The Smoluchowski-Kramers Approximation: What model describes a Brownian particle?

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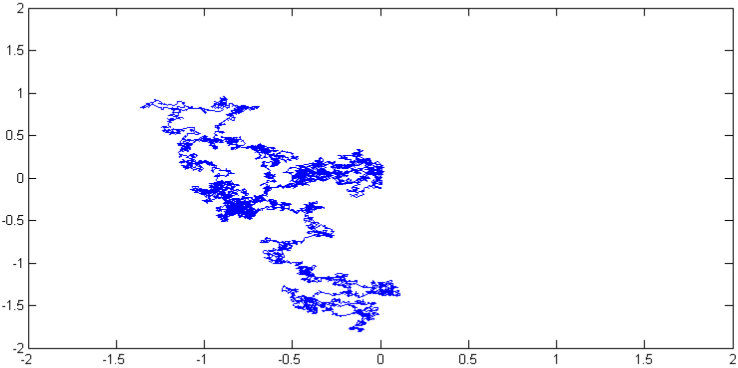
Brown observes a particle

1820s, botanist Robert Brown observes irregular motion of particle



Want to measure velocity.

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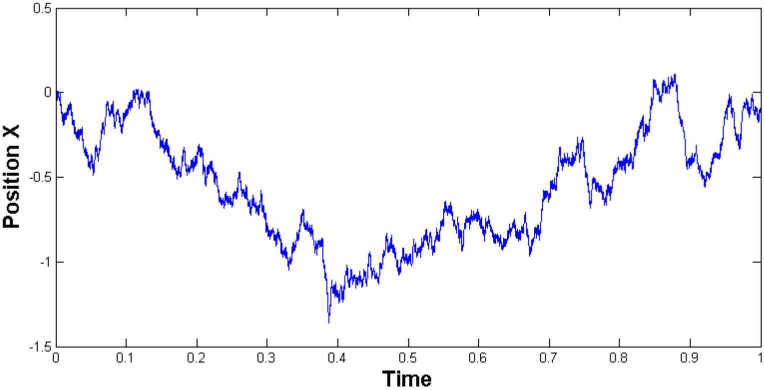


(Pictured, 1-D Wiener process $W_t(\omega)$ or Brownian motion, $E[W_t] = 0$, $E[(W_t - W_s)^2] = |t - s|$).

A dynamical theory for Brownian motion

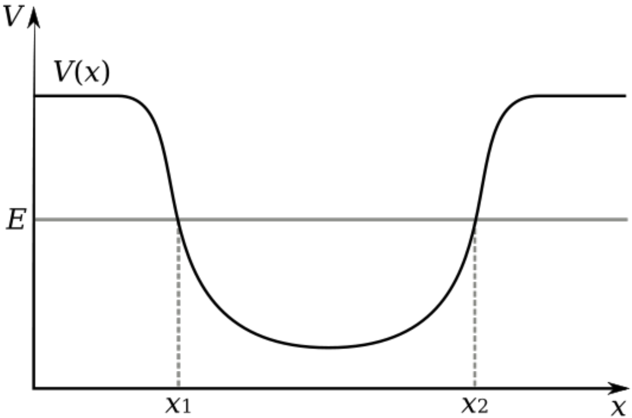
- Einstein and Smoluchowski derived the motion to be diffusive.
- Langevin and later Ornstein and Uhlenbeck (1930s) have dynamical theory.
- Newton's second law

$$
\begin{aligned}
dx_t^m &= v_t^m dt, \quad x_0^m = x \\
m dv_t^m &= b(x_t^m) - \gamma v_t^m dt + \sigma \, dW_t \quad v_0^m = v.
\end{aligned}
$$

b and γv_t^m are the drift forces, σ diffusion (noise) coefficient. Shorthand for

$$
\begin{aligned}
x_t^m &= x + \int_0^t v_s^m \, ds, \\
v_t^m &= v + \int_0^t \frac{b(x_s^m) - \gamma v_s^m}{m} \, ds + \int_0^t \frac{\sigma}{m} \, dW_s.
\end{aligned}
$$

Kramers



(en.wikipedia.org)

- Hendrick Kramers took $m = 0$ to simplify calculations to chemical reaction rates.

$$dx_t = \frac{b(x_t)}{\gamma} dt + \frac{\sigma}{\gamma} \, dW_t.$$

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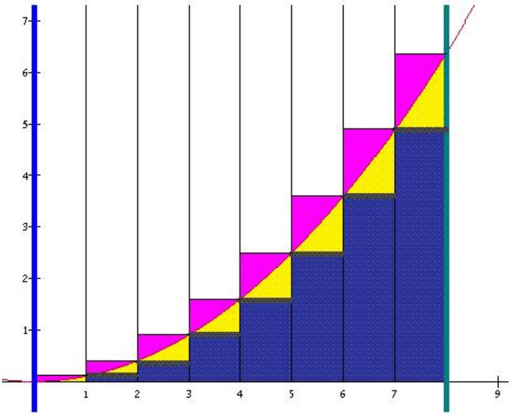
- Nelson showed $x_t^m \to x_t$ almost surely for $t \in [0, T],\ T < \infty$.
- How do we integrate

$$\int_0^t f(s, \omega)\, dW_s?$$

Riemann Sums



(conservapedia.com)

Stochastic Integral

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$$\lim_{N\to\infty} \phi_N(\alpha)_t = \lim_{N\to\infty} \sum_{i=1}^{N} f(t_i^*, \omega)(W_{t_i} - W_{t_{i-1}}),$$

W_t is the Wiener process.

$$t_i^* = \alpha t_i + (1-\alpha) t_{i-1}, \qquad \text{for all } 0 \leq \alpha \leq 1$$

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$$\int_0^t W_s\, d_\alpha W_s, = \frac{1}{2} W_t^2 - \left(\frac{1}{2} - \alpha\right) t$$

Special cases $\alpha = 0$ Itô, $\alpha = 1/2$ Stratonovich, $\alpha = 1$ anti-Itô.

Stochastic Integral

For f smooth ($E[|f(s,\omega) - f(t,\omega)|^2] \leq k|s-t|^{1+\epsilon}$),

$$\phi(\alpha)_t = \int_0^t f(s,\omega)\, dW_s, \qquad \text{for all } \alpha \in [0,1].$$

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For Kramers' equation

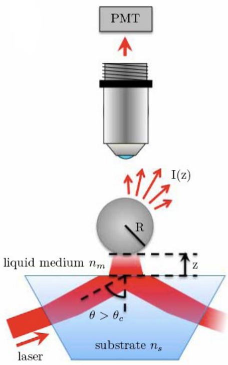
$$\begin{aligned} dx_t^m &= v_t^m\, dt \\ m dv_t^m &= b(x_t^m) - \gamma v_t^m\, dt + \sigma\, dW_t. \end{aligned}$$

Used the S-K approximation

$$dx_t = \frac{b(x_t)}{\gamma}\, dt + \frac{\sigma}{\gamma}\, dW_t.$$

Since σ and σ/γ constant, the integral is the same for all interpretations.

Experiment



(courtesy Giovanni Volpe)
Measure the drift forces

Model

$$dx_t^m = \frac{1}{\sqrt{m}} v_t^m \, dt$$
$$dv_t^m = \left(\frac{b(x_t^m)}{\sqrt{m}} - \frac{\gamma(x_t^m)}{m} v_t^m \right) \, dt + \frac{\sigma(x_t^m)}{\sqrt{m}} \, dW_t.$$

Approximated by the Smoluchowski-Kramers approximation

$$dx_t = \frac{b(x_t)}{\gamma(x_t)} \, dt + \text{``}\frac{\sigma(x_t)}{\gamma(x_t)} \, dW_t\text{''},$$

or

$$dx_t = \left[\frac{b(x_t)}{\gamma(x_t)} + \alpha \frac{\sigma(x_t)}{\gamma(x_t)} \frac{d}{dx_t} \left(\frac{\sigma(x_t)}{\gamma(x_t)} \right) \right] \, dt + \frac{\sigma(x_t)}{\gamma(x_t)} \, dW_t,$$

with the stochastic integral of the Itô form.

Results

- Freidlin studies $\gamma(x_t) = \gamma$ (purely mathematical?).

$$dx_t = \frac{b(x_t)}{\gamma} + \frac{\sigma(x_t)}{\gamma}\, dW_t, \text{(in Probability)}.$$

- Volpe/Wehr et al. use fluctuation dissipation theorem ($\gamma(x_t) = c\sigma(x_t)^2$),

$$dx_t = \left[\frac{b(x_t)}{c\sigma(x_t)^2}\right] dt + \frac{1}{c\sigma(x_t)}\, dW_t.$$

Measurements of forces not coinciding.

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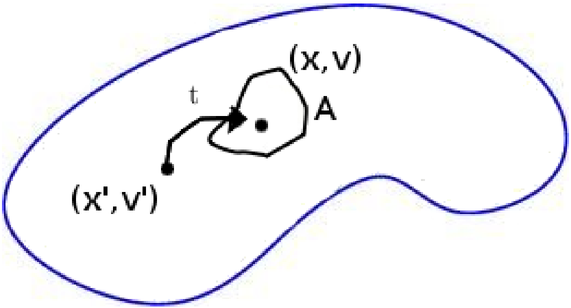
- $\alpha = 1$, anti-Itô!

PDE

- Recall that Einstein and Smoluchowski derived diffusion equation.



Probability transition function of (x_t, v_t), defined

$$P((x_t, v_t) \in A) = \int_A p(t; (x', v'), (x, v)) \, dxdv,$$

p is the density.

Connection to PDE

$$\begin{aligned} dx_t^m &= v_t^m \, dt \\ m dv_t^m &= b(x_t^m) - \gamma(x_t^m) v_t \, dt + \sigma(x_t^m) \, dW_t, \end{aligned}$$

Density p_m satisfies the *Fokker-Planck* (or *forward Kolmogorov*) equation

$$\begin{aligned} \frac{\partial p_m}{\partial t} &= \frac{1}{2} \frac{\partial^2}{\partial v^2} \left(\frac{\sigma(x)^2}{m} p_m \right) - \frac{\partial}{\partial x} (v p_m) - \frac{\partial}{\partial v} \left(\frac{(b(x) - \gamma(x) v)}{m} p_m \right) \\ &= L^*_{x,v} p, \end{aligned}$$

Also, for all $(x', x') \in \mathbb{R}^2$, p_m satisfies the *backward Kolmogorov* equation

$$\frac{\partial p_m}{\partial t} = L_{x',v'} p_m.$$

Heuristic calculation

Two scales, x_t^m of order 1 and v_t^m of order $1/\sqrt{m}$.

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$$\frac{\sigma(x)^2}{2\gamma(x)^2}\frac{\partial^2 p_0}{\partial x^2} + \left(\frac{b(x)}{\gamma(x)} - \frac{\sigma(x)^2}{2\gamma(x)^3}\frac{d(\gamma(x))}{dx}\right)\frac{\partial p_0}{\partial x} = \frac{\partial p_0}{\partial t}.$$

the BK equation satisfied by p_0.
Compare to the PDE of SK

$$\frac{\sigma(x)^2}{2\gamma(x)^2}\frac{\partial^2 p}{\partial x^2} + \left(\frac{b(x)}{\gamma(x)} + \alpha\left[-\frac{\sigma(x)}{\gamma(x)^3}\gamma'(x) - \frac{\sigma(x)^2}{\gamma(x)^2}\sigma'(x)\right]\right)\frac{\partial p}{\partial x} = \frac{\partial p}{\partial t}.$$

Equation for α

$$\alpha = \alpha(x_t) = \frac{\gamma'(x_t)\sigma(x_t)}{2(\gamma'(x_t)\sigma(x_t) - \gamma(x_t)\sigma'(x_t))}.$$

α constant iff $\gamma(q) = c\sigma(q)^\lambda$.

$$\alpha = \frac{\lambda}{2(\lambda - 1)}.$$

This coincides with Freidlin ($\lambda = 0 \implies \alpha = 0$) and Wehr/Volpe ($\lambda = 2 \implies \alpha = 1$).

Further work

$$\alpha = \frac{\lambda}{2(\lambda - 1)}.$$

- Properties of v_t as $\epsilon \to 0$.
- Consider the color noise case (W_t replaced by a differentiable process).
- Extend to $n-$dimensions.
- $\lambda = 1$ and its applications.

$$dx_t = \left(\frac{b(x_t)}{c\sigma(x_t)} - \frac{1}{2c^2\sigma(x_t)} \right) dt + \frac{1}{c} dW_t.$$

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Questions?