Random dynamics in a trap: killing versus survival

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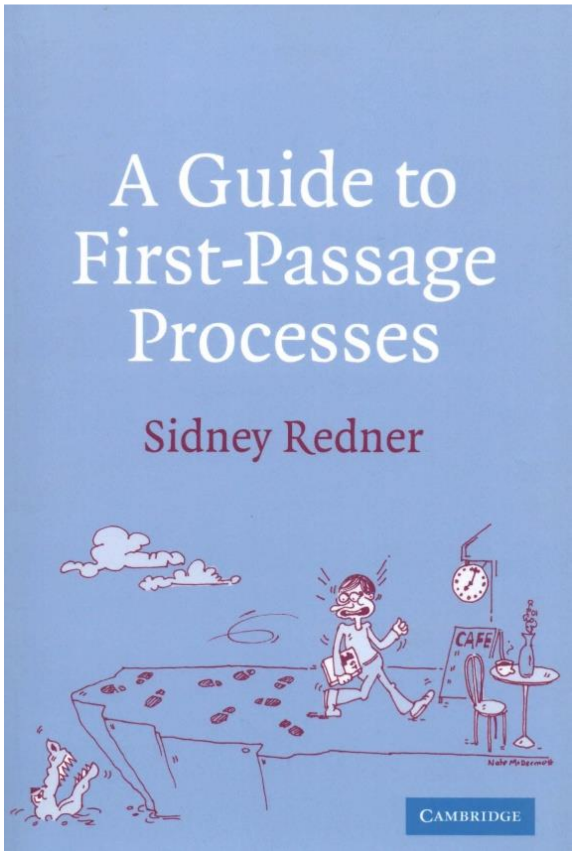


Direct pictorial inspiration

Diffusion in a **bounded domain** with absorbing boundaries **versus** permanently **trapped** diffusion process in the same bounded domain.

Departure point (inspirations):

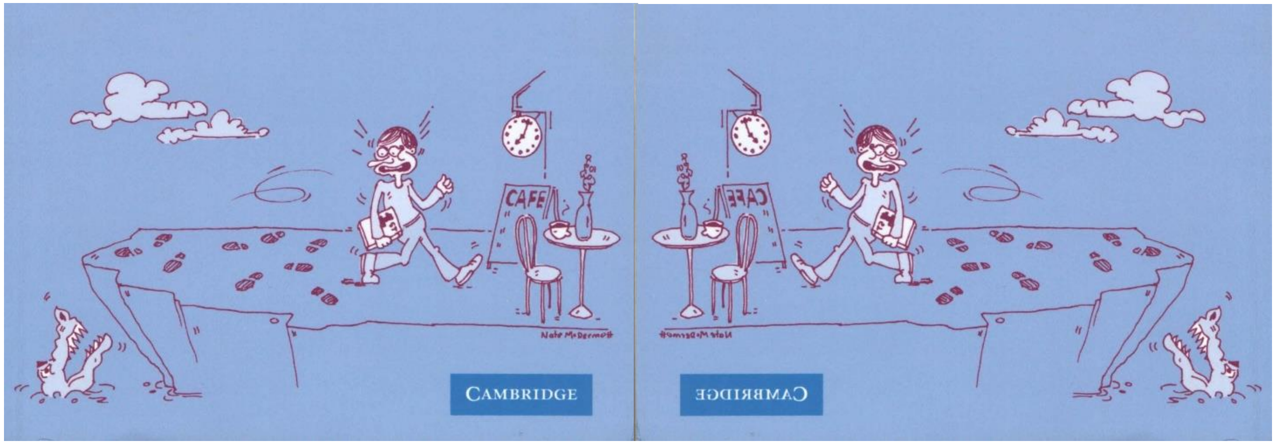
Fast power law-like decay for a diffusive system with absorbing borders, Michel Droz, **Andrzej Pękalski**, Physica A **470** (2017) 82–87

Cites:

[3] P. Blanchard, P. Garbaczewski, Phys. Rev. E 49 (1994) 3815. **Natural boundaries for the Smoluchowski equation and affiliated diffusion processes**

[5] T. Agranov, B. Meerson, A. Vilenkin, Phys. Rev. E 93 (2016) 012136. **Survival of interacting diffusing particles inside a domain with absorbing boundary**

Diffusion in **a bounded domain** (interval, disc, sphere) with **absorption (killing) at the boundary**. Inventory: first passage time, mean FPT**,** survival probability and its asymptotic **decay.** **How to make survival longer, ultimately eternal ?**



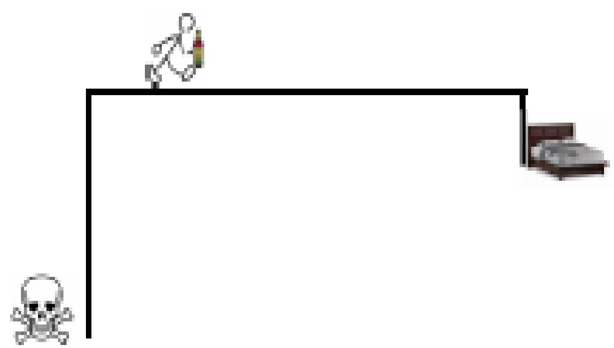
Interval with absorbing ends – directly from Redner's book

$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial x^2}.$$

$0 \le x \le L \qquad c(0,t) = c(L,t) = 0.$

$c(x, t=0) = \delta(x - x_0)$ with $0 < x_0 < L$,

$\int_0^L c(x, t=0)\,dx = 1$



Survival probability

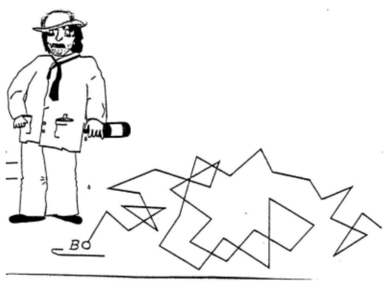
$$S(t) = \int_0^L c(x,t)\,dx$$

$$c(x,t) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi x}{L}\right) e^{-(\frac{n\pi}{L})^2 Dt}$$

$$S(t) \propto e^{\;D\pi^2 t/L^2} \equiv e^{-t/\tau_1}$$

The effect of these boundary conditions can be captured by setting c=0 on both boundaries: both act like perfectly absorbing walls.

Enforcing the long term survival (against the odds, taboo)



Brownian motion (**diffusion**) in a bounded domain with absorbing boundaries + fear (**conditioning)** = long term survival due to **conditioning (what that conditioned BM actually is ?**), Genuine random motion in a trap !

Some related hints (**how to increase the survival probability in a bounded domain**)

S. Redner, P. L. Krapivsky: „ ***Life and death at the edge of a windy cliff***" (1996)
(diffusing agent dies while reaching the edge, being subject to the strong „wind shear")

P.L. Krapivsky, S. Redner, „***Life and death in the cage and at the edge of the cliff***" (1999); („diffusing prisoner", expanding cage)

M. Li, N. D. Pearson, A. M. Poteshman, „***Conditional estimation of diffusion processes***", J. Financial Economics 74, (2004, 31-66; „time series of interest rate data, conditioned to remain between upper and lower boundaries"

M. Droz, A. Pękalski / Physica A 470 (2017) 82–87

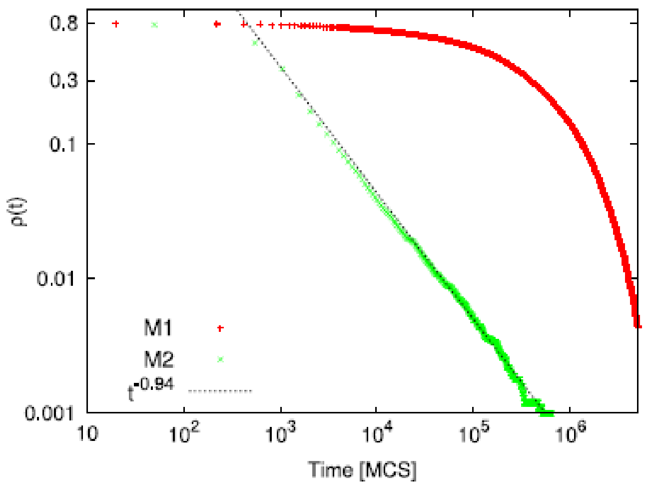


Fig. 1. Time dependence of the density for the M1 and M2 models. Colour online.

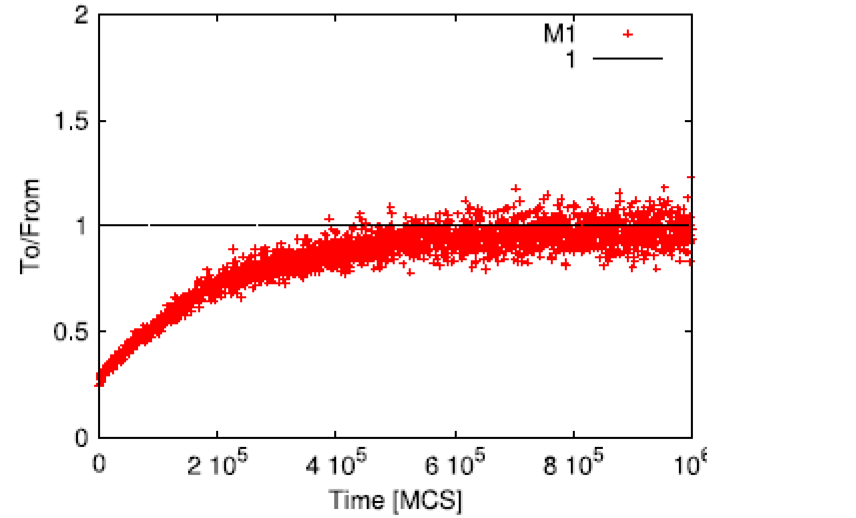


Fig. 3. Ratio of movements in the direction towards the sinks (To) and away from them (From)

„A special feature of Monte Carlo updating procedures is the direction of the average movements of the particles. **In the red-marked case they are moving away from the edges, towards the centre**, while in the other average jumps are directed towards the edges."

Recently, Agranov et al. considered the case where diffusing (dense gas of) particles, contained in a d-dimensional box, are absorbed when they reach the boundaries. In particular, they investigated, using macroscopic fluctuation theory, **the probability that no particle is absorbed during a time T and addressed an issue of large T.**

$$q(x) = 2n_0 \cos^2\left(\frac{\pi x}{2R}\right)$$ density profile $q(x,t)$ is stationary

$$v(x) = -\frac{\pi}{2R} \tan\left(\frac{\pi x}{2R}\right)$$ gradient (forward drift !) field,

Compare e.g. H. Risken's BM in a trap

Interval with absorbing ends, told anew

Free diffusion $\partial_t k = D\Delta k$ is considered within an interval $\Omega = [a, b] \subset R$, with absorbing boundary conditions at its end points a and b

Its time and space homogenous transition density, with $x, y \in (a, b)$, $0 \leq s < t$ and $b - a = L$ reads

$$k(x,t|y,s) = \frac{2}{L}\sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{L}(x-a)\right) \sin\left(\frac{n\pi}{L}(y-a)\right) \exp\left(-\frac{Dn^2\pi^2}{L^2}(t-s)\right)$$

We note that $\lim_{t\to s} k(x,t|y,s) \equiv \delta(x-y)$

From now on we employ the symmetric interval $[-c, c]$ with $L = 2c, c > 0$. We set $D = 1/2$

At this point we define a conditional transition probability density for the process "living" in $(-c, c)$ up to time T (might be interpreted as the a priori set survival time.

A conditional probability that no absorption takes place at the boundaries of $[-c, c]$, in a prescribed time interval $[0, T]$, can be rephrased in terms of a condition that $\max |X(\tau)| < c$ holds true for all times $t \leq [0, T]$.

Conditioning – towards taboo processes

$$p(y,s;x,t;u,T) = \frac{k(y,s|x,t)\,k(x,t|u,T)}{k(y,s|u,T)}$$

Note. We hereby answer the following question: assuming that the test particle originates from y at s, and terminates its route at (in the vicinity of) u at time T, what is the probability to find it in between x and $x + \Delta x$ at the intermediate time t, $s < t < T$.

For sufficiently large value of T,

$$k(x,t|u,T) \sim \sin[\frac{\pi}{L}(x+c)]\ \sin[\frac{\pi}{L}(u+c)]\ \exp\left(-\frac{\pi^2}{2L^2}(T-t)\right)$$

wit $k(y,s|u,T)$ obtained form $k(x,t|u,T)$ by replacements $x \to y$, $t \to s$.

Accordingly (remember about $T \gg t$ and $L = 2c$) we arrive at a conditioned transition density

$$p_{trap}(y,s|x,t) \sim k(y,s|x,t)\,\frac{\sin[\frac{\pi}{2c}(x+c)]}{\sin[\frac{\pi}{2c}(y+c)]}\,\exp\left(+\frac{\pi^2}{8c^2}(t-s)\right)$$

Instead of $\sim$ we actually reach an equality, if the limit $T \to \infty$ is executed.

We note that $\sin[\frac{\pi}{2c}(x+c) = cos(\frac{\pi}{2c}x)$

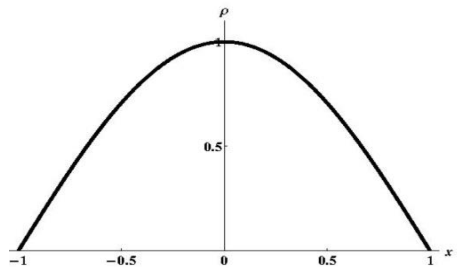
By general principles, we have thus arrived at the transition probability density of the diffusion process with inaccessible boundaries $\pm c$, whose forward drift reads

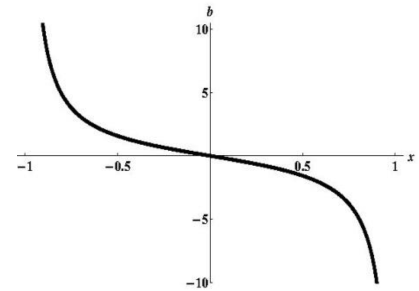
$$b(x) = \nabla \ln \cos(\frac{\pi}{2c}x) = -\frac{\pi}{2c}\tan(\frac{\pi}{2c}x)$$

and the corresponding Fokker-Planck equation has the form $\partial_t \rho = \frac{1}{2}\Delta\rho - \nabla(b\rho)$,

$dX_t = b(X_t)\,dt + dB_t$ provides a path-wise background

Visualization of the interval as a permanent trap for random motion: left, probability density, right the forward F-P eq. drift b(x)





More abstract setting: **eigenfunction expansions on the interval and on the disk**

We point out an obvious link with the standard (quantum mechanical by provenance) spectral problem for the operator $-\frac{1}{2}\Delta$ in an infinite well. Denoting λ_n, $n = 1, 2, \ldots$ the eigenvalues and $\phi_n, n = 1, 2, \ldots$ the orthonormal basis system composed of the eigenfunctions ϕ_n, we realize that $k(y, s|x, t)$ is the integral (Feynman-Kac) kernel of the semigroup operator $\exp \frac{1}{2}(t - s)\Delta_{\mathcal{D}})$, where the notation $\Delta_{\mathcal{D}}$ directly refers to the absorbing boundary data for the domain $\mathcal{D}$.

In the F-K formula context, it has become a classic to interpret $k(y,s|x,t)$ for the interval problem as a definition of $\Delta_{\mathcal{D}}$, while being determined entirely in terms of sample paths ω (here $\omega(s) = y$ while $\omega(t) = x$) that survive within the interval $(-c, c)$ up to time t, while being started within that interval at $s < t$

$$[\exp((t-s)\frac{1}{2}\Delta_{\mathcal{D}})](y,x) = \int d\mu_{s,y,x,t}(\omega) = \mu_{s,y,x,t}(\omega)$$

In parallel, a spectral decomposition of $\Delta_{\mathcal{D}}$ allows to rewrite $k(y,s|x,t)$ in a handy form:

$$k(y,s|x,t) = \sum_{n=1}^{\infty} e^{-\lambda_n(t-s)}\,\phi_n(x)\phi_n(y)$$

We can recast the previous conditional transition density $p(y,s;x,t;u,T)$ in terms of the eigenfunctions expanded kernels

It is clear that under suitable regularity assumptions concerning the $T \to \infty$ limit, specifically that $k(y,s|u,T) \sim \phi_1(y)\phi_1(u)\exp(-\lambda_1(T-s))$, we arrive at

$$p_{trap}(y,s|x,t) = k(y,s|x,t)\frac{\phi_1(x)}{\phi_1(y)}e^{+\lambda_1(t-s)}$$

as anticipated previously (setting e.g. $\lambda_1 = \frac{\pi^2}{2L^2}$ and $\phi_1(x) = \sqrt{\frac{2}{L}}\cos(\pi x/L)$).

$$p_{trap}(y,s|x,t) \sim (\phi_1(x))^2 = \rho(x) = \frac{2}{L}\cos^2(\pi x/L)$$

Back to the cliffy island (disk) with a fearful Brownian agent

Coming back to the "fearful" Brownian walker on the cliffy island, we should in fact consider (that is for simplicty) a domain in the regular disc shape, i.e. the circle of a fixed radius R. The spectral solution for such domain ($2D$ version of the previous $(-c, c)$ interval problem is well known, albeit somewhat murky form the casual (user friendly) point of view.

We know explicitly the spectral solution for the disk

$$k(y, s|x, t) = \sum_{n=1}^{\infty} e^{-\lambda_n (t-s)} \phi_n(x) \phi_n(y)$$

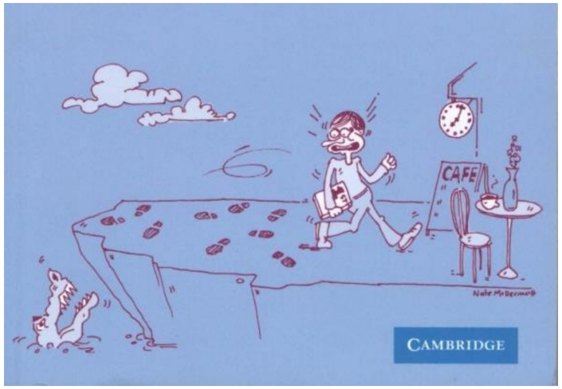
Coming back to the "fearful" Brownian walker on the cliffy island, we should in fact consider (that is for simplicty) a domain in the regular disc shape, i.e. the circle of a fixed radius R. The spectral solution for such domain ($2D$ version of the previous $(-c, c)$ interval problem is well known, albeit somewhat murky form the casual (user friendly) point of view.
Since we are interested in the long T duration of the conditioned process, we need basically the knowledge of the stationary density and the forward drift. In the present case these read respectively:

$$\rho(\mathbf{r}) \sim \frac{j_0^2\left(\frac{z_1 r}{R}\right)}{j_1^2(z_1)} = \phi_1^2(\mathbf{r})$$

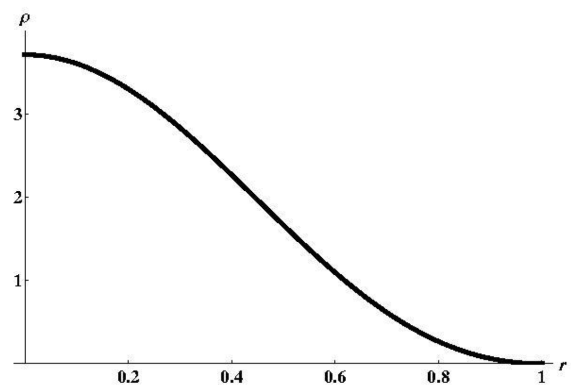
where $z_1 = 2.4048...$ is the first positive zero of the Bessel function $j_0(r)$, and (here $\hat{\mathbf{r}} = (1/r)(x, y, z)$)

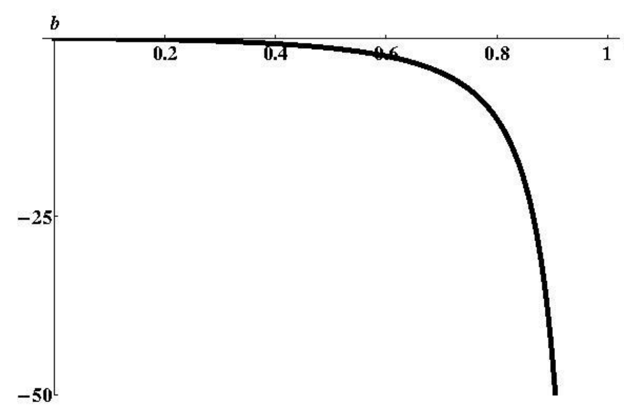
$$b(\mathbf{r}) = \nabla \ln \phi_1(\mathbf{r}) = -\frac{z_1 j_1\left(\frac{z_1 r}{R}\right)}{R j_0(z_1 r)}\,\hat{\mathbf{r}}$$

The Fokker-Planck operator takes the form: $(1/2)\Delta - \nabla b(\mathbf{r}), \cdot)$.



Visualization of **the disk (cliffy island**) as a permanent trap for random motion: left **- probability density,** right **- the forward Fokker-Planck equation drift b(x)**





General approach to stochastic processes with killing: towards an eternal life-time (suppression of killing means conditioning)

It is well known that operators of the form $\hat{H} = -\Delta + V \geq 0$ with $V \geq 0$ give rise to transition kernels of diffusion -type Markovian processes with killing (absorption), whose rate is determined by the value of $V(x)$ at $x \in R$. That interpretation stems from the celebrated Feynman-Kac (path integration) formula, which assigns to $\exp(-\hat{H}t)$ the positive integral kernel.

$$[\exp(-(t-s)(-\frac{1}{2}\Delta + V)](y,x) = \int \exp[-\int_s^t V(\omega(\tau))d\tau]\, d\mu_{s,y,x,t}(\omega)$$

In terms of Wiener paths that kernel is constructed as a path integral over paths that get killed at a point $X_t = x$ at time t in the time interval dt, with a probability $V(x)dt$ (note that physical dimensions of of V before scaling them out, were J/s, that is usually secured by a factor $1/2mD$ or $1/\hbar$). The killed path is henceforth remowed from the ensemble of on-going Wiener paths.

Given a discrete spectral solution for $\hat{H} = -\Delta + V$ with $V(x) \geq 0$, comprising the monotonically growing series of non-degenerate positive eignevalues, with real $L^2(R)$ eigenfunctions. The integral kernel of $\exp(-t\hat{H})$ has the time-homogeneous form

$$k(y,x,t) = k(x,y,t) = \sum_j \exp(-\epsilon_j t)\, \phi_j(y)\phi_j(x).$$

Consider the harmonic oscillator problem with $\hat{H} = (1/2)(-\Delta + x^2)$.

The integral kernel of $\exp(-t\hat{H})$ is given by a classic Mehler formula:

$$k(y,x,t) = [\exp(-t\hat{H})(y,x) = \frac{1}{\sqrt{\pi}} \exp[-(x^2+y^2)/2] \sum_{n=0}^{\infty} \frac{1}{2^n n!} H_n(y) H_n(x) \exp(-\epsilon_n\, t) =$$

$$\exp(-t/2)\, (\pi[1-\exp(-2t)])^{-1/2} \exp\left[-\frac{1}{2}(x^2-y^2) - \frac{(x-e^{-t}y)^2}{(1-e^{-2t})}\right] =$$

$$\frac{1}{(2\pi \sinh t)^{1/2}} \exp\left[-\frac{(x^2+y^2)\cosh t - 2xy}{2\sinh t}\right]$$

where $\epsilon_n = n + \frac{1}{2}$, $\phi_n(x) = [4^n (n!)^2 \pi]^{-1/4} \exp(-x^2/2)\, H_n(x)$ is the $L^2(R)$ normalized Hermite (eigen)function, while $H_n(x)$ is the n-th Hermite polynomial $H_n(x) = (-1)^n (\exp x^2) \frac{d^n}{dx^n} \exp(-x^2)$.

Conditioning: Let us define $\to T - t$ and accordingly consider $k(y,t|x,T) = k(T-t,x,y)$

$$p(y,s;x,t;u,T) = \frac{k(y,s|x,t)k(x,t|u,T)}{k(y,s|u,T)}$$

and investigate the $T \to \infty$ limit. Since we have

$$k(x,t|u,T) \sim \frac{1}{2\pi e^{-(T-t)/2}} \, e^{-\frac{1}{2}(x^2+u^2)}$$

we readily arrive at the transition probability density $p(y,s,x,t) = p_{t-s}(x|y)$ of the familiar Ornstein-Uhlenbeck process

$$p(y,s;x,t;u,T) \to p(y,s,x,t) = k(y,s,x,t)\, \frac{\exp(-x^2/2)}{\exp\left(-y^2/2\right)}\, e^{(t-s)/2} =$$

$$k(y,x,t)\, \frac{\phi_1(x)}{\phi_1(y)}\, e^{+\epsilon_1(t-s)} = [\pi(1-e^{-2(t-s)})]^{-1/2} \exp\left[-\frac{(x-e^{-(t-s)}y)^2}{(1-e^{-2(t-s)})}\right]$$

where $\phi_1(x) = \pi^{-1/2}\exp(-x^2/2)$ and $\epsilon_1 = 1/2$ have been accounted for.

Here the Fokker=Planck operator takes the form $L^* = (1/2)\Delta - \nabla[b(x)\,\cdot]$ and $b(x) = -x$. Clearly $b(x) = \nabla \ln \phi_1(x)$, as should be.

$$\rho(x) = \phi_1^2(x) = \frac{1}{\pi}\exp(-x^2)$$

About time rates to equilibrium in a trap (model independent statement)

$$k(y,x,t) \;=\; \sum_j \exp(-\lambda_j t)\, \phi_j(y)\phi_j(x).$$

Universal features

$$0 < k(y,x,t) \leq c_t \phi_1(y)\phi_(x)$$

$$p(y,x,t) = k(y,x,t)\, e^{+\lambda_1 t}\, \phi_1(x)/\phi_1(y)$$

Asymptotic

$$\lim_{t\to\infty} p(y,x,t) = \rho(x) = \phi_1^2(x)$$

We denote:

$$\tilde{k}(y,x,t) = e^{\lambda_1 t} k(y,x,t)/\phi_1(x)\phi_1(y).$$

We employ an estimate valid for t>1

$$|\tilde{k}(y,x,t) - 1| \leq C\, e^{-(\lambda_2 - \lambda 1)t}$$

The universal time rate formula !

(multiply both sides by $\rho(x) = \phi_1^2(x)$)

$$|p(y,x,t) - \rho(x)| \leq C\, e^{-(\lambda_2 - \lambda_1)t}\, \rho(x)$$

involves the energy gap $(\lambda_2 - \lambda_1)$ and the probability density $\rho(x) = \phi_1^2(x)$

About a semigroup transcript of the Fokker-Planck dynamics

Langevin equation $\frac{dx}{dt} = F(x) + \sqrt{2\nu} b(t)$ $F(x) = -dV(x)/dx$

Fokker-Planck equation $\partial_t \rho = \nu \partial_{xx} \rho - \partial_x (F\rho)$ With an asymptotic stationary density

Multiplicative decomposition $\rho(x,t) = \Psi(x,t) \exp[-V(x)/2\nu] = \Psi(x,t) \rho_*^{1/2}(x)$

$b(x) = \nu \nabla \ln \rho_*(x)$

Implies the semigroup evolution $\partial_t \Psi = \nu \partial_{xx} \Psi - \mathcal{V}(x) \Psi$ $\mathcal{V}(x) = \frac{1}{2}\left(\frac{F^2}{2\nu} + \partial_x F\right)$

for a real-valued function $\Psi(x,t)$. We tacitly presume the potential to be confining so that the positive definite ground state $\psi(x) \doteq \rho_*^{1/2}(x)$ exists and corresponds to the 0 eigenvalue of H. This can be always achieved by subtracting the lowest non-zero eigenvalue of H, if actually in existence, from the potential.

$\psi_1(x) \doteq \rho_*^{1/2}(x)$ corresponds to the zero eigenvalue of $H - E_1$

and we have $\Psi(x,t) = \exp(+E_1 t) \sum_{n=1}^{\infty} c_n \exp(-E_n t) \psi_n(x) \to \psi_1(x) = \rho_*^{1/2}(x)$

FPE can be rewritten: $\partial_t \rho = \left[\rho_*^{1/2} \Delta \left(\rho_*^{-1/2} \cdot\right) - \rho_*^{-1/2} \left(\Delta \rho_*^{1/2}\right)\right] \rho$

Back to conditioning and infinite life-times

The conditioning recipe examples in the above, directly involve integral (F-K) kernels of contracting semigroups, whose generators have purely discrete spectral solutions with the bottom eigenvalue being well separated from the rest of the spectrum.

The procedure will surely work for potentials that are bounded from below, since we can always redefine potentials with a bounded from below negative part, by adding to $V(x)$ a modulus of its minimal value $|V(x_{\min})|$ or a modulus of any of its multiple (identical) local minima: $V(x) \to V(x)+|V(x_{\min})|$ so arriving at $V(x) \geq 0$.

The redefined potential is nonnegative and gives rise to the diffusion-type process with killing, whose transition density $k(y,s|x,t)$ is given by the F-K formula.

How to handle absorption (i.e. to suppress killing) in case of the Brownian motion on a line with a single barrier ?

We need not to have a discrete spectral solution at hand. The employed conditioning formula appears to work properly also when the spectrum of the involved semigroup generator is continuous. This is the case e.g. for a single absorbing barrier problem in the $1D$ Brownian motion.

We set the sink at 0 and consider the Brownian motion as being restricted to the positive semi-axis ($x \in R^+$).
The pertinent transition density is obtained via the method of images, by employing the standard Brownian transition probability density (induced by $(1/2)\Delta$)

$$p(y,s|x,t) = [2\pi(t-s))]^{-1/2} \exp[-(x-y)^2/2\pi(t-s)]$$

Namely:

$$k(y,s,|x,t) = p(y,s|x,t) - p(-y,s|x,t) = \frac{2}{\sqrt{2\pi(t-s)}} \exp[-\frac{x^2+y^2}{2(t-s)}] \sinh\left(\frac{xy}{t-s}\right)$$

The large T behavior of $k(y,s|u,T)$ is easily inferred to imply:

$$k(y,s|u,T) \sim \frac{2}{\sqrt{2\pi T}} \exp[-\frac{y^2+u^2}{2T}] \frac{uy}{T}$$

Accordingly, the conditioned process has a transition probability density (that arises in the ultimate $T \to \infty$ limit):

$$p(y,s;x,t;u,T) \to p(y,s|x,t) = k(y,s|x,t)\ \frac{x}{y}$$

The forward drift of the process is calculable directly from the formula $b(x) = \nabla \ln x = 1/x$. The Fokker-Planck generator takes the familiar (Bessel process) form $L^* = (1/2)\Delta - [b(x)\cdot]$. We note that the point 0 is presently inaccessible for the process.

Links with Bessel processes

Told otherwise: the one-dimensional Brownian motion starting from $y > 0$, conditioned to remain positive up to time T, converges as $T \to \infty$ to the radial process of the three-dimensional Brownian motion, known a the Bessel process.

In the one-parameter family of Bessel processes, with drifts of the form $b(x) = (1 + 2a)/2x$, in case of $a \geq 0$, the point $x = 0$ is never reached from any $y > 0$ with probability one. To the contrary, for $a < 0$, the barrier at $x = 0$ is absorbing (sink).

Let us recall the backward generator of the process: $(1/2)\Delta + b(x)\nabla$ with $b(x) = (1 + 2a)/2x$. The one-parameter family of pertinent transition densities reads:

$$k_a(y, s|x, t) = \frac{y^{2a+1}}{t(xy)^a} \exp\left[-\frac{x^2 + y^2}{2t}\right] I_{|a|}\left(\frac{xy}{2t}\right)$$

Let us consider the special case of $a = \pm(1/2)$ for which the modified Bessel function takes a handy form

$$I_{1/2}(z) = \sqrt{\frac{2}{\pi z}} \sinh z$$

It is easy to verify that $k_{-1/2}(y, s|x, t)$ coincides with the transition density of the Brownian motion constrained to stay on $R+$, with a sink at 0. The generator simply is $(1/2)\Delta$ on R^+, with absorbing boundary at 0.

On the other hand $k_{+1/2}(y,s|x,t)$ is a transition probability density of the previously derived Bessel process with $b(x) = 1/x$ (e.g. the Brownian motion conditioned to never reach 0, if started from any $y > 0$). Its F-P generator reads $(1/2)\Delta - \nabla(b(x)\cdot)$, with $b(x) = \nabla \ln x$.

Out of time comments

Quiery: how much of that conditioning strategy can we extend to jump-type processes, specifically Levy-stable ones ?

Answer: Feynman-Kac kernels are computable, albeit basically without known explicit analytic forms. Conditioning itself can be imposed in exactly the same way (via Bernstein transition fucntions).

Link of the killed stochastic process and its "eternally living" partner can surely be established. However, the latter is surely **not** a drifted random motion, in sharp contrast to what we have met in the traditional Brownian motion context.

Thank you for attention

(Safe)   „Walk on the cliff" – Claude Monet