# Assignment: Preparatory Lectures

BSSP 2018

1. Consider the sum
$$S = \sum_{i=1}^{N^p} \exp(N\xi_i),$$
where $N > 0$, $p > 0$ and $\xi_i$ takes values within $0 < \xi \leq \xi_{max}$ . Find the following limit
$$\lim_{N\to\infty} \frac{\ln S}{N} = ?$$

2. Use saddle point approximation to derive Stirling's formula: $n! \approx \sqrt{2\pi n}\; e^{n\log(n)-n}$.

3. Consider a particle with equation of motion given by $\dot{x} = f(x)$. The equation describing the evolution of the probability density $\rho(x,t)$ is given by $\partial_t\rho(x,t) + \partial_x f(x)\rho(x,t) = 0$. Derive this continuity equation from the condition for conservation of particles which is $\rho(x,t)dx = \rho(x',t')dx'$ where $t' = t + dt$ and $x' = x(t + dt)$.

4. The moment generating function corresponding to a probability distribution$P(x)$ is defined as $Z(\lambda) = \langle e^{\lambda X}\rangle$. The cumulant generating function is defined as $\mu(\lambda) = \ln[Z(\lambda)]$. Use the Taylor series expansion of these generating functions to relate the first three cumulants $C_1, C_2, C_3$ to the first three moments $M_1, M_2, M_3$.

5. (a) Let $P_n$ be the probability that a discrete random variable $X$ takes a particular integer value $n$. Find out the corresponding moment generating function and cumulant generating function, if $P_n$ is a
i) Bernoulli distribution. Pmf : $P(k,p) = p^k(1-p)^{1-k},\ k = 0,1$
ii) Binomial distribution. Pmf : $P_N(n,p) = \ {}^N C_n p^n(1-p)^{N-n},\ n = 0,(1),N$
iii) Poisson distribution. Pmf : $P_\lambda(n) = \frac{\lambda^n}{n!}e^{-\lambda}$
Use them to evaluate the mean, variance, skewness and kurtosis of each of the distributions.

   (b) Let $P(x)$ be the probability density function for a continuous random variable $x$. Deduce expression for moment generating function and cumulant generating function if $P(x)$ is a
i) Gaussian distribution. Pdf : $P_\sigma(x) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{x^2}{2\sigma^2}}$
ii) Cauchy distribution. Pdf : $P_\gamma(x) = \frac{\gamma/\pi}{x^2+\gamma^2}$
iii) Levy stable distribution. Pdf : $P_\alpha(x) = \sqrt{\frac{\alpha}{2\pi}}\frac{e^{-\frac{\alpha}{2x}}}{x^{3/2}}$
Then determine first two moments and cumulants of each distribution. What is special about higher order cumulants of the Gaussian distribution ?

6. Consider $x$ be a continuous random variable with distribution $P(x) = \alpha\exp(-\alpha|x|)/2$ where $\alpha > 0$ is some parameter. Find the distribution $Q(g)$ of the random variable $g = x^2$.

7. Consider a box of volume $V$, containing $N$ non-interacting particles. Let us assume that the average density is $\rho = N/V$. Then,

(a) Find out the probability $P_N(n, v/V)$ of finding $n$ particles in a certain volume $v$.

(b) Evaluate average number of particles ($\mu = n$) occupied in volume v and the variance ($\sigma^2 = \langle n^2 \rangle - \langle n \rangle^2$) in the number fluctuations. Determine the standard deviation ($\sigma$) to mean ($\mu$) ratio ($\sigma/\mu$) and show that, the ratio goes as $N^{-1/2}$.

(c) Consider the following simple extension to interacting particles. Assume that the volume $V$ divided into $V$ number of cells of *unit* volume. Find the number of ways to distribute $N$ *indistinguishable* particles (with $0 \leq N \leq V$ ) within $V$ cells, such that each cell may be either empty or filled up by *only one* particle. Show that the entropy per particle $s(v)$ is given by

$$s(v) = K_B \; [v \ln v + (1 - v) \ln(1 - v)] \,, \quad \text{where} \;\; v = V/N.$$

From this expression also show that

$$\frac{p}{T} = -K_B \ln(1 - \rho),$$

where $p$ is the pressure, $T$ is the temperature and $\rho = 1/v$ is the density.

8. Let $\xi_i$'s (for $1 \leq i \leq n$) be a set of $n$ independent random variables chosen from certain distribution $\phi(\xi_i)$. $\mu$ and $\sigma$ be its mean and standard deviation respectively.

(a) Let use define a random variable $x$ in terms of $\xi$'s as follows

$$x = a \sum_{i=1}^{n} \xi_i$$

Find mean $\langle x(n) \rangle$ and variance $\langle x^2(n) \rangle - \langle x(n) \rangle^2$ of $x$ if,

$$(i) \qquad \xi_i = \begin{cases} 1 & \text{with probability } \frac{1}{2} \\ -1 & \text{with probability } \frac{1}{2} \end{cases} \qquad (\mu = 0, \sigma = 1)$$

and

$$(ii) \qquad \xi_i = \begin{cases} 0 & \text{with probability } \frac{1}{4} \\ 1 & \text{with probability } \frac{1}{4} \\ 2 & \text{with probability } \frac{1}{2} \end{cases} \qquad (\mu = 5/4, \sigma = 7/16)$$

(b) Let use define another random variable $y$ in terms of $\xi$'s as follows

$$y = \frac{\sum_{i=1}^{n} \xi_i - n\mu}{\sqrt{n}\sigma} \tag{1}$$

Show that in the limit $n \to \infty$, y has unit normal distribution [Gaussian with zero mean and unit variance, usually denoted as $\mathcal{N}(0, 1)$], irrespective of the form of $\phi(\xi)$.

9. Discrete time random walk on a lattice. The random walker started at $x = 0$ in time $t = 0$, takes a forward step with probability $p$ and backward step with probability $q = 1 - p$ after every fixed time interval $\tau$. Step size in both forward and backward direction is $\ell$.

(a) Determine the probability that the walker is at location $x = n\ell$ in time $t = N\tau$, where $N$ is the total number of steps taken and $n$ is an integer.

(b) Determine the limiting distributions in the following two limits (i) $p = q + \delta$ with $0 < \delta << 1/2$ and $N \to \infty$ [use Stirling's formula] (ii) $p \approx 0$ and $N \to \infty$ such that $Np =$ finite.

10. A random walker is moving on a one dimensional lattice. Starting from the origin, it takes a step towards right with probability $p$ and to the left with probability $q = 1 - p$. Show that the probability $R$ that the walker returns to the origin is given by $R = 1 - |p - q|$.

Hint: Note that $R$ can be written as $R = R_r p + R_\ell q$ where $R_r$ is the return probability to the origin given that the walker had taken its first step on the *right* side. Similarly, $R_\ell$ is the return probability to the origin given that the walker had taken its first step on the *left* side. Try to write down expression for $R_r$ by adding probabilities for different possibilities (events) as follows: Given that the the particle took the first step on the right side (*i.e.* it is at site 1), it can either come back immediately to origin with prob $q$ or it can take another step on the right side with $p$. Now given that it took another right step from the first site (site 1) it returns back to site 1 with prob $R_r$ and then it takes a left step to reach the origin. So the probability of this event is $(pR_r)q$. So, $R_r = q + (pR_r)q + ....$ Solving this equation one can get an expression of $R_r$. Similarly obtain an expression for $R_\ell$.

11. Continuous time random walk on a lattice. Consider a 1-D random walker jumps forward and backward with equal *rate* $r = 1$, with fixed jump length $\ell = 1$ on both side. Initial position of the random walker is $x_0 = 0$. Show that, $\langle x^2 \rangle = 2t$.

Write a computer program to numerically simulate this 1-D random walk and verify the above.

12. $P(x, t|x_0)$ is the probability distribution that a particle is at x in time t, given that it started from $x_0$ at $t = 0$ ($P(x, t|x_0)$ is also called as the propagator). For a particle undergoing diffusion, $P$ satisfies following equation:

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2} \tag{2}$$

where D is the diffusion constant.

(a) Solve for $P(x, t|x_0)$ from Eq.2 with an initial condition $P(x, t = 0) = \delta(x - x_0)$ and boundary conditions $P(x \to \pm\infty, t) = 0$. Check the normalization: $\int_{x=-\infty}^{\infty} P(x, t|x_0)dx = 1$. Show that $\langle x \rangle = x_0$ and $\langle x^2 \rangle - \langle x \rangle^2 = 2Dt$

(b) Solve Eq.2 with an initial condition $P(x, t = 0) = \delta(x - x_0)$, $(0 \leq x_0 \leq L)$ and reflecting boundaries at $x = 0$ and $x = L$. What happens to $P(x, t|x_0)$ as $t \to \infty$?

(c) Use method of images to find the solution Eq.2 with the same initial condition and (i) absorbing boundaries at $x = 0$ and $x = L$ (ii) reflecting boundaries at $x = 0$ and $x = L$.

13. The distribution for the first visiting times to some fixed point $x$, $q(x, t|x_0)$, is defined as, if a particle starts from $x = x_0$ at t=0, then $q$ is the probability that the particle reaches $x$ for the first time in time interval $t$ and $t+dt$. $q(x, t|x_0)$ and $P(x, t|x_0)$ are related through a renewal equation:

$$P(x', t|x_0) = \int_{\tau=0}^{t} q(x, \tau|x_0)P(x', t - \tau|x)d\tau \tag{3}$$

If one defines Laplace transform as $\tilde{g}(s) = \int_0^\infty e^{-st}g(t)dt$, then using the property of Laplace transform of a convolution, one can show that

$$\tilde{q}(x, s|x_0) = \frac{\tilde{P}(x', s|x_0)}{\tilde{P}(x', s|x)} \tag{4}$$

(a) Using the Laplace transform of $P$ determined in the previous question for diffusion process, find out $\tilde{q}(x, s|x_0)$.

(b) Using the properties of Laplace transforms, find out (i) what is the probability that the particle reaches $x$ ultimately, i.e. $\int_{t=0}^\infty q(x, t|x_0)dt$ and (ii) mean first passage time i.e. $\overline{T}(x|x_0) = \int_{t=0}^\infty tq(x, t|x_0)dt$.

(c) Using standard inverse Laplace transform formula, determine $q(x, t|x_0)$ from $\tilde{q}(x, s|x_0)$. How does $q(x, t|x_0)$ behave at large times?

14. Estimate the value of diffusion coefficient $D$ for a colloidal particle of radius $a = 1\mu m$ moving in water and in air.
How far does it travel (typical distance covered=$\sqrt{2D \times \text{time}}$) in a minute? and in an hour? Do the answers change if gravity is considered?
Consider temperature to be $20^0$C. In SI units, air density 1.205 $kg/m^3$ and viscosity $1.82 \times 10^{-5}$ $kg/ms$, water density 998.2 $kg/m^3$ and viscosity 0.001 $kg/ms$; gravitational acceleration 9.8 $m/s^2$).

15. Consider diffusion in a potential $U(x)$. Write the evolution equation for the probability distribution $P(x, t|x_0, 0)$.

a) Find the steady state distribution for continuous and bounding potentials ($\lim_{x\to\pm\infty} U(x) = 0$). What is the problem for unbounded potentials?

b) Consider a Brownian particle in a $1D$ box of length $L$. Inside the box we have a potential,

$$U(x) = \begin{cases} 0 & 0 < x < x_0 \\ U_0 & x_0 \leq x < L \\ \infty & \text{Otherwise} \end{cases}$$

What is the steady state distribution?

c) Show that the diffusion equation in a potential is equivalent to Schroedinger equation under suitable transformation. What is the effective 'quantum' potential?

16. The 'Master equation' is: $\frac{\partial P}{\partial t} = WP$.
Consider a spin in a constant magnetic field $h$. The spin have only two possible states, $s = 1, -1$. The spin can change the state via Metropolis dynamics characterised by the transition rate: $c = \min[1, exp(-\Delta E)]$, $\Delta E$ being the energy difference of the configurations before and after the transition.

(a) Find the $W$-matrix.

(b) Find the steady state.

(c) What is the relaxation time?

(d) Write a program to simulate the system and check (b) and (c).

17. Master equation for continuous time random walk on a lattice. Rate of jumping to the right is $p$ and to left is $q$. The configuration of the walker is specified by its position $x$ (discrete). The master equation is given by,

$$\frac{\partial P(x,t)}{\partial t} = pP(x-1,t) + qP(x+1,t) - (p+q)P(x,t).$$

(a) For a finite box of size $L = 3$, write the $W$-matrix. Use the boundary condition, $P(0,t) = P(L+1,t) = 0$.

(b) Find the eigenvalues and the left and right eigenvectors of $W$;

(c) (i) What is the steady state and relaxation time? (ii) Check the answers using simulation.

(d) Can we find the answer to the above questions for a general $L$?

(e) (i) What are the eigenvalues and eigenstates for random walk on an infinite lattice? Do we have a steady state in this case?
(ii) Find the probability P(x,t) for infinite line using simulation.

18. Under-damped Langevin equation for a particle of mass m moving in a fluid of temperature $T$ is given by:

$$\dot{x} = v \qquad m\dot{v} = -\gamma v + \sqrt{2\gamma k_B T}\,\eta(t) \tag{5}$$

where $\gamma$ is friction coefficient and $\eta(t)$ is a Gaussian white noise with $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = \delta(t-t')$. $k_B$ is Boltzmann's constant. If $x(t=0) = 0$ and $v(t=0) = 0$ are the initial conditions for the particle position and velocity respectively, then determine the behavior of $\langle v \rangle$, $\langle x \rangle$, $\langle v^2 \rangle$ and $\langle x^2 \rangle$ as a function of time.

19. Overdamped Langeving equation.

$$\frac{dx}{dt} = -\frac{1}{\gamma}\frac{\partial U}{\partial x} + \xi(t),$$

where the noise is characterised by, $\langle \xi(t) \rangle = 0,\ \langle \xi(t)\xi(t') \rangle = 2D\delta(t-t'),\ D = \frac{k_B T}{\gamma}$.

Check that, for $U = 0$, the time dependence as in question (11) is retrieved.
Consider potentials, (i) $U(x) = \frac{1}{2}kx^2$, (ii) $U(x) = -\frac{1}{2}kx^2 + \frac{1}{4}\lambda x^4$, $k$ and $\lambda > 0$. For initial condition $x(t=0) = x_0$, simulate the dynamics and plot,

(a) trajectories $x(t)$ vs $t$;
(b) $\langle x(t) \rangle,\ \langle x^2(t) \rangle$ vs $t$;
(c) Plot $P(x,t)$ vs $x$ for different $t$.

Note: For simulation, use the discretisation scheme: $x(t+\Delta t) = x(t) + \frac{F(x(t))}{\gamma}\Delta t + \sqrt{2D\Delta t}\,\eta,\ \eta$ is drawn at each time step from the unit normal distribution $\mathcal{N}(0,1)$.

A consequence of this discretisation. Define $x(t+) = \lim_{\Delta t\to 0} x(t+\Delta t)$ and $v(t,t+) = \lim_{\Delta t\to 0}(x(t+\Delta t) - x(t))/(\Delta t)$. Calculate the *ordered* average $\langle x(t+)v(t,t+) - v(t,t+)x(t) \rangle$.

20. Barrier crossing problem for overdamped Langevine particle.
Consider a potential, $U(x) = \frac{1}{2}ax^2 - \frac{1}{3}bx^3,\ a,\ b > 0$. It shall have a minima at $x = 0$ and maxima at $x_c = \frac{a}{b}$. Consider a large $N$ number of nonineracting browninan particles are released at $x = 0$ at the time $t = 0$. We consider a point $x_0$ beyond the *barrier*, i.e. $x_0 > x_c$.

(a) Let, $N_t$ is the number of particles at $x \geq x_0$ at time $t$. Averaging over a large number of realisations, numerically plot $\langle N_t \rangle$ vs $t$. The escape probability in time $t$ is approximately $P(x_0, t|0,0) \simeq \langle N_t \rangle / N$. Plot the escape rate $r = \frac{dP}{dt} = \frac{1}{N}\frac{d\langle N_t \rangle}{dt}$ with time.

(b) In a single realisation, find the escape time distribution $f(t, x_0|0,0)$ (probability density of crossing $x_0$ in the time interval $t$ to $t+dt$) by noting the escape time of each particle. Find the mean escape time and most probable escape time. How do they compare with the escape rate obtained in (a)?

(c) Can we theoretically explain the simulation results?