List 8

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Computer Simulations of Stochastic Processes

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Definition 1 (Mean square displacement)**.** Mean square displacement (MSD)

$$\text{EA-MSD}(\tau) \stackrel{def}{=} \mathbb{E}\left(X(\tau) - X(0)\right)^2,$$
$$\text{TA-MSD}(T,\tau) \stackrel{def}{=} \frac{1}{T-\tau}\int_0^{T-\tau} (X(t_0+\tau) - X(t_0))^2 dt_0$$

The main difference between both types of MSD is that the ensemble average is a number (it's just the expectation; also, in many applications $X(0) = x_0 = const.$, and it's just a variance when $\mathbb{E}X(t) = const$), while time average is a random variable.

We will calculate their estimators. Specifically, for N trajectories $[x_k(0), \ldots, x_k(n)], k = 1, 2, \ldots, N$ of length $n+1$, we calculate

$$\text{EA-MSD}(\tau) \stackrel{def}{=} \frac{1}{N}\sum_{k=1}^{N}(x_k(\tau) - x_k(0))^2, \quad \tau = 0, 1, \ldots, n$$
$$\text{TA-MSD}(k,\tau) \stackrel{def}{=} \frac{1}{n+1-\tau}\sum_{t_0=0}^{n-\tau}(x_k(t_0+\tau) - x_k(t_0))^2, \quad \tau = 0, 1, \ldots, n, k = 1, \ldots, N,$$
$$\text{EA-TA-MSD}(\tau) \stackrel{def}{=} \frac{1}{N}\sum_{k=1}^{N}\text{TA-MSD}(k,\tau), \quad \tau = 0, 1, \ldots, n.$$

N is the number of trajectories, n is their length, and τ is the parameter.

Problem 1. Implement MSD estimators. Apply them to already simulated processes.

Problem 2. Use applied MSD estimators to plot $\tau \mapsto$ (EA/TA/EA-TA)-MSD. Additionally, for TA-MSD consider its confidence interval for every lag τ.