

Stochastic methods in Mathematical Modelling

Lecture 10. Langevin vs Fokker-Planck approach. Examples. First-passage times

Skoltech Types of random processes

A random process (time could be continuous)

$$P(x_n,t_n|x_{n-1},t_{n-1};x_{n-2},t_{n-2};...;x_0,t_0)$$

1) Purely random

$$P(x_n,t_n|x_{n-1},t_{n-1};x_{n-2},t_{n-2};...;x_0,t_0)=P(x_n,t_n)$$

2) Markov Processes

$$P(x_n,t_n|x_{n-1},t_{n-1};x_{n-2},t_{n-2};...;x_0,t_0)=P(x_n,t_n|x_{n-1},t_{n-1})$$

3) General case

$$P(x_n,t_n|x_{n-1},t_{n-1};x_{n-2},t_{n-2};...;x_0,t_0)$$



How to describe a random process X(t)?

1) Simulate/calculate/determine the random variable itself X(t)

Stochastic Differential Equations (Langevin equation), Agent-based simulations

2) Simulate/calculate/determine PDF of the variable X(t)

Partial Differential Equations for the PDF such as Fokker-Planck equation



Skoltech Stochastic differential equations

One can conveniently use the SDEs to simulate the trajectory of a process

$$\dot{y} = A(y) + \xi(t)$$

$$\begin{cases} \langle \xi(t) \rangle = 0 \\ \langle \xi(t') \xi(t) \rangle = q \delta(t - t') \end{cases}$$

$$y(t+dt) = y(t) + A(y)dt + \sqrt{2qdt} Z$$

Z is random variable drawn from N(0,1)

Fast and precise algorithm for computer simulation of stochastic differential equations, R. Mannella, V. Palleschi, Phys Rev A, 3381 (1989)

$$\dot{x}_i = f_i(\mathbf{x}) + g_i(\mathbf{x})\xi(t), \quad i = 1, N$$

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(s) \rangle = \delta(t - s)$$

$$x(h)-x(0) = \sqrt{2D} Z_1 + fh + f'\sqrt{2D} Z_2 + \frac{1}{2}ff'h^2 + DZ_3f''$$
.



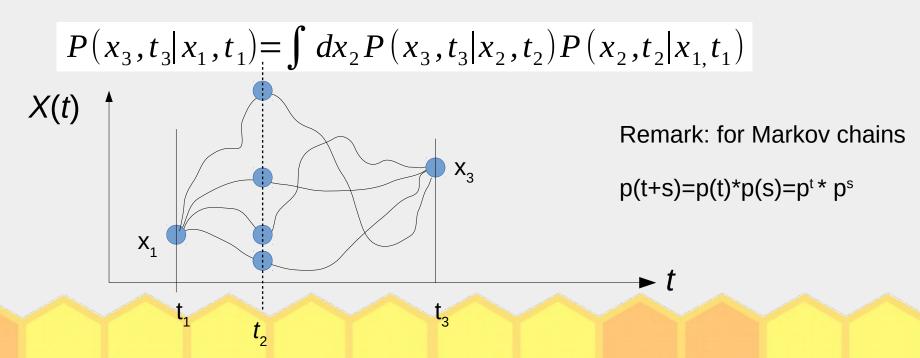
What is an alternative?

Answer: the use of Probability Distribution Functions!

For Markov processes

$$P(x_n,t_n|x_{n-1},t_{n-1};x_{n-2},t_{n-2};...;x_0,t_0)=P(x_n,t_n|x_{n-1},t_{n-1})$$

Chapman-Kolmogorov equation





Skoltech Kramers-Moyal expansion

$$P(x,t+\tau)-P(x,t)=\sum_{n=0}^{\infty}\left(-\frac{\partial}{\partial x}\right)^{n}\frac{M_{n}(x,t,\tau)}{n!}P(x,t),$$

where
$$M_n(x,t,\tau) = \int (x-x')^n P(x,t+\tau|x',t) dx'$$

Now, we expand the moments M_n into Taylor with respect to τ

$$M_n(x,t,\tau)/n! = D^{(n)}(x,t) \tau + O(\tau^2)$$

Finally we arrive at the equation for the pdf!

$$\frac{\partial P(x,t)}{\partial t} = \sum_{n=0}^{\infty} \left(- \frac{\partial}{\partial x} \right)^n D^{(n)}(x,t) P(x,t) = L_{KM} P(x,t)$$

If we stop the Kramers-Moyal expansion after 2 terms we get

$$\frac{\partial P(x,t)}{\partial t} = \left(-\frac{\partial}{\partial x}D^{(1)}(x,t) + \frac{\partial^2}{\partial x^2}D^{(2)}(x,t)\right)P(x,t) = L_{FP}P(x,t)$$

$$\frac{\partial P(x,t)}{\partial t} + \frac{\partial S(x,t)}{\partial x} = 0,$$

Probability current

$$S(x,t) = (D^{(1)}(x,t) - \frac{\partial}{\partial x}D^{(2)}(x,t))P(x,t)$$



Connection between descriptions in terms of variables and their PDFs

There is a connection between Langevin and Fokker-Planck (FP) equations

Case 1. Additive noise

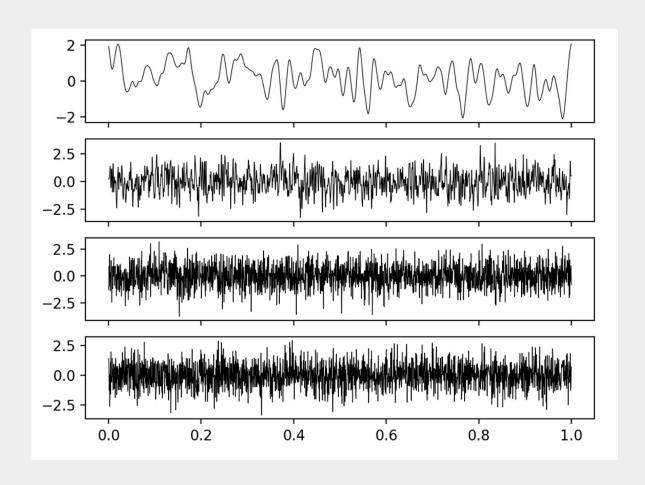
(1)
$$\dot{y} = A(y) + \xi(t)$$
 $\begin{cases} \langle \xi(t) \rangle = 0 \\ \langle \xi(t') \xi(t) \rangle = q \, \delta(t - t') \end{cases}$

(1) is equivalent to the following FP equation

$$\frac{\partial P(y,t)}{\partial t} = -\frac{\partial}{\partial y} A(y) P + \frac{q}{2} \frac{\partial^2 P}{\partial y^2}$$



Approaching white noise



The first three figures are draws from a Gaussian process with a finite correlation length with this length being decreased gradually. These have smooth, continuous paths. The bottom panel shows a draw from true white noise. As the length scale decreases, the finite correlation noise becomes increasingly similar to white noise, so we can think of white noise as an idealised limit of a series of smooth, continuous processes with increasingly small correlation time.

Properties of Ito stochastic integrals(SI)

1) Existence. Ito SI exists if G(t) is non-anticipating 16(t') DW(t') 6(t) is statistically undependent of W(s)-W(t) 6(+) is non-audicipating if + s, t; tc,s 2) $d(tw(t)) = [tw(t) + dw(t)]^n - w(t) = \sum_{r=1}^{\infty} {n \choose r} w(t)^{n-r} dw(t)^r =$ $= h w(t)^{-1} dw(t) + u(u-t) w(t)^{u-2} dt$ dw(+)2=olt, dw(+)~+2=0

3) $d\{e \times p(w(t))\} = e^{w(t)}[dw(t) + \frac{dt}{2}] = e^{w(t)}[dw(t)] + \frac{dw(t)}{2}$ $= e^{w(t)} + dw(t) - e^{+w(t)} = e^{w(t)}[dw(t)] + \frac{dw(t)}{2}$ 2 f [w(+),+] = 3 f dt + 1 3 f (dt) 2 3 f dw(+) + + 2 3 m2 [lw(4)] + 2 2 # dw(4) + 2 2 # dw(4) + () () = olt dftw/h/ = 3f + 1 22f - 3w dw(t).

dx(t) = a[x(b)]+)dt + b[xH,+] lw(t)_ $2f(x(t)) = f(x(t)) - f(x(t)) - f(x(t)) = f(x(t)) dx(t) + \frac{1}{2}f''(x(t)) dx(t)$ $= f([x k], +](a(x k), +]d+ f(x k), +)dw(+))+ \frac{1}{2}f''(x k) f(x k), +)(dw(+))$ I to for mula: dftx(t)] =[a(x(t)+) f' + = b2(x(t)) f'(x(t))]dt + ltx(t)+) f'(x(t))]dt + ltx(t)+) f'(x(t)) f' $\left(\frac{1}{at}\right) = \frac{1}{at}\left(\frac{1}{at}\right) = \left(\frac{1}{a}\left(\frac{1}{a}\left(\frac{1}{a}\right)\right) = \left(\frac{1}{a}\left(\frac{1}{a}\right)\right) = \left(\frac{1}{a}\left(\frac{1}{a}\right)\right)$ d ldx f(x) p(x,4)xo,56)= [dx[a(x,4)2x++2/2(x,4)2xx+]p(x,4)xo,56)

Idx f(x) $\partial_t P = \int dx f(x)(-\partial_x(\alpha p) + \frac{1}{2} \partial_x^2(b^2 p))$ $\partial_t P = -\partial_x(\alpha p) + \frac{1}{2} \partial_x^2(b^2 p)$ Since f is arbitrary.

Stratouvich

Stra $x(t) = x(t) + \int_{t}^{t} dt dt dt = x(t) + \int_{t}^{t} dw(t) dt = x(t) + \int_{t}^{t} dw(t$ s f dw (t) g t x (t), t = 2 f x (ti) + x (ti) - w (ti) $X(t_i) = X(t_{i-1}) + dx(t_{i-1})$ $ST = \frac{x(t_i) + x(t_{i-1})}{z}, t_{i-1} = S(x(t_{i-1}) + \frac{1}{z}dx(t_i), t_{i-1}) = \frac{1}{z}dx(t_i)$ $= \frac{g(t_{i-1}) + g(t_{i-1}) dx}{J + g(t_{i-1}) dx} dx(t_{i-1}) = ct[x(t_{i-1}), t_{i-1}](t_{i-1} t_{i-1}) + f[w(t_{i}) - w(t_{i-1})]$

$$= \beta(t_{i}) + [a(t_{i-1})dx]\beta(t_{i-1}) + \frac{1}{4} \beta^{2}(t_{i-1}) \frac{1}{2}(t_{i} - t_{i-1}) + \frac{1}{2} \beta(t_{i-1})dx\beta(t_{i-1}) + \frac{1}{4} \beta(t_{i-1}) + \frac{1}{2} \beta(t_{i-1})dx\beta(t_{i-1}) + \frac{1}{2} \beta(t_{i-1})dx\beta(t_{i-1})d$$

THO SDE dx=adt+bdw(t) 15 the same as Stratomovich SDE dx= Ta- 1 60x67 d+ +6dw (6) $\frac{\partial f}{\partial P(x, d)} = -\frac{\partial (x + \frac{1}{2} \beta \partial x \beta) P}{\partial (x + \frac{1}{2} \beta \partial x \beta) P} + \frac{1}{2} \frac{\partial x^2}{\partial (x^2 + \frac{1}{2} \beta \partial x \beta) P} =$ 3 (xp) + 1 2 7x [B 3x (Bp)]
Stratomyd form of F PE

Tho us Stratonovich example dx = Cxdu(t)y = lu × Ccx dy = cdw(+) 2 f [x (t)] = { a(x(t))+) f/(x,+) + } b^2[x(t),+] + (x,+)] d+ + + f[x(A)x] d (x(4) $2 \ln x = 30 + \frac{1}{2} (x) \frac{1}{2} \ln x = 30 + \frac{1}{2} (x) \frac{1}$ ly=clwH)- 22d+ =yH)=yH)+ ctw(+)-wbs)-

> x(t) = x (to) exp {c[w(4) - w (+o)] - \frac{1}{2} c^2 (t -40)} < x (4)>=(x(46)7 exp{-1 c2(+=+6) - 1 2(+=+6)} = (x (+6)) Stratonovich dy = c dw (+) $x(t) = x(t_0) exp {C(w(t) - w(t_0)]}$ $(x(t)) = (x(t_0)) - (xp[\frac{2}{2}c^2(4-t_0)]$



Connection between Ito and Stratonovich SDEs

There is a connection between Ito and Stratonovich SDEs

to SDE
$$dx_I = a(x_I(t),t)dt + b(x_I(t),t)dW(t)$$

The same solution will be produced by the following Stratonovich SDE

$$dx_{S} = \left(a(t) - \frac{1}{2}b(t)\frac{\partial b(t)}{\partial x}\right)dt + b(t)dW(t)$$

Where in the last expression

$$a(t)=a(x(t),t),b(t)=b(x(t),t)$$



Connection between descriptions in terms of variables and their PDFs

There is a connection between Langevin and Fokker-Planck (FP) equations

Multiplicative noise

(1)
$$\dot{y} = A(y) + C(y) \xi(t)$$
 $\langle \xi(t) \rangle = 0$ $\langle \xi(t) \rangle = q \delta(t - t')$

Now there is an ambiguity

Ito interpretation

$$\frac{\partial P(y,t)}{\partial t} = -\frac{\partial}{\partial y} (A(y)P(y,t)) + \frac{q}{2} \frac{\partial^2 (C^2(y)P)}{\partial y^2}$$

Stratonovich interpretation

$$\frac{\partial P(y,t)}{\partial t} = -\frac{\partial}{\partial y} (A(y)P(y,t)) + \frac{q}{2} \frac{\partial}{\partial y} (C(y) \frac{\partial}{\partial y} (C(y)P))$$

+other possibilities (*Klimontovich*, for instance)



Multivariate SDEs

$$d \mathbf{x} = \mathbf{A}(\mathbf{x}, t) dt + \mathbf{B}(\mathbf{x}, t) d \mathbf{W}(t)$$

x,A,B,dW are vectors now. dW is an n-variable Wiener process

Multivariate Fokker-Planck equation in Ito form

$$\frac{\partial P(\mathbf{x},t)}{\partial t} = -\sum_{i} \frac{\partial}{\partial x_{i}} A_{i}(\mathbf{x},t) P(\mathbf{x},t) + \frac{1}{2} \sum_{ij} \frac{\partial}{\partial x_{i}} \frac{\partial}{\partial x_{i}} ([\mathbf{B}(\mathbf{x},t)\mathbf{B}^{T}(\mathbf{x},t)]_{ij} P(\mathbf{x},t))$$

Multivariate Fokker-Planck equation in Stratonovich form

$$\frac{\partial P(x,t)}{\partial t} = -\sum_{i} \frac{\partial}{\partial x_{i}} A_{i}(x,t) P(x,t) +$$

+
$$\frac{1}{2}\sum_{ijk}\frac{\partial}{\partial x_i}([B_{ik}(x,t)\frac{\partial}{\partial x_j}B_{jk}(x,t)]P(x,t))$$



Coloured noise

What if the noise *y* is not delta-correlated?

$$\dot{x} = A(x) + C(x) y$$

Generation of y is necessary

An example

$$\dot{x} = A(x) + Cy$$

$$\langle y(t) \rangle = 0$$

$$\langle y(t')y(t) \rangle = \alpha \exp(-\alpha |t-t'|)$$

$$\dot{y} = -\alpha y + \xi(t)$$

$$\langle \xi(t) \rangle = 0 \quad \langle \xi(t')\xi(t) \rangle = q \delta(t-t')$$

$$\xi(t) \text{ is Gaussian}$$

Fast and precise algorithm for computer simulation of stochastic differential equations, R. Mannella V. Palleschi, Phys Rev A, 3381 (1989)

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How to solve Fokker-Planck equations

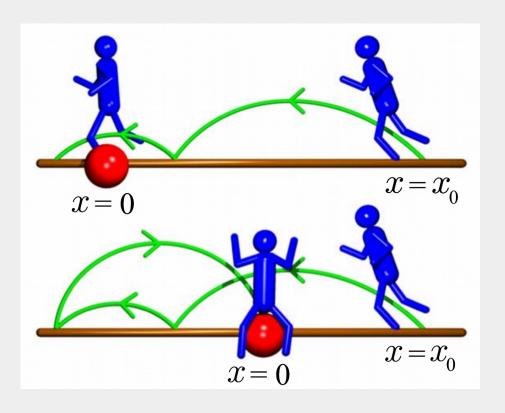
$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x} \left(-\frac{1}{m\eta} \frac{\partial V(x,t)}{\partial x} P(x,t)\right) + \frac{\partial^2}{\partial x^2} \left(D(x,t) P(x,t)\right)$$

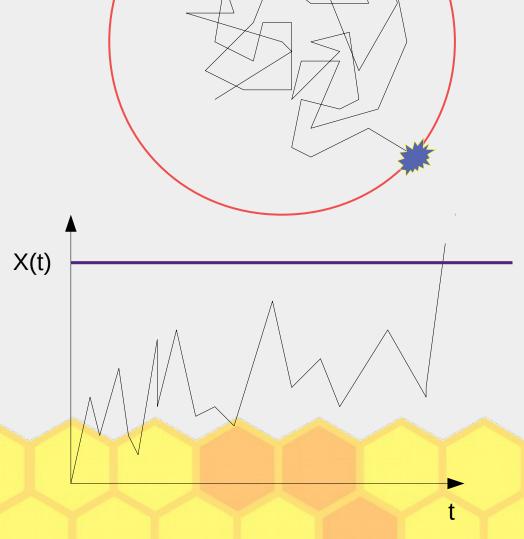
- 1. Eigenmode decomposition
- 2. Fourier-Laplace transform (if linear)
- 3. Numerical solution of PDE



First-passage phenomena

When do we cross a boundary/value for the first time?



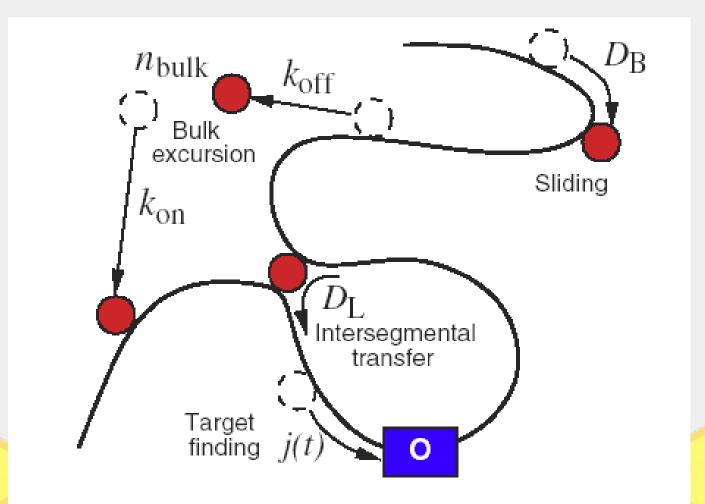




First-passage phenomena

Example. Reaction rates can be found within the first-passage approach

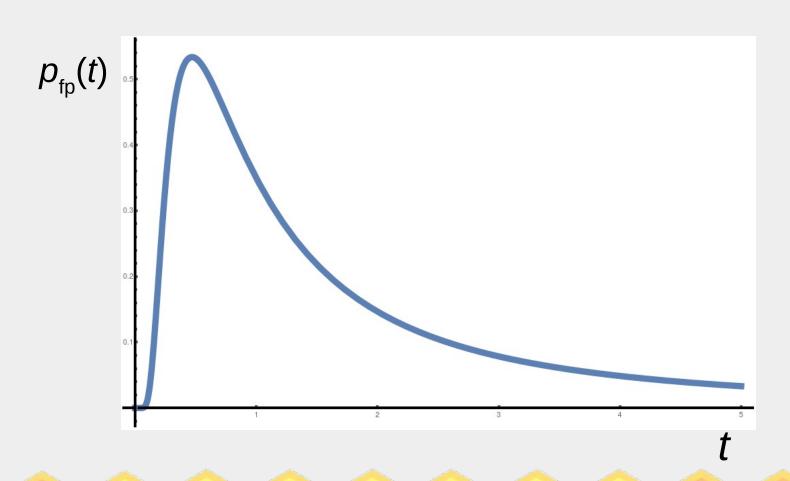
Berg - von Hippel model





SkoltechFirst-passage phenomena

Distribution of first-passage times

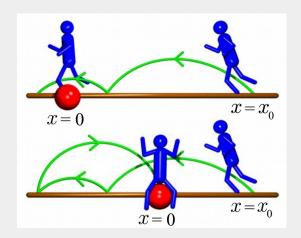




First-passage phenomena

First-passage time probability density function $p_{fo}(t)$

$$p_{fp}(s) = \int_0^\infty p_{fp}(t) e^{-st} dt = \int_0^\infty p_{fp}(t) (1 - st + \frac{1}{2} s^2 t^2 - \dots) dt = 1 - s \langle t \rangle + \frac{1}{2} s^2 \langle t^2 \rangle + \dots$$



Mean first-passage time

$$T = \langle t \rangle = \frac{\int_{0}^{\infty} t p_{fp}(t) dt}{\int_{0}^{\infty} p_{fp}(t) dt}$$

Survival probability

$$S(t)=1-\int_{0}^{t}p_{fp}(t')dt'$$
, i.e. $p_{fp}(t)=-\frac{dS(t)}{dt}$

Probability of eventual hitting

$$P = \int_0^\infty p_{fp}(t) dt \equiv p_{fp}(s=0)$$



First-passage on an interval

When do we cross a boundary/value for the first time?

$$T = \langle t \rangle = \frac{\int_{0}^{\infty} t p_{fp}(t) dt}{\int_{0}^{\infty} p_{fp}(t) dt}$$

$$\frac{\partial P(x,t)}{\partial t} = D \frac{\partial^{2} P(x,t)}{\partial x^{2}}, P(0,t) = P(1,t) = 0,$$

$$P(x_{0},0) = \delta(x-x_{0}), 0 \le x_{0} \le 1.$$

$$j(x,t) = -D \frac{\partial P(x,t)}{\partial x} \qquad p_{fp}(x=0,t) = j(x=0,t)$$
$$p_{fp}(x=1,t) = j(x=1,t)$$

Exercise: Compute analytically the probabilities of reaching the right and the left boundary as a function of initial position x_0 and mean first escape time (i.e. the sum of mean first-passage times to the right and to the left). Hint: obtain all the results in Laplace space.

Hint 2:
$$j(x=0,t)=-p_{fp}(x=0,t)$$
, $j(x=1,t)=p_{fp}(x=1,t)$

P_t = D P_{xx}

P(x=0,t) = F

| Variable transform | P(x=0,t) = F

| Variable transform | P(x,t=0) = D P''(x,s) | P(x,t=0) = D P''(x,t=0) | P(x,t=0) | P(x,t=0) = D P''(x,t=0) | P(x,t=0) | P(x, P(X=0,+)=P(x=1,+)=0 $P(x,+=0) = \delta(x-x_0)$ S = 0 6 11 $R(x,s) = A \sinh(\sqrt{s}x), \quad x < x_0$ $P_{2}(x,s) = B \sinh(\sqrt{s}(1-x)), \quad x > x_0$ $P(x,s) = A sinh(\sqrt{s} x_{x}) sinh(\sqrt{s} (1-x_{x}))$ $P'(x,s) = \int e^{-st} dt = \int e$ $X = M G \times (X, X_0)$ $X = M G \times (X, X_0)$ S P(X, S) $X = M G \times (X, X_0)$

$$\int_{S} P(x,s) - P(x,t=0) = DP'(x,s) \int_{S} dx$$

$$\int_{S} P(x,s) dx = \int_{X} S(x-x_0) = DP'(x_1s)$$

$$P(x,s) - P(x,s)|_{x=x_0} - D$$

$$P(x,s) = A \sin k \left(\sqrt{s} x \right) = A \sin k \left(\sqrt{s} x \right) = B \sin k \left(\sqrt{s} (1-x_0) \right) = B \sin k \left(\sqrt{s} (1-x_0) \right)$$

$$P(x,s) = \frac{\sin k \left(\sqrt{s} x \right) \sin k \left(\sqrt{s} (1-x_0) \right)}{\sqrt{s}D \sin k \left(\sqrt{s} (1-x_0) \right)}$$

$$P(x,s) = \frac{\sin k \left(\sqrt{s} x \right) \sin k \left(\sqrt{s} (1-x_0) \right)}{\sqrt{s}D \sin k \left(\sqrt{s} (1-x_0) \right)}$$

$$\int_{-\infty}^{\infty} \frac{1}{2\pi} dx = \frac{\sinh(\sqrt{5}(1-x_0))}{\sinh(\sqrt{5})}$$

$$\int_{-\infty}^{\infty} \frac{1}{2\pi} dx = \frac{\sinh(\sqrt{5}(1-x_0))}{\sinh(\sqrt{5}(1-x_0))}$$

$$\int_{-\infty}^{\infty} \frac{1}{2\pi} dx = \frac{\sinh(\sqrt{5}(1-x_0))}{\sinh(\sqrt{5}(1-x_0)}$$

$$\int_{-\infty}^{\infty} \frac{1}{2\pi} dx = \frac{1}{2\pi} \frac{1}{$$

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First-passage Skolkovo Institute of Science and Technology on a semi-infinite line. Method of images

$$\frac{\partial P(x,t)}{\partial t} = D \frac{\partial^2 P(x,t)}{\partial x^2}, P(0,t) = P(\infty,t) = 0$$

$$j(x,t) = -D \frac{\partial P(x,t)}{\partial x}$$

$$p_{fp}(x=0,t) = j(x=0,t)$$

$$p_{fp}(x=0,t) = \frac{x_0}{\sqrt{4 \pi D t^3}} \exp\left(-\frac{x_0^2}{4 D t}\right)$$
 $S(t) = erf\left(\frac{x_0}{\sqrt{4 D t}}\right)$



MFPT for the escape from an interval

$$A(x)\partial_x T(x) + \frac{1}{2} B(x)\partial_x^2 T(x) = -1$$

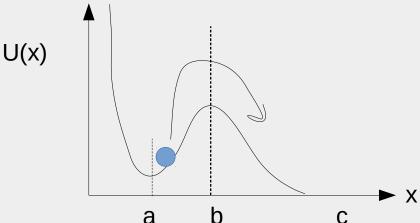
$$T(a) = T(b) = 0$$

$$\psi(x) = \exp\left\{\int_a^x dx' [2A(x')/B(x')]\right\}$$

$$T(x) = \frac{2\left[\left(\int_{a}^{x} \frac{dy}{\psi(y)}\right) \int_{x}^{b} \frac{dy'}{\psi(y')} \int_{a}^{y'} \frac{dz\psi(z)}{B(z)} - \left(\int_{x}^{b} \frac{dy}{\psi(y)}\right) \int_{a}^{x} \frac{dy'}{\psi(y')} \int_{a}^{y'} \frac{dz\psi(z)}{B(z)}\right]}{\int_{a}^{b} \frac{dy}{\psi(y)}}$$



Escape from a potential well. Kramers formula



Escape rate for BM

$$r \sim \sqrt{U''(a)U''(b)} \exp\left(-\frac{U(b)-U(a)}{k_B T}\right)$$

Mean first-passage (escape) time for BM

$$T_{MFPT} \sim \frac{1}{\sqrt{U''(a)U''(b)}} \exp\left(\frac{U(b)-U(a)}{k_B T}\right)$$

Survival probability for Brownian motion

$$p(t) \sim \exp(-rt)$$



Literature

- 1. A Guide to First-Passage Processes, S. Redner, Cambridge University Press, 2001 First-Passage Processes
- 2. N.G. Van Kampen, Stochastic Processes in Physics and Chemistry, 3rd Edition, Elsevier, 2007