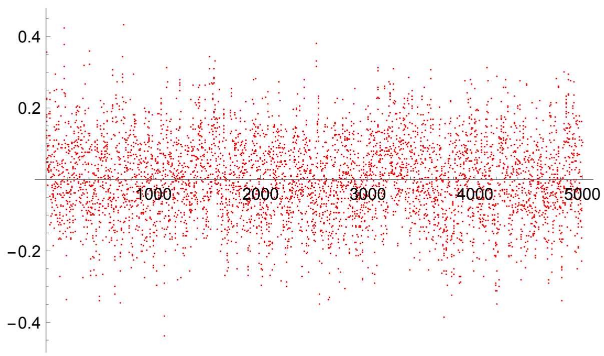
CBP Summer School
5 - 16 August, 2024

Physics Department, ASU

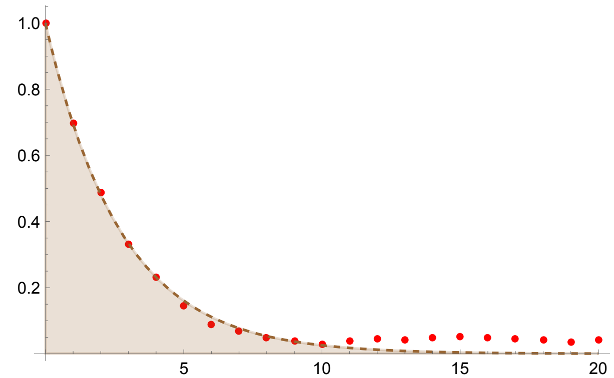
Lecture 9
Basics of the correlation functions

Stochastic process:

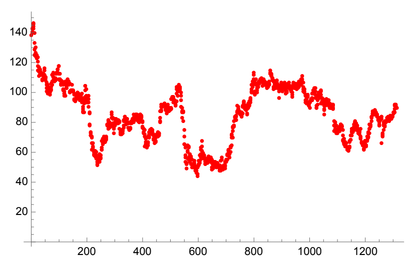


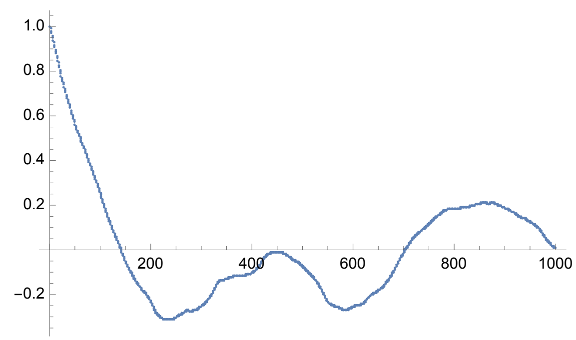
from Lecture9-1.nb

Time correlation function:



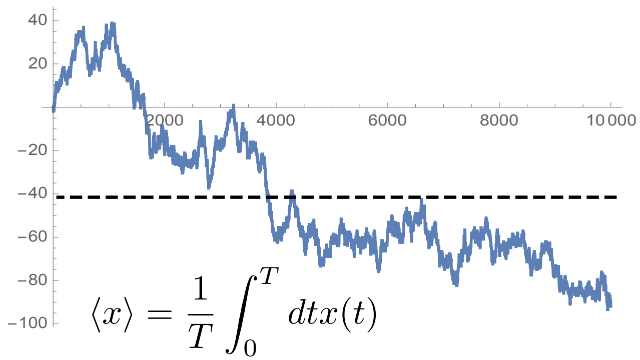
Price of GE stocks:





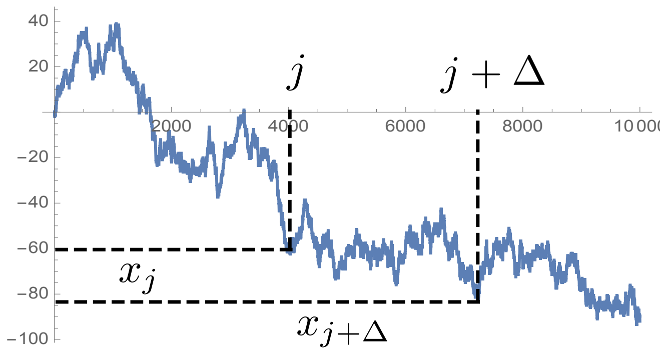
from Lecture9-2.nb

Time average



$$\langle x \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt x(t)$$

Correlation function



$$C_x(t = \tau\Delta) = \frac{1}{M}\sum_{i=1}^{M} \delta x_j \delta x_{j+\Delta}$$

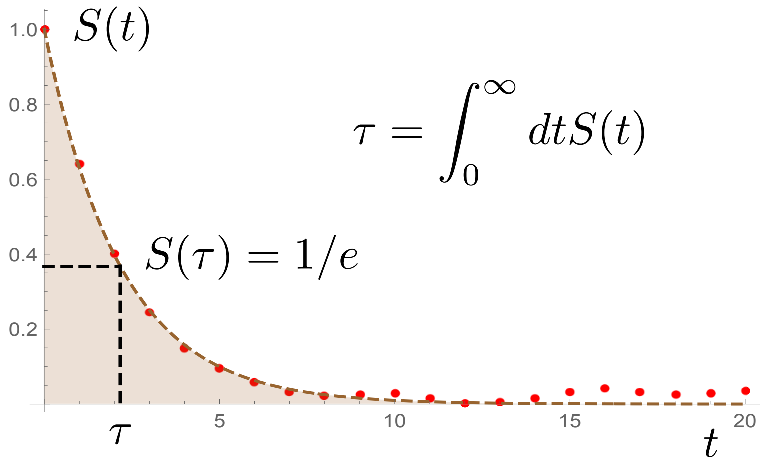
$$C_x(t) = \langle \delta x(t) \delta x(0) \rangle$$

$$\delta x(t) = x(t) - \langle x \rangle$$

deviation from the average

Normalized correlation function

$$S(t) = \frac{\langle \delta x(t) \delta x(0) \rangle}{\langle (\delta x(0))^2 \rangle}$$



relaxation time is the area under the S(t) curve

Mathematical properties

$$S_x(t) = \langle x(t)x(0)\rangle / \langle x(0)^2\rangle$$

$$S_x(0) = 1,$$
$$\dot{S}_x(0) = 0.$$

short times:

$$S_x(t) = e^{-\Omega^2 t^2/2} \simeq 1 - \Omega^2 t^2/2$$

Gaussian decay

$$S_x(\infty) = 0$$

loss of memory at long times

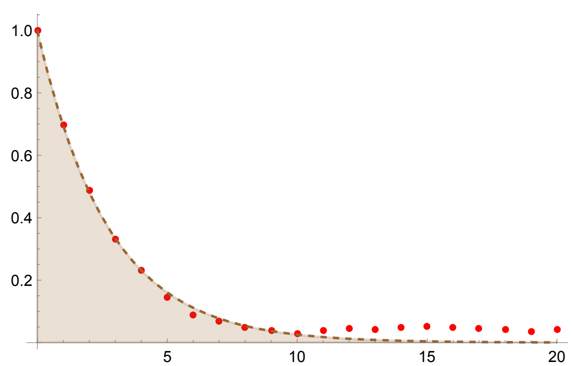
Exponential relaxation

$$\boxed{S(t) = e^{-t/\tau_r}.}$$

τ_r is the relaxation time

$$S_x(t) = e^{-t/\tau_r} \simeq 1 - t/\tau_r$$

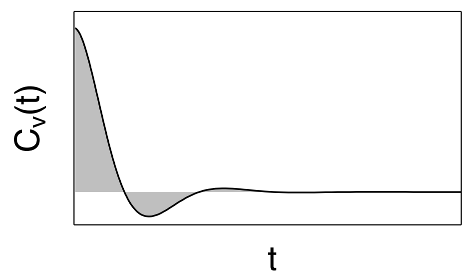
Gaussian decay is not satisfied



Velocity correlation function

$$C_v(t) = \langle \mathbf{v}(t) \cdot \mathbf{v} \rangle$$

$$\boxed{D = \frac{1}{3}\int_0^\infty dt \langle \mathbf{v}(t) \cdot \mathbf{v} \rangle.}$$



diffusion constant = area under the curve

Exponential relaxation

$$C_v(t) = \langle \mathbf{v}^2 \rangle e^{-t/\tau_v}$$

$$D = \frac{k_{\mathrm{B}}T}{m} \int_0^\infty dt e^{-t/\tau_v} = \frac{k_{\mathrm{B}}T}{m} \tau_v$$

From the known value of the diffusion constant one can estimate the relaxation time τ_v. Assume that a protein with $M = 10$ kDa (≈ 100 aa, 1 Da = 1 g/mol) has the diffusion constant of 10^3 μm^2/s. One obtains at $T = 300$ K ($R = 8.314$ J/(mol K) is the gas constant)

$$\tau_v = \frac{mD}{k_{\mathrm{B}}T} = \frac{MD}{RT} = \frac{10 \text{ kg} \times 10^{-9}\ m^2}{8.31 \times 300\ J \times s} = 4 \text{ ps.}$$