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Problem set 0: Computational Molecular Physics

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Statistical Mechanics

1. Binomial distribution describes the probability that in N independent trials an event that has a single trial probability p will occur exactly m times

$$P_N(m) = \binom{N}{m} \cdot p^m (1-p)^{N-m}$$

where $m = 0, 1, 2, ..., N$

a) Write a small code to calcualte the binomial distribution for $N = 50$, $p = 0.5$.

b) Plot the distribution for the limiting cases i.e.
1) $N>>1$ and finite p
2) $N>>1$ and $p<<1$

c) Comment on your observation.

2. For the following distributions.

(i) the uniform distribution $\rho(x) = \frac{1}{b-a}$ for $a \leq x \leq b$.
(ii) the Gaussian distribution $\rho(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[\frac{-x^2}{2\sigma^2}]$.
(iii) the Boltzmann distribution $\rho(x) = \exp[-\frac{x}{k_B T}]$

a) Write a programme to generate random numbers between 0 and 1.

b) Write a programme to draw $N = 10, 100, 1000, 10000$ samples x from each distribution.

c) Plot the histrogram of drawn samples for each N and each distribution.

d) Calculate the mean and variance from your samples. How do they compare to the actual values of mean and variance?

3. The file `data.txt` contains the dihedral angle (chiL) values of Alanine-Leucine (AL) obtained from the molecular dynamics simulation.

a) Plot the time series and normalized distribution.

b) Discretize and plot the data using different bin widths i.e. $5^0, 10^0, 15^0, 20^0, 15^0, 30^0$. Which bin width size do you think result in better discretization and why?

`[You can use any of your favourite programming language.]`