Lecture 13 : Correlation Fuctions

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March 23, 2001

Refer to the paper of G.I. Tayler on Proc. London Math Soc. Vol 20, 196 (1921).

Correlation coefficient of the two random variable X and Y is defined as

$$\rho = \mathrm{Corr}(X, Y) = \frac{\mathrm{Cov}(X, Y)}{\sigma_X \sigma_Y},$$

where $\mathrm{Cov}(X, Y)$ is a "two-variable variance" compared with the Var X:

$$\mathrm{Var}\ X = \sigma_X^2 = \langle (X - \langle X \rangle)^2 \rangle = \langle \triangle X^2 \rangle$$
$$\mathrm{Cov}(X, Y) = \langle (X - \langle X \rangle)\,(Y - \langle Y \rangle) \rangle = \langle \triangle X \triangle Y \rangle.$$

We know the following facts about ρ :

- $-1 \leq \rho \leq 1$
- When $\rho = 0$, X and Y are independent, because $\langle \triangle X \triangle Y \rangle = \langle \triangle X \rangle \langle \triangle Y \rangle = 0$.
- When $\rho = 1$, X and Y are perfectly correlated, that is $\triangle X/\sigma_X$ is an exact copy of $\triangle Y/\sigma_Y$.
- When $\rho = -1$, X and Y are anti-correlated, that is $\triangle X/\sigma_X$ is an exact copy of $-\triangle Y/\sigma_Y$.

1 Random walk with correlated steps

Correlation function is defined as

$$C(m, m') = \langle \triangle X_m \triangle X_{m'} \rangle = \mathrm{Cov}(\triangle X_m, \triangle X_{m'})$$

when $m,\ m'$ are part of a path $m \to m + 1 \to \cdots \to m'$.

When X_n are d-dimensional vectors, we can calculate the variance of X_n if $C(m, m')$ is known.

$$\overrightarrow{X}_n = \sum_{m=1}^{n} \overrightarrow{\triangle X}_m,$$
$$\langle \overrightarrow{X}_n^2 \rangle = \sum_{m=1}^{n} \sum_{m'=1}^{n} \langle \overrightarrow{\triangle X}_m \cdot \triangle \overrightarrow{X}_{m'} \rangle$$
$$= \sum_{m=1}^{n} \sum_{m'=1}^{n} C(m, m')$$

Now let us assume the correlation function is time-translationally invariant, that is

$$C(m, m') = C(|m - m'|) \text{ or } C(m) = \langle \triangle X_{m_0} \triangle X_{m_0+m} \rangle \text{ for all } m_0.$$

Noting that the variance of each step is $C(0) = \sigma^2$, we can calculate

$$\langle X_n^2 \rangle = nC(0) + 2(n-1)C(1) + 2(n-2)C(2) + \cdots + 2C(n-1)$$
$$= n\sigma^2 + 2\sum_{k=1}^{n-1} (n-k)C(k)$$

In continuum limit, when $m\tau = t$,

$$\frac{C(m)}{\tau^2} = \langle \frac{\overrightarrow{\triangle X}_{m_0}}{\tau} \cdot \frac{\overrightarrow{\triangle X}_{m_0+m}}{\tau} \rangle = \langle \vec{v}(0) \cdot \vec{v}(t) \rangle$$

Velocity auto-correlation function is defined as

$$\langle X^2(t) \rangle = \langle v^2(0) \rangle \, t\tau + 2 \int_0^t \langle \vec{v}(0) \cdot \vec{v}(t') \rangle \, (t - t')dt'$$
$$D = \lim_{t\to\infty} \frac{1}{2} \frac{d}{dt} \langle X^2(t) \rangle = \lim_{t\to\infty} \left[\frac{\langle \vec{v}(0)^2 \rangle \tau}{2} + \int_0^t \langle \vec{v}(0) \cdot \vec{v}(t') \rangle dt' \right]$$

When the correlation time t is much bigger than the time step τ, we can neglect the first term and get Green-Kubo formula :

$$D = \int_0^\infty \langle \vec{v}(0) \cdot \vec{v}(t') \rangle dt'.$$

Back to the discrete case, diffusion fall into different regimes according to the limiting behavior of $D \sim \sum_{m=1}^{n} C(m)$ as $n \to \infty$.

- If D goes to finite and non-zero value, we have "normal diffusion." Thus

$$\langle X_n^2 \rangle^{1/2} \sim \sqrt{n} \quad \text{or} \quad \langle X(t)^2 \rangle^{1/2} \sim \sqrt{2Dt}.$$

- If $D \to \infty$, we have "super diffusion."

$$\langle X(t)^2 \rangle^{1/2} \sim t^\alpha \text{ with } 1/2 < \alpha \leq 1.$$

- If $D \to 0$, we have "sub diffusion."

$$\langle X(t)^2 \rangle^{1/2} \sim t^\alpha \text{ with } 0 \leq \alpha < 1/2.$$

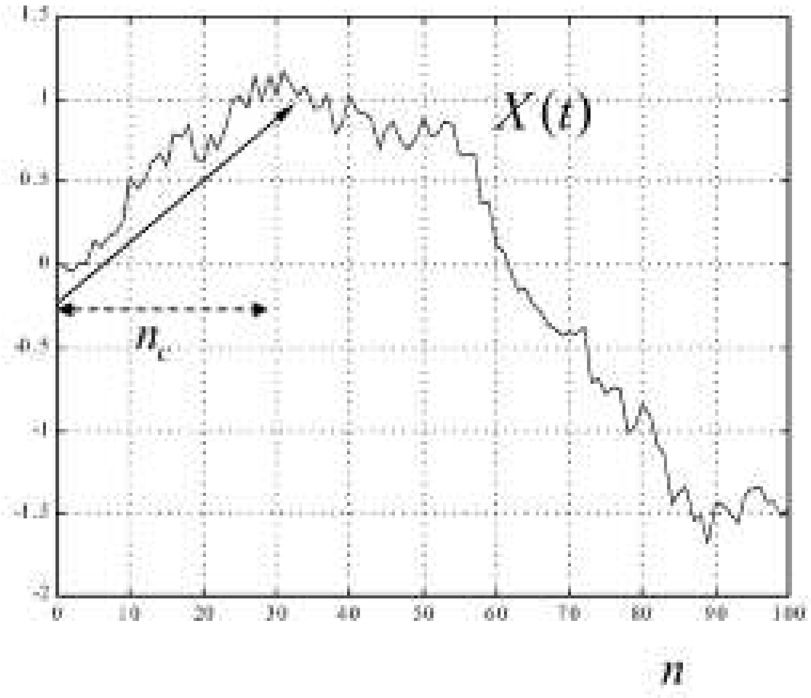

Figure 1: Renormalized Walk

2 Example : Exponentially Decaying Correlation Function

Suppose

$$C(n) = \rho^n \quad \text{with} \ -1 \leq \rho \leq 1$$
$$\text{or} \quad C(n) = e^{-2n/n_c} \quad \text{with } n_c = -2/\log\rho.$$

If $\rho \to 1$ (strongly positive correlation), $n_c \gg 1$ and we can think of n_c as "correlation time." looks like an independent walk taking n/n_c steps with big stepsize $n_c\sigma$.

Rather than X_n and n, we can consider "renormalized" or "homogenized" variables

$$\widetilde{X}^2 = \frac{\langle X_n^2\rangle}{(n_c\sigma)^2} \quad \text{and} \quad \widetilde{n} = \frac{n}{n_c}.$$

Then, by the dimensional argument we can infer that

$$\widetilde{X}^2 = \phi(\widetilde{n}) \quad \text{or} \quad \phi(\widetilde{n}, \frac{1}{n_c}).$$

Here ϕ is the function describing the independent walk and $1/n_c$ is typical time step.

To get ϕ, we have to calculate $\langle X_n^2 \rangle$. Assuming $\sigma = 1$ and $C(k) = \rho^k$,

$$\begin{aligned}
\langle X_n^2 \rangle &= n + 2\sum_{m=1}^{n}(n-m)\rho^m = -n + 2\sum_{m=0}^{n}(n-m)\rho^m \\
&= -n + 2n\sum_{m=0}^{n}\rho^m - 2\sum_{m=0}^{n} m\rho^m \\
&= -n + 2n\sum_{m=0}^{n}\rho^m - 2\rho\frac{d}{d\rho}\sum_{m=0}^{n} m\rho^m \\
&= -n + 2n\frac{1-\rho^{n+1}}{1-\rho} - 2\rho\frac{d}{d\rho}\left(\frac{1-\rho^{n+1}}{1-\rho}\right) \\
&= \frac{1+\rho}{1-\rho}n - \frac{2n\rho^{n+1}}{1-\rho} - 2\rho\frac{(\rho-1)(n+1)\rho^n - (\rho^{n+1}-1)}{(\rho-1)^n} \\
&= \frac{1+\rho}{1-\rho}n + 2\rho\frac{\rho^n - 1}{(\rho-1)^2}
\end{aligned}$$

Since $\langle X_n^2 \rangle \sim n$, we get a normal diffusion with

$$D = \frac{1+\rho}{1-\rho}\, D_0.$$

Now let ρ approach to 1. If $\rho = 1 - \varepsilon$,

$$\begin{aligned}
n_c &= -2/\log\rho \sim 2/\varepsilon \\
\frac{1+\rho}{1-\rho} &= \frac{2-\varepsilon}{\varepsilon} \sim \frac{2}{\varepsilon} = n_c \\
\frac{2\rho(\rho^n - 1)}{(\rho-1)^2} &\sim \frac{2(e^{-2n/n_c} - 1)}{\varepsilon^2} = \frac{n_c^2}{2}(\rho^{-2n/n_c} - 1)
\end{aligned}$$

Now we can get $\widetilde{X}$:

$$\begin{aligned}
\widetilde{X}^2 &= \frac{\langle X_n^2 \rangle}{n_c^2\sigma^2} = \frac{n}{n_c} + \frac{1}{2}(e^{-2n/n_c} - 1) \\
&= \widetilde{n} + \frac{1}{2}(e^{-2\widetilde{n}} - 1) = \phi(\widetilde{n}) \\
&\sim \begin{cases} \widetilde{n}^2 & \text{when } \widetilde{n} \ll 1 \ (1 \le n \ll n_c): \ \text{ballistic region} \\ \widetilde{n} & \text{when } 1 \ll \widetilde{n} \ (n_c \ll n): \text{diffusion region} \end{cases}
\end{aligned}$$

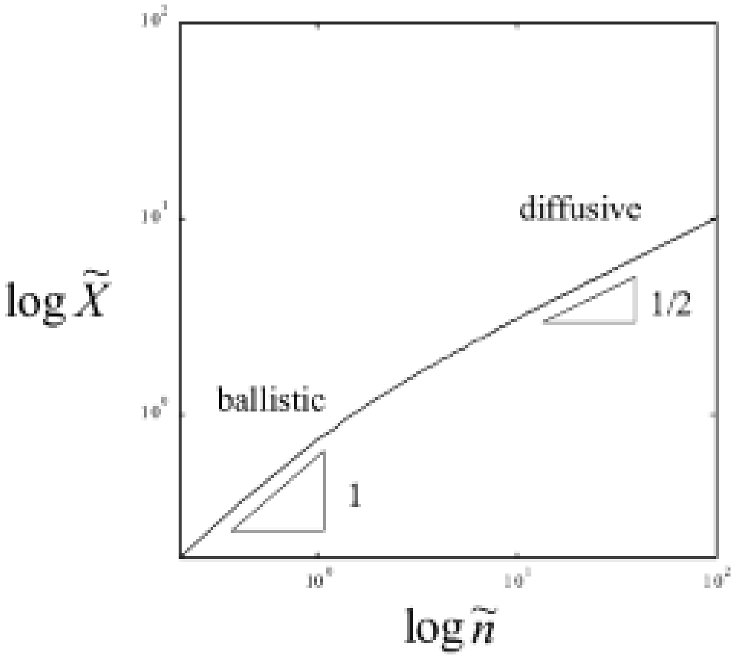

Figure 2: $\log \widetilde{X}$ vs. $\log \widetilde{n}$