Derivadas fracionárias em problemas de difusão anômala

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Introdução

O que é Cálculo Fracionário?

$$\frac{df(x)}{dx}, \quad \frac{d^2f(x)}{dx^2}, \quad \frac{d^3f(x)}{dx^3}, \quad \cdots \quad \frac{d^nf(x)}{dx^n} \quad n = \text{inteiro}$$

$$\frac{d^{\frac{1}{2}}f(x)}{dx^{\frac{1}{2}}} = ??????$$

Introdução

O que é Cálculo Fracionário?

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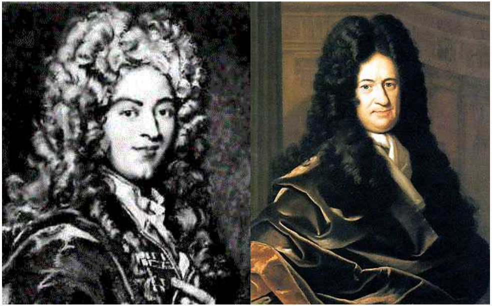
$$\frac{d^{\frac{1}{2}}f(x)}{dx^{\frac{1}{2}}} = \text{??????}$$

Um Pouco de História

l'Hospital e Leibniz (1695)



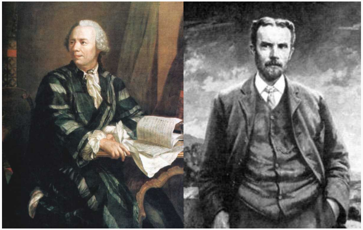
Em 1695 L'Hospital escreveu uma carta à Leibniz perguntando qual seria o significado de uma derivada de ordem $\frac{1}{2}$. Leibniz respondeu que "$d^{\frac{1}{2}}x$ deveria ser igual à $x\sqrt{dx : x}$".

Um Pouco de História

Euler (1730) e Heaviside (1893)

Generalização da fórmula de ordem inteira $n \leq m$

$$\frac{d^n x^m}{dx^n} = m(m-1)(m-2)\cdots(m-n+1)x^{m-n} = \frac{\Gamma(m+1)}{\Gamma(m-n+1)}x^{m-n},$$



para ordem real $\alpha \leq m$

$$\frac{d^\alpha x^m}{dx^n} = \frac{\Gamma(m+1)}{\Gamma(m-\alpha+1)}x^{m-\alpha}.$$

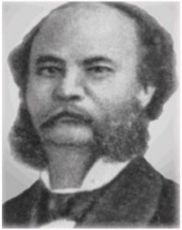
Um Pouco de História

Fourier (1820)

$$\frac{d^{\alpha}f(x)}{dx^{\alpha}} = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(t)\cos(ux - ut + \alpha\frac{\pi}{2})\,du\,dt$$

Um Pouco de História

Grünwald e Letnikov (1867)

$$\frac{d^{\alpha}f(x)}{d(x-a)^{\alpha}} = \lim_{N\to\infty}\left(\frac{x-a}{N}\right)^{-\alpha}\sum_{m=0}^{N-1}(-1)^m\binom{\alpha}{m}f\left(x+(\alpha-m)\frac{x-a}{N}\right)$$

Um Pouco de História

Grünwald e Letnikov (1867)

$$\frac{df(x)}{dx} = \lim_{h_1 \to 0} \frac{f(x+h_1) - f(x)}{h_1}$$

$$\begin{aligned}
\frac{d^2 f(x)}{dx^2} &= \lim_{h_2 \to 0} \frac{\frac{df(x+h_2)}{dx} - \frac{df(x)}{dx}}{h_2} \\
&= \lim_{h_2 \to 0} \lim_{h_1 \to 0} \frac{\frac{f(x+h_1+h_2)-f(x+h_2)}{h_1} - \frac{f(x-h_1)-f(x)}{h_1}}{h_2} \\
&= \lim_{h \to 0} \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2}
\end{aligned}$$

Um Pouco de História

Grünwald e Letnikov (1867)

$$\frac{d^2 f(x)}{dx^2} = \lim_{h_2 \to 0} \frac{\frac{df(x+h_2)}{dx} - \frac{df(x)}{dx}}{h_2}$$

$$= \lim_{h_2 \to 0} \lim_{h_1 \to 0} \frac{\frac{f(x+h_1+h_2)-f(x+h_2)}{h_1} - \frac{f(x-h_1)-f(x)}{h_1}}{h_2}$$

$$= \lim_{h \to 0} \frac{1 f(x+2h) - 2 f(x+h) + 1 f(x)}{h^2}$$

$$\frac{d^3 f(x)}{dx^3} = \lim_{h \to 0} \frac{1 f(x+3h) - 3 f(x+2h) + 3 f(x+h) - 1 f(x)}{h^3}$$

Um Pouco de História

Grünwald e Letnikov (1867)

$$\frac{d^n f(x)}{d(x-a)^n} = \lim_{N\to\infty}\left(\frac{x-a}{N}\right)^{-n}\sum_{m=0}^{N-1}(-1)^m\left(\begin{array}{c} n \\ m \end{array}\right) f(x+(n-m)\frac{x-a}{N})$$

$$\left(\begin{array}{c} n \\ m \end{array}\right) = 0 \;\; (m>n), \quad h = \frac{x-a}{N}$$

Generalizando para $\alpha \in \mathbb{R}$

$$\frac{d^\alpha f(x)}{d(x-a)^\alpha} = \lim_{N\to\infty}\left(\frac{x-a}{N}\right)^{-\alpha}\sum_{m=0}^{N-1}(-1)^m\left(\begin{array}{c} \alpha \\ m \end{array}\right) f(x+(\alpha-m)\frac{x-a}{N})$$

Um Pouco de História

Grünwald e Letnikov (1867)

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Um Pouco de História

Grünwald e Letnikov (1867)

Para $\alpha = n$ inteiro

$$\frac{d^{\alpha} f(x)}{d(x-a)^{\alpha}} = \begin{cases} \frac{d^n}{dx^n} f(x) & (n > 0) \\ f(x) & (n = 0) \\ \int_a^x f(t)(dt)^{-n} & (n < 0) \end{cases}$$

Um Pouco de História

Grünwald e Letnikov (1867)

Para $n=-1$ inteiro

$$\frac{d^{-1}f(x)}{d(x-a)^{-1}}=\lim_{N\to\infty}\left(\frac{x-a}{N}\right)\sum_{m=0}^{N-1}(-1)^m\left(\begin{array}{c}-1\\ m\end{array}\right)f(x-(1+m)\frac{x-a}{N})$$

$$\left(\begin{array}{c}-1\\ m\end{array}\right)=(-1)^m$$

$$\frac{d^{-1}f(x)}{d(x-a)^{-1}}=\lim_{N\to\infty}\sum_{m=0}^{N-1}\left(\frac{x-a}{N}\right)f(x-(1+m)\frac{x-a}{N})=\int_a^x f(t)dt$$

Um Pouco de História

Grünwald e Letnikov (1867)

Para $n = -1$ inteiro

$$\frac{d^{-1}f(x)}{d(x-a)^{-1}} = \lim_{N\to\infty}\left(\frac{x-a}{N}\right)\sum_{m=0}^{N-1}(-1)^m\left(\begin{array}{c}-1\\ m\end{array}\right)f(x-(1+m)\frac{x-a}{N})$$

$$\left(\begin{array}{c}-1\\ m\end{array}\right) = (-1)^m$$

$$\frac{d^{-1}f(x)}{d(x-a)^{-1}} = \lim_{N\to\infty}\sum_{m=0}^{N-1}\left(\frac{x-a}{N}\right)f(x-(1+m)\frac{x-a}{N}) = \int_a^x f(t)dt$$

Um Pouco de História

Riemann e Liouville (1832 - 1873)

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

e

$$\frac{d^{\alpha}f(x)}{d(b-x)^{\alpha}} = \frac{1}{\Gamma(n-\alpha)}\frac{d^n}{dx^n}\int_x^b \frac{f(t)}{(t-x)^{\alpha-n+1}}dt$$

onde

$$n-1 \leq \alpha < n$$

Um Pouco de História

Caputo (1967)

$$\frac{{}^{C}d^{\alpha}f(x)}{d(x-a)^{\alpha}} = \frac{1}{\Gamma(n-\alpha)} \int_{a}^{x} \frac{f^{(n)}(t)}{(x-t)^{\alpha-n+1}} dt$$

e

$$\frac{{}^{C}d^{\alpha}f(x)}{d(b-x)^{\alpha}} = \frac{1}{\Gamma(n-\alpha)} \int_{x}^{b} \frac{f^{(n)}(t)}{(t-x)^{\alpha-n+1}} dt$$

onde

$$n-1 \leq \alpha < n$$

O Cálculo Fracionário de Riemann-Liouville

O teorema de Cauchy para integração repetida

$$\int_a^x f(t)dt = \frac{1}{n!}\frac{d^n}{dx^n}\int_a^x (x-t)^n f(t)dt$$

$$\int_a^x f(t)(dt)^n = \int_a^x dt_n \int_a^{t_n} \cdots \int_a^{t_2} f(t_1)dt_1 = \frac{1}{(n-1)!}\int_a^x (x-t)^{n-1} f(t)dt$$

Da continuação analítica para $\alpha \in \mathbb{R}$ obtemos

$${}_aJ_x^{\alpha} f(t) = \int_a^x f(t)(dt)^{\alpha} = \frac{1}{\Gamma(\alpha)}\int_a^x \frac{f(t)}{(x-t)^{-\alpha+1}}dt$$

O Cálculo Fracionário de Riemann-Liouville

A proposta de Riemann-Liouville

Para $\alpha > 0$ com $\alpha \in \mathbb{R}$ temos

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

e

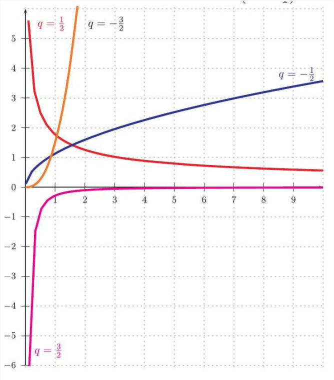
$$\frac{d^{\alpha} f(x)}{d(b-x)^{\alpha}} = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_x^b \frac{f(t)}{(t-x)^{\alpha-n+1}} dt,$$

onde

$$n-1 \leq \alpha < n$$

Derivada de algumas funções

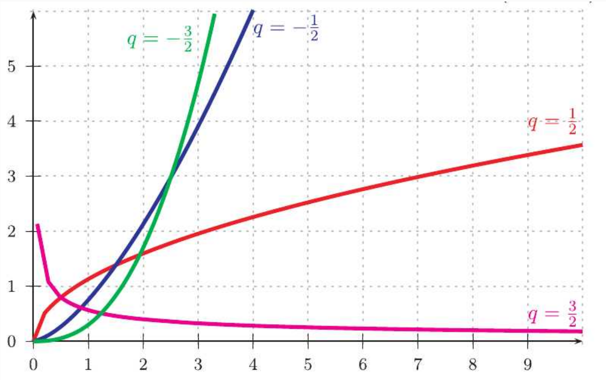
$$\frac{d^q 1}{dx^q} = \frac{x^{-q}}{\Gamma(1-q)}$$



O Cálculo Fracionário de Riemann-Liouville

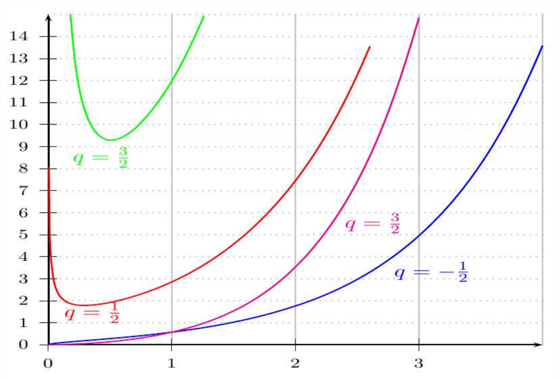
Derivada de algumas funções

$$\frac{d^q x}{dx^q} = \frac{x^{1-q}}{\Gamma(2-q)}$$



Derivada de algumas funções

$$\frac{d^q e^x}{dx^q} = \sum_{k=0}^{\infty} \frac{x^{k-q}}{\Gamma(k-q+1)}$$



Introdução

O Cálculo Fracionário e as derivadas de funções não diferenciáveis

Fractional differentiability of nowhere differentiable functions and dimensions

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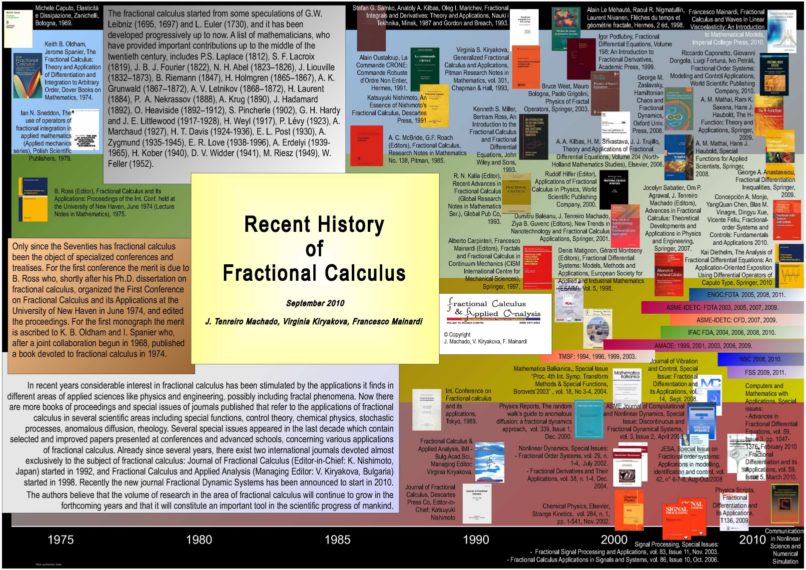
Department of Physics, University of Pune, Pune 411 007, India.

Abstract

Weierstrass's everywhere continuous but nowhere differentiable function is shown to be locally continuously fractionally differentiable everywhere for all orders below the 'critical order' $2-s$ and not so for orders between $2-s$ and 1, where s, $1<s<2$ is the box dimension of the graph of the function. This observation is consolidated in the general result showing a direct connection between local fractional differentiability and the box dimension/ local Hölder exponent. Lévy index for one dimensional Lévy flights is shown to be the critical order

Kolwankar and Gangal, Fractional differentiability of nowhere differentiable functions and dimensions, Chaos **6**, 505 (1996)

Introdução



Recent History of Fractional Calculus
September 2010
J. Tenreiro Machado, Virginia Kiryakova, Francesco Mainardi
The fractional calculus started from some speculations of G.W. Leibniz (1695, 1697) and L. Euler (1730), and it has been developed progressively up to now. A list of mathematicians, who have provided important contributions up to the middle of the twentieth century, includes P.S. Laplace (1812), S. F. Lacroix (1819), J. B. J. Fourier (1822), N. H. Abel (1823–1826), J. Liouville (1832–1873), B. Riemann (1847), H. Holmgren (1865–1867), A. K. Grunwald (1867–1872), A. V. Letnikov (1868–1872), H. Laurent (1884), P. A. Nekrassov (1888), A. Krug (1890), J. Hadamard (1892), O. Heaviside (1892–1912), S. Pincherle (1902), G. H. Hardy and J. E. Littlewood (1917-1928), H. Weyl (1917), P. Lévy (1923), A. Marchaud (1927), H. T. Davis (1924-1936), E. L. Post (1930), A. Zygmund (1935-1945), E. R. Love (1938-1996), A. Erdelyi (1939-1965), H. Kober (1940), D. V. Widder (1941), M. Riesz (1949), W. Feller (1952).
Only since the Seventies has fractional calculus been the object of specialized conferences and treatises. For the first conference the merit is due to B. Ross who, shortly after his Ph.D. dissertation on fractional calculus, organized the First Conference on Fractional Calculus and its Applications at the University of New Haven in June 1974, and edited the proceedings. For the first monograph the merit is ascribed to K. B. Oldham and J. Spanier who, after a joint collaboration begun in 1968, published a book devoted to fractional calculus in 1974.
In recent years considerable interest in fractional calculus has been stimulated by the applications it finds in different areas of applied sciences like physics and engineering, possibly including fractal phenomena. Now there are more books of proceedings and special issues of journals published that refer to the applications of fractional calculus in several scientific areas including special functions, control theory, chemical physics, stochastic processes, anomalous diffusion, rheology. Several special issues appeared in the last decade which contain selected and improved papers presented at conferences and advanced schools, concerning various applications of fractional calculus. Already since several years, there exist two international journals devoted almost exclusively to the subject of fractional calculus: Journal of Fractional Calculus (Editor-in-Chief: K. Nishimoto, Japan) started in 1992, and Fractional Calculus and Applied Analysis (Managing Editor: V. Kiryakova, Bulgaria) started in 1998. Recently the new journal Fractional Dynamic Systems has been announced to start in 2010.
The authors believe that the volume of research in the area of fractional calculus will continue to grow in the forthcoming years and that it will constitute an important tool in the scientific progress of mankind.
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1975
1980
1985
1990
2000
2010

O Cálculo Fracionário

O que ainda falta fazer?

- Novas formulações e suas relações
- Interpretação geométrica
- Cálculo vetorial fracionário
- Cálculo com derivadas imaginárias
- Cálculo com derivadas matriciais
- etc...

Aplicações do Cálculo Fracionário

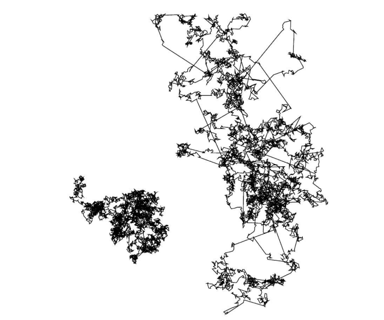
Algumas aplicações do Cálculo Fracionário

- Otmização em controle
- Mecânica clássica e física de partículas
- Eletrônica
- Processamento de sinais
- Biomatemática
- Sistemas Dinâmicos
- Processos Estocásticos
- Dinâmica de Fluídos
- etc

O que é difusão anômala?

Richardson em 1926

West *Rev. Modern Phys.* **86** (2014) 1169

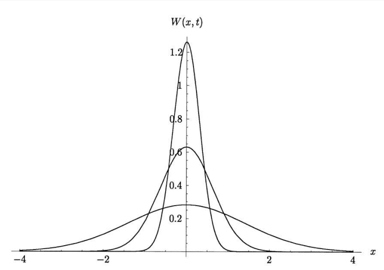


Voos de Levy

Metzler and Klafter *Phys. Rep.* **39** (2000) 1

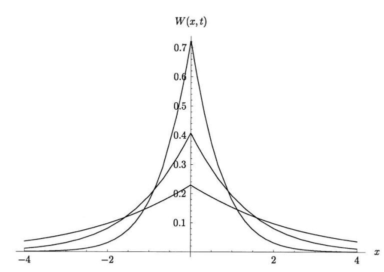
O Cálculo Fracionário em Difusão Anômala

O que é difusão anômala?



$$\langle x^2(t)\rangle = 2K_1 t$$

$$\frac{\partial W(x,t)}{\partial t} = K_1 \frac{\partial^2 W(x,t)}{\partial x^2}$$

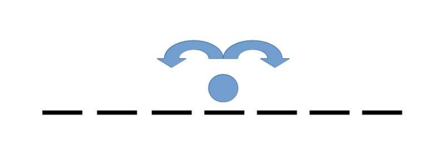


$$\langle x^2(t)\rangle = \frac{2K_\alpha}{\Gamma(\alpha+1)} t^\alpha$$

???

Difusão normal

Movimento Browniano no espaço discreto



$$W(i, t+\Delta t) = \frac{1}{2} W(i-1, t) + \frac{1}{2} W(i+1, t)$$

O Cálculo Fracionário em Difusão Anômala

Difusão normal

No limite do contínuo $\Delta x \to \infty$ e $\Delta t \to \infty$

$$W(i,t+\Delta t) = W(i,t) + \frac{\partial W(i,t)}{\partial t}\Delta t + O(\Delta t^2)$$

$$W(i\pm 1,t) = W(x,t) \pm \frac{\partial W(x,t)}{\partial x}\Delta x + \frac{\partial^2 W(x,t)}{\partial x^2}\frac{\Delta x^2}{2} + O(\Delta x^3)$$

Substituíndo em

$$W(i,t+\Delta t) = \frac{1}{2}W(i-1,t) + \frac{1}{2}W(i+1,t)$$

O Cálculo Fracionário em Difusão Anômala

Difusão normal

No limite do contínuo $\Delta x \to \infty$ e $\Delta t \to \infty$

$$W(i, t+\Delta t) = W(i,t) + \frac{\partial W(i,t)}{\partial t}\Delta t + O(\Delta t^2)$$

$$W(i \pm 1, t) = W(x,t) \pm \frac{\partial W(x,t)}{\partial x}\Delta x + \frac{\partial^2 W(x,t)}{\partial x^2}\frac{\Delta x^2}{2} + O(\Delta x^3)$$

Substituíndo em

$$W(i, t+\Delta t) = \frac{1}{2}W(i-1,t) + \frac{1}{2}W(i+1,t)$$

Difusão normal

Obtemos a equação de difusão

$$\frac{\partial W(x,t)}{\partial t} = K_1 \frac{\partial^2 W(x,t)}{\partial x^2}$$

onde

$$K_1 = \lim_{(\Delta x, \Delta t) \to (0,0)} \frac{\Delta x^2}{2\Delta t}$$

é o coeficiente de difusão

Difusão normal

Resolvendo a equação de difusão

$$\frac{\partial W(x,t)}{\partial t} = K_1 \frac{\partial^2 W(x,t)}{\partial x^2}$$

$$W(\pm\infty, t) = 0 \quad W(x, 0^+) = \delta(x)$$

$$W(x,t) = \frac{1}{\sqrt{4\pi K_1 t}} \exp\left(-\frac{x^2}{4K_1 t}\right) \Longrightarrow \langle x^2(t)\rangle = 2K_1 t$$

Difusão normal

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Difusão normal

Usando a transformada de Fourier

$$\frac{\partial W(k,t)}{\partial t} = -k^2 K_1 W(k,t)$$

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Usando a transfromada de Laplace

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Difusão normal

O desvio quadrático médio

$$\langle x^2(t) \rangle = -\mathcal{L}^{-1}\left\{ \lim_{k \to 0} \frac{\partial^2 W(k,s)}{\partial k^2} \right\} = 2K_1 t$$

Que $W(k,s)$ resulta no desvio quadrático médio da difusão anômala?

$$\langle x^2(t) \rangle = -\mathcal{L}^{-1}\left\{ \lim_{k \to 0} \frac{\partial^2 ?}{\partial k^2} \right\} = \frac{2K_\alpha}{\Gamma(\alpha+1)} t^\alpha$$

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Difusão anômala

Para a difusão anômala devemos ter

$$W(k,s) = \frac{W(k,0)}{s + k^2 K_\alpha s^{1-\alpha}}$$

Usando a relação

$$\mathcal{L}\left\{ {}_0J_t^\alpha f(t) \right\} = s^{-\alpha} f(s)$$

podemos inferir que a difusão anômala é descrita por

$$W(x,t) - W(x,0) = K_\alpha \, {}_0J_t^\alpha \left(\frac{\partial^2 W(x,t)}{\partial x^2} \right)$$

O Cálculo Fracionário em Difusão Anômala

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O Cálculo Fracionário em Difusão Anômala

Difusão anômala

Tomando a derivada de Riemann-Liouville obtemos

$$\frac{\partial^\alpha W(x,t)}{\partial t^\alpha} - \frac{1}{\Gamma(1-\alpha)}\frac{W(x,0)}{x^\alpha} = K_\alpha \frac{\partial^2 W(x,t)}{\partial x^2}$$

Finalmente a EDP fracionária da difusão anômala

$$\frac{{}^{C}\partial^\alpha W(x,t)}{\partial t^\alpha} = K_\alpha \frac{\partial^2 W(x,t)}{\partial x^2}$$

onde temos a derivada de Caputo

$$\frac{{}^{C}d^\alpha f(t)}{dt^\alpha} = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{1}{(t-u)^\alpha}\frac{df(u)}{du}du$$

O Cálculo Fracionário em Difusão Anômala

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Difusão de poluentes na atmosfera

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Fractional derivative models for atmospheric dispersion of pollutants

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HIGHLIGHTS

- The use of fractional derivatives to model diffusion of pollutants is investigated.
- Fractional differential equations for the concentration of pollutant are proposed.
- The solutions are compared with traditional models and with a real experiment.

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ABSTRACT

In the present work, we investigate the potential of fractional derivatives to model atmospheric dispersion of pollutants. We propose simple fractional differential equation models for the steady state spatial distribution of concentration of a non-reactive pollutant in Planetary Boundary Layer. We solve these models and we compare the solutions with a real experiment. We found that the fractional derivative models perform far better than the traditional Gaussian model and even better than models found in the literature where it is considered that the diffusion coefficient is a function of the position in order to deal with the anomalous diffusion.

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$$u\frac{{}^{C}\partial^{\alpha}\overline{c^{y}}(x,z)}{\partial x^{\alpha}} = K_z\frac{\partial^2\overline{c^{y}}(x,z)}{\partial z^2}$$

O Cálculo Fracionário em Difusão Anômala

Tabela: Observed and estimated crosswind-integrated concentrations for Copenhagen experiment.

Exp.	Distance (m)	Observed	α–Gaussian	Gaussian	α–SM	SM
1	1900	6.48	6.32	3.61	7.74	4.62
1	3700	2.31	4.97	2.72	4.20	2.30
2	2100	5.38	4.14	2.47	4.89	3.18
2	4200	2.95	3.27	1.76	2.79	1.58
3	1900	8.20	6.51	4.00	8.91	5.66
3	3700	6.22	5.22	3.73	5.03	2.88
3	5400	4.30	4.66	3.72	3.95	2.21
4	4000	11.7	10.60	10.25	8.21	5.93
5	2100	6.72	5.71	3.98	7.55	4.81
5	4200	5.84	4.70	3.93	4.28	2.43
5	6100	4.97	4.36	3.93	3.27	2.00
6	2000	3.96	2.90	1.72	3.90	2.63
6	4200	2.22	2.27	1.24	2.23	1.28
6	5900	1.83	2.08	1.12	1.79	0.90
7	2000	6.70	4.68	2.77	6.21	4.16
7	4100	3.25	3.65	1.95	3.50	2.03
7	5300	2.23	3.34	1.73	2.79	1.56
8	1900	4.16	5.75	3.51	7.32	4.87
8	3600	2.02	4.72	3.01	4.68	2.74
8	5300	1.52	4.18	2.95	3.39	1.84
9	2100	4.58	3.77	2.26	5.26	3.44
9	4200	3.11	2.99	1.61	3.07	1.74
9	6000	2.59	2.63	1.35	2.24	1.19

Tabela: Statistical indices to evaluate the performance of proposed models

Model	Cor	NMSE	FS	FB	FA2
α–Gaussian	0.83	0.07	0.30	0.001	0.87
Gaussian	0.82	0.23	0.27	-0.39	0.73
α–SM	0.83	0.08	0.17	0.03	0.83
SM	0.80	0.30	0.50	-0.44	0.74

$$\text{NMSE (normalized mean square error)} = \frac{\overline{(c_o - c_p)^2}}{\overline{c_o c_p}},$$

$$\text{Cor (correlation coefficient)} = \frac{\overline{(c_o - \overline{c_p})(c_p - \overline{c_p})}}{\sigma_o \sigma_p},$$

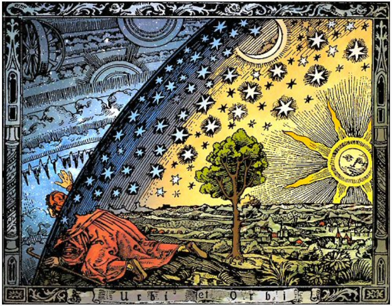
$$\text{FB (fractional bias)} = \frac{\overline{c_o - \overline{c_p}}}{0.5(\overline{c_o} + \overline{c_p})},$$

$$\text{FS (fractional standard deviations)} = \frac{\sigma_o - \sigma_p}{0.5(\sigma_o + \sigma_p)},$$

Aplicações do Cálculo Fracionário em Física

E futuro??

Leibniz - ”Segue que $d^{\frac{1}{2}}x$ é igual à $x\sqrt{dx : x}$, um aparente paradoxo, do qual algum dia poderemos tirar consequências úteis”



Obrigado!!