studeersnel

2016 - exam

Stochastic Simulation (Universiteit van Amsterdam)

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Gedownload door Nitai Nijholt (nitai1995@gmail.com)

Written exam stochastic simulation.

19 December 2016, 13.00 - 16.00, SP H.08

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

Assignment 1

Avoiding random walkers have the property that they can only visit a site once. Consider a one-dimensional *avoiding* random walker, which can either take a step of length l to the left or the right with equal probability q. Assume that the random walker starts on position $x = 0$.

1.1 Describe the dynamical behaviour you expect for this avoiding random walker, explain why.

We now lift the constraint of avoidance, and consider the same random walker but now as a *non-avoiding* random walker, so the random walker can visit a site more than once.

1.2 Describe the dynamical behaviour you expect for this non-avoiding random walker, explain why.

Assume next that the *non-avoiding* random walker can also take a step of $2l$ to the right with probability r. Denote with $p(x)$ the probability density that the random walker takes a step x from its current position.

1.3 Write a complete expression for $p(x)$.
1.4 How are the numbers q and r related?
1.5 Compute the mean displacement $E[x]$ and the variance $Var[x]$ after one step of the random walker. Try to simplify your expressions where possible.
1.6 Interpret your result of $E[x]$ and $Var[x]$ as a function of r in terms of the dynamics of the random walker.

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.

1.7 Derive a master equation for $P(x,t)$.
1.8 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 r.
1.9 How do D and c depend on r, and interpret this in terms of the dynamics of the underlying random walker.

Assignment 2

2.1 What is a Monte Carlo (MC) method in general terms? And where and how does stochasticity enter MC methods?

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Suppose that in some MC method you have generated n independent samples X_i with equal but unknown probability density function, with expected value Θ and variance σ^2. The sample mean is $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$.

2.2 Derive an expression Var[$\bar{X}$] as function of σ and n.

Now suppose you got the rather 'vague' requirement to estimate θ to an accuracy of 2% using this MC method.

2.3 Referring in detail to the theory behind MC methods, translate this requirement to a recipe for the simulations, and formulate a statistically sound way to report the final result of the simulations.

It may happen that you need to invoke advanced techniques known as Variance Reduction in your MC simulations.

2.4 What is Variance Reduction? Describe why you would need it.
2.5 One Variance Reduction technique is Importance Sampling. Explain this method.

Suppose we want to estimate $\int_0^1 e^{-x}dx$ using MC integration. A possible way for Variance Reduction for this integral could be antithetic variables.

2.6 Explain antithetic variables.
2.7 Would antithetic variables work for the MC integration problem stated above? Explain your answer.

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 $p_{ij} = P((X_{n+1} = j|X_{n+1} = i)$

3.1 When do we call such a Markov process irreducible?

Next, consider the simplest possible Ising spin model consisting of 2 spins, without an external field.

3.2 How many possible states does this model have, and list them all.

We first assume that all states in the Ising model have equal probability of occurring.

3.3 In which physical limit would this be possible?

We want to construct a Markov process that simulates the Ising model in the limit of all states occurring with equal probability.

3.4 What are the stationary probabilities π_i for this Markov process?
3.5 Derive for this situation the transition probabilities p_{ij}.

Turn over for continuation of third assignment.

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Next we consider the more complicated situation of a much larger Ising spin model with S spins at temperature T.

3.6 What is the probability of a specific spin state to occur?

We want to simulate the average magnetization $\langle M \rangle$ of this spin system, using a Metropolis algorithm.

3.7 Describe in some detail the Metropolis algorithm for this system (assume single spin flipping), including an equation for the transition probabilities.

3.8 Finally, explain how you would actually run the simulation (including a warm up period) and estimate $\langle M \rangle$, using a batch sampling method. How would you compute the errors in your estimate of $\langle M \rangle$?

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