends in applied mathematics: fractional calculus

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Introduction

- Almost everyone has probably wondered why n in

$$\frac{d^n}{dx^n}$$

has to be a positive integer.

- It can easily be grasped that n can also be 0, because

$$\frac{d^0}{dx^0} = Id.$$

- Then, we can argue that

$$\frac{d^{-n}}{dx^{-n}} \sim \underbrace{\int \dots \int}_{n}, \quad \text{because} \quad \frac{d^n}{dx^n} \underbrace{\int \dots \int}_{n} = Id.$$

But the last relation does not commute (why? - they "almost" commute). Hence we have written " $\sim$ " instead of " $=$ ".

Can we take n to be any **real** number?

- It turns out that this question dates back as far as to one of the fathers of the Calculus - Leibniz! Moreover, a number of the greatest mathematicians have taken up this topic.
- In 1695 de L'Hospital asked what would happen if we take $n = 1/2$. Leibniz replied [1] :
  "(...) an apparent paradox, from which one day useful consequences will be drawn."
- Euler introduced the famous Gamma function (which domain is equal to $\mathbb{C} - \{0, -1, -2, ...\}$) and proposed [2]

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

  which is a formal generalization of the elementary fact, that $\frac{d^n}{dx^n} x^m = \frac{m!}{(m-n)!} x^{m-n}$ for $m \geq n$.

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[1] G.W.Leibniz, Letter from Hannover, Germany. *Leibnizen Matematische Schriften* 2 (1695), 301-302.

[2] L. Euler, *De progressionibus transcendentibus seu quarum termini generales algebraice dari nequeunt*, Commentarii academiae scientiarum Petropolitanae 5 (1738), 36–57.

- In 1822 Fourier derives his integral representation

$$\frac{d^\mu}{dx^\mu}f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(s)ds \int_{-\infty}^{\infty} p^\mu \cos\left(px - ps + \frac{\mu\pi}{2}\right) dp,$$

  but underlines that μ can be "any quantity whatever, positive or negative." [3]
- Abel considered the tautochrone problem and posed his solution in terms of integral equation [4] . As it turns out, this equation is precisely what we call today the *fractional integral*. We will follow Abel's thoughts later on.
- Liouville considered functions that can be written as a series $f(x) \sim \sum_n a_n e^{\lambda_n x}$ and proposed the following form of fractional differentiation [5]

$$\frac{d^\alpha}{dx^\alpha}f(x) \sim \sum_n a_n \lambda_n^\alpha e^{\lambda_n x},$$

  as imposed from the fact that $\frac{d^n}{dx^n}e^{ax} = a^n e^{ax}$.

[3] J.B.J. Fourier, *Théorie Analitiue de la Chaleur*, Oeuvres de Fourier 1 (1822), 508, Didot, Paris.

[4] N.H.Abel, *Solution de quelques problémes á l'aide d'intégrales définites*, Ouvres Complétes 1 (1881,1823), 16-18.

[5] J. Liouville, *Mémoire sur quelques questions de geometrie et de mecanique, et sur un nouveau genre de calcul pour resoudre ces questions*, Journal de l'Ecole Polytechnique XIII:1 (1832).

- Liouville also derived the following integral representation as the candidate for the fractional integral

$$\frac{1}{(-1)^{\alpha}\Gamma(\alpha)}\int_0^{\infty} f(x+y)y^{\alpha-1}dy.$$

- Riemann in [6] proposes a different formula for fractional integration of order α

$$\frac{1}{\Gamma(\alpha)}\int_a^x (x-t)^{\alpha-1}f(t)dt+\sum_{n=1}^{\infty} C_n\frac{x^{n-\alpha}}{\Gamma(n-\alpha+1)},$$

where a and C_n are some constants. Then, he proposed to define a fractional derivative as the integer-order differentiation of the fractional integral. This is the basis of the modern definition.

Are all of these types of fractional operators consistent with each other?

[6]B. Riemann, *Versuch einer allgemeinen Auffassung der Integration und Differentiation*, (Januar 1847), In H. Weber, editor, Bernhard Riemann's gesammelte mathematische Werke und wissenschaftlicher Nachlass, page 353, Dover, 1953. Dover Publications

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Are all of these types of fractional operators consistent with each other?

No, they are not... But do not worry.

[6]B. Riemann, *Versuch einer allgemeinen Auffassung der Integration und Differentiation*, (Januar 1847), In H. Weber, editor, Bernhard Riemann's gesammelte mathematische Werke und wissenschaftlicher Nachlass, page 353, Dover, 1953. Dover Publications

Modern definitions

- The modern notion of the fractional differentiation originates from the formula for n-th integral (excerise)

$$\int_a^x \int_a^{x_1} \dots \int_a^{x_{n-1}} f(x_n) dx_1 dx_2 \dots dx_n = \frac{1}{(n-1)!} \int_a^x (x-t)^{n-1} f(t) dt.$$

- Why we do not replace n by α and $(n-1)!$ by $\Gamma(\alpha)$?
- We thus **define** the fractional integral of order $\alpha > 0$ by

$$I_a^\alpha f(x) := \frac{1}{\Gamma(\alpha)} \int_a^x (x-t)^{\alpha-1} f(t) dt.$$

- Notice that this definition depends on the lower terminal a, which accounts for various definitions of previous Authors (ex. Liouville: $a = -\infty$). Usually we choose $a = 0$.
- After Riemann we **define** the Riemann-Liouville fractional derivative of order $n - 1 < \alpha \leq n$ ($n \in \mathbb{N}$) as

$$D_a^\alpha f(x) := \frac{d^n}{dx^n} I_a^{n-\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_a^x (x-t)^{n-\alpha-1} f(t) dt.$$

Some basic identities

- For $0 < \alpha \leq 1$ the R-L derivative has the form

$$D_a^\alpha f(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_a^x (x-t)^{-\alpha} f(t) dt.$$

- It can be shown (exercise) that $I_a^\alpha f \to f$ pointwise for $\alpha \to 0$ (the same for the R-L derivative).
- The fractional integrals have the **semigroup** property

$$I_a^\alpha I_a^\beta f(x) = I_a^{\alpha+\beta} f(x) = I_a^\beta I_a^\alpha f(x).$$

- The above does not hold in general for R-L fractional derivative (contrary to the classical case!). Indeed, we have the following

$$D_a^\beta D_a^\alpha f(x) = D_a^{\alpha+\beta} f(x) - \sum_{k=1}^{n} D_a^{\alpha-k} f(a) \frac{(x-a)^{-\beta-k}}{\Gamma(1-\beta-k)},$$

for $n-1 < \alpha \leq n$, $m-1 < \beta \leq m$.

Some basic identities

- It can be shown that for $\alpha \neq \beta$ and $f^k(a) = 0$ for $k = 1, 2, ..., \max\{n-1, m-1\}$

$$D_a^\beta D_a^\alpha f(x) = D_a^{\alpha+\beta} f(x) = D_a^\alpha D_a^\beta f(x).$$

- The commutation is also valid for the ordinary, integer order derivatives

$$\frac{d^n}{dx^n} D_a^\alpha f(x) = D_a^{n+\alpha} f(x) = D_a^\alpha \frac{d^n}{dx^n} f(x).$$

- The composition with fractional integrals looks like the following

$$D_a^\alpha I_a^\alpha f(x) = f(x),$$

  but of course the opposite identity does not hold exactly

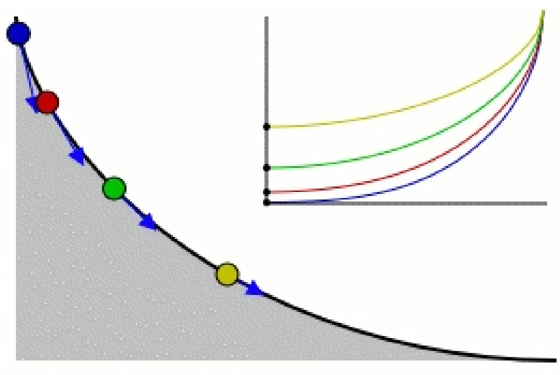
$$I_a^\alpha D_a^\alpha f(x) = f(x) - \sum_{k=1}^{n} D_a^{\alpha-k} f(a) \frac{(x-a)^{\beta-k}}{\Gamma(1+\beta-k)},$$

  where $n - 1 < \alpha \leq n$.
- We **do not** have the same formulas for the derivative of a product or composite functions!

An important application - the tautochrone problem

The problem

Find a curve with a property that a point, sliding on it only due to gravity (without friction), will reach the lowest point irrespective of the initial height chosen.



An important application - the tautochrone problem

Abel's solution

- From the conservation of energy we have

$$\frac{1}{2}m\left(\frac{ds}{dt}\right)^2 = mg(y_0 - y) \to dt = -\frac{1}{\sqrt{2g(y_0 - y)}}\frac{ds}{dy}dy,$$

  where s is arclength and y denotes height.

- The total time of the fall is (for $f(y) = (2g)^{-1/2}ds/dy$)

$$T = \int_0^{y_0} (y_0 - y)^{-\frac{1}{2}} f(y)dy,$$

  which is nothing else but a fractional integral of order $1/2$ (modulo the multiplicative constant $\Gamma(1/2) = \sqrt{\pi}$).

An important application - the tautochrone problem

- Let us apply the fractional integral on the both sides of our equation

$$I_0^{\frac{1}{2}} T = \sqrt{\pi} I_0^{\frac{1}{2}} I_0^{\frac{1}{2}} f(y_0) = \sqrt{\pi} I_0^1 f(y_0),$$

and differentiate to obtain

$$f = \frac{1}{\sqrt{\pi}} \frac{d}{dy_0} \int_0^{y_0} (y_0 - y)^{-\frac{1}{2}} T dy = D_0^{\frac{1}{2}} T$$

- Now we only need to calculate the fractional derivative of a constant (yes, a **derivative** of a constant)

$$D_0^{\frac{1}{2}} T = T \frac{1}{\sqrt{\pi}} \frac{d}{dy_0} \int_0^{y_0} (y_0 - y)^{-\frac{1}{2}} dy = \frac{2T}{\sqrt{\pi}} \frac{d}{dy_0} \sqrt{y_0} = \frac{T}{\sqrt{\pi y_0}}.$$

- Remember that $f(y) = (2g)^{-1/2} ds/dy$. Now, we easily arrive at

$$\frac{ds}{dy} = T \frac{\sqrt{2g}}{\pi} \frac{1}{\sqrt{y}},$$

which is a equation for a cycloid (and we renamed y_0 by y).

Some remarks

- As we have seen, the R-L fractional derivative of a constant is not zero. More generally, we have the following (exercise)

$$I_a^\alpha (x-a)^\beta = \frac{\Gamma(\beta+1)}{\Gamma(\beta+\alpha+1)}(x-a)^{\beta+\alpha}, \quad D_a^\alpha (x-a)^\beta = \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha+1)}(x-a)^{\beta-\alpha},$$

  for $\beta > -1$ (integrability). This is a rigorous result of what Euler and others thought about derivative of the power function.
- Abel integral equation is the one of the following form

$$\frac{1}{\Gamma(\alpha)}\int_0^x (x-t)^{\alpha-1} y(x)dx = f(x),$$

  what is $I_0^\alpha y = f$, which can be solved by applying the R-L fractional derivative on the both sides

$$y = D_0^\alpha f.$$

  This type of equation has many applications in astrophysics, computer tomography, geological surveying, ...

Another application - viscoelasticity

- This field is one of the most broadly investigated in fractional calculus due to extensive design of new materials (for ex. polymers).
- Some materials are mostly elastic (for ex. steel) while others show mainly viscous features (like honey).
- There are, though, many new materials that exhibit both of these characteristics.
- The modeling is done mainly by assuming constitutive dependence between the stress σ and strain ϵ

$$\text{Hooke's Law: } \sigma = E\epsilon, \quad \text{Newton's Law: } \sigma = \eta \frac{d\epsilon}{dt}.$$

- But what should we do, when a particular material is viscoelastic? There are models based on combining elastic and viscous elements in serial (Maxwell) or parallel (Voigt) combinations but are not satisfactory. Their refinements done by Kelvin (serial Hooke + Voigt) and Zener (parallel Hooke + Maxwell) work better but still leave some questions unanswered.

Another application - viscoelasticity

- Stress is proportional to the zeroth derivative of strain for elastic materials and to the first derivative for viscous.
- Maybe viscoelasticity can be modeled by an intermediate model? [7]

$$\sigma = E D_0^{\alpha} \epsilon, \quad 0 \leq \alpha \leq 1,$$

  with a material constant E.
- We can see that the continuous parameter α characterizes how much the material is viscous. It looks like a very natural application of the fractional derivative.
- There is also a possibility of taking into account the whole history of the process [8]

$$\sigma = \kappa D_{-\infty}^{\alpha} \epsilon, \quad 0 \leq \alpha \leq 1,$$

  where κ can be called as generalized viscosity.

[7] G. W. Scott Blair, *The role of psychophysics in rheology*, J. Colloid Science 2 (1947), 21-32.

[8] A.N. Gerasimov, *A generalization of linear laws of deformation and its application to inner friction problems*, Prikl. Mat. Mekh. 12 (1948), 251–259.

Fractional differential equations

- Viscoelasticity gave us constitutive equations containing fractional derivatives. If we wanted to obtain the dynamic behavior of those materials we would arrive at fractional differential equations.
- Two of the most important classes of ODEs are **relaxation** equation

$$y' = \lambda y + f,$$

  and **oscillation** equation

$$y'' = \lambda y + f.$$

- We are naturally led to consider the following fractional **relaxation-oscillation** equation

$$D_0^\alpha y = \lambda y + f, \quad 0 \leq \alpha \leq 2,$$

  where for simplicity we took 0 as the lower terminal.
- We know that the exponential function (of real or complex argument) is a fundamental solution of the classical equations. What about the fractional case?

Fractional differential equations

- To start, let us consider the following, homogeneous equation

$$D_0^\alpha y = y, \quad 0 < \alpha \leq 1.$$

- Let us look for a series solution $y(t) = t^\beta \sum a_n (t^\alpha)^n$, $\beta > -1$. Note that we anticipated the fact that the solution will be a function of t^α (which is consistent with $\alpha = 1$).
- Plugging the series into our equation we obtain (remember that $D_0^\alpha t^\mu = \Gamma(\mu+1)/\Gamma(\mu+1-\alpha)t^{\mu-\alpha}$)

$$\sum_{n=0}^{\infty} a_n \frac{\Gamma(n\alpha+\beta+1)}{\Gamma((n-1)\alpha+\beta+1)} t^{(n-1)\alpha+\beta} = \sum_{n=0}^{\infty} a_n t^{\alpha n+\beta}.$$

- Then, after equating terms we have

$$a_0 \frac{\Gamma(1+\beta)}{\Gamma(1+\beta-\alpha)} = 0, \quad a_n = a_{n-1} \frac{\Gamma((n-1)\alpha+\beta+1)}{\Gamma(n\alpha+\beta+1)}, \quad n \geq 1.$$

- The first condition is fulfilled for all a_0 for $\beta = \alpha - 1$.

Fractional differential equations

- Progressing recursively we have

$$a_n = a_{n-2}\frac{\Gamma((n-1)\alpha)}{\Gamma(n\alpha)}\frac{\Gamma(n\alpha)}{\Gamma((n+1)\alpha)} = \dots = a_0\frac{\Gamma(\alpha)}{\Gamma(n\alpha+\alpha)}.$$

- **Problem:** The unknown a_0 has to be determined from the initial conditions, but we cannot use $y(0)$ since $\lim_{t\to 0} y(t) = \infty$!
- Because $y(t) = a_0 t^{\alpha-1} + \dots$ we can see that in order to extract a_0 we have to take the derivative of order of $\alpha - 1$ (which is actually the fractional integral). We thus impose

$$D_0^{\alpha-1} y(0) = C,$$

which is a rather strange initial condition.
- We finally have $D_0^{\alpha-1} y(t) = a_0\Gamma(\alpha)/\Gamma(1) + O(t^\alpha)$, and the initial condition forces $a_0 = C/\Gamma(\alpha)$.
- The solution has the form

$$y(t) = Ct^{\alpha-1}\sum_{n=0}^{\infty}\frac{t^{\alpha n}}{\Gamma(\alpha n+\alpha)}.$$

Mittag-Leffler function

- The resulting function is an example of a special function known by the name of (generalized) Mittag-Leffler function

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

which is an entire function on the complex plane.
- The solution of our fractional problem can thus be written as

$$y(t) = Ct^{\alpha-1} E_{\alpha,\alpha}(t^\alpha).$$

- The special cases of the ML function include

$$E_{1,1}(z) = e^z, \quad E_{2,1}(z) = \cosh\sqrt{z}, \quad E_{1,2}(z) = \frac{e^z - 1}{z}, \quad E_{2,2}(z) = \frac{\sinh\sqrt{z}}{\sqrt{z}}.$$

Fractional differential equations

- Consider the general fractional differential Cauchy problem

$$D_0^{\alpha} y - \lambda y = f, \quad n-1 < \alpha \leq n, \quad D_0^{\alpha-k} y(0) = C_k, \quad k = 1, ..., n.$$

Then the solution can be expressed in terms of the ML function

$$y(t) = \sum_{i=1}^{n} C_k x^{\alpha-i} E_{\alpha,\alpha-i+1}(\lambda t^{\alpha}) + \int_0^t (t-s)^{\alpha-1} E_{\alpha,\alpha}(\lambda (t-s)^{\alpha}) f(s) ds.$$

The Caputo fractional derivative

- We have seen that solving the fractional differential problem required imposing some "'strange"' initial conditions (setting $D^{\alpha-1}y(0)$). In physical applications we measure mainly the value $y(0)$ or the velocity $y'(0)$. How to accommodate to that?
- The problem was solved by M.Caputo in [9] during his work on viscoelasticity.
- The idea is to exchange the order of the derivative and fractional integral operator

$$ {}^{C}D_a^{\alpha} y(x) := I^{n-\alpha} \frac{d^n}{dx^n} y(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x (x-t)^{n-\alpha+1} y^{(n)}(t) dt, $$

where $n-1 < \alpha \leq n$ (recall that the RL derivative had $D_a^{\alpha} y := d^n/dt^n \, I^{n-\alpha} y$).
- This of course requires much more regularity on y than the RL derivative (since first we differentiate and then integrate).

[9] M.Caputo, *Linear model of dissipation whose Q is almost frequency independent - II*, Geophys. J. R. Astr. Soc. 13 (1967), 529-539.

The Caputo fractional derivative

- It can be shown (exercise) that a similar formula for the derivative of a polynomial holds

$$ {}^{C}D_a^{\alpha}(x-a)^{\beta} = \frac{\Gamma(\beta+1)}{\Gamma(\beta+1-\alpha)}(x-a)^{\beta-\alpha}, $$

for $\beta > n$, where $n-1 < \alpha \leq n$ (for the RL derivative we required only $\beta > -1$).

- We also have the anticipated result that the derivative of a constant is zero. More generally,

$$ {}^{C}D_a^{\alpha}(x-a)^{k} = 0, \quad k = 0, ..., n-1. $$

- There is a relation between the RL and Caputo derivatives

$$ D_a^{\alpha}y(x) = {}^{C}D_a^{\alpha}y(x) + \sum_{i=0}^{n-1} \frac{y^{(i)}(a)}{\Gamma(i-\alpha+1)}(x-a)^{k-\alpha}, $$

thus the two types of derivative **coincide** for zero initial conditions.

The Caputo fractional derivative

- It can be shown that the solution of the following fractional problem

$$ {}^{C}D_0^{\alpha} y - \lambda y = f, \quad n-1 < \alpha \le n, \quad y^{(k)}(0) = C_k, \quad k = 0, ..., n-1. $$

  has the form

$$ y(t) = \sum_{i=0}^{n-1} C_k x^i E_{\alpha,i+1}(\lambda t^{\alpha}) + \int_0^t (t-s)^{\alpha-1} E_{\alpha,\alpha}(\lambda (t-s)^{\alpha}) f(s) ds. $$

- In particular (exercise), for $0 < \alpha \le 1$ and $f \equiv 0$

$$ y(t) = C_0 E_{\alpha}(\lambda t^{\alpha}), $$

  (where $E_{\alpha} := E_{\alpha,1}$).
- The Mittag-Leffler function is an **eigenfunction** of the Caputo derivative operator.

How to compute the fractional derivatives numerically?

- Due to physical applications, we will focus only on the Caputo derivative (but the reasoning is similar for RL).
- The first numerical discretization of the fractional derivative used the so-called Grünwald-Letnikov form. But in order keep the new material sufficiently compact, we will describe the **finite difference** methods.
- Recall that the Caputo derivative is defined by the formula ${}^{C}D_0^{\alpha} = I^{n-\alpha} d^n/dt^n$, so we only need learn how to discretize the fractional integral.
- Notice that the fractional integral is a **nonlocal** operator (in contrast with ordinary derivatives, which require knowledge of y only in a arbitrarly small neighbourhood). We expect that this will make the computation more expensive.

Simplest finite-difference scheme

- The simplest way of deriving a finite-difference scheme is to discretize the integral by a rectangular quadrature rule.
- Introduce the lattice: $0 = t_0 < t_1 < ... < t_n = T$, where $t_i = ih$, $h = T/n$ with n-number of grid-points and T is a fixed time. Denote $y(t_i) := y_i$.
- We can write

$$I_0^\alpha y(t_n) = \frac{1}{\Gamma(\alpha)} \int_0^{t_n} (t_n - s)^{\alpha-1} y(s) ds = \frac{1}{\Gamma(\alpha)} \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} (t_n - s)^{\alpha-1} y(s) ds.$$

- Now, approximate the value $y(t)$ on (t_{i-1}, t_i) by y_i (rectangular rule) and obtain the finite difference scheme

$$I_0^\alpha y(t_n) \approx \frac{1}{\Gamma(\alpha)} \sum_{i=1}^{n} y_i \int_{t_{i-1}}^{t_i} (t_n - s)^{\alpha-1} ds.$$

- Calculating the integral yields

$$I_0^\alpha y(t_n) \approx \frac{1}{\Gamma(1+\alpha)} \sum_{i=1}^{n} y_i \left((t_n - t_{i-1})^\alpha - (t_n - t_i)^\alpha \right).$$

Simplest finite-difference scheme

- Now, we can use the fact that $t_i = ih$, hence

$$I_0^\alpha y(t_n) \approx \frac{h^\alpha}{\Gamma(1+\alpha)} \sum_{i=1}^{n} y_i \left((n-i+1)^\alpha - (n-i)^\alpha\right).$$

  Notice the factor h^α, which is a verification that the integral is of order of α.

- **Finally**, our finite-difference for approximating the fractional integral has the form

$$I_0^\alpha y(t_n) \approx \frac{h^\alpha}{\Gamma(1+\alpha)} \sum_{i=1}^{n} a_{n,i}^\alpha y_i,$$

  where we denoted

$$a_{n,i}^\alpha := (n-i+1)^\alpha - (n-i)^\alpha.$$

Simplest finite-difference scheme

- The scheme for Caputo derivative can be obtained by using the backward approximation $y'(t_i) \approx h^{-1}(y_i - y_{i-1})$ (for simplicity we chose $0 < \alpha \leq 1$)

$$ {}^C D_0^\alpha y(t_n) = I_0^{1-\alpha} y'(t_n) \approx \frac{h^{-\alpha}}{\Gamma(2-\alpha)} \sum_{i=1}^{n} a_{n,i} \left(y_i - y_{i-1} \right). $$

- This formula, after changing the summation index can be transformed into the **finite-difference** for Caputo derivative

$$ {}^C D_0^\alpha y(t_n) \approx \frac{h^{-\alpha}}{\Gamma(2-\alpha)} \left(y_n - (n^{1-\alpha} - (n-1)^{1-\alpha}) y_0 + \sum_{i=1}^{n-1} b_{n,i}^{1-\alpha} \, y_i \right), $$

where

$$ b_{n,i}^\alpha := (n-i+1)^\alpha - 2(n-i)^\alpha + (n-i-1)^\alpha. $$

- Much more on finite difference schemes for fractional operators can be found in [10] .

[10] K. Diethelm, N.J. Ford and A.D. Freed, *A* predictor-corrector approach for the numerical solution of fractional differential equations, Nonlinear Dynamics 29 (2002), 3–22.

Numerical methods for fractional differential equations

- Previously derived finite differences can be used to solve fractional differential equations.
- Suppose we want to solve our simple example

$$ {}^{C}D_0^{\alpha} y = f(y,t), \quad 0 < \alpha \leq 1, $$

  with $y(0) = y_0$.
- For illustration, let us take the Euler explicit method (although all other can be used exactly in the same fashion) and discretize

$$ \frac{h^{-\alpha}}{\Gamma(2-\alpha)} \left(y_n - (n^{1-\alpha} - (n-1)^{1-\alpha}) y_0 + \sum_{i=1}^{n-1} b_{n,i}^{1-\alpha} \, y_i \right) = f(y_{n-1}, t_{n-1}). $$

- Transforming this yields

$$ y_n = (n^{1-\alpha} - (n-1)^{1-\alpha}) y_0 - \sum_{i=1}^{n-1} b_{n,i}^{1-\alpha} \, y_i + h^{\alpha} \Gamma(2-\alpha) f(y_{n-1}, t_{n-1}). $$

Laplace transform

- A large number of theoretical and practical results from fractional calculus come from utilizing the Laplace transform

$$F(s) = \mathcal{L}\left\{f(t)\right\}(s) := \int_0^\infty e^{-st} f(t)dt.$$

- Note the formula for a transform of a Laplace convolution $= \mathcal{L}\left\{f(t) * g(t)\right\}(s) = F(s)G(s)$, where $f(t) * g(t) = \int_0^t f(s)g(t-s)ds$.
- The fractional integral $I_0^\alpha y(t)$ is a Laplace convolution of y and $t^{\alpha-1}$, thus

$$\mathcal{L}\left\{I_0^\alpha y(t)\right\}(s) = s^{-\alpha}Y(s).$$

- We have

$$\mathcal{L}\left\{D_0^\alpha y(t)\right\}(s) = \mathcal{L}\left\{\frac{d^n}{dt^n} I_0^{n-\alpha} y(t)\right\}(s)$$

Laplace transform

- Recall also the formula for the Laplace transform of a derivative

$$\mathcal{L}\left\{f^{(n)}(t)\right\}(s) = s^n F(s) - \sum_{i=0}^{n-1} s^i f^{(n-i-1)}(0) = s^n F(s) - \sum_{i=0}^{n-1} s^{n-i-1} f^{(i)}(0)$$

- Using this formula we obtain

$$\mathcal{L}\left\{D_0^\alpha y(t)\right\}(s) = s^n \mathcal{L}\left\{I^{n-\alpha} y(t)\right\}(s) - \sum_{i=0}^{n-1} s^i D_0^{(\alpha-i-1)} y(0)$$

- Finally, the **Laplace transform of a RL derivative** have the form

$$\mathcal{L}\left\{D_0^\alpha y(t)\right\}(s) = s^\alpha Y(s) - \sum_{i=0}^{n-1} s^i D_0^{(\alpha-i-1)} y(0).$$

- Similarly, the **Laplace transform of a Caputo derivative** yields

$$\mathcal{L}\left\{{}^C D_0^\alpha y(t)\right\}(s) = s^\alpha Y(s) - \sum_{i=0}^{n-1} s^{\alpha-i-1} y^{(i)}(0).$$

Laplace transform

- Laplace transform method is particularly useful in dealing with fractional differential equations.
- Most of times, all we have to know are the formulas for the transform of a (fractional) derivative and the transform of a ML function

$$\mathcal{L}\left\{t^{\beta-1}E_{\alpha,\beta}(\pm\lambda t^{\alpha})\right\}(s) = \frac{s^{\alpha-\beta}}{s^{\alpha}\mp\lambda}$$

- Then, it is easy to obtain the formulas for the solutions to the fractional differential equations of arbitrary order (exercise).

Anomalous diffusion

- Of of the most prominent applications of the fractional calculus is the anomalous diffusion.
- Informally speaking, "anomalous" means that the diffusion front propagates slower or faster than the classical diffusion equation predicts.
- It has been observed in many fields such as: molecular dynamics, hydrology, financial systems, porous media analysis, charge transport, NMR and many more (for a concise review see [11]).
- The usual approach for modeling anomalous diffusion in by the stochastic Continuous Time Random Walk framework (see [11]). When we consider the Mean Squared Displacement (MSD) of a randomly walking particle we have

$$MSD \propto t^{\alpha}, \quad \text{where} \quad \begin{cases} \alpha < 1, & \text{subdiffusion;} \\ \alpha = 1, & \text{classical diffusion;} \\ \alpha > 1, & \text{superdiffusion.} \end{cases}$$

[11] R. Metzler and J. Klafter, *The randomwalk's guide to anomalous diffusion: a fractional dynamics approach*, Phys. Reports 339 (200), 1–77

Anomalous diffusion

- For a more concrete example consider a one-dimensional porous medium (a brick which one dimension is much bigger than others).
- Imagine a setting when a one side of the brick is held in constant concentration of water. During the time evolution the moisture will percolate into the medium. We ask at what pace.
- Mathematically, we impose the following initial-boundary conditions:

$$u(0,t) = C, \quad u(x,0) = 0,$$

where $u(x,t)$ is a concentration at x and t.
- **Self-similarity** - a characteristic feature of diffusion in our experiment. Moisture concentration $u(x,t)$ can be drawn on a single curve

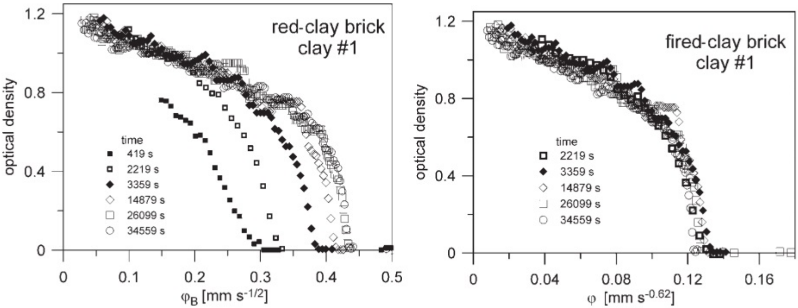
$$u(x,t) = U(\eta), \quad \eta = x/\sqrt{t},$$

for $U(0) = C$ i $U(\infty) = 0$.

Anomalous diffusion

- In a number of experiments (ex. [12]) the so-called Boltzmann scaling $\eta = x/t^{1/2}$ is not observed.
- A more appropriate and accurate is the **anomalous diffusion** scaling (Figure from [12])

$$u(x,t) = U(\eta), \quad \eta = x/t^{\alpha/2}, \quad 0 < \alpha < 2.$$



[12] Abd El-Ghany, El Abd and J.J. Milczarek, *Neutron radiography study of water absorption in porous building materials: anomalous diffusion analysis*, J. Phys. D.: Appl. Phys. 37 (2004) 2305–2313.

Anomalous diffusion

- What is a correct mathematical model of anomalous diffusion? Nobody knows for sure. But fractional derivatives provide a very elegant approach.
- It is mostly speculated that subdiffusive phenomena are caused by the fact that particles can be "trapped" in some regions of the medium. These **waiting times** cause that front propagates more slowly.
- Superdiffusion is in turn caused by nonlocal effects which shape the flux at some arbitrary point. For example we can think of a portion of fluid particles situated very far from considered point, which can move through this distance very quickly by **jumps** (ex. thin canals in porous medium).
- Both of these types of diffusion are modeled by assuming the power-law distribution for waiting times and/or jumps.
- We will provide a deterministic derivation of the resulting equation for subdiffusion.

Derivation of a subdiffusion equation

- Consider a porous medium with water percolating it. The mass is conserved, hence the continuity equation is fulfilled

$$u_t = -\nabla \cdot q(x,t),$$

where q is the flux.

- Suppose now that only a portion w_0 of the flux passes through our point, the rest w_1 stays trapped in some region for a time s. Then

$$u_t = -\left(w_0 \nabla \cdot q(x,t) + w_1 \nabla \cdot q(x,t-s)\right).$$

- This can be generalized for any number of waiting times s_i

$$u_t = -\sum_{i=1}^{n} w_i \, \nabla \cdot q(x, t-s_i).$$

- Introducing a weight density $w_i = w(s_i)\Delta s_i$ this can be generalized to a continuous distribution of waiting times

$$u_t = -\int_0^t w(s) \, \nabla \cdot q(x, t-s) ds.$$

Derivation of a subdiffusion equation

- By a change of the variable, we have

$$u_t = -\int_0^t w(t-s)\,\nabla\cdot q(x,s)ds.$$

- Now, we have to choose the weight in a way that it should reduce to the classical case in an appropriate limit. That is $w \to \delta$, where δ is a Dirac delta distribution.
- It is convenient to write

$$u_t = -\frac{\partial}{\partial t}\int_0^t k_\alpha(t-s)\,\nabla\cdot q(x,s)ds,$$

  where k_α is a **function** which encapsulates the limit passage (with α).
- The simplest choice is to take power function $k_\alpha(s) \propto s^{\alpha-1}$.
- Choosing appropriate constant (essentially immaterial) we get

$$u_t = -\frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t (t-s)^{\alpha-1}\,\nabla\cdot q(x,s)ds = -\partial_t^{\alpha-1}\nabla\cdot q,$$

  where $\partial_t^{\alpha-1}$ is a RL partial derivative.

Derivation of a subdiffusion equation

- It can be shown that for zero initial conditions, the time-fractional diffusion equation can be transformed into

$$ {}^{C}\partial_t^{\alpha} u = -\nabla \cdot q. $$

- For the simplest, Fickian case we have $q = -D\nabla u$. We thus obtain the linear equation

$$ {}^{C}\partial_t^{\alpha} u = D\nabla^2 u, $$

which fundamental solution can be obtained (with a help of a Laplace transform) and stated in terms of the Wright's function [13]

$$ G(x,t) = \frac{1}{2} t^{-\alpha/2} W_{-\alpha/2, 1-\alpha/2}\left(-\frac{|x|}{\sqrt{D} t^{\alpha/2}} \right), $$

where $W_{\mu,\nu}(z) := \sum_{n=0}^{\infty} \frac{z^n}{n!\Gamma(\mu n + \nu)}$ (only one-dimension for simplicity).

[13] F.Mainardi, Y.Luchko, G.Pagnini, *The fundamental solution of the space-time fractional diffusion equation* arXiv preprint cond-mat/0702419 (2007).

Space-time fractional diffusion equation

- The problem with a brick $u(x,0) = 0$, $u(0,t) = 1$ can be solved by

$$u(x,t) = W_{-\alpha/2,1}\left(-\frac{|x|}{\sqrt{D}t^{\alpha/2}}\right),$$

notice that this reduces to the classical solution of the Error function for $\alpha = 1$ (exercise).

- In a similar way as before we can derive the space-fractional equation which accounts for superdiffusion

$$u_t = -D\left(-\Delta_x\right)^{\frac{\alpha}{2}} u,$$

where $(-\Delta_x)^{\frac{\alpha}{2}}$ is the fractional Laplacian (or **Riesz fractional derivative**) defined by the Fourier transform

$$\mathcal{F}\left\{(-\Delta)^{\frac{\alpha}{2}} u(x)\right\}(\xi) = -|\xi|^{\alpha}\mathcal{F}\left\{u(x)\right\}(\xi).$$

- Solution of the space-fractional diffusion equation can be found in [13]

[13] F.Mainardi, Y.Luchko, G.Pagnini, *The fundamental solution of the space-time fractional diffusion equation* arXiv preprint cond-mat/0702419 (2007).

What I have not covered

- Stochastic processes (Levy walks etc.). This is a very broad field with numerous applications and interesting results.
- We have talked only about a small part of the world of anomalous diffusion. This is a rapidly evolving topic, where only linear equations are well-known. More on nonlinear anomalous diffusion can be found for ex. in my papers (on the webpage).
- Signal and Image processing.
- Fractional Models and Control.
- ...
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THANK YOU!

Now, on to the exercises :)

One more thing - some very useful monographs

- I. Podlubny, Fractional Differential Equations, Academic Press, 1999.
- A. Kilbas, H. Srivastava and J. Trujillo, Theory and applications of fractional differential equations, Elsevier Science, Amsterdam, 2006.
- K.S.Miller, B.Ross, An introduction to the fractional calculus and fractional differential equations, Wiley, 1993.

- And many, many more...