Concept of Fractional derivatives


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Where do fractional derivatives occur?

- Subdiffusive systems

\[ \frac{\partial}{\partial t} P(x, t) = 0 D_t^{1-\alpha} \kappa_\alpha \nabla^2 P(x, t) \]

- 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

PB302, PB304 – active groups attached to backbone

$G' \propto \omega^2, G'' \propto \omega$

$G' \propto \omega^\alpha, G'' \propto \omega^\beta$

$0 < \alpha, \beta < 1$

Graphs from Friedrich et al. (1999)
Role of fractional derivatives in constitutive equations

Assume:

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

\( E, \lambda, \beta \) are constants, \( 0 \leq \beta < 1 \)

Linear viscoelasticity

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

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

Gamma function

Interpolates factorial

\[ \Gamma(x) = \int_{0}^{\infty} t^{x-1} e^{-t} dt \]

\[ \Gamma(n) = (n-1)! \]

Rheological constitutive equation with fractional derivatives

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

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

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

\( \beta = 1, \quad \tau(t) = \eta \frac{d \gamma(t)}{dt}, \quad \) 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
First, define repeated integrals and fractional integrals:

\[ I^1 f(x) = \int_a^x f(y_1) dy_1 \]

\[ I^2 f(x) = \int_a^x (I^1 f(y_2)) dy_2 = \int_a^x \left( \int_a^{y_1} f(y_2) dy_2 \right) dy_1 \]

Similarly, integrating \( n \) times,

\[ I^n f(x) = \int_a^x \int_a^{y_1} \cdots \int_a^{y_{n-1}} f(y_n) dy_n \cdots dy_1 \]

By Cauchy’s Theorem for repeated integration,

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

\[ I^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x - y)^{\alpha-1} f(y) dy \quad \text{by generalizing to arbitrary } \alpha \]
Defining fractional derivatives – Part III

Notation: (potentially confusing!)

\[ a D_x^{-\alpha} f(x) \equiv \frac{1}{\Gamma(\alpha)} \int_a^x (x-y)^{\alpha-1} f(y)dy \quad \alpha > 0 \]

‘fractional integral of arbitrary order’

The fractional derivative!

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

‘\(\alpha\)-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

\[
\frac{d^\alpha}{dt^\alpha}
\]

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 \( \alpha > 0 \),

\[
\frac{d^\alpha}{dt^\alpha} = \frac{d^n}{dt^n} \left( \frac{d^{\alpha-n} f(t)}{dt^{\alpha-n}} \right) \quad n = [\alpha] + 1
\]

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: \( \frac{D^{1/2}}{0} 1 \)

\[ a = 0 \]
\[ \alpha = 0.5 \]
\[ n = 1 \]
\[ \alpha - n = -0.5 \]
\[ f(x) = 1 \]

\[ \frac{D^{1/2}}{0} x = \frac{d}{dx} \left( \frac{1}{\Gamma(1/2)} \int_{0}^{x} (x - y)^{-0.5} dy \right) \]

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

substitute \( x - y = z \)

\[ = \frac{d}{dx} \left( \frac{1}{\sqrt{\pi}} \int_{0}^{x} (z)^{-0.5} dz \right) \]

\[ = \frac{d}{dx} \left( \frac{2\sqrt{x}}{\sqrt{\pi}} \right) \]

\[ = \frac{1}{\sqrt{\pi x}} \]

Half-derivative of a constant is not 0!
Fractional derivatives of simple functions

Example 2: \( {}_0D^{1/2}x \)

\[
\begin{align*}
\alpha &= 0 \\
\alpha - n &= -0.5 \\
f(x) &= x \\
a &= 0 \\
n &= 1
\end{align*}
\]

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

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

substitute \( x - y = z \)

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

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

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

\[
= \frac{2\sqrt{x}}{\sqrt{\pi}}
\]

Liebniz Rule
More examples of fractional calculus

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### Examples of Fractional Calculus with $\alpha = \pm 1/2$

<table>
<thead>
<tr>
<th>Semi-integral</th>
<th>Function</th>
<th>Semi-derivative</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0 D_x^{-\frac{1}{2}} f(x) = \frac{d^{-\frac{1}{2}}}{dx^{-\frac{1}{2}}} f(x)$</td>
<td>$f(x)$</td>
<td>$0 D_x^{\frac{1}{2}} f(x) = \frac{d^{\frac{1}{2}}}{dx^{\frac{1}{2}}} f(x)$</td>
</tr>
<tr>
<td>$2C \sqrt{x/\pi}$</td>
<td>$C$, any constant</td>
<td>$C/\sqrt{\pi x}$</td>
</tr>
<tr>
<td>$\sqrt{\pi}$</td>
<td>$1/\sqrt{x}$</td>
<td>$0$</td>
</tr>
<tr>
<td>$x\sqrt{\pi}/2$</td>
<td>$\sqrt{x}$</td>
<td>$\sqrt{\pi}/2$</td>
</tr>
<tr>
<td>$4x^{3/2}/3\sqrt{\pi}$</td>
<td>$x$</td>
<td>$2\sqrt{x/\pi}$</td>
</tr>
<tr>
<td>$\frac{\Gamma(\mu+1)}{\Gamma(\mu+3/2)} x^{\mu+\frac{1}{2}}$</td>
<td>$x^\mu$, $\mu &gt; -1$</td>
<td>$\frac{\Gamma(\mu+1)}{\Gamma(\mu+1/2)} x^{\mu-\frac{1}{2}}$</td>
</tr>
<tr>
<td>$\exp(x) \text{erf}(\sqrt{x})$</td>
<td>$\exp(x)$</td>
<td>$1/\sqrt{\pi x} + \exp(x) \text{erf}(\sqrt{x})$</td>
</tr>
<tr>
<td>$2\sqrt{\pi x} [\ln(4x) - 2]$</td>
<td>$\ln x$</td>
<td>$\ln(4x)/\sqrt{\pi x}$</td>
</tr>
</tbody>
</table>

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**Fourier transform**

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

**Laplace transform**

$$\mathcal{L}\{0 D_t^\alpha f(t)\} = u^{-\alpha} \mathcal{L}\{f(\omega)\}$$

Eqn 10 in Freidrich et al. is probably incorrect

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

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

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From Sokolov et al. (2002)
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 $G$

$$\alpha = -\infty$$  
$$\alpha = \beta - 1 \quad 0 \leq \beta < 1$$

Definition of fractional derivative

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

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

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

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

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