Diffusion, fractional derivatives and inverse problems

Mikko Salo
University of Jyväskylä

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Outline

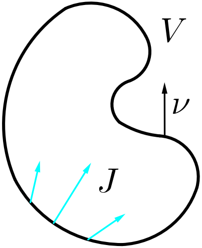
1. Normal diffusion / heat equation
2. Anomalous diffusion / fractional equations
3. Inverse problems

Diffusion

Diffusion describes the spreading out of particles or "intensity" from regions of high concentration to low.

Mathematical model

Let $u(x,t)$ be the intensity at point $x \in \mathbb{R}^n$ at time t. If $V \subset \mathbb{R}^n$ is a smooth subdomain,



$$\underbrace{\frac{\partial}{\partial t}\left[\int_V u(x,t)\,dx\right]}_{\text{intensity change in } V} = -\underbrace{\int_{\partial V} J(x,t)\cdot\nu(x)\,dS(x)}_{\text{total flux through } \partial V}$$

$$\implies \int_V \frac{\partial u}{\partial t}(x,t)\,dx = -\int_V \underbrace{\operatorname{div}_x J(x,t)}_{\sum_{j=1}^n \frac{\partial J_k}{\partial x_k}}\,dx \qquad \left(\begin{array}{c}\text{Gauss divergence}\\ \text{theorem}\end{array}\right)$$

$$\implies \frac{\partial u}{\partial t}(x,t) = -\operatorname{div}_x J(x,t). \qquad \left(V \text{ arbitrary}\right)$$

Mathematical model

In diffusion, the flux J is from regions of higher to lower concentration. The simplest model is

$$J(x,t) = -D\nabla_x u(x,t) \qquad (D > 0). \tag{$*$}$$

If u denotes the $\left\{ \begin{array}{c} \text{chemical concentration} \\ \text{temperature} \\ \text{electric potential} \end{array} \right\}$,

then $(*)$ is $\left\{ \begin{array}{c} \text{Fick's law of diffusion} \\ \text{Fourier's law of heat conduction} \\ \text{Ohm's law of electrical conduction} \end{array} \right\}$.

Mathematical model

Letting $D \equiv \frac{1}{2}$ and combining

$$\begin{cases} \frac{\partial u}{\partial t} = -\mathrm{div}_x J, \\ J = -\frac{1}{2}\nabla_x u \end{cases}$$

leads to the equations

$$\frac{\partial u}{\partial t} = \frac{1}{2}\Delta u, \qquad (\textit{heat equation})$$

$$\Delta u = 0. \qquad (\textit{Laplace equation})^1$$

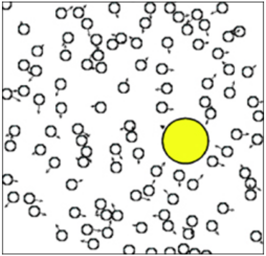
Here Δ is the *Laplace operator*

$$\Delta u = \mathrm{div}(\nabla u) = \sum_{j=1}^{n} \frac{\partial^2 u}{\partial x_j^2}.$$

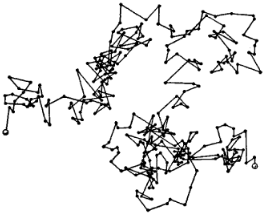
[1] steady state heat equation, where u is independent of t

Brownian motion

R. Brown (1827) observed the continuous jittery motion of microscopic particles suspended in water, due to the particle being pushed around by water molecules in thermal motion.



Molecular scale

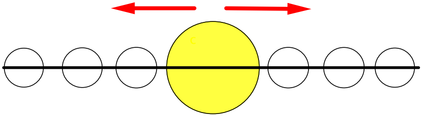


Microscopic

Macroscopic

Brownian motion

1D Brownian motion $(B_t)_{t\geq 0}$ is a scaling limit of random walk:



Suppose that when time increases from t to $t+\Delta t$, the particle is pushed Δx units either left or right. Then

$$B_{N\Delta t} \approx (\Delta x)(X_1 + \ldots + X_N)$$

where X_j are i.i.d. with $\mathbb{P}(X_j = \pm 1) = \frac{1}{2}$. If $\Delta t = \frac{1}{N}$, then

$$\mathbb{E}[\,|B_1|^2\,] \approx (\Delta x)^2 \mathbb{E}[\,(X_1 + \ldots + X_N)^2\,] = N(\Delta x)^2.$$

Normalizing B_1 to have variance 1 forces $\Delta x = \frac{1}{\sqrt{N}}$.

Brownian motion

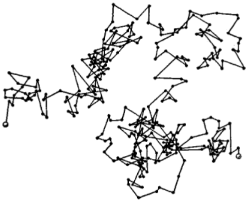
Try to define 1D Brownian motion $(B_t)_{t\geq 0}$ by

$$B_t = \lim_{N\to\infty} B_t^{(N)}, \qquad B_t^{(N)} = \frac{X_1 + \ldots + X_{\lfloor tN \rfloor}}{\sqrt{N}}.$$

Central limit theorem (connection to normal distribution $N(0,t)$)

$\implies$ limit exists (for each *fixed* t) and $B_t \sim N(0,t)$.

Donsker's theorem: $(B_t^{(N)})_{t\geq 0}$ converges in distribution to $(W_t)_{t\geq 0}$ (*Wiener process*), a process with independent Gaussian increments and almost surely continuous paths.



(In $\mathbb{R}^n$, treat each coordinate separately.)

Macroscopic picture

Let $u(x,t)$ be the density of Brownian particles at x at time t, if the initial density is $f(x)$. Heuristically,

$$\begin{aligned} u(x,t) &= \int_{\mathbb{R}^n} \#\{\text{particles jumping to } x \text{ in time } t \text{ from } y\}\, dy \\ &= \int_{\mathbb{R}^n} f(y) p_t(x-y)\, dy \end{aligned}$$

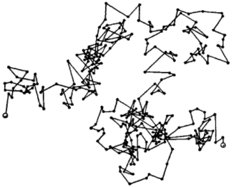
where $p_t(x) = \frac{1}{(2\pi t)^{n/2}} e^{-\frac{|x|^2}{2t}}$ is the probability density of B_t.

Thus $u(x,t)$ solves the *heat equation*

$$\begin{cases} \frac{\partial u}{\partial t} = \frac{1}{2}\Delta u & \text{in } \mathbb{R}^n \times \{t > 0\}, \\ u\big|_{t=0} = f. \end{cases}$$

Universality

Central limit and Donsker's theorems: microscopic particles follow Brownian motion, *no matter what the probability law* for the i.i.d. jumps X_j (assuming mean zero and finite variance).



Partly explains the success of the *normal diffusion* model, based on the heat and Laplace equations

$$\frac{\partial u}{\partial t} = \frac{1}{2}\Delta u,$$
$$\Delta u = 0.$$

Outline

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2. Anomalous diffusion / fractional equations
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Anomalous diffusion

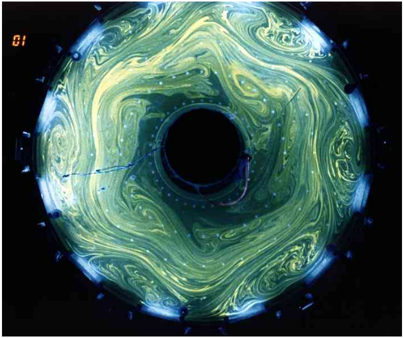
Normal diffusion arises in environments "close to equilibrium", and when the conditions of the Central Limit Theorem are met. In other cases, the diffusion will be called *anomalous*.

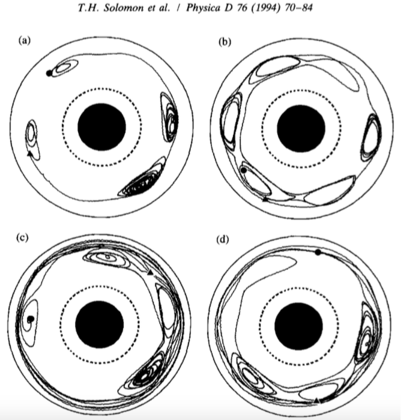
We will describe a model for anomalous diffusion that enjoys both a probabilistic and PDE interpretation.

- Probabilistically, this will involve random walks having *infinite variance* jumps, or where the waiting time between jumps is also random.
- Analytically, this will involve heat and Laplace type equations with fractional derivatives.

Turbulent fluids

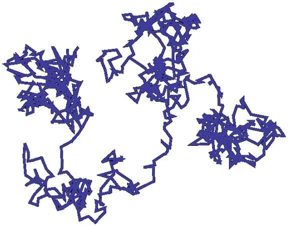
Trajectories of particles in a rotating annulus filled with water.



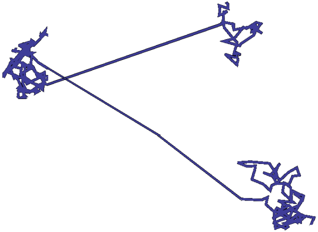


Lévy flight foraging hypothesis

Predators may follow Brownian motion in prey-abundant areas, but switch to Lévy flights in regions where prey is sparsely and unpredictably distributed.



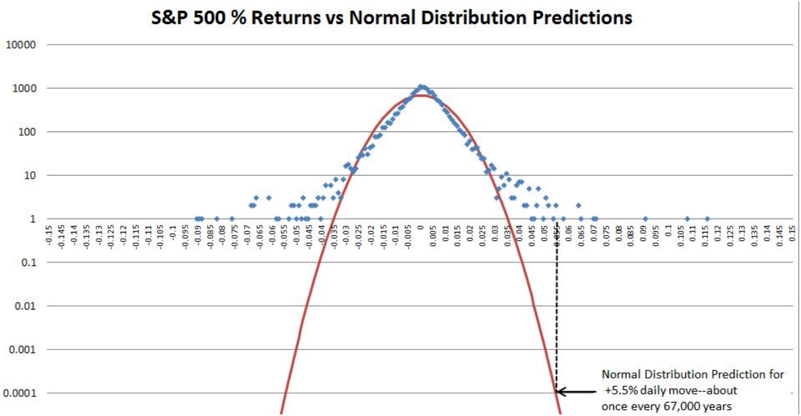
Brownian motion



Lévy flight

Financial modelling

Extreme events in financial markets seem to occur with a significant probability. B. Mandelbrot and E. Fama (1963) suggested heavy-tailed probability distributions, such as stable ones, to model stock market returns and prices.



Generalised central limit theorem

Random walk where jumps may have *infinite mean or variance*:

Theorem (Gnedenko-Kolmogorov 1949)

Let $X_1, X_2, \ldots$ be i.i.d. random variables. There are a_k, b_k with

$$\frac{X_1 + \ldots + X_k}{a_k} - b_k \xrightarrow{\mathrm{d}} Z$$

if and only if the limit Z has a *stable distribution*.

Stable distributions include the *symmetric* ones defined by

$$\mathbb{E}[e^{itZ}] = e^{-|t|^\alpha}, \qquad 0 < \alpha \leq 2.$$

If $\alpha = 2$ this is normal distribution, but if $\alpha < 2$ the probability density is $\sim |x|^{-1-\alpha}$ for large $|x| \implies$ *infinite variance*.

Generalised central limit theorem

Theorem. Let $X_1, X_2, \ldots$ be i.i.d. If for some a_n, b_n

$$\frac{X_1 + \ldots + X_n}{a_n} - b_n \xrightarrow{\mathrm{d}} Z, \qquad \text{then } Z \text{ has a } \textit{stable distribution}.$$

Proof idea. Let $Z_{nk} = \frac{X_1+\ldots+X_{nk}}{a_{nk}} - b_{nk}$. Break in k blocks:

$$\underbrace{\left[\frac{X_1 + \ldots + X_n}{a_n} - b_n\right]}_{Z_n^{(1)}} + \ldots + \underbrace{\left[\frac{X_{n(k-1)+1} + \ldots + X_{nk}}{a_n} - b_n\right]}_{Z_n^{(k)}} = c_{nk} \underbrace{Z_{nk}}_{\xrightarrow{\mathrm{d}} Z} + d_{nk}.$$

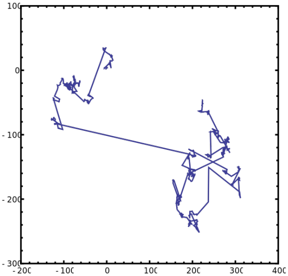
Here $Z_n^{(j)} \xrightarrow{\mathrm{d}} Z^{(j)}$ where $Z^{(j)}$ are i.i.d. copies Z. For such $Z^{(j)}$,

$$Z^{(1)} + \ldots + Z^{(k)} \stackrel{\mathrm{d}}{=} c_k Z + d_k \qquad (\textit{self-similarity!}).$$

Z infinitely divisible $\Longrightarrow \mathbb{E}[\, e^{itZ} \,]$ has special form [Lévy-Khintchine].

Lévy processes

The continuous-time version of the previous random walk is an example of a *Lévy process* $(X_t)_{t\geq 0}$. This is a process with independent stationary increments, but paths are in general discontinuous.



Consider $(X_t)_{t\geq 0}$ in $\mathbb{R}^n$ related to α-stable distribution,

$$\mathbb{E}[\, e^{-iX_t\cdot\xi}\,] = e^{-t|\xi|^\alpha}.$$

This induces an *anomalous diffusion*, where microscopic particles follow paths of X_t instead of Brownian motion. Next we derive the corresponding diffusion equation.

Fourier transform

If f is a nice function in $\mathbb{R}^n$, its *Fourier transform* is

$$\hat{f}(\xi) = \int_{\mathbb{R}^n} e^{-ix\cdot\xi} f(x)\, dx, \qquad \xi \in \mathbb{R}^n.$$

Example. If $p_t(x)$ is the probability density function of X_t, its Fourier transform is $\widehat{p_t}(\xi) = \mathbb{E}[\, e^{-iX_t\cdot\xi}\,] = e^{-t|\xi|^\alpha}$.

One can recover f from $\hat{f}$ (*Fourier inversion*), and

$$(\partial_j f)\hat{}(\xi) = i\xi_j \hat{f}(\xi), \qquad \begin{pmatrix}\text{derivatives}\\ \to \text{polynomials}\end{pmatrix}$$

$$\left[\int f(\cdot - y) g(y)\, dy\right]\hat{}(\xi) = \hat{f}(\xi)\hat{g}(\xi) \qquad \begin{pmatrix}\text{convolutions}\\ \to \text{products}\end{pmatrix}$$

In particular, $(-\Delta f)\hat{}(\xi) = |\xi|^2 \hat{f}(\xi) \quad \begin{pmatrix}\text{Laplacian}\\ \to |\xi|^2\end{pmatrix}$.

Diffusion equation

Let $u(x,t)$ be the density of Lévy particles at x at time t, if the initial density is $f(x)$. Heuristically,

$$u(x,t) = \int_{\mathbb{R}^n} f(y) p_t(x-y)\, dy$$

where $\widehat{p_t}(\xi) = e^{-t|\xi|^\alpha}$. Taking Fourier transforms in x,

$$\hat{u}(\xi,t) = \widehat{p_t}(\xi)\hat{f}(\xi) = e^{-t|\xi|^\alpha}\hat{f}(\xi)$$

$$\Longrightarrow \partial_t \hat{u}(\xi,t) = - \underbrace{|\xi|^\alpha \hat{u}(\xi,t)}_{\leftrightarrow \text{ fractional Laplacian } (-\Delta)^{\alpha/2}}$$

Thus $u(x,t)$ solves the *fractional heat equation*

$$\begin{cases} \frac{\partial u}{\partial t} + (-\Delta)^{\alpha/2} u = 0 & \text{in } \mathbb{R}^n \times \{t > 0\}, \\ u|_{t=0} = f. \end{cases}$$

Diffusion equation

Anomalous diffusion modelled by Lévy flights leads to *space-fractional* heat and Laplace equations

$$\begin{aligned} \frac{\partial u}{\partial t} + (-\Delta)^{\alpha/2} u &= 0, \\ (-\Delta)^{\alpha/2} u &= 0. \end{aligned}$$

Similarly, diffusion where waiting times between jumps follow a stable distribution leads to *time-fractional* diffusion equations

$$\partial_t^\alpha u - \Delta u = 0.$$

The study of such equations is currently an active topic in PDE.

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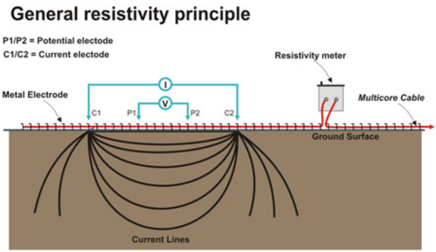
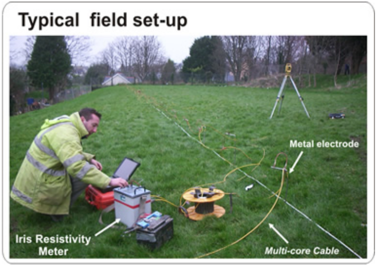
Calderón problem

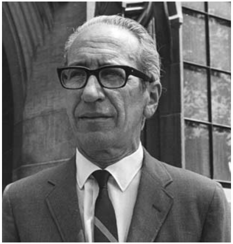
Electrical Resistivity Imaging in geophysics (1920's) [image: TerraDat]





A.P. Calderón (1980):

- mathematical formulation
- solution of the linearized problem
- exponential solutions



Calderón problem

Conductivity equation

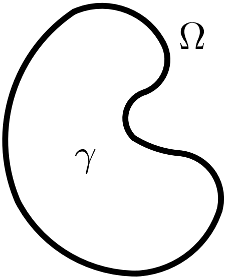
$$\begin{cases} \mathrm{div}(\gamma(x)\nabla u) = 0 & \text{in } \Omega, \\ u = f & \text{on } \partial\Omega \end{cases}$$

where $\Omega \subset \mathbb{R}^n$ bounded domain, $\gamma \in L^\infty(\Omega)$ positive scalar function (electrical conductivity).

Boundary measurements given by *Dirichlet-to-Neumann (DN) map*[1]

$$\Lambda_\gamma : f \mapsto \gamma \nabla u \cdot \nu|_{\partial\Omega}.$$

Inverse problem: given Λ_γ, determine γ.



[1] as a map $\Lambda_\gamma : H^{1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega)$

Schrödinger equation

Substitute $u = \gamma^{-1/2} v$, conductivity equation $\mathrm{div}(\gamma \nabla u) = 0$ reduces to Schrödinger equation $(-\Delta + q)v = 0$ where

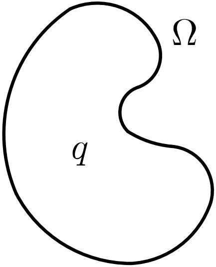
$$q = \frac{\Delta(\gamma^{1/2})}{\gamma^{1/2}}.$$

If $q \in L^\infty(\Omega)$, consider Dirichlet problem

$$\begin{cases} (-\Delta + q)u = 0 & \text{in } \Omega, \\ u = f & \text{on } \partial\Omega. \end{cases}$$

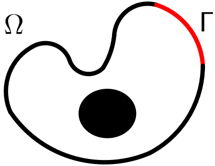
The DN map is $\Lambda_q : f \mapsto \partial_\nu u|_{\partial\Omega}$.

Inverse problem: given Λ_q, determine q.



Calderón problem

Uniqueness results, also for local data (measurements only on a subset $\Gamma \subset \partial\Omega$):



$n \geq 3$	$q \in L^\infty$	Sylvester-Uhlmann 1987
	local data	Kenig-S 2013, Kenig-Sjöstrand-Uhlmann 2007 (partial results)
$n = 2$	$q \in C^1$	Bukhgeim 2008
	local data	Imanuvilov-Uhlmann-Yamamoto 2010

Fractional Laplacian

We will study an inverse problem for the *fractional Laplacian*

$$(-\Delta)^s, \quad 0 < s < 1,$$

defined via the Fourier transform by

$$((-\Delta)^s u)\hat{}(\xi) = |\xi|^{2s} \hat{u}(\xi).$$

This operator is *nonlocal*, as opposed to the usual Laplacian:

- $(-\Delta)^s$ does not preserve supports
- computing $(-\Delta)^s u(x)$ needs values of u far away from x

Fractional Laplacian

Recall different models for diffusion:

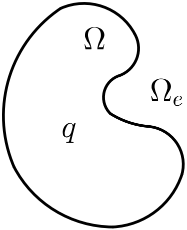
$\partial_t u - \Delta u = 0$	normal diffusion/BM
$\partial_t u + (-\Delta)^s u = 0$	superdiffusion/Lévy flight
$\partial_t^\alpha u - \Delta u = 0$	subdiffusion/CTRW

Many results for time-fractional inverse problems, very few for space-fractional [Jin-Rundell, survey 2015].

Fractional Laplacian

Let $\Omega \subset \mathbb{R}^n$ bounded, $q \in L^\infty(\Omega)$. Since $(-\Delta)^s$ is nonlocal, the boundary value problem becomes

$$\begin{cases} ((-\Delta)^s + q)u = 0 & \text{in } \Omega, \\ u = f & \text{in } \Omega_e \end{cases}$$



where $\Omega_e = \mathbb{R}^n \setminus \overline{\Omega}$ is the *exterior domain*.

Given f in Ω_e, look for a solution u in $\mathbb{R}^n$. DN map

$$\Lambda_q : H^s(\Omega_e) \to H^{-s}(\Omega_e), \quad \Lambda_q f = (-\Delta)^s u|_{\Omega_e}.^1$$

Inverse problem: given Λ_q, determine q.

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[1] the work required to maintain exterior data f in Ω_e

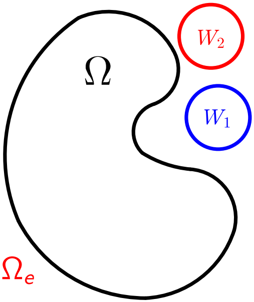
Main result

Theorem (Ghosh-S-Uhlmann 2016)

Let $\Omega \subset \mathbb{R}^n$ be a bounded open set, let $0 < s < 1$, and let $q_1, q_2 \in L^\infty(\Omega)$. If $W_j \subset \Omega_e$ are open sets, and if

$$\Lambda_{q_1} f|_{W_2} = \Lambda_{q_2} f|_{W_2}, \quad f \in C_c^\infty(W_1),$$

then $q_1 = q_2$ in Ω.



Main features:

- local data result for *arbitrary* $W_j \subset \Omega_e$
- the same method works for *all* $n \geq 2$
- new mechanism for solving (nonlocal) inverse problems

Main tools: uniqueness

The fractional equation has strong uniqueness properties:

Theorem

If $u \in H^{-r}(\mathbb{R}^n)$ for some $r \in \mathbb{R}$, and if both u and $(-\Delta)^s u$ vanish in some open set, then $u \equiv 0$.

Essentially due to [M. Riesz 1938], also have strong unique continuation results [Fall-Felli 2014, Rüland 2015].

Such a result could never hold for the Laplacian:
if $u \in C_c^\infty(\mathbb{R}^n)$, then both u and Δu vanish in a large set.

Main tools: uniqueness

Theorem

If $u \in H^{-r}(\mathbb{R}^n)$ for some $r \in \mathbb{R}$, and if $u|_W = (-\Delta)^s u|_W = 0$ for some open set $W \subset \mathbb{R}^n$, then $u \equiv 0$.

Proof (sketch). If u is nice enough, then

$$(-\Delta)^s u \sim \lim_{y \to 0} y^{1-2s} \partial_y w(\,\cdot\,, y)$$

where $w(x, y)$ is the *Caffarelli-Silvestre extension* of u:

$$\begin{cases} \mathrm{div}_{x,y}(y^{1-2s} \nabla_{x,y} w) = 0 & \text{in } \mathbb{R}^n \times \{y > 0\}, \\ w\big|_{y=0} = u. \end{cases}$$

Thus $(-\Delta)^s u$ is obtained from a *local equation*, which is degenerate elliptic with A_2 weight y^{1-2s}. Carleman estimates [Rüland 2015] and $u|_W = (-\Delta)^s u|_W = 0$ imply uniqueness. □

Main tools: approximation

Solutions of $\Delta u = 0$ (harmonic functions) in $\Omega \subset \mathbb{R}^n$ are *rigid*:

- if $n = 1$, then $u'' = 0 \implies u(x) = ax + b$
- u has no interior minima or maxima (*maximum principle*)
- if $u|_B = 0$ in $B \subset \Omega$, then $u \equiv 0$ (*unique continuation*)

Moreover, if $u_j \to f$ in $L^2(\Omega)$ where $\Delta u_j = 0$, then also $\Delta f = 0$ (harmonic functions can only approximate harmonic functions).

In contrast, solutions of $(-\Delta)^s u = 0$ turn out to be *flexible*.

Main tools: approximation

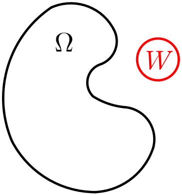
Theorem (Ghosh-S-Uhlmann 2016)

Any $f \in L^2(\Omega)$ can be approximated in $L^2(\Omega)$ by *solutions $u|_\Omega$*, where

$$((-\Delta)^s + q)u = 0 \text{ in } \Omega, \qquad \mathrm{supp}(u) \subset \overline{\Omega} \cup \overline{W}.$$

If everything is C^∞, can approximate in $C^k(\overline{\Omega})$.

Earlier [Dipierro-Savin-Valdinoci 2016]: C^k approximation by solutions of $(-\Delta)^s u = 0$ in B_1, but with no control over $\mathrm{supp}(u)$.



Main tools: approximation

The approximation property follows by duality from the uniqueness result.

This uses Fredholm properties of the solution operator for

$$\begin{cases} ((-\Delta)^s + q)u = F & \text{in } \Omega, \\ u = 0 & \text{in } \Omega_e, \end{cases}$$

mapping $F \in H^{\alpha-2s}(\Omega)$ to u in the *special space* $H^{s(\alpha)}(\overline{\Omega})$, adapted to the fractional Dirichlet problem, for $\alpha > 1/2$ [s-transmission property, Hörmander 1965, Grubb 2015]. One has

$$H^{\alpha}_{\mathrm{comp}}(\Omega) \subset H^{s(\alpha)}(\overline{\Omega}) \subset H^{\alpha}_{\mathrm{loc}}(\Omega)$$

but solutions in $H^{s(\alpha)}(\overline{\Omega})$ may have singularities near $\partial\Omega$.

Summary

1. Normal diffusion can be described either by the heat equation or by Brownian motion.
2. Anomalous diffusion gives rise to fractional differential equations.
3. The fractional operator $(-\Delta)^s$, $0 < s < 1$, is *nonlocal*. Boundary value problems are replaced by exterior problems.
4. Fractional equations may have *strong uniqueness and approximation properties*, replacing standard methods and leading to strong results in inverse problems.