

Deadline: Friday 28 October 2005

Question 1 *Random walk in 1 dimension*

A particle starts at $x = 0$ for $t = 0$ and then moves by Δ during the time interval δt . The values of Δ for different time steps are stochastically independent.

We expect the probability density function of the x -position X to spread according to the diffusion equation

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2},$$

which has the Green's function

$$G(x-x', t-t') = \frac{1}{\sqrt{4\pi D(t-t')}} e^{-\frac{(x-x')^2}{4D(t-t')}} \quad (1)$$

- (a) Assume $\Delta = \pm 1$, where the sign is randomly chosen for each time step. Plot the probability density function after $N_t = 1000$ steps and try to fit a Gaussian (1) to it. What is the diffusion constant D ? How can you test whether the broadening of the PDF is really described by Eq. (1)?
- (b) Repeat part (a) for $\Delta \sim \mathcal{U}(-0.5, 0.5)$.
- (c) Returning to $\Delta = \pm 1$, try to obtain the PDF of the *return time*, i.e. the time it takes for one particle to return to the origin for the first time. Will the average return time be finite?

Question 2 *Two-dimensional Ising model*

Program the two-dimensional Ising model

$$E = -\varepsilon \sum_{i=0}^{N-1} s_{ik} (s_{i-1,k} + s_{i+1,k} + s_{i,k-1} + s_{i,k+1})$$

for $N \times N$ spins. Assume periodic boundary conditions.

- (a) Vectorize the problem.
- (b) Using $N = 20$ points in each direction, plot energy per spin E/N and magnetization per spin as function of temperature T .
- (c) Plot the specific heat c_v as a function of temperature T .
- (d) Do you see indications of a phase transition?

Hints:

- You may need to increase N , but keep in mind that equilibration will take longer then.
- The IDL function `shift(array,n1,n2)` takes an array and performs a cyclic shift of its elements by n_1 in the first direction and n_2 in the second.

Question 3 *The travelling salesman problem*

A salesman starts from Calgary to a round trip through the following Canadian cities:

- Edmonton
 - Halifax
 - Montreal
 - Ottawa
 - Vancouver
 - (Calgary)
- (a) Use *simulated annealing* to find a sequence of these cities that tries to minimize the total mileage.
- (b) Increase the cooling ‘time’ and repeat the experiment to make sure you get consistent results.
- (c) How long is the round trip? Sketch the route.
- (d) Now assume that the Transcanada Highway is impassable between Calgary and Vancouver. How does the route change? [Assume that the other distances have not changed – which is quite inconsistent]

Hints:

- Number the cities and construct a distance matrix You can find the distances at <http://www.trailcanada.com/travel/gettingaround-distances.asp> or http://www.craigmarlatt.com/canada/geography&maps/distances_between_cities.html.
- Change the current route by interchanging an randomly picked pair of cities.