Langevin Dynamics

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Outline

References

Langevin Dynamics

Originally a reformulation of Einsteins theory of Brownian motion (BM) using stochastic differential equations (SDEs)

$$\frac{dx}{dt} = \eta(t), \quad \eta(t) \sim T(x, t|x', t')$$

For BM, $T(x, t|x', t') = \mathcal{N}(x', \sigma^2)$ where $\langle \eta(t)\eta(t') \rangle = \delta(t - t')$. If we have many x's, and $\eta(t)$ is uncorrelated over the ensemble we may write

$$\langle \eta(t)\eta(t') \rangle = \sigma^2 \delta_{ij} \delta(t - t')$$

Application to Brownian Motion

The solution to an SDE is a probability distribution $P(x, t)$ which obeys the Markov property

$$P(x, t') = \int T(x, t|x', t')P(x', t')dx'$$

With some effort this can be transformed into the Fokker-Planck equation

$$\frac{dP}{dt} = \frac{\sigma^2}{2}\frac{\partial^2 P}{\partial x^2} = D\frac{\partial^2 P}{\partial x^2}$$

which has a familiar non-stationary solution for $P(x, t)$ in BM:

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

Generalization to higher dimensions

When $\langle \eta_i(t)\eta_j(t)\rangle_t = \delta_{ij}$, the one-dimensional solution applies. Otherwise, $\langle \eta_i(t)\eta_j(t)\rangle_t = D_{ij} = \mathbf{\Sigma}/2$

$$\frac{d\boldsymbol{x}}{dt} = \sqrt{\mathbf{\Sigma}}\boldsymbol{\eta}(t)$$

where $\boldsymbol{D} = \mathbf{\Sigma}/2$ becomes a *diffusion tensor*. The Fokker-Planck equation for N-dimensional BM generalizes to

$$\frac{dP}{dt} = \sum_i \sum_j D_{ij} \frac{\partial P}{\partial x_i \partial x_j}$$

Diffusion in a harmonic potential: Ornstein-Uhlenbeck

A stochastic form of Newton's equation

$$\frac{d\boldsymbol{v}}{dt} = -\lambda \boldsymbol{v} + \boldsymbol{\eta}(t) - \boldsymbol{k} \cdot \boldsymbol{x}$$

Mean squared displacement

A common quantity measured experimentally is the mean-squared displacement (MSD). This is essentially the variance of $T(x, t|x', t')$

$$\begin{aligned}\mathrm{MSD}(\tau) &= \langle (x(t+\tau) - x(t))^2 \rangle \\ &= 4D\tau\end{aligned}$$

We would like to perform maximum likelihood estimation

$$\boldsymbol{k}^* = \underset{\boldsymbol{k}}{\mathrm{argmin}} - \log P(\boldsymbol{k}|\{\boldsymbol{x}\}_{i=1}^{N})$$

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