Concept of Fractional derivatives

1) Friedrich, C., H. Schiessel, et al. (1999). "Constitutive behavior modeling and fractional derivatives." Rheology Series: 429-466.

2) Sokolov, I. M., J. Klafter, et al. (2002). "Fractional Kinetics." Physics Today **55(11): 48-54.**

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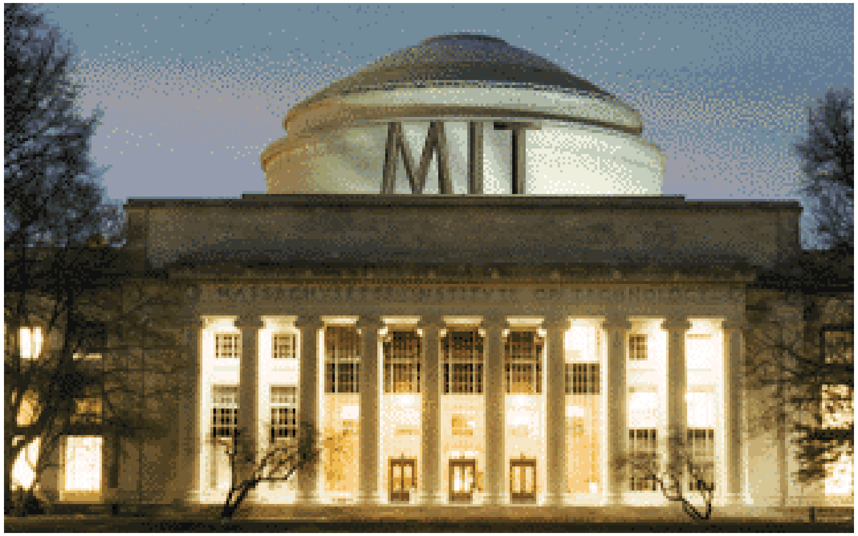
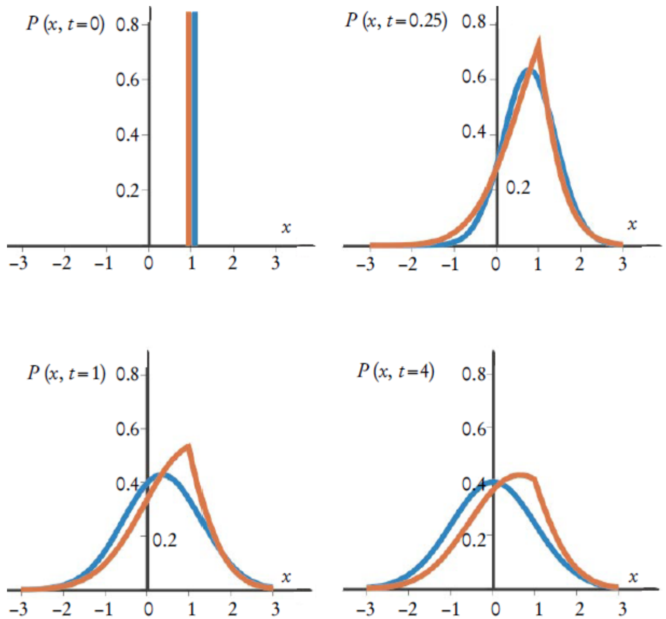


Where do fractional derivatives occur?

- Subdiffusive systems

$$\frac{\partial}{\partial t}P(x,t) = {}_0D_t^{1-\alpha}\kappa_\alpha \nabla^2 P(x,t)$$

- charge transport in anomalous semiconductors
- spread of contaminants in geological formations
- diffusing particle trapped in optical tweezers
-displacement of a monomer of the Rouse model in solvent



Subdiffusive system described by red curve. Singular cusp, slower relaxation

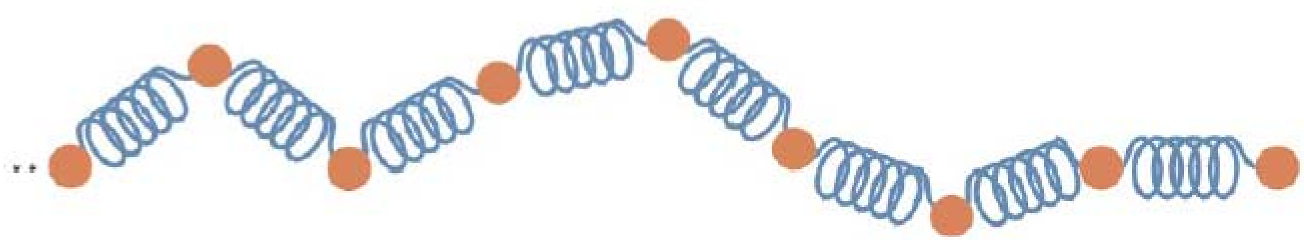


Image from sokolov et al. (2002)

Introduction – Power law behaviour

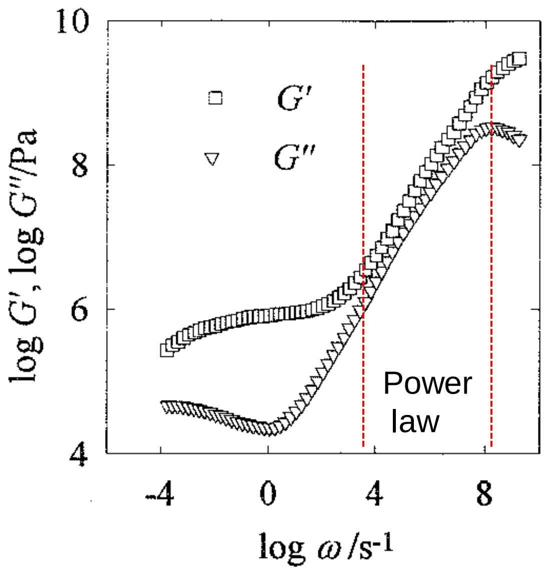


Fig 1(a). Storage modulus $G'(\omega)$ and loss modulus $G''(\omega)$ for polyisobutylene

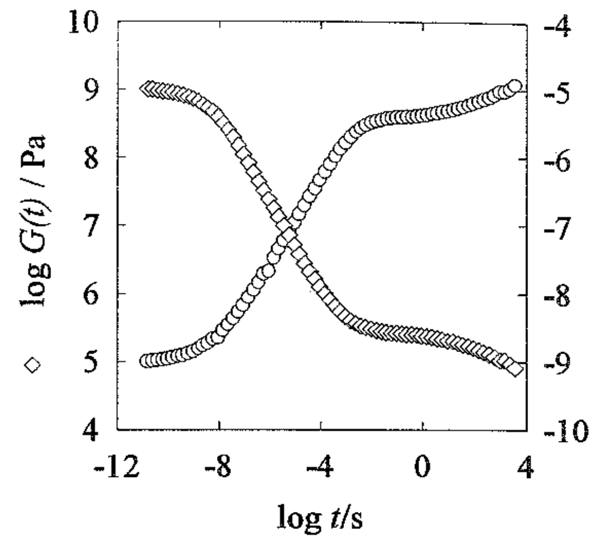


Fig. 1(b). Relaxation function $G(t)$ and creep function $J(t)$ for polyisobutylene

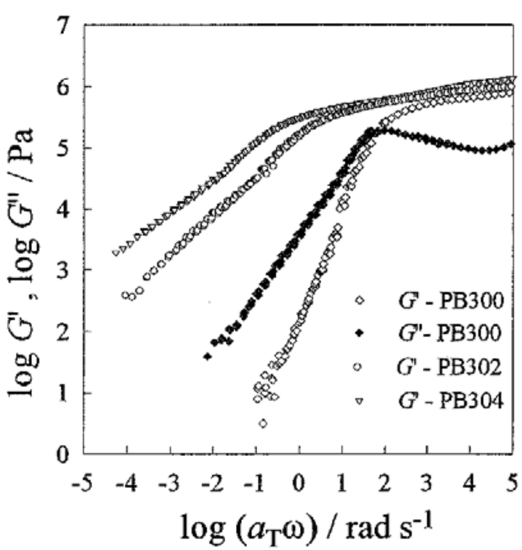


Fig 2. G' and G'' of substituted polybutadiene.

PB300 – unsubstituted → $G' \propto \omega^2, G'' \propto \omega$

PB302, PB304 – active groups attached to backbone → $G' \propto \omega^\alpha, G'' \propto \omega^\beta$

$0 < \alpha, \beta < 1$

Graphs from Friedrich et al. (1999)

Role of fractional derivatives in constitutive equations

Assume :

$$G(t) = \frac{E}{\Gamma(1-\beta)}\left(\frac{t}{\lambda}\right)^{-\beta}$$

E,λ,β are constants, $0\beta \leq 1$

Gamma function

Interpolates factorial

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

$$\Gamma(n) = (n-1)!$$

Linear viscoelasticity

$$\tau(t) = \int_{-\infty}^{t} G(t-t') \frac{d\gamma(t')}{dt'} dt'$$

$$\tau(t) = \frac{E\lambda^\beta}{\Gamma(1-\beta)} \int_{-\infty}^{t} dt'(t-t')^{-\beta} \frac{d\gamma(t')}{dt'}$$

Rheological constitutive equation with fractional derivatives

$$\tau(t) = E\lambda^\beta \frac{d^\beta \gamma(t)}{dt^\beta}$$

Can be written as a fractional derivative

$$\frac{d^\beta \gamma(t)}{dt^\beta} = \frac{1}{\Gamma(1-\beta)} \int_{-\infty}^{t} dt'(t-t')^{-\beta} \frac{d\gamma(t')}{dt'}$$

$\beta = 0, \quad \tau(t) = E\gamma(t),$ Hooke's law

$\beta = 1, \quad \tau(t) = \eta \frac{d\gamma(t)}{dt},$ Newton's law

Formal definitions – Part I

$$\frac{d^n}{dx^n} x^m = \frac{m!}{(m-n)!} x^{m-n}$$

Repeated integer differentiation of an integral power

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

Repeated integer differentiation of a fractional power

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

Fractional derivative of an arbitrary power

Can handle any function which can be expanded in a Taylor series

More general technique is using fractional integrals
Riemann-Liouville approach

Defining fractional derivatives – Part II

First, define repeated integrals and fractional integrals:

$$If(x) = \int_a^x f(y_1)dy_1$$

$$I^2 f(x) = \int_a^x (If)(y_2)dy_2 = \int_a^x \left(\int_a^{y_1} f(y_2)dy_2 \right) dy_1$$

Similarly, integrating n times,

$$I^n f(x) = \int_a^x \int_a^{y_1} \cdots \int_a^{y_{n-1}} f(y_n)dy_n \ldots \mathrm{dy}_1$$

By Cauchy's Theorem for repeated integration,

$$I^n f(x) = \frac{1}{(n-1)!} \int_a^x (x-y)^{n-1} f(y)dy$$ (Proof ?)

$$I^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-y)^{\alpha-1} f(y)dy$$ by generalizing to arbitrary α

Defining fractional derivatives – Part III

Notation: (potentially confusing!)

$$ {}_a D_x^{-\alpha} f(x) \equiv \frac{1}{\Gamma(\alpha)} \int_a^x (x-y)^{\alpha-1} f(y)\,dy \qquad \alpha > 0 $$

'fractional integral of arbitrary order'

The fractional derivative!

$$ {}_a D_x^{\alpha} \equiv \frac{d^n}{dx^n}\, {}_a D_x^{\alpha-n} \qquad n = [\alpha]+1, \quad \alpha > 0 $$

'α-th fractional derivative'

Example:

$$ {}_0 D_x^{7.4} = \frac{d^8}{dx^8}\, {}_0 D_x^{-0.6} $$

$a = 0$

$\alpha = 7.4$

$n = 8$

$\alpha - n = -0.6$

ie, to differentiate 7.4 times:

1) fractionally integrate first by 0.6
2) differentiate 8 times

Why integrate first?

Alternate Notation

$$\boxed{\frac{d^\alpha}{dt^\alpha}}$$

Used by Friedrich et al.

If $\alpha < 0,$ $$\frac{d^\alpha}{dt^\alpha} = \frac{1}{\Gamma(-\alpha)} \int_{-\infty}^{t} \frac{f(t')}{(t-t')^{\alpha+1}} dt'$$

If $\alpha > 0,$ $$\frac{d^\alpha}{dt^\alpha} = \frac{d^n}{dt^n}\left(\frac{d^{\alpha-n} f(t)}{dt^{\alpha-n}}\right) \qquad n = [\alpha]+1$$

Used in Rheological Constitutive Equations (RCE) because the lower limit of integration is $t' = -\infty$ where $\tau(t') = 0$

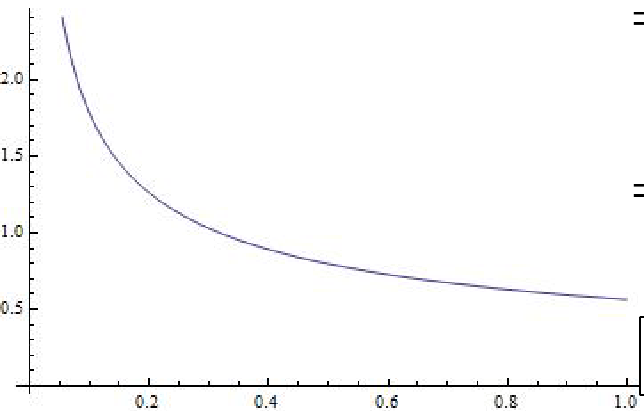
Fractional derivatives of simple functions

Example 1: $\color{red}{{}_0D^{1/2}1}$

$$
\begin{aligned}
a &= 0 \\
\alpha &= 0.5 \\
n &= 1 \\
\alpha - n &= -0.5 \\
f(x) &= 1
\end{aligned}
$$

$$
\begin{aligned}
{}_0D^{1/2}x &= \frac{d}{dx}\left(\frac{1}{\Gamma(1/2)}\int_0^x (x-y)^{-0.5}\,dy\right) \\
&= \frac{d}{dx}\left(\frac{-1}{\Gamma(1/2)}\int_x^0 (z)^{-0.5}\,dz\right) \\
&= \frac{d}{dx}\left(\frac{1}{\sqrt{\pi}}\int_0^x (z)^{-0.5}\,dz\right) \\
&= \frac{d}{dx}\left(\frac{2\sqrt{x}}{\sqrt{\pi}}\right) \\
&= \frac{1}{\sqrt{\pi x}}
\end{aligned}
$$

substitute $x - y = z$



Half-derivative of a constant is not 0 !

Fractional derivatives of simple functions

Example 2: ${}_0D^{1/2}x$

$a = 0$

$\alpha = 0.5$

$n = 1$

$\alpha - n = -0.5$

$f(x) = x$

$${}_0D^{1/2}x = \frac{d}{dx}\left(\frac{1}{\Gamma(1/2)}\int_0^x (x-y)^{-0.5} y\,dy\right)$$

$$= \frac{d}{dx}\left(\frac{-1}{\Gamma(1/2)}\int_x^0 (z)^{-0.5}(x-z)dz\right)$$

substitute $x - y = z$

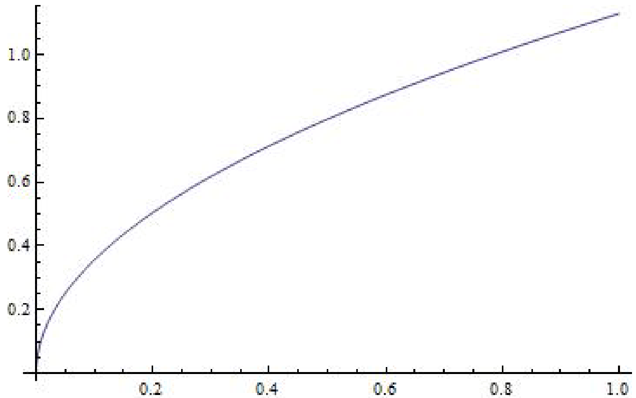
$$= \frac{d}{dx}\left(\frac{1}{\sqrt{\pi}}\int_0^x (z)^{-0.5}(x-z)dz\right)$$

$$= \frac{d}{dx}\left(\frac{1}{\sqrt{\pi}}\left[x\int_0^x z^{-0.5}dz - \int_0^x z^{0.5}dz\right]\right)$$

$$= \frac{1}{\sqrt{\pi}}\left(\int_0^x z^{-0.5}dz + x.x^{-0.5} - x^{0.5}\right)$$

Liebniz Rule

$$= \frac{2\sqrt{x}}{\sqrt{\pi}}$$



More examples of fractional calculus

Examples of Fractional Calculus with $\alpha = \pm 1/2$		
Semi-integral	**Function**	**Semi-derivative**
${}_0D_x^{-1/2} f(x) = \frac{d^{-1/2}}{dx^{-1/2}} f(x)$	$f(x)$	${}_0D_x^{1/2} f(x) = \frac{d^{1/2}}{dx^{1/2}} f(x)$
$2C\sqrt{x/\pi}$	C, any constant	$C/\sqrt{\pi x}$
$\sqrt{\pi}$	$1/\sqrt{x}$	0
$x\sqrt{\pi}/2$	$\sqrt{x}$	$\sqrt{\pi}/2$
$4x^{3/2}/3\sqrt{\pi}$	x	$2\sqrt{x/\pi}$
$\frac{\Gamma(\mu+1)}{\Gamma(\mu+3/2)} x^{\mu+1/2}$	$x^\mu,\ \mu > -1$	$\frac{\Gamma(\mu+1)}{\Gamma(\mu+1/2)} x^{\mu-1/2}$
$\exp(x)\,\mathrm{erf}(\sqrt{x})$	$\exp(x)$	$1/\sqrt{\pi x} + \exp(x)\,\mathrm{erf}(\sqrt{x})$
$2\sqrt{\pi/x}\,[\ln(4x) - 2]$	$\ln x$	$\ln(4x)/\sqrt{\pi x}$

Fourier transform

$$\mathcal{F}\{{}_{-\infty}D_t^\alpha f(t)\} = (i\omega)^\alpha f(\omega)$$

Laplace transform

$$\mathcal{L}\{{}_0D_t^{-\alpha} f(t)\} = u^{-\alpha}\mathcal{L}\{f(\omega)\}$$

Eqn 10 in Freidrich et al is probably incorrect

$$\frac{d^\mu}{dt^\mu}\frac{d^\nu f}{dt^\nu} \neq \frac{d^{\mu+\nu} f}{dt^{\mu+\nu}}$$

$$f = 1/\sqrt{x}, \mu = \nu = 1/2$$

From Sokolov et al. (2002)

Back to RCEs

For $G(t) = \frac{E}{\Gamma(1-\beta)}\left(\frac{t}{\lambda}\right)^{-\beta}$

$$\tau(t) = \frac{E\lambda^{\beta}}{\Gamma(1-\beta)}\int_{-\infty}^{t} dt'(t-t')^{-\beta}\frac{d\gamma(t')}{dt'}$$

CE for assumed form of G

$$\tau(t) = \frac{E\lambda^{\beta}}{\Gamma(-\alpha)}\int_{-\infty}^{t} dt' \frac{1}{(t-t')^{\alpha+1}}\frac{d\gamma(t')}{dt'}$$

Definition of fractional derivative

$$a = -\infty$$
$$\alpha = \beta - 1 \quad 0 \le \beta < 1$$

$$\tau(t) = E\lambda^{\beta}\frac{d^{\beta-1}}{dt^{\beta-1}}\frac{d\gamma(t)}{dt}$$

$$\tau(t) = E\lambda^{\beta}\frac{d^{\beta}\gamma(t)}{dt^{\beta}}$$

$G^{*}(\omega) = E(i\omega\lambda)^{\beta}$

For SAOS $\gamma(t) = \gamma_0 e^{i\omega t}$

$$\tau(t) = \int_{-\infty}^{t} G(t-t')\frac{d\gamma(t')}{dt'}$$

$$\tilde{\tau}(\omega) = G^{*}(\omega)\tilde{\gamma}(\omega)$$

$$\tilde{\tau}(\omega) = E(i\omega\lambda)^{\beta}\,\tilde{\gamma}(\omega)$$