Numerical Solution of Fractional PDEs — Beijing Computational Science Research Center, November 2015

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Part I

Fractional integrals and derivatives
Introduction

This lecture provides some key definitions and results from fractional calculus, needed for our study of fractional PDEs. The literature contains several concepts of fractional differentiation, but we focus only on the Riemann–Liouville and Caputo definitions, with a brief mention of the Grünwald–Letnikov approach.

In the sequel, we work almost exclusively with the Riemann–Liouville fractional integral and derivative.
Outline

Fractional integration

Fractional differentiation

Grünwald–Letnikov definition
Motivation: consider the $n$-fold integration operator $\mathcal{I}_{a+}^n$ based at $a$, defined recursively by

$$\mathcal{I}_{a+}^0 f(x) = f(x)$$

and

$$\mathcal{I}_{a+}^n f(x) = \int_a^x \mathcal{I}_{a+}^{n-1} f(y) \, dy \quad \text{for } n \geq 1.$$

We claim

$$\mathcal{I}_{a+}^n f(x) = \int_a^x \frac{(x - y)^{n-1}}{(n-1)!} f(y) \, dy \quad \text{for } n \geq 1.$$

The formula holds for $n = 1$ because $(x - y)^0 / 0! = 1$ and

$$\mathcal{I}_{a+}^1 f(x) = \int_a^x f(y) \, dy.$$
Easy proof by induction on $n$

Let $n \geq 1$ and assume

$$\mathcal{I}_a^n f(x) = \int_a^x \frac{(x - y)^{n-1}}{(n-1)!} f(y) \, dy.$$ 

Then

$$\mathcal{I}_a^{n+1} f(x) = \int_a^x \mathcal{I}_a^n f(z) \, dz = \int_a^x \int_y^z \frac{(z - y)^{n-1}}{(n-1)!} f(y) \, dy \, dz$$

$$= \int_a^x \int_y^x \frac{(z - y)^{n-1}}{(n-1)!} \, dz \, f(y) \, dy$$

$$= \int_a^x \frac{(x - y)^n}{n!} f(y) \, dy. \quad \Box$$
Gamma function

Recall that

\[ \Gamma(\alpha) = \int_0^\infty e^{-t} t^{\alpha-1} \, dt \quad \text{for } \alpha > 0, \]

and

\[ \Gamma(n + 1) = n! \quad \text{for any integer } n \geq 0. \]

For any real \( \alpha > 0 \), we define the left-sided, Riemann–Liouville fractional integration operator of order \( \alpha \) by

\[ I_{a+}^\alpha f(x) = \int_a^x \frac{(x - y)^{\alpha-1}}{\Gamma(\alpha)} f(y) \, dy \quad \text{for } x > a. \]

This definition is consistent with our earlier definition of \( I_{a+}^n \) when \( \alpha = n \).
Transposed operator

Putting

\[ \langle f, g \rangle = \int_{a}^{b} f(x)g(x) \, dx \]

we find that

\[ \langle I_{a+}^{\alpha} f, g \rangle = \langle f, I_{b-}^{\alpha} g \rangle, \]

where the right-sided, Riemann–Liouville fractional integration operator of order \( \alpha \) is given by

\[ I_{b-}^{\alpha} g(x) = \int_{x}^{b} \frac{(y - x)^{\alpha-1}}{\Gamma(\alpha)} g(y) \, dy \quad \text{for} \ x < b. \]
Semigroup property

From the recursive definition, we see that

$$\mathcal{I}_a^m \mathcal{I}_a^n = \mathcal{I}_a^{m+n} \quad \text{for all integers } m \geq 0, n \geq 0.$$

Key question: does

$$\mathcal{I}_a^\alpha \mathcal{I}_a^\beta = \mathcal{I}_a^{\alpha+\beta} \quad \text{for all } \alpha > 0 \text{ and } \beta > 0?$$

Consider

$$\mathcal{I}_a^\alpha \mathcal{I}_a^\beta f(x) = \int_a^x \frac{(x-z)^{\alpha-1}}{\Gamma(\alpha)} \int_a^z \frac{(z-y)^{\beta-1}}{\Gamma(\beta)} f(y) \, dy \, dz$$

$$= \int_a^x \int_y^x \frac{(x-z)^{\alpha-1}}{\Gamma(\alpha)} \frac{(z-y)^{\beta-1}}{\Gamma(\beta)} \, dz \, f(y) \, dy.$$
Putting \( t = (z - y)/(x - y) \), we have

\[
z = y + t(x - y), \quad x - z = (1 - t)(x - y), \quad z - y = t(x - y),
\]

so the Beta function identity

\[
\int_0^1 (1 - t)^{\alpha-1} t^{\beta-1} \, dt = B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)},
\]

gives

\[
\int_y^x \frac{(x - z)^{\alpha-1}}{\Gamma(\alpha)} \frac{(z - y)^{\beta-1}}{\Gamma(\beta)} \, dz
\]

\[
= \frac{(x - y)^{(\alpha-1)+ (\beta-1)+1}}{\Gamma(\alpha)\Gamma(\beta)} \int_0^1 (1 - t)^{\alpha-1} t^{\beta-1} \, dt
\]

\[
= \frac{(x - y)^{\alpha+\beta-1}}{\Gamma(\alpha + \beta)},
\]

implying the desired result.
Gel’fand–Shilov function

Let

\[ \Upsilon_\alpha(x) = \frac{x_+^{\alpha-1}}{\Gamma(\alpha)}, \]

where \( x_+ = \max(x, 0) \), and use the abbreviation

\[ I_\alpha = I_{0+}^\alpha \quad \text{for } \alpha > 0. \]

The fractional integral is given by the Laplace convolution

\[ I_\alpha f(x) = \int_0^x \Upsilon_\alpha(x - y)f(y) \, dy = \Upsilon_\alpha * f(x), \quad x > 0. \]

We easily see that

\[ \Upsilon_\alpha * \Upsilon_\beta = \Upsilon_{\alpha + \beta} \quad \text{for } \alpha > 0, \beta > 0. \]
In fact, since $\ast$ is associative,

$$(\Upsilon_\alpha \ast \Upsilon_\beta) \ast f = \Upsilon_\alpha \ast (\Upsilon_\beta \ast f) = \mathcal{I}^\alpha (\mathcal{I}^\beta f) = \mathcal{I}^{\alpha+\beta} f = \Upsilon_{\alpha+\beta} \ast f$$

for every continuous $f$.

It follows that

$$\mathcal{I}^\alpha \Upsilon_\beta = \Upsilon_{\alpha+\beta},$$

generalising the identity

$$\mathcal{I}^m \frac{x^n}{n!} = \frac{x^{m+n}}{(m + n)!}.$$
Shifted version

Let

\[ \gamma_{\beta,a}(x) = \gamma_{\beta}(x - a). \]

Using the substitution \( y = a + t \),

\[ I_{\alpha}^\alpha \gamma_{\beta,a}(x) = \int_x^a \gamma_{\alpha}(x - y) \gamma_{\beta}(y - a) \, dy \]

\[ = \int_0^{x-a} \gamma_{\alpha}(x - a - t) \gamma_{\beta}(t) \, dt \]

\[ = (\gamma_{\alpha} * \gamma_{\beta})(x - a) = \gamma_{\alpha+\beta}(x - a), \]

or in other words,

\[ I_{\alpha}^\alpha \gamma_{\beta,a}(x) = \gamma_{\alpha+\beta,a}(x), \quad x > a. \]
Fractional differentiation

Assume that

\[ n - 1 < \alpha \leq n \quad \text{for some } n \in \{1, 2, 3, \ldots \}, \]

and write \( \mathcal{D}^n = (d/dx)^n \).

The Riemann–Liouville fractional derivative is defined by

\[ \mathcal{D}_a^\alpha f(x) = \mathcal{D}^n \mathcal{I}_a^{n-\alpha} f(x) \quad \text{for } x > a. \]

whereas the Caputo fractional derivative is defined by

\[ ^C\mathcal{D}_a^\alpha f(x) = \mathcal{I}_a^{\alpha-n} \mathcal{D}^n f(x) \quad \text{for } x > a. \]

Lemma

For \( x > a \) and \( \beta > 0 \),

\[ (\mathcal{D}\mathcal{I}_a^\beta - \mathcal{I}_a^\beta \mathcal{D}) f(x) = f(a) \gamma_\beta(x - a). \]
Proof

Note that $\mathcal{D}\gamma_{\beta}(x) = \gamma_{\beta-1}(x)$ and $\gamma_1(x) = 1$.

By the fundamental theorem of calculus,

$$\mathcal{I}_{a+}\mathcal{D}f(x) = \int_a^x f'(y) \, dy = f(x) - f(a),$$

so

$$f(x) = \mathcal{I}_{a+}\mathcal{D}f(x) + f(a)\gamma_1(x - a),$$

Thus,

$$\mathcal{I}_{a+}^{\beta} f(x) = \mathcal{I}_{a+}^{\beta+1} \mathcal{D}f(x) + f(a)\gamma_{\beta+1}(x - a),$$

and finally

$$\mathcal{D}\mathcal{I}_{a+}^{\beta} f(x) = \mathcal{D}\mathcal{I}_{a+} \mathcal{I}_{a+}^{\beta} \mathcal{D}f(x) + f(a)\gamma_{\beta}(x - a). \quad \square$$
Relation between $\mathcal{D}^\alpha$ and $\mathcal{C}^\alpha\mathcal{D}^\alpha$

**Theorem**

*If* $n - 1 < \alpha < n$, *then*

$$
\mathcal{D}_a^\alpha f(x) = \mathcal{C}^\alpha\mathcal{D}_a^\alpha f(x) + \sum_{k=0}^{n-1} \mathcal{D}^k f(a) \frac{(x-a)^{k-\alpha}}{\Gamma(k+1-\alpha)}, \quad x > a.
$$

**Proof.**

In the case $n = 2$, we have $1 < \alpha < 2$ and the Lemma gives

$$
\mathcal{D}_a^\alpha f(x) = \mathcal{D}^2 \mathcal{I}_a^{2-\alpha} f(x) = \mathcal{D} \left( \mathcal{I}_a^{2-\alpha} \mathcal{D} f(x) + f(a) \mathcal{Y}_{2-\alpha}(x-a) \right)
$$

$$
= \mathcal{I}_a^{2-\alpha} \mathcal{D}^2 f(x) + \mathcal{D} f(a) \mathcal{Y}_{2-\alpha}(x-a) + f(a) \mathcal{Y}_{1-\alpha}(x-a)
$$

$$
= \mathcal{C}^\alpha\mathcal{D}_a^\alpha f(x) + f(a) \frac{(x-a)^{-\alpha}}{\Gamma(1-\alpha)} + \mathcal{D} f(a) \frac{(x-a)^{1-\alpha}}{\Gamma(2-\alpha)}.
$$

The general case follows in the same way.
Differentiating a shifted Gel’fand–Shilov function

Lemma
If $\alpha > 0$, $\beta > 0$ and $x > a$, then

$$\mathcal{D}_{a+}^{\alpha} \Upsilon_{\beta,a}(x) = \Upsilon_{\beta-\alpha,a}(x).$$

Proof.
If $n - 1 < \alpha < n$ then

$$\mathcal{D}_{a+}^{\alpha} \Upsilon_{\beta,a}(x) = \mathcal{D}^{n} \mathcal{I}_{a+}^{n-\alpha} \Upsilon_{\beta,a}(x) = \mathcal{D}^{n} \Upsilon_{n-\alpha+\beta,a}(x) = \Upsilon_{\beta-\alpha,a}(x).$$

In particular, since $\Upsilon_{1,a}(x) \equiv 1$, if $x > a$ then

$$\mathcal{D}_{a+}^{\alpha} 1(x) = \Upsilon_{1-\alpha,a}(x) = \frac{(x - a)^{-\alpha}}{\Gamma(1 - \alpha)} \quad \text{whereas} \quad c\mathcal{D}_{a+}^{\alpha} 1(x) = 0.$$
Relation between $\mathcal{D}^\alpha$ and $^c\mathcal{D}^\alpha$ restated

Since
\[
\frac{(x - a)^{k-\alpha}}{\Gamma(k + 1 - \alpha)} = \Upsilon_{k+1-\alpha, a}(x) = \mathcal{D}^\alpha_{a+} \Upsilon_{k+1, a}(x)
\]
the relation
\[
\mathcal{D}^\alpha_{a+} f(x) = \mathcal{D}^\alpha_{a+} f(x) + \sum_{k=0}^{n-1} \mathcal{D}^k f(a) \frac{(x - a)^{k-\alpha}}{\Gamma(k + 1 - \alpha)}, \quad x > a,
\]
may be re-stated in the form
\[
^c\mathcal{D}^\alpha_{a+} f(x) = \mathcal{D}^\alpha_{a+} \left( f(x) - \sum_{k=0}^{n-1} \mathcal{D}^k f(a) \frac{(x - a)^k}{k!} \right), \quad x > a,
\]
where $n - 1 < \alpha < n$, as before.
Alternative representation

Lemma

If $0 < \alpha < 1$ and $x > a$, then

$$\mathcal{D}^\alpha_{a^+} f(x) = f(x) \gamma_{1-\alpha}(x-a) + \int_a^x \gamma_{-\alpha}(x-y) [f(y) - f(x)] \, dy,$$

Proof.

Differentiate the identity

$$\mathcal{I}^{1-\alpha}_{a^+} f(x) = f(x) \gamma_{2-\alpha}(x-a) + \int_a^x \gamma_{1-\alpha}(x-y) [f(y) - f(x)] \, dy,$$

noting that the derivative of the integral on the right is

$$\int_a^x \gamma_{-\alpha}(x-y) [f(y) - f(x)] \, dx - \gamma_{2-\alpha}(x-a)f'(x).$$
Representation as a Hadamard finite-part integral

Assume $0 < \alpha < 1$ and $x > a$. Then

$$\int_a^x \Upsilon_{-\alpha}(x - y)[f(y) - f(x)] \, dy = \int_{x-\epsilon}^x \cdots \, dy$$

$$+ \int_a^{x-\epsilon} \Upsilon_{-\alpha}(x - y)f(y) \, dy + f(x)[\Upsilon_{1-\alpha}(\epsilon) - \Upsilon_{1-\alpha}(x - a)],$$

so

$$\mathcal{D}_{a+}^{\alpha} f(x) = \frac{f(x)\epsilon^{-\alpha}}{\Gamma(1-\alpha)} + \int_a^{x-\epsilon} \Upsilon_{-\alpha}(x - y)f(y) \, dy + O(\epsilon^{1-\alpha}).$$

and therefore

$$\mathcal{D}_{a+}^{\alpha} f(x) = \text{“} \mathcal{I}_{a+}^{-\alpha} f(x) \text{”} = \text{fp} \int_{\epsilon \downarrow 0}^{x-\epsilon} \Upsilon_{-\alpha}(x - y)f(y) \, dy.$$
Grünwald–Letnikov definition

Can we define a fractional derivative (or integral) directly, without using integer-order derivatives and integrals? Denote the backward difference by

$$\Delta_h f(x) = f(x) - f(x - h).$$

Can check by induction on $k$ that

$$\Delta_h^k f(x) = \sum_{j=0}^{k} \binom{k}{j} (-1)^j f(x - jh) \quad \text{for } k \in \{0, 1, 2, \ldots \}.$$ 

Hence define the fractional backward difference of order $\alpha$ by

$$\Delta_h^\alpha f(x) = \sum_{j=0}^{[n]} \binom{\alpha}{j} (-1)^j f(x - jh),$$

with

$$\binom{\alpha}{j} = \frac{\alpha}{1} \frac{\alpha - 1}{2} \ldots \frac{\alpha - j + 1}{j} = \frac{\Gamma(\alpha + 1)}{\Gamma(j + 1)\Gamma(\alpha - j + 1)}.$$
An induction on $k$ shows that
\[
\Delta^k_h f(x) = \int_0^h \cdots \int_0^h f^{(k)}(x - t_1 - \cdots - t_k) \, dt_1 \cdots dt_k,
\]
and thus
\[
f^{(k)}(x) = \lim_{h \to 0} \frac{\Delta^k_h f(x)}{h^k}.
\]
Given $x$ and $a$, we therefore define
\[
\text{GLD}^\alpha_{a+} f(x) = \lim_{h \to 0} \frac{\Delta^\alpha_{h,n} f(x)}{h^\alpha},
\]
where the limit is obtained by sending $n \to \infty$ and $h \to 0+$ keeping
\[
h = \frac{x - a}{n},
\]
so that $nh = x - a$ is constant.
Can show that if $m - 1 < \alpha < m$, then

$$GLD^{\alpha}_{a+} f(x) = \sum_{k=0}^{m-1} f^{(k)}(a) \frac{(x - a)^{k-\alpha}}{\Gamma(k + 1 - \alpha)}$$

$$+ \int_{a}^{x} \frac{(x - y)^{m-\alpha-1}}{\Gamma(m - \alpha)} f^{(m)}(y) \, dy,$$

which means that

$$GLD^{\alpha}_{a+} f(x) = CD^{\alpha}_{a+} f(x) + \sum_{k=0}^{m-1} f^{(k)}(a) \frac{(x - a)^{k-\alpha}}{\Gamma(k + 1 - \alpha)} = D^{\alpha}_{a+} f(x).$$

Furthermore,

$$GLD^{-\alpha}_{a+} f(x) = I^{\alpha}_{a+} f(x), \quad \alpha > 0.$$
Part II

Useful tools
Introduction

We will make extensive use of the Laplace transform (and some use of the Fourier transform), first to derive the fractional diffusion equation and then to study properties of the solution. Laplace transformation also plays a large role in some of the numerical methods we study, either as part of the method itself or for the error analysis.

This lecture also introduces some special functions that are arise in the study of fractional initial-boundary value problems.
Outline

Laplace transforms

Mittag–Leffler function

Wright functions
Laplace transforms

Notation:

\[ \hat{f}(z) = (\mathcal{L}f)(z) = \int_{0}^{\infty} e^{-zt} f(t) \, dt. \]

If \( f \) is locally integrable on \([0, \infty)\), and if

\[ |f(t)| \leq Ce^{\lambda t} \quad \text{for } t > 0, \]

then \( \hat{f}(z) \) exists and is analytic for \( \Re z > \lambda \), and we have the inversion formula

\[ f(t) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} e^{zt} \hat{f}(z) \, dz, \quad a > \lambda. \]
For $\alpha > 0$ and $z > 0$, the substitution $y = tz$ gives

\[
\hat{\Upsilon}_{\alpha}(z) = \frac{1}{\Gamma(\alpha)} \int_{0}^{\infty} e^{-zt} t^{\alpha-1} dt = \frac{1}{\Gamma(\alpha)} \int_{0}^{\infty} e^{-y \left(\frac{y}{z}\right)^{\alpha-1}} \frac{dy}{z} = \frac{z^{-\alpha}}{\Gamma(\alpha)} \int_{0}^{\infty} e^{-y} y^{\alpha-1} dy,
\]

that is,

\[
\hat{\Upsilon}_{\alpha}(z) = z^{-\alpha},
\]

consistent with

\[
z^{-\alpha-\beta} = \hat{\Upsilon}_{\alpha+\beta}(z) = \mathcal{L}(\Upsilon_\alpha \ast \Upsilon_\beta) = \hat{\Upsilon}_{\alpha}(z)\hat{\Upsilon}_{\beta}(z) = z^{-\alpha} z^{-\beta}.
\]
Laplace transform of an integral

Since

$$\mathcal{I}f(t) = \int_0^t f(s) \, ds = (\mathcal{Y}_1 \ast f)(t)$$

we have

$$\mathcal{L}\{\mathcal{I}f(t)\} = \hat{\mathcal{Y}}_1(z)\hat{f}(z) = z^{-1}\hat{f}(z).$$

In general, \( \mathcal{I}^n f = \mathcal{Y}_n \ast f \) so

$$\mathcal{L}\{\mathcal{I}^n f(t)\} = z^{-n}\hat{f}(z) \quad \text{for } n \in \{0, 1, 2, \ldots\}. $$
Laplace transform of a derivative

Integration by parts shows

\[ \mathcal{L}\{Df(t)\} = \int_0^\infty e^{-zt}Df(t) \, dt \]

\[ = \left[ e^{-zt}f(t) \right]_t=0^\infty - \int_0^\infty (-z)e^{-zt}f(t) \, dt \]

\[ = 0 - f(0) + z \int_0^\infty e^{-zt}f(t) \, dt, \]

so

\[ \mathcal{L}\{Df(t)\} = z\hat{f}(z) - f(0). \]

Easily verify by induction on \( n \) that

\[ \mathcal{L}\{D^n f(t)\} = z^n\hat{f}(z) - \sum_{k=0}^{n-1} z^{n-1-k}D^k f(0). \]
Laplace transform of a Caputo fractional derivative

If $n - 1 < \alpha < n$, then

$$\mathcal{C}D^\alpha f(t) = \mathcal{I}^{n-\alpha} g(t) \quad \text{where} \quad g(t) = D^n f(t),$$

so

$$\mathcal{L}\{\mathcal{C}D^\alpha f(t)\} = z^{-(n-\alpha)} \hat{g}(z)$$

$$= z^{\alpha-n} \left( z^n \hat{f}(z) - \sum_{k=0}^{n-1} z^{n-1-k} D^k f(0) \right)$$

and so

$$\mathcal{L}\{\mathcal{C}D^\alpha f(t)\} = z^{\alpha} \hat{f}(z) - \sum_{k=0}^{n-1} z^{\alpha-1-k} D^k f(0).$$
Laplace transform of a Riemann–Liouville fractional derivative

If $n - 1 < \alpha < n$, then

$$\mathcal{D}^\alpha f(t) = \mathcal{C}\mathcal{D}^\alpha f(t) + \sum_{k=0}^{n-1} \mathcal{D}^k f(0) \Gamma_{k+1-\alpha}(t),$$

and since $\hat{\Gamma}_{k+1-\alpha}(z) = z^{-(k+1-\alpha)}$ we have

$$\mathcal{L}\{\mathcal{D}^\alpha f(t)\} = \mathcal{L}\{\mathcal{C}\mathcal{D}^\alpha f(t)\} + \sum_{k=0}^{n-1} \mathcal{D}^k f(0) z^{\alpha-1-k},$$

that is,

$$\mathcal{L}\{\mathcal{D}^\alpha f(t)\} = z^\alpha \hat{f}(z).$$
Mittag–Leffler function

Problem: find $f(t)$ satisfying

$$\mathcal{D}^\alpha f(t) = f(t) \quad \text{for } t > 0, \quad \text{with } f(0) = 1.$$ 

If $\alpha = 1$ then $f(t) = e^t$.

If $0 < \alpha < 1$, then we claim

$$f(t) = \sum_{k=0}^{\infty} \frac{t^{k\alpha}}{\Gamma(1+k\alpha)}.$$ 

That is,

$$f(t) = E_\alpha(t^\alpha),$$

where the Mittag–Leffler function is

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1+k\alpha)}.$$
Proof

In fact, \( ^cD^\alpha \gamma_1 = 0 \) and for \( k \geq 1 \),

\[
^cD^\alpha \gamma_{1+k\alpha} = I^{1-\alpha}D\gamma_{1+k\alpha} = I^{1-\alpha}\gamma_{k\alpha} = \gamma_{1+(k-1)\alpha},
\]

so

\[
^cD^\alpha f = ^cD^\alpha (\gamma_1 + \gamma_{1+\alpha} + \gamma_{2+\alpha} + \gamma_{3+\alpha} + \cdots)
= 0 + \gamma_1 + \gamma_{1+\alpha} + \gamma_{2+\alpha} + \cdots = f.
\]

Also,

\[
\gamma_1(t) \equiv 1 \quad \text{and} \quad \gamma_{1+k\alpha}(0) = 0 \quad \text{for} \quad k \geq 1,
\]

so \( f(0) = 1 \).
Convergence?

We claim $E_\alpha(z)$ is an entire function of $z$. By the ratio test, it suffices to show that as $k \to \infty$,

$$
\left| \frac{z^{k+1}}{\Gamma(1 + (k + 1)\alpha)} \left/ \frac{z^k}{\Gamma(1 + k\alpha)} \right| = |z| \frac{\Gamma(1 + k\alpha)}{\Gamma(1 + k\alpha + \alpha)} \to 0.
$$

In fact, using Stirling’s approximation,

$$
\Gamma(x) = \sqrt{\frac{2\pi}{x}} \left( \frac{x}{e} \right)^x \left( 1 + O(x^{-1}) \right) \quad \text{as } x \to \infty,
$$

we find

$$
\frac{\Gamma(1 + k\alpha)}{\Gamma(1 + k\alpha + \alpha)} = \left( \frac{1}{1 + k\alpha + \alpha} \right)^\alpha \left( 1 + O(k^{-1}) \right).
$$
Mittag–Leffler function $E_\alpha(x)$ for $0 < \alpha \leq 1$
Mittag–Leffler function $E_\alpha(x)$ for $1 < \alpha \leq 2$
Special choices of $\alpha$

\[
E_0(x) = \sum_{k=0}^{\infty} z^k = \frac{1}{1 - z}.
\]

\[
E_{1/2}(x) = \exp(x^2) \text{erfc}(-x) = \frac{1}{\sqrt{2\pi}} \int_{-x}^{\infty} \exp(x^2 - t^2) \, dt.
\]

\[
E_1(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!} = \exp(x).
\]

\[
E_2(x) = \sum_{k=0}^{\infty} \frac{x^k}{(2k)!} = \cosh(\sqrt{x}), \quad x \geq 0.
\]

\[
E_2(-x) = \sum_{k=0}^{\infty} \frac{(-1)^k x^k}{(2k)!} = \cos(\sqrt{x}), \quad x \geq 0.
\]
Fractional relaxation equation

Problem: find \( u \) satisfying

\[
^C \mathcal{D}^\alpha u + \lambda u = 0 \quad \text{for } t > 0, \text{ with } u(0) = 1.
\]

We claim that the solution is

\[
u(t) = E_\alpha(-\lambda t^\alpha) = \sum_{k=0}^{\infty} \frac{(-\lambda)^k t^{k\alpha}}{\Gamma(1 + k\alpha)).
\]

In fact,

\[
^C \mathcal{D}^\alpha u(t) = \sum_{k=0}^{\infty} (-\lambda)^k \mathcal{C}_{1+k\alpha}(t)
\]

\[
= 0 + \sum_{k=1}^{\infty} (-\lambda)^k \mathcal{C}_{1+(k-1)\alpha}(t)
\]

\[
= -\lambda \sum_{k=1}^{\infty} (-\lambda)^{k-1} \mathcal{C}_{1+(k-1)\alpha}(t) = -\lambda u(t).
\]
Equivalent formulation

The function \( u(t) = E_{\alpha}(-\lambda t^\alpha) \) satisfies

\[
\mathcal{I}^{1-\alpha} D u(t) + \lambda u(t) = 0.
\]

To obtain an equation involving a Riemann–Liouville fractional derivative, apply \( D \mathcal{I}^\alpha \) and obtain

\[
D \mathcal{I}^{1} D u(t) + \lambda D \mathcal{I}^\alpha u(t) = 0.
\]

Therefore, since \( D \mathcal{I}^{1} f(t) = f(t) \),

\[
D u(t) + \lambda D^{1-\alpha} u(t) = 0.
\]

Taking Laplace transforms, \( z \hat{u}(z) - u(0) + \lambda z^{1-\alpha} \hat{u}(z) = 0 \), and thus \( (z + \lambda z^{1-\alpha}) \hat{u}(z) = 1 \), showing that

\[
\hat{u}(z) = \mathcal{L}\{E_{\alpha}(-\lambda t^\alpha)\} = \frac{1}{z + \lambda z^{1-\alpha}}.
\]
Fractional relaxation: \( u(t) = E_\alpha(-t^\alpha) \)
Integral representation

The reciprocal Gamma function has the representation

\[ \frac{1}{\Gamma(a)} = \frac{1}{2\pi i} \int_{-\infty}^{0^+} e^w w^{-a} \, dw, \]

where \( \int_{-\infty}^{0^+} \) means integration around a Hankel contour that encircles the negative real axis and has a counterclockwise orientation.

Theorem

*The Mittag–Leffler function admits the integral representation*

\[ E_\alpha(z) = \frac{1}{2\pi i} \int_{-\infty}^{0^+} \frac{e^w w^{\alpha-1}}{w^\alpha - z} \, dw \]

provided the Hankel contour encloses the disc \( |w| \leq |z|^{1/\alpha} \).
Proof

Since

\[
\frac{z^k}{\Gamma(1 + \alpha k)} = \frac{z^k}{2\pi i} \int_{-\infty}^{0^+} e^w w^{-1-\alpha k} \, dw,
\]

we see that

\[
E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{2\pi i} \int_{-\infty}^{0^+} e^w w^{-1-\alpha k} \, dw
\]

\[
= \frac{1}{2\pi i} \int_{-\infty}^{0^+} \frac{e^w}{w} \sum_{k=0}^{\infty} \left( \frac{z}{w^\alpha} \right)^k \, dw \quad \text{(if } |z| < |w|^{\alpha})
\]

\[
= \frac{1}{2\pi i} \int_{-\infty}^{0^+} \frac{e^w}{w} \cdot \frac{1}{1 - zw^{-\alpha}} \, dw
\]

\[
= \frac{1}{2\pi i} \int_{-\infty}^{0^+} \frac{e^w w^{\alpha-1}}{w^\alpha - z} \, dw. \quad \Box
\]
Another integral representation follows from the Laplace inversion formula,

\[ E_\alpha(-\lambda t^\alpha) = \frac{1}{2\pi i} \int_{0+}^{\infty} \frac{e^{zt} \, dz}{z + \lambda z^{1-\alpha}}, \quad t > 0. \]

By collapsing the Hankel contour onto the negative real axis, we find

\[ E_\alpha(-\lambda t^\alpha) = \frac{1}{\pi} \int_0^{\infty} \frac{e^{-rt} \lambda r^\alpha \sin \alpha \pi \, dr}{\left(r^\alpha + \lambda \cos \alpha \pi\right)^2 + \lambda^2 \sin^2 \alpha \pi}, \]

which shows that

\[ E_\alpha(-\lambda t^\alpha) > 0 \quad \text{and} \quad \frac{d}{dt} E_\alpha(-\lambda t^\alpha) < 0 \quad \text{for all} \quad t > 0. \]
Asymptotic behaviour

Since

\[ \frac{1}{z + z^{1-\alpha}} = \frac{z^{\alpha-1}}{1 + z^\alpha} = \frac{1}{z} \sum_{n=0}^{\infty} (-1)^n z^{(n+1)\alpha}, \quad |z| < 1, \]

we find that as \( t \to \infty \),

\[ E_\alpha(-t^\alpha) \sim \sum_{n=0}^{\infty} \frac{(-1)^n}{2\pi i} \int_{-\infty}^{0+} e^{zt} z^{(n+1)\alpha} \frac{dz}{z}, \]

and a substitution gives

\[ \frac{1}{2\pi i} \int_{-\infty}^{0+} e^{zt} z^{(n+1)\alpha} \frac{dz}{z} = \frac{t^{-(n+1)\alpha}}{2\pi i} \int_{-\infty}^{0+} e^{z} z^{(n+1)\alpha} \frac{dz}{z} \]

\[ = \frac{t^{-(n+1)\alpha}}{\Gamma(1 - (n + 1)\alpha)}. \]
Thus,

\[ E_\alpha(-t^\alpha) \sim \sum_{n=0}^{\infty} \frac{(-1)^n t^{-(n+1)\alpha}}{\Gamma(1 - (n + 1)\alpha)}, \]

that is,

\[ E_\alpha(-t^\alpha) \sim \sum_{n=1}^{\infty} \frac{(-1)^{n+1} t^{-n\alpha}}{\Gamma(1 - n\alpha)} = \frac{t^{-\alpha}}{\Gamma(1 - \alpha)} - \frac{t^{-2\alpha}}{\Gamma(1 - 2\alpha)} + \cdots. \]

The identity

\[ \frac{1}{\Gamma(1 - z)} = \frac{1}{\pi} \Gamma(z) \sin \pi z \]

yields an alternative form,

\[ E_\alpha(-t^\alpha) \sim \frac{1}{\pi} \sum_{n=1}^{\infty} (-1)^{n+1} t^{-n\alpha} \Gamma(n\alpha) \sin n\pi \alpha. \]

Notice what happens as \( \alpha \to 1 \).
Wright functions

The Wright function is defined by

$$W_{\lambda,\mu}(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!\Gamma(\lambda k + \mu)}, \quad \lambda > -1, \mu \in \mathbb{C}.$$ 

This series converges for all $z \in \mathbb{C}$ so $W_{\lambda,\mu}$ is an entire function.

Theorem

The Wright function has the integral representation

$$W_{\lambda,\mu}(z) = \frac{1}{2\pi i} \int_{-\infty}^{0+} \exp(w + zw^{-\lambda}) \frac{dw}{w^\mu}.$$
Proof

We once again use

$$\frac{1}{\Gamma(a)} = \frac{1}{2\pi i} \int_{-\infty}^{0^+} e^{w} w^{-a} \, dw,$$

and find

$$W_{\lambda,\mu}(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!} \frac{1}{2\pi i} \int_{-\infty}^{0^+} e^{w} w^{-\lambda k - \mu} \, dw$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{0^+} e^{w} w^{-\mu} \sum_{k=0}^{\infty} \frac{(zw^{-\lambda})^k}{k!} \, dw$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{0^+} \exp(w + zw^{-\lambda}) \frac{dw}{w^{\mu}}. \quad \square$$
Wright M-function

Our main concern is with the function

\[ M_\alpha(t) = \sum_{k=0}^{\infty} \frac{(-1)^k t^k}{k! \Gamma(1 - (k + 1)\alpha)}, \]

\(0 < \alpha < 1\), introduced by F. Mainardi in 1994. The identity

\[ \frac{1}{\Gamma(1 - z)} = \frac{1}{\pi} \Gamma(z) \sin \pi z \]

yields an alternative expression

\[ M_\alpha(t) = \frac{1}{\pi} \sum_{k=0}^{\infty} \frac{(-1)^k t^k}{k! \Gamma((k + 1)\alpha)} \sin \pi (k + 1)\alpha. \]

Two special cases: \((\text{Ai} = \text{Airy function})\)

\[ M_{1/2}(t) = \frac{\exp(-t^2/4)}{\sqrt{\pi}} \quad \text{and} \quad M_{1/3}(t) = 3^{2/3} \text{Ai}(t), \]
Wright M-function $M_\alpha(t)$
Integral representation and Laplace transform

Putting $\lambda = -\alpha$ and $\mu = 1 - \alpha$ in the integral representation of the Wright function, and replacing $t$ by $-t$, gives

$$M_\alpha(t) = \frac{1}{2\pi i} \int_{-\infty}^{0+} \exp(w - tw^\alpha) \frac{dw}{w^{1-\alpha}},$$

which allows us to prove the following result.

**Theorem**

*For $0 < \alpha < 1$, the Laplace transform of $M_\alpha$ is*

$$\hat{M}_\alpha(z) = E_\alpha(-z).$$
Proof

\[ \hat{M}_\alpha(z) = \int_0^\infty e^{-zt} M_\alpha(t) \, dt \]

\[ = \int_0^\infty e^{-zt} \frac{1}{2\pi i} \int_{-\infty}^{0+} \exp(w - tw^\alpha) \frac{dw}{w^{1-\alpha}} \, dt \]

\[ = \frac{1}{2\pi i} \int_{-\infty}^{0+} \frac{e^w}{w^{1-\alpha}} \int_0^\infty e^{-(z+w^\alpha)t} \, dt \, dw \]

\[ = \frac{1}{2\pi i} \int_{-\infty}^{0+} \frac{e^w}{w^{1-\alpha}} \frac{1}{z + w^\alpha} \, dw \]

\[ = \frac{1}{2\pi i} \int_{-\infty}^{0+} \frac{e^w w^{\alpha - 1}}{w^\alpha - (-z)} \, dw \]

\[ = E_\alpha(-z). \]
Fourier transform

Notation:

\[ \tilde{f}(\xi) = \mathcal{F}\{f(x)\} = \int_{-\infty}^{\infty} e^{-i\xi x} f(x) \, dx. \]

If \( f \in L_1(\mathbb{R}) \) then \( \tilde{f} \) is continuous on \( \mathbb{R} \) and \( \tilde{f}(\xi) \to 0 \) as \( |\xi| \to \infty \).

Plancherel theorem: Fourier transform extends uniquely to a bounded linear operator \( \mathcal{F} : L_2(\mathbb{R}) \to L_2(\mathbb{R}) \) satisfying

\[ \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathcal{F}f(\xi) \overline{\mathcal{F}g(\xi)} \, d\xi = \int_{-\infty}^{\infty} f(x) \overline{g(x)} \, dx. \]

Inversion formula:

\[ f(x) = \frac{1}{2\pi} \lim_{R \to \infty} \int_{-R}^{R} e^{i\xi x} \tilde{f}(\xi) \, d\xi, \quad -\infty < x < \infty. \]
Symmetric Wright M-function

We will require the Fourier transform of $M_\alpha(|x|)$.

**Lemma**

*For* $\kappa > -1$ *and* $0 < \alpha < 1$,*

$$\int_{0}^{\infty} t^\kappa M_\alpha(t) \, dt = \frac{\Gamma(\kappa + 1)}{\Gamma(\alpha\kappa + 1)}.$$

**Theorem**

*For* $0 < \alpha < 1$,*

$$\mathcal{F}\{M_\alpha(|x|)\} = 2E_{2\alpha}(-\xi^2).$$
Proof of the lemma

\[
\int_0^\infty t^\kappa M_\alpha(t) \, dt = \int_0^\infty t^\kappa \frac{1}{2\pi i} \int_{-\infty}^0 \exp(w - tw^\alpha) \frac{dw}{w^{1-\alpha}} \, dt
\]

\[
= \frac{1}{2\pi i} \int_{-\infty}^0 e^w \int_0^\infty t^\kappa e^{-tw^\alpha} \, dt \frac{dw}{w^{1-\alpha}}
\]

and

\[
\int_0^\infty t^\kappa e^{-tw^\alpha} \, dt = \Gamma(\kappa + 1) \int_0^\infty e^{-tw^\alpha} \Upsilon_{\kappa+1}(t) \, dt
\]

\[
= \Gamma(\kappa + 1) \hat{\Upsilon}_{\kappa+1}(w^\alpha) = \Gamma(\kappa + 1)(w^\alpha)^{-(\kappa+1)}
\]

so

\[
\int_0^\infty t^\kappa M_\alpha(t) \, dt = \frac{\Gamma(\kappa + 1)}{2\pi i} \int_{-\infty}^0 e^w w^{-(\alpha\kappa+1)} \, dw = \frac{\Gamma(\kappa + 1)}{\Gamma(\alpha\kappa + 1)}.
\]
Proof of the theorem

\[ \mathcal{F}\{M_\alpha(|x|)\} = \int_{-\infty}^{\infty} e^{-i\xi x} M_\alpha(|x|) \, dx \]
\[ = 2 \int_{0}^{\infty} M_\alpha(x) \cos \xi x \, dx \]
\[ = 2 \int_{0}^{\infty} M_\alpha(x) \sum_{k=0}^{\infty} (-1)^k \frac{(\xi x)^{2k}}{(2k)!} \, dx \]
\[ = 2 \sum_{k=0}^{\infty} (-1)^k \frac{\xi^{2k}}{(2k)!} \int_{0}^{\infty} x^{2k} M_\alpha(x) \, dx \]
\[ = 2 \sum_{k=0}^{\infty} (-1)^k \frac{\xi^{2k}}{(2k)!} \frac{\Gamma(2k + 1)}{\Gamma(2\alpha k + 1)} \]
\[ = 2 \sum_{k=0}^{\infty} \frac{(-\xi^2)^k}{\Gamma(1 + 2\alpha k)} = 2 E_{2\alpha}(-\xi^2). \]
Part III

Anomalous diffusion
The classical diffusion equation,

$$u_t - K \nabla^2 u = 0,$$

describes how the concentration $u$ of a substance evolves over time if, at the microscopic scale, its particles exhibit Brownian motion. The equation can also be derived from a purely macroscopic argument based on conservation of mass and Fick’s law, which states that the mass flux vector equals $-K \nabla u$.

In this lecture, we study continuous-time random walks, which provide a generalization of Brownian motion. When the waiting-time distribution obeys a power law, the particles experience trapping and their macroscopic behaviour is said to be subdiffusive. The mean-square displacement of such a particle is proportional to $t^\alpha$ for a characteristic exponent in the range $0 < \alpha < 1$. 


With the help of Fourier and Laplace transformation, we show that the macroscopic concentration obeys a time-fractional PDE,

\[ u_t - \partial_t^{1-\alpha} K_\alpha \nabla^2 u = 0, \]

where it is convenient to write \( \partial_t^{1-\alpha} = D_{0+}^{1-\alpha} \) for the Riemann–Liouville fractional derivative with respect to \( t \). The constant \( K_\alpha > 0 \) is a generalized diffusivity, and the classical diffusion equation then arises as the limiting special case when \( \alpha \to 1 \).
Outline

Continuous-time random walks

Rescaling

Subdiffusion
Continuous-time random walks

A walker moves along the $x$-axis, starting at position $x_0$ at time $t_0 = 0$. At time $t_1$ the walker jumps to $x_1$, then at time $t_2$ jumps to $x_2$, and so on. We assume that the increments

$$\Delta t_n = t_n - t_{n-1} \quad \text{and} \quad \Delta x_n = x_n - x_{n-1}$$

are independent, identically distributed random variables with probability density functions $\psi(t)$ and $\lambda(x)$, respectively. That is,

$$P(a < \Delta t_n < b) = \int_a^b \psi(t) \, dt \quad \text{for } 0 < a < b < \infty,$$

and

$$P(a < \Delta x_n < b) = \int_a^b \lambda(x) \, dx \quad \text{for } -\infty < a < b < \infty.$$

Aim: determine the probability that the particle lies in a given spatial interval at time $t$. 
An example

Suppose that the waiting-time distribution is exponential with parameter $\tau > 0$,

$$\psi(t) = \tau^{-1} e^{-t/\tau} \quad \text{for } 0 < t < \infty,$$

and that the jump-length distribution is normal with mean 0 and variance $\sigma^2$,

$$\lambda(x) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right) \quad \text{for } -\infty < x < \infty.$$

Thus,

$$E(\Delta t_n) = \tau, \quad E(\Delta t_n^2) = \tau^2, \quad E(\Delta x_n) = 0, \quad E(\Delta x_n^2) = \sigma^2.$$

The position $x(t)$ of the walker is a step function.
Typical path \((\tau = 1, \sigma = 1, x_0 = 2)\)
Random walk in 3D ($\sigma_x = \sigma_y = \sigma_z = 1$)
Convolutions and probability

We denote the Fourier convolution of $f$ and $g$ by

\[ f \ast g(z) = \int_{-\infty}^{\infty} f(z - y)g(y) \, dy, \quad \text{for } -\infty < z < \infty. \]

If $f(x) = 0$ for $x < 0$ and $g(y) = 0$ for $y < 0$ then this integral equals the Laplace convolution

\[ f \ast g(z) = \int_{0}^{z} f(z - y)g(y) \, dy \quad \text{for } z > 0. \]

Theorem

If $X$ and $Y$ are independent random variables with probability density functions $f$ and $g$, respectively, then the sum $Z = X + Y$ has probability density function $f \ast g$. 
Probability distribution of $t_n$

Let $\psi_n(t)$ denote the probability density function of the random variable

$$t_n = \Delta t_1 + \Delta t_2 + \cdots + \Delta t_n,$$

that is,

$$P(a < t_n < b) = \int_a^b \psi_n(t) \, dt \quad \text{for } 0 < a < b < \infty.$$

By the theorem quoted above,

$$\psi_n(t) = (\psi_{n-1} \ast \psi)(t) = \int_0^t \psi_{n-1}(s) \psi(t - s) \, ds,$$

so

$$\psi_n = \underbrace{\psi \ast \psi \ast \cdots \ast \psi}_{\text{n factors}} \quad \text{with} \quad \psi_0 = \delta.$$
Survival probability

Let $\Psi(t)$ denote the survival probability, that is, the probability of the walker not jumping within a time $t$, or equivalently, the probability of remaining stationary for at least a duration $t$. Then,

$$\Psi(t) = \int_t^\infty \psi(s) \, ds = 1 - \int_0^t \psi(s) \, ds \quad \text{for } 0 < t < \infty.$$ 

It follows that the probability of taking exactly $n$ steps up to time $t$ is

$$\chi_n(t) = \int_0^t \psi_n(s) \Psi(t - s) \, ds \quad \text{for } 0 < t < \infty.$$
Probability distribution of $x_n - x_0$

Let $\lambda_n(x)$ denote the probability density function of the random variable

$$x_n - x_0 = \Delta x_1 + \Delta x_2 + \cdots + \Delta x_n,$$

that is,

$$P(a < x_n - x_0 < b) = \int_a^b \lambda_n(x) \, dx \text{ for } -\infty < a < b < \infty.$$

Since

$$\lambda_n(x) = (\lambda_{n-1} \ast \lambda)(x) = \int_{-\infty}^{\infty} \lambda_{n-1}(y) \lambda(x - y) \, dy,$$

we have

$$\lambda_n = \underbrace{\lambda \ast \lambda \ast \cdots \ast \lambda}_{n \text{ factors}} \text{ with } \lambda_0 = \delta.$$
Characteristic functions

Terminology from probability theory: the characteristic function of \( \psi(t) \) is just its Laplace transform,

\[
\hat{\psi}(z) = \mathcal{L}\psi(z) = \int_0^\infty e^{-zt} \psi(t) \, dt,
\]

whereas the characteristic function of \( \lambda(x) \) is its Fourier transform,

\[
\tilde{\lambda}(\xi) = \mathcal{F}\lambda(\xi) = \int_{-\infty}^{\infty} e^{-i\xi x} \lambda(x) \, dx.
\]

Since \( \psi_n \) and \( \lambda_n \) are \( n \)-fold convolutions of \( \psi \) and \( \lambda \), respectively,

\[
\hat{\psi}_n(z) = \hat{\psi}(z)^n \quad \text{and} \quad \tilde{\lambda}_n(\xi) = \tilde{\lambda}(\xi)^n \quad \text{for} \quad n \geq 0.
\]

The characteristic function for the survival probability \( \Psi = 1 - \mathcal{I}^{1/2} \psi \) is

\[
\hat{\Psi}(z) = z^{-1} - z^{-1} \hat{\psi}(z) = \frac{1 - \hat{\psi}(z)}{z}
\].
Probability density

Let \( p(x, t) \) denote the probability density function for the position of the particle at time \( t \), that is,

\[
P(a < x(t) - x_0 < b) = \int_a^b p(x, t) \, dx.
\]

Since \( \chi_n(t) \) is the probability of taking \( n \) steps up to time \( t \),

\[
p(x, t) = \sum_{n=0}^{\infty} \lambda_n(x) \chi_n(t).
\]

Recalling that \( \chi_n = \psi_n \ast \Psi \),

\[
\hat{\chi}_n(z) = \hat{\psi}_n(z) \hat{\Psi}(z) = \hat{\psi}(z)^n \frac{1 - \hat{\psi}(z)}{z}.
\]
Characteristic function

Denote the Fourier–Laplace transform of $p$ by

$$\hat{p}(\xi, z) = \mathcal{LF}p(\xi, z) = \int_0^\infty e^{-zt} \int_{-\infty}^{\infty} e^{-i\xi x} p(x, t) \, dx \, dt.$$ 

Using the results derived above,

$$\hat{p}(\xi, z) = \sum_{n=0}^{\infty} \tilde{\lambda}_n(\xi) \hat{\chi}_n(z)$$

$$= \sum_{n=0}^{\infty} \tilde{\lambda}(\xi)^n \hat{\psi}(z)^n \frac{1 - \hat{\psi}(z)}{z}$$

$$= \frac{1 - \hat{\psi}(z)}{z} \sum_{n=0}^{\infty} \left[ \tilde{\lambda}(\xi) \hat{\psi}(z) \right]^n.$$
Geometric series

Since \( \lambda \) is a probability density function,

\[
\tilde{\lambda}(0) = \int_{-\infty}^{\infty} \lambda(x) \, dx = 1,
\]

and likewise

\[
\hat{\psi}(0) = \int_{0}^{\infty} \psi(t) \, dt = 1.
\]

But if \( \xi \neq 0 \) or \( z > 0 \), then \( |\tilde{\lambda}(\xi)\hat{\psi}(z)| < 1 \) so

\[
\sum_{n=0}^{\infty} [\tilde{\lambda}(\xi)\hat{\psi}(z)]^n = \frac{1}{1 - \tilde{\lambda}(\xi)\hat{\psi}(z)}
\]

and hence

\[
\hat{p}(\xi, z) = \frac{1 - \hat{\psi}(z)}{z} \frac{1}{1 - \tilde{\lambda}(\xi)\hat{\psi}(z)}.
\]
Earlier example

If
\[ \psi(t) = \tau^{-1}e^{-t/\tau} \quad \text{and} \quad \lambda(x) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right), \]

we find that
\[ \hat{\psi}(z) = \frac{1}{1 + \tau z} \quad \text{and} \quad \tilde{\lambda}(\xi) = e^{-\sigma^2\xi^2/2}, \]

so
\[ \frac{1 - \hat{\psi}(z)}{z} = \frac{\tau}{1 + \tau z}, \]
\[ 1 - \hat{\psi}(z)\tilde{\lambda}(\xi) = \frac{1 + \tau z - \exp(-\sigma^2\xi^2/2)}{1 + \tau z}, \]

and thus
\[ \hat{p}(\xi, z) = \frac{\tau}{1 + \tau z - \exp(-\sigma^2\xi^2/2)}. \]
Uncertain initial position

Instead of assuming $x(0) = x_0$ is known, we can treat $x_0$ as a random variable with probability density $p_0(x)$, so that

$$P(a < x_0 < b) = \int_a^b p_0(x) \, dx \quad \text{for } -\infty < a < b < \infty.$$  

Let $\lambda_n$ denote the probability density function for $x_n$ (rather than $x_n - x_0$, as before), so

$$P(a < x_n < b) = \int_a^b \lambda_n(x) \, dx \quad \text{for } -\infty < a < b < \infty.$$  

Since

$$x_n = x_0 + \Delta x_1 + \cdots + \Delta x_n,$$

we have

$$\lambda_n = p_0 \ast \lambda \ast \lambda \ast \cdots \ast \lambda.$$  

$n$ factors
In particular, $\lambda_0 = p_0$ (rather than $\delta$),

Using

$$[\tilde{\lambda}(\xi)]^n \tilde{p}_0(\xi)$$

in the preceding analysis leads to

$$\hat{p}(\xi, z) = \frac{1 - \hat{\psi}(z)}{z} \frac{\tilde{p}_0(\xi)}{1 - \tilde{\lambda}(\xi)\hat{\psi}(z)},$$

that is, the only change is to introduce a factor $\tilde{p}_0(\xi)$.

Formally, put $p_0(x) = \delta(x - x_0)$ to recover the case when $x_0$ is known with certainty.
Rescaling

Assume now that the probability density functions $\psi(t)$ and $\lambda(x)$ are normalized to satisfy

$$
\int_0^\infty t \psi(t) \, dt = 1, \quad \int_{-\infty}^\infty x \lambda(x) \, dx = 0, \quad \int_{-\infty}^\infty x^2 \lambda(x) \, dx = 1.
$$

Let $\tau > 0$ and $\sigma > 0$, and let the random variables $\Delta t_n$ and $\Delta x_n$ now have the rescaled probability density functions

$$
\psi_\tau(t) = \frac{1}{\tau} \psi\left(\frac{t}{\tau}\right) \quad \text{and} \quad \lambda_\sigma(x) = \frac{1}{\sigma} \lambda\left(\frac{x}{\sigma}\right),
$$

so that

$$
E(\Delta t_n) = \tau, \quad E(\Delta x_n) = 0, \quad E(\Delta x_n^2) = \sigma^2.
$$

We want to investigate what happens as $\tau$ and $\sigma$ tend to zero.
Typical path ($\sigma = 0.1$, $\tau = 0.005$)
Detailed view of inset
Moments

We saw earlier that $\hat{\psi}(0) = 1 = \tilde{\lambda}(0)$. Since

$$
\frac{d^k \hat{\psi}}{dz^k} = \int_0^\infty e^{-zt}(-t)^k \psi(t) \, dt
$$

we have

$$
\psi'(0) = - \int_0^\infty t \psi(t) \, dt = -1.
$$

Similarly,

$$
\frac{d^k \tilde{\lambda}}{d\xi^k} = \int_{-\infty}^\infty e^{-i\xi x}(-ix)^k \lambda(x) \, dx
$$

so

$$
\tilde{\lambda}'(0) = -i \int_{-\infty}^\infty x \lambda(x) \, dx = 0,
$$

$$
\tilde{\lambda}''(0) = - \int_{-\infty}^\infty x^2 \lambda(x) \, dx = -1.
$$
Characteristic functions

Since
\[ \hat{\psi}_\tau(z) = \hat{\psi}(\tau z) \quad \text{and} \quad \tilde{\lambda}_\sigma(\xi) = \tilde{\lambda}(\sigma \xi), \]
we have
\[ \hat{p}(\xi, z; \sigma, \tau) = \frac{1 - \hat{\psi}(\tau z)}{z} \frac{1}{1 - \hat{\psi}(\tau z) \tilde{\lambda}(\sigma \xi)}. \]

The Taylor expansion
\[ \hat{\psi}(z) = \hat{\psi}(0) + \hat{\psi}'(0) z + \cdots = 1 - z + O(z^2) \quad \text{as} \quad z \to 0, \]
implies that
\[ \frac{1 - \hat{\psi}(\tau z)}{z} = \frac{\tau z + O(\tau^2 z^2)}{z} = \tau (1 + O(\tau z)) \quad \text{as} \quad \tau \to 0. \]
Assume for simplicity that $\lambda(-x) = \lambda(x)$. Then $\tilde{\lambda}'''(0) = 0$ and

$$\tilde{\lambda}(\xi) = \tilde{\lambda}(0) + \tilde{\lambda}'(0)\xi + \frac{1}{2} \tilde{\lambda}''(0)\xi^2 + \cdots = 1 - \frac{1}{2}\xi^2 + O(\xi^4).$$

Thus,

$$\hat{\psi}(\tau z)\tilde{\lambda}(\sigma \xi) = [1 - \tau z + O(\tau^2 z^2)] [1 - \frac{1}{2}\sigma^2\xi^2 + O(\sigma^4\xi^4)]$$

$$= 1 - \tau z - \frac{1}{2}\sigma^2\xi^2 + O(\tau^2 z^2 + \sigma^4\xi^4)$$

and

$$1 - \hat{\psi}(\tau z)\tilde{\lambda}(\sigma \xi) = (\tau z + \frac{1}{2}\sigma^2\xi^2) [1 + O(\tau z + \sigma^2\xi^2)],$$

so

$$\hat{\rho}(\xi, z; \sigma, \tau) = \frac{\tau}{\tau z + \frac{1}{2}\sigma^2\xi^2} \times \frac{1 + O(\tau z)}{1 + O(\tau z + \sigma^2\xi^2)}.$$
Limiting probability density

Now send $\sigma \to 0$ and $\tau \to 0$ while keeping

$$\frac{\sigma^2}{2\tau} = K,$$

for a fixed $K > 0$, and obtain

$$\hat{p}(\xi, z) = \lim_{\tau \to 0} \frac{\tau}{\tau z + \frac{1}{2} \sigma^2 \xi^2} = \frac{1}{z + K \xi^2}.$$

Inverting the Laplace transform, we find

$$\tilde{p}(\xi, t) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} \frac{e^{zt} \, dz}{z + K \xi^2} = e^{-K \xi^2 t},$$

and then inverting the Fourier transform,

$$p(x, t) = \frac{1}{\sqrt{4\pi K t}} \exp\left(-\frac{x^2}{4Kt}\right).$$
Snapshots of $p(x, t)$
Partial differential equation for $p$

Notice that

$$
\mathcal{L}F(p_t - Kp_{xx}) = z\hat{p}(\xi, z) - \tilde{p}(\xi, 0) + K\xi^2\hat{p}(\xi, z) \\
= (z + K\xi^2)\hat{p}(\xi, z) - \tilde{p}(\xi, 0) \\
= 1 - \tilde{p}(\xi, 0) = 0,
$$

where the final step follows because $p(x, 0) = \delta(x)$ and so $\tilde{p}(\xi, 0) = 1$.

Therefore, $p(x, t)$, the probability density for $x(t) - x_0$, the position (relative to $x_0$) of the walker at time $t$, satisfies the partial differential equation

$$
p_t - Kp_{xx} = 0 \quad \text{for } 0 < t < \infty \text{ and } -\infty < x < \infty.
$$
Uncertain initial position

When $x_0$ is uncertain,

$$
\hat{p}(\xi, z; \sigma, \tau) = \frac{\tau \tilde{p}_0(\xi)}{\tau z + \frac{1}{2} \sigma^2 \xi^2} \times \frac{1 + O(\tau z)}{1 + O(\tau z + \sigma^2 \xi^2)},
$$

so in the scaling limit,

$$
\hat{p}(\xi, z) = \frac{\tilde{p}_0(\xi)}{z + K \xi^2}
$$

and thus

$$
\mathcal{L}\mathcal{F} \left( p_t - K p_{xx} \right) = z \hat{p}(\xi, z) - \tilde{p}(\xi, 0) + K \xi^2 \hat{p}(\xi, z) \\
= (z + K \xi^2) \hat{p}(\xi, z) - \tilde{p}(\xi, 0) \\
= \tilde{p}_0(\xi) - \tilde{p}(\xi, 0) = 0,
$$

since $p(x, 0) = p_0(x)$. 
Subdiffusion

Let $0 < \alpha < 1$, and suppose now that the waiting time probability density function is a power law:

$$\psi(t) \sim \frac{A}{t^{1+\alpha}} \text{ as } t \to \infty,$$

for some constant $A > 0$. It follows that

$$\int_0^\infty t\psi(t)\,dt = +\infty,$$

so the preceding analysis of the random walk breaks down. We make no change to our assumptions on $\lambda(x)$.

Example

$$\psi(t) = \frac{\alpha}{(1 + t)^{1+\alpha}} \quad \text{and} \quad \lambda(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right).$$
Power law ($\alpha = 0.75$) vs Exponential ($\tau = 1$) distributions
Typical path ($\alpha = 0.75, \sigma = 1$)
Behaviour of the characteristic function as $z \to 0$

Assume there exists $T > 0$ such that

$$|t^{1+\alpha}\psi(t) - A| \leq Ct^{-1} \quad \text{for } T \leq t < \infty,$$

and let $0 < z \leq T^{-1}$ (so $Tz \leq 1$). Since we know $\hat{\psi}(0) = 1$, consider

$$1 - \hat{\psi}(z) = \int_0^\infty (1 - e^{-zt})\psi(t) \, dt = l_1 + l_2 + l_3,$$

where

$$l_1 = \int_0^T (1 - e^{-zt})\psi(t) \, dt,$$

$$l_2 = \int_T^\infty (1 - e^{-zt})(\psi(t) - At^{-1-\alpha}) \, dt,$$

$$l_3 = \int_T^\infty (1 - e^{-zt})At^{-1-\alpha} \, dt.$$
Since
\[ 0 \leq 1 - e^{-y} \leq \min(1, y) \quad \text{for } 0 \leq y \leq 1, \]
we immediately see that
\[ 0 \leq l_1 \leq \int_0^T zt\psi(t)\,dt \leq zT \int_0^\infty \psi(t)\,dt = Tz. \]

Also, the substitution \( t = y/z \) gives
\[
|l_2| \leq \int_T^\infty (1 - e^{-zt})Ct^{-2-\alpha}\,dt \leq Cz^{1+\alpha} \int_{Tz}^\infty (1 - e^{-y})y^{-2-\alpha}\,dy
\leq Cz^{1+\alpha} \left( \int_{Tz}^1 y^{-1-\alpha}\,dy + \int_1^\infty y^{-2-\alpha}\,dy \right)
= Cz^{1+\alpha} \left( \frac{(Tz)^{-\alpha} - 1}{\alpha} + \frac{1}{1 + \alpha} \right) \leq C_{\alpha, Tz}.\]
The same substitution \( t = y/z \) yields

\[
l_3 = \int_T^\infty (1 - e^{-zt}) A t^{-1-\alpha} \, dt = A z^\alpha \int_T^{\infty} \frac{1 - e^{-y}}{y^{1+\alpha}} \, dy = B_\alpha z^\alpha + l_4,
\]

where

\[
B_\alpha = A \int_0^\infty \frac{1 - e^{-y}}{y^{1+\alpha}} \, dy \quad \text{and} \quad l_4 = -A z^\alpha \int_0^{Tz} \frac{1 - e^{-y}}{y^{1+\alpha}} \, dy.
\]

Since

\[
|l_4| \leq Az^\alpha \int_0^{Tz} y^{-\alpha} \, dy = \frac{AT^{-\alpha}z}{1 - \alpha},
\]

we have shown that

\[
|1 - \hat{\psi}(z) - B_\alpha z^\alpha| = |l_1 + l_2 + l_4| \leq C_{T,\alpha} z \quad \text{for } 0 < z \leq T^{-1}.
\]
Integrating by parts,
\[
\int_0^\infty \frac{1 - e^{-y}}{y^{1+\alpha}} \, dy = \int_0^\infty (1 - e^{-y}) \, d(-\alpha^{-1}y^{-\alpha}) \\
= \left[-\frac{1 - e^{-y}}{\alpha y^\alpha}\right]_0^\infty + \alpha^{-1} \int_0^\infty e^{-y}y^{-\alpha} \, dy \\
= \alpha^{-1} \Gamma(1 - \alpha) = -\Gamma(-\alpha),
\]
which completes the proof of the following result.

**Theorem**

If
\[
\psi(t) = At^{-1-\alpha} + O(t^{-2-\alpha}) \quad \text{as } t \to \infty,
\]
then, with \( B_\alpha = A\alpha^{-1} \Gamma(1 - \alpha) \),

\[
\hat{\psi}(z) = 1 - B_\alpha z^\alpha + O(z) \quad \text{as } z \to 0.
\]
Rescaling

As before, normalize $\lambda(x)$ so that

$$
\int_{-\infty}^{\infty} x \lambda(x) \, dx = 0 \quad \text{and} \quad \int_{-\infty}^{\infty} x^2 \lambda(x) \, dx = 1,
$$

but now suppose

$$
\psi(t) \sim \frac{A}{t^{1+\alpha}} \quad \text{as } t \to \infty.
$$

Define the rescaled probability density functions

$$
\psi_\tau(t) = \frac{1}{\tau} \psi\left(\frac{t}{\tau}\right) \quad \text{and} \quad \lambda_\sigma(x) = \frac{1}{\sigma} \lambda\left(\frac{x}{\sigma}\right),
$$

and notice $\psi_\tau$ is again a power law,

$$
\psi_\tau(t) \sim \frac{A_\tau^\alpha}{t^{1+\alpha}} \quad \text{as } t \to \infty.
$$
Characteristic functions

Hence,

\[ E(\Delta t_n) = +\infty, \quad E(\Delta x_n) = 0, \quad E(\Delta x_n^2) = \sigma^2. \]

As before,

\[
\hat{p}(\xi, z; \sigma, \tau) = \frac{1 - \hat{\psi}(\tau z)}{z} \cdot \frac{1}{1 - \hat{\psi}(\tau z)\tilde{\lambda}(\sigma \xi)},
\]

with

\[ \tilde{\lambda}(\xi) = 1 - \frac{1}{2} \xi^2 + O(\xi^4) \quad \text{as} \quad \xi \to 0, \]

but this time

\[ \hat{\psi}(z) = 1 - B_\alpha z^\alpha + O(z) \quad \text{as} \quad z \to 0, \]

where \( B_\alpha = A\alpha^{-1}\Gamma(1 - \alpha). \)
Thus,

\[
\frac{1 - \hat{\psi}(\tau z)}{z} = \frac{B_\alpha \tau^\alpha z^\alpha + O(\tau z)}{z} = B_\alpha \tau^\alpha z^{\alpha-1} [1 + O(\tau^{1-\alpha} z^{1-\alpha})].
\]

Likewise,

\[
\hat{\psi}(\tau z)\tilde{\lambda}(\sigma \xi) = \left[1 - B_\alpha \tau^\alpha z^\alpha + O(\tau z)\right] \left[1 - \frac{1}{2} \sigma^2 \xi^2 + O(\sigma^4 \xi^4)\right]
= 1 - B_\alpha \tau^\alpha z^\alpha - \frac{1}{2} \sigma^2 \xi^2 + O(\tau z + \tau^{2\alpha} z^{2\alpha} + \sigma^4 \xi^4)
\]

so

\[
1 - \hat{\psi}(\tau z)\tilde{\lambda}(\sigma \xi) = B_\alpha \tau^\alpha z^\alpha + \frac{1}{2} \sigma^2 \xi^2 + O(\tau z + \tau^{2\alpha} z^{2\alpha} + \sigma^4 \xi^4)
= \left[B_\alpha \tau^\alpha z^\alpha + \frac{1}{2} \sigma^2 \xi^2\right] \left[1 + O(\tau^{1-\alpha} z^{1-\alpha} + \tau^\alpha z^\alpha + \sigma^2 \xi^2)\right].
\]
Limiting probability density

Therefore,

\[
\hat{p}(\xi, z; \sigma, \tau) = \frac{B_\alpha \tau^\alpha z^{\alpha-1}}{B_\alpha \tau^\alpha z^\alpha + \frac{1}{2} \sigma^2 \xi^2} \frac{1 + O(\tau^{1-\alpha} z^{1-\alpha})}{1 + O(\tau^{1-\alpha} z^{1-\alpha} + \tau^\alpha z^\alpha + \sigma \xi)}. 
\]

Once again, send \( \sigma \to 0 \) and \( \tau \to 0 \), but now keep

\[
\frac{\sigma^2}{2B_\alpha \tau^\alpha} = K_\alpha,
\]

for a fixed \( K_\alpha > 0 \), and obtain

\[
\hat{p}(\xi, z) = \lim \frac{B_\alpha \tau^\alpha z^{\alpha-1}}{B_\alpha \tau^\alpha z^\alpha + \frac{1}{2} \sigma^2 \xi^2} = \frac{z^{\alpha-1}}{z^\alpha + K_\alpha \xi^2}.
\]

Notice that we recover the earlier formula by putting \( \alpha = 1 \).
Typical path \((\alpha = 0.75, \sigma = 0.1, \tau^\alpha = \sigma^2/2, N = 800)\)
Detailed view of inset
Recall that
\[ \mathcal{L}_{t \to z}\{E_\alpha(-\lambda t^\alpha)\} = \frac{1}{z + \lambda z^{1-\alpha}} \]
and
\[ \mathcal{F}_{x \to \xi}\{M_{\alpha/2}(|x/\mu|)\} = 2\mu E_\alpha(-\mu^2 \xi^2). \]

Since
\[ \hat{p}(\xi, z) = \frac{z^{\alpha-1}}{z^\alpha + K_\alpha \xi^2} = \frac{1}{z + \lambda z^{1-\alpha}} \quad \text{if } \lambda = K_\alpha \xi^2, \]
we see that
\[ \tilde{p}(\xi, t) = E_\alpha(-K_\alpha t^\alpha \xi^2) = E_\alpha(-\mu^2 \xi^2) \quad \text{if } \mu = \sqrt{K_\alpha t^\alpha}. \]

Thus,
\[ p(x, t) = \frac{1}{2\sqrt{K_\alpha t^\alpha}} \ M_{\alpha/2}\left(\frac{|x|}{\sqrt{K_\alpha t^\alpha}}\right). \]
Snapshots of $p(x, t)$ when $\alpha = 2/3$. 
Fractional partial differential equation for $p$

We have

\[ \mathcal{L} \mathcal{F} \{ p_t - K_\alpha D^{1-\alpha} p_{xx} \} = z \hat{p}(\xi, z) - \tilde{p}(\xi, 0) + K_\alpha z^{1-\alpha} \xi^2 \hat{p}(\xi, z) \]

\[ = (z + K_\alpha z^{1-\alpha} \xi^2) \hat{p}(\xi, z) - \tilde{p}(\xi, 0) = 0 \]

since

\[ \hat{p}(\xi, z) = \frac{z^{\alpha-1}}{z^\alpha + K_\alpha \xi^2} = \frac{1}{z + K_\alpha z^{1-\alpha} \xi^2} \quad \text{and} \quad \tilde{p}(\xi, 0) = \tilde{\delta}(\xi) = 1. \]

Thus, $p$ satisfies the time-fractional diffusion equation,

\[ p_t - K_\alpha D^{1-\alpha} p_{xx} = 0 \quad \text{for} \ 0 < t < \infty \ \text{and} \ -\infty < \xi < \infty. \]
Mean-square displacement

Let

\[ V(t) = E((x(t) - x_0)^2) = \int_{-\infty}^{\infty} x^2 p(x, t) \, dx \quad \text{for } t > 0. \]

Since

\[ \hat{V}(z) = \int_{-\infty}^{\infty} x^2 \hat{p}(x, z) \, dx = -\left. \frac{d^2}{d\xi^2} \hat{p}(\xi, z) \right|_{\xi=0} \]

\[ = -\left. \frac{d^2}{d\xi^2} \left( z + K_\alpha z^{1-\alpha} \xi^2 \right)^{-1} \right|_{\xi=0} = 2K_\alpha z^{-1-\alpha}, \]

it follows that \( V(t) = 2K_\alpha \gamma_{1+\alpha}(t), \) that is,

\[ E((x(t) - x_0)^2) = \frac{2K_\alpha t^\alpha}{\Gamma(1 + \alpha)} \propto t^\alpha. \]
Part IV

The time-fractional diffusion equation
We have shown that in 1D the probability density function for the location of a subdiffusive particle at time $t$ obeys a time-fractional PDE. The concentration $u = u(x, t)$ of a large number of such particles evolves in the same way. Moreover, the 1D analysis can be generalized to higher dimensions to yield the time-fractional diffusion equation

$$u_t - K_\alpha \partial_t^{1-\alpha} \nabla^2 u = 0.$$  

As in the classical case $\alpha = 1$, the solution $u$ in a bounded spatial domain (and subject to homogeneous boundary conditions) can be constructed by separation of variables to yield a series expansion involving the eigenfunctions of $-\nabla^2$. We use this representation of $u(x, t)$ to investigate its behaviour.
Outline

Initial-boundary value problem

Smoothing property of fractional diffusion

Positivity
Initial-boundary value problem

Let \( \Omega \) denote a bounded, Lipschitz domain in \( \mathbb{R}^2 \) or \( \mathbb{R}^3 \). We seek \( u = u(x, t) \) satisfying

\[
  u_t - K_\alpha \partial_t^{1-\alpha} \nabla^2 u = f(x, t) \quad \text{for } x \in \Omega \text{ and } t > 0,
\]

\[
  u = u_0(x) \quad \text{for } x \in \Omega, \text{ when } t = 0,
\]

and impose homogeneous boundary conditions, either Dirichlet

\[
  u = 0 \quad \text{for } x \in \partial \Omega \text{ and } t > 0,
\]

or else Neumann,

\[
  \frac{\partial u}{\partial n} = 0 \quad \text{for } x \in \partial \Omega \text{ and } t > 0,
\]

where \( n \) is the outward unit normal to \( \Omega \).
Abstract initial-value problem

Let $A$ be a linear operator with dense domain $D(A)$ in a Hilbert space $\mathcal{H}$ with inner product $\langle u, v \rangle$ and norm $\|u\| = \sqrt{\langle u, u \rangle}$. Given $u_0 \in \mathcal{H}$ and $f : [0, \infty) \to \mathcal{H}$ we seek $u : [0, \infty) \to \mathcal{H}$ satisfying

$$\dot{u} + \partial_t^{1-\alpha} Au = f(t) \quad \text{for } t > 0,$$

with $u(0) = u_0$, where $\dot{u} = u_t = \partial u / \partial t$.

Standard example:

$$\mathcal{H} = L_2(\Omega), \quad Au = -K_\alpha \nabla^2 u, \quad D(A) = H^2(\Omega) \cap H_0^1(\Omega).$$

Integrate to obtain an equivalent Volterra equation in $\mathcal{H}$,

$$u(t) + \int_0^t \gamma_\alpha(t - s) Au(s) \, ds = u_0 + \int_0^t f(s) \, ds, \quad t > 0.$$
Eigenfunction expansion

Assume that $A$ is self-adjoint and positive-semidefinite, with a complete orthonormal eigensystem, say

$$A \phi_m = \lambda_m \phi_m \quad \text{for} \ m = 0, 1, 2, \ldots,$$

with $\langle \phi_m, \phi_n \rangle = \delta_{mn}$. Number the eigenvalues so that

$$0 \leq \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \cdots.$$

(These assumptions hold for our standard example.) Thus,

$$u(t) = \sum_{m=0}^{\infty} u_m(t) \phi_m \quad \text{where} \ u_m(t) = \langle u(t), \phi_m \rangle.$$

Likewise, putting $f_m(t) = \langle f(t), \phi_m \rangle$ and $u_{0m} = \langle u_0, \phi_m \rangle$, we have

$$f(t) = \sum_{m=0}^{\infty} f_m(t) \phi_m \quad \text{and} \quad u_0 = \sum_{m=0}^{\infty} u_{0m} \phi_m.$$
Dirichlet boundary conditions in 1D

Take $\Omega = (0, L)$ and $A = -K_\alpha d^2/dx^2$ with homogeneous Dirichlet boundary conditions. Then,

$$\phi_m(x) = \sqrt{\frac{2}{L}} \sin \frac{m\pi}{L} x \quad \text{and} \quad \lambda_m = K_\alpha \left(\frac{m\pi}{L}\right)^2,$$

for $m \in \{1, 2, 3, \ldots\}$, so

$$v(x) = \sum_{m=1}^{\infty} v_m \phi_m(x)$$

is just the sine series expansion of $v$, where

$$v_m = \langle v, \phi_m \rangle = \sqrt{\frac{2}{L}} \int_0^L v(x) \sin \frac{m\pi}{L} x \, dx.$$
Neumann boundary conditions in 1D

Again take $\Omega = (0, L)$ and $A = -K_\alpha d^2/dx^2$, but now impose homogeneous Neumann boundary conditions. Then,

$$\phi_0(x) = \frac{1}{\sqrt{L}} \quad \text{and} \quad \lambda_0 = 0,$$

with

$$\phi_m(x) = \sqrt{\frac{2}{L}} \cos \frac{m\pi}{L} x \quad \text{and} \quad \lambda_m = K_\alpha \left( \frac{m\pi}{L} \right)^2 \quad \text{for} \ m \geq 1,$$

so

$$v(x) = \sum_{m=0}^{\infty} v_m \phi_m(x)$$

is just the cosine series expansion of $v$. 

Separation of variables

The function $u$ satisfies

$$\dot{u} + \partial_t^{1-\alpha} Au = f(t) \quad \text{for } t > 0, \text{ with } u(0) = u_0.$$  

iff the $m$th eigenmode satisfies

$$\dot{u}_m + \lambda_m \partial_t^{1-\alpha} u_m = f_m(t) \quad \text{for } t > 0, \text{ with } u_m(0) = u_{0m},$$

for $m = 0, 1, 2, \ldots$. Laplace transformation gives

$$z \hat{u}_m(z) - u_m(0) + \lambda_m z^{1-\alpha} \hat{u}_m(z) = \hat{f}_m(z)$$

so

$$\hat{u}_m(z) = \frac{u_{0m} + \hat{f}_m(z)}{z + \lambda_m z^{1-\alpha}}.$$
Duhamel formula and the mild solution

Recall that

\[ \mathcal{L}\{E_\alpha(-\lambda t^\alpha)\} = \frac{1}{z + \lambda z^{1-\alpha}}, \]

so

\[ u_m(t) = E_\alpha(-\lambda_m t^\alpha)u_0 + \int_0^t E_\alpha(-\lambda_m (t-s)^\alpha) f_m(s) \, ds. \]

Define the solution operator for the homogeneous problem,

\[ \mathcal{E}(t) v = \sum_{m=0}^{\infty} E_\alpha(-\lambda_m t^\alpha) \langle v, \phi_m \rangle \phi_m \quad \text{for } t > 0 \text{ and } v \in \mathbb{H}, \]

then the **mild solution** of the abstract initial-value problem is

\[ u(t) = \mathcal{E}(t)u_0 + \int_0^t \mathcal{E}(t-s)f(s) \, ds, \quad t > 0. \]

Caution: \( \mathcal{E}(t + s) \neq \mathcal{E}(t)\mathcal{E}(s) \) if \( 0 < \alpha < 1 \).
Stability in $\mathbb{H}$

Recall that $E_\alpha(-\lambda t^\alpha)$ is positive and decreasing for $t > 0$, and equals 1 at $t = 0$, so

$$0 < E_\alpha(-\lambda t^\alpha) \leq 1 \quad \text{for } 0 \leq t < \infty \text{ and any } \lambda \geq 0.$$ 

Thus, using Parseval’s identity,

$$\|\mathcal{E}(t)v\|^2 = \sum_{m=0}^{\infty} E_\alpha(-\lambda_m t^\alpha)^2 \langle v, \phi_m \rangle^2 \leq \sum_{m=0}^{\infty} \langle v, \phi_m \rangle^2 = \|v\|^2,$$

and therefore

$$\|\mathcal{E}(t)v\| \leq \|v\| \quad \text{for } t \geq 0 \text{ and } v \in \mathbb{H}.$$

Hence, the mild solution satisfies the stability estimate

$$\|u(t)\| \leq \|u_0\| + \int_0^t \|f(s)\| \, ds \quad \text{for } t \geq 0.$$
Smoothing property of fractional diffusion

For $0 \leq r < \infty$, define the norm

$$\|v\|_r^2 = \|(I + A)^{r/2}v\|^2 = \sum_{m=0}^{\infty} (1 + \lambda_m)^r \langle v, \phi_m \rangle^2$$

and the corresponding closed subspace

$$\mathbb{H}_r = \{ v \in \mathbb{H} : \|v\|_r < \infty \},$$

which is a Hilbert space with respect to the inner product that induces $\| \cdot \|_r$.

For our standard example $\mathbb{H} = L_2(\Omega)$ and $A = -K_\alpha \nabla^2$, write $\mathbb{H}_r = \mathbb{H}_r^D(\Omega)$ or $\mathbb{H}_r^N(\Omega)$ to indicate the choice of Dirichlet or Neumann boundary conditions.
Dirichlet boundary conditions and Sobolev spaces

Can prove the following via interpolation and elliptic regularity.

**Theorem**

*Suppose that* \( \partial \Omega \) *is* \( C^\infty \). *If* \( 0 \leq r < \frac{1}{2} \), *then* \( \mathbb{H}_D^r(\Omega) = H^r(\Omega) \), *however if* \( 2j - \frac{3}{2} < r < 2j + \frac{1}{2} \) *for* \( j \in \{1, 2, 3, \ldots\} \), *then*

\[
\mathbb{H}_D^r(\Omega) = \{ v \in H^r(\Omega) : v = Av = \cdots = A^{j-1}v = 0 \text{ on } \partial \Omega \}.
\]

*In the exceptional case* \( r = 2j - \frac{3}{2} \), *the condition* \( A^{j-1}v = 0 \text{ on } \partial \Omega \) *must be replaced by* \( A^{j-1}v \in \tilde{H}^{1/2}(\Omega) \).

*If* \( \Omega \) *is Lipschitz, then the conclusions still hold for* \( r \leq 1 \), *and in particular* \( \mathbb{H}_D^1 = H^1_0(\Omega) = \{ u \in H^1(\Omega) : u = 0 \text{ on } \partial \Omega \} \).

*If* \( \Omega \) *is convex or* \( C^{1,1} \), *then* \( r \leq 2 \) *is OK, and in particular* \( \mathbb{H}_D^2 = H^2(\Omega) \cap H^1_0(\Omega) = \{ u \in H^2(\Omega) : u = 0 \text{ on } \partial \Omega \} \).
Neumann boundary conditions and Sobolev spaces

Theorem
Suppose that $\partial \Omega$ is $C^\infty$. If $0 \leq r < \frac{3}{2}$, then $H^r_N(\Omega) = H^r(\Omega)$, however if $2j - \frac{1}{2} < r < 2j + \frac{3}{2}$ for $j \in \{1, 2, 3, \ldots\}$, then

$$H^r_N(\Omega) = \{ v \in H^r(\Omega) : \partial_n v = \partial_n Av = \cdots = \partial_n A^{j-1} v = 0 \text{ on } \partial \Omega \}.$$

In the exceptional case $r = 2j - \frac{1}{2}$, the condition $\partial_n A^{j-1} v = 0$ on $\partial \Omega$ must be replaced by $\partial_n A^{j-1} v \in \tilde{H}^{1/2}(\Omega)$.

If $\Omega$ is Lipschitz, then the conclusions still hold if $r \leq 1$, and in particular $H^1_N(\Omega) = H^1(\Omega)$.

If $\Omega$ is convex or $C^{1,1}$, then $r \leq 2$ is OK, and in particular $H^2_N(\Omega) = \{ u \in H^2(\Omega) : \partial_n u = 0 \text{ on } \partial \Omega \}$. 
A 1D example

Consider $v(x) = 1$ for $x \in \Omega = (0, L)$. Since

$$\int_0^L v(x) \sin \frac{m\pi}{L} x \, dx = L \frac{1 - (-1)^m}{m\pi}$$

and $(1 + \lambda_m)^r \sim (1 + m^2)^r$, we see that

$$\|v\|_r < \infty \iff \sum_{p=0}^{\infty} (1 + 2p)^{2r-2} < \infty,$$

so $v \in \mathbb{H}_D^r(\Omega)$ iff $2r - 2 < -1$, that is, $r < \frac{1}{2}$. However, $v \in \mathbb{H}_N^r(\Omega)$ for all $r \geq 0$ because

$$\int_0^L v(x) \cos \frac{m\pi}{L} x \, dx = 0 \quad \text{for all } m \geq 1.$$
Smoothing property of classical diffusion

If $\alpha = 1$ then $E_\alpha(-t^\alpha) = e^{-t}$ so

$$E(t) v = \sum_{m=0}^{\infty} e^{-\lambda_m t} \langle v, \phi_m \rangle \phi_m$$

and thus

$$\|E(t)v\|_{r+\mu}^2 = \sum_{m=0}^{\infty} (1 + \lambda_m)^{r+\mu} (e^{-\lambda_m t} \langle v, \phi_m \rangle)^2.$$  

If $0 < t \leq T$ and $\lambda \geq 0$, then

$$(1 + \lambda)^{\mu} (e^{-\lambda t})^2 \leq t^{-\mu} (T + \lambda t)^{\mu} e^{-2\lambda t} \leq C_{T,\mu} t^{-\mu}$$

and so

$$\|E(t)v\|_{r+\mu} \leq C_{T,\mu} t^{-\mu/2} \|v\|_r \quad \text{for } \mu \geq 0.$$
Weaker smoothing property for subdiffusion

The theorem below shows that if \( v \in \mathbb{H}^r \) then \( \mathcal{E}(t)v \in \mathbb{H}^{r+2} \) for each \( t > 0 \), but \( \|\mathcal{E}(t)v\|_{r+2} \) may blow up as \( t \to 0+ \).

**Lemma**

\( 0 < E_\alpha(-t^\alpha) \leq C \min(1, t^{-\alpha}) \) for \( 0 < t < \infty \).

**Proof.**

Follows because

\[
E_\alpha(-t^\alpha) = \begin{cases} 
1 + O(t^\alpha) & \text{as } t \to 0+, \\
\frac{t^{-\alpha}}{\Gamma(1 - \alpha)} + O(t^{2-\alpha}) & \text{as } t \to \infty.
\end{cases}
\]

**Theorem**

*Let \( 0 \leq \mu \leq 2 \) and \( 0 \leq r < \infty \). If \( v \in \mathbb{H}^r \), then*

\[
\|\mathcal{E}(t)v\|_{r+\mu} \leq C_T t^{-\alpha\mu/2} \|v\|_r \quad \text{for } 0 < t \leq T.
\]
Proof of theorem

Put $g(t) = E_\alpha(-t^\alpha)$. Since $g(\lambda^{1/\alpha} t) = E(-\lambda t^\alpha)$, we have

$$\|E(t)v\|^2_{r+\mu} = \sum_{m=0}^{\infty} (1 + \lambda_m)^{r+\mu} g(\lambda_m^{1/\alpha} t)^2 \langle v, \phi_m \rangle^2.$$  

The lemma implies that (assuming $0 \leq \mu \leq 2$)

$$0 < g(t) \leq C(1 + t^\alpha)^{-\mu/2} \quad \text{for } 0 < t < \infty,$$

so, for $0 < t \leq T$,

$$g(\lambda^{1/\alpha} t)^2 \leq C(1 + \lambda t^\alpha)^{-\mu} = C t^{-\mu \alpha} (t^{-\alpha} + \lambda)^{-\mu} \leq C_T t^{-\mu \alpha} (1 + \lambda)^{-\mu}$$

and thus

$$\|E(t)v\|^2_{r+\mu} \leq C_T \sum_{m=0}^{\infty} (1 + \lambda_m)^r \langle v, \phi_m \rangle^2 = C_T t^{-\alpha \mu} \|v\|^2_r.$$  \(\square\)
Regularity in time

Let \( q \in \{1, 2, 3, \ldots \} \). Similar arguments yield the following estimates.

**Lemma**

The function \( g(t) = E_\alpha(-t^\alpha) \) satisfies

\[
t^q |g^{(q)}(t)| \leq C_q \min(t^\alpha, t^{-\alpha}) \quad \text{for } 0 < t < \infty.
\]

**Theorem**

Let \(-2 \leq \mu \leq 2, 0 \leq r < \infty \) and \( q \in \{1, 2, 3, \ldots \} \). If \( v \in H^r \), then

\[
t^q \|E^{(q)}(t)v\|_{r+\mu} \leq C_{q,T} t^{-\alpha\mu/2} \|v\|_r \quad \text{for } 0 < t \leq T.
\]
Detailed behaviour as $t \to 0^+$

Since

$$E_\alpha(-\lambda t^\alpha) = \sum_{p=0}^{M-1} \frac{(-1)^p t^{\alpha p}}{\Gamma(1 + \alpha p)} \lambda^p + O(\lambda^M t^{\alpha M}) \quad \text{as } t \to 0^+,$$

and $\lambda^p_m \langle v, \phi_m \rangle = \langle A^p v, \phi_m \rangle$, we can show the following.

**Theorem**

Let $0 \leq r < \infty$ and $M \in \{1, 2, 3, \ldots\}$. If $v \in \mathbb{H}^{r+2M}$, then

$$\mathcal{E}(t)v = v + \sum_{p=1}^{M-1} \frac{(-1)^p t^{\alpha p}}{\Gamma(1 + \alpha p)} A^p v + R_M(t)A^M v,$$

where, given $0 \leq \mu \leq 2$, the remainder operator satisfies

$$\|R_M(t)v\|_{r+\mu} \leq C_M, T t^{M\alpha - \alpha\mu/2} \|v\|_r \quad \text{for } 0 < t \leq T.$$
Behaviour of an eigenmode

If the initial data is an eigenfunction of $A$, say $u_0 = \phi_m$, then the solution of the homogeneous problem is

$$u(t) = \mathcal{E}(t)\phi_m = E_\alpha(-\lambda_m t^\alpha)\phi_m,$$

so

$$u(x, t) = \left(1 - \frac{\lambda_m t^\alpha}{\Gamma(1 + \alpha)} + O(t^{2\alpha})\right)\phi_m(x) \quad \text{as } t \to 0^+.$$

This example makes clear the fact that the time derivative $\dot{u} = O(t^{\alpha - 1})$ is unbounded as $t \to 0^+$ no matter how regular the initial data (so long as it is not zero, but in that case $u \equiv 0$).

Contrast this behaviour with that of the classical diffusion equation ($\alpha = 1$): if $u_0 = \phi_m$ then $u(x, t) = e^{-\lambda_m t}\phi_m(x)$ is $C^\infty$ for $t \geq 0$. 

The inhomogeneous problem

The function $u(t) = \mathcal{E}(t)u_0$ solves the homogeneous problem

$$\dot{u} + \partial_t^{1-\alpha} Au = 0 \quad \text{for } t > 0, \text{ with } u(0) = u_0.$$

Now consider

$$u(t) = \mathcal{E} \ast f(t) = \int_0^t \mathcal{E}(t - s)f(s) \, ds,$$

which solves the inhomogeneous problem with vanishing initial data:

$$\dot{u} + \partial_t^{1-\alpha} Au = f(t) \quad \text{for } t > 0, \text{ with } u(0) = 0.$$

Theorem

For $0 \leq r < \infty$ and $q \in \{0, 1, 2, \ldots\}$, the function $u = \mathcal{E} \ast f$ satisfies

$$t^q \|u^{(q)}(t)\|_r \leq C_q \sum_{j=0}^q \int_0^t s^j \|f^{(j)}(s)\|_r \, ds \quad \text{for } 0 < t < \infty.$$
Positivity

If we write

$$u_+(t) = \begin{cases} 0, & t < 0, \\ u(t), & t \geq 0, \end{cases},$$

then the Laplace transform of $u$ is related to the Fourier transform of $u_+$ by

$$\hat{u}(iy) = \hat{u}_+(y) = \int_0^\infty e^{-iyt} u(t) \, dt.$$

Thus, the Parseval–Plancherel identity,

$$\int_{-\infty}^{\infty} f(t) g(t) \, dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(\xi) \tilde{g}(\xi) \, d\xi,$$

implies that

$$\int_{0}^{\infty} u(t) \overline{v(t)} \, dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{u}(iy) \overline{\hat{v}(iy)} \, dy.$$
We can now show that the operator $\partial_t^{1-\alpha}$ is positive semidefinite.

**Theorem**

If $0 < \beta < 1$ and if $u$ is real-valued, then

$$\int_0^\infty (\partial_t^\beta u) u \, dt = \frac{\cos \frac{1}{2} \pi \beta}{\pi} \int_0^\infty y^\beta |\hat{u}(iy)|^2 \, dy \geq 0.$$  

**Proof.**

Since $\mathcal{L}\{\partial_t^\beta u(t)\} = z^\beta \hat{u}(z)$,

$$\int_0^\infty (\partial_t^\beta u) u \, dt = \frac{1}{2\pi} \int_{-\infty}^\infty (iy)^\beta |\hat{u}(iy)|^2 \, dy.$$  

The result follows because $\overline{\hat{u}(iy)} = \hat{u}(-iy)$ and for $y > 0$,

$$(\pm iy)^\beta = (e^{\pm i\pi/2} y)^\beta = y^\beta (\cos \frac{1}{2} \pi \beta \pm i \sin \frac{1}{2} \pi \beta).$$
H-valued case

Lemma

For $0 < \alpha < 1$ and suitable $u : (0, \infty) \to \mathbb{H}$,

$$
\int_0^\infty \langle \partial_t^{1-\alpha} Au, u \rangle \, dt = \frac{\sin \frac{1}{2} \pi \alpha}{\pi} \int_0^\infty y^{1-\alpha} \|A^{1/2} \hat{u}(iy)\|^2 \, dy \geq 0.
$$

Proof.

$$
\int_0^\infty \langle \partial_t^{1-\alpha} Au, u \rangle \, dt = \int_0^\infty \sum_{m=0}^\infty \lambda_m \langle \partial_t^{1-\alpha} u_m, u_m \rangle \, dt
$$

$$
= \sum_{m=0}^\infty \lambda_m \frac{\cos \frac{1}{2} \pi (1 - \alpha)}{\pi} \int_0^\infty y^{1-\alpha} |\hat{u}_m(iy)|^2 \, dy.
$$
Digression: fractional derivative at a jump discontinuity

Suppose that

\[ v(t) = \begin{cases} 
  v_1(t), & 0 \leq t < a, \\
  v_2(t), & t > a,
\end{cases} \]

where \( v_1 : [0, a] \to \mathbb{R} \) and \( v_2 : [a, \infty) \to \mathbb{R} \) are \( C^1 \) functions. If \( 0 < t < a \), then differentiating the formula

\[ \mathcal{I}^\alpha v(t) = \mathcal{G}_\alpha * v(t) = \int_0^t \mathcal{G}_\alpha(s)v(t - s) \, ds \]

gives

\[ \partial_t^{1-\alpha} v(t) = \mathcal{D}\mathcal{I}^\alpha v_1(t) = v_1(0)\mathcal{G}_\alpha(t) + \int_0^t \mathcal{G}_\alpha(s)v_1'(t - s) \, ds \]

\[ = v(0^+)\mathcal{G}_\alpha(t) + \int_0^t \mathcal{G}_\alpha(t - s)v'(s) \, ds. \]
However, if \( t > a \) then

\[
I^\alpha v(t) = \int_0^a \gamma_\alpha(t - s)v_1(s) \, ds + \int_a^t \gamma_\alpha(t - s)v_2(s) \, ds
\]

\[
= \int_{t-a}^t \gamma_\alpha(s)v_1(t - s) \, ds + \int_0^{t-a} \gamma_\alpha(s)v_2(t - s) \, ds
\]

so

\[
\partial^{1-\alpha} v(t) = v_1(0)\gamma_\alpha(t) - v_1(a)\gamma_\alpha(t - a) + v_2(a)\gamma_\alpha(t - a)
\]

\[
+ \int_{t-a}^t \gamma_\alpha(s)v'_1(t - s) \, ds + \int_0^{t-a} \gamma_\alpha(s)v'_2(t - s) \, ds
\]

and therefore, with \([v]_a = v_2(a) - v_1(a) = v(a^+) - v(a^-)\),

\[
\partial^{1-\alpha} v(t) = v(0^+)\gamma_\alpha(t) + [v]_a\gamma_\alpha(t - a)
\]

\[
+ \int_a^a \gamma_\alpha(t - s)v'(s) \, ds + \int_a^t \gamma_\alpha(t - s)v'(s) \, ds.
\]
Example
Stability via an energy argument

Consider the homogeneous equation,

\[
\dot{u}(t) + \partial_t^{1-\alpha} Au(t) = 0.
\]

Take the inner product with \( u(t) \) and integrate to obtain

\[
\int_0^T \langle \dot{u}, u \rangle \, dt + \int_0^T \langle \partial_t^{1-\alpha} Au, u \rangle \, dt = 0.
\]

Letting

\[
u_*(t) = \begin{cases} u(t), & 0 < t < T, \\ 0, & t > T, \end{cases}
\]

we have

\[
\int_0^T \langle \partial_t^{1-\alpha} Au, u \rangle \, dt = \int_0^\infty \langle \partial_t^{1-\alpha} Au_*, u_* \rangle \, dt \geq 0.
\]
Thus,
\[ \int_0^T \langle \dot{u}, u \rangle \, dt \leq 0. \]

But
\[ \int_0^T \langle \dot{u}, u \rangle \, dt = \left[ \frac{1}{2} \langle u, u \rangle \right]_{t=0}^T = \frac{1}{2} \| u(T) \|^2 - \frac{1}{2} \| u(0) \|^2, \]
so \( \| u(T) \| \leq \| u(0) \| \), which again shows that
\[ \| \mathcal{E}(t)u_0 \| \leq \| u_0 \| \quad \text{for } t > 0. \]
Part V

Simple finite difference schemes
Introduction

We begin our study of numerical methods for fractional diffusion problems by considering simple explicit and implicit finite difference (and quadrature) schemes in the 1D case:

\[ u_t - K_\alpha \partial_t^{1-\alpha} u_{xx} = f(x, t). \]

These schemes generalize the forward and backward Euler methods for the heat equation. As in the classical setting, the explicit scheme is stable only if the time step is sufficiently small, but the implicit scheme is unconditionally stable.

Unlike the classical Euler methods, the grid stencils extend back through all preceding time levels resulting in a dramatically higher computational cost.
Outline

Explicit Euler method for a fractional ODE

Explicit Euler method for a fractional PDE

Implicit Euler method
Consider first the scalar problem \( A = \lambda > 0 \)

\[ \dot{u} + \lambda \partial_t^{1-\alpha} u = f(t) \quad \text{for } 0 < t < T, \text{ with } u(0) = u_0, \]

where \( \lambda > 0 \). Put \( \Delta t = T/N \) and define grid points

\[ t_n = n\Delta t \quad \text{for } 0 \leq n \leq N. \]

We want to compute

\[ U^n \approx u(t_n). \]
Time-stepping

Integrating the ODE gives

\[ u(t_{n+1}) - u(t_n) + \lambda \int_{t_n}^{t_{n+1}} \partial_t^{1-\alpha} u(t) \, dt = \int_{t_n}^{t_{n+1}} f(t) \, dt, \]

which suggests the time-stepping scheme

\[ U^{n+1} - U^n + \lambda \int_{t_n}^{t_{n+1}} \partial_t^{1-\alpha} U(t) \, dt = f^n \Delta t, \]

where \( f^n = f(t_n) \) and \( U \) is the piecewise-constant function

\[ U(t) = U^n \quad \text{for} \ t_n \leq t < t_{n+1}. \]
Approximation of the fractional derivative

Recalling $\partial_t^{1-\alpha} v = (\mathcal{V}_\alpha \ast v)_t$, we have

$$
\int_{t_n}^{t_{n+1}} \partial_t^{1-\alpha} U(t) \, dt = (\mathcal{V}_\alpha \ast U)(t_{n+1}) - (\mathcal{V}_\alpha \ast U)(t_n)
$$

$$
= \int_{t_n}^{t_{n+1}} \mathcal{V}_\alpha(t_{n+1} - t) U^n \, dt
$$

$$
+ \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} \left[ \mathcal{V}_\alpha(t_{n+1} - t) - \mathcal{V}_\alpha(t_n - t) \right] U^j \, dt
$$

$$
= \Delta t^\alpha \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha + 1)} \sum_{j=0}^{n} w_{n-j} U^j.
$$
Weights

Here,

\[ \int_{t_n}^{t_{n+1}} \Gamma_\alpha(t_{n+1} - t) \, dt = \Gamma_\alpha+1(\Delta t) = \frac{\Delta t^\alpha}{\Gamma(\alpha + 1)} \]

so \( w_0 = 1 \), and for \( 0 \leq j \leq n - 1 \),

\[ \frac{\Delta t^\alpha}{\Gamma(\alpha + 1)} w_{n-j} = \int_{t_j}^{t_{j+1}} \left[ \Gamma_\alpha(t_{n+1} - t) - \Gamma_\alpha(t_n - t) \right] U^j \, dt. \]

Find that

\[ w_j = (j + 1)^\alpha - 2j^\alpha + (j - 1)^\alpha \text{ for } j \geq 1. \]

Note that \( w_j < 0 \) for \( j \geq 1 \), with \( w_j \approx \alpha(\alpha - 1)j^{\alpha-2} \) for large \( j \).
Weights when $\alpha = 1/2$
Implementation

In this way, we arrive at

\[ U^{n+1} - U^n + \frac{\lambda \Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=0}^{n} w_{n-j} U^j = f^n \Delta t. \]

Thus, starting from \( U^0 = u_0 \) we compute

\[ U^{n+1} = U^n + f^n \Delta t - \frac{\lambda \Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=0}^{n} w_{n-j} U^j \]

for \( n = 0, 1, 2, \ldots, N \).
Classical Euler method

In the limiting case $\alpha = 1$ we have $w_j = 0$ for $j \geq 1$ so

$$\frac{\lambda \Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=0}^{n} w_{n-j} U^j = \lambda \Delta t U^n$$

and therefore

$$U^{n+1} - U^n + \lambda \Delta t U^n = f^n \Delta t,$$

or equivalently,

$$\frac{U^{n+1} - U^n}{\Delta t} + \lambda U^n = f^n.$$
Conditional stability

Since $w_0 = 1$ we have

$$U^{n+1} = \left(1 - \frac{\lambda \Delta t^\alpha}{\Gamma(\alpha + 1)}\right)U^n + f^n \Delta t - \frac{\lambda \Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=0}^{n-1} w_{n-j} U^j,$$

and we can prove the following discrete analogue of the stability estimate for the continuous problem:

$$|u(t)| \leq |u_0| + \int_0^t |f(s)| \, ds \quad \text{for } t > 0.$$

Theorem

If

$$\frac{\lambda \Delta t^\alpha}{\Gamma(\alpha + 1)} \leq 1$$

then

$$|U^n| \leq |U^0| + \sum_{j=0}^{n-1} |f^n| \Delta t \quad \text{for } 1 \leq n \leq N.$$
Proof

Put $\rho = \lambda \Delta t^\alpha / \Gamma(\alpha + 1) \leq 1$, then

$$|U^{n+1}| \leq (1 - \rho)|U^n| + |f^n| \Delta t + \rho \sum_{j=0}^{n-1} \left| w_{n-j} \right||U^j|$$

and we find

$$\sum_{j=0}^{n-1} \left| w_{n-j} \right| = - \sum_{j=1}^{n} w_j = 1 + n^\alpha - (n + 1)^\alpha \leq 1,$$

so

$$|U^{n+1}| \leq (1 - \rho)|U^n| + |f^n| \Delta t + \rho \max_{0 \leq j \leq n-1} |U^j|$$

$$\leq |f^n| \Delta t + \max_{1 \leq j \leq n} |U^j|.$$
Example: $\alpha = 1/2, \lambda = 1, f \equiv 0, N = 25, \rho = 0.3192$
Example: $\alpha = 1/2$, $\lambda = 4$, $f \equiv 0$, $N = 25$, $\rho = 1.2766$
Explicit Euler method for a PDE

Consider $\Omega = (0, L)$ in 1D with boundary $\partial \Omega = \{0, L\}$. We seek $u = u(x, t)$ satisfying

$$u_t - K_\alpha \partial^{1-\alpha}_t u_{xx} = f(x, t) \quad \text{for } x \in \Omega \text{ and } 0 < t < T,$$

$$u = u_0(x) \quad \text{for } x \in \Omega, \text{ when } t = 0,$$

$$u = 0 \quad \text{for } x \in \partial \Omega \text{ and } 0 < t < T.$$

Put $\Delta x = L/P$ and $\Delta t = T/N$, and define grid points

$$(x_p, t_n) = (p \Delta x, n \Delta t) \quad \text{for } 0 \leq p \leq P \text{ and } 0 \leq n \leq N.$$

We want to compute

$$U^n_p \approx u(x_p, t_n).$$
Second central difference in space

Using the approximation

\[ u_{xx}(x_p, t_n) \approx \frac{U_{p+1}^n - 2U_p^n + U_{p-1}^n}{\Delta x^2} \]

and letting \( f_p^n = f(x_p, t_n) \), we discretize in time as before and arrive at the scheme

\[ U_{p+1}^n - U_p^n - \frac{K_\alpha \Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=0}^{n} w_{n-j} \frac{U_{p+1}^j - 2U_p^j + U_{p-1}^j}{\Delta x^2} = f_p^n \Delta t \]

for \( 0 \leq n \leq N - 1 \) and \( 1 \leq p \leq P - 1 \), with the initial conditions

\[ U_0^0 = u_0(x_p) \quad \text{for} \quad 0 \leq p \leq P, \]

and boundary conditions

\[ U_0^n = 0 = U_P^n \quad \text{for} \quad 1 \leq n \leq N. \]
Stencil
Matrix–vector formulation

Let

\[ U^n = \begin{bmatrix} U^n_1 \\
U^n_2 \\
\vdots \\
U^n_{P-2} \\
U^n_{P-1} \end{bmatrix} \quad \text{and} \quad A = \frac{K_\alpha}{\Delta x^2} \begin{bmatrix} 2 & -1 \\
-1 & 2 & -1 \\
\vdots & \vdots & \vdots \\
-1 & 2 & -1 \\
-1 & 2 \end{bmatrix} \]

so that

\[ U^{n+1} - U^n + \frac{\Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=0}^{n} w_{n-j} AU^j = \Delta t f^n \]

and hence

\[ U^{n+1} = U^n + \Delta t f^n - \frac{\Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=0}^{n} w_{n-j} AU^j. \]
Eigenvectors

Recall that

$$\phi_m(x) = \sin \frac{m\pi}{L} x \quad \text{and} \quad \lambda_m = K_\alpha \left( \frac{m\pi}{L} \right)^2$$

satisfy

$$-K_\alpha \frac{d^2}{dx^2} \phi_m = \lambda_m \phi_m \quad \text{for} \ x \in \Omega = (0, L),$$

with $$\phi_m(0) = 0 = \phi_m(L)$$. Putting

$$\Phi_m = \begin{bmatrix} \phi_m(x_1) \\ \phi_m(x_2) \\ \vdots \\ \phi_m(x_{P-1}) \end{bmatrix} \quad \text{and} \quad \Lambda_m = \frac{K_\alpha}{\Delta x^2} \left( 2 \sin \frac{m\pi}{2L} \Delta x \right)^2,$$

we find that

$$A \Phi_m = \Lambda_m \Phi_m.$$
Discrete $L_2$-inner product and -norm

For $U, V \in \mathbb{R}^{P-1}$ define

$$\langle U, V \rangle = \sum_{p=1}^{P-1} U_p V_p \Delta x$$

and

$$\| U \| = \sqrt{\langle U, U \rangle}.$$ 

We find that $\Phi_1, \Phi_2, \ldots, \Phi_{P-1}$ form an orthogonal basis for $\mathbb{R}^{P-1}$,

$$\langle \Phi_m, \Phi_{m'} \rangle = 0 \text{ if } m \neq m' \text{ and } m, m' \in \{1, 2, \ldots, P - 1\},$$

and, with $\theta = m\pi/P$,

$$\| \Phi_m \|^2 = \sum_{p=1}^{P-1} \left( \sin \frac{m\pi}{L} x_p \right)^2 \Delta x = \frac{L}{P} \sum_{p=1}^{P} \sin^2 p\theta$$

$$= \frac{L}{P} \left( \frac{P}{2} - \frac{\cos(P + 1)\theta \sin P\theta}{2 \sin \theta} \right) = \frac{L}{2}.$$
Stability of the discrete Fourier modes

Define the discrete Fourier coefficients

\[ \tilde{U}_m^n = \frac{\langle U^n, \Phi_m \rangle}{\| \Phi_m \|^2}, \quad 1 \leq m \leq P - 1, \]

so that

\[ U^n = \sum_{m=1}^{P-1} \tilde{U}_m^n \Phi_m. \]

For \( 1 \leq m \leq P - 1 \),

\[ \tilde{U}_m^{n+1} - \tilde{U}_m^n + \frac{\Lambda_m \Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=0}^{n-1} w_{n-j} \tilde{U}_m^j = \tilde{f}_m^n \Delta t, \]

with \( \tilde{U}_m^0 = \tilde{u}_{0m} \), so our earlier analysis gives

\[ |\tilde{U}_m^n| \leq |\tilde{U}_m^0| + \sum_{j=0}^{n-1} |\tilde{f}_m^j| \Delta t \quad \text{provided} \quad \frac{\Lambda_m \Delta t^\alpha}{\Gamma(\alpha + 1)} \leq 1. \]
Stability of the full solution

Since

\[ \| \mathbf{U} \|^2 = \sum_{m=1}^{P-1} |\tilde{U}_m|^2 \| \Phi_m \|^2 = \frac{L}{2} \sum_{m=1}^{P-1} |\tilde{U}_m|^2, \]

and \( \Lambda_m \leq 4K_\alpha/\Delta x^2 \), we can show the following.

**Theorem**

If

\[ \rho \equiv \frac{4K_\alpha \Delta t^\alpha}{\Gamma(\alpha + 1) \Delta x^2} \leq 1 \]

then

\[ \| \mathbf{U}^n \|^2 \leq 2 \| \mathbf{U}^0 \|^2 + 2t_n \sum_{j=0}^{n-1} \| f^j \|^2 \Delta t \quad \text{for } 1 \leq n \leq N. \]
Problem if $\alpha$ is small

The stability restriction $\rho \leq 1$ means that the time step must be chosen so that

$$
\Delta t^\alpha \leq \frac{\Gamma(\alpha + 1)}{4K_\alpha} \Delta x^2.
$$

This is a severe restriction if $\alpha$ is small.

Example

Suppose $\alpha = 1/5$, $K_\alpha = \Gamma(\alpha + 1)$ and $\Delta x = 2 \times 10^{-3}$, then we require

$$
\Delta t \leq (\Delta x/2)^{10} = 10^{-30}.
$$

Therefore natural to consider implicit methods.
Implicit Euler method

Again start with the ODE

\[ \dot{u} + \lambda \partial_t^{1-\alpha} u = f(t) \quad \text{for } 0 < t < T, \text{ with } u(0) = u_0, \]

but now integrate over \((t_{n-1}, t_n)\) to obtain

\[ u(t_n) - u(t_{n-1}) + \lambda \int_{t_{n-1}}^{t_n} \partial_t^{1-\alpha} u(t) \, dt = \int_{t_{n-1}}^{t_n} f(t) \, dt, \]

and compute \( U^n \approx u(t_n) \) via

\[ U^n - U^{n-1} + \lambda \int_{t_{n-1}}^{t_n} \partial_t^{1-\alpha} U(t) \, dt = f^n \Delta t, \]

where

\[ U(t) = U^n \quad \text{for } t_{n-1} < t \leq t_n. \]
Weights

We find that

\[
\int_{t_{n-1}}^{t_n} \partial_t^{1-\alpha} U(t) \, dt = (\Gamma_\alpha \ast U)(t_n) - (\Gamma_\alpha \ast U)(t_{n-1})
\]

\[
= \int_{t_{n-1}}^{t_n} \Gamma_\alpha(t_n - t) U^n \, dt
\]

\[
+ \sum_{j=1}^{n-1} \int_{t_{j-1}}^{t_j} \left[ \Gamma_\alpha(t_n - t) - \Gamma_\alpha(t_{n-1} - t) \right] U^j \, dt
\]

\[
= \frac{\Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=1}^{n} \omega_{n-j} U^j,
\]

where, as before \( \omega_0 = 1 \) and

\[
\omega_j = (j + 1)^\alpha - 2j^\alpha + (j - 1)^\alpha \quad \text{for} \ j \geq 1.
\]
Unconditional stability

In this way,

\[ U^n - U^{n-1} + \rho \sum_{j=1}^{n} w_{n-j} U^j = f^j \Delta t, \quad \rho = \frac{\lambda \Delta t^\alpha}{\Gamma(\alpha + 1)}. \]

Thus, starting from \( U^0 = u_0 \), we compute \( U^n \) for \( n = 1, 2, \ldots, N \) by solving

\[ (1 + \rho) U^n = U^{n-1} + f^n \Delta t - \rho \sum_{j=1}^{n-1} w_{n-j} U^j. \]

Theorem

\[ |U^n| \leq |U^0| + \sum_{j=1}^{n} |f^j| \Delta t \quad \text{for} \quad 1 \leq n \leq N. \]
Proof

We have
\[\sum_{j=1}^{n-1} |w_{n-j}| = \sum_{j=1}^{n-1} |w_j| = -\sum_{j=1}^{n-1} w_j = 1 + (n - 1)^\alpha - n^\alpha \leq 1\]

so
\[(1 + \rho)|U^n| \leq |U^{n-1}| + |f^n| \Delta t + \rho \max_{1 \leq j \leq n-1} |U^j|\]

and therefore
\[|U^n| \leq |f^n| \Delta t + \frac{|U^{n-1}|}{1 + \rho} + \frac{\rho}{1 + \rho} \max_{1 \leq j \leq n-1} |U^j|\]
\[\leq |f^n| \Delta t + \max_{1 \leq j \leq n-1} |U^j|.

The desired estimate follows using induction on $n$. \qed
Example: $\alpha = 1/2, \, \lambda = 1, \, f \equiv 0, \, N = 25$
Convergence behaviour
Put

\[ E_1(N) = \max_{1 \leq n \leq N} |U^n - u(t_n)|, \]

\[ E_2(N) = \max_{0.5 \leq t_n \leq T} |U^n - u(t_n)|. \]

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<tr>
<td>5120</td>
<td>4.998e-04</td>
<td>6.602e-05</td>
</tr>
<tr>
<td>10240</td>
<td>2.688e-04</td>
<td>3.310e-05</td>
</tr>
</tbody>
</table>
Remark on computing the weights

Recall that if we compute a sum with $M$ terms,

\[ S = \sum_{m=1}^{M} A_m \]

in a system of floating-point arithmetic with unit roundoff $\epsilon$, then

\[ |\text{fl}(S) - S| \leq \frac{M\epsilon}{1 - M\epsilon} \sum_{m=1}^{M} |A_m|. \]

Thus, for $w_j = (j + 1)^\alpha - 2j^\alpha + (j - 1)^\alpha$ and $j$ large,

\[ |\text{fl}(w_j) - w_j| \leq \epsilon j^\alpha \quad \text{whereas} \quad w_j \approx \alpha(1 - \alpha)j^{\alpha-2} \]

so the relative rounding error $|\text{fl}(w_j) - w_j|/|w_j|$ is of order $\epsilon j^2$. 
By writing \( w_j = \Delta_j - \Delta_{j-1} \) and using `expm1` and `log1p` to evaluate

\[
\Delta_j \equiv (j + 1)^\alpha - j^\alpha = j^\alpha [(1 + j^{-1})^\alpha - 1] = j^\alpha \left( \exp \left[ \alpha \log(1 + j^{-1}) \right] - 1 \right),
\]

we can reduce somewhat the rounding error in \( \text{fl}(w_j) \) for large \( j \).

When we compute

\[
S = \rho \sum_{j=1}^{n} w_{n-j} U^j
\]

the estimates above yield

\[
|\text{fl}(S) - S| \lesssim n\epsilon \sum_{j=1}^{n} (n - j)^\alpha |U^j| \lesssim n^{\alpha+2}\epsilon \max_{1 \leq j \leq n} |U^j|,
\]

which suggests that roundoff might become a problem once

\[
n^{\alpha+2} \geq \epsilon^{-1}.
\]
For $\Omega = (0, L)$, we again consider the initial-boundary value problem

$$u_t - K_\alpha \partial_t^{1-\alpha} u_{xx} = f(x, t) \quad \text{for } x \in \Omega \text{ and } 0 < t < T,$$

$$u = u_0(x) \quad \text{for } x \in \Omega, \text{ when } t = 0,$$

$$u = 0 \quad \text{for } x \in \partial \Omega \text{ and } 0 < t < T.$$

The implicit time-stepping scheme leads to

$$U^n_p - U^{n-1}_p - \frac{K_\alpha \Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=1}^n w_{n-j} \frac{U^j_{p+1} - 2U^j_p + U^j_{p-1}}{\Delta x^2} = f^n_p \Delta t$$

for $1 \leq n \leq N$ and $1 \leq p \leq P - 1$, with

$$U^0_p = u_0(x_p) \quad \text{and} \quad U^0_0 = 0 = U^0_P.$$
Stencil
Matrix–vector formulation

We have

\[ U^n - U^{n-1} + \frac{\Delta t^\alpha}{\Gamma(\alpha + 1)} \sum_{j=1}^{n} w_{n-j} A U^j = \Delta t f^n \]

so

\[ (I + B)U^n = U^{n-1} + \Delta t f^n - \sum_{j=1}^{n-1} w_{n-j} B U^j \]

where

\[ B = \frac{\Delta t^\alpha}{\Gamma(\alpha + 1)} \quad A = \frac{K_\alpha \Delta t^\alpha}{\Gamma(\alpha + 1) \Delta x^2} \]

\[
\begin{align*}
&\begin{bmatrix}
2 & -1 \\
-1 & 2 & -1 \\
& \cdot & \cdot & \cdot \\
& & \cdot & \cdot & \cdot \\
& & & -1 & 2 & -1 \\
& & & & -1 & 2
\end{bmatrix},
\end{align*}
\]
Computational cost

At the \( n \)th time step, evaluation of the RHS costs \( O(nP) \) flops, and the elliptic solve costs \( O(P) \) flops. Since

\[
\sum_{n=1}^{N} n \approx \frac{N^2}{2},
\]

the overall cost of \( N \) time steps is \( O(N^2P) \).

Also, the \( n \)th time step requires \( O(nP) \) active memory locations.

Contrast this with using the implicit Euler method to solve the classical diffusion equation (the case \( \alpha = 1 \)): each time step requires \( O(P) \) flops and \( O(P) \) active memory locations, and \( N \) time steps requires \( O(NP) \) flops.

Conclusion: cost when \( 0 < \alpha < 1 \) is \( N \) times the cost when \( \alpha = 1 \).
Comparison with direct simulation

Let $u = u(x, t)$ be the solution of

$$u_t - K_\alpha \partial_t^{1-\alpha} u_{xx} = f(x, t) \quad \text{for } x \in \Omega = (-L, L) \text{ and } 0 < t < T,$$

$$u = \delta(x) \quad \text{for } x \in \Omega, \text{ when } t = 0,$$

$$u = 0 \quad \text{for } x \in \partial\Omega = \{-L, L\} \text{ and } 0 < t < T.$$

We can approximate $u$ using the implicit Euler method, or by simulating CTRWs with

$$\psi(t) = \frac{\alpha}{(1 + t)^\alpha} \quad \text{and} \quad \lambda(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2).$$

In this case $\psi(t) \sim A/t^{1+\alpha}$ as $t \to \infty$, with $A = \alpha$, so

$$B_\alpha = A\alpha^{-1}\Gamma(1 - \alpha) = \Gamma(1 - \alpha)$$

and we must rescale in such a way that

$$\frac{\sigma^2}{2\Gamma(1 - \alpha)\tau^\alpha} = K_\alpha.$$
Implicit Euler solutions ($\alpha = 2/3$)
Probability densities of CTRWs (15,000 samples)
Part VI

Spatial discretization via finite elements
The finite element method provides the simplest approach for discretization of a fractional diffusion problem on a spatial domain of general shape. In the classical method of lines for the heat equation, such a spatial discretization leads to a large, stiff system of first-order ODEs in time, that can be integrated using an appropriate black-box routine. For a time-fractional diffusion problem, we instead obtain a system of fractional-order ODEs.

In this lecture, we seek to estimate the errors from the spatial discretization assuming that the time integration is performed exactly. Suitable approaches for the time discretization include the implicit Euler method described previously and the more accurate schemes addressed in subsequent lectures.
Outline

Method of lines

Error estimates

Non-smooth data
Method of lines

Spatial domain $\Omega \subseteq \mathbb{R}^d$ ($d = 1, 2$ or $3$); for simplicity a convex polygon or polyhedron so the elliptic problem is $H^2$-regular.

With $0 < \alpha < 1$, let $u = u(x, t)$ be the mild solution of

$$u_t - K_\alpha \partial_t^{1-\alpha} \nabla^2 u = f(x, t) \quad \text{for } x \in \Omega \text{ and } t > 0,$$

$$u = u_0(x) \quad \text{for } x \in \Omega, \text{ when } t = 0,$$

subject to homogeneous Dirichlet boundary conditions

$$u = 0 \quad \text{for } x \in \partial \Omega \text{ and } t > 0.$$

We wish (for now) to discretize in space only.
Weak formulation

Put

$$Au = -K_\alpha \nabla^2 u \quad \text{and} \quad a(u, v) = \int_\Omega K_\alpha \nabla u \cdot \nabla v \, dx.$$ 

First Green identity:

$$\int_\Omega Au \, v \, dx = a(u, v) - \int_{\partial \Omega} K_\alpha \frac{\partial u}{\partial n} \, v \, ds.$$ 

Thus,

$$\langle u_t, v \rangle + a(\partial_t^{1-\alpha} u, v) = \langle f, v \rangle \quad \text{for } v \in H^1_0(\Omega),$$

and also

$$\langle u_t, v \rangle + \partial_t^{1-\alpha} a(u, v) = \langle f, v \rangle \quad \text{for } v \in H^1_0(\Omega).$$
Finite element space

Family of triangulations $\mathcal{T}_h$ of $\Omega$, where as usual

$$h = \max_{K \in \mathcal{T}_h} \text{diam}(K).$$

Let $V_h$ denote the space of real-valued functions on $\Omega$ that are continuous piecewise polynomials of degree at most $p \geq 1$ with respect to $\mathcal{T}_h$, and which vanish on $\partial\Omega$. Hence,

$$V_h \subseteq H^1_0(\Omega).$$

Seek a finite element solution $u_h : [0, \infty) \rightarrow V_h$ satisfying

$$\langle u_{ht}, \chi \rangle + \partial_t^{1-\alpha} a(u_h, \chi) = \langle f, \chi \rangle \quad \text{for} \ \chi \in V_h \ \text{and} \ t > 0,$$

with $u_h(0) = u_{0h} \approx u_0$ for a suitable $u_{0h} \in V_h$. 
Alternative formulation

Define the discrete elliptic operator $A_h : V_h \to V_h$ by

$$\langle A_h \psi, \chi \rangle = a(\psi, \chi) \quad \text{for } \psi, \chi \in V_h,$$

and the $L_2$-projector $P_h : L_2(\Omega) \to V_h$ by

$$\langle P_h v, \chi \rangle = \langle v, \chi \rangle \quad \text{for } v \in L_2(\Omega) \text{ and } \chi \in V_h.$$

Since

$$\partial_t^{1-\alpha} a(u_h, \chi) = \partial_t^{1-\alpha} \langle A_h u_h, \chi \rangle = \langle \partial_t^{1-\alpha} A_h u_h, \chi \rangle,$$

we see that

$$\langle u_{ht} + \partial_t^{1-\alpha} A_h u_h, \chi \rangle = \langle f, \chi \rangle = \langle P_h f, \chi \rangle \quad \text{for all } \chi \in V_h,$$

and thus

$$u_{ht} + \partial_t^{1-\alpha} A_h u_h = P_h f \quad \text{for } t > 0.$$
Nodal equations

Construct a nodal basis $\chi_1, \chi_2, \ldots, \chi_N$ for $V_h$ so that

$$\chi_j(x_k) = \delta_{jk},$$

where $x_1, x_2, \ldots, x_N$ are the free (interior) nodes. Thus,

$$u_h(x, t) = \sum_{k=1}^{N} U_k(t) \chi_k(x) \quad \text{where} \quad U_k(t) = u_h(x_k, t).$$

Define the mass matrix $M$, stiffness matrix $S$ and load vector $f$ by

$$M_{jk} = \langle \chi_k, \chi_j \rangle, \quad S_{jk} = a(\chi_k, \chi_j), \quad f_k(t) = \langle f(t), \chi_k \rangle$$

then the nodal vector $U = [U_k(t)]$ satisfies the system of ordinary integro-differential equations

$$M \frac{dU}{dt} + \partial_t^{1-\alpha} SU = f(t) \quad \text{for} \ t > 0.$$
Discrete eigensystem

The finite dimensional linear operator $A_h : V_h \to V_h$ is symmetric and positive-definite, so $V_h$ has an orthonormal basis $\phi_1^h, \phi_2^h, \ldots, \phi_N^h$ consisting of eigenfunctions of $A_h$. Thus,

$$A_h \phi_m^h = \lambda_m^h \phi_m^h \quad \text{for } 1 \leq m \leq N,$$

with $\langle \phi_m^h, \phi_n^h \rangle = \delta_{mn}$, and consequently

$$u_h(t) = \mathcal{E}_h(t)u_{0h} + \int_0^t \mathcal{E}_h(t-s)P_h f(s) \, ds,$$

where the discrete solution operator for the homogeneous problem is defined by

$$\mathcal{E}_h(t)\chi = \sum_{m=1}^N E_\alpha(\lambda_m^h t^\alpha) \langle \chi, \phi_m^h \rangle \phi_m^h \quad \text{for } \chi \in V_h.$$
Stability

Theorem
The finite element solution is stable in $L_2(\Omega)$:

$$\|u_h(t)\| \leq \|u_0h\| + \int_0^t \|P_hf(s)\| \, ds \quad \text{for } t \geq 0.$$  

Proof.
Since $0 < E_\alpha(-s) \leq 1$ for $0 \leq s < \infty$,

$$\|E_h(t)\chi\|^2 = \sum_{m=1}^N |E_\alpha(-\lambda_m^ht^\alpha)\langle \chi, \phi_m^h \rangle|^2 \leq \sum_{m=1}^N |\langle \chi, \phi_m^h \rangle|^2 = \|\chi\|^2,$$

so $\|E_h(t)\chi\| \leq \|\chi\|$ and the desired estimate follows from the Duhamel formula above. \qed
Error estimates

We wish to estimate the error \( u_h(t) - u(t) \) in \( L_2(\Omega) \) and in \( H^1_0(\Omega) \).

Our assumption that \( \Omega \) is convex implies that the elliptic problem,

\[ -\nabla^2 u = f \quad \text{in } \Omega, \text{ with } u = 0 \text{ on } \partial\Omega, \]

is \( H^2 \)-regular, that is, the weak solution \( u \in H^1_0(\Omega) \), given by

\[ a(u, v) = \langle f, v \rangle \quad \text{for all } v \in H^1_0(\Omega), \]

necessarily belongs to \( H^2(\Omega) \) and

\[ \|u\|_2 \leq C\|f\|. \]

Caution: in this lecture, \( \|v\|_r \) denotes the norm in \( H^r(\Omega) \), so \( \|v\|_r < \infty \) does not guarantee \( v \in H^r_0(\Omega) \) unless \( v \) vanishes appropriately on \( \partial\Omega \).
Error in the elliptic problem

Let \( u_h \in V_h \) be the finite element solution of the elliptic problem above, so that

\[
a(u_h, \chi) = \langle f, \chi \rangle \quad \text{for all } \chi \in V_h.
\]

Since the symmetric bilinear form \( a(u, v) \) is bounded and coercive on \( H_0^1(\Omega) \), and using an appropriate quasi-interpolant, we have

\[
\| u_h - u \|_1 \leq C \inf_{\chi \in V_h} \| \chi - u \|_1 \leq Ch^{r-1} \| u \|_r \quad \text{for } 1 \leq r \leq p + 1.
\]

The usual duality argument (which relies on \( H^2 \)-regularity) then implies that

\[
\| u_h - u \| \leq Ch \inf_{\chi \in V_h} \| \chi - u \|_1 \leq Ch^r \| u \|_r \quad \text{for } 1 \leq r \leq p + 1.
\]
It is convenient to define $R_h : H^1_0(\Omega) \to V_h$ by $R_h u = u_h$, or equivalently,

$$a(R_h v, \chi) = a(v, \chi) \quad \text{for all} \ \chi \in V_h.$$ 

It follows that $R^2_h = R_h$, with

$$\|v - R_h v\| \leq Ch^r \|v\|_r \quad \text{and} \quad \|v - R_h v\|_1 \leq Ch^{r-1}\|v\|_r$$ 

for $1 \leq r \leq p + 1$. Also, since

$$\langle P_h Av, \chi \rangle = \langle Av, \chi \rangle = a(v, \chi) = a(R_h v, \chi) = \langle A_h R_h v, \chi \rangle$$ 

for all $v \in H^1_0(\Omega)$ and $\chi \in V_h$, we see that

$$P_h A = A_h R_h : H^1_0(\Omega) \to V_h.$$
Equation for the error

Returning to the time-dependent case, we split the error into two terms

\[ u_h(t) - u(t) = \vartheta(t) + \varrho(t), \quad \vartheta = u_h - R_hu, \quad \varrho = R_hu - u. \]

Then for all \( \chi \in V_h, \)

\[
\langle \vartheta_t, \chi \rangle + \partial^{1-\alpha}_t a(\vartheta, \chi) \\
= \langle u_{ht}, \chi \rangle + \partial^{1-\alpha}_t a(u_h, \chi) - \langle R_hu_t, \chi \rangle - \partial^{1-\alpha}_t a(R_hu, \chi) \\
= \langle f, \chi \rangle + \langle R_hu_t, \chi \rangle - \partial^{1-\alpha}_t a(u, \chi) \\
= \langle u_t, \chi \rangle + \partial^{1-\alpha}_t a(u, \chi) - \langle R_hu_t, \chi \rangle - \partial^{1-\alpha}_t a(u, \chi)
\]

so \( \vartheta : [0, \infty) \rightarrow V_h \) satisfies an equation of the same form as the one for \( u_h \) (with \( u_t - R_hu_t \) playing the role of \( f \))

\[
\langle \vartheta_t, \chi \rangle + \partial^{1-\alpha}_t a(\vartheta, \chi) = \langle u_t - R_hu_t, \chi \rangle.
\]
Estimate for $\vartheta = u_h - R_h u$

**Lemma**

For $1 \leq r \leq p + 1$,

$$\| \vartheta(t) \| \leq \| u_{0h} - R_h u_0 \| + C h^r \int_0^t \| u_t \|_r \, ds$$

**Proof.**

Stability in $L_2(\Omega)$ gives

$$\| \vartheta(t) \| \leq \| \vartheta(0) \| + \int_0^t \| P_h(u_t - R_h u_t) \| \, ds,$$

and here $\vartheta(0) = u_{h0} - R_h u_0$ with

$$\| P_h(u_t - R_h u_t) \| \leq \| u_t - R_h u_t \| \leq C h^r \| u_t \|_r.$$
Estimate for $\varrho = R_h u - u$

Lemma

For $1 \leq r \leq p + 1$,

$$\|\varrho(t)\| \leq Ch^r \left( \|u_0\|_r + \int_0^t \|u_t\|_r \, ds \right).$$

Proof.

Write

$$\varrho(t) = \varrho(0) + \int_0^t \varrho_t(s) \, ds$$

and use

$$\|\varrho_t\| = \|u_t - R_h u_t\| \leq Ch^r \|u_t\|_r$$

together with

$$\|\varrho(0)\| = \|R_h u_0 - u_0\| \leq Ch^r \|u_0\|_r.$$
The finite element solution of the time-fractional diffusion equation satisfies

\[ \| u_h(t) - u(t) \| \leq \| u_{0h} - R_h u_0 \| + Ch^r \left( \| u_0 \|_r + \int_0^t \| u_t(s) \|_r \, ds \right) \]

for \( 1 \leq r \leq p + 1 \).

In practice, this bound is unlikely to be useful for \( r > 2 \) because \( u \) will not be sufficiently smooth for \( (\cdots) \) on the RHS to be finite.
Realistic smoothness

Consider the homogeneous problem with \( f \equiv 0 \) so that \( u(t) = \mathcal{E}(t)u_0 \), and choose \( p = 1 \) (piecewise-linear).

For sufficiently small \( \epsilon > 0 \), if \( u_0 \in H^{2+\epsilon}(\Omega) \) and \( u_0 = 0 \) on \( \partial\Omega \), then \( u_0 \in H_{D}^{2+\epsilon}(\Omega) \) so by our earlier regularity theorem,

\[
\|tu_t\|_2 \leq Ct^{\epsilon\alpha/2}\|u_0\|_{2+\epsilon},
\]

implying that \( \|u_t\|_2 = O(t^{\epsilon\alpha/2-1}) \) as \( t \to 0 \). Choosing \( u_{0h} = R_hu_0 \) for simplicity, we obtain

\[
\|u_h(t) - u(t)\| \leq Ch^2\|u_0\|_{2+\epsilon} \quad \text{for} \ 0 \leq t \leq T,
\]

with \( C = C(T, \alpha, \epsilon, \Omega) \).
Estimate for $\|v(t)\|_1$

We saw that

$$\langle v_t, \chi \rangle + a(\partial_t^{1-\alpha} v, \chi) = \langle -\rho_t, \chi \rangle$$

for all $\chi \in V_h$.

Choosing $\chi = A_h v(t)$, we have

$$\langle v_t, A_h v \rangle = \frac{1}{2} \frac{d}{dt} \langle v, A_h v \rangle = \frac{1}{2} \frac{d}{dt} a(v, v)$$

with

$$a(\partial_t^{1-\alpha} v, A_h v) = \langle \partial_t^{1-\alpha} A_h v, A_h v \rangle$$

and

$$\langle -\varrho_t, A_h v \rangle = -\langle \varrho_t, P_h A_h v \rangle = -\langle P_h \varrho_t, A_h v \rangle = -a(P_h \varrho_t, v).$$

Thus,

$$\frac{1}{2} \frac{d}{dt} a(v, v) + \langle \partial_t^{1-\alpha} A_h v, A_h v \rangle = -a(P_h \varrho_t, v).$$
Integrating from $t = 0$ to $t = T$ and using
\[
\int_0^T \langle \partial_t^{1-\alpha} A_h \vartheta, A_h \vartheta \rangle \, dt \geq 0,
\]
we have
\[
a(\vartheta(T), \vartheta(T)) - a(\vartheta(0), \vartheta(0)) \leq -2 \int_0^T a(P_{h\varrho_t}, \vartheta) \, dt
\]
Since $a(v, v)$ is equivalent to $\|v\|_1^2$,
\[
\|\vartheta(T)\|_1 \leq C \left( \|\vartheta(0)\|_1 + \int_0^T \|P_{h\varrho_t}\|_1 \, dt \right).
\]
Choose $t^*$ such that
\[
\|\vartheta(t^*)\|_1 = \max_{0 \leq t \leq T} \|\vartheta(t)\|_1,
\]
then
\[
\|\vartheta(T)\|_1 \|\vartheta(t^*)\|_1 \leq \|\vartheta(t^*)\|_1^2
\]
\[
\leq C \|\vartheta(0)\|_1^2 + C \int_0^{t^*} \|P_h \varrho_t\|_1 \|\vartheta\|_1 \, dt
\]
\[
\leq C \left( \|\vartheta(0)\|_1 + \int_0^T \|P_h \varrho_t\|_1 \, dt \right) \|\vartheta(t^*)\|_1
\]
so
\[
\|\vartheta(T)\|_1^2 \leq C \|\vartheta(0)\|_1^2 + C \int_0^T \|P_h \varrho_t(t)\|_1 \|\vartheta(t)\|_1 \, dt
\]
Quasi-optimal error bound in $H^1(\Omega)$

Assume now that $\mathcal{T}_h$ is such that the $L_2$-projector $P_h$ is stable in $H^1(\Omega)$, that is,

$$\|P_h v\|_1 \leq C \|v\|_1 \quad \text{for} \ v \in H^1(\Omega).$$

For instance, it suffices to assume that $\mathcal{T}_h$ is quasi-uniform.

**Theorem**

*The finite element solution of the time-fractional diffusion equation satisfies*

$$\|u_h(t) - u(t)\|_1 \leq C \|u_0h - R_h u_0\|_1 + Ch^{r-1} \left( \|u_0\|_r + \int_0^t \|u_t(s)\|_r \, ds \right)$$

for $2 \leq r \leq p + 1$. 
Proof

Recall that \( u_h - u = \vartheta + \varrho \) and

\[
\| \vartheta(t) \|_1 \leq C \left( \| \vartheta(0) \|_1 + \int_0^t \| P_h \varrho_t(s) \|_1 \, dt \right).
\]

Here,

\[
\| \vartheta(0) \|_1 = \| u_0 h - R_h u_0 \|_1,
\]

and since \( P_h \) is stable in \( H^1(\Omega) \),

\[
\| P_h \varrho_t(s) \|_1 \leq C \| u_t(s) - R_h u_t(s) \|_1 \leq Ch^{r-1} \| u_t(s) \|_r.
\]

The error bound follows because

\[
\| \varrho(t) \|_1 \leq \| \varrho(0) \|_1 + \int_0^t \| \varrho_t(s) \|_1 \, ds
\]

\[
= \| u_0 - R_h u_0 \|_1 + \int_0^t \| u_t(s) - R_h u_t(s) \|_1 \, ds
\]

\[
\leq Ch^{r-1} \left( \| u_0 \|_1 + \int_0^t \| u_t(s) \|_1 \, ds \right).
\]

\( \square \)
Non-smooth data

Define the closed sector

\[ \Sigma_{\psi} = \{ z \in \mathbb{C} : z \neq 0 \text{ and } |\arg z| \leq \psi \} \cup \{0\}. \]

Our aim now is to prove the following error bound, which does not require any spatial regularity for \( u_0 \) or \( f \).

**Theorem**

Assume that \( u_{0h} = P_h u_0 \), and fix \( \varphi \) such that \( 0 < \varphi < \pi/2 \). Then,

\[
\| u_h(t) - u(t) \| \leq C t^{-\alpha} h^2 \left( \| u_0 \| + \sup_{z \in \partial \Sigma_{\pi - \varphi}} \| \hat{f}(z) \| \right)
\]

for \( 0 < t \leq T \).
Under Laplace transformation, our problem

\[ u_t + \partial_t^{1-\alpha} Au = f(t) \quad \text{for } t > 0, \quad \text{with } u(0) = u_0, \]

becomes

\[ z\hat{u}(z) - u_0 + z^{1-\alpha} A\hat{u}(z) = \hat{f}(z), \]

so

\[ (z^\alpha I + A)\hat{u}(z) = z^{\alpha - 1} g(z) \quad \text{where } g(z) = u_0 + \hat{f}(z). \]

Similarly, for \( u_h \) we have

\[ (z^\alpha I + A_h)\hat{u}_h(z) = z^{\alpha - 1} g_h(z) \quad \text{where } g_h(z) = u_{0h} + P_h\hat{f}(z). \]

Notice that \( g_h(z) = P_h g(z) \) because we assume \( u_{0h} = P_h u_0 \).
Resolvent estimate for $A$

Recall that $A\phi_m = \lambda_m \phi_m$ with $0 \leq \lambda_1 < \lambda_2 < \cdots$.

**Theorem**

Let $\varphi$ satisfy $0 < \varphi \leq \pi/2$ and put

$$M = \frac{1}{\sin \varphi}.$$

If $z \in \Sigma_{\pi - \varphi}$ then

$$\| (zI + A)^{-1} \| \leq \frac{M}{|z|} \leq \left(1 + \frac{2}{\lambda_1}\right) \frac{M}{1 + |z|}.$$
Proof

Let \( z = re^{i\theta} \) with \( |\theta| \leq \pi - \varphi \) and \( r > 0 \).

If \( 0 \leq |\theta| \leq \pi/2 \) then \( |z| \leq |z + \lambda_m| \) because

\[
0 \leq \Re z \leq \Re(z + \lambda_m) \quad \text{and} \quad \Im z = \Im(z + \lambda_m)
\]

If \( \pi/2 \leq |\theta| \leq \pi - \varphi \) then \( |z| \leq M|z + \lambda_m| \) because

\[
|z| \sin \varphi \leq |z| \sin |\theta| = |\Im z| = |\Im(z + \lambda_m)| \leq |z + \lambda_m|.
\]

Therefore, since \( M \geq 1 \),

\[
\frac{1}{|z + \lambda_m|} \leq \frac{M}{|z|}
\]

and so \((zl + A)^{-1}\) exists with

\[
(zl + A)^{-1}v = \sum_{m=1}^{\infty} \frac{\langle v, \phi_m \rangle}{z + \lambda_m} \phi_m \quad \text{for} \quad v \in L_2(\Omega).
\]
Hence, Parseval’s identity yields the first estimate:

\[
\|(zI + A)^{-1}v\|^2 = \sum_{m=1}^{\infty} \left| \frac{\langle v, \phi_m \rangle}{z + \lambda_m} \right|^2 \leq \left( \frac{M}{|z|} \right)^2 \sum_{m=1}^{\infty} |\langle v, \phi_m \rangle|^2 = \left( \frac{M}{|z| \|v\|} \right)^2.
\]

If \(|z| \leq \lambda_1/2\), then \(|z + \lambda_m| \geq \lambda_1 - |z| \geq \lambda_1/2\) so

\[
\frac{1 + |z|}{|z + \lambda_m|} \leq \frac{1 + \lambda_1/2}{\lambda_1/2} = 1 + \frac{2}{\lambda_1}.
\]

If \(|z| \geq \lambda_1/2\), then

\[
\frac{1 + |z|}{|z + \lambda_m|} \leq \frac{2|z|/\lambda_1 + |z|}{|z| \sin \varphi} = M\left(1 + \frac{2}{\lambda_1}\right),
\]

and the second estimate follows at once.
Resolvent estimate for $A_h$

**Theorem**

Let $\varphi$ satisfy $0 < \varphi \leq \pi/2$ and put $M = 1/\sin \varphi$. If $z \in \Sigma_{\pi-\varphi}$ then

$$
\| (zI + A_h)^{-1} \| \leq \frac{M}{|z|} \leq \left( 1 + \frac{2}{\lambda_1} \right) \frac{M}{1 + |z|}.
$$

**Proof.**

The same proof shows that the conclusion holds with $\lambda_1^h$ in place of $\lambda_1$. But

$$
\lambda_1^h = \min_{\chi \in V_h} \frac{\langle A_h \chi, \chi \rangle}{\| \chi \|^2} = \min_{\chi \in V_h} \frac{\langle A \chi, \chi \rangle}{\| \chi \|^2}
$$

$$
\geq \min_{v \in H^1_0(\Omega)} \frac{\langle Av, v \rangle}{\| v \|^2} = \lambda_1,
$$

so $2/\lambda_1^h \leq 2/\lambda_1$.  \qed
Integral representations

Since

\[ \hat{u}(z) = z^{\alpha-1}(z^{\alpha} I + A)^{-1} g(z) \]

and

\[ \hat{u}_h(z) = z^{\alpha-1}(z^{\alpha} I + A_h)^{-1} P_h g(z) \]

the Laplace inversion formula gives

\[ u(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} z^{\alpha-1}(z^{\alpha} I + A)^{-1} g(z) \, dz \]

and

\[ u_h(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} z^{\alpha-1}(z^{\alpha} I + A_h)^{-1} P_h g(z) \, dz, \]

where

\[ \Gamma = \{ a + iy : -\infty < y < \infty \} \quad \text{for any } a > 0. \]
Thus, 

\[ u_h(t) - u(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} z^{\alpha-1} G_h(z) g(z) \, dz \]

where 

\[ G_h(z) = (z^\alpha I + A_h)^{-1} P_h - (z^\alpha I + A)^{-1} = G_h^1(z) + G_h^2(z), \]

with 

\[ G_h^1(z) = (z^\alpha I + A_h)^{-1} P_h - P_h(z^\alpha I + A)^{-1}, \]

\[ G_h^2(z) = (P_h - I)(z^\alpha I + A)^{-1}. \]
Lemma
For $z \in \Sigma_{\pi-\varphi}$,

$$\|A(z^\alpha I + A)^{-1}v\| \leq C\|v\| \quad \text{and} \quad \|(z^\alpha I + A_h)^{-1}A_h\chi\| \leq C\|\chi\|.$$  

Proof.
The identity

$$A(z^\alpha I + A)^{-1} = (z^\alpha I + A - z^\alpha I)(z^\alpha I + A)^{-1} = I - z^\alpha(z^\alpha I + A)^{-1}$$

implies that

$$\|A(z^\alpha I + A)^{-1}\| \leq 1 + |z^\alpha| \frac{M}{|z^\alpha|} \leq C.$$  

Similarly,

$$(z^\alpha I + A_h)^{-1}A_h = I - z^\alpha(z^\alpha I + A_h)^{-1}.$$
Estimate for $G_h^1(z)$

Lemma
\[ \| G_h^1(z)v \| \leq Ch^2\| v \| \text{ for } z \in \Sigma_{\pi-\varphi}. \]

Proof.
Recall that $P_hA = A_hR_h$, so

\[
G_h^1(z) = (z^\alpha I + A_h)^{-1}P_h - P_h(z^\alpha I + A)^{-1} \\
= (z^\alpha I + A_h)^{-1}[P_h(z^\alpha I + A) - (z^\alpha I + A_h)P_h](z^\alpha I + A)^{-1} \\
= (z^\alpha I + A_h)^{-1}A_h(R_h - P_h)(z^\alpha I + A)^{-1},
\]

$H^2$-regularity of the elliptic problem gives

\[
\| G_h^1(z)v \| \leq C\| (R_h - P_h)(z^\alpha I + A)^{-1}v \| \leq Ch^2\| (z^\alpha I + A)^{-1}v \|_2 \\
\leq Ch^2\| A(z^\alpha I + A)^{-1}v \| \leq Ch^2\| v \|. 
\]
Lemma
\[ \| G_h^2(z)v \| \leq C h^2 \| v \| \text{ for } z \in \Sigma_{\pi-\varphi}. \]

Proof.
As above,
\[
\| G_h^2(z)v \| = \| (P_h - I)(z^\alpha I + A)^{-1}v \|
\leq C h^2 \| (z^\alpha I + A)^{-1}v \|_2
\leq C h^2 \| A(z^\alpha I + A)^{-1}v \|
\leq C h^2 \| v \|.
\]
\[\square\]
Thus, we have shown that

$$u_h(t) - u(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} z^\alpha G_h(z) g(z) \, dz$$

with \( \| G_h(z)v \| \leq Ch^2 \| v \| \) for \( z \in \Sigma_{\pi - \varphi} \).

Deform the integration contour \( \Gamma \) to \( \partial \Sigma_{\pi - \varphi} = \Gamma_+ - \Gamma_- \), where

$$\Gamma_{\pm} = \{ se^{\pm i(\pi - \varphi)} : 0 < s < \infty \},$$

so that \( u_h(t) - u(t) = l_+ - l_- \) where

$$l_{\pm} = \frac{1}{2\pi i} \int_{\Gamma_{\pm}} e^{zt} z^\alpha G_h(z) g(z) \, dz.$$
The substitution \( z = se^{\pm i(\pi - \varphi)} = s(-\cos \varphi \pm i \sin \varphi) \) gives

\[
\| l_{\pm} \| \leq Ch^2 \left( \| u_0 \| + \sup_{z \in \Gamma_{\pm}} \| \hat{f}(z) \| \right) \int_0^\infty e^{-st \cos \varphi} s^\alpha \frac{ds}{s}.
\]

A second substitution \( s = w(t \cos \varphi)^{-1} \) shows that the integral on the right equals

\[
\int_0^\infty e^{-w} \left( \frac{w}{t \cos \varphi} \right)^\alpha \frac{dw}{w} = C_{\alpha,\varphi} t^{-\alpha}.
\]
Part VII

Methods based on the Laplace transform
Introduction

The Laplace inversion formula yields a contour integral representation of the finite element solution $u_h(t)$ to the time-fractional diffusion equation. Applying a quadrature approximation [Lopez-Fernandez+Palencia-2004] leads to a fully discrete solution $U_{N,h}(t)$. The main cost of the method is the computation of $\hat{u}_h(z_j)$ at the quadrature point $z_j$ for $|j| \leq N$, which requires the solution of a system of finite element equations involving the complex parameter $z_j$.

The main advantages of the this approach are high accuracy and easy parallel implementation. A key disadvantage is that the method imposes severe limitations on form of the source term $f(t)$. We outline a modified approach [McLean+Thomee-2010] that sacrifices some accuracy to relax the requirements on $f(t)$.
Outline

Contour integral and quadrature

Parallel-in-time algorithm

A more flexible approach
Contour integral and quadrature

Once again consider

\[ \dot{u} + \partial_t^{1-\alpha} Au = f(t) \quad \text{for } t > 0, \quad \text{with } u(0) = u_0, \]

and recall that

\[ u(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} z^{\alpha-1} (z^\alpha I + A)^{-1} g(z) \, dz, \]

where

\[ g(z) = u_0 + \hat{f}(z). \]

We now choose for \( \Gamma \) a contour of the form

\[ z = z(\xi) = \mu(1 - \sin(\delta - i\xi)) \quad \text{for } -\infty < \xi < \infty, \]

where the parameters \( \mu \) and \( \delta \) satisfy

\[ \mu > 0 \quad \text{and} \quad 0 < \delta < \frac{\pi}{2}. \]
Hyperbola

Since

\[ \sin(\delta - i\xi) = \sin\delta \cosh\xi - i \cos\delta \sinh\xi, \]

we have

\[ x(\xi) = \Re z(\xi) = \mu (1 - \sin\delta \cosh\xi), \]
\[ y(\xi) = \Im z(\xi) = \mu \cos\delta \sinh\xi, \]

so \( \Gamma \) is the left branch of the hyperbola

\[ \left( \frac{x - \mu}{\mu \sin\delta} \right)^2 - \left( \frac{y}{\mu \cos\delta} \right)^2 = 1. \]

Notice that the asymptotes are

\[ y = \pm (x - \mu) \cot \delta. \]
Parameterised integral

We have

\[ u(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} z^{\alpha-1} (z^\alpha I + A)^{-1} g(z) \, dz \]

\[ = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{z(\xi)t} z(\xi)^{\alpha} (z(\xi)^\alpha I + A)^{-1} g(z(\xi)) \frac{z'(\xi)}{z(\xi)} \, d\xi \]

with

\[ z(\xi) = \mu(1 - \sin(\delta - i\xi)) = \mu(1 - \sin \delta \cosh \xi + i \cos \delta \sinh \xi), \]
\[ z'(\xi) = i\mu \cos(\delta - i\xi) = \mu(-\sin \delta \sinh \xi + i \cos \delta \cosh \xi). \]

Find that

\[ \left| \frac{z'(\xi)}{z(\xi)} \right|^2 = \frac{\cosh^2 \xi - \sin^2 \delta}{(\cosh \xi - \sin \delta)^2} = \frac{\cosh \xi + \sin \delta}{\cosh \xi - \sin \delta} < \frac{1}{1 - \sin \delta}. \]
Double exponential decay

Key factor in the behaviour of the integrand is

\[ |e^{z(\xi)t}| = e^{x(\xi)t} = \exp(\mu t (1 - \sin \delta \cosh \xi)), \]

and since \( \cosh \xi \geq \frac{1}{2} \exp(|\xi|) \),

\[ |e^{z(\xi)t}| \leq \exp(\mu t - \frac{1}{2} \mu t \sin \delta \exp(|\xi|)). \]
Discretisation error

For $\Delta \xi > 0$, let

$$Q_\infty(v) = \sum_{j=-\infty}^{\infty} v(j \Delta \xi) \Delta \xi.$$  

Theorem ([Trefethen+Weideman-2014])

Let $r_\pm > 0$ and assume

1. $v(\zeta)$ is analytic on the strip $-r_- \leq \Im \zeta \leq r_+$;
2. $\int_{-r_-}^{r_+} |v(\xi + i\eta)| \, d\eta \to 0$ as $|\xi| \to \infty$;
3. $\int_{-\infty}^{\infty} |v(\xi \pm i r_\pm)| \, d\xi \leq M_\pm$.

Then

$$\left| Q_\infty(v) - \int_{-\infty}^{\infty} v(\xi) \, d\xi \right| \leq \text{DE}_+ + \text{DE}_-$$

where

$$\text{DE}_\pm = \frac{M_\pm}{\exp(2\pi r_\pm/\Delta \xi) - 1}.$$
Conformal mapping

The formula

\[ z = \Phi(\zeta) = \mu(1 - \sin(\delta - i\zeta)) \]

defines conformal mapping that takes the line \( \Re\zeta = \eta \) to the left branch of the hyperbola

\[ \left(\frac{x - \mu}{\mu \sin(\delta + \eta)}\right)^2 - \left(\frac{y}{\mu \cos(\delta + \eta)}\right)^2 = 1. \]

Need to ensure

\[ 0 < \delta + \eta < \frac{\pi}{2} \]

so that the hyperbola crosses into the left half-plane.
Truncation error

In practice, compute

\[ Q_N(v) = \sum_{j=-N}^{N} v(j \Delta \xi) \Delta \xi, \]

so need to estimate

\[ \text{TE} = \sum_{|j| > N} v(j \Delta \xi) \Delta \xi \]

then the triangle inequality gives

\[ \left| Q_N(v) - \int_{-\infty}^{\infty} v(\xi) \, d\xi \right| \leq |\text{DE}_+| + |\text{DE}_-| + |\text{TE}|. \]
In our application, if $\zeta = \xi + i\eta$ then

$$|v(\zeta)| \leq C|e^{\Phi(\zeta)t}| \leq C \exp(\mu t(1 - \sin(\delta + \eta) \cosh \xi)).$$

Lemma ([Lopez-Fernandez+Palencia-2004])

For $a > 0$ and $0 < b \leq 1$,

$$\int_{0}^{\infty} e^{a(1-b \cosh \xi)} d\xi \leq Ce^{a(1-b)}L(ab)$$

where

$$L(x) = \begin{cases} 1, & x \geq 1, \\ \log \frac{e}{x}, & x \leq 1. \end{cases}$$
Proof

Since \( a(1 - b \cosh \xi) = a(1 - b) + ab(1 - \cosh \xi) \) it suffices to estimate

\[
I \equiv \int_0^\infty e^{ab(1-\cosh \xi)} \, d\xi = \int_0^\infty \frac{e^{-aby} \, dy}{\sqrt{y(y + 2)}} = \int_0^\infty \frac{e^{-x} \, dx}{\sqrt{x(x + 2ab)}},
\]

where we used the substitution \( y = \cosh \xi - 1 \) followed by \( x = aby \). If \( ab \geq 1 \) then

\[
I \leq \int_0^\infty x^{-1/2} e^{-x} \, dx < \infty,
\]

whereas if \( ab \leq 1 \), then

\[
I \leq \int_0^1 \, dx \frac{dx}{\sqrt{x(x + 2ab)}} + \int_1^\infty e^{-x} \, dx
\]

and the substitution \( x = abt/e \) gives

\[
\int_0^1 \frac{dx}{\sqrt{x(x + 2ab)}} = \int_0^{e/(ab)} \frac{dt}{\sqrt{t(t + 2e)}} \leq C + \log \frac{e}{ab}. \quad \Box
\]
Thus, taking $a = \mu t$ and $b = \sin(\delta \pm r_{\pm})$ in the lemma,

$$\int_{-\infty}^{\infty} |v(\xi \pm ir_{\pm})| \, d\xi \leq M_{\pm} = Ce^{\mu t(1-\sin(\delta \pm r_{\pm}))} L(\mu t \sin(\delta \pm r_{\pm})),$$

so

$$|DE_{\pm}| \leq \frac{M_{\pm}}{e^{2\pi r_{\pm}/\Delta \xi} - 1} \leq M_{\pm} e^{-2\pi r_{\pm}/\Delta \xi} \leq CL(\mu t \sin(\delta \pm r_{\pm})) \exp\left[\mu t (1 - \sin(\delta \pm r_{\pm})) - 2\pi r_{\pm}/\Delta \xi\right].$$

At the same time,

$$|TE| \leq \sum_{|j| > N} |v(j \Delta \xi)| \Delta \xi \lesssim 2|v(N \Delta \xi)| \Delta \xi \leq C \exp(\mu t(1 - \sin \delta \cosh(N \Delta \xi)) \Delta \xi.$$
Choice of parameters

To balance $\text{TE}_+$, $\text{TE}_-$ and $\text{DE}$, we want

$$
\mu t(1 - \sin(\delta + r_+)) - \frac{2\pi r_+}{\Delta \xi} = \mu t(1 - \sin(\delta - r_-)) - \frac{2\pi r_-}{\Delta \xi} \\
= \mu t(1 - \sin(\delta - r_-)) - \frac{2\pi r_-}{\Delta \xi} \\
= \mu t(1 - \sin \delta \cosh(N \Delta \xi)),
$$

while satisfying

$$
0 < \delta - r_- < \delta + r_+ < \frac{\pi}{2}.
$$

The limiting choices $r_+ = \pi/2 - \delta$ and $r_- = \delta$ give

$$
- \frac{2\pi}{\Delta \xi} \left( \frac{\pi}{2} - \delta \right) = \mu t - \frac{2\pi \delta}{\Delta \xi} = \mu t(1 - \sin \delta \cosh(N \Delta \xi)),
$$

so

$$
\mu t = \frac{\pi}{\Delta \xi} (4\delta - \pi) \quad \text{and} \quad \mu t \sin \delta \cosh(N \Delta \xi) = \frac{2\pi \delta}{\Delta \xi}.
$$
Eliminating $\mu t$,

$$\sin \delta \cosh(N \Delta \xi) = \frac{2\delta}{4\delta - \pi},$$

so we define

$$b(\delta) = \cosh^{-1} \left( \frac{2\delta}{(4\delta - \pi) \sin \delta} \right)$$

and obtain

$$\Delta \xi = \frac{b(\delta)}{N} \quad \text{and} \quad \mu = \frac{\pi(4\delta - \pi)}{b(\delta)} \frac{N}{t}.$$ 

In this case,

$$-\frac{2\pi}{\Delta \xi} \left( \frac{\pi}{2} - \delta \right) = -B(\delta)N \quad \text{where} \quad B(\delta) = \frac{\pi(\pi - 2\delta)}{b(\delta)},$$

and the error bound for the quadrature rule is

$$|\text{DE}_+| + |\text{DE}_-| + |\text{TE}| \leq \text{CL}(\cdots)e^{-B(\delta)N}.$$
Optimal choice of $\delta$
We find that $B(\delta)$ has a unique maximum in the interval $\pi/4 < \delta < \pi/2$, namely, at

$$\delta_* = 1.17210423, \quad \text{(near } 3\pi/8 = 1.17809724)$$

and the maximum value is

$$B(\delta_*) = 2.31565403.$$ 

Given $N$ and $t$, the corresponding optimal parameters are

$$\Delta \xi_* = \frac{1.08179214}{N} \quad \text{and} \quad \mu_* = 4.49207528 \frac{N}{t},$$

leading to an error bound with the decay factor

$$e^{-B(\delta_*)N} = e^{-2.3157N} = 10.1315^{-N}.$$
Scalar test problem

For $\lambda > 0$, recall that

$$\mathcal{L}\{e^{-\lambda t}\} = \int_{0}^{\infty} e^{-(z+\lambda)t} \, dt = (z + \lambda)^{-1}.$$ 

We consider

$$e^{-\lambda t} = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} (z + \lambda)^{-1} \, dz$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{z(\xi)t} (z(\xi) + \lambda)^{-1} z'(\xi) \, d\xi$$

$$\approx Q_N = \frac{1}{2\pi i} \sum_{j=-N}^{N} e^{z_j t} (z_j + \lambda)^{-1} z'_j \Delta \xi,$$

where

$$z_j = z(j \Delta \xi) \quad \text{and} \quad z'_j = z'(j \Delta \xi).$$
Convergence behaviour
Quadrature points for different $N$ (with $t = 1$)
Quadrature points for different $t$ (with $N = 15$)
Fixed points with varying $t$

Given $N$ and $\tau > 0$, suppose we choose $\Delta \xi^*$ and $\mu^*$ as above for $t = \tau$. What if we use the approximation

$$e^{-\lambda t} \approx \frac{1}{2\pi i} \sum_{j=-N}^{N} e^{zt}(z_j + \lambda)^{-1}z'_j \Delta \xi$$

for $t$ near $\tau$?

In the fractional PDE case, we can solve one set of elliptic problems for $\hat{u}_h(z_j)$ at the $z_j$ optimized for $t = \tau$ and use them not just at $t = \tau$ but for several values of $t$ in an interval around $\tau$. The $z_j$ are then slightly sub-optimal but we avoid having to compute a new set of $\hat{u}_h(z_j)$ for each $t$. 
Error for the scalar example with $\tau = 1$
Parallel-in-time algorithm

Combining the above approach to numerical inversion of the Laplace transform with a spatial discretisation by finite elements leads to a fully discrete numerical method that involves no time stepping.

The method is particularly suited to applications in which the solution is required for only a few values of $t$.

In addition to its high, spectral-order accuracy in time, the method is embarrassingly parallel.
Method-of-lines solution

Recall that the semidiscrete finite element solution $u_h : [0, \infty) \rightarrow V_h$ satisfies

$$\langle u_{ht}, \chi \rangle + \partial_t^{1-\alpha} a(u_h, \chi) = \langle f(t), \chi \rangle \quad \text{for } \chi \in V_h \text{ and } t > 0,$$

or equivalently,

$$u_{ht} + \partial_t^{1-\alpha} A_h u_h = P_h f(t) \quad \text{for } t > 0,$$

with $u_h(0) = u_{0h} \approx u_0$.

Under Laplace transformation in time, we obtain

$$z \hat{u}_h + z^{1-\alpha} A_h \hat{u}_h = g_h(z)$$

where $g_h(z) = u_{0h} + P_h \hat{f}(z)$. 
Fully-discrete solution

If we solve the (complex) finite element equations for $\hat{u}_h(z)$ at each quadrature point $z = z_j$, then we can compute

$$U_{N,h}(t) = \frac{1}{2\pi i} \sum_{j=-N}^{N} e^{z_j t} \hat{u}_h(z_j) z_j' \Delta \xi$$

as an approximation to

$$u_h(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} \hat{u}_h(z) \, dz = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{z(\xi) t} \hat{u}_h(z(\xi)) z'(\xi) \, d\xi.$$

The computational cost is dominated by solving the elliptic problems, and a key advantage of the method is that (unlike in a time-stepping scheme) these elliptic solves can easily be performed in parallel.
Halving the computational cost

Assuming that \( u_0 \) and \( f \) are real-valued, it follows that \( u_h \) is real-valued and so
\[
\hat{u}_h(z) = \hat{u}_h(\bar{z}).
\]
Since
\[
z(-\xi) = \overline{z(\xi)} \quad \text{and} \quad z'(-\xi) = -\overline{z'(\xi)},
\]
so
\[
z_{-j} = \overline{z_j}, \quad \hat{u}_h(z_{-j}) = \overline{\hat{u}_h(z_j)}, \quad z'_{-j}/i = \overline{z'_j/i}
\]
and therefore
\[
\frac{1}{2\pi i} \sum_{j=-N}^{-1} e^{z_j^t} \hat{u}_h(z_j) z'_j \Delta \xi = \frac{1}{2\pi i} \sum_{j=1}^{N} e^{z_j^t} \hat{u}_h(z_j) z'_j \Delta \xi.
\]
Since \( y_0 = 0 \) and \( x'_0 = 0 \), it follows that

\[
U_{N,h}(t) = \frac{1}{2\pi} e^{x_0 t} \hat{u}_h(x_0) y'_0 \Delta \xi + \frac{1}{\pi} \sum_{j=1}^{N} \Re( e^{z_j t} \hat{u}_h(z_j) z'_j / i ) \Delta \xi.
\]

In particular, it suffices to compute \( \hat{u}_h(z_j) \) for \( 0 \leq j \leq N \).

In matrix terms, we solve the \( N + 1 \) linear systems

\[
(z_j^{\alpha} M + S) \hat{U}(z_j) = z_j^{\alpha-1} \hat{G}(z_j), \quad 0 \leq j \leq N,
\]

where \( M \) and \( S \) are the mass and stiffness matrices, \( \hat{U}(z) \) is the vector of nodal values of \( \hat{u}_h(z) \), and \( \hat{G}(z_j) \) is the load vector for \( g_h(z) \).
Quadrature error

To estimate $DE_{\pm}$ we must bound

$$M_{\pm} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left\| e^{z(\xi + i\eta)} \hat{u}_h(z(\xi + i\eta)) z'(\xi + i\eta) \right\| d\xi$$

for $\eta = \delta \pm r_{\pm}$ where $0 < r_- < \delta < r_+ < \pi/2$. We saw earlier that

$$\| (zI + A_h)^{-1} v \| \leq \frac{\| v \|}{|z| \sin \varphi} \quad \text{for } z \in \Sigma_{\pi - \varphi} \text{ and } v \in V_h,$$

and

$$\left| \frac{z'(\xi + i\eta)}{z(\xi + i\eta)} \right| \leq \sqrt{\frac{1 + \sin(\delta + \eta)}{1 - \sin(\delta + \eta)}} = \frac{2}{\cos(\delta + \eta)}.$$
Since 

\[(z^\alpha I + A_h)\hat{u}_h(z) = z^{\alpha-1}g_h(z),\]

we have

\[\|\hat{u}_h(z)\| = \|z^{\alpha-1}(z^\alpha I + A_h)^{-1}g_h(z)\| \leq \frac{\|g_h(z)\|}{|z| \sin \varphi}\]

for \(z^\alpha \in \Sigma_{\pi-\varphi}\), that is, for \(z \in \Sigma_{(\pi-\varphi)/\alpha}\) and hence for \(z \in \Sigma_{\pi-\varphi}\).

Therefore,

\[M_{\pm} \leq \frac{1}{2\pi \sin \varphi} \int_{-\infty}^{\infty} |e^{z(\xi \pm ir_\pm)t}| \left\| g_h(z(\xi \pm ir_\pm)) \right\| \frac{|z'(\xi \pm ir_\pm)|}{|z(\xi \pm ir_\pm)|} d\xi\]

\[\leq \frac{1}{\pi \sin \varphi \cos(\delta \pm r_\pm)} \int_{-\infty}^{\infty} |e^{z(\xi \pm ir_\pm)t}| \left\| g_h(z(\xi \pm ir_\pm)) \right\| d\xi,\]

and similarly for TE.
Conclusion: if $\hat{f}(z)$ is analytic with

$$\|\hat{f}(z)\| \leq C_{f,\varphi} \quad \text{for } z \in \Sigma_{\pi-\varphi},$$

so that

$$\|g_h(z)\| \leq \|u_0\| + \|P_h \hat{f}(z)\| \leq \|u_0\| + C_{f,\varphi} \quad \text{for } z \in \Sigma_{\pi-\varphi},$$

then we may estimate the quadrature error as before and obtain

$$\|U_{N,h}(t) - u_h(t)\| \leq Ce^{-B(\delta)N}L(ct).$$

Thus, by the triangle inequality,

$$\|U_{N,h}(t) - u(t)\| \leq \|U_{N,h}(t) - u_h(t)\| + \|u_h(t) - u(t)\|$$

$$= O(L(ct)e^{-B(\delta)N}) + O(t^{-\alpha}h^2).$$
In practice, roundoff means that we compute

\[ U_{N,h}^*(t) = \frac{1}{2\pi i} \sum_{j=-N}^{N} e^{z_j t} \hat{u}_h(z_j) z_j' (1 + \epsilon_j) \Delta \xi \]

with \( \|\epsilon_j\|_{L_\infty(\Omega)} \leq \varepsilon \), leading to an additional perturbation

\[ \|U_{N,h}^*(t) - U_{N,h}(t)\| \leq \frac{\varepsilon}{2\pi} \sum_{j=-N}^{N} |e^{z_j t}| \|\hat{u}_h(z_j)\| |z_j'| \Delta \xi \leq \frac{\varepsilon}{\pi \sin \varphi \cos \delta} \sum_{j=-N}^{N} |e^{z_j t}| \|g_h(z_j)\| \Delta \xi \]
Since
\[
\sum_{j=-N}^{N} |e^{z_j}t| \Delta \xi = \sum_{j=-N}^{N} \exp(\mu t(1 - \sin \delta \cosh(j \Delta \xi)) \Delta \xi
\]
\[
\approx \int_{-N \Delta \xi}^{N \Delta \xi} e^{\mu t(1 - \sin \delta \cosh \xi)} d\xi \leq C e^{\mu(1 - \sin \delta)} L(\mu t \sin \delta)
\]
we conclude that
\[
\| U_{N, h}(t) - U_{N, h}(t) \| \leq C e^{\mu t(1 - \sin \delta)} L(\mu t \sin \delta) \max_{-N \leq j \leq N} \| g(z_j) \|.
\]

The optimal choices
\[
\delta_\ast = 1.1721 \quad \text{and} \quad \mu_\ast = 4.4921 N/t
\]
lead to
\[
e^{\mu_\ast t(1 - \sin \delta_\ast)} = e^{1.4224 N} = 1.422^N.
\]
Example
Suppose $h = 10^{-3}$ and $\varepsilon = 2^{-52} \approx 2.22 \times 10^{-16}$. Then

$$\varepsilon 1.422^N \geq h^2 = 10^{-6}$$

when

$$N \geq \frac{\log(10^{-6}/\varepsilon)}{\log 1.422} = 63.14.$$ 

So roundoff probably not an issue.

However, “optimal” parameter values might be problematic if a high-accuracy spatial discretisation (say a spectral method) were used. We do not want $\mu$ to be too large.
Behaviour of $\hat{f}(z)$

Example
If $f(x, t) = g(x)e^{-at}\cos \omega t$, then

$$\hat{f}(x, z) = g(x) \frac{z + a}{(z + a)^2 + \omega^2},$$

which has simple poles at $z = -a \pm i\omega$.

Example
If

$$f(x, t) = \begin{cases} g(x), & 1 < t < 2, \\ 0, & \text{otherwise}, \end{cases}$$

then

$$\hat{f}(x, z) = \int_1^2 e^{-zt} g(x) \, dt = g(x) \frac{e^{-z} - e^{-2z}}{z},$$

and

$$|e^{-2z(\xi)}| = e^{\mu(\sin \delta \cosh \xi - 1)}.$$
A more flexible approach [McLean+Thomee-2010]

Now drop the assumption that \( \hat{f}(z) \) is analytic and bounded for \( z \in \Sigma_{\pi-\varphi} \). We will describe a method based on Duhamel’s formula,

\[
    u(t) = \mathcal{E}(t)u_0 + \int_0^t \mathcal{E}(t - s)f(s) \, ds, \quad t > 0.
\]

Recall that \( \mathcal{E}(t) \), the solution operator for the homogeneous fractional diffusion equation has the series representation

\[
    \mathcal{E}(t)v = \sum_{m=0}^{\infty} E_\alpha(-\lambda_m t^\alpha) \langle v, \phi_m \rangle \phi_m, \quad A\phi_m = \lambda_m \phi_m,
\]

and the integral representation

\[
    \mathcal{E}(t)v = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} \hat{E}(z) v \, dz, \quad \hat{E}(z) = z^{\alpha-1}(z^\alpha I + A)^{-1}.
\]
Noting that
\[
\int_0^t \mathcal{E}(t - s)f(s)\, ds = \int_0^t \frac{1}{2\pi i} \int_{\Gamma} e^{z(t-s)} \hat{\mathcal{E}}(z)f(s)\, dz\, ds
\]
\[
= \frac{1}{2\pi i} \int_{\Gamma} \hat{\mathcal{E}}(z) \int_0^t e^{z(t-s)} f(s)\, ds\, dz,
\]
we define
\[
g(z, t) = e^{zt} u_0 + \int_0^t e^{z(t-s)} f(s)\, ds
\]
and deduce
\[
u(t) = \frac{1}{2\pi i} \int_{\Gamma} \hat{\mathcal{E}}(z) g(z, t)\, dz.
\]
Notice that \(g(z, t)\) is an entire function of \(z\), with
\[
\|g(z, t)\| \leq \|u_0\| + \int_0^t \|f(s)\|\, ds \quad \text{for } \Re z \leq 0 \text{ and } t \geq 0.
\]
Since $\hat{\mathcal{E}}(z) \sim z^{-1} l$ as $|z| \to \infty$ with $z \in \Sigma_{\pi - \varphi}$, we expect

$$\hat{\mathcal{E}}_0(z) = \hat{\mathcal{E}}(z) - z^{-1} l$$

to decay more rapidly than $\hat{\mathcal{E}}(z)$, which is needed to compensate for the disappearance of the factor $e^{zt}$ in the integrand.

**Theorem**
If $0 \leq \sigma \leq 1$ and $v \in D(A^\sigma)$, then

$$\|\hat{\mathcal{E}}_0(z)v\| \leq C_{\varphi,\sigma} \frac{\|A^\sigma v\|}{|z|^{1+\alpha \sigma}} \text{ for } z \in \Sigma_{\pi - \varphi},$$

where

$$C_{\varphi,\sigma} = \left(1 + \frac{1}{\sin \varphi}\right)^{1-\sigma} \left(\frac{1}{\sin \varphi}\right)^{\sigma}.$$
Proof

We have

\[ \hat{\mathcal{E}}_0(z) = \hat{\mathcal{E}}(z) - zI \]
\[ = z^{\alpha-1}(z^{\alpha}I + A)^{-1} - z^{-1}(z^{\alpha}I + A)(z^{\alpha}I + A)^{-1} \]
\[ = [z^{\alpha-1}I - z^{-1}(z^{\alpha}I + A)](z^{\alpha}I + A)^{-1} \]
\[ = -z^{-1}A(z^{\alpha}I + A)^{-1} \]
\[ = -z^{-1}[A(z^{\alpha}I + A)^{-1}]^{1-\sigma} [(z^{\alpha}I + A)^{-1}]^{\sigma} A^{\sigma} \]

and

\[ A(z^{\alpha}I + A)^{-1} = [(z^{\alpha}I + A) - z^{\alpha}](z^{\alpha}I + A)^{-1} \]
\[ = I - z^{\alpha}(z^{\alpha}I + A)^{-1}. \]
For $z \in \Sigma_{\pi - \varphi}$, our resolvent estimate gives

$$\| (z^\alpha I + A)^{-1} \| \leq \frac{1}{|z|^\alpha \sin \varphi},$$

so

$$\| \left[ (z^\alpha I + A)^{-1} \right]^\sigma \| \leq \| (z^\alpha I + A)^{-1} \|^\sigma \leq \left( \frac{1}{|z|^\alpha \sin \varphi} \right)^\sigma$$

and

$$\| \left[ A(z^\alpha I + A)^{-1} \right]^{1-\sigma} \| \leq \left( 1 + \frac{1}{\sin \varphi} \right)^{1-\sigma}.$$

Thus,

$$\| \hat{E}_0(z)v \| \leq \frac{1}{|z|} \left( 1 + \frac{1}{\sin \varphi} \right)^{1-\sigma} \left( \frac{1}{|z|^\alpha \sin \varphi} \right)^\sigma \| A^\sigma v \|. \quad \square$$
Since $\hat{E}(z) = z^{-1}I + \hat{E}_0(z)$ and

$$\frac{1}{2\pi i} \int_G z^{-1}g(z, t) \, dt = \text{res}_{z=0} \frac{g(z, t)}{z} = g(0, t) = u_0 + \int_0^t f(s) \, ds,$$

we have

$$u(t) = g(0, t) + \frac{1}{2\pi i} \int_G w_0(z, t) \, dz$$

where

$$w_0(z, t) = \hat{E}_0(z)g(z, t) = w(z, t) - z^{-1}g(z, t).$$

and $w(z, t) = \hat{E}(z)g(z, t)$ denotes the solution of the (complex) elliptic problem

$$(z^\alpha I + A)w(z, t) = z^{\alpha-1}g(z, t).$$
Similarly, if we define the spatially discrete operators

\[ \hat{\mathcal{E}}_h(z) = z^{\alpha - 1} (zI + A_h)^{-1} \quad \text{and} \quad \hat{\mathcal{E}}_0h(z) = \mathcal{E}_h(z) - z^{-1}I \]

and put

\[ g_h(z, t) = e^{zt} u_{0h} + \int_0^t e^{z(t-s)} P_h f(s) \, ds, \]

then

\[ u_h(t) = g_h(0, t) + \frac{1}{2\pi i} \int_\Gamma \hat{\mathcal{E}}_0h(z) g_h(z, t) \, dz \]

\[ = u_{0h} + \int_0^t P_h f(s) \, ds + \frac{1}{2\pi i} \int_\Gamma w_{0h}(z, t) \, dz \]

where \( w_{0h}(z, t) = \hat{\mathcal{E}}_0h(z) g_h(z, t) = w_h(z, t) - z^{-1} g_h(z, t) \), and \( w_h(z, t) \) is computed by solving the (complex) finite element equations

\[ (z^\alpha I + A_h) w_h(z, t) = z^{\alpha - 1} g_h(z, t). \]
Fully-discrete scheme

The equal-weight quadrature approximation

\[
\int_{\Gamma} w_{0h}(z, t) \, dz \approx \sum_{j=-N}^{N} w_{0h}(z_j, t) z'_j \Delta \xi
\]

leads to

\[
U_{N,h}(t) = g_h(0, t) + \frac{1}{2\pi i} \sum_{j=-N}^{N} w_{0h}(z_j, t) z'_j \Delta \xi.
\]

Lemma

If \( z = z(\xi + i\eta) \) and \( z' = z'(\xi + i\eta) \), then for \( 0 < \sigma_1 + \alpha^{-1} = \sigma \leq 1 \),

\[
\| w_h(z, t)z' \| \leq \frac{2C_{\varphi,\sigma,\sigma_1}}{\cos(\delta + \eta)} \frac{e^{\mu t(1-\sin \delta)}}{|z|^{\alpha \sigma}} \left( \| A_{h}^{\sigma} u_{0h} \| + \| A_{h}^{\sigma_1} P_{h} f(0) \| + \int_{0}^{t} \| A_{h}^{\sigma_1} P_{h} f'(s) \| \, ds \right).
\]
Outline of Proof

Integrating by parts, we find that

\[ w_h(z, t) = \hat{E}_{0h}(z) (e^{zt} u_{0h}) + \hat{E}_{0h}(z) \left( \frac{e^{zt} - 1}{z} P_h f(0) + \int_0^t \frac{e^{z(t-s)} - 1}{z} P_h f'(s) \, ds \right) \]

with

\[ \| \hat{E}_{0h}(z) u_{0h} z' \| \leq C_{\varphi, \sigma} |z'| \frac{\| A_{h}^{\sigma} u_{0h} \|}{|z|^{1+\alpha\sigma}} = C_{\varphi, \sigma} \frac{|z'|}{|z|} \frac{\| A_{h}^{\sigma} u_{0h} \|}{|z|^{\alpha\sigma}} \]

and, since \( 2 + \alpha \sigma_1 = 1 + \alpha (\sigma_1 + \alpha^{-1}) = 1 + \alpha \sigma \),

\[ \| z^{-1} \hat{E}_{0h}(z) P_h f(0) z' \| \leq C_{\varphi, \sigma_1} |z'| \frac{\| A_{h}^{\sigma_1} u_{0h} \|}{|z|^{2+\alpha\sigma_1}} = C_{\varphi, \sigma_1} \frac{|z'|}{|z|} \frac{\| A_{h}^{\sigma_1} u_{0h} \|}{|z|^{\alpha\sigma}} . \]

Now recall that \( |z'/z| \leq 2/\cos(\delta + \eta) \). \[ \square \]
Quadrature error

We saw previously that

$$|z(\xi + i\eta)| = \mu (\cosh \xi - \sin(\delta + \eta)),$$

and since

$$\frac{\cosh \xi - \sin \delta}{\frac{1}{2} e|\xi|} = 1 + e^{-2|\xi|} - 2e^{-|\xi|} \sin \delta$$

$$= (1 - e^{-|\xi|} \sin \delta)^2 + e^{-2|\xi|} \cos^2 \delta$$

$$\geq (1 - \sin \delta)^2,$$

it follows that

$$\frac{1}{|z(\xi + i\eta)|^{\alpha\sigma}} \leq \left( \frac{2}{1 - \sin(\delta + \eta)} \right)^{\alpha\sigma} \frac{e^{-\alpha\sigma|\xi|}}{\mu^{\alpha\sigma}}.$$
Set \( r = r_\pm \) such that \( 0 < \delta - r < \delta + r < \pi/2 \), and estimate

\[
\int_{-\infty}^{\infty} \| w(z(\xi \pm ir)) z'(\xi \pm ir) \| \ d\xi \leq C \frac{e^{\mu t(1-\sin \delta)}}{\mu^{\alpha \sigma}} \int_0^{\infty} e^{-\alpha \sigma \xi} \ d\xi
\]

so

\[
|DE_\pm| \leq C \frac{e^{\mu t(1-\sin \delta)}}{\mu^{\alpha \sigma}} e^{-2\pi r/\Delta \xi}.
\]

At the same time,

\[
\sum_{|j| > N} \| w_h(z_j, t) z'_j \| \Delta \xi \leq C \frac{e^{\mu t(1-\sin \delta)}}{\mu^{\alpha \sigma}} \sum_{j=N+1}^{\infty} e^{-\alpha \sigma j \Delta \xi} \Delta \xi
\]

so

\[
|TE| \leq C \frac{e^{\mu t(1-\sin \delta)}}{\mu^{\alpha \sigma}} e^{-\alpha \sigma N \Delta \xi}.
\]
Setting $2\pi r/\Delta \xi = \alpha \sigma N \Delta \xi$, and choosing $\mu > 0$ to minimise $e^{\mu t(1-\sin \delta)}/\mu^{\alpha \sigma}$, we arrive at the following estimate.

**Theorem**

*For the flexible scheme described above, if*

$$\Delta \xi = \sqrt{\frac{2\pi r}{\alpha \sigma N}} \quad \text{and} \quad \mu = \frac{\alpha \sigma}{t(1 - \sin \delta)},$$

*then*

$$\| U_{N,h}(t) - u_h(t) \| \leq Ct^{\alpha \sigma} \exp(-\sqrt{2\pi r \alpha \sigma N}).$$

*The error bound suggests choosing $\delta = \pi/4$ and $r$ slightly less than $\pi/4$.***
Example

Taking

\[ r = \frac{\pi}{4}, \quad \alpha = \frac{1}{2}, \quad \sigma = 1 \]

gives \( 2\pi r \alpha \sigma = \frac{\pi^2}{4} \) so the decay factor in the error bound is of order

\[ e^{-\frac{1}{2} \pi \sqrt{N}} = e^{-1.5708 \sqrt{N}}, \]

compared to

\[ e^{-B(\delta_*)N} = e^{-2.3157N} = 10.1315^{-N} \]

for our earlier method.
Part VIII

Convolution Quadrature
Introduction

Convolution quadrature [Lubich-1988, Lubich-2004] refers to an approximation of the form

\[
\int_0^{t_n} K(t_n - s)f(s) \, ds \approx \sum_{j=0}^n w_{n-j} f(t_j), \quad t_j = j \Delta t,
\]

where the convolution weights \(w_n = w_n(\Delta t)\) are computed directly from the Laplace transform \(\hat{K}(z)\) rather than the kernel \(K(t)\). This approach can be advantageous if \(\hat{K}(z)\) is simpler than \(K(t)\).

Convolution quadrature can be used to approximate any function of the form \(K \ast f\), and in particular the fractional integral \(I^\alpha f = \Upsilon_\alpha \ast f\).
Outline

Contour integrals again

Operational calculus

Application to fractional diffusion
Contour integrals again

Assume that $\hat{K}(z)$ is analytic and satisfies

$$|\hat{K}(z)| \leq C|z|^{-\mu} \quad \text{for } z \in \Sigma_{\pi-\varphi}, \text{ where } \mu > 0.$$  

Then, as before,

$$K(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} \hat{K}(z) \, dz, \quad t > 0.$$  

Since

$$\int_0^t K(t - s)f(s) \, ds = \int_0^t \left( \frac{1}{2\pi i} \int_{\Gamma} e^{z(t-s)} \hat{K}(z) \, dz \right) f(s) \, ds,$$

by reversing the order of integration we obtain

$$K \ast f(t) = \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z) \int_0^t e^{z(t-s)} f(s) \, ds \, dz.$$
The associated ODE

Put

\[ y(t; z) = \int_{0}^{t} e^{z(t-s)} f(s) \, ds \]

so that

\[ K \ast f(t) = \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z)y(t; z) \, dz. \]

Notice that

\[ \frac{dy}{dt} = f(t) + z \int_{0}^{t} e^{z(t-s)} f(s) \, ds \]

so \( y \) is the solution of the initial-value problem

\[ \frac{dy}{dt} - zy = f(t) \quad \text{for} \ t > 0, \ \text{with} \ y(0) = 0. \]
Implicit Euler method

Compute

\[ Y^n = Y^n(z) \approx y(t_n; z) \quad \text{where } t_n = n \Delta t, \]

by solving

\[ \frac{Y^n - Y^{n-1}}{\Delta t} - zY^n = F^n \quad \text{for } n \geq 1, \text{ with } Y^0 = 0, \]

where \( F^n = f(t_n) \). Then,

\[ K \ast f(t_n) = \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z)y(t_n; z) \, dz \]

\[ \approx \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z)Y^n(z) \, dz. \]
Generating function

Let

\[ \tilde{Y}(\zeta) = \tilde{Y}(\zeta; z) = \sum_{n=0}^{\infty} Y^n(z)\zeta^n. \]

Putting \( Y^{-1} = 0 \), we have

\[ \sum_{n=0}^{\infty} (Y^n - Y^{n-1})\zeta^n = \sum_{n=0}^{\infty} Y^n\zeta^n - \sum_{n=-1}^{\infty} Y^n\zeta^{n+1} = (1 - \zeta)\tilde{Y}(\zeta), \]

so the finite difference equation implies that

\[ \frac{1 - \zeta}{\Delta t} \tilde{Y}(\zeta) - z\tilde{Y}(\zeta) = \tilde{F}(\zeta). \]

Thus,

\[ \tilde{Y}(\zeta; z) = \frac{\tilde{F}(\zeta)}{\delta(\zeta)\Delta t^{-1} - z} \quad \text{where} \quad \delta(\zeta) = 1 - \zeta. \]
Recall

\[(K \ast f)(t_n) \approx \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z) Y^n(z) \, dz.\]

For $\Delta t$ and $|\zeta|$ sufficiently small, $\Gamma$ passes to the left of the pole at $z = \delta(\zeta)\Delta t^{-1}$, and

\[
\sum_{n=0}^{\infty} (K \ast f)(t_n)\zeta^n \approx \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z) \tilde{Y}(\zeta; z) \, dz
\]

\[
= -\frac{1}{2\pi i} \int_{\Gamma} \frac{\hat{K}(z) \, dz}{z - \delta(\zeta)\Delta t^{-1}} \tilde{F}(\zeta).
\]

Here, the integrand is $O(|z|^{-1-\mu})$ so Cauchy’s theorem gives

\[-\frac{1}{2\pi i} \int_{\Gamma} \frac{\hat{K}(z) \, dz}{z - \delta(\zeta)\Delta t^{-1}} = \hat{K}(\delta(\zeta)\Delta t^{-1}).\]

Thus,

\[\tilde{K} \ast f(\zeta) \approx \hat{K}(\delta(\zeta)\Delta t^{-1}) \tilde{F}(\zeta).\]
Weights

Define $w_n = w_n(\Delta t)$ by

$$\hat{K}(\delta(\zeta) \Delta t^{-1}) = \tilde{w}(\zeta) = \sum_{n=0}^{\infty} w_n \zeta^n,$$

then because

$$\hat{K}(\delta(\zeta) \Delta t^{-1}) \tilde{F}(\zeta) = \left( \sum_{n=0}^{\infty} w_n \zeta^n \right) \left( \sum_{m=0}^{\infty} F^m \zeta^m \right)$$

$$= \sum_{n=0}^{\infty} \left( \sum_{j=0}^{n} w_{n-j} F^j \right) \zeta^n,$$

we conclude that

$$(K \ast f)(t_n) \approx \sum_{j=0}^{n} w_{n-j} F^j = \sum_{j=0}^{n} w_j F^{n-j}.$$
Example

Suppose $K(t) = \gamma_\alpha(t)$ and so $\hat{K}(z) = z^{-\alpha}$. Then

$$\hat{K}(\delta(\zeta)\Delta t^{-1}) = ((1 - \zeta)\Delta t^{-1})^{-\alpha} = \Delta t^\alpha (1 - \zeta)^{-\alpha}$$

$$= \Delta t^\alpha \sum_{n=0}^{\infty} \binom{-\alpha}{n} (-1)^n \zeta^n,$$

showing that

$$w_n(\Delta t) = \Delta t^\alpha \binom{-\alpha}{n} (-1)^n.$$

Note that $w_n > 0$ because $w_0 = \Delta t^\alpha$ and, for $n \geq 1$,

$$\binom{-\alpha}{n} (-1)^n = \frac{-\alpha}{1} \times \frac{-\alpha - 1}{2} \times \cdots \times \frac{-\alpha - n + 1}{n} (-1)^n$$

$$= \frac{\alpha}{1} \times \frac{\alpha + 1}{2} \times \cdots \times \frac{\alpha + n - 1}{n} = \binom{\alpha + n - 1}{n}.$$
Weights when $\alpha = 1/2$ and $\Delta t = 1$
Higher-order methods

To improve on the implicit Euler method, recall that the polynomial

\[ Y^n + \frac{\Delta Y^n}{\Delta t} (t - t_n) + \frac{1}{2} \frac{\Delta^2 Y^n}{\Delta t^2} (t - t_n)(t - t_{n-1}) + \cdots + \frac{1}{p!} \frac{\Delta^p Y^n}{\Delta t^p} (t - t_n) \cdots (t - t_{n-p+1}) \]

of degree \( p \) takes the value \( Y^j \) at \( t = t_j \) for \( n - p \leq j \leq n \), where \( \Delta Y^n = Y^n - Y^{n-1} \) denotes the backward difference. Differentiating with respect to \( t \) and setting \( t = t_n \) leads to the backward differentiation formula (BDF)

\[ y'(t_n) \approx \frac{\Delta Y^n}{\Delta t} + \frac{1}{2} \frac{\Delta^2 Y^n}{\Delta t^2} \Delta t + \cdots + \frac{1}{p!} \frac{\Delta^p Y^n}{\Delta t^p} (\Delta t)(2\Delta t) \cdots ((p - 1)\Delta t). \]
Simplifying:

\[ y'(t_n) \approx \frac{\Delta Y^n}{\Delta t} + \frac{1}{2} \frac{\Delta^2 Y^n}{\Delta t} + \cdots + \frac{1}{p} \frac{\Delta^p Y^n}{\Delta t} \]

\[ = \frac{1}{\Delta t} \sum_{\ell=1}^{p} \frac{\Delta^\ell Y^n}{\ell}. \]

Compute \( Y^n(z) \approx y(t_n; z) \) by solving

\[ \frac{1}{\Delta t} \sum_{\ell=1}^{p} \frac{\Delta^\ell Y^n}{\ell} - zY^n = F^n \quad \text{for } n \geq 1, \]

with starting values \( Y^0 = Y^{-1} = \cdots = Y^{-p} = 0. \) Generating function still satisfies

\[ \frac{\delta(\zeta)}{\Delta t} \tilde{Y}(\zeta) - z\tilde{Y}(\zeta) = \tilde{F}(\zeta) \quad \text{but now} \quad \delta(\zeta) = \sum_{\ell=1}^{p} \frac{(1 - \zeta)^\ell}{\ell}. \]
\( A(\alpha) \)-Stability

The BDF of order \( p \) has the property that

\[
| \arg \delta(\zeta) | \leq \pi - \alpha \quad \text{for } |\zeta| < 1,
\]

for the following values of \( \alpha \).

\[
\begin{array}{cc}
p & \alpha \\
1 & 90^\circ \\
2 & 90^\circ \\
3 & 86^\circ \\
4 & 73^\circ \\
5 & 51^\circ \\
6 & 17^\circ \\
\end{array}
\]
Operational calculus

Notation:

\[ \hat{K}(\partial)f(t) = K \ast f(t) = \int_0^t K(t - s)f(s)\,ds \quad \text{for } t > 0. \]

In this way, since

\[ \mathcal{L}\{K \ast f\} = \hat{K}(z)\hat{f}(z), \]

we have

\[ \hat{K}(\partial)f(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} \hat{K}(z)\hat{f}(z)\,dz. \]

Explanation: if \( K(t) = 1 \) then \( \hat{K}(z) = z^{-1} \) so

\[ \partial^{-1}f(t) = \int_0^t f(s)\,ds \quad \text{and} \quad \mathcal{L}\{\partial^{-1}f\} = z^{-1}\hat{f}(z). \]
Example
For $K(t) = \gamma_{\alpha}(t) = t^{\alpha-1}/\Gamma(\alpha)$ we have $\hat{K}(z) = z^{-\alpha}$ and so

$$\partial^{-\alpha} f(t) = \gamma_{\alpha} * f(t) = \mathcal{I}^{\alpha} f(t)$$

is the fractional integral of order $\alpha > 0$, with

$$\mathcal{L}\{\partial^{-\alpha} f\} = z^{-\alpha}\hat{f}(z).$$

Example
If $K(t) = e^{at}$ then $\hat{K}(z) = (z - a)^{-1}$ so

$$(\partial - a)^{-1} f(t) = \int_{0}^{t} e^{a(t-s)} f(s) \, ds$$

with

$$\mathcal{L}\{(\partial - a)^{-1} f\} = (z - a)^{-1}\hat{f}(z).$$
Theorem

\[ \hat{K}(\partial) = \frac{1}{2\pi i} \int_\Gamma \hat{K}(z)(\partial - z)^{-1} \, dz. \]

Proof.

\[ \hat{K}(\partial)f(t) = (K \ast f)(t) = \int_0^t K(t - s)f(s) \, ds \]
\[ = \int_0^t \frac{1}{2\pi i} \int_\Gamma e^{z(t-s)} \hat{K}(z) \, dz \, f(s) \, ds \]
\[ = \frac{1}{2\pi i} \int_\Gamma \hat{K}(z) \int_0^t e^{z(t-s)} f(s) \, ds \, dz \]
\[ = \frac{1}{2\pi i} \int_\Gamma \hat{K}(z)(\partial - z)^{-1}f(t) \, dz. \]
Discrete operational calculus

Notation:

\[ \hat{K}(\partial_{\Delta t})f(t) = \sum_{0 \leq t_j \leq t} w_j(\Delta t)f(t - t_j) \quad \text{for } t > 0. \]

In particular, at \( t = t_n \),

\[ \hat{K}(\partial_{\Delta t})f(t_n) = \sum_{j=0}^{n} w_j f(t_n - t_j) = \sum_{j=0}^{n} w_j f(t_{n-j}), \]

or equivalently,

\[ \hat{K}(\partial_{\Delta t})F^n = \sum_{j=0}^{n} w_j F^{n-j} = \sum_{j=0}^{n} w_{n-j} F^j. \]
Example

If $K(t) = 1$ then $\hat{K}(z) = z^{-1}$ so

$$\hat{K}(\delta(\zeta)\Delta t^{-1}) = \left(\frac{1 - \zeta}{\Delta t}\right)^{-1} = \frac{\Delta t}{1 - \zeta} = \Delta t \sum_{n=0}^{\infty} \zeta^n$$

for $|\zeta| < 1$, showing that $w_j = \Delta t$ and hence

$$\partial_{\Delta t}^{-1} f(t) = \sum_{0 \leq t_j \leq t} f(t - t_j) \Delta t$$

$$\approx \int_0^t f(t - s) \, ds = \int_0^t f(s) \, ds = \partial^{-1} f(t).$$
Example

The function

\[ y(t) = (\partial - a)^{-1} f(t) = \int_0^t e^{a(t-s)} f(s) \, ds \]

is the solution of the initial-value problem

\[ \dot{y} - ay = f(t) \quad \text{for } t > 0, \quad \text{with } y(0) = 0. \]

The BDF solution \( Y^n \) satisfies

\[ (\delta(\zeta) \Delta t^{-1} - a) \tilde{Y}(\zeta) = \tilde{F}(\zeta), \quad F^n = f(t_n), \]

so if

\[ (\delta(\zeta) \Delta t^{-1} - a)^{-1} = \sum_{n=0}^{\infty} w_n \zeta^n, \]

then

\[ Y^n = \sum_{j=0}^{n} w_{n-j} F^j = (\partial_{\Delta t} - a)^{-1} f(t_n). \]
Example
For the BDF of order $p = 2$,

$$y'(t_n) \approx \frac{\Delta Y^n}{\Delta t} + \frac{1}{2} \frac{\Delta^2 Y^n}{\Delta t}$$

and

$$\delta(\zeta) = (1 - \zeta) + \frac{1}{2}(1 - \zeta)^2 = \frac{3}{2}(1 - \zeta)(1 - \frac{1}{3}\zeta).$$

Recalling that

$$(1 - \zeta)^{-\alpha} = \sum_{n=0}^{\infty} \binom{\alpha + n - 1}{n} \zeta^n$$

we see that the weights for $\partial_{\Delta t}^{-\alpha}$ are

$$w_n = \left(\frac{2}{3}\right)^\alpha \sum_{j=0}^{n} \binom{\alpha + n - j - 1}{n - j} \binom{\alpha + j - 1}{j} 3^{-j}.$$
Integral representation of the weights

Since

\[ \hat{K}(\delta(\zeta)\Delta t^{-1}) = \sum_{n=0}^{\infty} w_n \zeta^n, \]

for any sufficiently small \( \epsilon > 0 \) we have

\[ w_n = \frac{1}{2\pi i} \oint_{|\zeta|=\epsilon} \frac{\hat{K}(\delta(\zeta)\Delta t^{-1})}{\zeta^{n+1}} d\zeta. \]

We can use this representation to show the following result.

**Theorem**

\[ \hat{K}(\partial_{\Delta t}) = \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z)(\partial_{\Delta t} - z)^{-1} dz. \]
Proof

We have

\[ w_n = \frac{1}{2\pi i} \int_{|\zeta| = \epsilon} \frac{\hat{K}(\delta(\zeta)\Delta t^{-1})}{\zeta^{n+1}} d\zeta \]

and

\[ \hat{K}(\delta(\zeta)\Delta t^{-1}) = \frac{1}{2\pi i} \int_{\Gamma} \frac{\hat{K}(z) dz}{\delta(\zeta)\Delta t^{-1} - z} d\zeta \]

so

\[ w_n = \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z) \frac{1}{2\pi i} \int_{|\zeta| = \epsilon} \frac{(\delta(\zeta)\Delta t^{-1} - z)^{-1}}{\zeta^{n+1}} d\zeta \ dz. \]

\[ w^*_n(\Delta t; z) \]
Since

$$(\delta(\zeta)\Delta t^{-1} - z)^{-1} = \sum_{n=0}^{\infty} w^*_n(\Delta t; z)\zeta^n,$$

it follows that

$$\hat{K}(\partial_{\Delta t})f(t) = \sum_{0 \leq t_j \leq t} w_j f(t - t_j)$$

$$= \sum_{0 \leq t_j \leq t} \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z)w^*_j(\Delta t; z)\,dz f(t - t_j)$$

$$= \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z) \sum_{0 \leq t_j \leq t} w^*_j(\Delta t; z)f(t - t_j)\,dz$$

$$= \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z)(\partial_{\Delta t} - z)^{-1}f(t)\,dz. \quad \Box$$
\( \hat{K}(\partial)f(t) = \int_0^t K(t - s)f(s) \, ds = \frac{1}{2\pi i} \int_\Gamma e^{zt} \hat{K}(z)\hat{f}(z) \, dz \)

\[ = \frac{1}{2\pi i} \int_\Gamma \hat{K}(z)y(t; z) \, dz = \frac{1}{2\pi i} \int_\Gamma \hat{K}(z)(\partial - z)^{-1}f(t) \, dz. \]

\[ \hat{w}(\zeta) = \sum_{n=0}^{\infty} w_n \zeta^n = \hat{K}(\delta(\zeta)\Delta t^{-1}). \]

\[ \hat{K}(\partial_{\Delta t})F^n = \sum_{j=0}^n w_{n-j}F^j = \frac{1}{2\pi i} \oint_{|\zeta|=\epsilon} \hat{w}(\zeta)\tilde{F}(\zeta) \frac{1}{\zeta^{n+1}} \, d\zeta \]

\[ = \frac{1}{2\pi i} \int_\Gamma \hat{K}(z)Y^n(z) \, dz = \frac{1}{2\pi i} \int_\Gamma \hat{K}(z)(\partial_{\Delta t} - z)^{-1}f(t) \, dz. \]
Accuracy of convolution quadrature

Since

\[ \hat{K}(\partial_{\Delta t})f(t) = \sum_{j=0}^{\infty} w_j f(t - t_j) \chi(t - t_j), \quad \chi(t) = \begin{cases} 1, & t > 0, \\ 0, & t < 0, \end{cases} \]

we have, with \( \zeta = e^{-z \Delta t} \),

\[ \mathcal{L}\{\hat{K}(\partial_{\Delta t})f\} = \int_0^{\infty} e^{-zt} \sum_{j=0}^{\infty} w_j f(t - t_j) \chi(t - t_j) \, dt \]

\[ = \sum_{j=0}^{\infty} w_j \int_{t_j}^{\infty} e^{-zt} f(t - t_j) \, dt \]

\[ = \sum_{j=0}^{\infty} w_j \int_0^{\infty} e^{-z(t + t_j)} f(t) \, dt = \sum_{j=0}^{\infty} w_j \zeta^j \int_0^{\infty} e^{-zt} f(t) \, dt \]

\[ = \hat{K}(\delta(e^{-z \Delta t} \Delta t^{-1}) \hat{f}(z). \]
The BDF of order $p$ satisfies

$$\delta(e^{-h})h^{-1} = 1 + O(h^p) \quad \text{as } h \to 0,$$

so

$$\delta(e^{-z\Delta t})\Delta t^{-1} = z\delta(e^{-h})h^{-1}, \quad h = z\Delta t,$$

$$= z + O(z^{p+1}\Delta t^p)$$

and thus

$$\mathcal{L}\{\hat{K}(\partial_{\Delta t})f\} = \hat{K}(z + O(z^{p+1}\Delta t^p))\hat{f}(z).$$

Notice also

$$\hat{K}(\partial_{\Delta t})f(t) - \hat{K}(\partial)f(t)$$

$$= \frac{1}{2\pi i} \int_{\Gamma} \hat{K}(z)[(\partial_{\Delta t} - z)^{-1} - (\partial - z)^{-1}]f(t) \, dz.$$
(A1) There exist $0 < \varphi < \pi/2$ and $-\infty < \mu < \infty$ such that the function $G(z)$ is analytic with $|G(z)| \leq C|z|^{-\mu}$ for $|\arg z| < \pi - \varphi$.

(A2) The linear multistep method is strongly A-stable of order $p \geq 1$, that is,

1. $\delta(\zeta)$ is analytic in a neighbourhood of the closed unit disk $|\zeta| \leq 1$,
2. for $\zeta$ in this neighbourhood, $\delta(\zeta) = 0$ iff $\zeta = 1$,
3. there exists $\varphi_1 > \varphi$ such that $|\arg \delta(\zeta)| \leq \pi - \varphi_1$ for $|\zeta| < 1$,
4. $h^{-1}\delta(e^{-h}) = 1 + O(h^p)$ as $h \to 0$.

Theorem ([Lubich-2004])

If assumptions (A1) and (A2) hold, then for $0 < t < \infty$,

$$
|G(\partial_{\Delta t})t^{\beta-1} - G(\partial)t^{\beta-1}| \leq \begin{cases} 
Ct^{\mu-1+\beta-p}\Delta t^p, & p \leq \beta, \\
Ct^{\mu-1}\Delta t^\beta, & 0 < \beta \leq p.
\end{cases}
$$
Multiplication property

Notice that since

\[ K_1 \ast (K_2 \ast f) = (K_1 \ast K_2) \ast f \quad \text{and} \quad \mathcal{L}\{K_1 \ast K_2\} = \hat{K}_1(z)\hat{K}_2(z), \]

we have

\[ \hat{K}_1(\partial)\hat{K}_2(\partial) = (\hat{K}_1\hat{K}_2)(\partial), \]

so in particular \( \hat{K}_1(\partial) \) commutes with \( \hat{K}_2(\partial) \).

The analogous identity holds in the discrete case.

Theorem

\[ \hat{K}_1(\partial_{\Delta t})\hat{K}_2(\partial_{\Delta t}) = (\hat{K}_1\hat{K}_2)(\partial_{\Delta t}). \]
Proof

On the one hand,

$$\hat{K}_1(\partial_{\Delta t})\hat{K}_2(\partial_{\Delta t})f(t) = \sum_{0 \leq t_j \leq t} w_j^1 \hat{K}_2(\partial_{\Delta t})f(t - t_j)$$

$$= \sum_{0 \leq t_j \leq t} w_j^1 \sum_{0 \leq t_k \leq t - t_j} f(t - t_j - t_k)$$

$$= \sum_{0 \leq t_n \leq t} \sum_{j + k = n} w_j^1 w_k^2 f(t - t_{j+k})$$

$$= \sum_{0 \leq t_n \leq t} \left( \sum_{j=0}^{n} w_j^1 w_{n-j}^2 \right) f(t - t_n).$$
On the other hand,

\[
\hat{K}_1 (\delta (\zeta) \Delta t^{-1}) \hat{K}_2 (\delta (\zeta) \Delta t^{-1}) = \sum_{j=0}^{\infty} w_j^1 \zeta^j \sum_{k=0}^{\infty} w_k^2 \zeta^k
\]

\[
= \sum_{n=0}^{\infty} \sum_{j+k=n} w_j^1 w_k^2 \zeta^{j+k}
\]

\[
= \sum_{n=0}^{\infty} \left( \sum_{j=0}^{n} w_j^1 w_{n-j}^2 \right) \zeta^n
\]

\[
= \sum_{n=0}^{\infty} w_n \zeta^n.
\]

Example

\[
\partial_{\Delta t}^{-\alpha} \partial_{\Delta t}^{-\beta} = \partial_{\Delta t}^{-\alpha+\beta}.
\]
Associativity

Associativity of the Laplace convolution means that

\[ K \ast (f \ast g) = (K \ast f) \ast g, \]

or equivalently,

\[ \hat{K}(\partial)(f \ast g) = (\hat{K}(\partial)f) \ast g. \]

The analogous identity holds in the discrete case,

\[ \hat{K}(\partial_{\Delta t})(f \ast g) = (\hat{K}(\partial_{\Delta t})f) \ast g, \]

because

\[ \mathcal{L}\{\hat{K}(\partial_{\Delta t})(f \ast g)\} = \hat{K}(\delta(e^{-z\Delta t})\Delta t^{-1})\hat{f}(z)\hat{g}(z). \]
Remark

Taylor expansion gives

\[ f(t) = \sum_{k=0}^{p-1} \frac{f^{(k)}(0)}{k!} t^k + \frac{1}{(p-1)!} \int_0^t (t-s)^{p-1} f^{(p)}(s) \, ds \]

\[ = \sum_{k=0}^{p-1} f^{(k)}(0) \gamma_{k+1}(t) + (\gamma_p \ast f^{(p)})(t), \]

so

\[ G(\partial) f(t) = \sum_{k=0}^{p-1} f^{(k)}(0) G(\partial) t^k + (G(\partial) \gamma_p) \ast f^{(p)}(t), \]

and the same formula holds with \( \partial \) replaced by \( \partial_{\Delta t} \). Hence,

\[ \left| [G(\partial_{\Delta t}) - G(\partial)] f(t) \right| \leq C t^{\mu-1} \sum_{k=0}^{p-1} |f^{(k)}(0)| \Delta t^{k+1} \]

\[ + C \Delta t^p \int_0^t (t-s)^{\mu-1} |f^{(p)}(s)| \, ds. \]
Correction terms

If $p \geq 2$, put

$$G(\partial_{\Delta t}) \tilde{f}(t_n) = G(\partial_{\Delta t}) f(t_n) + \sum_{j=0}^{p-2} w_{nj} f(t_j)$$

and choose the extra weights $w_{nj}$ so that the modified quadrature rule is exact for polynomials up to degree $p - 2$:

$$\sum_{j=1}^{p-1} w_{nj} \gamma_k(t_j) = G(\partial) \gamma_k(t_n) - G(\partial_{\Delta t}) \gamma_k(t_n)$$

for $1 \leq k \leq p - 1$. Unfortunately, the matrix $[\gamma_k(t_j)]$ is badly conditioned.

An alternative approach works if $t_n$ is bounded away from 0.
Application to fractional diffusion

For simplicity, we suppose $f \equiv 0$ so that, after integrating in time, our initial-value problem takes the form

$$u + \partial^{-\alpha}Au = u_0,$$

or equivalently,

$$(I + \partial^{-\alpha}A)u = (I + \partial^{-\alpha}A)u_0 - \partial^{-\alpha}Au_0.$$

Thus,

$$u = u_0 - (I + \partial^{-\alpha}A)^{-1} \partial^{-\alpha}Au_0,$$

which suggests seeking $U(t) \approx u(t)$ such that

$$U = u_0 - (I + \partial^{-\alpha}_t A)^{-1} \partial^{-\alpha}Au_0.$$
Thus,

\[ U = u_0 + W \quad \text{where} \quad (I + \partial_{\Delta t}^{-\alpha} A)W = -\partial_{\Delta t}^{-\alpha} Au_0, \]

which leads to the implicit scheme

\[
W^n + \sum_{j=0}^{n} w_{n-j}AW^j = -\gamma_{1+\alpha}(t_n)Au_0 \quad \text{for } n \geq 1,
\]

with \( W^0 = 0 \), where the weights \( w_n = w_n(\Delta t) \) are given by

\[
[\delta(\zeta)\Delta t^{-1}]^{-\alpha} = \sum_{n=0}^{\infty} w_n \zeta^n.
\]

Fully-discrete version: \( U_h = u_{0h} + W_h \) where \( W_h^0 = 0 \) and

\[
W_h^n + \sum_{j=0}^{n} w_{n-j}A_hW_h^j = -\gamma_{1+\alpha}(t_n)A_hu_{0h} \quad \text{for } n \geq 1.
\]
Error bound for nonsmooth initial data

Since

\[ u - u_0 = -(I + \partial^{-\alpha} A)\partial^{-\alpha} A u_0, \]
\[ U - u_0 = -(I + \partial_{\Delta t}^{-\alpha} A)\partial^{-\alpha} A u_0, \]

the error from the time discretization is

\[ U - u = [G(\partial) - G(\partial_{\Delta t})] \partial^{-\alpha} u_0, \]

where

\[ G(z) = (I + z^{-\alpha} A)^{-1} A. \]

**Theorem ([Cuesta+Lubich+Palencia-2006])**

For \( t > 0, \)

\[ \| U(t) - u(t) \| \leq \begin{cases} 
Ct^{-1}\Delta t \| u_0 \|, & p = 1, \\
Ct^{-1-\alpha}\Delta t^{1+\alpha} \| u_0 \|, & p \geq 2.
\end{cases} \]
Proof

Since
\[
G(z) = (I + z^{-\alpha}A)^{-1}A = z^\alpha(z^\alpha I + A)^{-1}A \\
= z^\alpha(z^\alpha I + A)^{-1}[(z^\alpha I + A) - z^\alpha I] \\
= z^\alpha[I - z^\alpha(z^\alpha I + A)^{-1}]
\]
and \(\|(z^\alpha I + A)^{-1}\| \leq C|z|^{-\alpha}\), we have
\[
\|G(z)\| \leq C|z|^\alpha \quad \text{for } z \in \Sigma_{\pi-\varphi}.
\]

Noting that \(\partial^{-\alpha}u_0 = \Gamma_{1+\alpha}(t)u_0 = t^\alpha u_0/\Gamma(1 + \alpha)\), we apply the theorem with \(\mu = -\alpha\) and \(\beta = 1 + \alpha\) to conclude
\[
\|U(t) - u(t)\| = \|[G(\partial)t^\beta - G(\partial_\Delta t)t^\beta]u_0\|/\Gamma(1 + \alpha) \\
\leq C\|u_0\| \times \begin{cases} 
& t^{-p}\Delta t^p, \quad p \leq 1 + \alpha, \\
& t^{-\alpha-1}\Delta t^{1+\alpha}, \quad p \geq 1 + \alpha.
\end{cases}
\]
Error bound for smooth initial data

Recall that

\[ u(t) = E(t)u_0 = u_0 - \frac{t^\alpha}{\Gamma(1 + \alpha)} Au_0 + \cdots \quad \text{as } t \to 0, \]

and observe that

\[
(l + \partial^{-\alpha} A) \left[ u(t) - u_0 + \gamma_{1+\alpha}(t) Au_0 \right] \\
= u_0 - (l + \partial^{-\alpha} A)u_0 + (l + \partial^{-\alpha} A)\gamma_{1+\alpha}(t) Au_0 \\
= \gamma_{1+2\alpha}(t) A^2 u_0,
\]

so

\[
u(t) = u_0 - \gamma_{1+\alpha}(t) Au_0 + (l + \partial^{-\alpha} A)^{-1} \gamma_{1+2\alpha}(t) A^2 u_0.
\]

We therefore consider

\[
U(t) = u_0 - \gamma_{1+\alpha}(t) Au_0 + (l + \partial^{-\alpha} A)^{-1} \gamma_{1+2\alpha}(t) A^2 u_0.
\]
The error is

\[ U(t) - u(t) = \left[ (I + \partial_{\Delta t}^{-\alpha} A)^{-1} - (I + \partial^{-\alpha} A)^{-1} \right] \gamma_{1+2\alpha}(t) A^2 u_0 \]

\[ = \left[ G(\partial_{\Delta t}) - G(\partial) \right] \gamma_{1+2\alpha}(t) A u_0, \]

where, once again, \( G(z) = (I + z^{-\alpha} A)^{-1} A \). Applying the theorem with \( \mu = -\alpha \) and \( \beta = 1 + 2\alpha \) we have

\[ \| U(t) - u(t) \| \leq C \| A u_0 \| \times \begin{cases} t^{\alpha-p} \Delta t^p, & p \leq 1 + 2\alpha, \\ t^{-1-\alpha} \Delta t^{1+2\alpha}, & p \geq 1 + 2\alpha. \end{cases} \]

For instance, if \( p = 2 \) and \( 1/2 \leq \alpha < 1 \), then

\[ \| U(t) - u(t) \| \leq C t^{\alpha-2} \Delta t^2 \| A u_0 \|. \]
Part IX

Discontinuous Galerkin methods for time stepping
We consider a class of time-stepping methods in which $u(t)$ is approximated by a piecewise polynomial $U$ in $t$. Continuity across the time levels is enforced only weakly. These fully implicit methods are flexible and robust, and can achieve high accuracy, but are rather complicated to implement in general and have a somewhat higher computational cost than many simpler time-stepping schemes. Crucially, they allow the use of highly non-uniform grids.

Once again, we largely ignore the spatial discretization.
Outline

Discontinuous piecewise-polynomial approximation in time

Stability

Convergence
Discontinuous piecewise-polynomial approximation in time

Let \( \mathbf{t} = (t_n)_{n=0}^N \) be a vector of time levels satisfying
\[
0 = t_0 < t_1 < t_2 < \cdots < t_N = T,
\]
and denote the \( n \)th open subinterval and its length by
\[
I_n = (t_{n-1}, t_n) \quad \text{and} \quad \Delta t_n = t_n - t_{n-1} \quad \text{for } 1 \leq n \leq N.
\]

For each \( n \), choose a closed subspace \( S_n \subset H_0^1(\Omega) \) and an integer \( p_n \geq 0 \), and write \( \mathbf{S} = (S_n)_{n=0}^N \) and \( \mathbf{p} = (p_n)_{n=1}^N \).

We define our trial space \( \mathcal{W} = \mathcal{W}(\mathbf{t}, \mathbf{S}, \mathbf{p}) \) to consist of those functions \( U : (0, T) \to H_0^1(\Omega) \) such that \( U|_{I_n} \) is a polynomial of degree at most \( p_n \) in \( t \) with coefficients in \( S_n \) for \( 1 \leq n \leq N \).
Example
Choose $S_n = H^1_0(\Omega)$ and $p_n = p$ independent of $n$.

Example
Choose $S_n = V_h$ to be the usual continuous piecewise-linear finite element space with respect to a triangulation $T_h$ of $\Omega$ and enforcing a homogeneous Dirichlet boundary condition.

Thus, our methods are conforming in space but non-conforming in time.

For $U \in \mathcal{W}$, we denote the one-sided limits and the jumps at $t_n$ by

$$U_{\pm}^n = U(t_{\pm}^n) = \lim_{t \to t_{\pm}^n} U(t) \quad \text{and} \quad [U]^n = U_+^n - U_-^n$$

for $0 \leq n \leq N$, with the convention that $U_0^- \in S_0$ (even though $I_0$ is undefined).
Weak formulation

Recall that the mild solution $u$ of our initial-boundary value problem for the fractional diffusion equation satisfies

$$\langle \dot{u}(t), v \rangle + a(\partial_t^{1-\alpha} u(t), v) = \langle f(t), v \rangle \quad \text{for all } v \in H^1_0(\Omega),$$

where $\dot{u} = u_t = \partial u/\partial t$. Hence, for suitable $v : I_n \to H^1_0(\Omega)$,

$$\int_{I_n} [\langle \dot{u}(t), v(t) \rangle + a(\partial_t^{1-\alpha} u(t), v(t))] \, dt = \int_{I_n} \langle f(t), v(t) \rangle \, dt.$$

In the discontinuous Galerkin (DG) method we seek $U \in \mathcal{W}$ satisfying, for all $X \in \mathcal{W}$ and for $1 \leq n \leq N$,

$$\langle U^{n-1}_+, X^{n-1}_+ \rangle + \int_{I_n} [\langle \dot{U}(t), X(t) \rangle + a(\partial_t^{1-\alpha} U(t), X(t))] \, dt$$

$$= \langle U^{n-1}_-, X^{n-1}_+ \rangle + \int_{I_n} \langle f(t), X(t) \rangle \, dt.$$
In addition, we require that $U_0 = U^0$ for a suitable approximation $U^0 \in S_0$ to the given initial data $u_0$.

**Example**

Take $p_n = 0$ and $S_n = V_h$ for all $n$, so that $U$ and $X$ are piecewise constant in time. Writing $U^n = U^n_-$ and $\chi = X^n_-$, we have

$$U(t) = U^n = U^n_- \quad \text{and} \quad X(t) = \chi = X^n_- \quad \text{for all} \ t \in I_n,$$

with $\dot{U} = 0$ on $I_n$, so

$$\langle U^n - U^{n-1}, \chi \rangle + \int_{I_n} a(\partial_t^{1-\alpha} U(t), \chi) \, dt$$

$$= \int_{I_n} \langle f(t), \chi \rangle \, dt \quad \text{for all} \ \chi \in S_n,$$

which is essentially the implicit Euler scheme we considered earlier, but using finite elements instead of finite differences in space.
Fully implicit time stepping

If $\psi_0^n, \psi_1^n, \ldots, \psi_p^n$ is a basis for the space of polynomials of degree at most $p_n$, and if $\chi_1, \chi_2, \ldots, \chi_{M_n}$ is a basis for $S_n$ (so $M_n = \dim S_n$), then we can write

$$U(x, t) = \sum_{r=0}^{p_n} \sum_{l=1}^{M_n} U_{lr}^n(t) \psi_r^n(t) \chi_l(x) \quad \text{for } x \in \Omega \text{ and } t \in I_n.$$  

Starting from the known (approximate) initial data

$$U_0^0(x) = U^0(x) = \sum_{l=1}^{M_0} U_{l0}^0 \chi_l^0(x) \quad \text{for } x \in \Omega,$$

we compute the unknown $U_{lr}^n$ by solving the $[(p_n + 1)M_n] \times [(p_n + 1)M_n]$ linear system determined by the DG equations on $I_n$ for successive $n = 1, 2, \ldots, N$. 
Stability

We now prove a series of technical lemmas that will establish unconditional stability of DG time stepping. This robustness is a key benefit of the method, and helps justify its relatively high computational cost. The stability estimate below also shows that most of the jumps $[U]^i$ must be small for large $N$.

**Theorem**

If $U_0 = U^0 \in \mathbb{H}$ and $f \in L_2((0, T); \mathbb{H})$ then there exists a unique DG solution $U \in \mathcal{W}$, and for $1 \leq n \leq N$,

\[
\|U^n\|^2 + \sum_{j=1}^{n-1} \|U^j\|^2 + \int_0^{t_n} a(\partial_t^{1-\alpha} U, U) \, dt \\
\leq \|U^0\|^2 + \int_0^{t_n} \langle A^{-1} f, I^{1-\alpha} f \rangle \, dt.
\]
Global bilinear form

By rewriting the $n$th DG equation as

$$
\langle [U]^{n-1}, X^{n-1} \rangle + \int_{I_n} \left[ \langle \dot{U}, X \rangle + a(\partial_t^{1-\alpha} U, X) \right] dt = \int_{I_n} \langle f, X \rangle dt,
$$

and summing over $n$, we see that $U \in \mathcal{W}$ is the DG solution iff

$$
G_N(U, X) = \langle U^0, X^0 \rangle + \int_0^{t_N} \langle f(t), X(t) \rangle dt \quad \text{for all } X \in \mathcal{W},
$$

where the bilinear form $G_N$ is defined by

$$
G_N(U, X) = \langle U^0_-, X^0_+ \rangle + \sum_{n=1}^{N} \langle [U]^{n-1}, X^{n-1} \rangle
$$

$$
+ \sum_{n=1}^{N} \int_{I_n} \left[ \langle \dot{U}(t), X(t) \rangle + a(\partial_t^{1-\alpha} U(t), X(t)) \right] dt.
$$
Lemma

\[
\langle [U]^{n-1}, U_+^{n-1} \rangle + \int_{I^n} \langle \dot{U}, U \rangle \, dt = \frac{1}{2} \left( \| [U]^{n-1} \|_2^2 + \| U_+^n \|_2^2 - \| U_-^{n-1} \|_2^2 \right).
\]

Proof.

Since \( \langle \dot{U}, U \rangle = (d/dt)^{\frac{1}{2}} \| U \|_2^2 \), twice the LHS equals

\[
2\langle [U]^{n-1}, U_+^{n-1} \rangle + \| U_-^n \|_2^2 - \| U_+^{n-1} \|_2^2
\]

\[
= \langle [U]^{n-1}, [U]^{n-1} + U_+^{n-1} + U_-^{n-1} \rangle + \| U_-^n \|_2^2 - \| U_+^{n-1} \|_2^2
\]

\[
= \| [U]^{n-1} \|_2^2 + \| U_-^{n-1} \|_2^2 - \| U_+^{n-1} \|_2^2 + \| U_-^n \|_2^2 - \| U_+^{n-1} \|_2^2
\]

\[
= \| [U]^{n-1} \|_2^2 + \| U_-^n \|_2^2 - \| U_-^{n-1} \|_2^2.
\]
Lemma

\[ G_N(U, U) = \frac{1}{2} \| U_0 \|^2 + \frac{1}{2} \| U_N \|^2 + \frac{1}{2} \sum_{n=1}^{N-1} \|[U]^n\|^2 \]

\[ + \int_0^{t_N} a(\partial_t^{1-\alpha} U, U) \, dt. \]

Proof.

\[ \langle U_0^0, U_0^0 \rangle + \sum_{n=1}^{N} \left( \langle [U]^{n-1}, U_+^{n-1} \rangle + \int_{I_n} \langle \dot{U}, U \rangle \, dt \right) \]

\[ = \langle U_0^0, U_0^0 \rangle + \frac{1}{2} [U]^0 - \frac{1}{2} \| U_0^0 \|^2 + \frac{1}{2} \| U_N \|^2 + \frac{1}{2} \sum_{n=1}^{N-1} \|[U]^n\|^2. \]
To prove the next lemma, recall the identities

\[ \int_0^\infty (\partial_t^\beta u) \bar{v} \, dt = \int_{-\infty}^\infty (iy)^\beta \hat{u}(iy) \bar{\hat{v}}(iy) \, dy \]

and, when \( u \) is real-valued,

\[ \int_0^\infty (\partial_t^\beta u) u \, dt = \frac{\cos \frac{1}{2} \pi \beta}{\pi} \int_0^\infty y^\beta |\hat{u}(iy)|^2 \, dy \geq 0. \]

**Lemma**

*For* \( 0 < \beta < 1 \), and real-valued \( u \) and \( v \),

\[ \left| \int_0^\infty (\partial_t^\beta u) v \, dt \right| \leq \frac{1}{\cos \frac{1}{2} \pi \beta} \left( \int_0^\infty (\partial_t^\beta u) u \, dt \right)^{1/2} \left( \int_0^\infty (\partial_t^\beta v) v \, dt \right)^{1/2}. \]
Proof

Noting that \( \hat{u}(-iy) = \hat{u}(iy) \) and \( \hat{v}(-iy) = \hat{v}(iy) \), and using the Cauchy–Schwarz inequality, we have

\[
\left| \int_0^\infty (\partial_t^\beta u) v \, dt \right| \leq \frac{1}{2\pi} \int_{-\infty}^{\infty} |y|^{\beta} |\hat{u}(iy)| |\hat{v}(iy)| \, dy
\]

\[
= \frac{1}{\pi} \int_0^\infty \left( y^{\beta/2} |\hat{u}(iy)| \right) \left( y^{\beta/2} |\hat{v}(iy)| \right) \, dy
\]

\[
\leq \frac{1}{\pi} \left( \int_0^\infty y^{\beta} |\hat{u}(iy)|^2 \, dy \right)^{1/2} \left( \int_0^\infty y^{\beta} |\hat{v}(iy)|^2 \, dy \right)^{1/2}
\]

\[
= \frac{1}{\cos \frac{1}{2}\pi \beta} \left( \int_0^\infty (\partial_t^\beta u) u \, dt \right)^{1/2} \left( \int_0^\infty (\partial_t^\beta v) v \, dt \right)^{1/2}.
\]

\[\square\]
**Lemma**

*For* $0 < \beta < 1$,

$$2 \left| \int_0^T \langle \partial_t^\beta u, v \rangle \, dt \right| \leq \int_0^T \langle \partial_t^\beta u, u \rangle \, dt + \frac{1}{\cos^2 \frac{1}{2} \pi \beta} \int_0^T \langle \partial_t^\beta v, v \rangle \, dt.$$

**Proof.**

Extend $u$ and $v$ by zero. For any $\mu > 0$, the $m$th Fourier coefficients satisfy

$$2 \int_0^T (\partial_t^\beta u_m) v_m \, dt = 2 \int_0^\infty (\partial_t^\beta u_m) v_m \, dt$$

$$\leq \frac{1}{\cos \frac{1}{2} \pi \beta} \left( \mu \int_0^T (\partial_t^\beta u_m) u_m \, dt + \frac{1}{\mu} \int_0^T (\partial_t^\beta v_m) v_m \, dt \right),$$

and the result follows by summing over $m$, using Parseval’s identity and choosing $\mu = \cos \frac{1}{2} \pi \beta$. 

\[\square\]
Proof of the stability theorem

The DG solution $U$ satisfies

$$G_N(U, X) = \langle U^0, X^0_+ \rangle + \int_0^{t_N} \langle f(t), X(t) \rangle dt$$

for all $X \in \mathcal{W}$,

and by choosing $X = U$ the second lemma gives

$$\frac{1}{2} \| U_+^0 \|^2 + \frac{1}{2} \| U^-_N \|^2 + \frac{1}{2} \sum_{n=1}^{N-1} \| [U]^n \|^2$$

$$+ \int_0^{t_N} a(\partial_t^{1-\alpha} U, U) dt = \langle U^0, U^0_+ \rangle + \int_0^{t_N} \langle f(t), U(t) \rangle dt.$$

Now use $\langle U^0, U^0_+ \rangle \leq \frac{1}{2} \| U^0 \|^2 + \frac{1}{2} \| U^0_+ \|^2$ and cancel the term $\frac{1}{2} \| U^0_+ \|^2$. 
Thus,
\[
\|U_N\|^2 + \sum_{n=1}^{N-1} \|[U]^n\|^2 \\
+ 2 \int_0^{t_N} a(\partial_t^{1-\alpha} U, U) \, dt = \|U^0\|^2 + 2 \int_0^{t_N} \langle f(t), U(t) \rangle \, dt.
\]

Write \(\langle f(t), U(t) \rangle = \langle \partial_t^{1-\alpha} g(t), v(t) \rangle\) where
\[
g(t) = \mathcal{I}^{1-\alpha} A^{-1/2} f(t) \quad \text{and} \quad v(t) = A^{1/2} U(t),
\]
so that
\[
2 \int_0^{t_N} \langle f(t), U(t) \rangle \, dt \leq \int_0^{t_N} a(\partial_t^{1-\alpha} U, U) \, dt \\
+ \frac{1}{\cos^2 \frac{1}{2} \pi \beta} \int_0^{t_N} \langle A^{-1} f(t), \mathcal{I}^{1-\alpha} f(t) \rangle \, dt.
\]
Piecewise-constant case

If $p_n = 0$ then $\|U(t)\| \leq \|U_{n^*}\| = \max_{0 \leq n \leq N} \|U^n\|$ for $0 \leq t \leq t_N$.

Since

$$\|U_{n^*}\|^2 \leq \|U_{n^*}\|^2 + \sum_{n=1}^{n^*-1} \|[U]^n\|^2$$

$$+ 2 \int_0^{t_{n^*}} a(\partial_t^{1-\alpha} U, U) \, dt = \|U^0\|^2 + 2 \int_0^{t_{n^*}} \langle f(t), U(t) \rangle \, dt$$

and $U^0 = U_0$, we have

$$\|U_{n^*}\||U_-|| \leq \|U_{n^*}\|^2 \leq \left(\|U^0\| + \int_0^{t_{n^*}} \|f(t)\| \, dt\right)\|U_{n^*}\|,$$

so

$$\|U^n\| \leq \|U^0\| + 2 \int_0^{t_n} \|f(t)\| \, dt, \quad 0 \leq n \leq N.$$
If $p_n = 1$ for all $n$, then

$$\| U \|_{I_n} \equiv \sup_{t \in I_n} \| U(t) \| = \max \{ \| U_{n-1}^+ \|, \| U_n^- \| \}.$$ 

For the first subinterval,

$$\| U \|_{I_1}^2 \leq \| U_0^+ \|^2 + \| U_1^- \|^2 \leq 2 \langle U_0^+, U_0^- \rangle + 2 \int_0^{t_1} \langle f(t), U(t) \rangle \, dt$$

so

$$\| U \|_{I_1} \leq 2 \| U^0 \| + 2 \int_0^{t_1} \| f(t) \| \, dt.$$
For $n \geq 2$, since $U^{n-1}_n = U^{n-1}_1 + [U]^{n-1}$,

$$\|U^{n-1}_+\|^2 \leq 2\|U^{n-1}_-\|^2 + 2\|[U]^{n-1}\|^2$$

$$\leq (2 + 2)
\left(2\langle U^0, U^0_+ \rangle + 2 \int_0^{t_n} \langle f(t), U(t) \rangle \, dt \right),$$

and by choosing $n_*$ such that $\|U\|_{I_{n_*}} = \max_{1 \leq n \leq N} \|U\|_{I_n}$ we see

$$\|U\|_{I_n} \leq 8 \left(\|U^0\| + \int_0^{t_n} \|f(t)\| \, dt \right) \quad \text{for } 1 \leq n \leq N.$$  

However, for $p \geq 2$ we have not been able to prove such an $L_{\infty}(L_2)$ stability bound that mimics the one for the continuous problem:

$$\|u(t)\| \leq \|u_0\| + \int_0^t \|f(s)\| \, ds, \quad 0 \leq t \leq T.$$
Convergence

For simplicity, assume now that $S_n = H^1_0(\Omega)$ for all $n$ (so no spatial discretization). We decompose the DG error as

$$U - u = \vartheta + \varrho, \quad \vartheta = U - \Pi u, \quad \varrho = \Pi u - u,$$

where the quasi-interpolant $\Pi u \in \mathcal{W}(t, S, p)$ is defined by the conditions

$$(\Pi u)_n = u(t^-_n) \quad \text{and} \quad \int_{I_n} (u - \Pi u)t^{q-1} dt = 0$$

for $1 \leq q \leq p_n$ and $1 \leq n \leq N$, with $(\Pi u)_0^- = u(0)$.

Example

If $p_n = 0$ then $(\Pi u)(t) = u(t_n)$ for $t \in I_n$. 
Example
If $p_n = 1$ then

$$(\Pi u)(t) = u(t_n) + \frac{u(t_n) - \text{avg}_{I_n}(u)}{\Delta t_n/2}(t - t_n) \quad \text{for } t \in I_n,$$

where $\text{avg}_{I_n}(u) = \Delta t_n^{-1} \int_{I_n} u\,dt$. Can show that

$$(\Pi u)(t) - u(t) = \int_{t_n}^{t} u'(s)\,ds - 2\frac{t_n - t}{\Delta t_n^2} \int_{I_n} (s - t_{n-1})u'(s)\,ds$$

$$= \int_{t}^{t_n} (t - s)u''(s)\,ds + \frac{t_n - t}{\Delta t_n^2} \int_{I_n} (s - t_{n-1})^2u''(s)\,ds,$$

for $t \in I_n$, and hence

$$\|u - \Pi u\|_{I_n} \leq 2\int_{I_n} \|u'(t)\|\,dt \leq 2\Delta t_n\|u'\|_{I_n},$$

$$\|u - \Pi u\|_{I_n} \leq 3\Delta t_n \int_{I_n} \|u''(t)\|\,dt \leq 3\Delta t_n^2\|u''\|_{I_n}.$$
In the general case we have the following estimate.

**Theorem ([Schoetzau+Schwab-2000])**

For $0 \leq q \leq p_n$,

$$\int_{I_n} \| (u - \Pi u)'(t) \|^2 dt \leq C \epsilon(p_n, q) \left( \frac{\Delta t_n}{2} \right)^{2q} \int_{I_n} \| u^{(q+1)}(t) \|^2 dt,$$

where

$$\epsilon(p, q) = \frac{(p - q)!}{(p + q)!}.$$

Notice that

$$\epsilon(p, p) = \frac{1}{(2p)!}.$$
Recall

\[
G_N(U, X) = \langle U_0^0, X_0^0 \rangle + \sum_{n=1}^{N-1} \langle [U]^n, X^n_+ \rangle \\
+ \sum_{n=1}^N \int_{I_n} \left[ \langle \dot{U}(t), X(t) \rangle + a(\partial_t^{1-\alpha} U(t), X(t)) \right] \, dt.
\]

Integration by parts yields a dual representation

\[
G_N(U, X) = \langle U_N^0, X_N^0 \rangle - \sum_{n=1}^{N-1} \langle U^n_-, [X]^n_+ \rangle \\
+ \sum_{n=1}^N \int_{I_n} \left[ -\langle U(t), \dot{X}(t) \rangle + a(\partial_t^{1-\alpha} U(t), X(t)) \right] \, dt.
\]
For all $X \in \mathcal{W}(t, p, S)$, the DG solution satisfies

$$G_N(U, X) = \langle U^0, X^0_+ \rangle + \int_0^t \langle f(t), X(t) \rangle \, dt,$$

and, since $[u]^n = 0$, the exact solution satisfies

$$G_N(u, X) = \langle u_0, X^0_+ \rangle + \int_0^t \langle f(t), X(t) \rangle \, dt.$$

Furthermore, the construction of $\Pi$ ensures

$$\varrho^n_- = 0 \quad \text{and} \quad \int_{l_n} \langle \varrho, \dot{X} \rangle \, dt = 0 \quad \text{for} \ 1 \leq n \leq N,$$

so

$$G_N(\varrho, X) = \int_0^{t_N} a(\partial_t^{1-\alpha} \varrho, X) \, dt.$$
Thus,
\[ G_N(U - u, X) = \langle U^0 - u_0, X_+^0 \rangle, \]
and since \( U - u = \vartheta + \varrho \) we have
\[ G_N(\vartheta, X) = G_N(U - u - \varrho, X) = G_N(U - u, X) - G_N(\varrho, X). \]

Therefore,
\[ G_N(\vartheta, X) = \langle U^0 - u_0, X_+^0 \rangle + \int_0^{t_N} \langle -A\partial_t^{1-\alpha} \varrho, X \rangle \, dt \]
for all \( X \in \mathcal{W}(t, p, S) \), showing that \( \vartheta \) is the DG solution with initial data \( U^0 - u_0 \) and source term \(-\partial_t^{1-\alpha} A \varrho\). By applying the stability result to \( \vartheta \) it is possible to prove the following error estimate.
h-Version accuracy

Theorem ([Mustapha-2015])

Let $\gamma \geq 1$ and $\sigma > 0$. If

$$t_n = \left(\frac{n}{N}\right)^\gamma T \quad \text{and} \quad p = (1, p, p, \ldots, p)$$

and

$$\|u^{(j)}(t)\|_1 \leq Ct^{\sigma-j} \quad \text{for } 0 < t \leq T \text{ and } 1 \leq j \leq p + 1,$$

then

$$\|U(t) - u(t)\| \leq C\Delta t_N^r \leq CN^{-r} \quad \text{for } 0 \leq t \leq T,$$

where

$$r = \begin{cases} 
\min\{\gamma(\sigma + \frac{1}{2}\alpha - \frac{1}{2}), 2 + \frac{1}{2}\alpha - \frac{1}{2}\}, & p = 1, \\
\min\{\gamma(\sigma + \frac{1}{2}\alpha - \frac{1}{2}), p + 1 + \frac{1}{2}\alpha - \frac{1}{2}\} - \frac{1}{2}, & p \geq 2.
\end{cases}$$
Piecewise-constants on a uniform mesh

Theorem ([McLean+Mustapha-2015])

Suppose \( f \equiv 0, \ t_n = n \Delta t \) and \( p_n = 0 \) for all \( n \).

1. For \( 0 < \alpha < 1 \), if \( u_0 \in H \) then

\[
\| U^n - u(t_n) \| \leq C t^{-1}_n \Delta t \| u_0 \|.
\]

2. for \( 0 < \alpha \leq 1/2 \), if \( A^2 u_0 \in H \) then

\[
\| U_n - u(t_n) \| \leq C t^{2\alpha - 1}_n \Delta t \| A^2 u_0 \|.
\]

3. for \( 1/2 \leq \alpha < 1 \), if \( A^{1/\alpha} u_0 \in H \) then

\[
\| U_n - u(t_n) \| \leq C \Delta t \| A^{1/\alpha} u_0 \|.
\]

Corollary

\[
\| U^n - u(t_n) \| \leq C t^{r\alpha - 1}_n \Delta t \| A^r u_0 \| \text{ for } 0 \leq r \leq \min\{2, 1/\alpha\}.
\]
Part X

Further reading


William McLean and Kassem Mustapha. Time-stepping error bounds for fractional diffusion problems with non-smooth initial data.
William McLean and Vidar Thomee.  
Numerical solution via laplace transforms of a fractional order evolution equation.  

Kassem Mustapha.  
Time-stepping discontinuous galerkin methods for fractional diffusion problems.  

Dominik Schötzau and Christoph Schwab.  
Time discretization of parabolic problems by the hp-version of the discontinuous galerkin method.  

Lloyd N. Trefethen and J. A. C. Weideman.  
The exponentially convergent trapezoidal rule.  

J. A. C. Weideman and L. N. Trefethen.
Parabolic and hyperbolic contours for computing the bromwich integral.