Optimal Parameter Estimation for Mean Squared Displacement

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Outline

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:

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

Time-averaged mean squared displacement

A common dynamical quantity measured for a single particle trajectory is the mean-squared displacement (MSD)

$$\begin{aligned}\mathbf{MSD}(\Delta t) &= \langle |\tilde{\boldsymbol{r}}(t+\Delta t) - \tilde{\boldsymbol{r}}(t)|^2 \rangle \\ &= \frac{1}{M}\sum_{n=1}^{M} |\tilde{\boldsymbol{r}}(t+n\tau) - \tilde{\boldsymbol{r}}(t)|^2\end{aligned}$$

Each lag time $\Delta t = n\tau$ has an associated histogram $T(d^2)$ with $M = \binom{N}{n}$ samples. The $\mathbf{MSD}$ is essentially the variance over M samples

Time averaged MSD: Brownian motion

$\mathbf{MSD} = 4D\Delta t$ for Brownian motion. However our measurement $\tilde{\boldsymbol{r}}(t)$ is generally not equal to the true value $\boldsymbol{r}(t)$ due to localization error

Time averaged MSD: Brownian motion

$\tilde{\boldsymbol{r}}(t) = \boldsymbol{r}(t) + \epsilon$ where ϵ is normally distributed $\epsilon \sim \mathcal{N}(0, \sigma^2)$

Our uncertainty σ of the particle position is related to experimental parameters by

$$\sigma = a\sqrt{\left(1 + \frac{\tilde{D} t_E}{s^2}\right) \cdot \frac{1}{2\pi I_0}}$$

where s and I_0 parameterize a symmetric Gaussian PSF and t_E is the exposure time

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