Optimization with respect to order in a fractional diffusion model

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Outline

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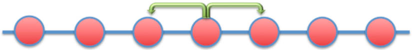
Local jump random walk

- We consider a random walk of a particle along the real line.
- $h\mathbb{Z} = \{hz : z \in \mathbb{Z}\}$ — possible states of the particle.
- $u(x,t)$ — probability of the particle to be at $x \in h\mathbb{Z}$ at time $t \in \tau\mathbb{N}$.
- Local jump random walk: at each time step of size τ, the particle jumps to the left or right with probability $1/2$.



$$u(x, t+\tau) = \frac{1}{2}u(x+h, t) + \frac{1}{2}u(x-h, t)$$

If we consider $\tau = 2h^2$, then we obtain

$$\frac{u(x,t+\tau) - u(x,t)}{\tau} = \frac{u(x+h,t) + u(x-h,t) - 2u(x,t)}{h^2}$$

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$$u_t - \Delta u = 0$$

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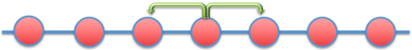

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Long jump random walk

- The probability that the particle jumps from the point $hk \in h\mathbb{Z}$ to the point $hm \in h\mathbb{Z}$ is $\mathcal{K}(k-m) = \mathcal{K}(m-k)$.

$$u(x, t+\tau) = \sum_{k\in\mathbb{Z}} \mathcal{K}(k) u(x+hk, t),$$

since $\sum_{k\in\mathbb{Z}} \mathcal{K}(k) = 1$, this yields

$$u(x, t+\tau) - u(x,t) = \sum_{k\in\mathbb{Z}} \mathcal{K}(k) \left(u(x+hk, t) - u(x,t)\right)$$

- Let $\mathcal{K}(y) \sim |y|^{-(1+2s)}$ with $s \in (0,1)$.
- Choose $\tau = h^{2s}$, then $\frac{\mathcal{K}(k)}{\tau} = h\mathcal{K}(kh)$.

Let $h, \tau \downarrow 0$,

$$\partial_t u = \int_{\mathbb{R}} \frac{u(x+y,t) - u(x,t)}{|y|^{1+2s}} \, \mathrm{d}y \Leftrightarrow \partial_t u = -(-\Delta)^s u$$

Long jump random walk

Question: What were the fundamental ingredients that led to a fractional heat equation?

- $\mathcal{K}(y) \sim |y|^{-(1+2s)}$ with $s \in (0,1)$, but the construction would have worked with another kernel, thus obtaining another nonlocal operator.
- $\tau = h^{2s}$. The space and time must have a particular scaling!

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Outline

The model problem

- The data:
  - $\Omega \subset \mathbb{R}^n$, open, convex and with Lipschitz boundary.
  - $\mathsf{f}, \mathsf{u}_d : \Omega \to \mathbb{R}$, "nice" enough.
- The problem: Find $(\bar{s}, \bar{\mathsf{u}})$ that minimize

$$J(s,u) = \frac{1}{2}\|u - \mathsf{u}_d\|^2_{L^2(\Omega)} + \varphi(s)$$

  subject to $(-\Delta)^s u = \mathsf{f}$.
- Where:
  - For $0 \leq \alpha < \beta \leq 1$, $\varphi \in C^2(\alpha, \beta)$ is nonnegative, convex and

$$\lim_{s \downarrow \alpha} \varphi(s) = \lim_{s \uparrow \beta} \varphi(s) = +\infty.$$

    For instance,

$$\varphi(s) = (s-\alpha)^{-1}(\beta - s)^{-1}, \qquad \varphi(s) = (s-\alpha)^{-1} e^{(\beta - s)^{-1}}.$$

  - $(-\Delta)^s$ denotes the fractional powers of the Dirichlet Laplacian.

The model problem

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  subject to

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Question: What are we trying to model here?

- Given some "observations/measurements" u_d, can we find the order of fractional diffusion s that best represents them?

Comment: This problem was originally considered by (Sprekels, Valdinoci 2016) for the fractional heat operator $\partial_t + (-\Delta)^s$, the authors show existence of solutions and optimality conditions.

Outline

Spectral theory 101

We consider the definition of $(-\Delta)^s$ based on spectral theory:

- $-\Delta : H^2(\Omega) \cap H_0^1(\Omega) \subset L^2(\Omega) \to L^2(\Omega)$ is symmetric, closed and unbounded and its inverse is compact.
- The eigenpairs $\{\lambda_k, \varphi_k\}$, i.e.

  $$-\Delta\varphi_k = \lambda_k\varphi_k, \qquad \varphi_k|_{\partial\Omega} = 0$$

  form an orthonormal basis of $L^2(\Omega)$.
- For u sufficiently smooth:

  $$u = \sum_{k=1}^{\infty} u_k\varphi_k \longmapsto (-\Delta)^s u := \sum_{k=1}^{\infty} u_k\lambda_k^s\varphi_k$$

- $(-\Delta)^s : \mathbb{H}^s(\Omega) \to \mathbb{H}^{-s}(\Omega)$, $\mathbb{H}^s(\Omega) = [H_0^1(\Omega), L^2(\Omega)]_{1-s}$.

The control to state map

- For $\mathsf{f} = \sum_k \mathsf{f}_k \varphi_k \in \mathbb{H}^{-s}(\Omega)$ the solution to the state equation is
$$\mathsf{u} = \sum_k \lambda_k^{-s} \mathsf{f}_k \varphi_k.$$
- This defines: $(0,1) \ni s \mapsto \mathcal{S}(s) = \sum_k \lambda_k^{-s} \mathsf{f}_k \varphi_k \in L^2(\Omega)$.

Theorem (properties of $\mathcal{S}$)

For $\mathsf{f} \in L^2(\Omega)$ the control to state map $\mathcal{S}$ is bounded
$\|\mathcal{S}(s)\|_{L^2(\Omega)} \lesssim 1$,
and three times Fréchet differentiable:

$$\mathcal{S}'(s) = -\sum_k \lambda_k^{-s} \ln(\lambda_k) \mathsf{f}_k \varphi_k =: \mathsf{u}'(s)$$
$$\mathcal{S}''(s) = \sum_k \lambda_k^{-s} \ln^2(\lambda_k) \mathsf{f}_k \varphi_k =: \mathsf{u}''(s)$$

with
$$\|\mathcal{S}^{(k)}(s)\|_{\mathbb{R} \to L^2(\Omega)} \lesssim s^{-k}, \ k = 1, 2, 3.$$

Existence

Since the state equation always has a solution, we introduce the reduced cost

$$f(s) = J(s, \mathcal{S}(s)).$$

Theorem (existence)

There is an optimal pair $(\bar{s}, \bar{\mathrm{u}} = \mathcal{S}(\bar{s})) \in (\alpha, \beta) \times \mathbb{H}^{\bar{s}}(\Omega)$ *for which*

$$f(\bar{s}) \leq f(s), \quad \forall s \in (\alpha, \beta).$$

Proof.

- The function f in continuous on (α, β).
- Consider sequences $\alpha_k \downarrow \alpha$, $\beta_k \uparrow \beta$ and seek for

$$s_k = \underset{s \in [\alpha_k, \beta_k]}{\operatorname{argmin}} f(s).$$

- Any accumulation point of $\{s_k\}_{k \geq 1}$ is a minimizer.

Optimality conditions

Theorem (optimality conditions)

- *First order necessary condition: If $(\bar{s}, \bar{\mathsf{u}}(\bar{s}))$ is optimal, then*

$$(\bar{\mathsf{u}}(\bar{s}) - \mathsf{u}_d, \bar{\mathsf{u}}'(\bar{s}))_{L^2(\Omega)} + \varphi'(\bar{s}) = 0 \qquad (f'(\bar{s}) = 0).$$

- *second order sufficient condition: If $(\bar{s}, \bar{\mathsf{u}}(\bar{s}))$ satisfies the first order condition and, in addition,*

$$\|\bar{\mathsf{u}}'(\bar{s})\|^2_{L^2(\Omega)} + (\bar{\mathsf{u}}(\bar{s}) - \mathsf{u}_d, \bar{\mathsf{u}}''(\bar{s}))_{L^2(\Omega)} + \varphi''(\bar{s}) > 0, \quad (f''(\bar{s}) > 0)$$

  then the pair is optimal.

- In essence, we are dealing with the unconstrained minimization of a twice differentiable function over an open set.

What about (local) uniqueness?

Assume that φ is strongly convex, i.e., there is $\xi > 0$

$$(\varphi'(s_1) - \varphi'(s_2)) \cdot (s_1 - s_2) \geq \xi |s_1 - s_2|^2, \forall s_1, s_2 \in (\alpha, \beta)$$

then we have:

Theorem (local uniqueness)

Assume that φ is strongly convex, $\|\mathsf{f}\|_{L^2(\Omega)}$ and $\|\mathsf{u}_d\|_{L^2(\Omega)}$ are small enough. If $\bar{s}$ is optimal, there is $\delta > 0$ and $\eta > 0$ such that

$$f(s) \geq f(\bar{s}) + \eta |s - \bar{s}|^2, \quad \forall s \in (\alpha, \beta) \cap (\bar{s} - \delta, \bar{s} + \delta).$$

- This implies local uniqueness.

Outline

Disclaimer

Up to now we could have

$$\alpha = 0 \qquad \beta = 1$$

from now on we require

$$\alpha > 0 \qquad \beta < 1$$

Discretization in s

- For $\sigma > 0$ introduce the centered difference operator

$$d_\sigma \psi(s) = \frac{1}{2\sigma} \left(\psi(s+\sigma) - \psi(s-\sigma) \right).$$

- Recall that, for $\psi \in C^3$

$$|\psi'(s) - d_\sigma \psi(s)| = \mathcal{O}(\sigma^2).$$

- We will discretize the first order optimality condition and seek for $s_\sigma \in (\alpha, \beta)$ such that

$$j_\sigma(s_\sigma) = (\mathsf{u}(s_\sigma) - \mathsf{u}_d, d_\sigma \mathsf{u}(s_\sigma))_{L^2(\Omega)} + \varphi'(s_\sigma) = 0.$$

How do we find s_σ?

```
0 < σ ≪ 1 and set s_l, s_r ∈ (α, β), with s_l < s_r;                ▷ Initialization
                                         ▷ We take care of possible degenerate cases
if j_σ(s_l) = 0 then
    s_σ = s_l;
end if
if j_σ(s_r) = 0 then
    s_σ = s_r;
end if
                                                                   ▷ Root isolation
while j_σ(s_r) < 0 do
    s_r := s_r + σ;
end while
while j_σ(s_l) > 0 do
    s_l := s_l − σ;
end while
                                                                        ▷ Bisection
k = 1;
repeat
    s_k = (1/2)(s_l + s_r);
    if j_σ(s_k) = 0 then
        s_σ = s_k;
        break;                                       ▷ The solution has been found
    end if
    if j_σ(s_l) j_σ(s_k) > 0 then                                      ▷ Sign check
        s_l = s_k;
    else
        s_r = s_k;
    end if
    k = k + 1;
until forever
```

Bisection method

Does the root isolation step finish?

Lemma (root isolation)

If σ is sufficiently small there are $s_l, s_r \in (\alpha, \beta)$ for which

$$j_\sigma(s) < 0 \; s \in (\alpha, s_l), \qquad j_\sigma(s) > 0 \; s \in (s_r, \beta).$$

A standard argument then yields

Lemma (convergence of bisection)

The bisection method generates a sequence $\{s_k\}_{k\geq 1}$ that satisfies

$$|s_\sigma - s_k| \lesssim 2^{-k}.$$

With $j_\sigma(s_\sigma) = 0$.

What about convergence of s_σ?

- The optimal $\bar{s}$ need not be unique. Thus, we do not expect convergence of the whole family s_σ to s.
- The following statement is the best we can hope for.

Lemma (convergence of s_σ)

The family $\{s_\sigma\}_{\sigma>0}$ has a convergent subsequence and any accumulation point satisfies the first order condition.

- If we focus on one of these subsequences we can establish a rate.

Theorem (rate in σ)

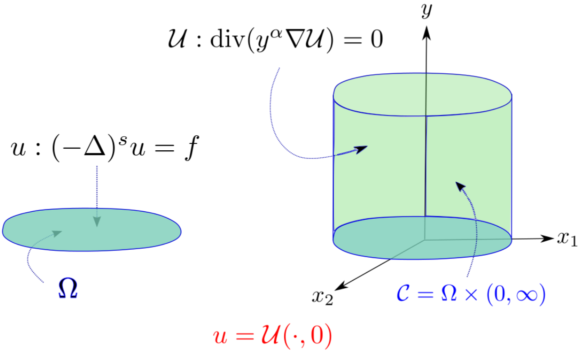
If σ is sufficiently small we have

$$|\bar{s} - s_\sigma| \lesssim \sigma^2.$$

Outline

The α-harmonic extension

Molčanov, Ostrovskiĭ (1969), Caffarelli, Silvestre (2007), Cabré, Tan (2010), Capella et al. (2011), Stinga Torrea (2010–2012).



- $s \in (0,1)$ and $\alpha = 1 - 2s \in (-1,1)$.
- $\partial_{\nu^\alpha} \mathcal{U} = -\lim_{y \downarrow 0} y^\alpha \partial_y \mathcal{U}$ on $\Omega \times \{0\}$.
- $d_s = 2^\alpha \Gamma(1-s)/\Gamma(s)$.

The α-harmonic extension

- Recall that $\alpha = 1 - 2s \in (-1, 1)$, y^α is degenerate $(\alpha > 0)$ or singular $(\alpha < 0)$!
- But y^α is a Muckenhoupt weight.
- The domain $\mathcal{C} = \Omega \times (0, \infty)$ is infinite!
- We can consider a truncated version and incur in an exponentially small error:

$$\|\mathcal{U} - \mathcal{V}\|_{\mathring{H}^1_L(y^\alpha, \mathcal{C}_\Upsilon)} \lesssim e^{-\sqrt{\lambda_1}\Upsilon/4}.$$

- The solution has a rather bad behavior $\mathcal{U}_{yy} \approx y^{-\alpha-1}$ as $y \approx 0^+$.
- We use anisotropic meshes.

Discretization

- Denote: $\mathscr{T}_\mathcal{Y}$ the mesh and $\mathbb{V}(\mathscr{T}_\mathcal{Y})$ the discrete space. Then

$$\|\mathcal{V} - V_{\mathscr{T}_\mathcal{Y}}\|_{\mathring{H}^1_L(y^\alpha, \mathcal{C}_\mathcal{Y})} = \inf_{W \in \mathbb{V}(\mathscr{T}_\mathcal{Y})} \|\mathcal{V} - W\|_{\mathring{H}^1_L(y^\alpha, \mathcal{C}_\mathcal{Y})},$$

  and set $W = \Pi\mathcal{V} \in \mathbb{V}(\mathscr{T}_\mathcal{Y})$. We need to construct a suitable interpolation operator.

  N. O. S. *Piecewise polynomial interpolation in Muckenhoupt weighted Sobolev spaces*. Numer. Math 2016.

- If the mesh is suitably graded:

$$\begin{aligned}\|u - V_{\mathscr{T}_\mathcal{Y}}(\cdot, 0))\|_{\mathbb{H}^s(\Omega)} &\le \|\nabla(\mathcal{U} - V_{\mathscr{T}_\mathcal{Y}})\|_{L^2(y^\alpha, \mathcal{C})} \\ &\lesssim |\log \#\mathscr{T}_\mathcal{Y}|^s \#\mathscr{T}_\mathcal{Y}^{-\frac{1}{n+1}}.\end{aligned}$$

  which is near optimal estimate in terms of degrees of freedom.

  N. O. S. *A PDE approach to fractional diffusion*. Found. Comp. Math. 2015.

- This formulation allows us to devise multigrid methods

  L. Chen, N. O. S. *Multilevel methods for nonuniformly elliptic equations*. Math. Comp. 2016.

The discrete control to state map

- All the hidden constants in the previous discussion depend on s, but since $s \in (\alpha, \beta) \Subset (0,1)$ they are uniformly controlled.
- Define $S_{\mathscr{T}} : (\alpha, \beta) \to \mathbb{U}(\mathscr{T}_\Omega)$ by $s \mapsto U_{\mathscr{T}_\Omega} = V_{\mathscr{T}_\mathcal{Y}}(\cdot, 0)$

Lemma (continuity of $S_{\mathscr{T}}$)

For every $\mathscr{T}_\mathcal{Y}$ the map $S_{\mathscr{T}}$ is continuous on (α, β).

- All norms in finite dimensions are equivalent.

Fully discrete scheme

Define

$$j_{\sigma,\mathscr{T}}(s) = (U_{\mathscr{T}_\Omega}(s) - \mathsf{u}_d, d_\sigma U_{\mathscr{T}_\Omega}(s))_{L^2(\Omega)} + \varphi'(s).$$

We seek for $s_{\sigma,\mathscr{T}}$ such that

$$j_{\sigma,\mathscr{T}}(s_{\sigma,\mathscr{T}}) = 0.$$

- The continuity of $S_{\mathscr{T}}$ implies that we can find it by using bisection as before.

Error estimates

- As before, we can only expect that a subsequence of $\{s_{\sigma,\mathscr{T}}\}_{\mathscr{T}}$ converges to a s_σ.
- If we extract this subsequence then we have.

Theorem (rate of convergence)

If $\mathsf{f} \in \mathbb{H}^{1-\epsilon}(\Omega)$ *for all* $\epsilon > 0$ *we have*

$$|\bar{s} - s_{\sigma,\mathscr{T}}| \lesssim \sigma^{-1} |\log(\#\mathscr{T}_{\mathcal{Y}})|^2 \, (\#\mathscr{T}_{\mathcal{Y}})^{-1/(n+1)} + \sigma^2.$$

Corollary (explicit rate)

Choose $\sigma \approx |\log(\#\mathscr{T}_{\mathcal{Y}})|^{2/3} \, (\#\mathscr{T}_{\mathcal{Y}})^{-\frac{1}{3(n+1)}}$ *then*

$$|\bar{s} - s_{\sigma,\mathscr{T}}| \lesssim |\log(\#\mathscr{T}_{\mathcal{Y}})|^{2/3} \, (\#\mathscr{T}_{\mathcal{Y}})^{-\frac{2}{3(n+1)}}$$

Outline

Generalities

- $\Omega = (0,1)^2$
- $\mathscr{Y} = 1 + \frac{1}{3}(\#\mathscr{T}_\Omega)$
- $\sigma = \frac{1}{2.5}\left(\#\mathscr{T}_{\mathscr{Y}}\right)^{-1/9}$
- The initial bounds are $s_l = 0.3$ and $s_r = 0.9$

In this geometry we have

$$\lambda_{k,l} = \pi^2(k^2 + l^2), \qquad \varphi_{k,l}(x,y) = \sin(k\pi x)\sin(l\pi y).$$

So if, for $s \in (0,1)$

$$\mathsf{f} = \lambda_{2,2}^s \varphi_{2,2} \implies \mathsf{u} = \varphi_{2,2}$$

Example 1: $\bar{s} = 1/2$

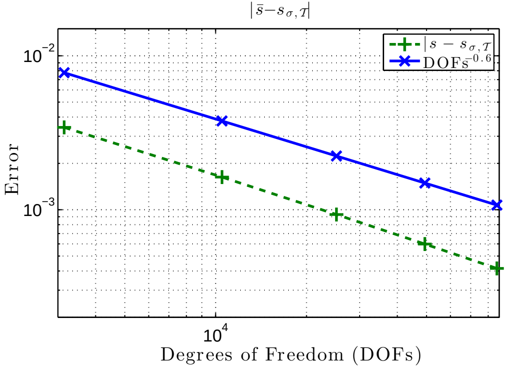
Set

$$\varphi(s) = \frac{1}{s(1-s)}$$

The following table shows the computed value of $s_{\sigma,\mathscr{T}}$ and the number of bisection iterations.

$\#\mathscr{T}_{\mathcal{Y}}$	$s_{\sigma,\mathscr{T}}$	$j_{\sigma,\mathscr{T}}(s_{\sigma,\mathscr{T}})$	N
3146	4.96572e-01	-8.89011e-14	53
10496	4.98371e-01	-8.38218e-14	53
25137	4.99069e-01	3.49235e-14	53
49348	4.99402e-01	1.52327e-12	53
85529	4.99585e-01	6.28221e-12	53

Example 1: $\bar{s} = 1/2$. Convergence rate



- The rate of convergence is $\mathcal{O}(\#\mathscr{T}_{\mathcal{Y}}^{-0.6})$ which is better than the predicted rate of -0.22!

Example 2: $\bar{s} = (3 - \sqrt{5})/2$

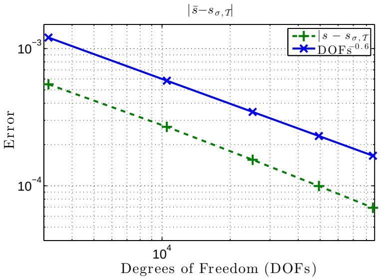
Set

$$\varphi(s) = \frac{1}{s} e^{\frac{1}{(1-s)}}$$

The following table shows the computed value of $s_{\sigma,\mathscr{T}}$ and the number of bisection iterations.

$\#\mathscr{T}_{\mathcal{Y}}$	$s_{\sigma,\mathscr{T}}$	$j_{\sigma,\mathscr{T}}(s_{\sigma,\mathscr{T}})$	N
3146	3.81417e-01	9.99201e-16	46
10496	3.81697e-01	-2.52812e-13	53
25137	3.81811e-01	1.36418e-12	53
49348	3.81866e-01	2.66251e-12	53
85529	3.81897e-01	3.53083e-12	53

Example 2: $\bar{s} = (3 - \sqrt{5})/2$. Convergence rate



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Example 3. Unknown solution

$$
\begin{aligned}
\varphi(s) &= \frac{1}{s} e^{\frac{1}{(1-s)}}, \\
\mathsf{u}_d &= \max\left\{0, \frac{1}{2} - \sqrt{|x - \frac{1}{2}|^2 + |y - \frac{1}{2}|^2}\right\}, \\
\mathsf{f} &= 10 \notin \mathbb{H}^{\mu}(\Omega),\ \mu \geq \frac{1}{2}
\end{aligned}
$$

We do not know the solution, but we can still compute.
The following table shows the computed value of $s_{\sigma,\mathscr{T}}$ and the number of bisection iterations.

$\#\mathscr{T}_{\mathcal{Y}}$	$s_{\sigma,\mathscr{T}}$	$j_{\sigma,\mathscr{T}}(s_{\sigma,\mathscr{T}})$	N
3146	4.44005e-01	4.22951e-12	53
10496	4.47239e-01	2.97451e-11	53
25137	4.48182e-01	-3.20792e-11	53
49348	4.48544e-01	4.83542e-11	53
85529	4.48690e-01	2.68390e-10	53

Outline

Recap

- Parameter identification problem: The parameter is the order of the fractional elliptic operator.
- Existence and optimality conditions: Local uniqueness under smallness assumptions.
- Semidiscrete scheme: Convergence up to subsequences. Rate of convergence for subsequences.
- Fully discrete scheme: ídem.

Open questions

- Can we let $\alpha = 0$ and $\beta = 1$? The numerics seem to indicate that this is not an issue.
- Modulo technicalities we can also handle the time dependent problem, where the state equation is $\partial_t u + (-\Delta)^s u = \mathsf{f}$.
- Completely open: Space time fractional $\partial_t^\gamma u + (-\Delta)^s u = \mathsf{f}$ and optimize in s and γ.
- Ongoing: Consider the integral version of $(-\Delta)^s$ (with M. D'Elia).