

Simulation of diffusion processes with discontinuous coefficients

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Divergence form operators in modelling

In many problems, a concentration, pressure, size of a population, ... is given by a partial differential equation (PDE) that follows from

$$\int_V (C(t + \Delta t, x) - C(t, x)) dx = \Delta t \int_{\partial V} \mathbf{J}(t, x) d\sigma(x)$$

with

- V volume
- $\mathbf{J}(t, x)$ flux
- $C(t, x)$ concentration

Then

$$\frac{\partial C(t, x)}{\partial t} = \text{div}(\mathbf{J}(t, x))$$

In general, the flux can be related to the concentration itself by

$$\mathbf{J}(t, x) = a(x)\nabla C(t, x)$$

for a matrix $a(x)$ (diffusivity/permeability/...), which leads to

$$\frac{\partial C(t, x)}{\partial t} = \text{div}(a(x)\nabla C(t, x)) \text{ or } \text{div}(a(x)\nabla C(x)) = f(x) \text{ (steady state)}$$

Under the assumption (**uniform ellipticity**) that for some constants $\lambda, \Lambda > 0$,

$$\lambda|\xi|^2 \leq a(x)\xi \cdot \xi \leq \Lambda|\xi|^2, \quad \forall \xi \in \mathbb{R}^d, \quad \forall x \in \mathbb{R}^d$$

and a is measurable (no continuity assumption !) the PDE

$$\begin{cases} \frac{\partial u(t, x)}{\partial t} = \frac{1}{2} \operatorname{div}(a(x)\nabla u(t, x)) \\ u(0, x) = g(x) \end{cases}$$

has a unique solution (in the weak sense), that is

$$\begin{aligned} \int_{\mathbb{R}^d} \phi(0, x)g(x) dx + \int_0^T \int_{\mathbb{R}^d} \frac{\partial \phi(t, x)}{\partial t} u(t, x) dt \\ = \frac{1}{2} \int_0^T \int_{\mathbb{R}^d} a(x)\nabla u(t, x)\nabla \phi(t, x) dx dt \end{aligned}$$

for all $\phi \in \mathcal{C}^{\infty, \infty}([0, T]; \mathbb{R}^d)$, $\phi(T, x) = 0$.

This solution is $(\alpha/2, \alpha)$ -Hölder continuous and weakly differentiable, but one cannot expect **better regularity** in general.

However, if a is locally regular, then u is also be locally regular.

Consider the case where S is a surface smooth enough, and a is smooth on each sides S_+ and S_- of S .

Then, for x on S ,

$$u(t, x+) = u(t, x-)$$

$$\text{and } \underbrace{a(x+)\mathbf{n}_+ \cdot \nabla u(t, x+) = a(x-)\mathbf{n}_- \cdot \nabla u(t, x-)}_{\text{continuity of the flux}}$$

Examples of models with discontinuities/interfaces:

- Concentration of a fluid in a porous media (Darcy's law) with different type of rocks
- Diffusion of species in several type of habitats
- Composite materials
- ...

Divergence form op. and diffusion processes

There exists a **fundamental solution** $p(t, x, y)$ for the differential operator $\frac{1}{2} \operatorname{div}(a \nabla \cdot)$ so that the solution to

$$\begin{cases} \frac{\partial u(t, x)}{\partial t} = \frac{1}{2} \operatorname{div}(a(x) \nabla u(t, x)) \\ u(0, x) = g(x) \end{cases}$$

may be written

$$u(t, x) = \int_{\mathbb{R}^d} p(t, x, y) g(y) dy.$$

In addition, $0 \leq p(t, x, y)$, $\int_{\mathbb{R}^d} p(t, x, y) dy = 1$ and

$$p(t, x, y) \leq \frac{C_1}{t^{d/2}} \exp\left(-\frac{C_2 |y - x|^2}{2t}\right) \quad (\text{Nash-Aronson estimate})$$

$\implies \frac{1}{2} \operatorname{div}(a \nabla \cdot)$ is the infinitesimal generator of a strong Markov, continuous stochastic process X .

Link with solutions of SDEs

If a is of class \mathcal{C}^1 , then

$$L = \frac{1}{2} \operatorname{div}(a \nabla \cdot) = \frac{1}{2} \sum_{i,j=1}^d a_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i,j=1}^d \frac{1}{2} \frac{\partial a_{i,j}}{\partial x_i} \frac{\partial}{\partial x_j}$$

and then X is solution to the SDE

$$X_t = x + \int_0^t \sigma(X_s) dB_s + \int_0^t \frac{1}{2} \nabla a(X_s) ds$$

with $\sigma \sigma^T = a$ and B is a Brownian motion.

In general, X is **not** a semi-martingale, because ∇a has no meaning.

However, the differential operator acts locally, so that in the region where a is smooth, X behaves like a “good” diffusion.

What happens at the surface of discontinuity?

Divergence and non-divergence form operators

$$D = \frac{1}{2} \operatorname{div}(a \nabla \cdot)$$

- There always exists a process associated to D , as soon as a is measurable, uniformly elliptic bounded.
- Gaussian estimates are the keys
- Difficult to simulate
- Martingale + something
- Natural class of functions: Sobolev spaces

$$N = \frac{1}{2} \sum_{i,j=1}^d a_{i,j} \partial_{i,j}^2$$

- Existence and uniqueness is provided under regularity of a (Hölder continuity) or on restrictive conditions on the discontinuities.
- Uniqueness may fail with discontinuous coefficients
- Easy to simulate
- Semi-Martingales
- Natural class of functions: \mathcal{C}^2

Note: The special case of $N = \frac{1}{2} a_{i,j} \partial_{i,j}^2$ with $a(x) = \rho(x) \operatorname{Id}$, $\rho : \mathbb{R}^d \rightarrow \mathbb{R}$ can be understood as a special case of divergence form operator with invariant measure ρ and then regularity assumptions on ρ may be dropped.

A simple case: $d = 1$

From now, we work under the simple case of $d = 1$.

☹ It is too **restrictive** to understand what happens when $d > 1$, which is the case for most of real-world problems.

☺ But it allows one to have a **better understanding** on what happens.

From now, we consider

$$L = \frac{\rho}{2} \nabla (a \nabla \cdot)$$

where

- ρ, a are measurable
- $\lambda \leq \rho(x) \leq \Lambda$ for all $x \in \mathbb{R}$
- $\lambda \leq a(x) \leq \Lambda$ for all $x \in \mathbb{R}$
- a and ρ are piecewise smooth and have a left/right limit at any point

Our choice of L covers both the case of divergence and non-divergence form operators

Remark 1: the drift is not a problem

If one wishes to consider

$$L = \frac{\rho}{2} \nabla(a \nabla \cdot) + b \nabla$$

with a measurable, bounded b , one has only to remark that

$$L = \frac{\rho e^{-\Phi}}{2} \nabla(a e^{\Phi} \nabla \cdot)$$

with

$$\Phi(x) = 2 \int^x \frac{b(y)}{a(y)\rho(y)} dy$$

and $a e^{\Phi}$ and $\rho e^{-\Phi}$ satisfy locally the previous hypotheses.

Thus, it is not a problem to consider a drift, or to set $b = 0$.

Remark 2: on the transmission condition

A function f in the domain $\text{Dom}(L)$ of L satisfies

$$f(x-) = f(x+) \text{ and } a(x-)\nabla f(x-) = a(x+)\nabla f(x+)$$

at any point x where a or ρ is discontinuous.

If a and ρ are continuous on $(-\infty, \beta)$ and on $(\beta, +\infty)$, set

$$\tilde{a}(x) := \begin{cases} \lambda a(x) & \text{on } (-\infty, \beta) \\ a(x) & \text{otherwise} \end{cases} \text{ and } \tilde{\rho}(x) := \begin{cases} \rho(x)/\lambda & \text{on } (-\infty, \beta) \\ \rho(x) & \text{otherwise} \end{cases}$$

so that

$$\tilde{L} = \frac{\tilde{\rho}}{2} \nabla(\tilde{a} \nabla)$$

is such that

$$\tilde{L}f(x) = Lf(x) \text{ for } x \in (-\infty, \beta) \cup (\beta, +\infty)$$

but for f in $\text{Dom}(\tilde{L})$,

$$f(x-) = f(x+) \text{ and } \lambda a(x-)\nabla f(x-) = a(x+)\nabla f(x+)$$

On one-dimensional diffusion processes

The operator L is the infinitesimal generator of a strong Markov process with continuous paths.

This process can be constructed either as the process associated to the divergence-form operator L , or by its scale function and its speed measure (or by other means).

Scale function: There exists a continuous, increasing function S (unique up to additive and multiplicative constants) such that for $x < y < z$

$$\mathbb{P}_y [\tau_x < \tau_z] = \frac{S(z) - S(y)}{S(z) - S(x)}$$

Speed measure: There exists a measure μ such that

$$\mathbb{E}_y [\tau_{[x,z]}] = \int_x^z G_{x,z}(y, u) \mu(du)$$

for the Green function $G_{x,y}(y, u)$ on $[-x, z]$ of L (given by a simple expression).

On one-dimensional diffusion processes

The scale function is related to the probability that the diffusion reaches a given point x before another given point y , while the speed measure gives an indication to the average times it takes to exit from some interval.

If B is a Brownian motion, the processes $t \mapsto B_t$ and $t \mapsto B_{2t}$ have the same scale function $S(x) = x$ but different speed measures.

In dimension one, any diffusion process X is **fully characterized** by its scale function S and its speed measure μ

There exists a random time change T related to m such that

$$X_t = S(B_{T(t)}).$$

Convergence results

If a^n , b^n and ρ^n are such that

$$\frac{1}{a^n} \xrightarrow[n \rightarrow \infty]{L^2_{\text{loc}}(\mathbb{R})} \frac{1}{a}, \quad \frac{1}{\rho^n} \xrightarrow[n \rightarrow \infty]{L^2_{\text{loc}}(\mathbb{R})} \frac{1}{\rho} \quad \text{and} \quad \frac{b^n}{a^n \rho^n} \xrightarrow[n \rightarrow \infty]{L^2_{\text{loc}}(\mathbb{R})} \frac{b}{a\rho}$$

then the process X^n associated to $L^n = \frac{\rho^n}{2} \nabla(a^n \nabla \cdot) + b^n \nabla$ converges in distribution to the process X associated to $L = \frac{\rho}{2} \nabla(a \nabla \cdot) + b \nabla$ for any starting point.

A way to deal with the problem of discontinuous coefficients consists in using a sequence of mollifiers to regularize the coefficients, but

☹ From the numerical point of view, it does not work very well

☹ From the theoretical point of view, there is nothing to understand

Instead, we will assume that a and ρ are **piecewise constant**, which can be a good approximation of piecewise smooth function by adding a lot of small jumps.

Local behavior of the process

If a and ρ are constant on the intervals (x_i, x_{i+1}) then for $f \in \text{Dom}(L)$,

$$\begin{cases} Lf(x) = \frac{1}{2}\rho(x_i+)a(x_i+)f''(x) \text{ on } (x_i, x_{i+1}), \\ f \in \mathcal{C}^2((x_i, x_{i+1})), \quad \forall i \\ f(x_i-) = f(x_i+), \\ (1 - q_i)\nabla f(x_i-) = (1 + q_i)\nabla f(x_i+) \text{ with } q_i = \frac{a(x_i+) - a(x_i-)}{a(x_i+) + a(x_i-)}. \end{cases}$$

With the remark on the transmission condition above (multiply a by λ on (x_i, x_{i+1}) and ρ by $1/\lambda$ on (x_i, x_{i+1})), the problem consists in finding the local behavior of a process X such that

- It is a Brownian motion with a given speed on (x_{i-1}, x_i)
- It is a Brownian motion with a given speed on (x_i, x_{i+1})
- The functions in the domain of its infinitesimal generator satisfy $(1 - q_i)\nabla f(x_i-) = (1 + q_i)\nabla f(x_i+)$ and $f(x_i-) = f(x_i+)$ at x_i

A simple case

Assumption: a and ρ are constant on \mathbb{R}_-^* and \mathbb{R}_+^* .

It can be showned (by several means) that

$$X_t = x + \int_0^t \sqrt{a(X_s)\rho(X_s)} dB_s + \underbrace{\frac{a(0+) - a(0-)}{a(0+) + a(0-)}}_{\in(-1,1)} L_t^0(X),$$

where

- B is a Brownian motion
- $L_t^0(X)$ is the symmetric **local time** at 0 of X :

$$L_t^0(X) = \lim_{\epsilon \rightarrow 0} \frac{1}{2\epsilon} \int_0^t \mathbf{1}_{[-\epsilon, \epsilon]}(X_s) ds$$

The local time characterizes the time spend by X at 0.

$t \mapsto L_t^0(X)$ is continuous and non-decreasing. However, it increases only on $\{t \geq 0 \mid X_t = 0\}$ which has a Lebesgue measure equal to 0!

The local time has an effect only when X reaches 0. Otherwise, X behaves like a Brownian motion with diffusion coefficient $a\rho/2$.

A simple case: why such an SDE?

Heuristic: consider a function of class $\mathcal{C}_b^2(\mathbb{R} \setminus \{0\}) \cap \mathcal{C}(\mathbb{R})$ with $a(0+)\nabla f(0+) = a(0-)\nabla f(0-)$

Itô-Tanaka formula \implies

$$\begin{aligned}
 f(X_t) = f(x) &+ \underbrace{\int_0^t \frac{1}{2} (f'(X_s+) + f'(X_s-)) dX_s}_{\int_0^t f'(X_s) \sqrt{\sigma(X_s)a(X_s)} dB_s + K} \\
 &+ \underbrace{\frac{1}{2} \int_0^t (f'(X_s+) - f'(X_s-)) dL_t^0(X_s)}_{=-K} + \frac{1}{2} \int_0^t \sigma(X_s) a(X_s) f''(X_s) ds
 \end{aligned}$$

so that $M_t = f(X_t) - f(x) - \int_0^t \frac{1}{2} \int_0^t \sigma(X_s) a(X_s) f''(X_s) ds$ is a martingale with brackets $\langle M \rangle_t = \int_0^t a(X_s) \sigma(X_s) f'(X_s)^2 ds$

\implies characterization of the infinitesimal generator of X .

SDE with local time

Conditions for strong existence and convergence results for SDE of type

$$X_t = x + \int_0^t \sigma(X_s) dB_s + \int_{\mathbb{R}} \nu(dy) L_t^y(X)$$

have been provided to J.-F. Le Gall in the 80's.

In our case, we consider measures of type

$$\nu(dx) = g(x) dx + \sum_i \alpha_i \delta_{x_i}$$

With the occupation density formula,

$$\int_{\mathbb{R}} g(x) L_t^x(X) dx = \int_0^t \sigma(X_s)^2 g(X_s) ds$$

so that one can consider measures of type $\nu(dx) = \sum_i \alpha_i \delta_{x_i}$.

This class of SDE is stable under application of one-to-one mappings Φ

such that $\Phi \in \mathcal{C}(\mathbb{R}) \cap \mathcal{C}^2(\mathbb{R} \setminus \{z_i\})$ with

$$(1 + q_i) \nabla \Phi(z_i+) = (1 - q_i) \nabla \Phi(z_i-).$$

The Skew Brownian motion

The **Skew Brownian motion** is a generalization of the Brownian motion that depends on a parameter $\alpha \in [-1, 1]$.

$$a = \begin{cases} a_+ & \text{on } \mathbb{R}_+ \\ a_- & \text{on } \mathbb{R}_-, \end{cases}, \quad \rho = \begin{cases} 1/a_+ & \text{on } \mathbb{R}_+ \\ 1/a_- & \text{on } \mathbb{R}_- \end{cases} \quad \text{and } \alpha = \frac{a_+}{a_+ + a_-}$$

The process X is solution to the SDE (Harrison-Shepp)

$$X_t = x + B_t + \beta L_t^0(X) \quad \text{with } \beta = 2\alpha - 1.$$

 A possible **construction** of the Skew Brownian motion (Itô-McKean)

- Consider the excursions of a reflected Brownian motion
- Change the sign of each excursion with independent Bernouilli random variables of parameter α

Constructions of the Skew Brownian motion

Another possible construction of the Skew Brownian motion (N. Portenko, 78') it is the process whose infinitesimal generator is

$$L = \frac{1}{2}\Delta + \alpha\delta_0\nabla$$

Yet another construction of the Skew Brownian motion (Harrison-Shepp) consider a simple random walk S_n on \mathbb{Z} such that

$$\mathbb{P}[S_{n+1} = 1 | S_n = 0] = \alpha. \text{ Then } n^{-1/2}S_{nt} \xrightarrow[n \rightarrow \infty]{\text{dist.}} \text{SBM}(\alpha)$$

We have also a simple expression for the density of the SBM.

There are indeed many ways to construct a SBM, and some schemes follows easily from these constructions.

The Skew Brownian motion is the basic element to understand SDE with local time.

An apparent paradox?

What can be done in the case of $L = \frac{\rho}{2} \nabla(a \nabla \cdot)$?

Heuristically, the discontinuity may be interpreted as **permeable barrier**: the particle goes to one side or the other with a given probability.



However, the situation is more complex.

Consider

$$a(x) = \begin{cases} a_+ & \text{if } x \geq 0, \\ a_- & \text{if } x < 0, \end{cases} \text{ and } \rho = 1.$$

Then for any $h > 0$,

$$\mathbb{P}_0 [\tau_h < \tau_{-h}] = \frac{a_+}{a_+ + a_-}$$

Yet for any $t > 0$,

$$\mathbb{P}_0 [X_t > 0] = \frac{\sqrt{a_+}}{\sqrt{a_+} + \sqrt{a_-}}$$

Simulation techniques

In order to get simulation techniques for

$$L = \frac{\rho}{2} \nabla (a \nabla \cdot)$$

a possible approach consists in using well-chosen one-to-one mapping to change the process.

Suppression of the local time

$Y_t = S(X_t)$ with $S'(x) = 1/a(x)$ is solution to

$$Y_t = \int_0^t \sqrt{\frac{\rho \circ S^{-1}(Y_s)}{a \circ S^{-1}(Y_s)}} dB_s$$

Simulation: Euler scheme for SDE with discontinuous coefficients

iL. Yan, *Ann. Appl. Probab.* 2002 for the convergence of the Euler scheme with discontinuous coeff.

iM. Martinez, Ph.D. thesis, 2004 for application to divergence form operators and computation of the rate of convergence.

Reduction to the SBM

$$\Psi(x) = \int^x \frac{1}{\sqrt{\rho(y)a(y)}} dy$$

then $Y_t = \Psi(X_t)$ is solution to

$$Y_t = \Phi(x) + B_t + \underbrace{\frac{\sqrt{a(0+)/\rho(0+)} - \sqrt{a(0-)/\rho(0-)}}{\sqrt{a(0+)/\rho(0+)} + \sqrt{a(0-)/\rho(0-)}}}_{2\alpha-1} L_t^{\Psi(0)}(Y)$$

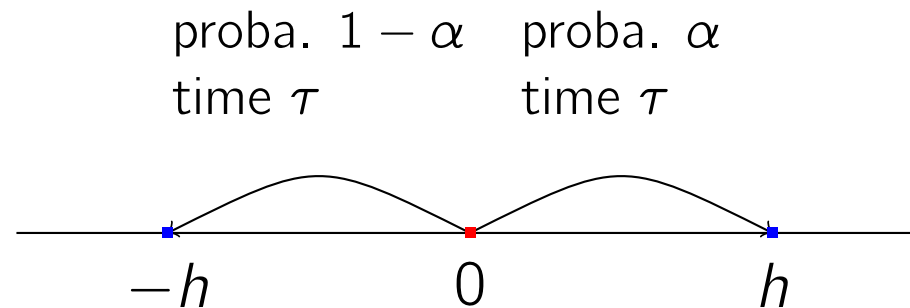
(To simplify, we assume only one point of discontinuity at 0)

The process Y is then (locally if there are more than one point of discontinuity) a skew Brownian motion.

If at time t the process is at 0 and

$$\tau = \inf \{ s > t \mid X_s = \pm h \}$$

then τ and Y_τ are independent, $\mathbb{P} [Y_\tau = h] = \alpha$ and τ is distributed as the first exit time of the Brownian motion from $[-h, h]$



Simulation: At 0 (or any point of discontinuity), one can re-inject the particle in $-h$ or h by simulating Y_τ and increasing the time by τ .

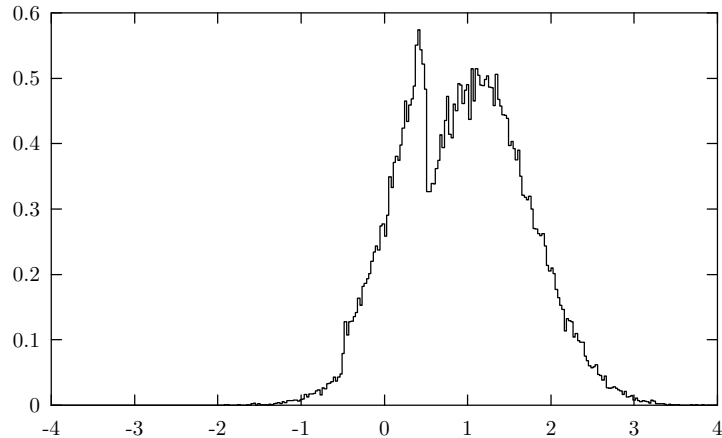
It is also possible to simulate exactly $(\tau \wedge T, Y_{\tau \wedge T})$.

This method becomes costly unless the coefficients are piecewise constant with not too many points of discontinuities.

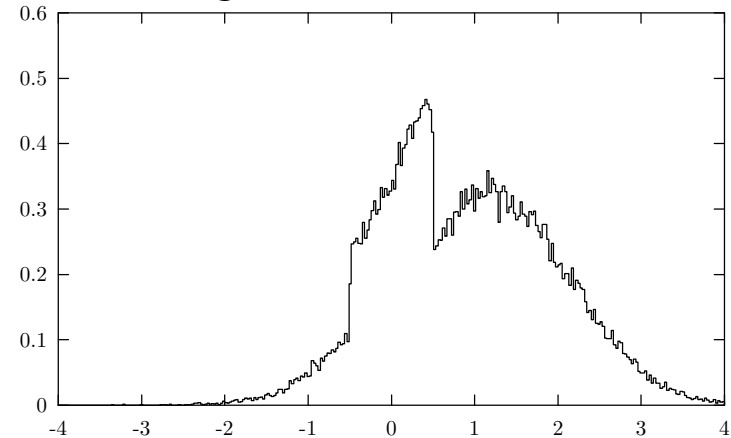
 A.L. & M. Martinez, *Ann. Appl. Probab.*, 2005.

A numerical example: doubly SBM

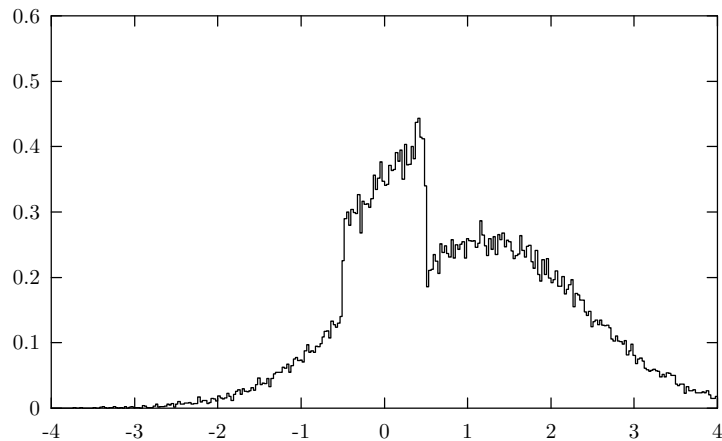
$$X_t = 1 + B_t + \frac{2}{3}L_t^{-1/2}(X) - \frac{2}{3}L_t^{1/2}(X)$$



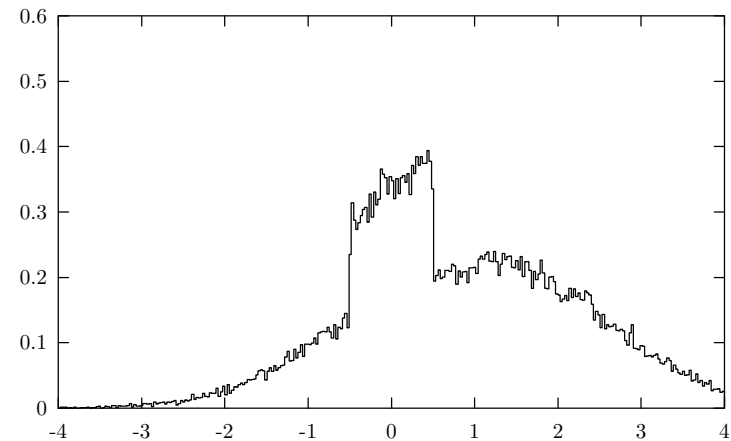
$t = 1/2$



$t = 1$



$t = 3/2$



$t = 2$

Approximation by a random walk I

If a and ρ are piecewise constant, up to a small perturbation of the positions of the points of discontinuities, it is possible to assume that there are contained $\{x_i\}_{i \in \mathbb{Z}}$ with $\Psi(x_i) = ih$ for a given step h , where

$$\Psi(x) = \int_0^x \frac{1}{\sqrt{\rho(y)a(y)}} dy.$$

$Y := \Psi(X)$ is solution to

$$Y_t = \Psi(x) + B_t + \sum_{i \in \mathbb{Z}} \beta_i L_t^{ih}(Y).$$

where

$$\beta_i = \frac{\sqrt{a(x_i+)/\rho(x_i+)} - \sqrt{a(x_i-)/\rho(x_i-)}}{\sqrt{a(x_i+)/\rho(x_i+)} + \sqrt{a(x_i-)/\rho(x_i-)}}$$

Simulation: walk on the grid $\{ih\}_{i \in \mathbb{Z}}$

- Perform a random walk (ξ_k) with

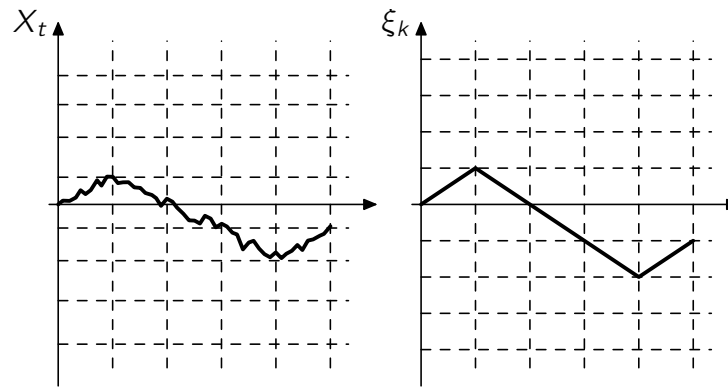
$$\mathbb{P}[\xi_{k+1} = (i+1)h \mid \xi_k = ih] = \frac{1 + \beta_i}{2}$$

- At each step, increase the time by

$$h^2 = \mathbb{E}[\tau_i \mid \xi_k = ih, \xi_{k+1} = (i+1)h] = \mathbb{E}[\tau_i \mid \xi_k = ih, \xi_{k+1} = (i-1)h]$$

with $\tau_i = \inf \{ t > 0 \mid |Y_t - \xi_i| = h \}$

- ☞ The position $\Psi^{-1}(\xi_k)$ represents an approximation of the position of X_t at time $t = kh^2$.



Rate of convergence as in Donsker's theorem

📖 P. Étoré, *Electron. J. Probab.*, 2006

Approximation by a random walk II

The difficulty with the previous method is that the grid depends on the coefficients.

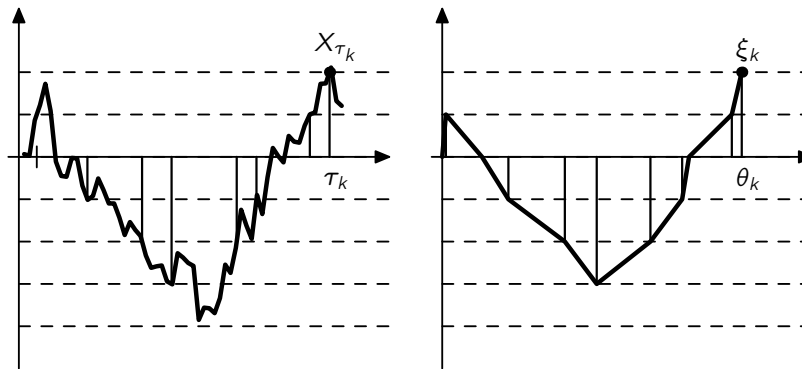
Consider a process X with infinitesimal generator $L = \frac{\rho}{2} \nabla (a \nabla \cdot)$ whose coefficients are uniformly elliptic and bounded (this method does not use SDE with local times)

Consider a grid $\mathcal{G} = \{x_i\}_i$ with $x_{i-1} < x_i$ for all i .

Set

$$\delta_i = \inf \{ t > 0 \mid X_t \in \mathcal{G} \setminus \{X_{\tau_i}\} \}, \quad \tau_{i+1} = \tau_i + \delta_i$$

The τ_i 's represent the time at which X reaches successive levels.



Simulation: random walk on the grid \mathcal{G}

- Perform a random walk with

$$\mathbb{P} [\xi_{k+1} = x_{i+1} \mid \xi_k = x_i] = \mathbb{P}_{x_i} [X_{\tau_k} = x_{i+1}] = u(x_i)$$

with

$$\begin{cases} Lu = 0 \text{ on } (x_{i-1}, x_{i+1}), \\ u(x_{i+1}) = 1, \quad u(x_{i-1}) = 0. \end{cases}$$

- At each step, increment the time by

$$t_k := \mathbb{E} [\tau_k \mid \xi_k = x_i, \xi_{k+1}] = v(x_i)/w(x_i) \text{ with}$$

$$\begin{cases} Lv = -w & \text{on } (x_{i-1}, x_{i+1}) \\ v(x_{i-1}) = v(x_{i+1}) = 0 \end{cases}$$

with

$$w = \begin{cases} u & \text{if } \xi_i = x_k, \quad \xi_{i+1} = x_{k+1}, \\ 1 - u & \text{if } \xi_i = x_k, \quad \xi_{i+1} = x_{k-1}. \end{cases}$$

👉 At time $\theta_i = \sum_{j < i} t_j$, (θ_i, ξ_i) is an approximation of (τ_i, X_{τ_i}) .

📖 P. Étoré & A.L., *ESAIM Probab. Stat.*, 2007.

Other approaches and related works

- ★ J. M. Ramirez, E.A. Thomann & E.C. Waymire (Oregon State University) used the multi-skew Brownian motion in a geophysical context.
- ★ M. Decamps, A. De Scheeper, M. Goovaerts & W. Schoutens (Catholic University of Leuven) have proposed some “self-exciting threshold interest rates models” in finance that relies on the SBM and numerical methods using perturbation formulas of the density of the SBM.
- ★ N. Limić (University of Zagreb) have proposed a scheme for $d > 1$ where the infinitesimal generator of a continuous time Markov process is constructed from a finite-volume scheme.