

1.) Random Numbers

Create a program which calculates the average of N random numbers taken from a uniform random number distribution. The program must run for $N=10,100,1000,10000,100000,1000000$ random numbers. Plot the mean value as a function of N (it's preferable that the axis of N is logarithmic). Describe your conclusions from the results. As initial seed use your record number (as in all following problems).

2.) Trapping

- a. Create a program which constructs a lattice of one (1) dimension and 100000 sites. In this lattice put at random positions a number of trap molecules, which will have concentration c . Put 1 particle in a random position on the lattice and let it perform a random walk. In this walk you will not place a time restriction, namely you will not declare a specific number of steps. The walk will stop when the particle falls on a trap. The time needed for this to happen is the trapping time. Perform 100000 runs, save the trapping times and make the distribution of these times. From this distribution calculate the survival probability $\Phi(c,n)$. Run this program for $c=10^{-1}$, 10^{-2} and 10^{-3} . Put the 3 survival probabilities in the same graph and compare them with the Rosenstock approximation. After that plot the survival probability $\Phi(c,n)$ as a function of the combination $x=cn^{1/2}$. Describe your conclusions.
- b. As in (a) but use a two (2) dimensional lattice of size 1000×1000 . Calculate the survival probability for $c=10^{-2}$ and 10^{-3} and compare it with the Rosenstock approximation. Beware of boundary conditions. When the particle reaches the borders of the lattice it shouldn't be allowed to escape from it but to remain in the lattice, either by returning on it former position or by being placed in the opposite site of the lattice

3.) Networks

Create a network with N nodes. Use $N=10000$ and $N=100000$ for:

- Random distribution of connections. Use the rule that for every possible connection between two (2) nodes there is a probability of $1/6$. Find the k of every node, where k is its number of connections. Make the distribution of $P(k)$ and plot $P(k)$ vs k on a graph.
- Power law distribution which results in a scale-free network. Use the distribution $P(k) \sim k^{-\gamma}$, where γ is constant. Here use $\gamma=2, 2.5, 3$. Use the values $k_{\min}=1$ and $k_{\max}=N$. On a graph (with logarithmic axes) create the distributions $P(k)$ vs k for the three values of γ .

The data will be the average of 100 runs.

4.) Percolation

Create a two (2) dimensional lattice of size $N \times N$. N should take different values and usually be in the interval $100 < N < 1000$. The lattice sites will be 0 or 1 with a probability p to be 1 and $(1-p)$ to be 0. After that, apply the CMLT algorithm to find the distribution of clusters. Change p from 0.1 to 0.8, initially with $\Delta p=0.1$ but near the critical point p_c with $\Delta p=0.01$.

Calculate the quantity:

$$I_{av} = \sum_{m=1}^{m_{\max}} \frac{i_m m^2}{pN^2}$$

where m is the size of clusters and i_m is the number of clusters of size m . Afterwards calculate I'_{av} which is the same as I_{av} , but without the bigger cluster. Plot I_{av} vs p and I'_{av} vs p . All the results must be averages, so 1000 runs are needed.

Calculate P_{\max} and plot P_{\max} vs p .

$$P_{\max} = \frac{m_{\max}}{pN^2}$$

From the equations:

$$I_{\alpha\nu}(p) = k|p - p_c|^{-\gamma}, p < p_c$$

$$I'_{\alpha\nu}(p) = k'|p - p_c|^{-\gamma'}, p > p_c$$

$$P_{\infty}(p) = k^n|p - p_c|^{-\beta}$$

find the critical exponents b, γ, γ'

5.) Molecular Dynamics

In all exercises we assume units in which $\sigma = \varepsilon = m = 1$.

a. The Lennard-Jones potential is given:

$$\phi(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} + \left(\frac{\sigma}{r} \right)^6 \right]$$

which describes the interaction potential between two atoms A and B which are at distance r . We assume that their initial positions are (4,2) and (3,1), when their velocities are (1,-2) and (1,-2).

- i. What is the force applied between the two atoms?
- ii. Which will be their position the moment $t_1 = \Delta t$ where $\Delta t = 0.2$?
- iii. Which will be their velocity the moment t_1 ?
- iv. Calculate the problems (ii) and (iii) for $t_2 = t_1 + \Delta t$ until $t_{50} = t_{49} + \Delta t$. Create a graphical representation of the orbits of the two atoms until t_{50} .

For the calculation of the positions and velocities use the Verlet algorithm for velocities.

- b. We consider a liquid with density $\rho = 0.7$. We simulate a system of $N = 256$ atoms. The initial positions of the atoms are in a lattice with small random displacements. The assignment of initial velocities is random, so that the magnitude of the initial velocities varies from 0 to 0.5 (alternatively all velocities may be $v_i(t=0) = 0$). We calculate the interactions between atoms only if their distance is $r < R_c = 2.5\sigma$. We have cyclic boundary conditions.

- i. Calculate the potential energy $V(t)$ of the system, the kinetic energy:
$$K(t) = \frac{1}{2} \sum m_i [v_i(t)]^2$$
, as well as the total energy $E(t)=V(t)+K(t)$ as a function of time.
 - ii. Afterwards plot in a graph the temperature as a function of time for the same time interval, using the equation $K = 3/2 Nk_B T$.
 - iii. Calculate the mean square displacement of the atoms as a function of time $\langle R^2(t) \rangle$.
- c. Molecular Dynamics under constant temperature. We use the conditions of the previous exercise but now the temperature is constant. Calculate the kinetic, potential and total energy as a function of time, as well as the temperature. Begin with $T=0.2$ and repeat for $T=0.5$ and $T=1.0$.

6. Correlation Coefficient Matrix of Stock Market prices.

Analyzing the correlation coefficient matrix is of great importance to many scientific fields dealing with multivariate time series. One such field is that of EconoPhysics. In the file “prices.zip” you will find the daily closing prices $P_i(t)$ of a group 20 of stocks from the Athens Stock Exchange for the year 2004. Thus you have a total of 253 closing prices for each stock. From these prices calculate:

- The logarithmic returns, using the formula: $r(t) = \ln P_i(t) - \ln P_i(t-1)$.
Hint: The result should be a vector with 252 return values for each stock.
- The correlation coefficient matrix, where every matrix element i, j will be calculated using the linear (Pearson's) cross-correlation formula:

$$\rho_{ij} = \frac{\langle r_i r_j \rangle - \langle r_i \rangle \langle r_j \rangle}{\sqrt{(\langle r_i^2 \rangle - \langle r_i \rangle^2)(\langle r_j^2 \rangle - \langle r_j \rangle^2)}}, \text{ where } \langle \dots \rangle \text{ stands for the time average over}$$

all the investigated period.

Hint : The result should be a 20x20 matrix with values ranging from -1 to 1.

- The distance matrix, which is calculated by applying the transformation $d_{ij} = \sqrt{2(1 - \rho_{ij})}$ to all the elements of the correlation coefficient matrix.

Hint : The result should be a 20x20 matrix with values ranging from 0 to 2.