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Stochastic methods in Mathematical Modelling

Lecture 9. Tools for modelling and understanding of random processes. SDE vs Fokker-Planck approach

Types of random processes

A random process (time could be continuous)

$$P\left(x_n, t_n \middle| x_{n-1}, t_{n-1}; x_{n-2}, t_{n-2}; \ldots; x_0, t_0\right)$$

1) Purely random

$$P\left(x_n, t_n \middle| x_{n-1}, t_{n-1}; x_{n-2}, t_{n-2}; \ldots; x_0, t_0\right) = P\left(x_n, t_n\right)$$

2) Markov Processes

$$P\left(x_n, t_n \middle| x_{n-1}, t_{n-1}; x_{n-2}, t_{n-2}; \ldots; x_0, t_0\right) = P\left(x_n, t_n \middle| x_{n-1}, t_{n-1}\right)$$

3) General case

$$P\left(x_n, t_n \middle| x_{n-1}, t_{n-1}; x_{n-2}, t_{n-2}; \ldots; x_0, t_0\right)$$

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

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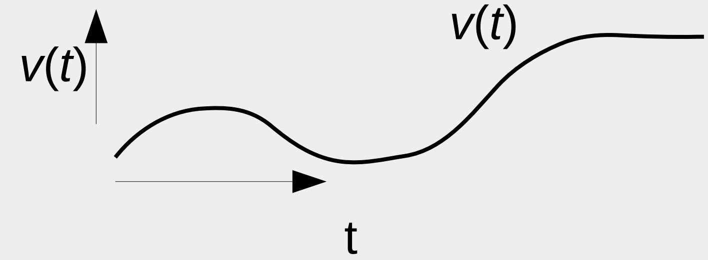
Stochastic differential equations

Deterministic diff. equation

$$\frac{dv(t)}{dt} = a$$



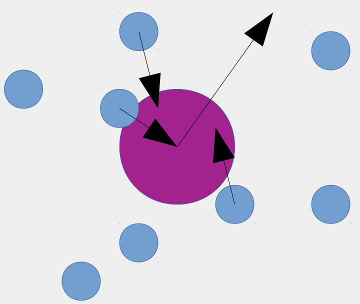
Example: $a = g$ (gravity constant). Then: v(t)=v(0)+gt

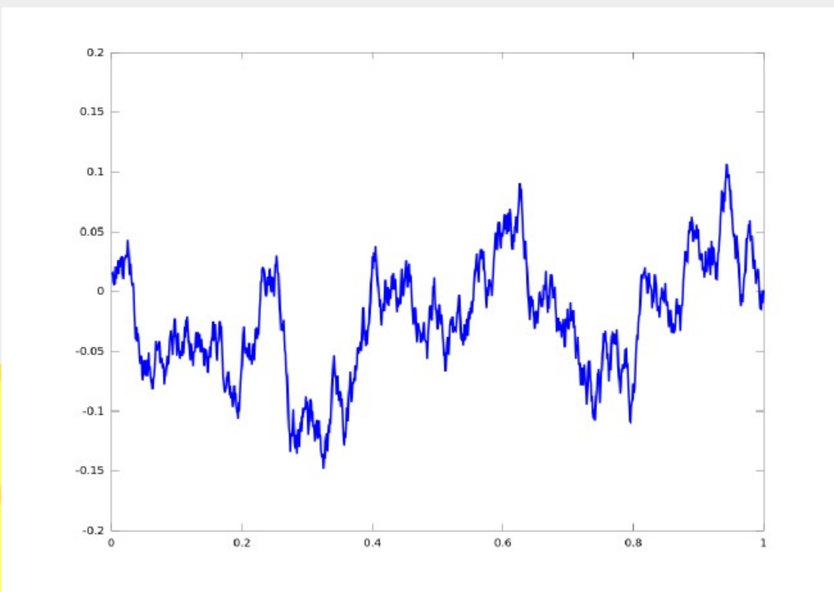
Stochastic diff. equation

$$m\frac{dv(t)}{dt} = F_{rand}(t)$$

random force (noise)

Brownian motion





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Stochastic differential equations

$$m\frac{dv(t)}{dt}=\underbrace{F(t)}_{\text{deterministic force}}+\underbrace{F_{rand}(t)}_{\text{random force (noise)}}$$

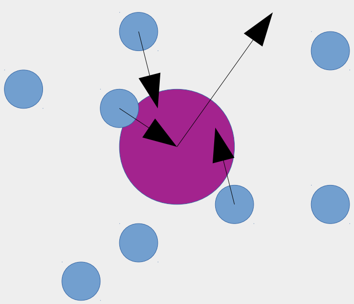
For a Brownian particle in a viscous solution. No external fields. Assumption m = 1

$$F(t)=-\gamma v$$

$$\langle F_{rand}(t)\rangle=0$$

$$\langle F_{rand}(t')F_{rand}(t)\rangle=q\,\delta(t-t')$$

Brownian motion



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Stochastic differential equations

Langevin equation

$$m\dot{v}+\gamma v=F_{rand}(t)$$

$$\langle F_{rand}(t)\rangle=0$$

$$\langle F_{rand}(t')F_{rand}(t)\rangle=q\,\delta(t-t')$$

Overdamped Langevin equation

$$m\dot{v}\ll\gamma v$$

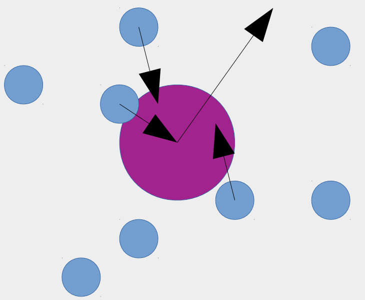
$$\dot{x}=\xi(t)$$

noise

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

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

Brownian motion



Stochastic differential equations

Solution of Langevin equation

$$m\dot{v}+\gamma v=F_{rand}(t)$$

$$\langle F_{rand}(t)\rangle=0$$

$$\langle F_{rand}(t')F_{rand}(t)\rangle=q\,\delta(t-t')$$

$$v(t)=v_0 e^{\frac{-\gamma}{m}t}+\frac{e^{\frac{-\gamma}{m}t}}{m}\int_0^t e^{\frac{\gamma}{m}t'}F_{rand}(t')\,dt'$$

Qs: 1. $\langle v(t)\rangle-?$

2. $\langle v^2(t)\rangle-?$

Solution of LE

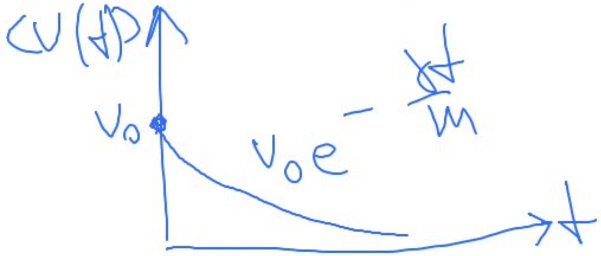
$$\frac{dv}{dt} = -\frac{\gamma}{m} v(t) + \frac{1}{m}\xi(t)$$

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

$$\langle \xi_1(t)\, \xi_2(t) \rangle = g\, \delta(t_2 - t_1)$$

$$v(t) = v_0 e^{-\frac{\gamma t}{m}} + \frac{e^{-\frac{\gamma t}{m}}}{m} \int_0^t e^{\frac{\gamma t_1}{m}} \xi(t')\, dt'$$

1. $$\langle v(t) \rangle = v_0 e^{-\frac{\gamma t}{m}} + \frac{e^{-\frac{\gamma t}{m}}}{m} \int_0^t e^{\frac{\gamma t_1}{m}} \overbrace{\langle \xi(t') \rangle}^{=0}\, dt' = v_0 e^{-\frac{\gamma t}{m}}$$



2) Correlation function

$$\langle v(t_2)\, v(t_1)\rangle_\xi = \Big\langle \Big[v_0 e^{-\frac{\gamma t_2}{m}} + \frac{1}{m}\int_0^{t_2} ds_2\, e^{-\frac{\gamma}{m}(t_2-s_2)}\,\xi(s_2)\, ds_2\Big] \times$$

$$\times \Big[v_0 e^{-\frac{\gamma t_1}{m}} + \frac{1}{m}\int_0^{t_1} ds_1\, e^{-\frac{\gamma}{m}(t_1-s_1)}\,\xi(s_1)\, ds_1\Big]\Big\rangle_\xi =$$

$$g\,\delta(s_2-s_1)$$

$$= v_0^2 e^{-\frac{\gamma(t_1+t_2)}{m}} + 0 + 0 + \frac{1}{m^2}\int_0^{t_2} ds_2 \int_0^{t_1} ds_1\, e^{-\frac{\gamma}{m}(s_1-t_1)}\, e^{-\frac{\gamma}{m}(s_2-t_2)} \langle \xi(s_2)\,\xi(s_1)\rangle_\xi =$$

$t_1 \geq t_2$

$$= v_0^2 e^{-\frac{\gamma(t_1+t_2)}{m}} + \frac{g}{m}\int_0^{\min(t_1,t_2)} e^{-\frac{\gamma}{m}(t_1+t_2-2s_1)}\, ds_1 =$$

$t_2 \geq t_1$

$$= v_0^2 e^{-\frac{\gamma(t_1+t_2)}{m}} + \frac{g}{m} e^{-\frac{\gamma}{m}(t_1+t_2)} \int_0^{t_1} e^{\frac{2 s_1 \gamma}{m}}\, ds_1 =$$

$$= v_0^2 (t_1+t_2) + \frac{g}{2m\gamma}\Big(e^{-\frac{\gamma(t_2-t_1)}{m}} - e^{-\frac{\gamma(t_1+t_2)}{m}}\Big)$$

$t_1 = t_2 = t$

$$\langle v^2(t) \rangle = \frac{g}{2m\gamma} + \left(v_0^2 - \frac{g}{2m\gamma}\right) e^{-\frac{2\gamma t}{m}}$$

$$\langle v^2(t) \rangle = \frac{g}{2m\gamma}$$

$$\langle E \rangle = \frac{1}{2} m \langle v^2(t) \rangle = \frac{1}{2}\cancel{m} \frac{g}{2\gamma \cancel{m}} = \frac{1}{2} k_B T$$

$$\downarrow g = 2\gamma k_B T$$

Stochastic differential equations

More generally there are two types of stochastic diff equations

Additive noise

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

"Linear". Markovian process (no memory). Unambiguous solution

Multiplicative noise

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

"Non-linear". Non-Markovian process (with memory).
Solution depends on interpretation!!!

SDEs with multiplicative noise

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

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

$$\langle \xi(t)\xi(t') \rangle = 2\delta(t-t')$$

Transformation of variables

$$A(y,t) = A(y)$$

$$C(y,t) = C(y)$$

$$\dot{\eta} = \frac{\dot{y}}{C(y)} = \frac{A(y)}{C(y)} + \xi(t) = h_1(\eta) + \xi(t)$$

$$\eta = f(y) = \int^{y} \frac{dy'}{C(y')} \qquad y = f^{-1}(\eta)$$

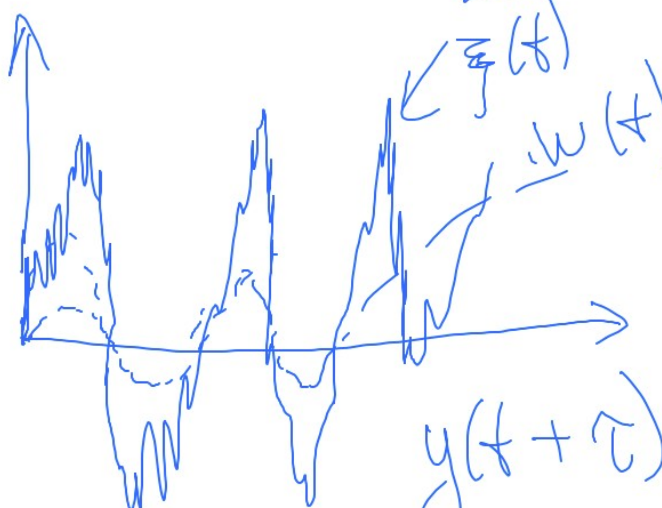
What if we have a time-dependent $C(y,t)$

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

$$y_{n+1} - y_n = A_n + C(y_n, n)\,\xi_n$$

ε

$$\dot{w}(t) = \xi(t)$$



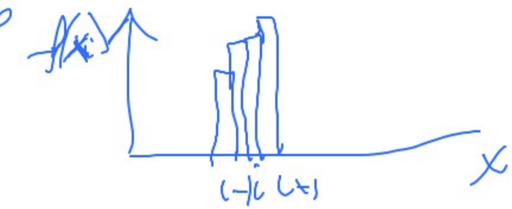
$$w(t) = \int_0^t \xi(t')\,dt'$$

$$y(t+\tau) = y(t) + \underbrace{\int_t^{t+\tau} A(y,t')\,dt'}_{\text{Riemann integral}} + \underbrace{\int_t^{t+\tau} C(y,t')\,dw(t')}_{\text{Stiltjes integral}}$$

Stiltjes integral

Riemann integral

$$\lim_{n\to\infty} \sum f(x_i)\,(x_i - x_{i-1})$$



$$S = \int_a^b f(x)\,dg(x)$$

$$\int f(x)\,dg(x) = \lim_{n\to\infty} \sum_{i=1}^{n} f(c_i)\,[g(x_i) - g(x_{i-1})]$$

$$\Rightarrow \forall c_i \in [x_{i-1}, x_i]$$

$$\left| \sum_{i=1}^{\infty} f(c_i)\,[g(x_i) - g(x_{i-1})] - A \right| < \varepsilon$$

$$\int_0^1 x\,dx^2 \overset{\text{Riemann}}{=} 2/3$$

$$\int_0^1 x\,dx^2 \overset{\text{Stieltjes}}{=} \lim_{n\to\infty}\sum_{i=0}^{n} \frac{i}{n}\left[\frac{i^2}{n^2}-\frac{(i-1)^2}{n^2}\right] = \lim_{n\to\infty}\sum_{i=0}^{\infty}\frac{i}{n^3}\left(i^2-i^2+2i-1\right) =$$

$$= \lim_{n\to\infty}\left(\sum_{i=1}^{n} \frac{2i^2}{n^3} - \sum_{i=1}^{n} \frac{i}{n^3}\right) = \lim_{n\to\infty}\left(2\,\frac{n(n+1)(2n+1)}{6n^3} - \overset{\to 0}{\frac{1}{n^3}\,\frac{n(n+1)}{2}}\right) = 2/3.$$

Stieltjes integral in probability theory

$$E[f(x)] = \int f(x)\,p(x)\,dx = \int f(x)\,dF_x(x)$$

PDF — CDF

for SDEs $\dot{W} = \xi(t)$: problem

$$\psi(\tau) = W(t+\tau) - W(t) = \int_t^{t+\tau} dW(t) = \int_t^{t+\tau} \xi(t')\,dt'$$

Prop: $\psi(t)$ is a Wiener process or Brownian motion

$$\psi(0) = 0$$

$$\langle \psi(\tau) \rangle = 0$$

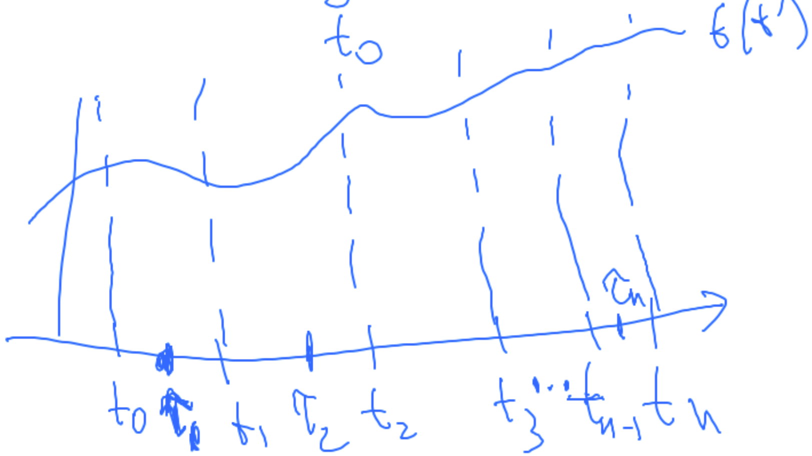
$$\langle \psi(\tau_1)\,\psi(\tau_2) \rangle = \int_t^{t+\tau_1}\int_t^{t+\tau_2} \langle \xi(s_1)\,\xi(s_2) \rangle\, ds_1\, ds_2 = 2\int_t^{t+\tau_1}\int_t^{t+\tau_2} \delta(s_1 - s_2)\, ds_1\, ds_2$$

$$= 2\min(\tau_2, \tau_1) = \begin{cases} 2\tau_2, & \tau_1 > \tau_2 \\ 2\tau_1, & \tau_2 > \tau_1 \end{cases}$$

Stochastic integrals

$$\int_{t_0}^{t} G(t')\,dW(t') \;\longrightarrow\; S_n = \sum_{i=1}^{n} G(\tau_i)\left[W(t_i) - W(t_{i-1})\right]$$

what if $W(\tau_i)$



$$\tau_i = \alpha t_i + (1-\alpha) t_{i-1}$$

$$0 \le \alpha \le 1$$

$$\langle S_n \rangle = \left\langle \sum_{i=1}^{n} W(\tau_i)\left[W(t_i) - W(t_{i-1})\right]\right\rangle =$$

$$= \sum_{i=1}^{n}\left[\min(\tau_i, t_i) - \min(\tau_i, t_{i-1})\right] =$$

$$= \sum_{i=1}^{n} (\tau_i - t_{i-1})$$

We have a few choices now

$$\langle S_n \rangle = \sum_{i=1}^{n} (\tau_i - t_{i-1})$$

$\tau_i = \alpha t_i + (1-\alpha) t_{i-1}$

~~Choice 1~~ $\cancel{\tau_i = t_{i-1}}$

$$\langle S_n \rangle = \sum_{i=1}^{n} (t_i - t_{i-1}) \alpha = (t - t_0) \alpha$$

Choice 1 $\quad \tau_i = t_{i-1}, \quad \alpha = 0$

Îto stochastic integral

Choice 2 $\quad \tau_i = \dfrac{t_{i-1} + t_i}{2}, \quad \alpha = 1/2$

Stratonovich integral

Îto stochastic integral

$$I\int_{t_0}^{t} G(t')\,dW(t') = \left\langle \operatorname*{ms\,lim}_{n\to\infty} \sum_{i=1}^{n} G(t_{i-1})\left[W(t_i) - W(t_{i-1})\right] \right\rangle$$

Example:

$$\int_{t_0}^{t} W(t')\,dW(t') = \left\langle \operatorname*{ms\,lim}_{n\to\infty} \sum_{i=1}^{n} W_{i-1}\underbrace{(W_i - W_{i-1})}_{\Delta W_i} \right\rangle$$

$$S_n = \sum_{i=1}^{n} W_{i-1}\Delta W_i = \frac{1}{2}\sum_i\left[(W_{i-1}+\Delta W_i)^2 - (W_{i-1})^2 - (\Delta W_i)^2\right] =$$

$$= \frac{1}{2}\left[W^2(t) - W^2(t_0)\right] - \frac{1}{2}\sum_{i=1}^{n}(\Delta W_i)^2$$

$$\left\langle \sum (\Delta W_i)^2 \right\rangle = \sum \left\langle (W_i - W_{i-1})^2 \right\rangle = \sum_i (t_i - t_{i-1}) = \underline{t - t_0},$$

$$I\int_{t_0}^{t} W(t')\,dW(t') = \frac{1}{2}\left[W^2(t) - W^2(t_0)\right] - \frac{1}{2}(t - t_0)$$

1) Ito integration is different from Riemannian integration

2) The rules are different

Choice 2 $\quad \alpha = 1/2 \quad \underline{W(t)} = \frac{1}{2}\left[W(t_i) + W(t_{i-1})\right]$

$$S\int_{t_0}^{t} W(t')\,dW(t') = \frac{1}{2}\left[W^2(t) - W^2(t_0)\right]$$

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Stochastic differential equations

Alternatively, in probability theory&finance the SDEs are written as

$$dX(t)=\mu(X(t),t)\,dt+\sigma(X(t),t)\,dW(t)$$

cf. $\gamma v=F_{det}(t)+F_{rand}(t)$

Measure of a random process
(for instance, Wiener measure)

Formally, a process *X*(t) satisfies a stochastic differential equation

$$dX(t)=\mu(X(t),t)\,dt+\sigma(X(t),t)\,dW(t),\quad t\in[0,T]$$

iff it satisfies the following stochastic integral equation

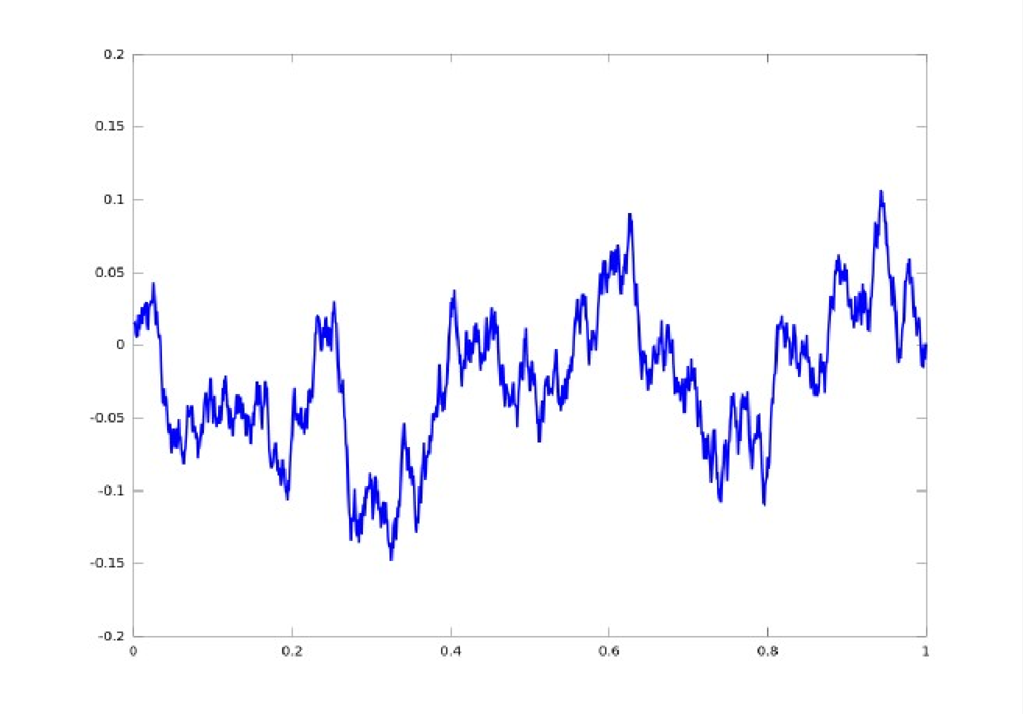
$$X(t)=X(0)+\int_0^t \mu(X(s),s)\,ds+\int_0^t \sigma(X(s),s)\,dW(s)$$

$$t\in[0,T]$$

Stochastic differential equations

Wiener process (Brownian motion)

$$d\,X(t) = \sigma dW(t)$$



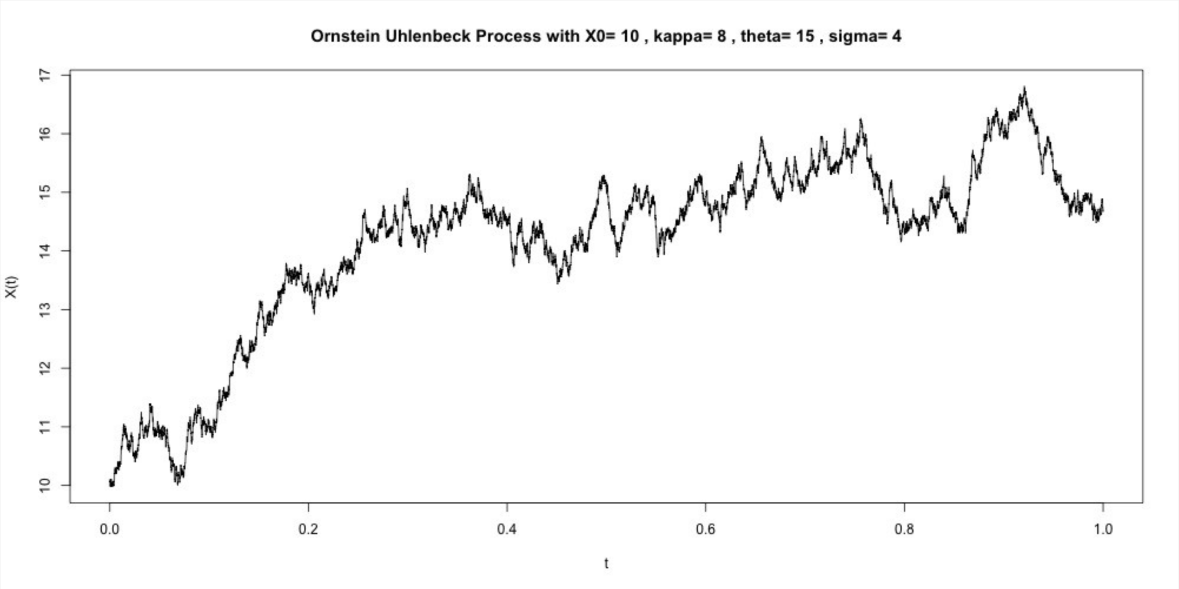
$$X(t) = \sigma W(t)$$

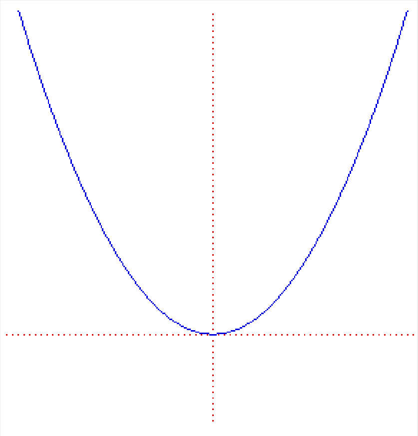
Stochastic differential equations

Ornstein-Uhlenbeck process

$$dX = -\gamma X\,dt + \sigma dW$$

Diffusion in a harmonic potential





$$X(t) = e^{-\gamma t} X(0) + \sigma \int_0^t \exp(-\gamma(t-s))\,dW,$$

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Stochastic differential equations

Geometric Brownian motion example
(Black–Scholes model for option pricing)

$$\frac{dS}{S} = \mu(S(t), t)\,dt + \sigma(S(t), t)\,dW(t)$$

Samuelson (1965) and Merton (1973)

price

return on the stock

Ito calculus solution

$$S(t) = S(0)\exp\left(\int_0^t (\mu(s) - \sigma^2(s)/2)\,ds + \int_0^t \sigma(s)\,dW(s)\right)$$

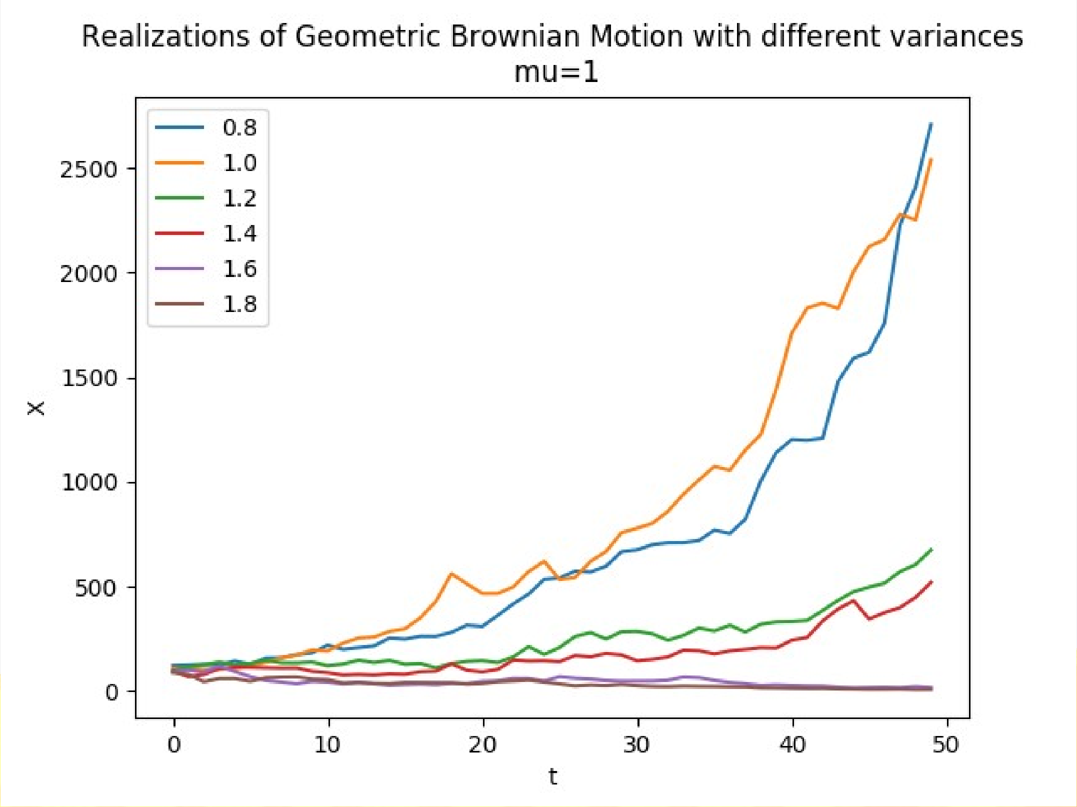
$$if\ \mu(s) = const,\ \sigma(s) = const$$

$$S(t) = S(0)\exp((\mu - \sigma^2/2)t + \sigma W(t))$$

Stochastic differential equations

Geometric Brownian motion example
(Black–Scholes model for option pricing)

$$S(t) = S(0)\exp\left(\left(\mu - \sigma^2/2\right)t + \sigma W(t)\right)$$



Stochastic differential equations

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

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

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

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

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

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)

What is an alternative?

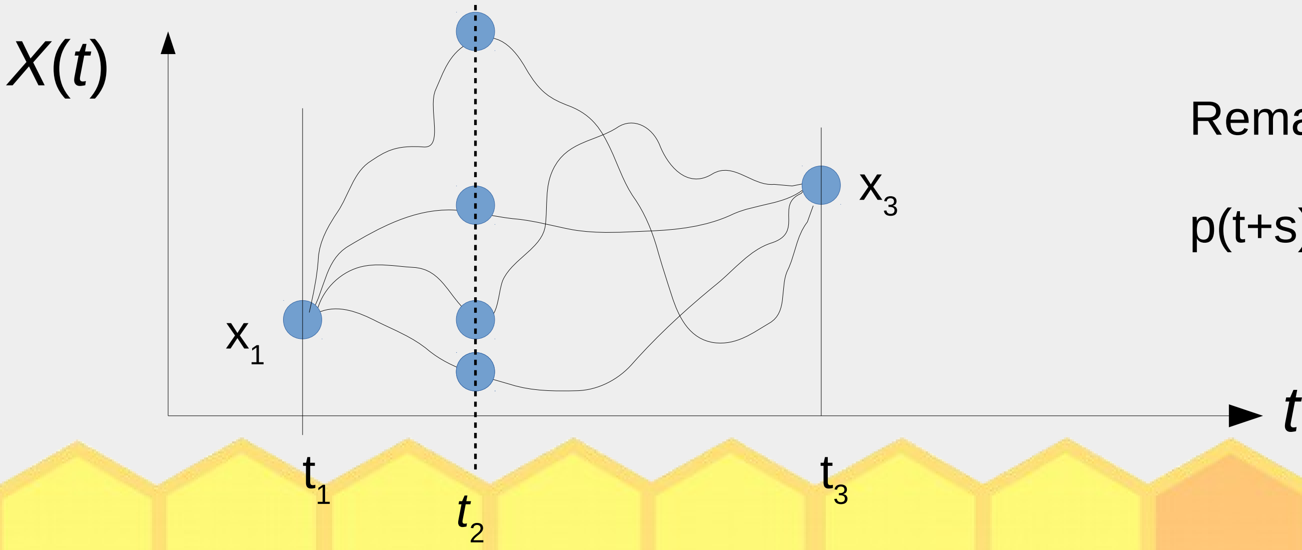
Answer: the use of Probability Distribution Functions!

For Markov processes

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

Chapman-Kolmogorov equation

$$P(x_3, t_3 | x_1, t_1) = \int dx_2 P(x_3, t_3 | x_2, t_2) P(x_2, t_2 | x_1, t_1)$$



Remark: for Markov chains

p(t+s)=p(t)*p(s)=$p^t * p^s$

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What is an alternative?

$$P(x_3,t_3|x_1,t_1)=\int dx_2 P(x_3,t_3|x_2,t_2)P(x_2,t_2|x_{1,}t_1)$$

(1) $$P(x,t+\tau|0,0)=P(x,t+\tau)=\int dx' P(x,t+\tau|x',t)P(x',t)$$

Introducing Δ=x-x’ and performing Taylor expansion

(2) $$P(x,t+\tau|x',t)P(x',t)=P(x-\Delta+\Delta,t+\tau|x-\Delta,t)P(x-\Delta,t)=$$

$$=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Delta^n\left(\frac{\partial}{\partial x}\right)^n P(x+\Delta,t+\tau|x,t)P(x,t)$$

Inserting (2) into (1) and integrating we get (see the next slide):

Kramers-Moyal expansion

$$P(x,t+\tau)-P(x,t)=\sum_{n=1}^{\infty}\left(-\frac{\partial}{\partial x}\right)^n \frac{M_n(x,t,\tau)}{n!}P(x,t),$$

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!

$$\boxed{\frac{\partial P(x,t)}{\partial t}=\sum_{n=1}^{\infty}\left(-\frac{\partial}{\partial x}\right)^n D^{(n)}(x,t)P(x,t)=L_{KM}P(x,t)}$$

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The Fokker-Planck equation

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

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

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

PDF

Probability current

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

The Fokker-Planck equation

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

Examples

Wiener process

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

initial condition $P(x,t|x',t) = \delta(x - x')$

The Fokker-Planck equation

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

Examples

Wiener process

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

initial condition $P(x,t|x',t) = \delta(x-x')$

$$P(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left(\frac{-x^2}{4Dt}\right)$$

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The Fokker-Planck equation

Examples

Ornstein-Uhlenbeck process

$$\frac{\partial P(x,t|x',t')}{\partial t} = -\gamma \frac{\partial}{\partial x}(x P(x,t|x',t')) + D \frac{\partial^2}{\partial x^2} P(x,t|x',t')$$

initial condition $P(x,t|x',t) = \delta(x-x')$

$$P(x,t|x',t') = \sqrt{\frac{\gamma}{2\pi D(1-\exp(-2\gamma(t-t')))}} \exp\left(-\frac{\gamma(x-\exp(-\gamma(t-t')x'))^2}{2D(1-\exp(-2\gamma(t-t')))}\right)$$

Q How does one find the solution of the equation?

$$P_{st}(x) = \sqrt{\frac{\gamma}{2\pi D}} \exp\left(-\gamma \frac{x^2}{2D}\right)$$

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

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

(1) is equivalent to the following FP equation

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

Q. Starting from dy/dt=-γ y+ξ(t) obtain the FP equation for Ornstein-Uhlenbeck process

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Connection between descriptions in terms of variables and their PDFs

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

Case 2. Multiplicative noise

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

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

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)

Literature

1. C. Gardiner, Stochastic Methods, A Handbook for the Natural and Social Sciences, 4th Edition, Springer, 2009
2. N.G. Van Kampen, Stochastic Processes in Physics and Chemistry, 3rd Edition, Elsevier, 2007.
3. H. Risken, The Fokker-Planck Equation, Springer, 1989