2017

Stochastic Simulation (Universiteit van Amsterdam)

Written exam stochastic simulation.

21 December 2017, 13.00 - 16.00, SP D1.115 & D1.116

This exam has 3 assignments, and each assignment has equal weight.

Assignment 1

Consider a non-avoiding one dimensional random walker, which can either take a step of length l to the left or the right with equal probability p, take a step on length 0 with probability q, and take a step of length $2l$ with probability r. Denote with $P(x)$ the probability density that the random walker takes a step x from its current position.

1.1 Write a complete expression for $P(x)$.
1.2 How are the numbers p, q and r related?
1.3 Compute the mean displacement $E[x]$ and the variance $Var[x]$ after one step of the random walker, where the initial position is a $x = 0$.
1.4 Interpret your result of $E[x]$ and $Var[x]$ for $r = 0$ and $r = 1$ in terms of the dynamics of the random walker.
1.5 For any other value of r, describe the dynamical behaviour you expect for this random walker, explain why.

Assume that the time for one step of the random walker is τ, N is the number of steps taken and then define the time t as $N\tau$. Moreover, the current position of the random walker is denoted by x. Finally define $P(x,t)$ as the probability that on time t the random walker is on position x.

1.6 Derive a master equation for $P(x,t)$.
1.7 Show that for small enough l and τ the probability $P(x,t)$ is governed by an advection-diffusion equation, so
$$\partial P(x,t)/\partial t + c\,\partial P(x,t)/\partial x = D\,\partial^2 P(x,t)/\partial x^2$$
and derive an expression for the diffusion coefficient D and the advection velocity c as a function of l, τ, and p, q, and r.
1.8 What happens in the limit of $r = 1$ (as in 1.4), reinterpret your result in 1.7

Assignment 2

2.1 What is variance reduction, and why is this needed?
2.2 One example of variance reduction is using antithetic variables. Explain how this variance reduction method works.
2.3 What is stratified sampling?

Call $\overline{X}$ the sample mean and $\mathcal{E}$ the stratified estimator of $E[X]$, and Y the discrete random variable that was used to stratify X. Using conditional variances, we can derive that $Var[\overline{X}] - \mathrm{Var}[\mathcal{E}] = \frac{1}{n} Var[E[X|Y]]$ where n is the total number of samples.

2.4 Interpret this equation, what does this mean when simulating $E[X]$ using stratified sampling of X with Y?

Suppose that X is defined on the interval (0,1). Also suppose that f(X), the pdf of X, is such that $\int_{0.4}^{0.6} f(X)dx = 0.99$.

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2.5 Propose a stratified sampling for this situation, and write an equation for the probability mass function of the discrete random variable Y that is used to stratify X.

Assignment 3

Consider a discrete random variable X which can take N possible values. Consider a Markov process and denote by X_n the value of X at time n. Finally define transition probabilities as $p_{ij} = P(X_{n+1} = j | X_n = i)$

Suppose $N = 4$ and the transition matrix is $\begin{bmatrix} 0.8 & 0.2 & 0 & 0 \\ 0.2 & 0.8 & 0 & 0 \\ 0 & 0 & 0.6 & 0.4 \\ 0 & 0 & 0.4 & 0.6 \end{bmatrix}$.

3.1 Is this Markov process irreducible? Explain why.
3.2 For a general Markov process, what are the stationary distribution and what are the limiting probabilities, and under what conditions are they the same?
3.3 Now assume that you have a Markov process where the stationary distribution is the same as the limiting probabilities. Explain why this property is so important for simulations

Now consider a 2-dimensional Ising system of $N \times N$ spins. Consider the case without an external magnetic field. The energy of a microstate is now given by $E = -J \sum_{<ij>} s_i s_j$ where s_i is the spin state of spin i, and $<ij>$ denotes summation of nearest neighbours. Finally, assume that the temperature is T.

3.4 What is the probability p_s to find the Ising system in a specific microstate s?

Next, we perturb the system by randomly selecting one spin and flipping it.

3.5 What is the maximum change of energy of the Ising system after such spin flip, and why?

Suppose we want to estimate the specific heat of the Ising system as a function of temperature, using the fact that the specific heat is proportional to the variance of the energy fluctuations.

3.6 How would you simulate this, describe in some detail the algorithms you would use, and explain why they sample correctly the fluctuations in the energy?
3.7 Finally, when you simulate the specific heat with the algorithm proposed in 3.6, you are estimating the variance of the energy fluctuations. Describe a clear procedure to how to communicate the quality of your result.