Modeling with the fractional diffusion equation

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Mark M. Meerschaert
Department of Statistics and Probability
Michigan State University

mcubed@stt.msu.edu
http://www.stt.msu.edu/users/mcubed

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Abstract

The advection dispersion model in ground water hydrology uses random fields to interpolate sparse data on hydraulic conductivity. This partial differential equation is used to model flow and transport in porous media, and typically solved by numerical methods. The fractional advection dispersion equation provides a convenient upscaling.

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Traditional model for groundwater flow and transport [B72]

Step 1: Measure *hydraulic conductivity* $\boldsymbol{K}(\boldsymbol{x})$, a tensor field that codes how easily water can flow through a porous medium.

Step 2: Compute the hydraulic head (pressure) $h(\boldsymbol{x}, t)$ by numerically solving the groundwater flow equation

$$\frac{\partial h(\boldsymbol{x}, t)}{\partial t} = a\nabla \cdot \boldsymbol{K}(\boldsymbol{x})\nabla h(\boldsymbol{x}, t) + f(\boldsymbol{x}, t),$$

where $f(\boldsymbol{x}, t)$ is a source/sink term.

Step 3: Compute the velocity field $\boldsymbol{v}(\boldsymbol{x}, t)$ using Darcy's Law

$$\boldsymbol{v}(\boldsymbol{x}, t) = -b\boldsymbol{K}(\boldsymbol{x})\nabla h(\boldsymbol{x}, t).$$

Groundwater flow and transport (continued)

Step 4: Compute solute concentration $C(\boldsymbol{x},t)$ by numerically solving the advection-dispersion equation

$$\frac{\partial C(\boldsymbol{x},t)}{\partial t} = -\nabla \cdot \boldsymbol{v}(\boldsymbol{x},t)C(\boldsymbol{x},t) + \nabla \cdot \boldsymbol{D}(\boldsymbol{x},t)\nabla C(\boldsymbol{x},t) + F(\boldsymbol{x},t),$$

where $F(\boldsymbol{x},t)$ is a source/sink term and $\boldsymbol{D}(\boldsymbol{x},t)$ is the dispersivity tensor (normal covariance matrix).

Typical simplifying assumptions:

1. Steady state hydraulic head $h(\boldsymbol{x})$
2. Steady state velocity field $\boldsymbol{v}(\boldsymbol{x})$
3. Scalar dispersion $\boldsymbol{D}(\boldsymbol{x}) = \lambda\|\boldsymbol{v}(\boldsymbol{x})\|\boldsymbol{I}$
4. Scalar hydraulic conductivity $\boldsymbol{K}(\boldsymbol{x}) = K(\boldsymbol{x})\boldsymbol{I}$
5. Gaussian $\ln K$ field with isotropic exponential correlation

Data requirements

Consider a bounded (rectangular) domain in $\mathbb{R}^2$ or $\mathbb{R}^3$

Establish (or assume) boundary conditions for hydraulic head h

Measure **hydraulic conductivity** K at some points (expensive!)

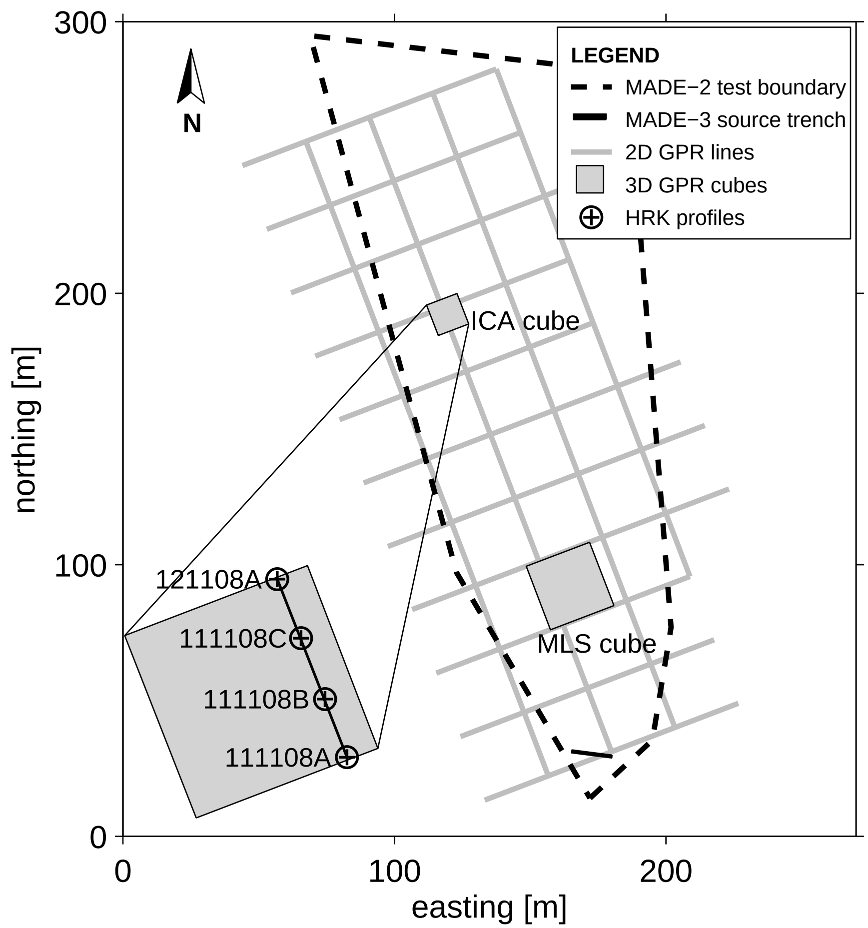
Extrapolate K field to all ($> 10^6$) grid points in the domain

Typically, we have just a few vertical columns of K data

Each vertical column contains **100 to 500 data points**

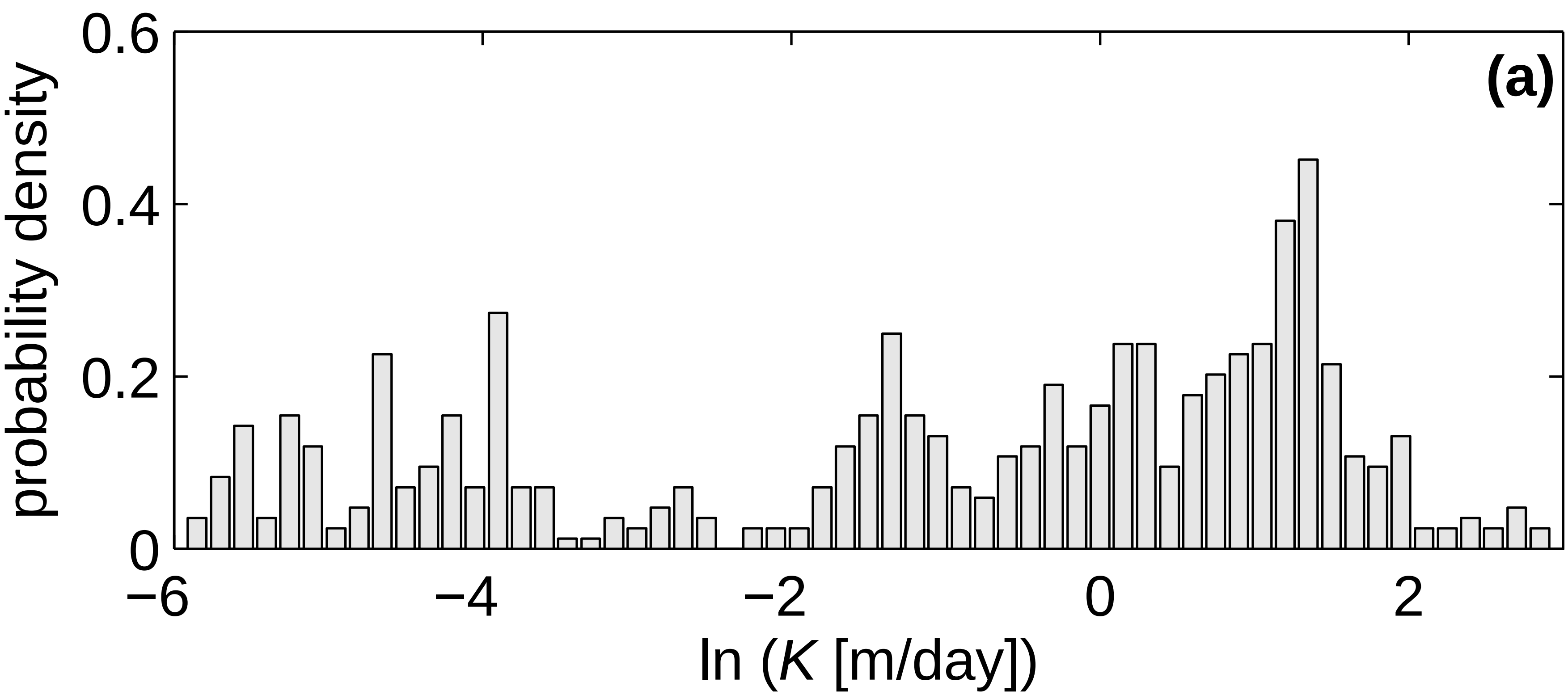
Data source: The MADE site [MDDHB13]

MAcroDispersion Experimental Site (MADE) in Columbus MS.



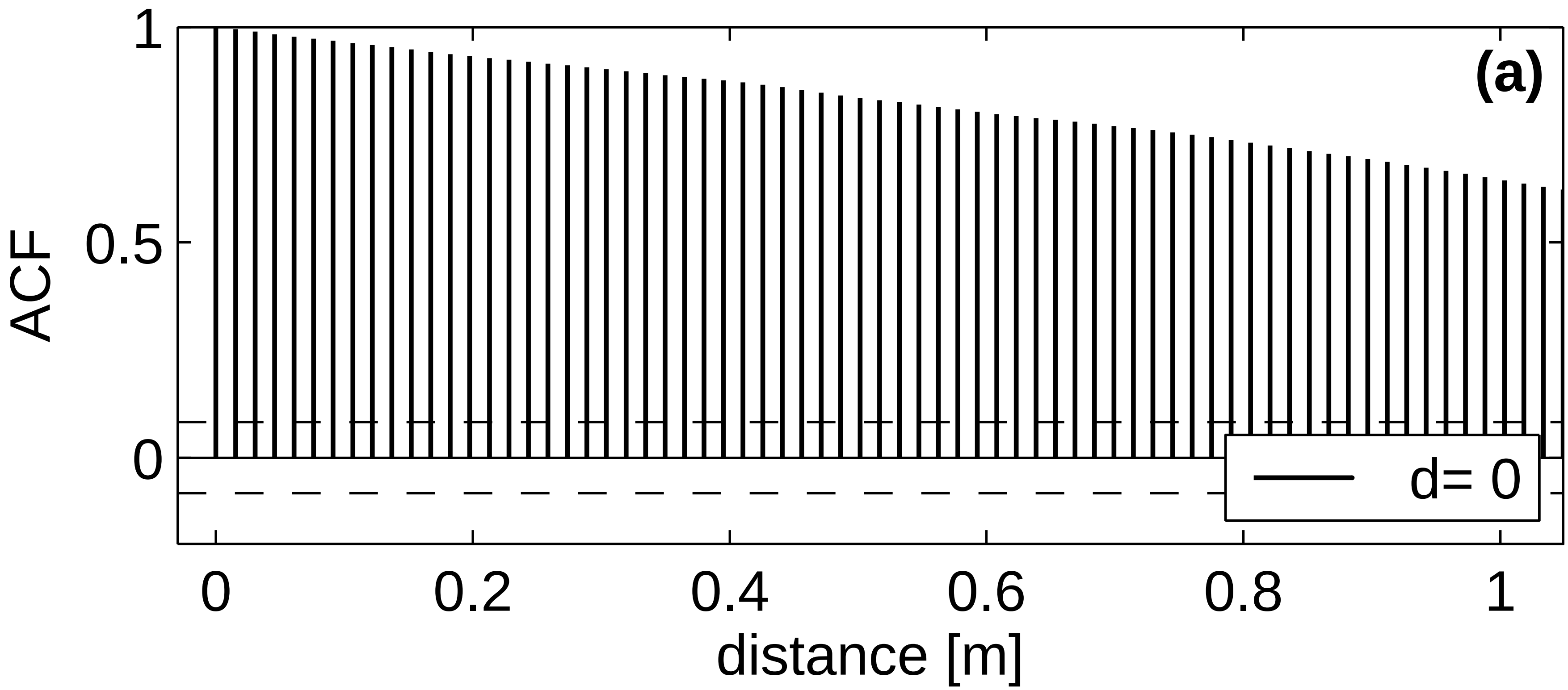
Hydraulic conductivity data distribution [MDDHB13]

Histogram of measured $\ln K$ data (one column, $n = 561$).



Hydraulic conductivity data correlation [MDDHB13]

Autocorrelation function for one column of $\ln K$ data ($n = 561$).



Fractional difference (fractal filter) [MDDHB13]

Apply a fractional difference filter to the data $X_n = \ln K(x, y, z_n)$ to obtain an uncorrelated sequence

$$Z_n = \sum_{j=0}^{\infty} (-1)^j \binom{d}{j} X_{n-j}$$

where the fractional binomial coefficients

$$\binom{d}{j} = \frac{\Gamma(d+1)}{j!\Gamma(j-d+1)}$$

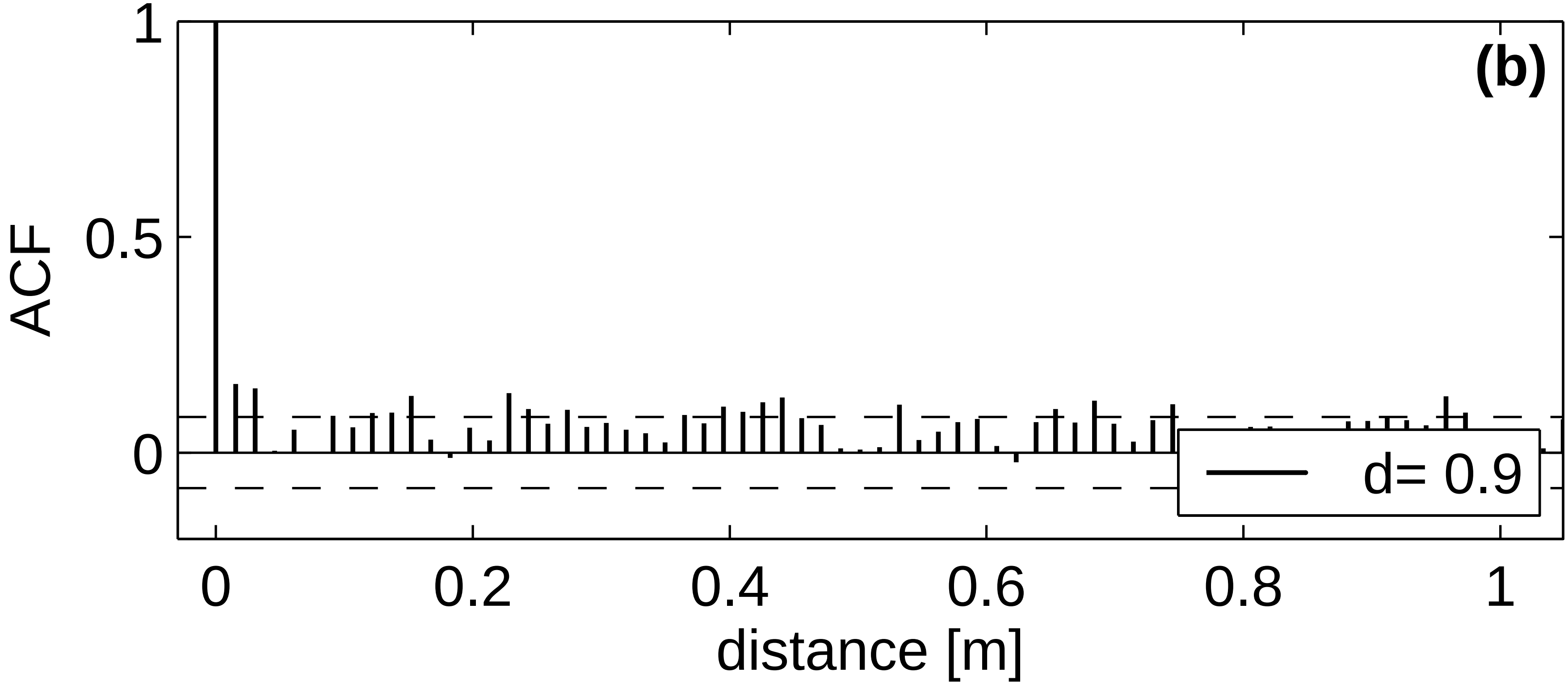
for some $d > 0$. Then X_n is a fractionally integrated white noise.

If $d = 1$ then $Z_n = X_n - X_{n-1}$, so that $X_n = Z_1 + \cdots + Z_n$.

If Z_n is Gaussian and $0.5 < d < 1.5$, then X_n is an fBm with Hurst index $H = d - 0.5$ sampled at equally spaced points.

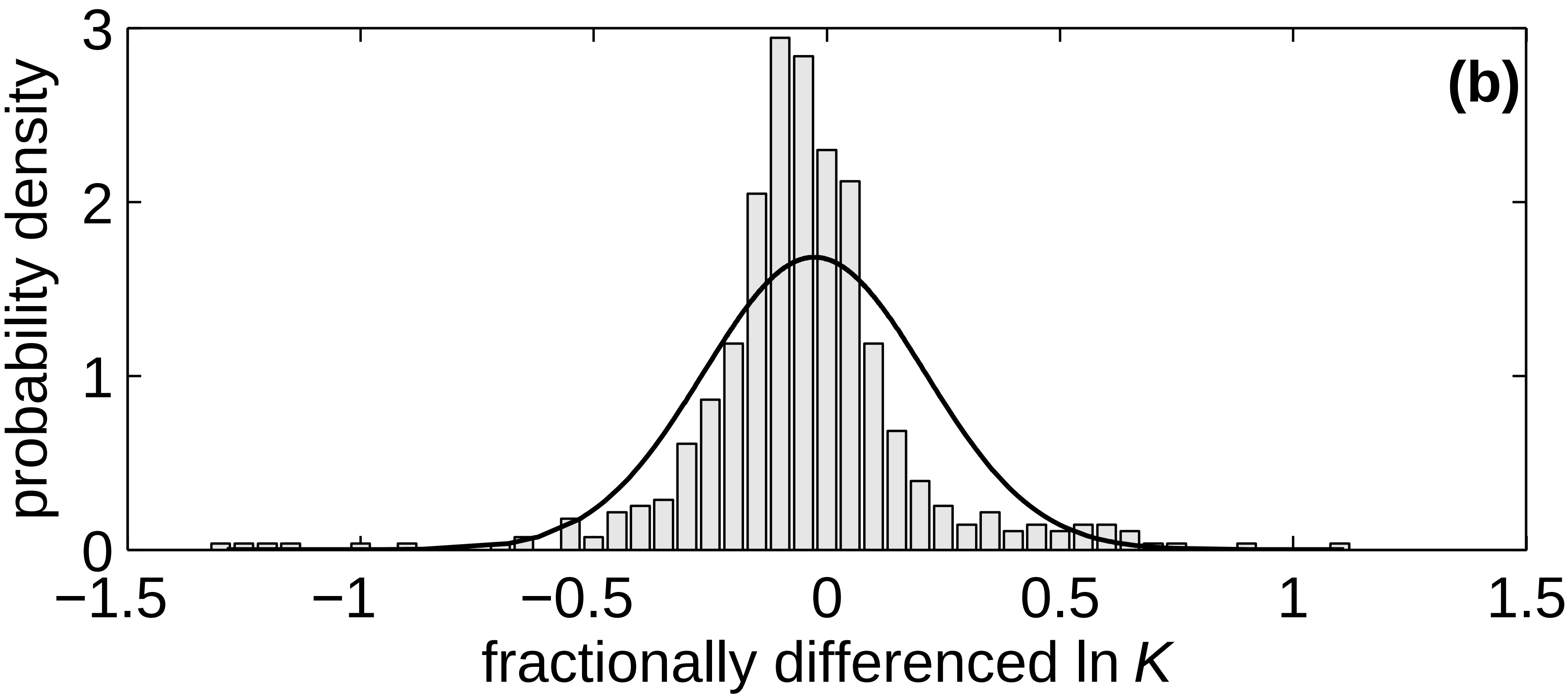
Filtering out the data correlation [MDDHB13]

A fractional difference with $d = 0.9$ removes the correlation.



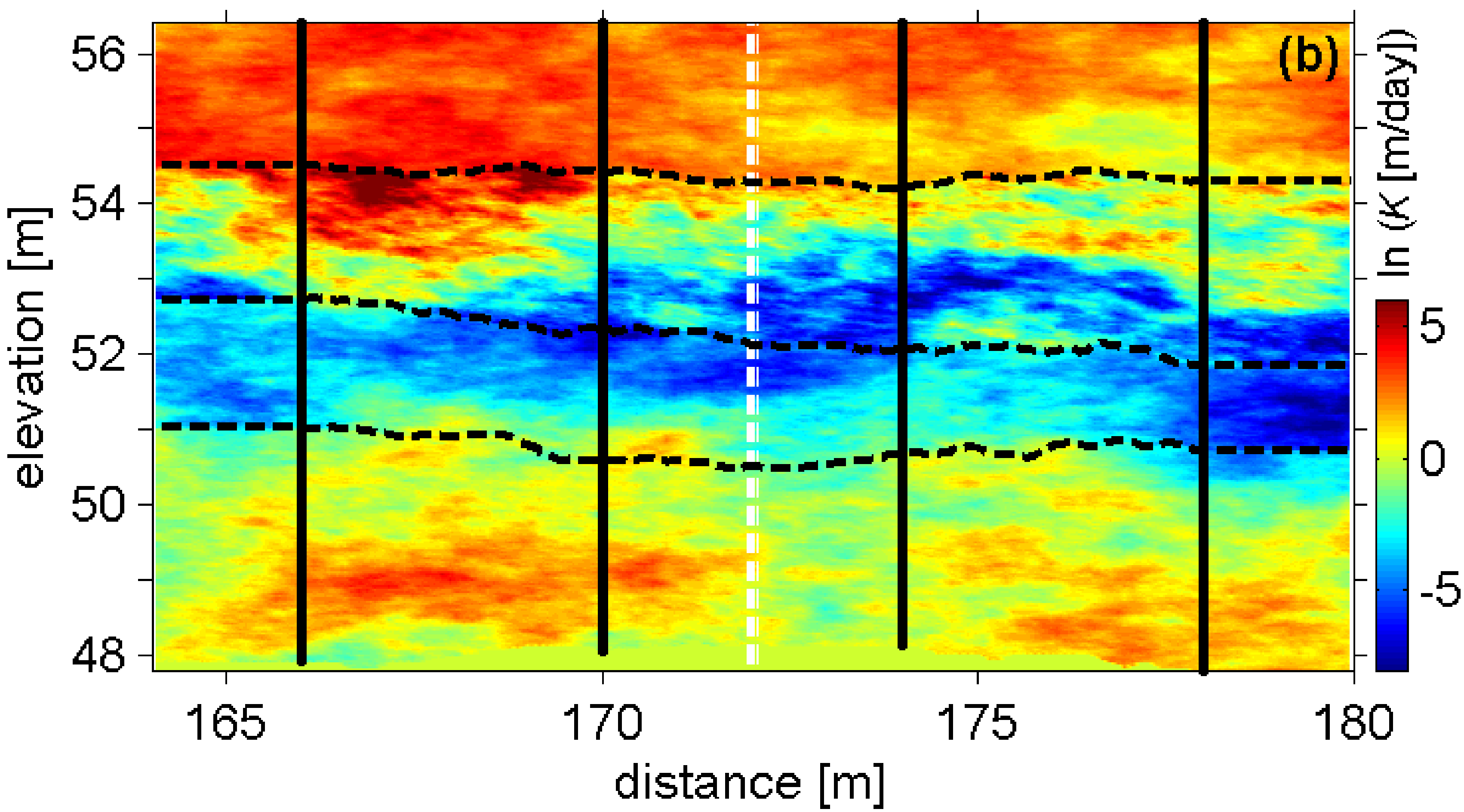
Distribution of the filtered data [MDDHB13]

A fractional difference with $d = 0.9$ reveals that the underlying distribution has heavier tails and a sharper peak than the best fitting Gaussian.



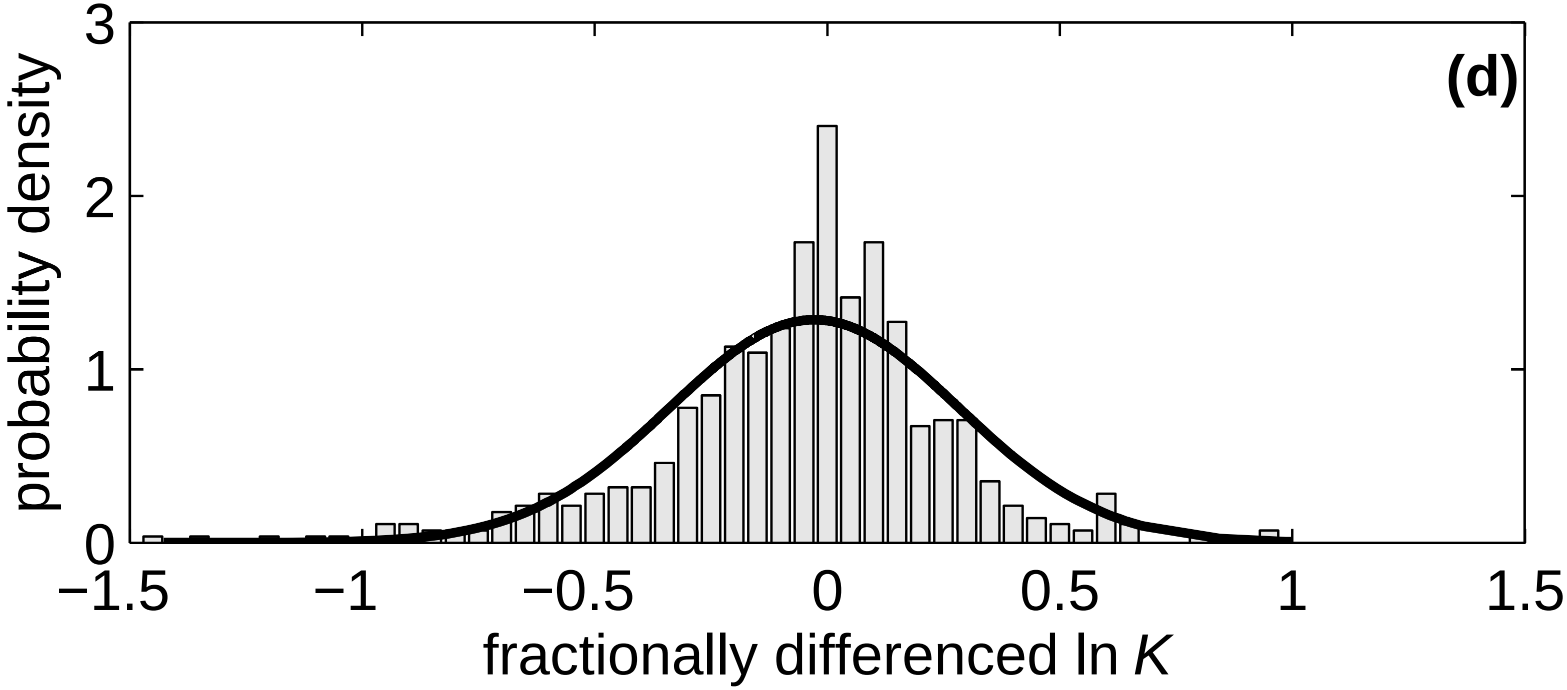
Our model for $\ln K$ [MDDHB13]

We simulate an anisotropic Gaussian $\ln K$ field in each layer, conditional on the observed data (solid black lines) and sample one column (white dotted line) for model validation.



Simulated column of ln K data [MDDHB13]

The simulated ln K data in a single column (white dotted line) is a Gaussian mixture, resembling the ln K data.



Parameterizing the ADE [MS12]

Apply the Fourier transform

$$\widehat{C}(\boldsymbol{k},t) = \int_{\boldsymbol{x}\in\mathbb{R}^d} e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} C(\boldsymbol{x},t)\,d\boldsymbol{x}$$

in the constant coefficient ADE with $F(\boldsymbol{x},0) = \delta(\boldsymbol{x})$ to get

$$\frac{d\widehat{C}(\boldsymbol{k},t)}{dt} = -(i\boldsymbol{k})\cdot\boldsymbol{v}\ \widehat{C}(\boldsymbol{k},t) + (i\boldsymbol{k})\cdot\boldsymbol{D}(i\boldsymbol{k})\ \widehat{C}(\boldsymbol{k},t)$$

with initial condition $C(\boldsymbol{k},0) = 1$. Then obviously

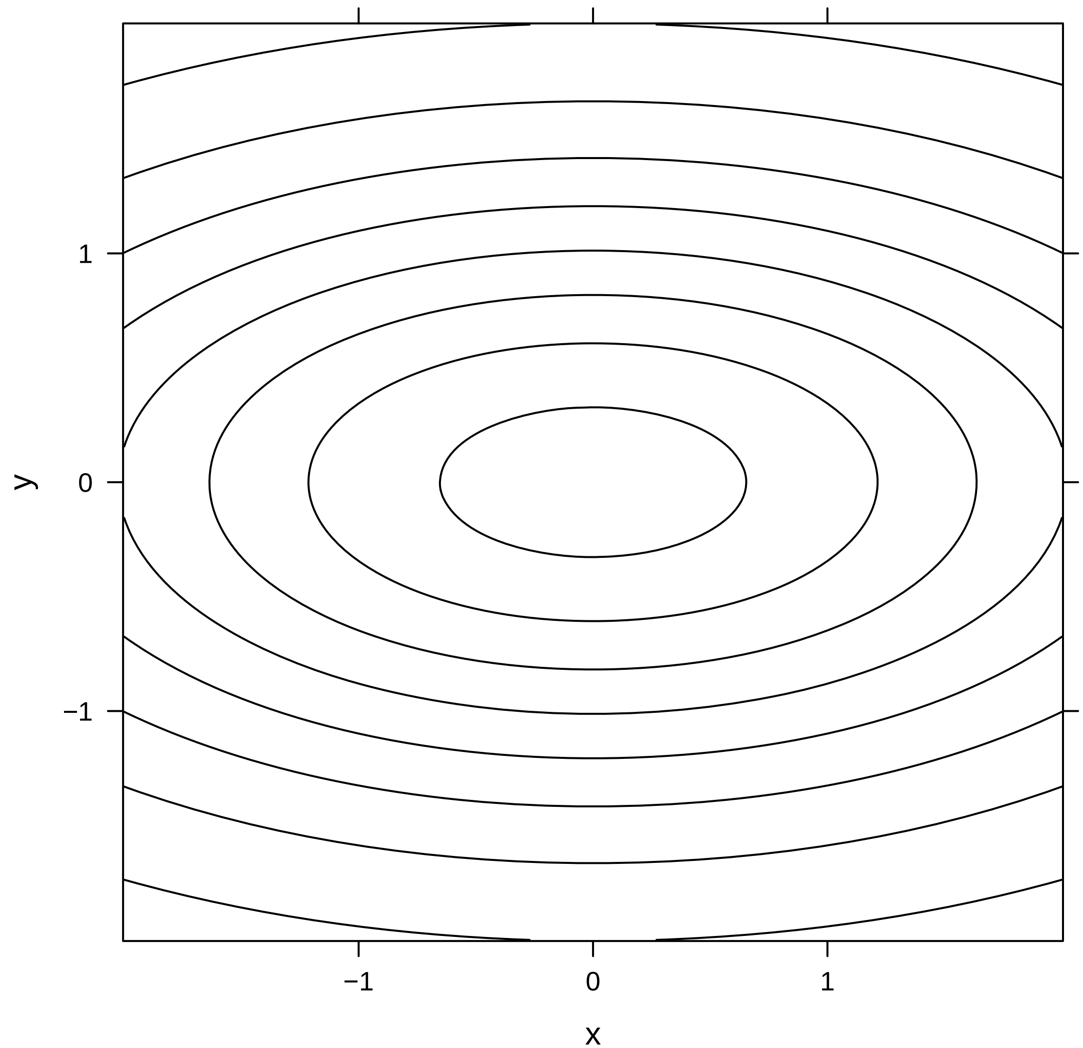
$$\widehat{C}(\boldsymbol{k},t) = \exp\Big[-(i\boldsymbol{k})\cdot\boldsymbol{v}t + (i\boldsymbol{k})\cdot\boldsymbol{D}(i\boldsymbol{k})t\Big]$$

which inverts to a multivariate Gaussian PDF with mean $\boldsymbol{v}t$ and covariance matrix $2\boldsymbol{D}t$.

Sums of IID particle jumps with mean $\boldsymbol{v}$ and covariance matrix $2\boldsymbol{D}$ converge to this PDF.

Solution to the ADE with constant coefficients [MS12]

Level sets are ellipses whose principal axes are the eigenvectors of the covariance matrix, centered at the mean.



Fractional advection dispersion equation [MS12]

A convenient upscaling model

$$\frac{\partial C(\boldsymbol{x},t)}{\partial t} = -\nabla \cdot \boldsymbol{v}(\boldsymbol{x},t)C(\boldsymbol{x},t) + a\nabla_M^\alpha C(\boldsymbol{x},t) + F(\boldsymbol{x},t),$$

where the fractional derivative $\nabla_M^\alpha C(\boldsymbol{x},t)$ has Fourier transform

$$\int_{\|\theta\|=1} (i\boldsymbol{k}\cdot\boldsymbol{\theta})^\alpha M(d\boldsymbol{\theta})\ \widehat{C}(\boldsymbol{k},t)$$

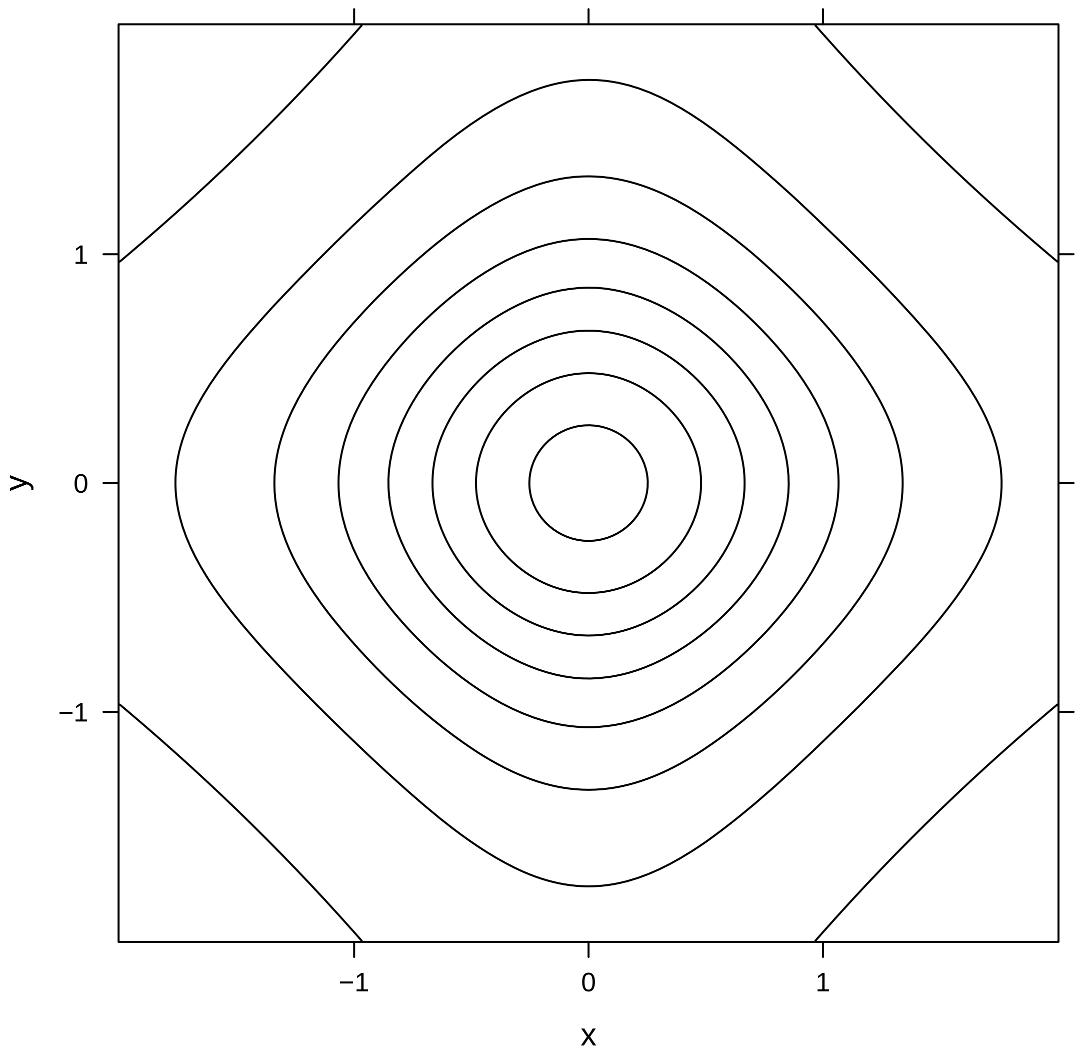
and $M(d\boldsymbol{\theta})$ is the PDF of a random unit vector.

Now $C(\boldsymbol{x},t)$ is the PDF of an α-stable random vector. If Θ has PDF $M(d\boldsymbol{\theta})$ and $P(R > r) = Cr^{-\alpha}$ then sums of IID particle jumps $R\Theta$ converge to this stable random vector.

Strongly correlated jumps in the ADE lead to the FADE.

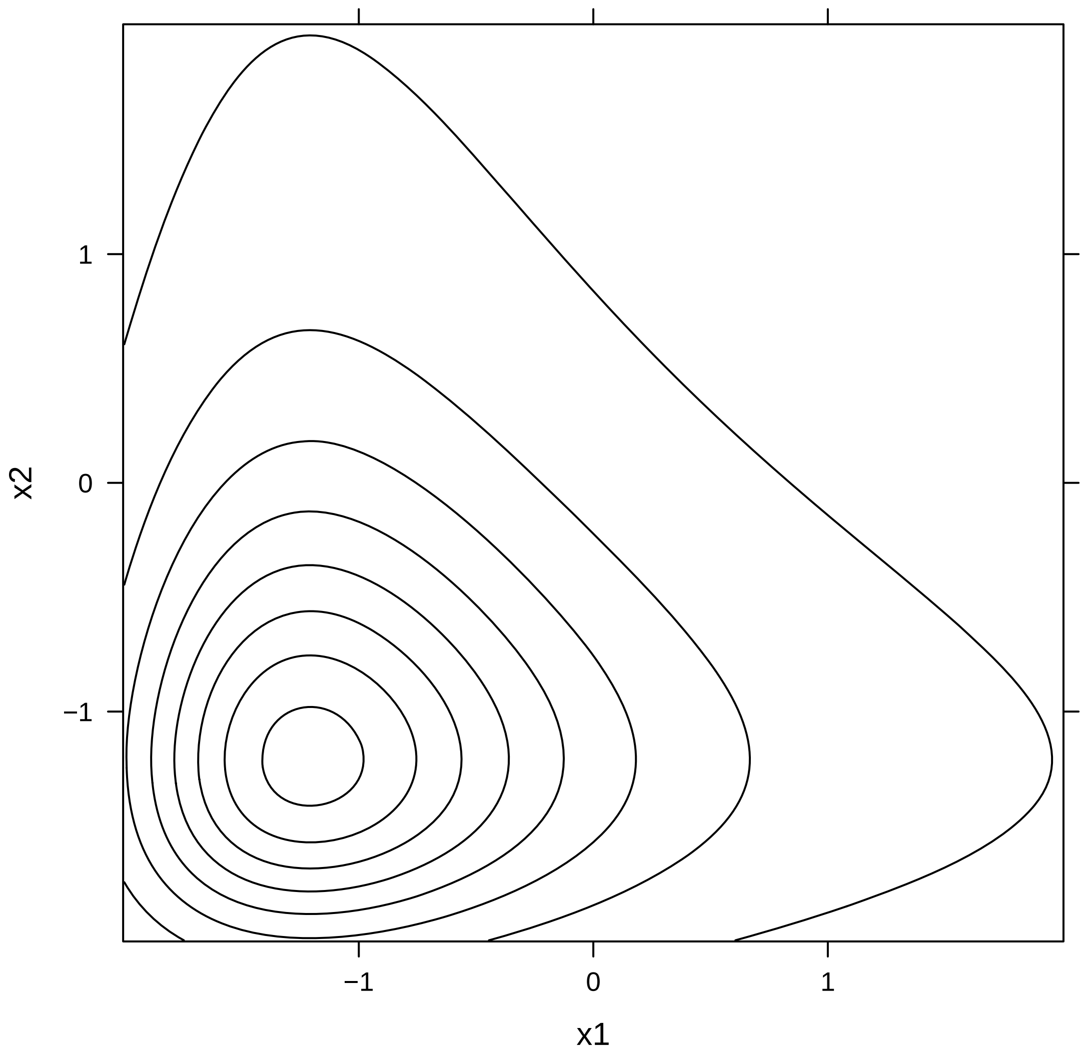
Solution to the fractional ADE: Case 1 [MS12]

Jump direction $M(d\boldsymbol{\theta})$ along the coordinate axes.



Solution to the fractional ADE: Case 2 [MS12]

Jump directions $M(d\boldsymbol{\theta})$ along the positive coordinate axes.



A richer class of models [MS12]

If jump direction PDF $M(d\boldsymbol{\theta})$ is uniform over the sphere, level sets are also spheres (fractional Laplacian).

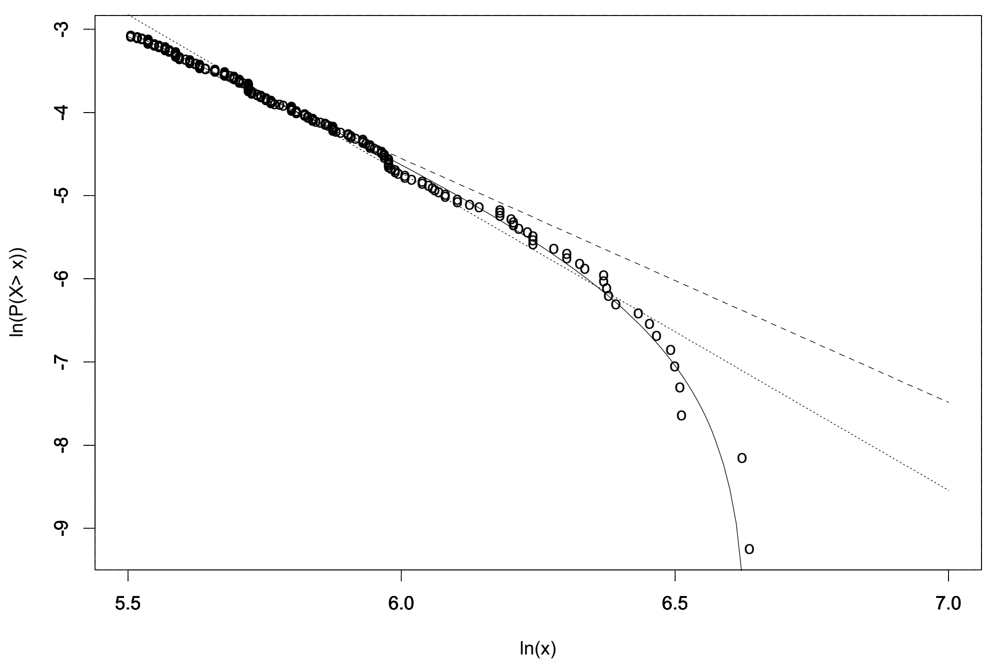
Fourier symbols for the three cases:

$$(ik_1)^\alpha + (ik_2)^\alpha \neq -|k_1|^\alpha - |k_2|^\alpha \neq -\|\boldsymbol{k}\|^\alpha$$

except in the very special case $\alpha = 2$ (traditional ADE).

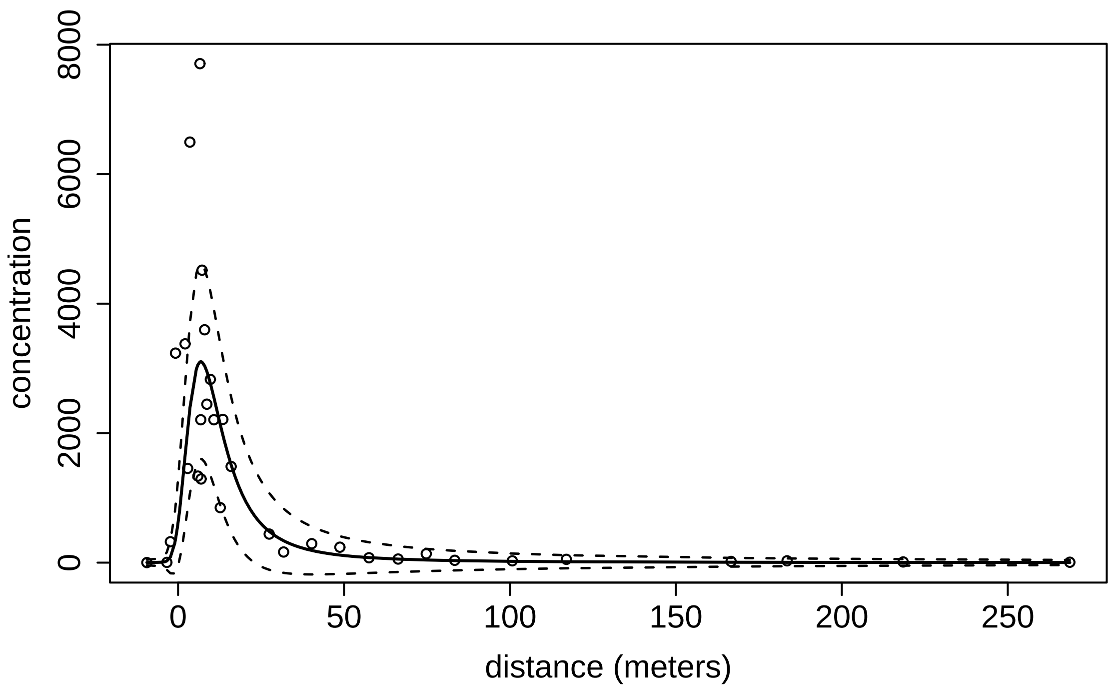
Parameter estimation: Method 1 [AMP06]

Hydraulic conductivity K data fits a (possibly truncated) power law PDF $\Rightarrow$ fractional parameter $\alpha \approx 1.1$. Spreadsheet tool for fitting at `www.stt.msu.edu/users/mcubed/TahoeTruncPareto.xls`



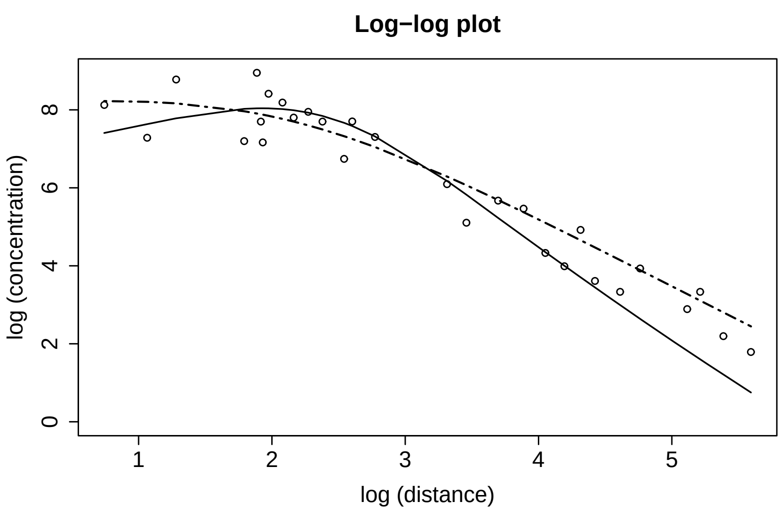
Parameter estimation: Method 2 [CML09]

Fit a stable PDF to measured concentration data in 1-D, with 95% confidence bands. Note retention at injection site. We now have a Matlab code for fitting.



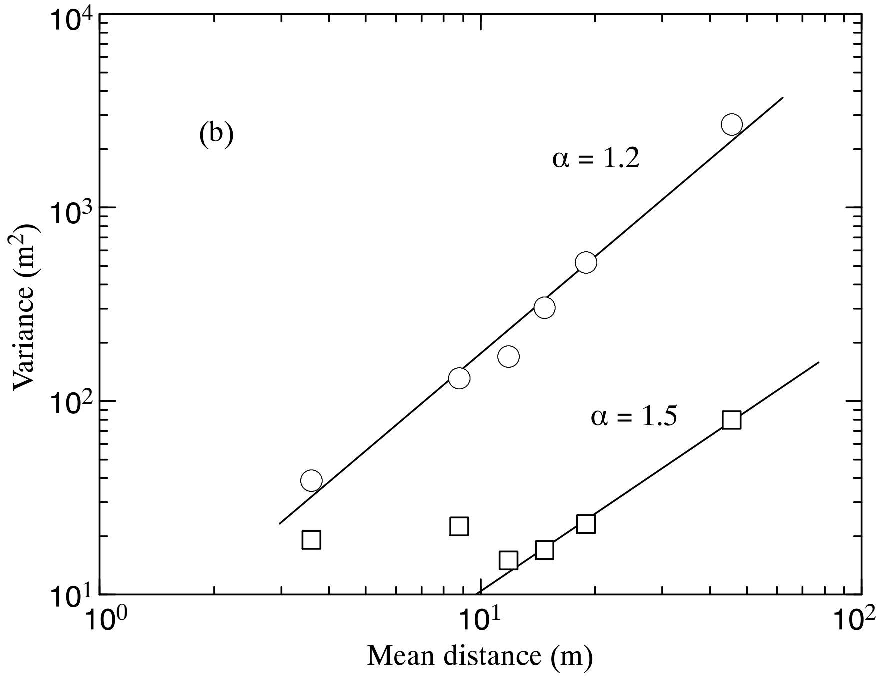
Parameter estimation: Method 2 [CML09]

Log-log plot reveals the power law tail $\alpha \approx 1.1$. Alternative fit with $\alpha = 0.7$ (dotted line) is also shown.



Vector parameter estimation [MS12]

Spreading rate $t^{1/\alpha}$ varies with direction in 2-D data.



Strongly anisotropic fractional diffusion equation [MS12]

The simplest model with $\alpha_1 \neq \alpha_2$ is

$$\frac{\partial}{\partial t}C(x,y,t) = D_1 \frac{\partial^{\alpha_1}}{\partial x^{\alpha_1}}C(x,y,t) + D_2 \frac{\partial^{\alpha_2}}{\partial y^{\alpha_2}}C(x,y,t)$$

The random walk model is $R^E\Theta$ where $M(d\theta)$ is concentrated on the positive coordinate axes, $P(R > r) = Cr^{-1}$ and E is a diagonal matrix with entries $1/\alpha_i$.

The eigenvectors of the covariance matrix of particle location data provide a consistent estimator of the correct coordinate vectors. The eigenvalues can also be used to estimate the fractional parameters α_i [MS99].

Stochastic differential equations [ZBMS06,C09]

If X_t is an α-stable Lévy process and

$$|a(y)|^2 + |b(y)|^2 \leq C(1 + |y|^2) \quad \text{(growth condition)}$$

$$|a(y_1) - a(y_2)|^2 + |b(y_1) - b(y_2)|^2 \leq C|y_1 - y_2|^2 \quad \text{(Lipschitz)}$$

then there exists a unique solution to $dY_t = a(Y_t)dt + b(Y_t)dX_t$, a Markov process whose PDF solves

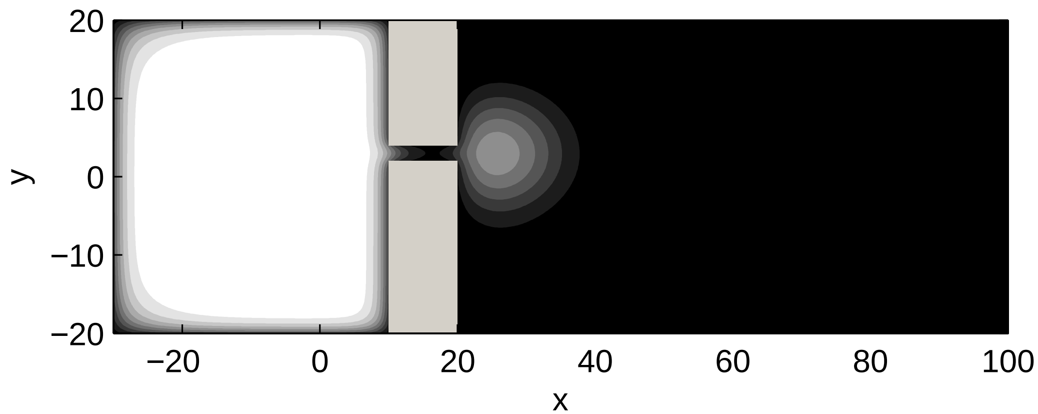
$$\frac{\partial C(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[a(x)C(x,t)\right] + pD\frac{\partial^\alpha}{\partial x^\alpha}\left[b(x)^\alpha C(x,t)\right] + qD\frac{\partial^\alpha}{\partial(-x)^\alpha}\left[b(x)^\alpha C(x,t)\right]$$

These conditions are sometimes violated in practice [BKMSS16].

Reaction-diffusion equations in Ecology [BKM08]

Traditional model for population growth and dispersal

$$\frac{\partial P}{\partial t} = C\frac{\partial^2 P}{\partial x^2} + D\frac{\partial^2 P}{\partial y^2} + rP\left(1 - \frac{P}{K}\right)$$

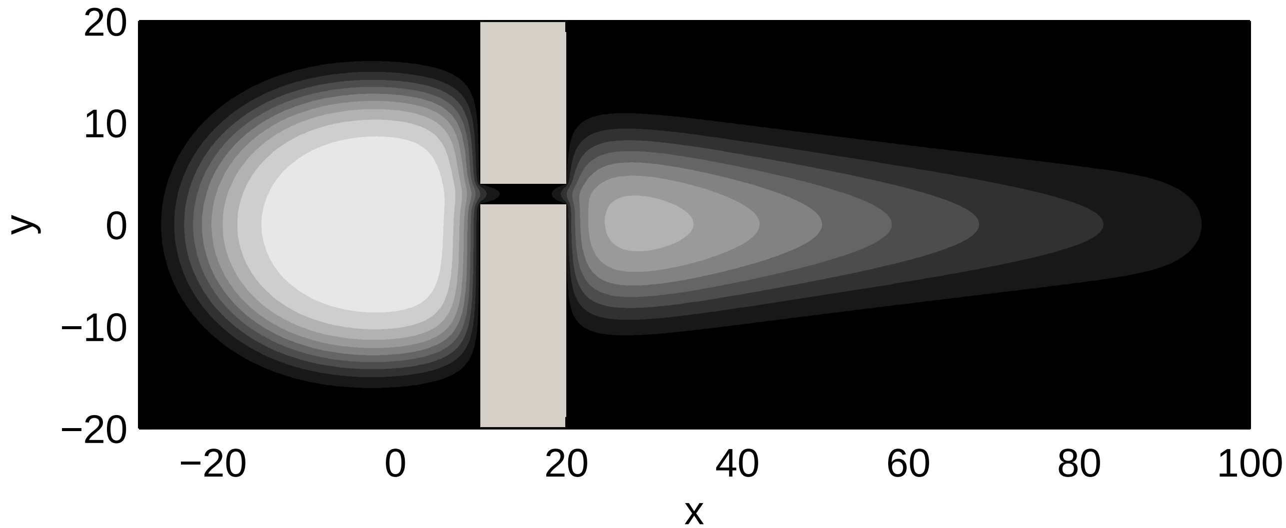


Note slow growth across the barrier.

Fractional reaction-diffusion equation [BKM08]

Fractional derivatives model fast spreading via long movements.

$$\frac{\partial P}{\partial t} = C\frac{\partial^{1.7} P}{\partial x^{1.7}} + D\frac{\partial^2 P}{\partial y^2} + rP\left(1 - \frac{P}{K}\right)$$



Fractional diffusion jumps the barrier.

Real invasive species data shows this behavior.

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