Numerical Solution of Fractional Diffusion Equations

William McLean, UNSW, Sydney
Kassem Mustapha, KFUPM, Dharan

Bob Anderssen's 70th Birthday,
Canberra, January 2009

Fractional Diffusion

Random walk model (Metzler and Klafter, 2000): write

$$x_j = x(t_j^+), \quad x_{j+1} = x_j + \Delta x_j, \quad t_{j+1} = t_j + \Delta t_j$$

and assume probability distributions

$$\lambda_\sigma(x) = \sigma^{-1}\lambda(x/\sigma), \quad \psi_\tau(t) = \tau^{-1}\psi(t/\tau)$$

such that

$$P[a < \Delta x_j < b] = \int_a^b \lambda_\sigma(x)\,dx, \qquad -\infty < a < b < \infty,$$

$$P[a < \Delta t_j < b] = \int_a^b \psi_\tau(t)\,dt, \qquad 0 < a < b < \infty.$$

Require λ and ψ to satisfy

$$\lambda(-x) = \lambda(x) \qquad \text{for } -\infty < x < \infty,$$
$$\psi(t) \sim \frac{\text{const}}{t^{1+\nu}} \qquad \text{as } t \to \infty,$$

with $0 < \nu < 1$. Fourier transform $\hat{\lambda}$ and Laplace transform ψ^* then satisfy

$$\hat{\lambda}(\xi) = 1 - C\xi^2 + O(\xi^4), \qquad \text{as } \xi \to 0,$$
$$\psi^*(\eta) = 1 - D\eta^\nu + O(\eta), \qquad \text{as } \eta \to 0.$$

If $\sigma \to 0$ and $\tau \to 0$ with fixed ratio $K = \dfrac{C\sigma^2}{D\tau^\nu}$ then limiting density of particles $u = u(x, t)$ satisfies

$$\eta\hat{u}^* - \hat{u}(0) + K\eta^{1-\nu}\xi^2\hat{u}^*(\xi) = 0.$$

Invert transforms to get fractional diffusion equation

$$\partial_t u - K\partial_t^{1-\nu}\nabla^2 u = 0.$$

Here, $\partial^{-\nu} = \mathcal{B}_\nu$, the Riemann–Liouville fractional integration operator,

$$\mathcal{B}_\nu u(t) = \int_0^t \omega_\nu(t-s)u(s)\,ds, \qquad \omega_\nu(t) = \frac{t^{\nu-1}}{\Gamma(\nu)}.$$

Sub-diffusion observed via mean-square displacement of particle: if $\hat{u}(0) = 1$ then

$$\hat{u}^*_{\xi\xi}(0,\eta) = 2K\eta^{-\nu-1},$$

so after Laplace inversion,

$$E[x(t)^2] = \int_{-\infty}^{\infty} x^2 u(x,t)\,dt = -\hat{u}_{\xi\xi}(0,t) = \frac{2K\,t^\nu}{\Gamma(\nu+1)}.$$

Numerical solutions:

Finite Differences Henry and Langlands 2005.

Convolution Quadrature Cuesta, Lubich and Palencia 2006

Contour Integration McLean and Thomée 2009(?),
López-Fernandez, Palencia and Schädle 2006.

Write $\alpha = \nu - 1$ (so $-1 < \alpha < 0$) and

$$\mathcal{B}_\alpha u = (\mathcal{B}_{1+\alpha} u)' = (\mathcal{B}_\nu u)' = \partial_t^{1-\nu},$$

and consider abstract inhomogeneous problem

$$u' + \mathcal{B}_\alpha A u = f \quad \text{for } 0 < t < T, \text{ with } u(0) = u_0,$$

where A is a positive-semidefinite, selfadjoint linear operator with compact inverse in a real Hilbert space $\mathbb{H}$.
Energy arguments show that we have a unique (mild) solution satisfying

$$\|u(t)\| \le \|u_0\| + 2 \int_0^t \|f(s)\| \, ds \quad \text{for } t > 0.$$

Discontinuous Galerkin Method

Set up a mesh

$$0 = t_0 < t_1 < t_2 < \cdots < t_N = T,$$

and choose finite-dimensional subspaces $S_n \subseteq D(A^{1/2})$.
Let $\mathcal{W}_q$ denote the space of trial functions of the form

$$X(t) = \sum_{\ell=1}^{q} t^{\ell-1} V_\ell, \qquad V_\ell \in S_n, \quad t \in I_n = (t_{n-1}, t_n],$$

for $1 \le n \le N$, and write

$$U^n = U(t_n^-), \quad U_+^n = U(t_n^+), \quad [U]^n = U_+^n - U^n.$$

Weak formulation:

$$\langle u', v \rangle + A(\mathcal{B}_\alpha u, v) = \langle f, v \rangle$$

for any continuous $v : [0, T] \to D(A^{1/2})$.
We seek $U \in \mathcal{W}_q$ such that

$$\langle U_+^{n-1}, X_+^{n-1} \rangle + \int_{I_n} \big[\langle U', X \rangle + A\big(\mathcal{B}_\alpha U, X\big) \big] \, dt = \langle U^{n-1}, X_+^{n-1} \rangle + \int_{I_n} \langle f, X \rangle \, dt$$

for all $X \in \mathcal{W}_q$ and $1 \le n \le N$, with initial condition

$$U(0) = U^0 \quad \text{for a suitable } U^0 \approx u_0.$$

Now restrict to the special case $q = 1$ (piecewise constants). Let

$$k_n = t_n - t_{n-1}, \qquad \bar{f}^n = \frac{1}{k_n} \int_{I_n} f(t)\, dt,$$

and

$$\bar{\mathcal{B}}_\alpha^n v = \frac{1}{k_n} \int_{I_n} \mathcal{B}_\alpha v(t)\, dt = \frac{1}{k_n} \big[(\mathcal{B}_{1+\alpha} v(t_n) - \mathcal{B}_{1+\alpha} v(t_{n-1}) \big].$$

Since $U_+^{n-1} = U^n$ we find that

$$\left\langle \frac{U^n - U^{n-1}}{k_n}, V \right\rangle + A\big(\bar{\mathcal{B}}_\alpha^n U, V\big) = \langle \bar{f}^n, V \rangle \quad \text{for all } V \in S_n.$$

Nonlocal finite difference approximation to the fractional derivative:

$$\mathcal{B}_\alpha v(t_n) \approx \bar{\mathcal{B}}_\alpha^n V = k_n^{-1}\left(\beta_{nn} V^n - \sum_{j=1}^{n-1} \beta_{nj} V^j\right) \quad \text{if } v \approx V \in \mathcal{W}_1,$$

with weights

$$\beta_{nn} = \int_{I_n} \omega_{1+\alpha}(t_n - s)\, ds = \omega_{2+\alpha}(k_n) = k_n^{1+\alpha}/\Gamma(2+\alpha),$$

$$\beta_{nj} = \int_{I_j} \big[\omega_{1+\alpha}(t_{n-1} - s) - \omega_{1+\alpha}(t_n - s)\big]\, ds > 0, \quad 1 \le j \le n-1.$$

Implicit time-stepping scheme:

$$\langle U^n, V\rangle + \beta_{nn} A(U^n, V) = \langle U^{n-1} + k_n \bar{f}^n, V\rangle + \sum_{j=1}^{n-1} \beta_{nj} A(U^j, V).$$

An Error Bound

Energy argument shows unconditional stability.

Theorem

Given $U^0 \in \mathbb{H}$ and $f \in L_1\big((0,T);\mathbb{H}\big)$, the piecewise-constant ($q=1$) DG method has a unique solution $U \in \mathcal{W}_1$. Furthermore, $U^n \in D(A^{1/2})$ for $n \geq 1$, with

$$\|U^n\| \leq \|U^0\| + 2\sum_{n=1}^{N} \|\bar{f}^n\| \quad \text{for } 0 \leq n \leq N.$$

Now restrict further to the case $S_n = D(A^{1/2})$, that is, no "spatial" discretization, and let

$$k = \max_{1 \leq n \leq N} k_n.$$

The following error bound is $O(k^{1+\alpha})$ is u if $Au' \in L_1$.

Theorem

$$\|U^n - U^{n-1}\| \le \|U^0 - u_0\| + C_\alpha \sum_{j=1}^{n} \int_{I_j} (t - t_{j-1})^{1+\alpha} \|Au'(t)\|\, dt.$$

Sketch of Proof: write $U - u = \theta + \eta$ where

$$\theta(t) = U^n - u(t_n) \quad \text{and} \quad \eta(t) = u(t_n) - u(t) \quad \text{for } t \in I_n,$$

and note that $\theta \in \mathcal{W}_1$. The exact solution satisfies

$$\langle u(t_n) - u(t_{n-1}), V\rangle + k_n A(\bar{\mathcal{B}}_\alpha^n u, V) = k_n \langle \bar{f}^n, V\rangle$$

for all $V \in D(A^{1/2}$, whereas

$$\langle U^n - U^{n-1}, V\rangle + k_n A(\bar{\mathcal{B}}_\alpha^n U, V) = k_n \langle \bar{f}^n, V\rangle.$$

Subtracting, we see that

$$\begin{aligned}\langle \theta^n - \theta^{n-1}, V\rangle + k_n A(\bar{\mathcal{B}}^n_\alpha \theta, V) &= -k_n A(\bar{\mathcal{B}}^n_\alpha \eta, V)\\ &= -k_n \langle \bar{\mathcal{B}}^n_\alpha A\eta, V\rangle,\end{aligned}$$

so stability gives

$$\|U^n - u(t_n)\| = \|\theta^n\| \le \|\theta^0\| + 2\sum_{j=1}^{n} k_j \|\bar{\mathcal{B}}^n_\alpha A\eta\|.$$

We can determine $\delta_n(t)$ such that

$$\bar{\mathcal{B}}^n_\alpha A\eta = \int_0^{t_n} \delta_n(t) A u'(t)\, dt,$$

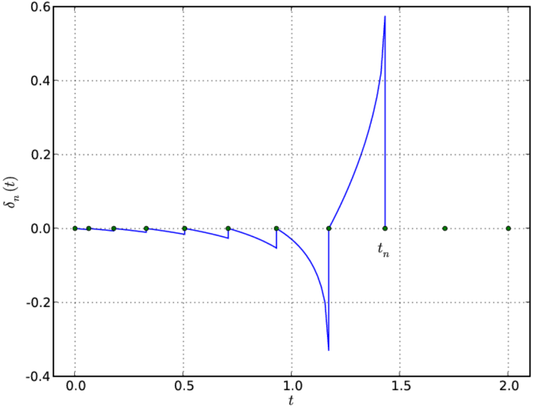
and then estimate

$$\begin{aligned}\sum_{j=1}^{n} k_j \|\bar{\mathcal{B}}^n_\alpha A\eta\| &\le \sum_{j=1}^{n}\sum_{i=1}^{j}\int_{I_i} |\delta_j(t)| \|Au'(t)\|\, dt\\ &= \sum_{i=1}^{n}\int_{I_i}\sum_{j=i}^{n} |\delta_j(t)| \|Au'(t)\|\, dt.\end{aligned}$$

Stated error bound follows from estimate

$$\sum_{j=i}^{n} |\delta_j(t)| \leq 2\omega_{2+\alpha}(t - t_{i-1}) \quad \text{for } t \in I_i,$$

but we can do better by exploiting the sign of δ_n.



First-Order Accuracy

Assume that the mesh satisfies

$$k_n \geq k_{n-1} \quad \text{and} \quad \frac{k_j}{t_n - t_j} \geq \frac{k_{n-1}}{t_{n-1} - t - j - 1} \tag{1}$$

for $3 \leq j \leq n-1$; for example, take

$$t_n = (n/N)^\gamma T, \qquad \text{with } \gamma \geq 1.$$

Theorem

The condition (1) *implies*

$$\|U^n - u(t_n)\| \leq \|U^0 - u_0\| + C_\alpha \biggl(\int_{I_1} t^{1+\alpha} \|Au'(t)\| \, dt + k_n t_n^{1+\alpha} \|Au'(t_n)\| + \sum_{j=2}^{n} k_j t_j^{1+\alpha} \int_{I_j} \|Au''(t)\| \, dt \biggr).$$

Proof uses integration by parts:

$$\int_{t_1}^{t_j} \delta_j(t) A u'(t)\, dt = -\Delta_j(t_j) A u'(t_j) + \int_{t_1}^{t_j} \Delta_j(t) A u''(t)\, dt,$$

with

$$\Delta_j(t) = -\int_{t_1}^{t} \delta_j(t)\, dt, \quad t_1 < t < t_j.$$

The condition (1) ensures $\Delta_j(t_j) < 0$.
Assuming we have $M > 0$ and $0 < \sigma < 1$ such that

$$t^{1+\alpha} \|A u'(t)\| + t^{2+\alpha} \|A u''(t)\| \le M t^{\sigma - 1} \quad \text{for } 0 < t \le T,$$

we find

$$\|U^n - u(t_n)\| \le \|U^0 - u_0\| + CM \begin{cases} k^{\gamma\sigma}, & 1 \le \gamma < 1/\sigma, \\ k \log(t_n/t_1), & \gamma = 1/\sigma, \\ t_n^{\sigma - 1/\gamma} k, & \gamma > 1/\sigma. \end{cases}$$