Advanced Statistical Mechanics (Part III Minor Topic)

Q o g s

Prerequisites

There are no formal prerequisites, as all students are expected to have attended the Part II Thermal & Statistical Physics course (or equivalent, for the MASt cohort). It would be helpful to have attended the Part II Soft Condensed Matter option; for those who have not, the lectures cover the essential material.

Learning Outcomes and Assessment

This is a theoretical course that focuses on the microscopic processes that drive fluctuations, examining the fundamentals and modern techniques of statistical mechanics, with applications in non-equilibrium thermal physics, diffusion and viscoelasticity, genetics and evolution, and stock markets. However, the in-depth topics are all “physical”, covering the mean first-passage time, non-Markov noise and anomalous diffusion, and the crossover between quantum and statistical uncertainty.

Synopsis

ol ar fl: Equilibrium statistical mechanics revised via partition functions / free energy, and via rates / detailed balance.

l e p f mol pp p: Markov process, Poisson and Wiener processes, Stochastic differential equations; conversion from Langevin to Fokker-Planck and Smoluchowski equations; Example 1 – Black-Scholes equation for the price of stocks. Detailed balance; Correlation functions; Fluctuation-dissipation theorem.

mmif fl p l c I d sf av j f p: Diffusion in shear flow. Example 2 – viscosity of a simple fluid. Ornstein-Uhlenbeck theory; Diffusion in external potentials; Periodic and random potentials; Kramers escape theory and mean first-passage time. Example 3 – “hitting a small target”.

o ifp a I d sf av j f p: Covariant formulation of multi-variable stochastic processes; Fokker-Planck and Smoluchowski equations; Non-Markov stochastic process, viscoelasticity and memory functions; Generalised (viscoelastic) Langevin equation and anomalous diffusion; Dissipation as coupling to an ensemble of oscillators; Mori equation; Liouville equation for dynamical variable and for distribution function (Heisenberg and Schrodinger formalisms). Example 4 – Kubo formula.

r rj ol ppl s o: Quantum and stochastic probabilities; statistics of the density matrix; Dissipation as coupling to an ensemble of oscillators. Example 5 – Marcus equation for electron transfer. Example 6 – rate of escape over and tunnelling under the potential barrier

KEY BOOKS

Nonequilibrium Statistical Mechanics, Zwanzig R. (OUP 2001)
Introduction to Stochastic Processes, 2nd Edition, Lawler G. F. (Chapman & Hall 2006)
Brownian Motion: Fluctuations, Dynamics, and Applications, Mazo R. (OUP 2002)
Fokker-Planck Equation, Risken H. (Springer 1996)

Advanced Statistical Mechanics (2024)

Lecture 1

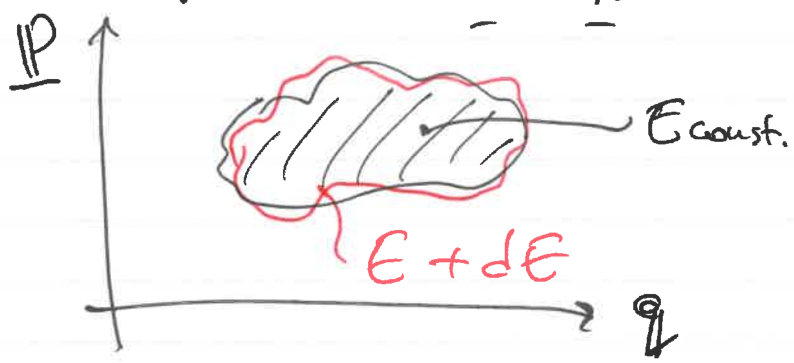
Brief recap of "Statistical physics"

- Microcanonical Ensemble

"phase space" $(\underline{p}, \underline{q})$

Hamiltonian $H(\underline{p}, \underline{q})$

Mean $H = E$



Find area: $\int d\underline{p}\, d\underline{q}$

$$E < H(\underline{p}, \underline{q}) < E + dE$$

$$= \int \left(\Theta[E + dE - H] - \Theta[E - H] \right) d\underline{p}\, d\underline{q}$$

step-functions $\Theta(x)$

$$= dE \int \frac{d}{dE} \Theta(E - H)\, d\underline{p}\, d\underline{q}$$

$\frac{d}{dx}\Theta(x) = \delta(x)$

Define: $\Omega(E) = \int \delta(E - H)\, d\underline{p}\, d\underline{q}$

(E) is the number of states with $H(p,q) = E$ fixed E)

De 'ne $S(E) = k \quad (E)$

the entropy o this microstate (with constant E)

D 'ne probabil: (E) :

Mean $X(p,q)$ = ~~$\int X(p,q) \rho(E)$~~

$$= \frac{\int X(p,q)\, \delta(E - H(p,q))\, dp\, dq}{\Omega(E)}$$

Hence $(E) = \dfrac{\delta(E - H(p,q))}{\Omega(E)}$ of a state within the microstate (E)

Normalised!

Eas to :

$$\Omega(E) \equiv \Omega(E_1) \quad (E - E_1)\, dE_1$$

Since $\Omega(E)$ is <u>not</u> Normalised, there is an extra $\int \Omega(E)\, dE$

⊙ Canonical ensemble

of many microstates exchanging energy between

Define $e^{-\beta E}$ "weight"

Define probability — but first: its Normalisation factor

$$Z = \sum_{\text{all states}} e^{-\beta E} = \int dp\,dq\; e^{-\beta H(p,q)}$$

$\left(\int dp\,dq\right)$

re-order this summation: over microstates

$$Z = \sum_{\substack{\text{Microstates}\\(E)}} e^{-\beta E} \cdot \Omega(E) \quad \rightarrow e^{\ln \Omega}$$

$Z = \sum$ [illegible] $e^{-\beta(E - k_B T \ln \Omega(E))}$

P [illegible] microstates (E)

Probabili[illegible] free

$$p(E) = \frac{1}{Z} e^{-\beta(E - TS(E))}$$

This effect of multiplicity of states $\Omega(E)$, or $S(E)$, increases the probability $\rho(E)$

Maximum (mode) probability is when

(in a large system this is also the average and median)

$E - TS(E)$ is minimal

v

min E for equilibrium

max $S(E)$ for equilibrium

S high

E low

" " is switch between two trends

Findi equilibrium

E

$F(E)$

$\mathbb{P}$

How fast?

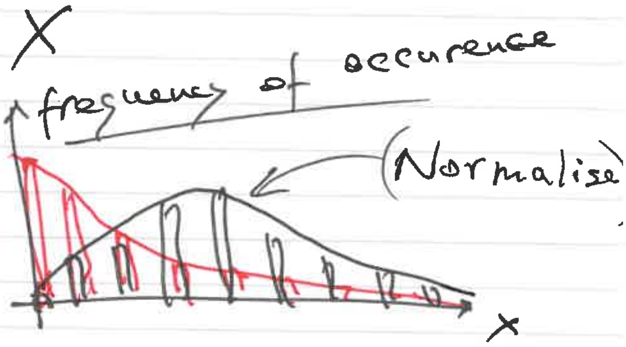
Barriers (metastability)?

Mechanism of this?

Lecture 2 — Basic terms and definitions of probability theory.

⊙ "Random", or "Stochastic" variable: X

Probability $P(x)$: such that



$$\langle x \rangle = \int x \, P(x) \, dx \qquad \int P(x)\, dx = 1$$

Also $\langle \Delta x^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 \equiv \sigma^2$ Variance

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⊙ Characteristic function (of X)

$$\phi_X(k) \overset{\text{def.}}{=} \left\langle e^{ikx} \right\rangle_{P(x)}$$

This is just a FT of $P(x)$:

$$\phi_X(k) = \int e^{ikx} P(x) \, dx$$

$$= \int \sum_n \frac{1}{n!} (ikx)^n P(x) \, dx$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} (ik)^n \langle x^n \rangle$$

← Moments of $P(x)$

Separately, define:

$$\phi_x(k) = \exp\left[\sum_{m=0}^{\infty} \frac{(ik)^m}{m!} C_m\right]$$

cumulants of $P(x)$

So that

$$C_n = \frac{d^n}{d(ik)^n} \phi_x(k) \Big|_{=0}$$

ow compare ...

$$n=1 \qquad C_1 = \frac{d}{d(ik)} \sum_n \frac{(ik)^n}{n!} C_n \Big|_{k=0} \qquad (1)$$

$$n=1$$

$$- \frac{d}{d(ik)} \sum_n \frac{1}{n!}(ik)^n \langle x^n \rangle \qquad (2)$$

cancel {n} and renumber the sum in numerator

$$= \frac{\sum_n n\cdot\frac{(ik)^{n-1}}{n!} \langle x^n \rangle}{\sum_n (ik)^n \langle x^n \rangle} = \langle x^1 \rangle = \langle x \rangle$$

Check yourself:

[redacted]

If $P(x)$ is Gaussian,

$\phi_x(k)$ is also ... $P(x) \sim e^{-\frac{(x-x_0)^2}{2\sigma^2}}$

⊙ If there is a ~~[illegible]~~ linked sequence of random variables:

$$Y_N = X_1 + X_2 + \dots X_N$$

Each of these has same $P(x)$

→ is called "Random walk" or "Stochastic process"

Then: $\langle Y_N \rangle = N \langle x \rangle$

Variance: $\langle \Delta Y_N^2 \rangle = \langle Y_N^2 \rangle - \langle Y_N \rangle^2$

$$= \sum_{i,j} \langle x_i x_j \rangle - \sum_i \langle x_i \rangle \sum_j \langle x_j \rangle$$

$$= \sum_i \langle x_i^2 \rangle + \sum_{i \neq j} \langle x_i x_j \rangle - N^2 \langle x \rangle^2$$

$$= N \langle x^2 \rangle + N(N-1) \langle x \rangle^2 - N^2 \langle x \rangle^2$$

$$= N \left(\langle x^2 \rangle - \langle x \rangle^2 \right) = N \sigma^2$$

⊙ Central Limit Theorem

Take a "normalised" random walk

$$S_N = \frac{Y_N}{N} \quad \text{such that} \quad \langle S_N \rangle = \langle x \rangle$$

and Variance $= \frac{\sigma^2}{N}$

for large N: $P(S_N)$ converges to a Gaussian

Proof via characteristic function:

$$\phi_S(k) = \left\langle e^{iks} \right\rangle_{P(s)} = \left\langle e^{\frac{ik}{N}\sum_m x_m} \right\rangle$$

product of N exponentials

$$= \left\langle e^{\frac{ik}{N}x} \right\rangle_{P(x)}^{N}$$

But this is the characteristic function $\phi_x(k/N)$ raised to N ...

Separately:

$$\phi_S(k) = \exp\left[\sum_{m=0}^{\infty} \frac{(ik)^m}{m!} C_m(s)\right]$$

$$= \left[\phi_x(k/N)\right]^N$$

Now, [redacted]

...

[redacted]

product of exponentials ....

→ $n=1$ $\exp\left(ik\, c_1(x)\right)$

→ $n=2$ $\exp\left(-\frac{k^2}{2N} c_2(x)\right)$

See the added "note" at the end

No need to go further if $N \gg 1$...

this cuts out the range of possible "k" when $|k| > \sqrt{N}$, this $\exp(-k^2/N) \to 0$

Then:

$$\phi_s(k) = \exp\left(N + ik\, c_1(x) - \frac{k^2}{2N} c_2(x)\right)$$

[redacted]

(irrelevant if $|k| < \sqrt{N}$)

def. $\int$ [redacted]

over the range $|k| < \sqrt{N}$

$$P(s) \approx \int e^{-iks + ik\langle x\rangle} \cdot e^{-\frac{k^2}{2N}\sigma^2} \, dk$$

$$= \text{const} \cdot e^{-\frac{(s-\langle x\rangle)^2}{2\sigma^2/N}}$$

Extend range (k) to ∞, ignoring higher terms

So it is Gaussian with

$$\langle S\rangle = \langle x\rangle$$

$$\text{var}(S) = \sigma^2/N$$

⊙ Replace N with time t

→ Stochastic process $y(t)$

(random walk $y_N = \sum_{m=0}^{N} x_m$)

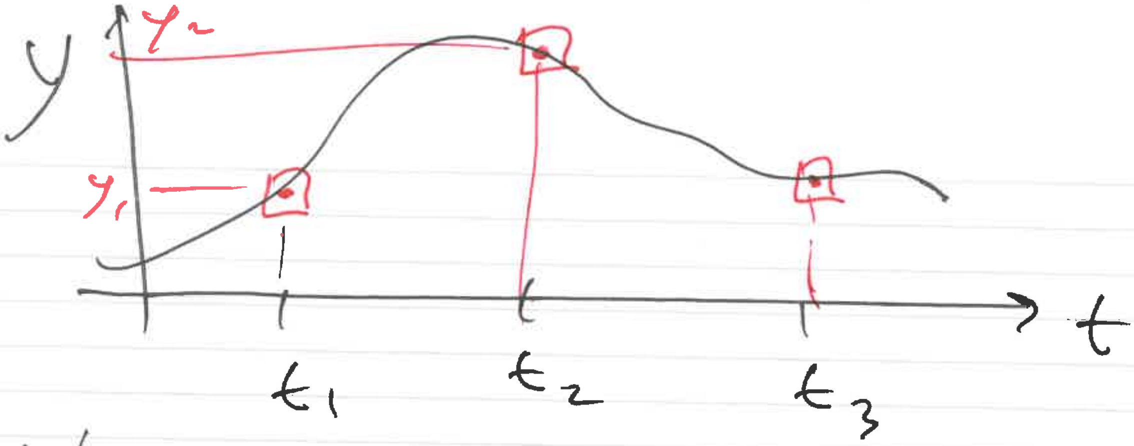
and stay with continuous t...

Define set of probabilities:

$P_1(y, t)$: reach value y in t

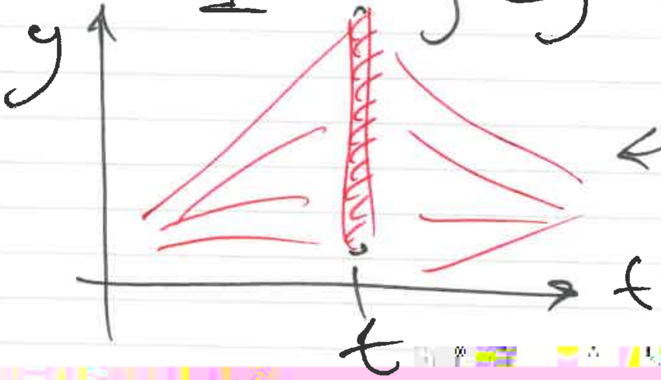
$P_2(y_1, y_2 \mid t_1, t_2)$: (simultaneous) y_1 at t_1 and y_2 at t_2

etc.



Normalisation:

$$1 = \int dy\, P(y,t)$$



Also:

$$1 = dy_1 dy_2 \dots P(y_1, y_2 \dots t_1 t_2 \dots)$$

⊙ Reduction:

$$dy_N\, P_N(y_1 y_2 \; y_N \; \dots) = P_{N-1}(y_1 y_2 \dots y_{N-1})$$

i.e. $$dy_2\, P_2(y_1 y_2 \; t_1 t_2) = P_1(y_1 t$$

⊙ Correlation function:

$$\langle y(t) \rangle = \int y \cdot P(y,t)\, dy$$

$$\langle y_1(t_1)\, y_2(t_2) \rangle = \int dy_1\, dy_2\, y_1 y_2\, P_2(\;, 2)$$

etc...

- Stationary process $y(t)$ is when $P(y,t)$ is invariant with time shift $t \to t + \Delta t$

$\langle y(t) \rangle$ is not t-dependent

$\langle y(t_1)\, y(t_2) \rangle \sim f(t_1 - t_2)$ (so that $t_1 + \Delta t$ and $t_2 + \Delta t$)

etc.

- Conditional probability = Propagator

$$P_2(y_1\, y_2 \,|\, t_1, t_2) = G[2|1]\, P_1(y_1 | t_1)$$

→ Simultaneous (pair) probability $P(1,2)$

⊙ Markov process (without memory)

fully determined by $P_1(y,t)$ and $G(y_2 y_1 | t_2 t_1)$

⊙ Evolution relation

$$P_1(y_2, t_2) = \int G[y_2 y_1 | t_2 t_1] P_1(y_1 | t_1) \, d$$

⊙ Kolmogorov Chapman relation

$$G[y_2 y_1 | t_2 t_1] = \int G[y_2 \tilde{y} | t_2 \tilde{t}] \, G[\tilde{y} \, y_1 | \tilde{t} \, t_1] \, d\tilde{y}$$

(difference with "Evolution" is that we retain (track) the initial condition $y_1(t_1)$ here

A Note about C.L.T.

We expand in exponent:

$$\phi_S(k) = \left[\phi_x(k/N)\right]^N$$

$$= \exp\left[1 + (ik)\langle x\rangle - \frac{k^2}{N}c_2(x) + \frac{ik^3}{N^2}c_3 + \ldots \frac{k^n}{N^{n-1}}c_n + \ldots\right]$$

$$e^{ik\langle x\rangle} \cdot e^{-\frac{k^2}{N}c_2} \cdot e \ldots e^{-\frac{k^n}{N^{n-1}}c_n}$$

$|k| \sim \sqrt{N}$

$|k| \sim N^{1-1/N}$ almost... (wider)

$-\sqrt{N}$ ⟷ $+\sqrt{N}$

$e^{\frac{1}{N^x}} \approx 1$

Hence only the k^2 term matters

→ Gaussian $e^{-\frac{k^2}{2N}c_2}$ is the

leading non-trivial term (eff...

Lecture 3 Stationary Markov process(es)

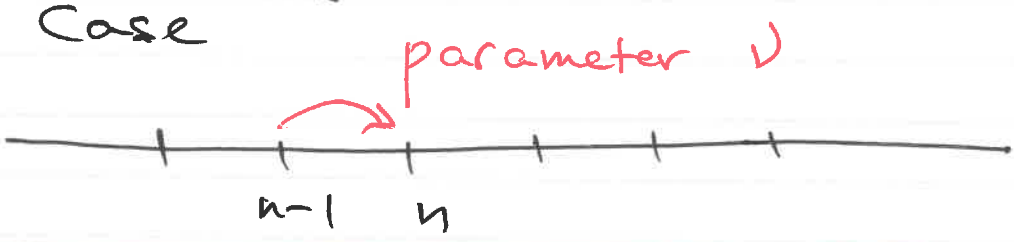
with the propagator

$$G(y_2 y_1 \mid t_2 - t_1)$$

Two of these processes are especially important in Physics

Wiener process	Poisson process
independent steps	independent steps
≠ equal — Must step	only forward — or not
Gaussian step distribution	"number of hits in a fixed target"

1D case



ν : rate of a single step

probability to make a step in time dt

$$p_+ = \nu \, dt$$

The whole stochastic process: $n(t)$

Still within a single step:

$(n-1) \longrightarrow (n)$

- What is the total (cumulative) probability to make this step in time t: $W(t)$
- Or equivalently, what is the "survival probability" to still not step in time t:

$$S(t) = 1 - W(t)$$

Then: $S(t+dt) = S(t) - \nu\, dt \cdot S(t)$

$$\frac{dS}{dt} = -\nu S$$

if $t=0$, $S(t)=1$

$$S(t) = e^{-\nu t}$$

Now define probability density:

$$w = \frac{\partial W(t)}{\partial t} = -\frac{\partial S(t)}{\partial t} = \nu e^{-\nu t}$$

So we can evaluate integrals:

Average time $(n-1) \rightarrow (n)$: $\langle t \rangle_{step} = \int_0^\infty t\, w(t)\, dt = 1/\nu$

Also $\langle t^2 \rangle - \langle t \rangle^2 = 1/\nu^2$, etc.

Exercise (simulation):

fix time of step Δt, and "flip a biased coin":

$p_+ = \nu \Delta t$ and $p_0 = 1 - \nu dt$

When do we reach a point (k) after a time $t = N\Delta t$. make k steps

This is a binomial distribution

$$P(k, N) = \frac{N!}{k!(N-k)!} p_+^k \, p_0^{N-k}$$

to reach (k) after (N) steps

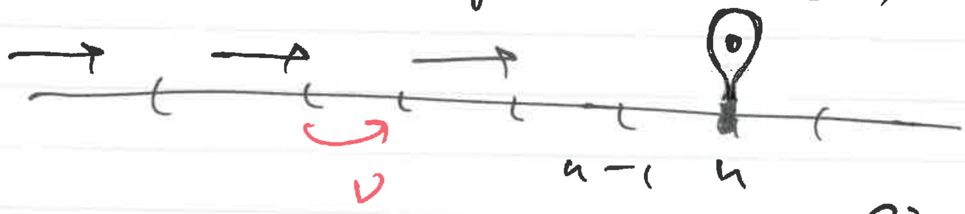
At large N, with Np constant λ reduces to

$$p(k, \lambda) = \frac{\lambda^k}{k!} e^{-\lambda}$$

this is "Poisson"

Now lets ~~derive~~ understand it.

- What is the probability to reach a position (n) after time



(t), given step

[redacted]

The

[redacted]

Stay at (n)

[redacted]

Step from (n−1)

[redacted]

This is often called the "Master Equation"

$$\dot{P} = \text{rate in} - \text{rate out}$$

Recall we saw "characteristic function"

$$\phi_x(k) = \langle e^{ikx} \rangle_{P(x)}$$

Similar logic employs the "generating function"

$$g(k,t) = \sum_{n=0}^{\infty} P(n,t)\, k^n$$

Now: $$\frac{\partial g(k,t)}{\partial t} = \sum_{n=0}^{\infty} k^n \cdot \nu \left[P(n-1,t) - P(n,t) \right]$$

renumber the sum $$= \sum_{n=0}^{\infty} \nu \left(k^{n+1} - k^n \right) P(n,t)$$

$$= \nu (k-1) \sum_{n=0}^{\infty} k^n P(n,t)$$

but this is the definition of $g(k,t)$

$$\boxed{\frac{\partial g}{\partial t} = \nu (k-1) \cdot g}$$

At $t=0$

$$P(n,0) = \delta_{n,0}$$

$$g(k,0) = 1$$

$$g(k) = e^{\nu (k-1) t}$$

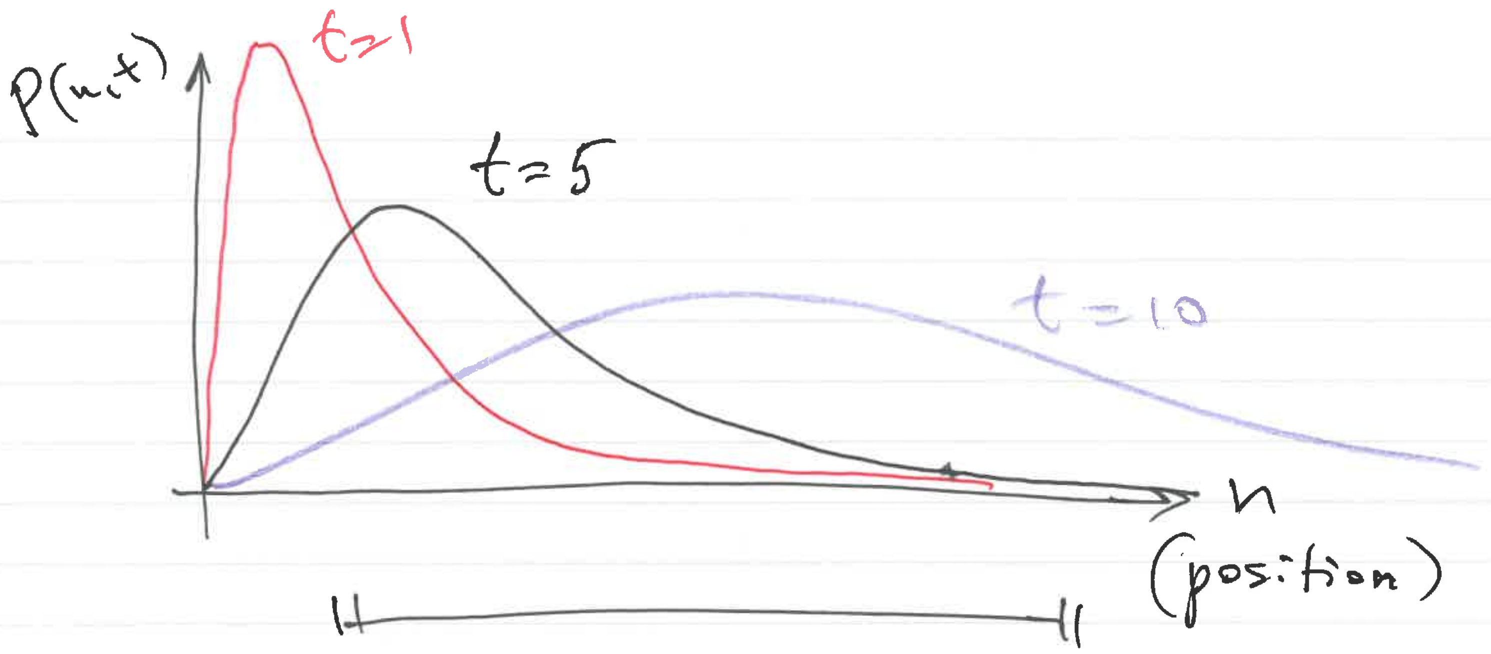
Now expand this exponential: (to isolate $\sum_n k^n (\dots)$)

$$g(k,t) = e^{-\nu t} \sum_{n=0}^{\infty} \frac{(\nu k t)^n}{n!} = \sum_{n=0}^{\infty} k^n \left(\frac{(\nu t)^n}{n!} e^{-\nu t} \right)$$

this is the Poisson distribution

$$\boxed{P(n,t) = \frac{1}{n!} (\nu t)^n e^{-\nu t}}$$

Before we had $\lambda = Np$, now use (νt) as the "time" parameter



⊙ Average time of the 10^{th} step

$n=10$

each step is independent!

$$\langle t_{10} \rangle = 10 \langle t_1 \rangle = 10/\nu$$

⊙ Probability that 10^{th} step $(n=10)$ occurs after time t.

$P(t_{10} > t)$ or $P(n(t) < 10)$

↓

9 events at t', then step

$$\int_t^\infty \frac{(\nu t')^9}{9!} e^{-\nu t'} \cdot \nu dt'$$

(the step #10 occurs: $t' > t$)

↓

Sum of $0 \div 9$ steps at t:

$$\sum_{n=0}^{9} P(n,t)$$

$$= \sum_{n=0}^{9} \frac{(\nu t)^n}{n!} e^{-\nu t}$$

They better be equal!

A comment about Master Equation

⊙ Evolution:

$$P(n, t+\Delta t) = \sum_m G(n, t+\Delta t \,|\, m, t)\, P(m,t)$$

Subtract $P(n,t)$ from both sides

$$\frac{\partial P(n,t)}{\partial t} = \frac{1}{\Delta t}\Big[\sum_m G(n, t+\Delta t | m,t)\, P(m,t) - P(n,t)\cdot \sum_m G(m\, t+\Delta t | n,t)\Big]$$

$= 1$

$$= \sum_m \frac{G(n, t+\Delta t | m,t)}{\Delta t} \cdot P(m,t)$$

"flux in" ($\forall m \to n$)

$$- \sum_m \frac{G(m, t+\Delta t | n,t)}{\Delta t} \cdot P(n,t)$$

"flux out" ($n \to \forall m$)

So:

$$\frac{\partial P(n,t)}{\partial t} = \sum_m \left[w_{nm} P(m,t) - w_{mn} P(n,t) \right]$$

transition probabilities....

Not necessary to have $n > m$....

It is so for Poisson process, but the Evolution relation is more general.

Lecture 4 : Wiener process

random variable X : $p(x)$
Stochastic process $y_X \to y(t)$

} when independent steps each have Gaussian probability → $W(t)$

- Increment $\Delta W = W(t+\Delta t) - W(t)$

  has $$p(\Delta W) = \frac{1}{\sqrt{2\pi\Delta t}} e^{-\frac{\Delta W^2}{2\Delta t}}$$

  (Normalise if: Variance $= \Delta t$)

- Characteristic function of ΔW

$$\phi(k,t) = \langle e^{ik\Delta W} \rangle_{p(\Delta W)}$$

$$= e^{i W_0} \cdot e^{-\frac{1}{2}k^2(\Delta t - t_0)}$$

if we had a condition W_0 at $t = t_0$

- Scaling: $V(t) = \frac{1}{c} W(ct)$ is also a Wiener

Could we find the full probability of the process $W(t)$: $P(w,t)$?

Let's start from Evolution eq:

$$\odot \quad P(w+\Delta w, t+\Delta t) = \int G\left(\overset{(w+\Delta w)-w}{\Delta W}\,\Big|\,\Delta t\right) P(w,t)\,dw$$

propagator : ste ΔW

or it could be Kolmogorov–Chapman:

$$P\left(w+\Delta w, t+\Delta t \,\middle|\, w_0, t_0\right) =$$

$$= G(\Delta W|\Delta t)\, P(w,t \,|\, w_0 t_0)$$

Change variable: $\Delta W = W(t+\Delta t) - W(t)$

$dw \to (-) d_\Delta W$ from $dw \to -d(\Delta W)$

$$P\left(w+\Delta w \,\middle|\, t_1+\Delta t\right) = (-)\int G(\Delta w|\Delta t)\, P\left(W(t+\Delta t) - \Delta W, t\right) (-) d_\Delta W$$

change the limits of integral back

Small ΔW : Taylor expansion

0-order:

$$P(w+\Delta w, t+\Delta t) = \int G(\Delta w / \Delta t) \cdot P(w(t+\Delta t), t) \, d_\Delta w$$

$1 = \int G \, dw$

1st order:

$$- \int G(\Delta w / \Delta t) \cdot \frac{\partial P}{\partial W} \Delta W \, d_\Delta W$$

Gaussian: $\int w G \, dw = 0$

2nd order:

$$+ \int G(\Delta w / \Delta t) \, \frac{1}{2} \frac{\partial^2 P(w,t)}{\partial W^2} \Delta W^2 \, d_\Delta w$$

! variance of G

(+ ... stop)

All together this makes:

$$\frac{P(..\, t+\Delta t) - P(..\, t)}{\Delta t} = \frac{1}{2} \frac{(\text{variance})}{\Delta t} \cdot \frac{\partial^2 P}{\partial W^2}$$

$$\boxed{\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial W^2}} \leftarrow$$

$$D = \frac{(\text{Variance})}{2 \Delta t}$$

Equivalently

$$\frac{\partial P}{\partial t} = -\operatorname{div} J$$

flux: prob. current $J = -D \frac{\partial P}{\partial W}$

Equations of this nature, for full $P(w,t)$, or $\phi_k(w)$, are called "kinetic" or macroscopic.

On the microscopic level of $w(t)$ we have "stochastic differential equation" (SDE)

1905 Einstein, Smoluchowski

→ 1911 Langevin equation

We saw this in simple Brownian motion:

$$m\frac{dv}{dt} = \sum \text{forces} = -\gamma v + \ldots(t)$$

More generally:

SDE
$$\frac{dx}{dt} = F(x) + \ldots x \, \xi(t)$$

drift term — diffusion term — stochastic force

or noise

Wiener process

$\to D = \frac{1}{2}\sigma^2$

Mathematical format of SDE

[redacted]

drift diffusion

Gaussian $P(dW)$ Wiener

Example of SDE:

Geometric Brownian Motion

Multiplicative Wiener

SDE: $$dS_t = (\mu \cdot S_t)\,dt + (\sigma \cdot S_t)\,dW_t$$

constant.

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

looks like $d(\ln S)$

looks like simple Brownian motion...

But we discover that a lot is hidden

[redacted]

Itoh Lemma

if we have a stochastic process $X(t)$, with SDE

$$dX_t = \mu\, dt + \sigma\, dW_t$$

and there is a function $f(x)$, then what is its SDE?

$$df = f(x+dx) - f(x)$$

chain rule

[redacted] $\frac{\partial^2 f}{\partial x^2} dx^2$

$+ \dots$

none there

We only want terms linear in (dt), not higher-order.

$$= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial x} (\mu\, dt + \sigma\, dW)$$

$$+ \frac{1}{2} \frac{\partial^2 f}{\partial x^2} \left(\mu^2 dt^2 + 2\mu\sigma\, dt\, dW + \sigma^2 dW^2 \right)$$

→ 0 (dt^2), small ($dt\,dW$)

$$\approx \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial x} (\mu\, dt + \sigma\, dW)$$

$$+ \frac{1}{2} \frac{\partial^2 f}{\partial x^2} \sigma^2 dW^2 \dots$$

$\sim \langle dW^2 \rangle = dt$

assume fast steps

So we have:

$$df = \left(\frac{\partial f}{\partial t} + \mu \frac{\partial f}{\partial x} + \frac{1}{2}\sigma^2 \frac{\partial^2 f}{\partial x^2}\right) dt$$

drift term

$$+ \sigma \frac{\partial f}{\partial x} dW$$

diffusion term

Itoh! Lemma

Now: GBM

$$dS = \mu S\, dt + \sigma S\, dW$$

and $f(S) = \ln(S)$

$$d[\ln(S)] = \frac{\partial f}{\partial S} dS + \frac{1}{2}\frac{\partial^2 f}{\partial S^2} dS^2$$

$$= \frac{dS}{S} - \frac{1}{2S^2} dS^2$$

$$= \frac{dS}{S} - \frac{1}{2S^2}\left(\mu^2 S^2 dt^2 + 2\mu\sigma S^2 dt\,dW + \sigma^2 S^2 dW^2\right)$$

$dW^2 \to dt$

$$d[\ln(S)] = \left(\mu - \frac{1}{2}\sigma^2\right) dt + \sigma\, dW$$

gives

$$S = S_0\, e^{\left(\mu - \frac{\sigma^2}{2}\right)t + \sigma W}$$

Look here!

Still stochastic

Stochasticity (σ) can reduce, or even revert exponential growth $e^{\mu t}$...

Lecture 5

We just did "Itoh Lemma" and looked at "GBM" $dS = \mu S dt + \sigma S dW$

Entry level of financial application:
"Black-Scholes equation"
→ Nobel Prize 1997 (also to Merton)

Analysis of dynamics and prediction of option prices in a volatile market.

How to decide on a "portfolio" to buy: exchange risk for cash

Crisis 1987 → Traders colluded to punish the early adopters of B-S.

Crisis 2008 → Too much trust into B-S analysis, incorrect use of it.

"Stock" $S(t)$: value of shares

$$dS = S\,dt + \sigma S\,dW$$

"Option" is a contract when

on (seller) agree to sell

some stock $S(t)$ at a

ture time t, at a

current price (s)

buyer have to a a

fee for this : $V(s)$.

Obviously $V(s,t)$ and $V(t=0)=0$

① How to estimate best $V(s)$

"Portfolio" of this transaction

is what buyer has:

cash $$\Pi = -V(s) + \alpha S$$

(paid) ↘ ... ↗ (cash is some stock)

is called "hedging"

In continuous trading, we have small increments

$$\Delta\Pi = -\Delta V(s) + \alpha \Delta S$$

Itoh Lemma Says:

$$dV(S) = \left(\frac{\partial V}{\partial t}dt + \frac{\partial V}{\partial S}dS + \frac{1}{2}\frac{\partial^2 V}{\partial S^2}dS^2\right)$$

$$dV = \left(\frac{\partial V}{\partial t} + \mu S\frac{\partial V}{\partial S} + \frac{1}{2}\sigma^2 S^2\frac{\partial^2 V}{\partial S^2}\right)dt$$

$$+ \sigma S\frac{\partial V}{\partial S}dW$$

Now put this back into $d\Pi$:

[illegible]

$$+\left(\alpha\sigma S - \sigma S\frac{\partial V}{\partial S}\right)dW$$

fluctuating part

We can choose the factor α such that the bracket $= 0$!

$$\alpha = \frac{\partial V}{\partial S}$$

⊙ Then no volatility left in $d\Pi$

Now we wish to build the equation for $V(S)$, using some model Π.

Determine the l.h.s. $d\Pi$:

we need to make a decision on what we want to achieve:

$$d\Pi = r \cdot \Pi \, dt$$

we "deal in" the rate of growth.

What is the lowest risk-free rate of growth?

l.h.s. r.h.s.

$$r(\alpha S - V)\,\cancel{dt} = \left(-\frac{\partial V}{\partial t} - \cancel{\mu S \frac{\partial V}{\partial S}} - \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + \cancel{\alpha \mu S}\right)\cancel{dt}$$

$$\left(\alpha = \frac{\partial V}{\partial S}\right)$$

Finally we have: with initial $V(t=0)=0$

$$\frac{\partial V(S,t)}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} = V - S\frac{\partial V}{\partial S}$$

is is B-S equation for $V(S,t)$. To solve it we need to know [illegible] and σ, but note that has disappeared ...

1) Consider the simplest: $r=0$

$$\frac{\partial V}{\partial t} + \frac{\sigma^2}{2} S^2 \frac{\partial^2 V}{\partial S^2} = 0$$

has known solutions

⊙ re we certain we know σ?
All of the modern science is about more accurate

2 Some standard maths of B-S eq.

A substitution: S – stock now ($t=0$)

E – stock at the end ($t=T$)

define $x = \ln S/E$

or $S = E e^x$ [illegible]

(c) Then call

$$u(x,\tau) = Z(x,\tau)\cdot e^{\beta x + \gamma \tau}$$

enter new parameters (β,γ)

then

$$\frac{\partial u}{\partial \tau}$$ [redacted] $$(\beta,\gamma)\cdot\frac{\partial u}{\partial x} + B(\beta,\gamma)\cdot u = 0$$

Choose β,γ such that $A=0,\ B=0$

$$\beta = r/\sigma^2 - 1/2$$

$$\gamma = r/2 + \frac{\sigma^2}{8} + r^2/2\sigma^2$$

then just simple diffusion eq.

$$\boxed{\frac{\partial u}{\partial \tau} = \frac{\sigma^2}{2}\frac{\partial^2 u}{\partial x^2}}$$

via Green's function

$$u(x,\tau) = \int \frac{1}{\sqrt{2\pi\sigma^2\tau}}\, e^{-\frac{(x-w)^2}{2\sigma^2\tau}} \cdot u(w,0)\, dw$$

when $x(\tau=0) = w$

then roll back substitutions!

first $Z(x,\tau)$ from $u(x,\tau)$,

then $V(S,t)$

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The Heston Model – The Physics of Stochastic Volatility Models

Date **Friday, 9 February**
Time **11:00 a.m. - 12:00 p.m.**
Room **Bragg Building, Small Lecture Theather**

Open to all Cambridge students

Join us for an exclusive lecture by Optiver on financial modeling. Dive into the complexities of the Heston model, a cornerstone in stochastic volatility modeling, and discover how it revolutionizes our understanding of financial markets.

Key agenda points

- Comprehensive overview of the Heston model's dynamic properties
- In-depth analysis of the affine structure inherent to the model
- Partial Differential Equations (PDEs) and Ordinary Differential equations (ODEs) of the model
- Practical application: Characteristic function in option pricing

About the lecturer

Fabio Maggioni is an Optiver quantitative researcher working on the development and improvement of new pricing models and techniques. The focus of his research is around the impact of rate and volatility term structure and dividend uncertainty on the early exercise of American options. He joined Optiver after earning a Master's Degree in Mathematical Engineering at Polytechnic University of Milan.

Heston model

The physics of stochastic volatility models

Cambridge University   Fabio Maggioni, 08.02.2024

Heston model

The physics of stochastic volatility models

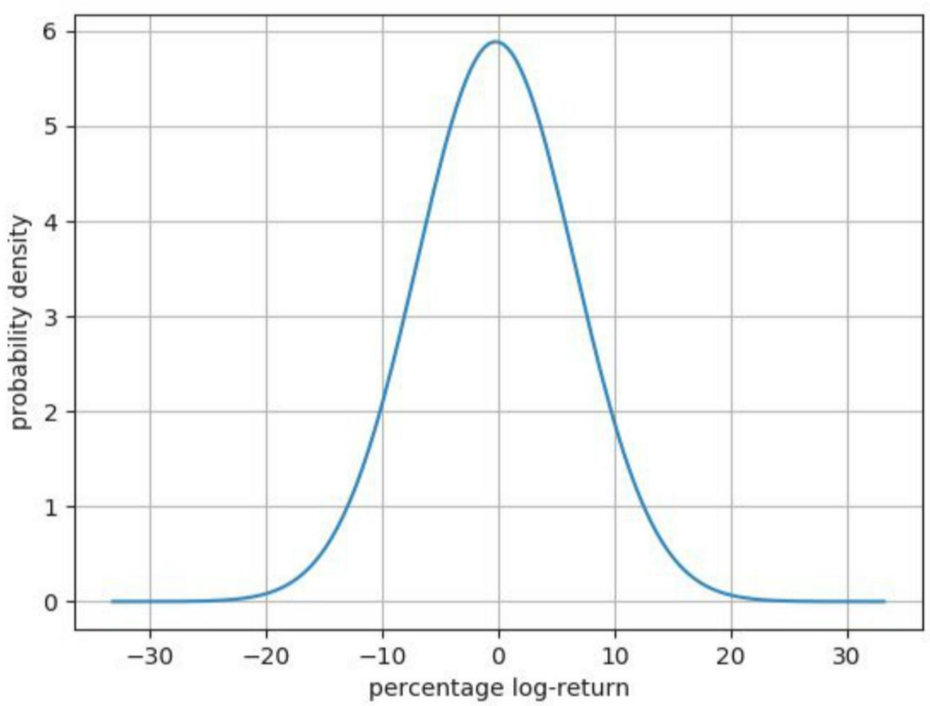
- Beyond Black-Scholes assumptions
- Definition
- Dynamics
- Partial Differential Equation
- Characteristic function

Beyond Black-Scholes

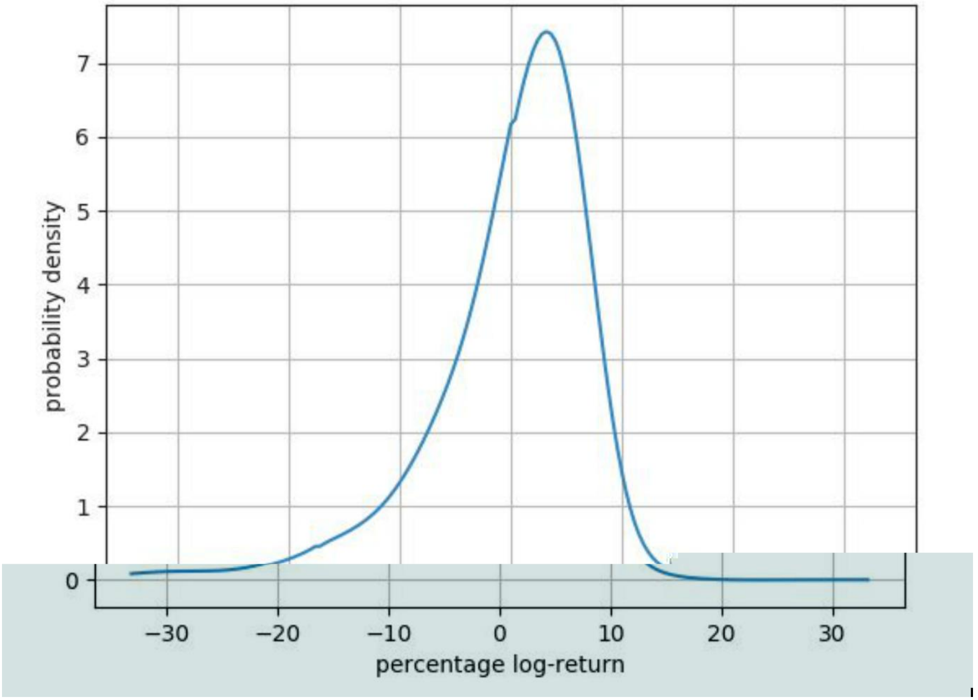
Pros	Cons	Market
Closed form solution for option prices Mathematical tractability Great for communication	Uncorrelated log-returns Gaussian log-returns	Persistence of variability (high vol and low vol periods) Spot-vol correlation Fat tailed log-return (kurtosis and skew)

Log-return distribution

Black-Scholes



Financial markets

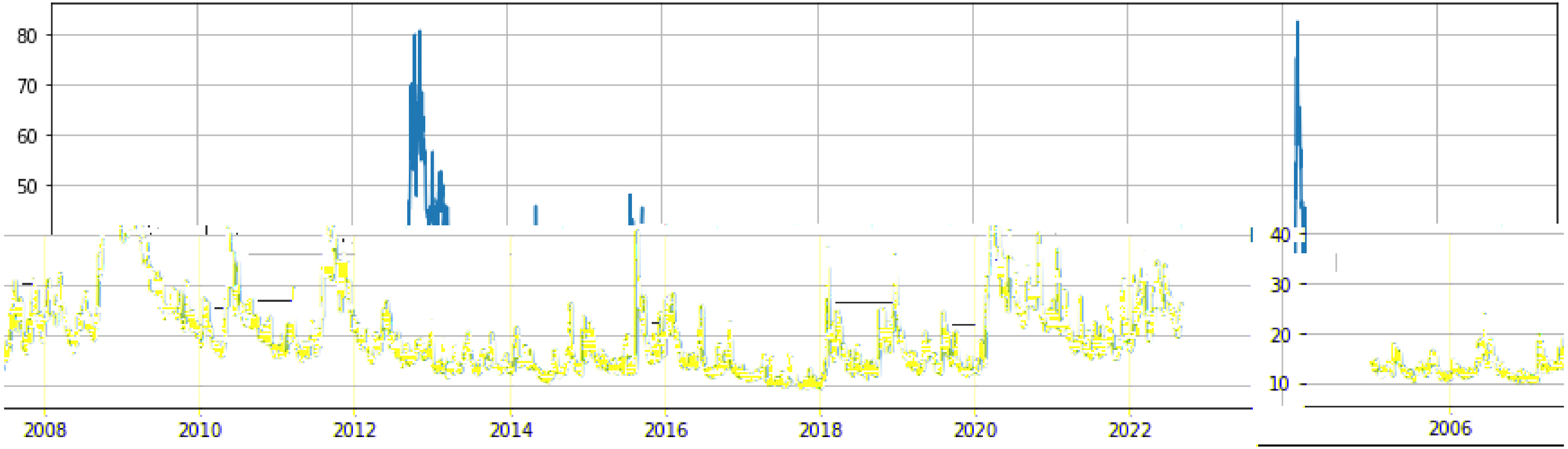


More complex models

$$dS_t = rS_t\, dt + \sigma_t S_t\, dW_t$$

Deterministic time dependent volatility does not improve over normality of log returns

Looking at Volatility Index we can guess that volatility is a good place to start: stochastic volatility models!



Stochastic volatility models

Setting:

$$dS_t = rS_t\,dt + \sigma_t S_t\,dW_t^1$$
$$d\sigma_t = a(t,\sigma_t)dt + b(t,\sigma_t)\,dW_t^2$$

With dW^1 and dW^2 being possibly correlated (ρ) random increments and a b

According to the structure of functions a and b we can produce all sort of dynamics for the vol.

Which one is appropriate?

Heston

$$
\begin{cases}
dS_t = rS_t\,dt + S_t\sqrt{v_t}\,dW_t^1 \\
dv_t = \kappa(\bar{v} - v_t)\,dt + \gamma\sqrt{v_t}\,dW_t^2 \\
\mathrm{S}_{\mathrm{t}_0} = \mathrm{S}_0 \\
\mathrm{v}_{\mathrm{t}_0} = \mathrm{v}_0 \\
\mathrm{E}\left[dW_t^1\,dW_t^2\right] = \rho\,dt
\end{cases}
$$

$\kappa = speed\ of\ mean\ reversion\ in\ years$

$\bar{v} = long\ term\ variance$

$v_0 = short\ term\ variance$

$\gamma = vol\ of\ vol$

$\rho = spot - variance\ correlation$

Heston

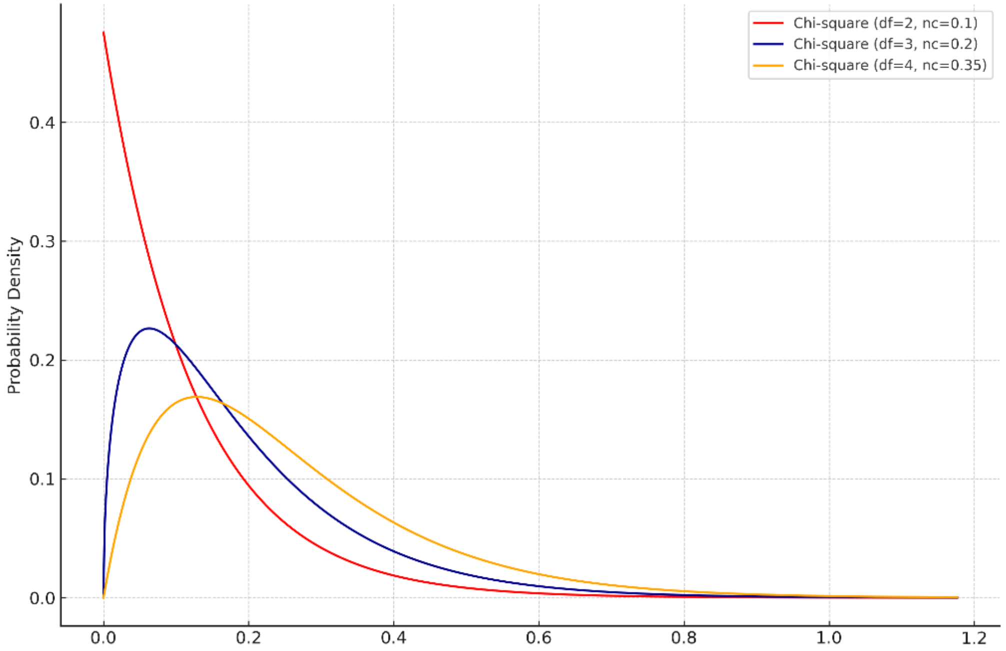
$$\begin{cases} dS_t = rS_t\,dt + S_t\sqrt{v_t}\,dW_t^1 \\ dv_t = \kappa(\bar{v} - v_t)\,dt + \gamma\sqrt{v_t}\,dW_t^2 \end{cases}$$

Instantaneous variance v_t is mean reverting

Instantaneous volatility $\sqrt{v_t}$ has 2 sources of randomness:

- Spot level via correlation ρ
- Exogenous variance process guided by vol of vol γ

Variance is distributed as a scaled Non central Chi square



Dynamics at the limit

Let's look at some key quantities of the Heston model for an expiry time T.

$$E[v_T|v_0] = v_0 e^{-\kappa T} + \bar{v}\left(1 - e^{-\kappa T}\right)$$

$$Var[v_T|v_0] = v_0 \frac{\gamma^2}{\kappa}\left(e^{-\kappa T} - e^{-2\kappa T}\right) + \frac{\bar{v}\gamma^2}{2\kappa}\left(1 - e^{-\kappa T}\right)^2$$

For $\kappa \to \infty$, $E[v_t|v_0] \to \bar{v}$, $Var[v_t|v_0] \to 0$, Heston → Black&Scholes with $\sigma^2 = \bar{v}$

For $\gamma \to 0$, $E[v_t|v_0] = v_0 e^{-\kappa t} + \bar{v}(1 - e^{-\kappa t})$, $Var[v_t|v_0] \to 0$, Heston → Black&Scholes with deterministic term structure

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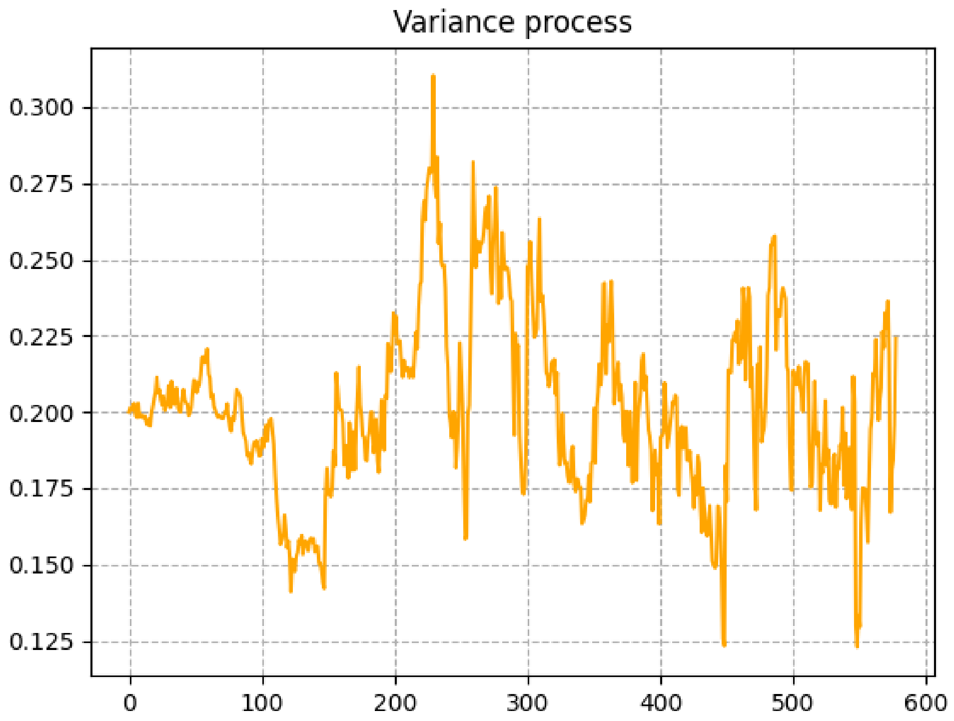
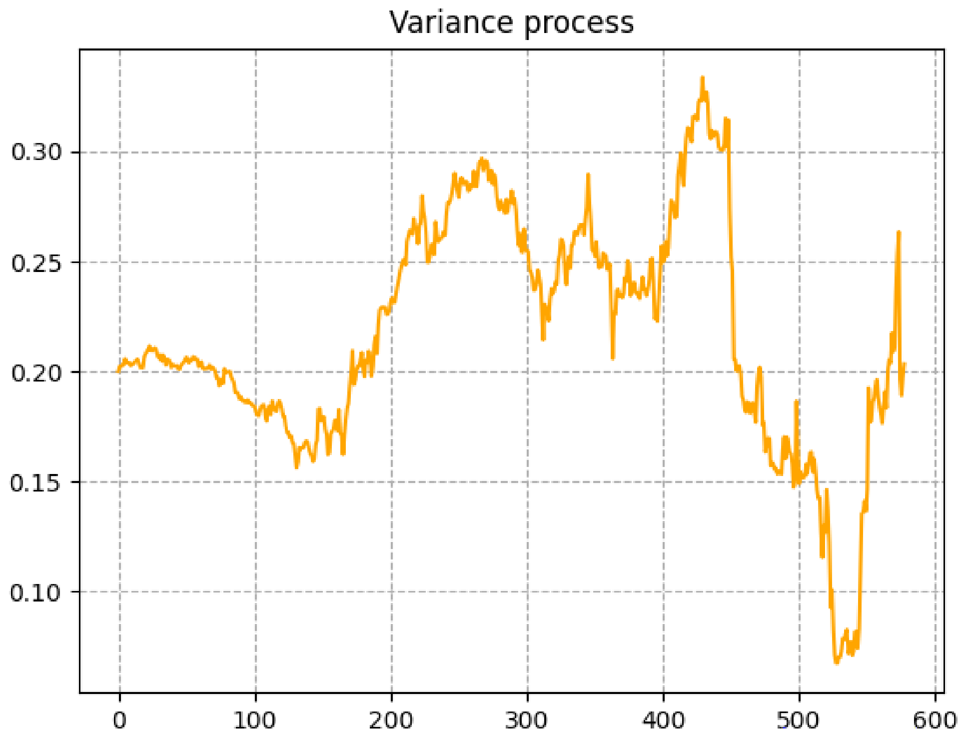
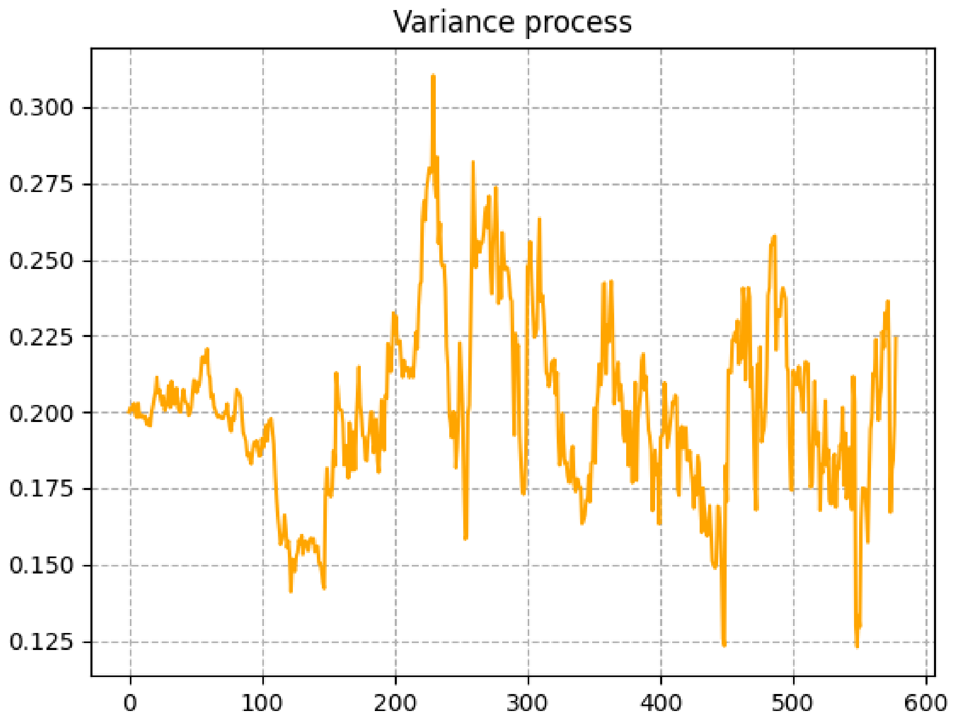
Variance dynamics

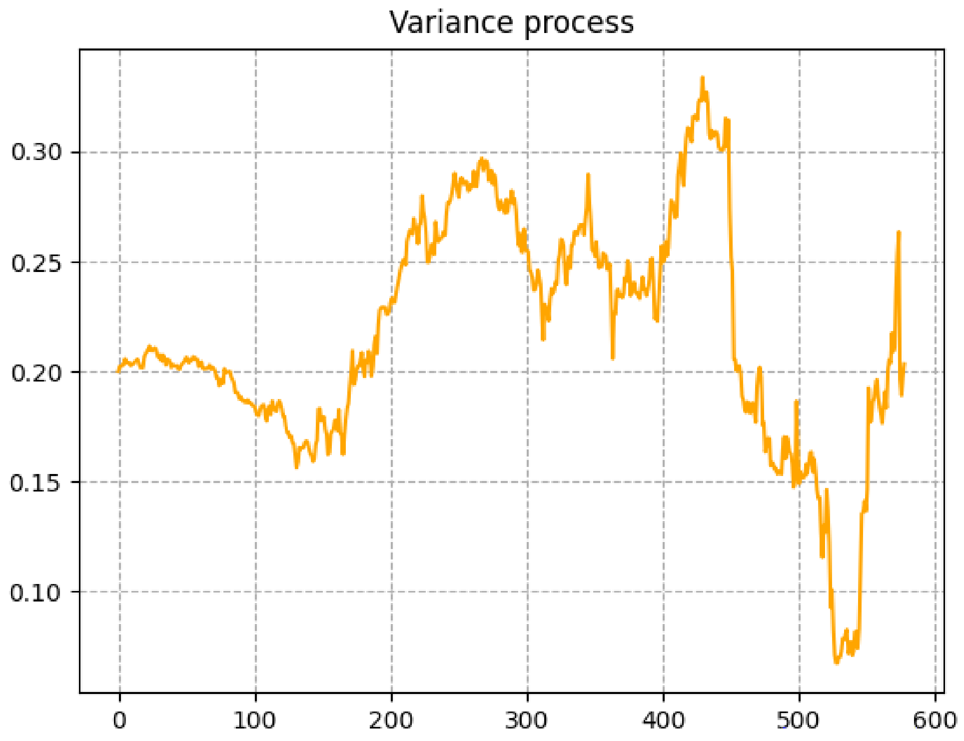




Variance dynamics

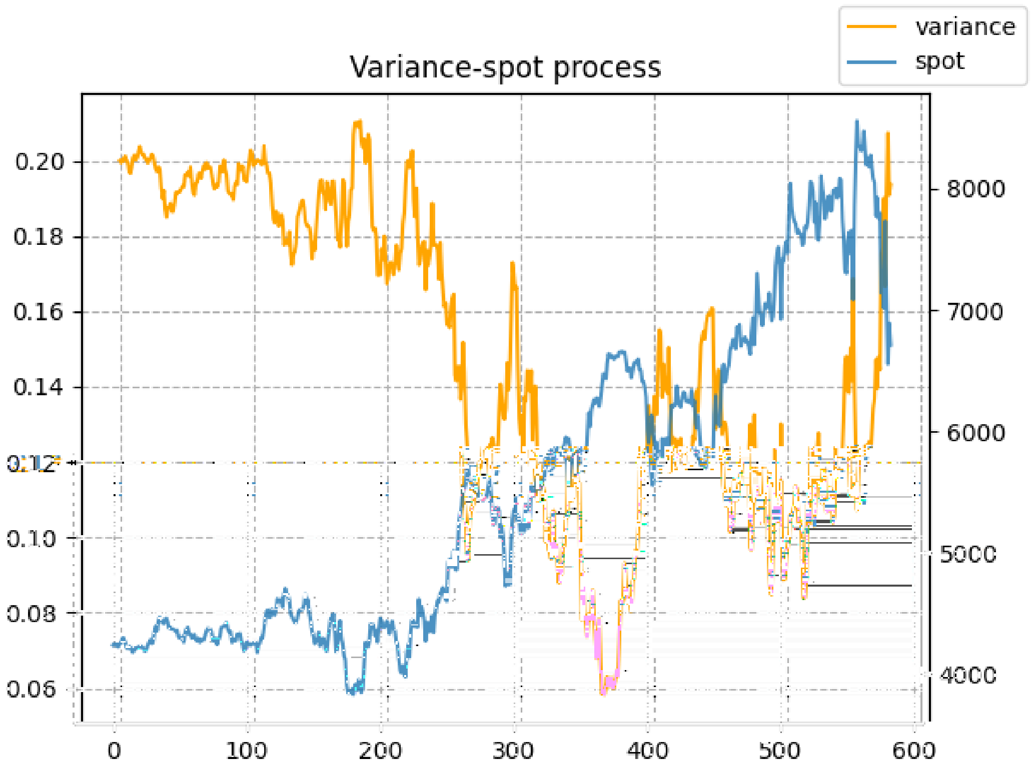


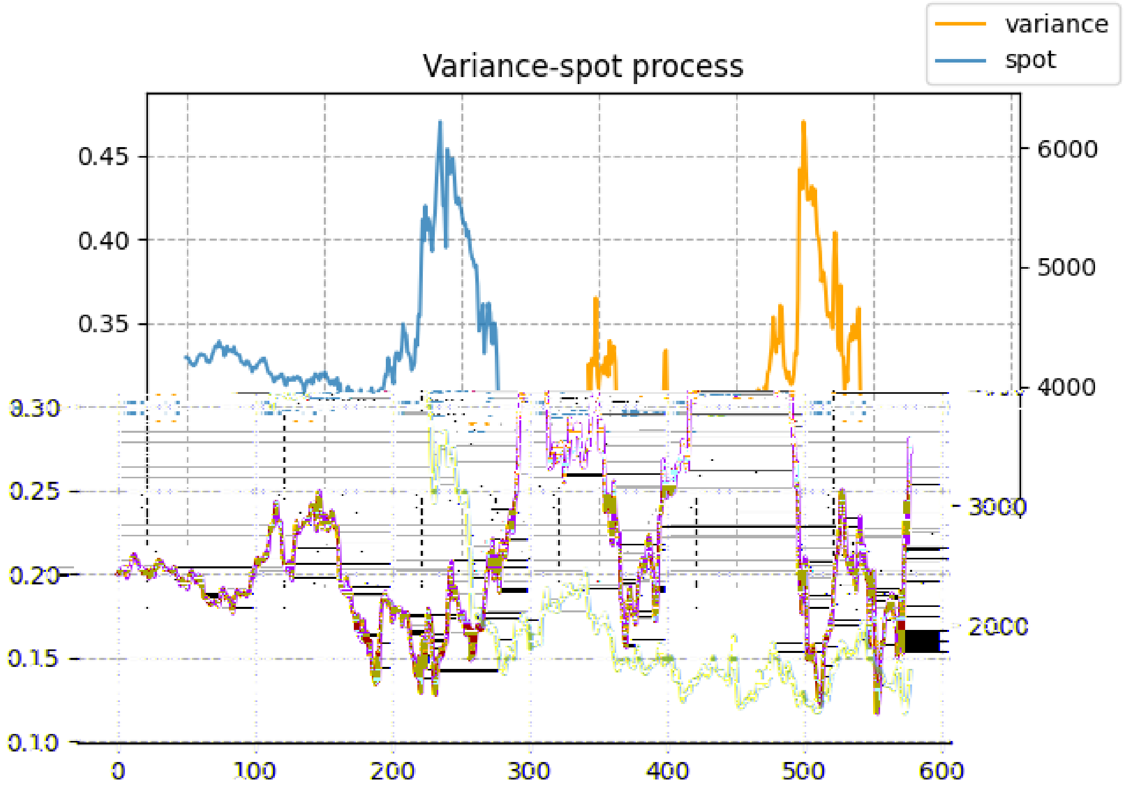
High mean reversion



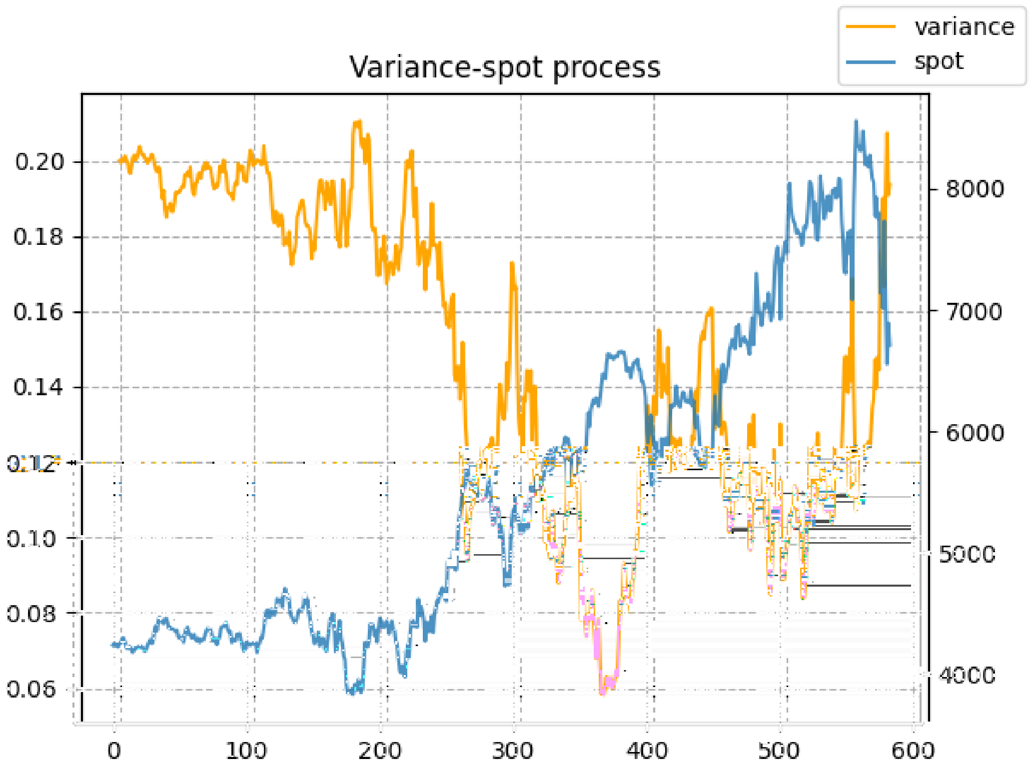
Low mean reversion

The Joint dynamics

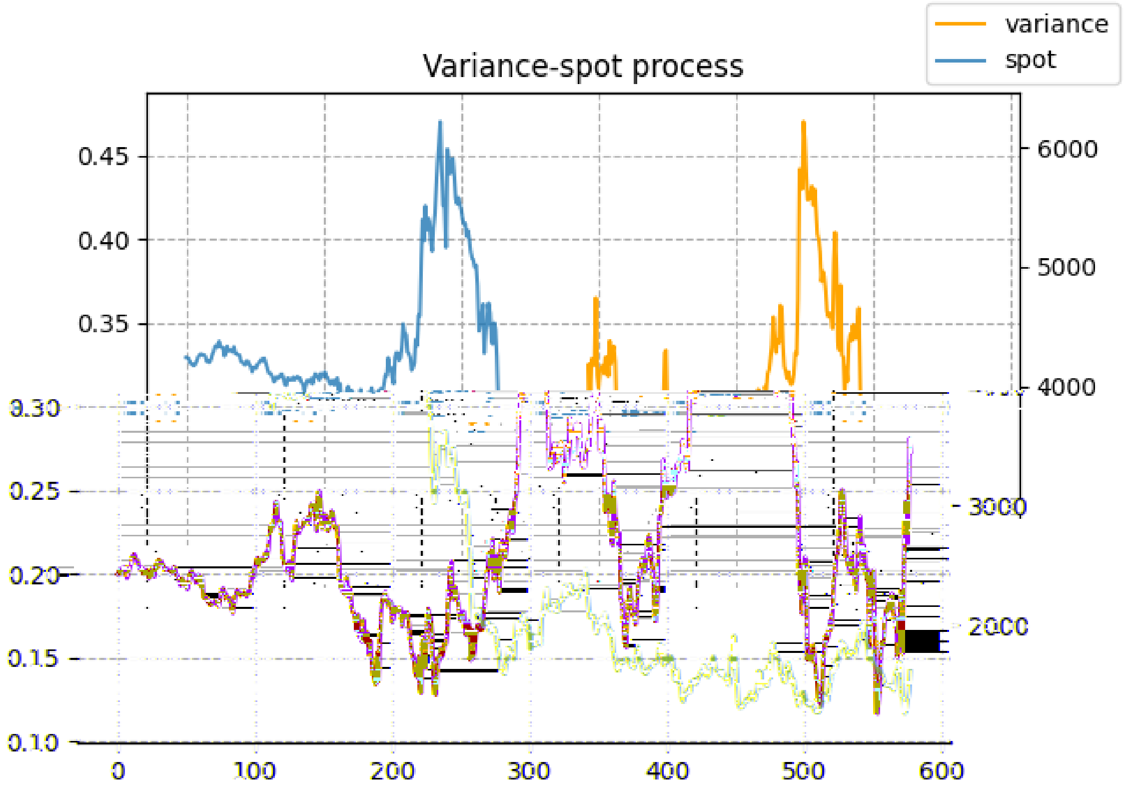




The Joint dynamics

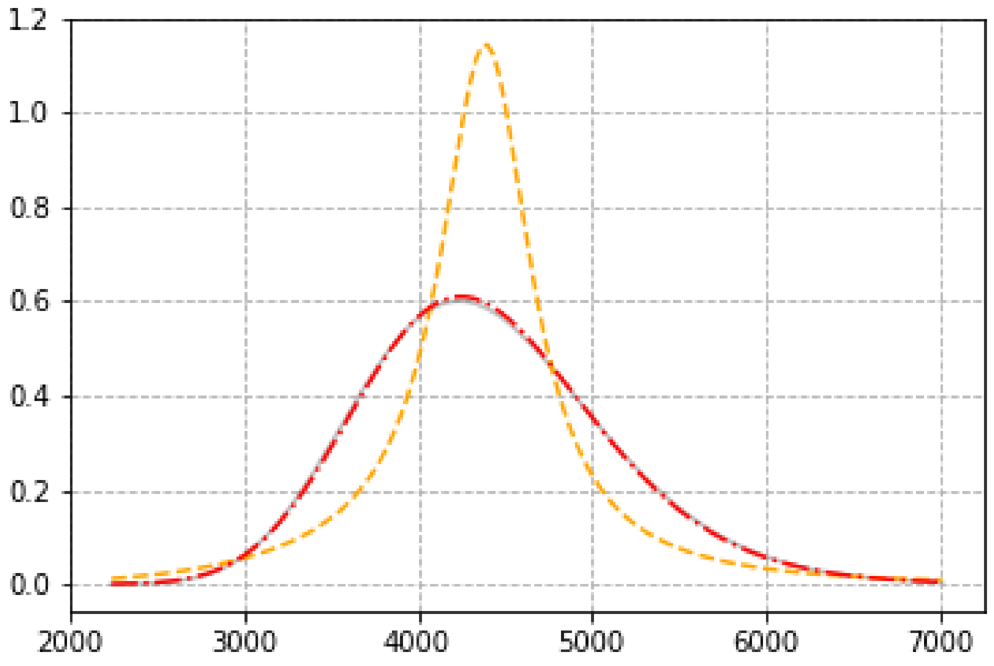


Variance-spot correlation

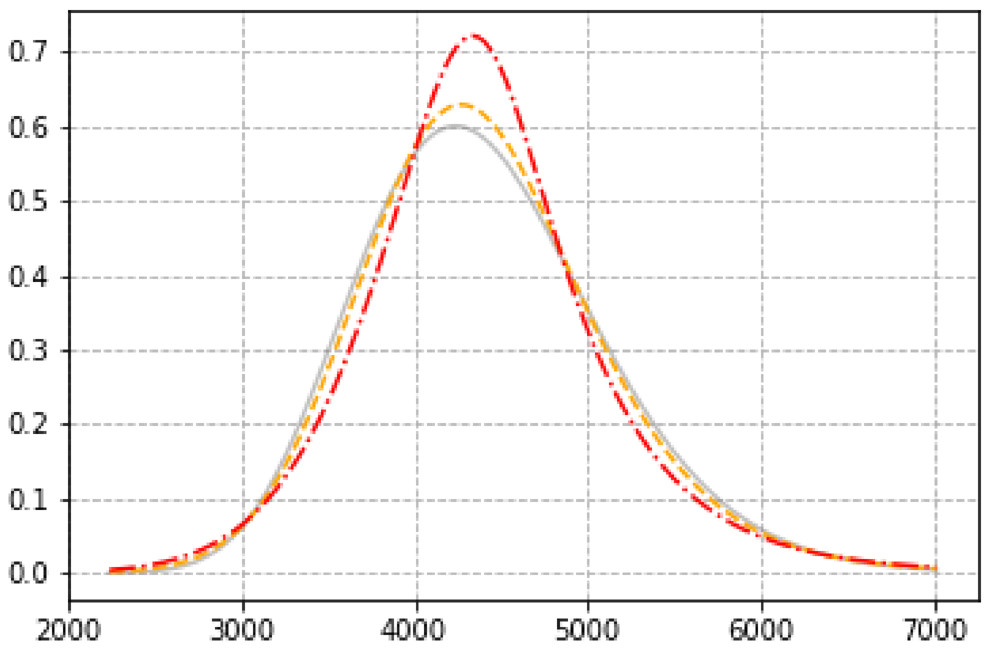


No variance-spot correlation

Heston stock distribution

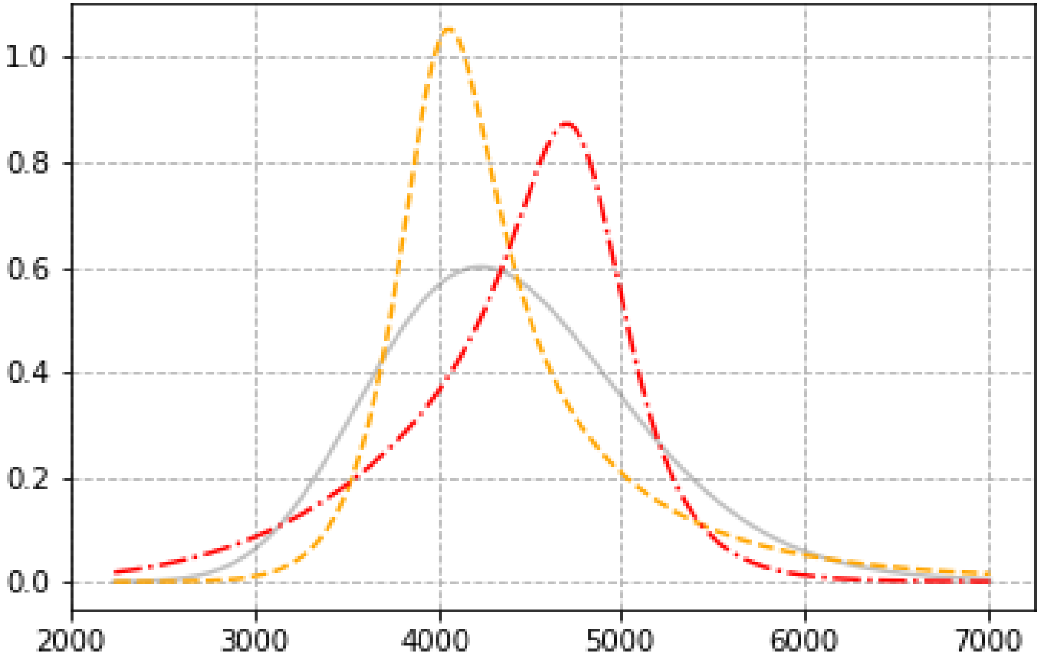


Vol of vol = 0.1
Vol of vol = 0.7

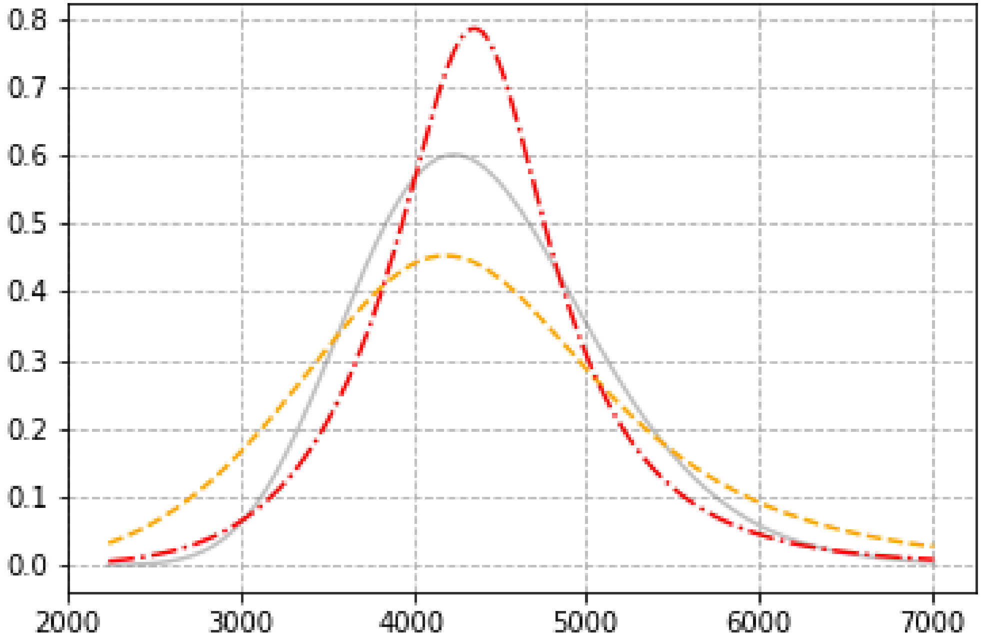


Mean reversion = 0.1
Mean reversion = 0.3

Heston stock distribution

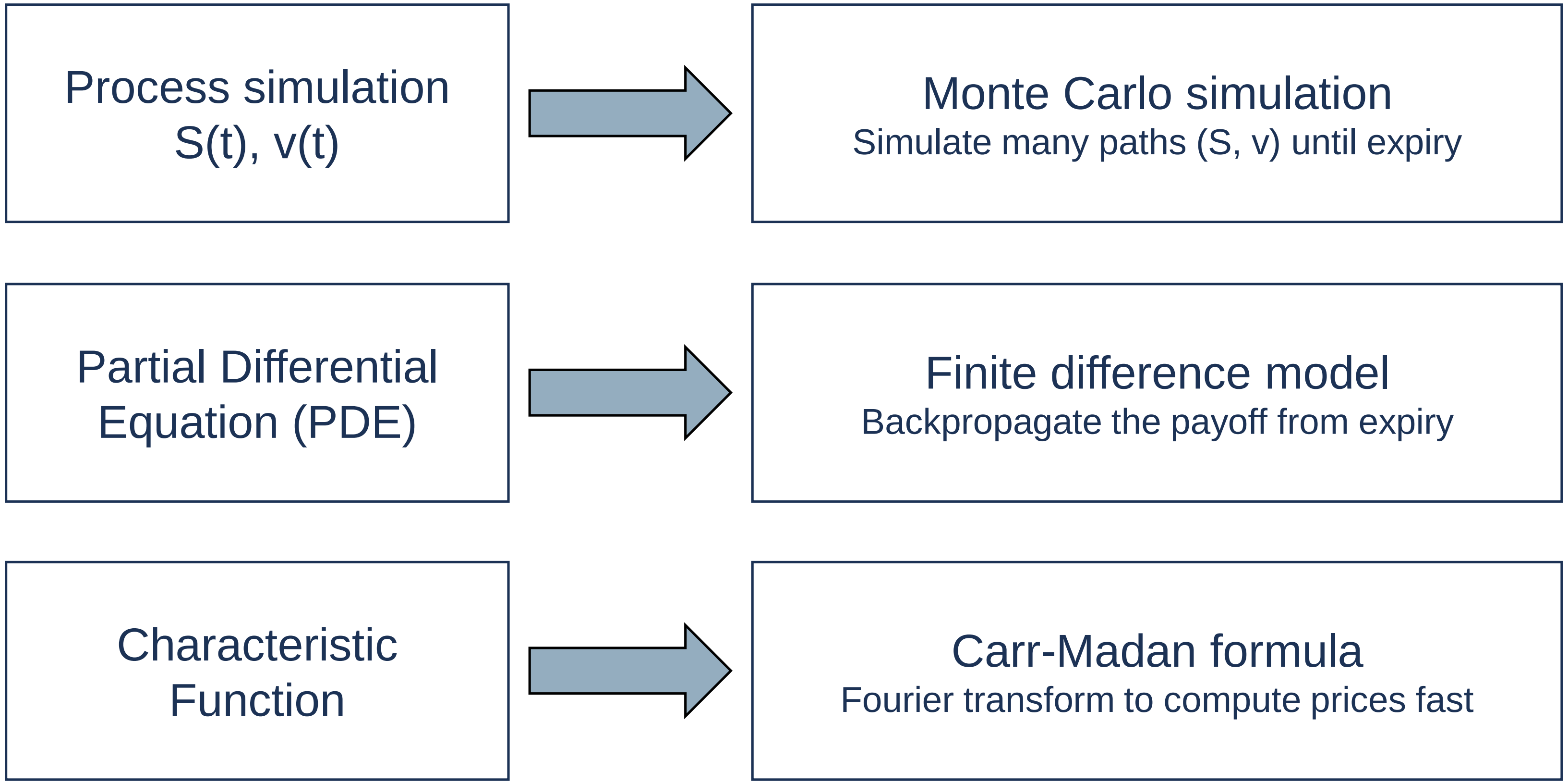


$\rho = -0.7$ Left skew
$\rho = 0.7$ Right skew



$v_0 = 0.04$
$v_0 = 0.1$

Heston model – How to deal with it?



Heston model

Black-Scholes model 2 parameters, 1d process:

$$dS = rS\,dt + \sigma S\,dW$$
$$S(t=0) = S_0$$

Heston model dynamics 6 parameters, 2d process:

$$dS = rS\,dt + \sqrt{v}S\,dW_S$$
$$dv = \kappa(\bar{v} - v)\,dt + \gamma\sqrt{v}\,dW_v$$
$$\mathrm{E}[dW_S dW_v] = \rho\,dt$$
$$S(t=0) = S_0$$
$$v(t=0) = v_0$$

Decorrelating correlated Brownian motions

$$dW_S = dW_1$$

Expectation and variance matches, so far so good

$$dW_v = a\,dW_1 + b\,dW_2$$

Expectation:

$$E[dW_v] = E[a\,dW_1 + b\,dW_2] = aE[dW_1] + bE[dW_2] = 0 + 0 = 0$$

Variance:

$$Var(dW_v) = Var(a\,dW_1 + b\,dW_2) = E\left[a^2 dW_1^2 + 2ab\,dW_1 dW_2 + b^2 dW_2^2\right] = a^2 dt + b^2 dt \Rightarrow a^2 + b^2 = 1$$

Covariance:

$$Cov(dW_S, dW_v) = Cov(dW_1, a\,dW_1 + b\,dW_2) = E\left[a\,dW_1^2 + b\,dW_1 dW_2\right] = a\,dt \Rightarrow a = \rho \Rightarrow b = \sqrt{1-\rho^2}$$

Decorrelating correlated Brownian motions

Matrix notation:

$$\begin{pmatrix} 1 & 0 \\ \rho & \sqrt{1-\rho^2} \end{pmatrix} \begin{pmatrix} dW_1 \\ dW_2 \end{pmatrix} = \begin{pmatrix} dW_S \\ dW_v \end{pmatrix}$$

Monte Carlo simulation discretizing:

$$\left| \begin{aligned} dS &= rS\,dt + \sqrt{v}S\,dW_1 \\ dv &= \kappa(\bar{v} - v)dt + \gamma\sqrt{v}(\rho\,dW_1 + \sqrt{1-\rho^2}\,dW_2) \end{aligned} \right.$$

Heston PDE derivation

Heston model SDE:

$$\begin{cases} dS = rS\,dt + \sqrt{v}S\,dW_1 \\ dv = \kappa(\bar{v} - v)dt + \gamma\sqrt{v}(\rho\,dW_1 + \sqrt{1-\rho^2}\,dW_2) \end{cases}$$

Option price should change over time (on expectation) same as value of money   martingale (no-arbitrage):

$$e^{-rt}V(t, S(t), v(t)) = e^{-rT}E[V(T, S(T), v(T))]$$

$$d(e^{-rt}V) = e^{-rt}dV - re^{-rt}Vdt$$
$$= e^{-rt}\left(\frac{\partial V}{\partial t}dt + \frac{\partial V}{\partial S}dS + \frac{1}{2}\frac{\partial^2 V}{\partial S^2}dS^2 + \frac{\partial V}{\partial v}dv + \frac{1}{2}\frac{\partial^2 V}{\partial v^2}dv^2 + \frac{\partial^2 V}{\partial S \partial v}dSdv\right) - re^{-rt}Vdt$$

Heston PDE derivation

$$\begin{cases} dS = rS\,dt + \sqrt{v}S\,dW_1 \\ dv = \kappa(\bar{v} - v)\,dt + \gamma\sqrt{v}(\rho\,dW_1 + \sqrt{1-\rho^2}\,dW_2) \end{cases}$$

$$d(e^{-rt}V) = e^{-rt}\left(\frac{\partial V}{\partial t}dt + \frac{\partial V}{\partial S}dS + \frac{1}{2}\frac{\partial^2 V}{\partial S^2}dS^2 + \frac{\partial V}{\partial v}dv + \frac{1}{2}\frac{\partial^2 V}{\partial v^2}dv^2 + \frac{\partial^2 V}{\partial S\partial v}dSdv\right) - re^{-rt}Vdt =$$

$$= e^{-rt}\left(\frac{\partial V}{\partial t}dt + \frac{\partial V}{\partial S}\left(rS\,dt + \sqrt{v}S\,dW_1\right) + \frac{1}{2}\frac{\partial^2 V}{\partial S^2}vS^2\,dt + \frac{\partial V}{\partial v}(\kappa(\bar{v} - v)\,dt + \gamma\sqrt{v}(\rho\,dW_1 + \sqrt{1-\rho^2}\,dW_2))\right.$$
$$\left. + \frac{1}{2}\frac{\partial^2 V}{\partial v^2}\gamma^2 v\,dt + \frac{\partial^2 V}{\partial S\partial v}\gamma v S\rho\,dt\right) - re^{-rt}V\,dt$$

On expectation this change should equal zero. $\mathrm{E}[dW] = 0$, so we only need to take care of dt terms:

$$\frac{\partial V}{\partial t} + \frac{\partial V}{\partial S}rS + \frac{1}{2}\frac{\partial^2 V}{\partial S^2}vS^2 + \frac{\partial V}{\partial v}\kappa(\bar{v} - v) + \frac{1}{2}\frac{\partial^2 V}{\partial v^2}\gamma^2 v + \frac{\partial^2 V}{\partial S\partial v}\gamma v S\rho - rV = 0$$

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Affine processes

Given a d dimensional process X

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

Characteristic function exponentially affine:

$$\phi(v, t, T) = E[e^{-\int_t^T r(s)ds + iu^T X(T)}] = e^{A(u,T-t) + B^T(u,T-t)X(T)}$$

Necessary condition:

$$\mu(t, X) = a^0 + a^1 X$$

$$[\sigma(t, X)\sigma^T(t, X)]_{ij} = c_{ij}^0 + \sum_k c_{ij}^1{}_k X_k$$

Drift and covariance matrix at most linear in all coefficients

Heston – affine process in log(S)

$X = \log(S)$

$$d\begin{pmatrix} X \\ v \end{pmatrix} = \begin{pmatrix} r - \frac{1}{2}v \\ \kappa\bar{v} - \kappa v \end{pmatrix} dt + \begin{pmatrix} \sqrt{v} & 0 \\ \rho\gamma\sqrt{v} & \gamma\sqrt{1-\rho^2}\sqrt{v} \end{pmatrix} d\begin{pmatrix} W_1 \\ W_2 \end{pmatrix}$$

$$\sigma\sigma^T = \begin{pmatrix} v & \rho\gamma v \\ \rho\gamma v & \gamma^2 v \end{pmatrix}$$

PDE in terms of X and $\tau = T - t$:

$$-\frac{\partial V}{\partial \tau} + \left(r - \frac{1}{2}v\right)\frac{\partial V}{\partial X} + \frac{1}{2}v\frac{\partial^2 V}{\partial X^2} + \kappa(\bar{v} - v)\frac{\partial V}{\partial v} + \frac{1}{2}\gamma^2 v\frac{\partial^2 V}{\partial v^2} + \gamma v\rho\frac{\partial^2 V}{\partial X \partial v} - rV = 0$$

Heston model characteristic function

Chf:

$$e^{-rt}\phi(u,t,T) = e^{-rT}E\left[e^{iuX(T)}\right]$$

Solution ansatz:

$$\phi(u,t,T) = e^{A(u,\tau)+B(u,\tau)X+C(u,\tau)v}$$

Initial (final) conditions:

$$\phi(u,T,T) = e^{iuX(T)} \Rightarrow A(u,0) = C(u,0) = 0, B(u,0) = iu$$

$$\frac{dB}{d\tau} = 0$$

$$\frac{dC}{d\tau} = \frac{1}{2}B(B-1) - (\kappa - \gamma\rho B)C + \frac{1}{2}\gamma^2 C^2$$

$$\frac{dA}{d\tau} = \kappa\bar{v}C + r(B-1)$$

Call option price and characteristic function

Call price:

$$C(K) = E[\max(S_T - K, 0)] = \int_0^{+\infty} \max(s - K)\, f(s) ds$$

We know the characteristic function in close form, but not the density. Using the Fourier Transform:

$$C(K) = F_\alpha^{-1}\big[F_\alpha[C]\big](k) = \frac{e^{-\alpha k}}{2\pi} \int_{-\infty}^{+\infty} e^{-ivk} \frac{\phi\big(v - i(\alpha + 1)\big)}{(\alpha + iv)(\alpha + iv + 1)} dv$$

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Thank you!

Do you have any questions?

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Lecture 7 "back to physics" ...

Ornstein - Uhlenbeck process

General SDE: $dx_t = \mu(x,t)\,dt + \sigma(x,t)\,dW$

Normalised Wiener process

O-U process is when

$$dx_t = -\theta(x - x_0)\,dt + \sigma\,dW$$

constants

we are familiar with

$$m\dot{v} = -\gamma v + \sqrt{2kT\gamma}\cdot\xi(t)$$

friction   thermal noise

Also overdamped:

$$\gamma\dot{x} = -k(x - x_0) + \sqrt{2kT\gamma}\,\xi(t)$$

spring force

All physical systems near equilibrium....
So standard form

$$dx_t = -\frac{k}{\gamma}(x - x_0)\,dt + \sqrt{\frac{2kT}{\gamma}}\,dW$$

Note: $X(t) = \int_0^t V(s)\,ds$

$$\langle x^2(t)\rangle = \int_0^t ds_1 \int_0^t ds_2 \,\langle V(s_1)V(s_2)\rangle$$

$$\frac{d}{dt}\langle x^2(t)\rangle = 2\int_0^t ds\,\langle V(t)V(s)\rangle$$

ensemple averaging at fixed t.

for free diffusion
$\langle x^2\rangle = 2Dt$

$$D = \int_0^t \langle V(t)\,V(s)\rangle\,ds = \int_0^t \langle V(\tilde{s})V(0)\rangle\,d\tilde{s}$$

depends on $t-s=\tilde{s}$

Also: go back to free-diffusion SDE
multiply it by $V_0 = \text{const}$, $\langle \ldots \rangle$

$$m\frac{d}{dt}\langle V(t)\cdot V_0\rangle = -\gamma\langle V(t)V_0\rangle \,,$$ hence

$\langle V_0 \xi\rangle = 0$

$$\langle V(t)V(0)\rangle = V_0^2\cdot e^{-\gamma/m\, t}$$

$\langle V_0^2\rangle$: ensemble average with $P(v)$

"Memory" of initial velocity V_0 decays with $\tau_v = m/\gamma$

Then...

$$D = \langle v_0^2 \rangle \int_0^t ds\, e^{-\frac{\gamma}{m}s} = \langle v_0^2 \rangle \frac{m}{\gamma}\left(1 - e^{-\frac{\gamma}{m}t}\right)$$

"Diffusion" is constant only at $t \gg m/\gamma$, then

$$D = \langle v_0^2 \rangle \frac{m}{\gamma} = \frac{k_B T}{\gamma}$$

But $\left\langle \frac{mv^2}{2} \right\rangle = \frac{1}{2} kT$

This is called Green-Kubo formula

$$D = \int_0^\infty \langle v(t) v(0) \rangle dt$$

Multiple variables in O-U proc.

$$dx_i = -\theta_{ik} x_k\, dt + \sigma_{ik}\, dW_k$$

(or equivalently $\frac{d}{dt} x_i = -\theta_{ik} x_k + \sigma_{ik} \xi_k$)

Don't need to be symmetric

Just like we did in 1D diffusion, solve this SDE set via Green's function:

$$X_i(t) = \int_0^t e^{-\theta_{ik}(t-s)} \sigma_{kl} \, \xi_l(s) \, ds$$

initial

$-\theta_{11}(t-s)$

[redacted]

Check by differentiation!

Consider a correlation function

$$M_{ik} = X_i(t) \, X_k(t) \quad \langle \xi_b(s_1) \, \xi_q(s_2) \rangle$$

$$M_{ik} = \int_0^t \int_0^t ds_1 \, ds_2 \, e^{-\theta_{ia}(t-s_1)} \sigma_{ab} \, e^{-\theta_{kp}(t-s_2)} \sigma_{pq}$$

So we have

$$M_{ik} = \int_0^t ds\, e^{-\theta_i (t-s)} \sigma_{ip} \sigma^T_{bp}\, e^{-\theta^T_{pk}(t-s)}$$

(Recall $\int_0^t ds \langle v_0^2 \rangle e^{-\frac{\gamma}{m} t}$)

Call $t - s \to \tilde{s}$

$$M_{ik} = \int_0^t d\tilde{s}\, e^{-\underline{\underline{\theta}} \tilde{s}} \sigma \sigma^T e^{-\underline{\underline{\theta}}^T \tilde{s}}$$

take this to ∞

for 1D case: $M = \langle x^2 \rangle = \int_0^\infty dt\, e^{-2\theta t} \cdot \sigma^2 = \frac{\sigma^2}{2\theta}$

⊙ $m\dot{v} = -\gamma v + A(t)$ $\quad \sqrt{2kT\gamma}\, \xi(t)$

↓

$$\langle v_\infty^2 \rangle = \frac{2kT\gamma}{m^2 \cdot 2\gamma/m} = \frac{kT}{m}$$ ✓

⊙ $\gamma \dot{x} = -\varkappa x + \sqrt{2kT\gamma}\, \xi(t)$

↓

$$\langle x^2 \rangle = \frac{2kT\gamma}{\gamma^2 \cdot 2\varkappa/\gamma} = \frac{kT}{\varkappa}$$ ✓

in potential well

Let us construct

$$\underline{\underline{\Theta}} \cdot \underline{\underline{M}} + \underline{\underline{M}} \cdot \underline{\underline{\Theta}}^T$$

$$= \int_0^\infty \left(\underline{\underline{\Theta}} \cdot e^{-\underline{\underline{\Theta}} t} \cdot \underline{\underline{\sigma}}\,\underline{\underline{\sigma}}^T \cdot e^{-\underline{\underline{\Theta}}^T t} + e^{-\underline{\underline{\Theta}} t} \underline{\underline{\sigma}}\,\underline{\underline{\sigma}}^T e^{-\underline{\underline{\Theta}}^T t} \underline{\underline{\Theta}}^T \right) dt$$

this is the full $\frac{d}{dt}\left(e^{-\Theta t} \sigma\sigma^T e^{-\Theta^T t}\right)$

$$= -\int_0^\infty dt \frac{d}{dt}\left(e^{-\underline{\underline{\Theta}} t} \underline{\underline{\sigma}}\,\underline{\underline{\sigma}}^T e^{-\underline{\underline{\Theta}}^T t} \right) = \underline{\underline{\sigma}}\,\underline{\underline{\sigma}}^T$$

only at lower limit

General (multi-variable) form of Fluctuation-Dissipation relation

$$\Theta_{ik} \langle X_k X_l \rangle_{eq.} + \langle X_i X_k \rangle_{eq.} \Theta_{lk} = \sigma_{ik} \sigma_{lk}$$

il

Lecture 8 ... still on O-U process

$$dX = -\theta x\, dt + \sigma\, dW$$

It is hard to solve (or even comprehend) an SDE...

Instead, it would be better if we had $P(x,t)$

then normal calculus rules

How to systematically derive $P(x,t)$ from the SDE.

Start with Evolution Eq.

$$P(x, t+dt) = \int G_{x,t+dt\; y,t}\, P(y,t)\, dy$$

Normally we think of a propagator $G(x,y)$ with fixed initial y, variable x.

Here, variable is y...

To address this, take $\Delta x = x - y$,

so $y = x - \Delta x$

$$P(x, t+\Delta t) = \int G(\overbrace{x - \Delta x}^{x} + \Delta x, t+\Delta t \mid x - \Delta x, t)\, P(x-\Delta x, t)\, d(-\Delta x)$$

uniform shift:

⊙ G "steps" from $(x-\Delta x)$ into $(x-\Delta x) + \Delta x$: step Δx

⊙ We have a uniform function of $(x - \Delta x)$

Taylor expand it:

$$P(x, t+\Delta t) = \int \sum_{n=0}^{\infty} \frac{(-\Delta x)^n}{n!} \frac{\partial^n}{\partial x^n} G(x+\Delta x \mid x)\, P(x)\, d(\Delta x)$$

whole range!

Define moments:

$\langle \Delta x^0 \rangle = 1$: G normalised for O–U

$\langle \Delta x^1 \rangle = \int \Delta x\, G(x+\Delta x \mid x)\, d\Delta x \rightarrow -\theta x \cdot dt$

$\langle \Delta x^2 \rangle = \int \Delta x^2\, G(x+\Delta x \mid x)\, d\Delta x \rightarrow \sigma^2 dt$

. . . . .

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

terms ~ dt

(no more)

Now substitute moments:

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\theta x \cdot P(x,t)\right) + \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}P(x,t)$$

for O-U process. (limit $dt \to 0$)

No more terms $\sim dt$ in r.h.s.

θx → external force

$\frac{\sigma^2}{2}$ → diffusion constant

$D = \frac{1}{2}\sigma^2$

...'s was an example of using "Kramers–Moyal expansion"

Evolution → Expand kernel in powers of "step"

identify moments in the PDE for $P(x,t)$

Kramers-Moyal Expansion (general)

Evolution

$$P(x, t+\Delta t) = \int G(x, t+\Delta t \,|\, y, t)\, P(y, t)\, dy$$

or it could be Kolmogorov-Chapman if we care about the initial condition:

$$P(x, t+\Delta t \,|\, x_0, t_0) = G(x, t+\Delta t \,|\, y, t)\, P(y, t \,|\, x_0, t_0)\, dy$$

Again: $\Delta x = x - y$, so $y = x - \Delta x$

ep

shifted argument

Then we have:

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

for $\forall$ SDE, not necessarily Wiener, or ....

$$\frac{\partial P}{\partial t} = \hat{L}_{KM} P(x,t)$$

← K.-M. operator

$D^{(n)}(x)$ carry all information about the nature of stochastic proc.

(for Wiener process, there are only two non-zero K-M coeffs)

Practice:

①

$$\dot{v} = -\frac{\gamma}{m} v + \frac{\sqrt{2kT\gamma}}{m} \xi(t)$$

$$dv = -\frac{\gamma}{m} v\, dt + \frac{\sqrt{2kT\gamma}}{m} dw$$

standard O-U format

$$\langle dv \rangle = -\frac{\gamma}{m} v\, dt$$

$$\langle dv^2 \rangle = \frac{2kT\gamma}{m^2} \langle dw^2 \rangle \quad (\langle dw^2 \rangle = dt)$$

then:

$$\frac{\partial P(v,t)}{\partial t} = \frac{\gamma}{m} \frac{\partial}{\partial v} (v \cdot P) + \frac{kT\gamma}{m^2} \frac{\partial^2 P}{\partial v^2}$$

This equation describes relaxation of P(v,t) towards the equilibrium Maxwell distribution test the steady state (eq.):

$$0 = \frac{\partial}{\partial v}\left[\frac{\gamma}{m} v \cdot P + \frac{kT\gamma}{m^2} \frac{\partial P}{\partial v} \right]$$

$$\frac{\partial P}{\partial v} = \frac{m^2}{kT\gamma}\left(-\frac{\gamma}{m} v \cdot P \right)$$

$$\frac{dP}{P} = -\frac{m}{kT} v \, dv$$

rmostat equili. $P_e = \text{norm}\, e^{-\frac{mv}{2kT}}$

2 Relaxation to a fixed equilibrium (in a harmonic potential V(x))

over damped limit

will test later

$$\gamma \dot{x} = \theta (x - x_0) + 2kT\gamma \cdot \xi(t)$$

$$dx = -\frac{\theta}{\gamma}(x - x_0) + \frac{2kT}{\gamma} dW$$

standard O-U format

$$\frac{\partial P(x,t)}{t} = \frac{\partial}{\partial x} \frac{\theta}{\gamma}(x - x_0) P + \frac{2kT}{\square} \frac{\partial^2 P}{\partial x^2}$$

Smoluchowski equation:

(diffusion with external force)

test: steady state: $\frac{dP}{dx} = -\frac{\theta}{kT}(x - x_0) P$: $P = P_0 e^{-\frac{\frac{\theta}{2}(x-x_0)^2}{kT}}$

i.e. Boltzmann distr.

③ GBM $dS = \mu S\,dt + \sigma S\,dW$

$\langle dS \rangle = \mu S\,dt$

$\langle dS^2 \rangle = \sigma^2 S^2 \langle dW^2 \rangle = dt$

$$\frac{\partial P(S,t)}{\partial t} = -\frac{\partial}{\partial S}\left(\mu S\,P(S,t)\right) + \frac{\sigma^2}{2}\frac{\partial^2}{\partial S^2}\left(S^2 P\right)$$

4 Multi-variable process.

(see the last lecture for 'matrix notation')

rownian motion with force

$v(t)$, $x(t)$

$m\dot{v} = -\gamma v - \theta(x - x_0) + 2kT\gamma\,\xi(t)$

$\dot{x} = v$

linear drift terms.

O-U rocess

Matrices: $\underline{\underline{\theta}} = \begin{pmatrix} \frac{\gamma}{m} & \frac{\theta}{m} \\ -1 & 0 \end{pmatrix}$; $\underline{\underline{\sigma}} = \begin{pmatrix} \frac{\sqrt{2kT\gamma}}{m} & 0 \\ 0 & 0 \end{pmatrix}$

et us work out the PDE

$P(v, x, t)$ ...

1st K-M coefficient 2nd K-M coefficient

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta_{ik} x_k \cdot P\right) + \frac{1}{2}\left(\sigma\sigma^T\right)_{ik} \frac{\partial^2 P}{\partial x_i \partial x_k}$$

$$= \frac{\partial}{\partial v} \frac{\gamma}{m} v \cdot P + \frac{\partial}{\partial v} \frac{\theta}{m}(x - x_0) P - \frac{\partial}{\partial x} v P) + \frac{kT\gamma}{m^2} \frac{\partial^2 P}{\partial v^2}$$

full force

$$\frac{\partial P(v,x,t)}{\partial t} + \frac{\partial}{\partial x}(v \cdot P) = \frac{\partial}{\partial v} \frac{\gamma v + \theta(x-x_0)}{m} \cdot P$$

convective derivative

$$+ \frac{kT\gamma}{m^2} \frac{\partial^2 P}{\partial v^2}$$

eneral Fokker-Planck equation

Brownian motion in pot.

Lecture 9

In the last lecture ...

Chain rule :

$$\frac{d f(x,t)}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{\partial x}{\partial t}$$

$$\Rightarrow \dot{f} + (\underline{v} \cdot \underline{\nabla}) f$$

convective derivative

(or is it $\underline{\nabla}(\underline{v} f)$?)

In K-M expansion :

$$\frac{\partial^n}{\partial x^n} \int (\Delta x)^n \, G(x+\Delta x / x) \, P(x,t) \, d\Delta x$$

$$\Rightarrow \frac{\partial^n}{\partial x^n} \left(D^{(n)}(x) \, P(x,t) \right)$$

(definitely under $\frac{\partial}{\partial x}$)

We have seen the Smoluchowski equation in harmonic potential (for O-U process)

What if the force $f(x)$ is arbitrary: $f = -\frac{\partial V(x)}{\partial x}$

SDE

(overdamped limit) $\gamma \dot{x} = f(x) + \sqrt{2kT\gamma}\, \xi(t)$

will derive soon...

via K.-M. expansion:

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(\frac{f(x)}{\gamma} P(x,t)\right) + \frac{1}{2}\frac{2kT\gamma}{\gamma^2} P'' \quad (*)$$

$$= -\frac{\partial}{\partial x}\left(\frac{f(x)}{\gamma} P\right) + \frac{kT}{\gamma}\frac{\partial^2 P}{\partial x^2}$$

diffusion in ∀ force.

$D = \frac{kT}{\gamma} = \frac{1}{2}\sigma^2$

Write it in an alternative equivalent form:

$$\frac{\partial P}{\partial t} = -\nabla J(x,t)$$

where the "flux" or "current of probability"

in multi-dimensions: $\operatorname{div} J$

$$J = -D\frac{\partial P}{\partial x} + \frac{f(x)}{\gamma} P(x,t)$$

"Fick's Law"

Another equivalent form: $D = \frac{kT}{\gamma}$

$$J(x,t) = -D\, e^{-\beta V(x)} \frac{\partial}{\partial x}\left[e^{\beta V(x)} P(x,t) \right]$$

In all cases, we see a general "flux" $\underline{J} = \rho \underline{v}$, and

Continuity equation: $\dot{P} = -\operatorname{div} \underline{J}$

for conserved field $\int P\, dx = 1$

What if we have an x-dependent noise: $\sigma(x)$?

$$dx = \mu(x,t)\, dt + \sigma(x,t)\, dW$$

Then we "probably" would still have following Itoh's maths!

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\Big(\mu(x,t) P \Big) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\Big(\sigma^2(x,t) P \Big)$$

from K.M. expansion.

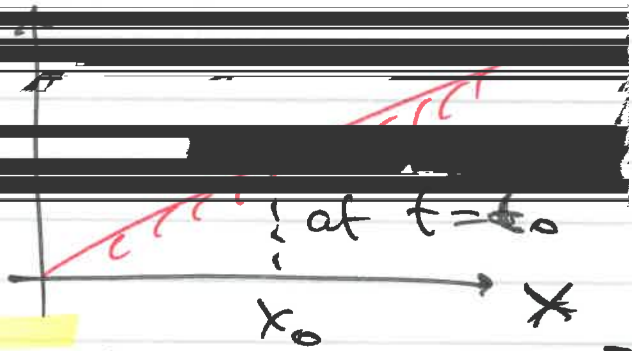
[redacted]

To finish the O-U section:

two examples:

1) Diffusion in constant force

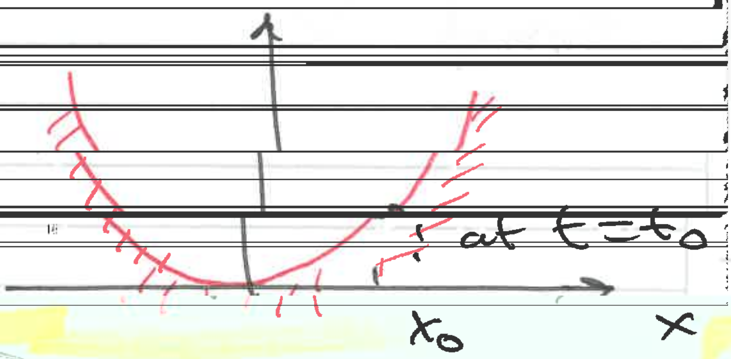
[redacted]



$\Downarrow$

$$P(x,t) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left[-\frac{\left(x-x_0+\frac{f}{\gamma}(t-t_0)\right)^2}{4D(t-t_0)}\right]$$

[redacted]



$$P(x,t) = \frac{1}{\sqrt{2\pi kT\, S(t)/\alpha}} \exp\left[-\frac{\alpha}{2}\frac{\left(x-x_0 e^{-\frac{\alpha}{\gamma}(t-t_0)}\right)^2}{kT\, S(t)}\right]$$

with [redacted]

Convection Diffusion

[redacted]

e is a background flow with velocity u), diffusion on top of ...

Recall $\partial P(x,t)$ (∂ [redacted]) + [ ]

Now, when $u(x)$ is present: extra flux $u \cdot P$

$$\frac{\partial P}{\partial t} = D \underline{\nabla}\left(e^{-\beta V} \underline{\nabla}\left[e^{\beta V} \cdot P\right]\right) - \underline{\nabla}(\underline{u} \cdot P)$$

Or re-write:

$$\frac{\partial P}{\partial t} + \underline{\nabla}(\underline{u}(x) \cdot P) = \text{"old r.h.s."}$$

$$= -\frac{\partial}{\partial x}\left(\frac{f(x)}{\gamma} P\right) + D \frac{\partial^2 P}{\partial x^2}$$

r.h.s. of Smoluchowski

if div $\underline{u} = 0$

convective derivative

$$\frac{\partial P}{\partial t} + (\underline{u} \cdot \underline{\nabla}) P = \ldots\ldots$$

Many implications, since $u(x)$ adds to the potential $V(x)$

$$\frac{\partial P}{\partial t} = -\nabla\left(\left(f(x) + u(x)\right)P\right) + D\frac{\partial^2 P}{\partial x^2}$$

New structure emerging.

What if $u = \text{const}$:

$$\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x} = D\frac{\partial^2 P}{\partial x^2}$$

Similar to diffusion under constant force.

so if $t=0$ $P = \delta(x)$

easy!

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

But if $x=0$ $P=P_0$ (Boundary Condition)

after a long time

$$P(x,t) = \tfrac{1}{2}P_0\left[\mathrm{Erfc}\left(\frac{x-ut}{\sqrt{4Dt}}\right) + e^{\frac{u\cdot x}{D}}\,\mathrm{Erfc}\left(\frac{x-ut}{\sqrt{4Dt}}\right)\right]$$

"Dispersivity" parameter

Lecture 10 Mean First Passage Time (MFPT).

Examples Class #1 at 2pm today — Here.

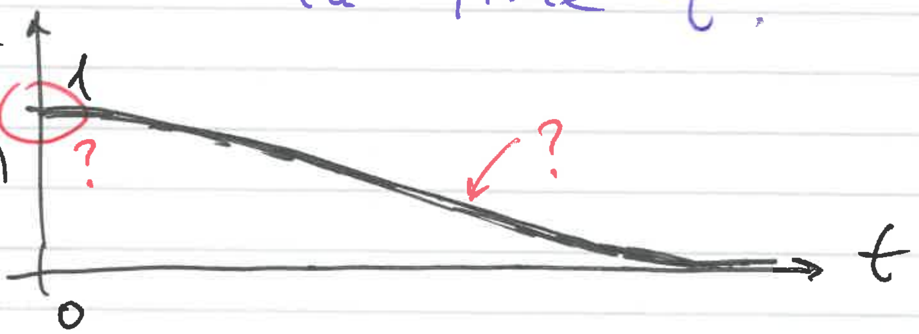
- What is the probability of escape in time t ?
- Mean time of escape?

(For ∀ stochastic process)

Approach #1 : via Survival probability

$S(t)$ that it did not escape in time t.

Expect $S(t)$



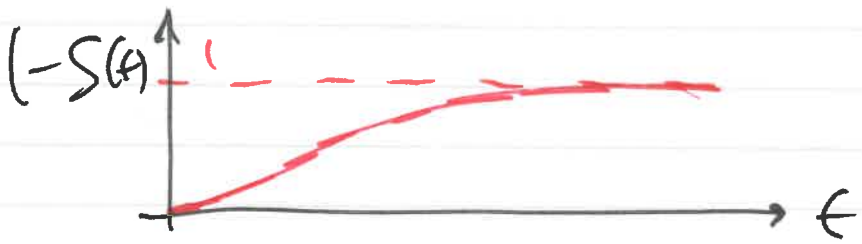
If we knew the full process probability $P(x,t)$, then

$$S(t) = \int_{\text{all values } x} P(x,t)\,dx$$

Non-equilibrium process.

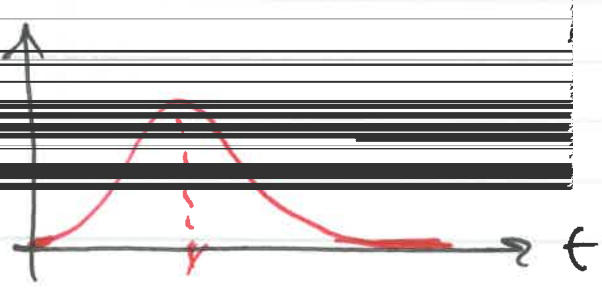
$\int P(x,t)\,dx = 1$ if normalised

Then $1-S(t)$ is the probability to have escaped in time t.



Consider a small step Δt:

$S(t) - S(t+\Delta t)$: number [redacted]



then $\langle t \rangle = \int_0^\infty t \, f(t) \, dt$

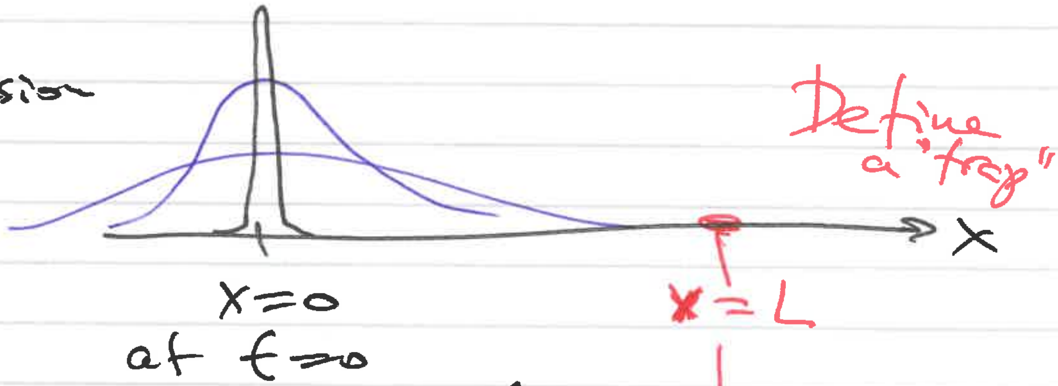
average time to escape

(by parts...)

$$\langle t \rangle = \int S(t) \, dt$$

Let's test a simple example

1D diffusion



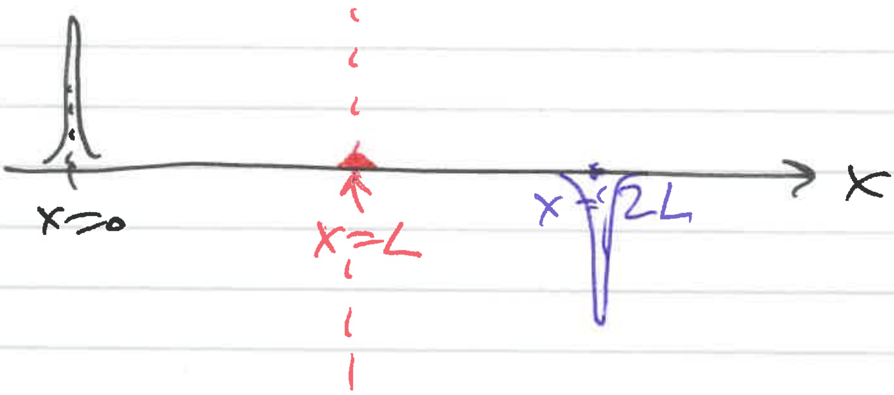
$$P(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}$$

Absorbing Boundary Condition

$P(L,t) = 0$

We must find the correct $P(x,t)$ satisfying this B.C.

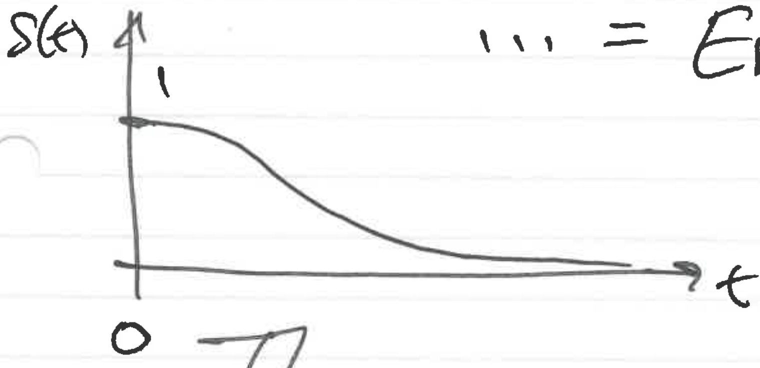
Here we can use Method of Images!



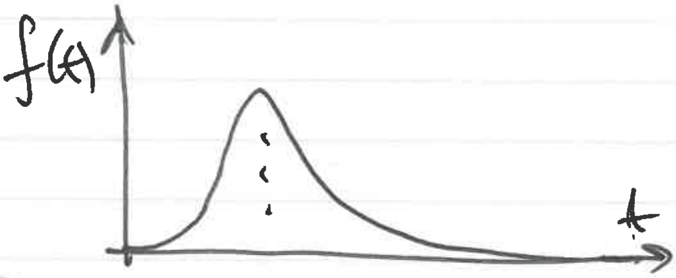
Find $P(x,t) = \frac{1}{\sqrt{4\pi D t}}\left(e^{-\frac{x^2}{4Dt}} - e^{-\frac{(x-2L)^2}{4Dt}}\right)$

Then $S(t) = \int_{-\infty}^{L} P(x,t)\,dx$ All available space!

$\ldots = \mathrm{Erf}\left[L/\sqrt{4Dt}\right]$



Then we find $f(t) = -\frac{\partial S}{\partial t}$



$f(t) = \frac{L}{\sqrt{4\pi D t^3}} e^{-\frac{L^2}{4Dt}}$

$$MFPT = \langle t \rangle = \int_0^\infty t \frac{L}{\sqrt{4\pi D t^3}} e^{-\frac{L}{4Dt}}\,dt$$

$$\sim \int^\infty \frac{1}{\sqrt{t}}\,dt \rightarrow \infty \quad ✓$$

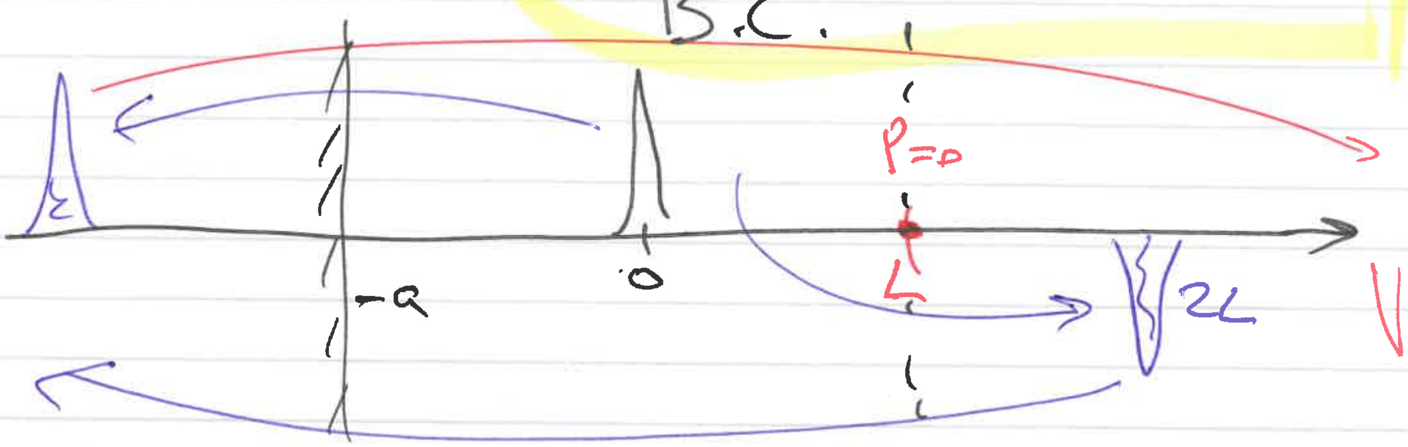
This is not a well-posed problem

(∞ time of travel to $x \rightarrow -\infty$ and back)

Make it well-posed:

i.e. $\frac{\partial p}{\partial x} = 0$

How to find $P(x,t)$ that satisfies both B.C.



⊙ Build an ∞ series of ± images reflecting $e^{-\frac{x^2}{4Dt}}$

OR...

⊙ Just solve the diffusion equation $\dot{p} = Dp''$ with these two B.C.

→ ∞ series of $\sum_n \sin\left(\frac{n\pi x}{L+a}\right) e^{-?Dt}$

....

Once $P(x,t)$ is found

$\rightarrow \quad S(t) = \int_{-a}^{L} P(x,t)\,dx$ All available space

$\downarrow$

$$\text{MFPT} = \frac{L(L+2a)}{2D}$$ for start at $x=0$

if $a=0$ | $\text{MFPT} = L^2/2D$ } Diffusion time (mean) over L

But if the initial condition is an arbitrary $x = x_0$ (at $t=0$), then MFPT is a function of x_0 (E.g. if $x_0 = L$ MFPT $= 0$)

• Now a different approach to MFPT, for Wiener process.

#2: Via Adjoint Fokker-Planck operator

We saw the Smoluchowski equation (a case of Fokker-Planck equation set)

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(\frac{f(x)}{\gamma} p\right) + D\frac{\partial^2 p}{\partial x^2}$$

$$\left(\text{or } -\frac{\partial}{\partial x}\left(\mu(x,t)\, p\right) + \frac{\sigma^2}{2}\frac{\partial^2 p}{\partial x^2} \right)$$

Define a Fokker-Planck operator acting on X.

$$\frac{\partial p}{\partial t} = -\hat{L}_{FP}\, P(x,t)$$

We saw the alternative form of it:

$$\hat{L}_x = D\frac{\partial}{\partial x}\left(e^{-\beta V(x)}\frac{\partial}{\partial x}\left[e^{\beta V(x)} p(x,t)\right]\right)$$

this operator acts on X!

$$P(x,t) = e^{-\hat{L}_x t}\, p(x,0)$$

If we want MFPT:

$$MFPT = \int_0^\infty S(t)\, dt$$

$$= \int_0^\infty dt \int_{\text{vol.}} dx\, P(x,t \mid x_0, 0)$$

initial condition

$$\equiv \tau(x_0)$$

Could we find an equation that would return $\tau(x_0)$?

To find that, we need operators that act on the initial condition

(that's not what we are used to)

Need Kolmogorov - Chapman

$$P(x,t \mid x_0, 0) = \int G(x,t \mid y, t')\, P(y,t' \mid x_0, 0)\, dy$$

Here

Since $\frac{\partial P}{\partial t} = -$ [redacted]

Kolmogorov–Chapman

Let me differentiate w.r.t. t'

$$\frac{\partial}{\partial t'} P(x,t|x_0,0) \equiv 0$$

$$0 = \int \left[G(x,t|y,t') \frac{\partial P(y,t'|x_0,0)}{\partial t'} + P(y,t'|x_0,0) \frac{\partial G(x,t|y,t')}{\partial t'} \right] dy$$

$$= \int G(x,t|y,t') \cdot \left[- \hat{L}_y P(y,t'|x_0,0) \right]$$

Continue next ....

deal with this...

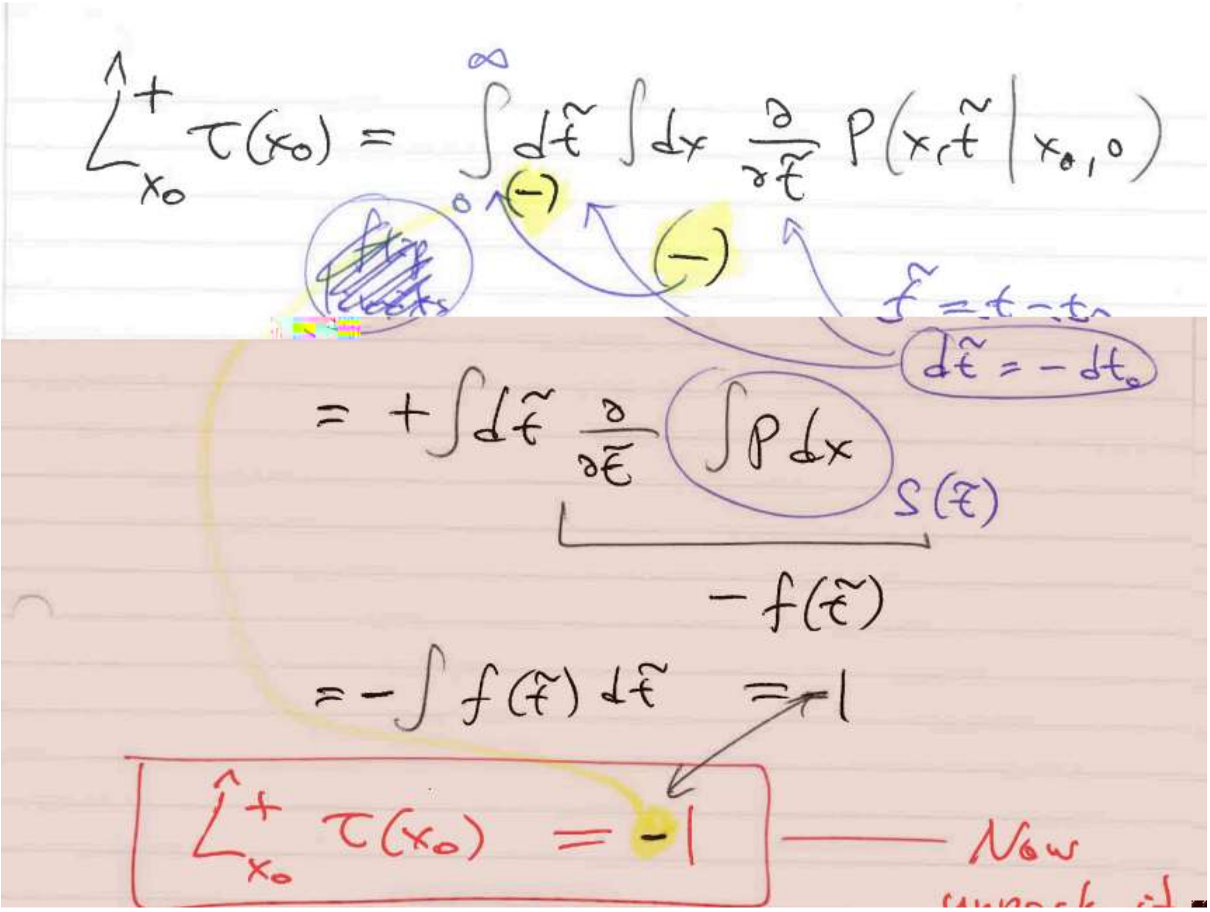
Adjoint Fokker-Planck Derivation of MFPT

Patrick Collins <pac74@cam.ac.uk>
Tue 4/2/2024 5:16 PM
To:Eugene Terentjev <emt1000@cam.ac.uk>
Cc:Vivian Perez <oap22@cam.ac.uk>

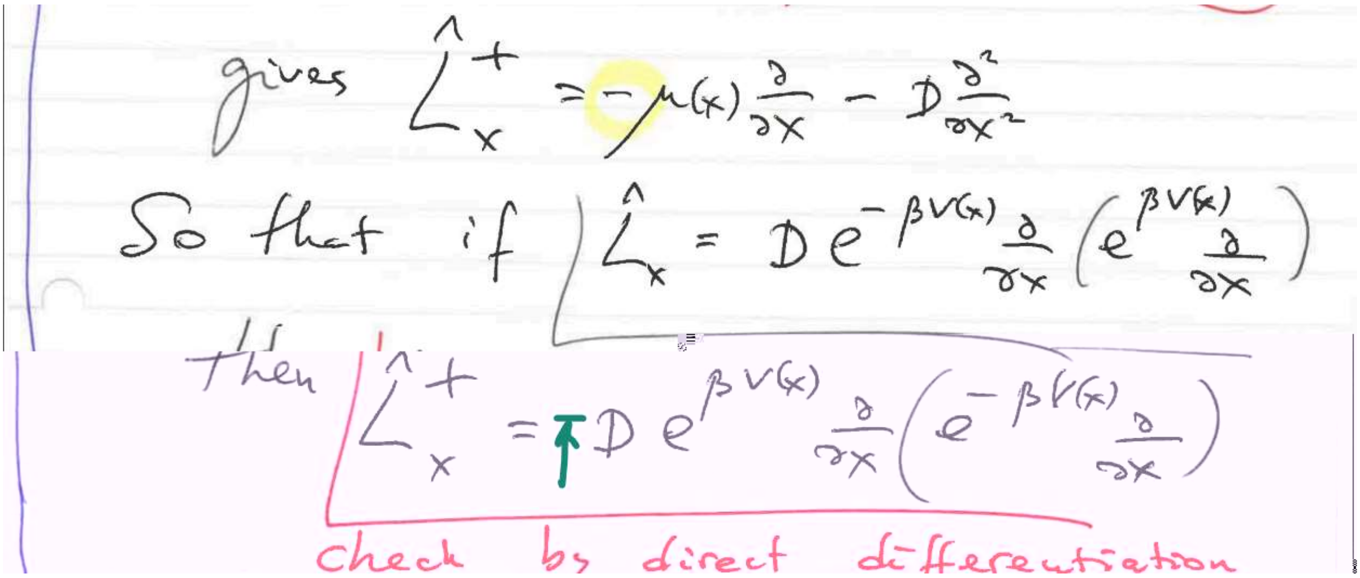
1 attachments (2 MB)
Adjoint FP MFPT derivation.docx;

Dear Professor Terentjev,

My colleague and I have been looking over the derivation for the MFPT from the adjoint Fokker-Planck operator. We weren't sure on the origin of the - sign here in your notes:



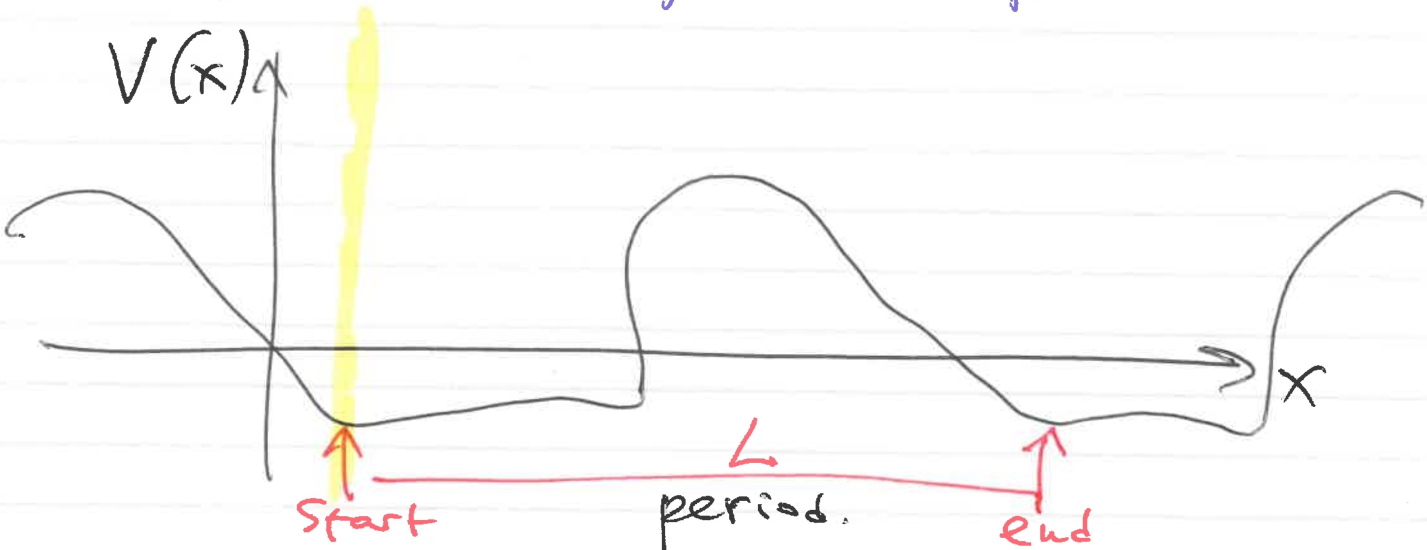
We have worked through this and believe it should be +1. Furthermore, the definition of the adjoint Fokker-Planck operator earlier in the notes seems to miss a - sign, which corrects for the - previously.



We believe that combining these two corrections leads to the correct result. We have attached the workings in a word document to these email, please let us know if you would like us to rewrite them in a neater format. Do you think our approach to this is correct?

Lecture 12 – finishing MFPT ...

⊙ Diffusion in periodic potential



MFPT from "start" to "end"

$$\tau = \frac{1}{D}\int_0^L dx\, e^{\beta V(x)} \int_0^x e^{-\beta V(y)}\, dy$$

(lower limit of the first integral: 0 = start; lower limit of the second integral: 0 = left boundary)

Define "effective diffusion" in time τ:

$$L^2 = 2 D_{eff} \cdot \tau,$$

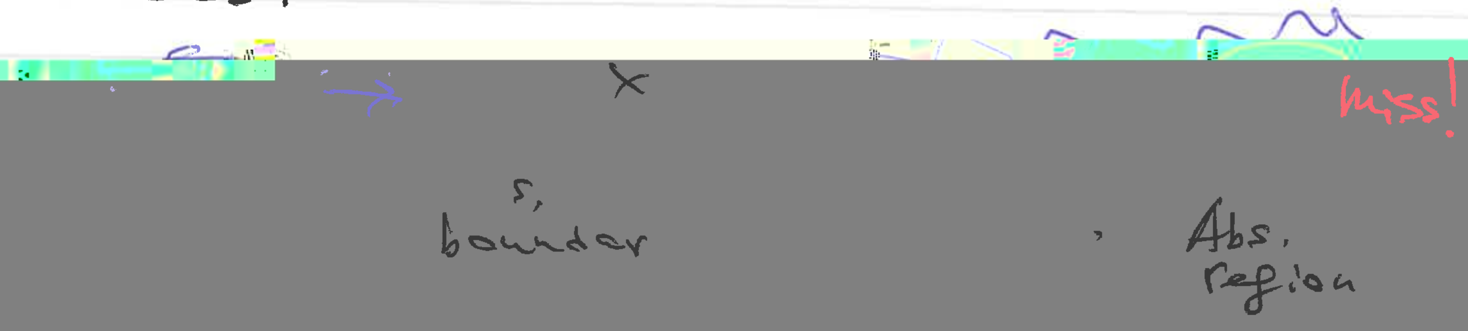
So
$$D_{eff} = \frac{L^2}{2} D \frac{1}{\int_0^L e^{\beta V(x)} \int_0^x e^{-\beta V(y)}\, dy}$$

Always big ...

Any potential: $D_{eff} \ll D$

What we did in MFPT was strictly 1D ...

In higher-Dimensions, the issue arises!



! MFPT must de d on the size target

Examples

① "Formi a fi" size ε

→ Szabo et. al. 1980

② "Narrow escape" size ε

→ Holcman et. al. 2000

How long it takes to make contact?

MFPT: 1D $\tau \sim \frac{L^2}{D}$

2D $\tau \sim \frac{L^2}{D} \ln(1/\varepsilon)$

3D $\tau \sim \frac{L^3}{D\varepsilon}$

Last topic

"Multiplicative Noise"

i.e., $dx = \mu(x,t)\,dt + \sigma(x)\,dW$

(E.g. in GBM)

Corresponding F.-P. equation

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

2nd Kramers-Moyal cf.

or is it $\frac{\sigma^2(x)}{2}\frac{\partial^2 P}{\partial x^2}$

or is it $\frac{1}{2}\sigma(x)\frac{\partial}{\partial x}\sigma(x)\frac{\partial P}{\partial x}$

or something else

Let's re-examine the Kramers-Moyal process: evaluate $\langle \Delta x^n \rangle$ first

$$\langle \Delta x \rangle = \int_t (\mu + \xi)\,ds$$

Average in another way: time average

slow variation

$$= \mu(x,t)\,\Delta t + \sigma(x[t])\int \xi(s)\,ds$$

Wiener?...

We need to decide at which

[redacted]

Mathematically consistent (Itoh)

- version is: evaluate at t, (start of interval)

$$\underbrace{G(x[t])}\int_t^{t+\Delta t} \underbrace{dW}$$

Statistically independent!

- Stratonovich version: evaluate at the middle

$$\int G(x[t+\tfrac{1}{2}\Delta t])\,\xi(t)\,dt$$

- More recently: evaluate at an arbitrary point

and compare with experiment

$$G(x[t+\alpha\Delta t])$$

Itoh: $\alpha=0$

Stratonovich: $\alpha=\frac{1}{2}$

Lau-Lubensky: $\alpha=1$ (end of...)

If we follow Itoh process:

$\alpha = 0$

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

If we follow Stratonovich process:

$\alpha = 1/2$

$$\text{——— '' ———} \quad \frac{1}{2}\frac{\partial}{\partial x}\left(\sigma(x)\frac{\partial}{\partial x}\left[\sigma(x) P\right]\right)$$

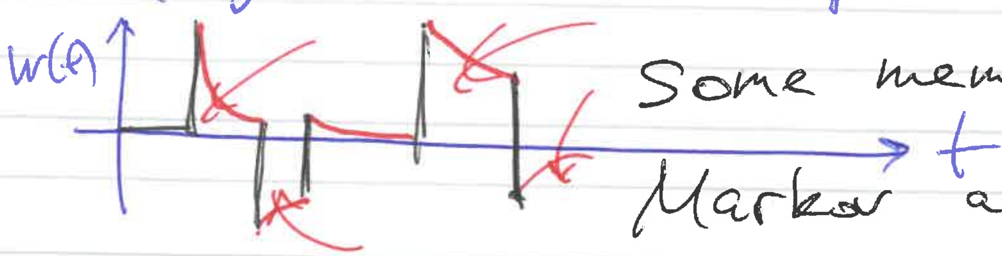
If we follow Lau-Lubensky:

$\alpha = 1$

$$\text{——— '' ———} \quad \frac{1}{2}\frac{\partial}{\partial x}\left(\sigma^2(x)\frac{\partial P}{\partial x}\right)$$

The formal accepted resolution of this is via a more careful look at the approximation leading to the Wiener process ...

Physical (e.g. thermal noise) process



Some memory?

Markov assumption

Wong-Zakai Theorem:

[applies when a physical process behind the approximate $W(t)$ is a sequence of deterministic events "W_n"

→ we must modify the SDE

$$dx = \left(\mu(x,t) + \frac{1}{2}\sigma(x)\frac{\partial \sigma}{\partial x}\right)$$ [redacted]

[Must have an additive drift term

We then work with proper Itoh process (statistically independent $\sigma(x)$ and dW)

$$\rightarrow \frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}(\mu \cdot P) - \frac{1}{2}\frac{\partial}{\partial x}\left(\sigma\frac{\partial \sigma}{\partial x}\cdot P\right)$$

1st Kramers-Moyal term

$$+\frac{1}{2}\frac{\partial^2}{\partial x^2}\left(\sigma^2(x) P\right)$$

2nd Kramers-Moyal

Simple algebra gives:

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\Big(\mu(x,t)\,P\Big) + \frac{1}{2}\frac{\partial}{\partial x}\left[\sigma(x)\frac{\partial}{\partial x}\Big(\sigma(x)P\Big)\right]$$

exactly the Stratonovich version!

when $\sigma = \text{const}$: $D = \frac{1}{2}\sigma^2$, we had

$$J = -De^{-\beta V(x)}\frac{\partial}{\partial x}\left(e^{\beta V(x)}P(x,t)\right)$$

Now we have the flux:

$$J = -\frac{1}{2}\sigma(x)e^{-\beta V(x)}\frac{\partial}{\partial x}\left(\sigma(x)\cdot e^{\beta V(x)}\cdot P\right)$$

As long as we identify the "friction constant" as

$$\gamma(x) = \frac{2kT}{\sigma^2(x)}$$

a version of F.D.T.

then $D(x) = \frac{kT}{\gamma(x)} = \frac{1}{2}\sigma^2(x)$ is still valid.