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THE NATIONAL UNIVERSITY OF IRELAND MAYNOOTH

MATHEMATICAL PHYSICS

SEMESTER 1
2018–2019

Computational Physics 2
MP468C

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Time allowed: 2 hours

Answer ALL questions

All questions carry equal marks

1. (a) Assuming a generator of uniform pseudo-random numbers between 0 and 1 is given, use the transformation method to construct a recipe for obtaining pseudo-random numbers in the interval $[a, b]$, with the following probability distribution.

$$p(y) = \frac{y^6}{N}, \tag{1.1}$$

where N is a normalisation constant. **[10 marks]**

(b) Given a generator of pseudo-random numbers distributed according to $g(x) = \frac{1}{N}\exp(-4x^2)$, where N is a normalisation constant, use the rejection method to construct a recipe for obtaining pseudo-random numbers distributed over the real line according to

$$f(x) = \frac{e^{-4x^2}}{M(x^2+1)}, \tag{1.2}$$

where is M a normalisation constant. You may assume C is a positive constant such that $f(x) \leq Cg(x)$ for all $x \in \mathbb{R}$. **[10 marks]**

(c) Assuming you have a random number generator to generate pseudo-random numbers x with the following distribution:

$$p(x) = \frac{2x}{x^2+1}, \quad x \in [0, \sqrt{e-1}\,]. \tag{1.3}$$

explain how you would use Monte Carlo integration with importance sampling to compute the following integral:

$$I = \int_0^{\sqrt{e-1}} \frac{4x^3}{3x^2+3} dx \tag{1.4}$$

[10 marks]

(d) Derive the master equation for a Markov chain,

$$P(X, t_{n+1}) - P(X, t_n) = \sum_Y [P(Y, t_n)T(Y \to X) - P(X, t_n)T(X \to Y)]. \tag{1.5}$$

Using this, derive the detailed balance condition for a stationary Markov chain,

$$P(X)T(X \to Y) = P(Y)T(Y \to X). \tag{1.6}$$

[10 marks]

(e) List the key steps of the Metropolis algorithm for creating an ergodic Markov chain which leads to the stationary distribution $P(X)$. Prove the detailed balance condition is satisfied by the resultant Markov chain. **[10 marks]**

2. (a) Consider the matrix equation

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b}, \tag{2.1}$$

where $\mathbf{A}$ is a known $N \times N$ matrix, $\mathbf{b}$ is a known vector of length N, and $\mathbf{x}$ is a vector of N unknowns $x_i, i = 1, \cdots, N$. Explain how this equation may be solved using gaussian elimination. **[10 marks]**

(b) Show that the number of floating point operations (multiplication, division, addition, subtraction) required to obtain the solution this way grows like N^3 as N increases.

[10 marks]

(c) Using symmetric finite difference equations for the first and second derivative, show that the discretised version of the differential equation for the unknown function $y(x)$

$$\frac{\partial^2 y}{\partial x^2}(x) + g(x)\frac{\partial y}{\partial x}(x) + h(x)y(x) = f(x), \quad y(a) = c_1,\ y(b) = c_2, \tag{2.2}$$

where $g(x), h(x)$ and $f(x)$ are known functions of x, can be written in the form $\mathbf{A} \cdot \mathbf{y} = \mathbf{b}$, where A is a tridiagonal matrix and b is a known vector. **[12 marks]**

(d) Consider the $1 + 1$ dimensional diffusion equation

$$\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2}. \tag{2.3}$$

Write down the Forward Time Centred Space discretisation scheme for this equation, assuming a lattice spacing δx in the space direction and a spacing Δt in the time direction.

[12 marks]

(e) Using von Neumann stability analysis, derive the stability criterion for this scheme

$$\Delta t \leq \frac{(\delta x)^2}{2D} \tag{2.4}$$

[6 marks]

Solutions: Question 1

(a) We want to find a function f such that, given X is uniformly distributed between 0 and 1, $Y = f(X)$ is distributed in the interval $[a, b]$ according to

$$p(y) = \frac{y^6}{N}. \tag{0.5}$$

We know that

$$\begin{aligned} \text{Probability } X \in [\epsilon, \delta] &= \text{Probability } Y \in [f(\epsilon), f(\delta)], && (0.6)\\ \implies \int_\epsilon^\delta P_X(x)dx &= \int_{f(\epsilon)}^{f(\delta)} P_Y(y)dy, && (0.7)\\ \implies \int_0^x dx' &= \int_0^y \frac{(y')^6}{N} dy', && (0.8)\\ \implies x &= \frac{1}{N}\left[\frac{y^7}{7} - \frac{a^7}{7}\right]. && (0.9) \end{aligned}$$

Inverting this gives

$$y = \sqrt[7]{7Nx + a^7}. \tag{0.10}$$

Hence, generating a uniformly distributed number X between 0 and 1 and applying the function $f(x) = \sqrt[7]{7Nx + a^7}$ produces a number Y which is distributed according to (0.5). **[10 marks]**

(b) Given a constant $C \in \mathbb{R}$, the following three steps will produce a random number Y distributed according to $g(x)$ given generators for producing random numbers u distributed uniformly between 0 and 1 and X distributed according to $f(x)$.

(a) Generate a random number X according to $g(x)$.
(b) Generate a uniformly distributed random number u between 0 and 1.
(c) If $u < f(X)/Cg(X)$, accept $Y = X$. Other wise reject X and execute these three steps again.

[7 marks]

Using the expressions for $f(x)$ and $g(x)$ given in the question, these steps become the following

(a) Generate a random number X according to $g(x)$.
(b) Generate a uniformly distributed random number u between 0 and 1.

(c) If $u < \frac{N}{CM(X^2+1)}$, accept $Y = X$. Other wise reject X and execute these three steps again.

[3 marks]

(c) Rewritting the integrand yields

$$I = \int_0^{\sqrt{e-1}} \frac{4x^3}{3x^2+3} dx \tag{0.11}$$

$$= \int_0^{\sqrt{e-1}} \frac{2x^2}{3} \frac{2x}{x^2+1} dx \tag{0.12}$$

$$= \int_0^{\sqrt{e-1}} \frac{2x^2}{3} p(x) dx \tag{0.13}$$

Hence, to compute I using Monte Carlo integration with importance sampling one can generate N pseudo-random numbers x_i distributed under $p(x)$ and compute

$$I = \frac{2}{3N} \sum_{i=1}^{N} x^2 \tag{0.14}$$

[10 marks]

(d) If the probability of being in state X at time t_n is $P(X, t_n)$ and the transition probabilities of the Markov chain are denoted by $T(X \to Y)$, then the probability of being in state X at time t_{n+1} is

$$P(X, t_{n+1}) = \sum_Y P(Y, t_n) T(Y \to X). \tag{0.15}$$

Also, we know

$$\sum_Y T(X \to Y) = 1 \implies P(X, t_n) = P(X, t_n) \sum_Y T(X \to Y). \tag{0.16}$$

Subtracting the equation for $P(X, t_{n+1})$ and $P(X, t_n)$ to get the change in probability of being in state X after one step of the Markov chain yields the master equation:

$$P(X, t_{n+1}) - P(X, t_n) = \sum_Y [P(Y, t_n) T(Y \to X) - P(X, t_n) T(X \to Y)]. \tag{0.17}$$

For a stationary Markov chain, the probabilities $P(X, t)$ don't change in time and so the left hand side of the master equation is zero. To ensure the Markov chain is stationary for the probabilities $P(X)$, we may require that each term in the sum on the right hand side of the master equation is zero. This gives the condition of detailed balance:

$$P(Y)T(Y \to X) - P(X)T(X \to Y) = 0 \implies P(X)T(X \to Y) = P(Y)T(Y \to X). \quad (0.18)$$

[10 marks]

(e) We first choose a Markov chain where each step of the process can be separated into two steps: a trial step where a new state Y is proposed to be the new state, given the current state X, and an acceptance step where the proposed state Y is accepted as the new state with probability $A_{X,Y}$, other wise the system remains in state X. The transition probabilities of such a process can be factored into a trial probability $\omega_{X,Y}$ (the probability of choosing the state Y given the current state X), which we choose to be symmetric in X and Y, and an acceptance probability $A_{X,Y}$.

$$T(X \to Y) = \omega_{X,Y} A_{X,Y}. \quad (0.19)$$

The Metropolis algorithm is the following choice of acceptance probability.

$$A_{X,Y} = \begin{cases} 1 \text{ if } P(X) \leq P(Y) \\ \frac{P(Y)}{P(X)} \text{ if } P(Y) \leq P(X) \end{cases}. \quad (0.20)$$

[6 marks]

To see this Markov chain satisfies the condition of detailed balance we can look at the following quotient.

$$\frac{T(X \to Y)}{T(Y \to X)} = \frac{\omega_{X,Y} A_{X,Y}}{\omega_{Y,X} A_{Y,X}} = \frac{A_{X,Y}}{A_{Y,X}} = \frac{P(Y)}{P(X)}. \quad (0.21)$$

This is the detailed balance condition. **[4 marks]**

Solutions: Question 2

(a) The equation $\mathbf{A} \cdot \mathbf{y} = \mathbf{b}$ can be solved by repeatedly replacing rows of the equation with a linear combination of themselves and another row in the following way.

  (a) First divide the first row by its first element so that the top left element is 1.
  (b) Subtract the first row from the remaining $N - 1$ rows so that the first element in each is 0.
  (c) repeat (i) and (ii) on the remaining $(N - 1) \times (N - 1)$ sub-matrix.
  (d) Continue until the matrix $\mathbf{A}$ is in upper triangular form.
  (e) the vector $\mathbf{x}$ can then be found by back substitution.

[10 marks]

(b) In the first step of Gaussian elimination on an $N \times N$ matrix we must perform N division to ($N-1$ elements of $\mathbf{A}$ and the first element of $\mathbf{b}$). Then there are $N(N-1)$ multiplications and $N(N-1)$ subtractions to be made so that the first element of each of the $N-1$ remaining rows is zero. So there are $N + 2N(N-1) = N(2N-1)$ operations in total in the first step. This procedure is then repeated in the second step in the $(N-1)\times(N-1)$ sub-matrix. Hence, the total number of operations is

$$\sum_{n=1}^{N} n(2n-1) \approx N^3. \tag{0.22}$$

[10 marks]

(c) The symmetric finite difference equation for the first derivative of a function f is

$$f'(x) = \frac{f(x+a) - f(x-a)}{2a}. \tag{0.23}$$

The symmetric finite difference equation for the second derivative of a function f is

$$f''(x) = \frac{f(x+a) - 2f(x) + f(x-a)}{a^2}. \tag{0.24}$$

We discretise an interval of the real line, $[a, b]$ into a set of $N+2$ points separated by a spacing dx. For a function $y(x)$ on the interval we write

$$y(x) = y(x_0 + idx) = y_i, \tag{0.25}$$

where $i, j = 0 \cdots N+1$. Similarly $f(x) = f(x_i) = f_i$. The first and second derivatives at points away from the boundary are then given by

$$\frac{\partial y}{\partial x}(x) = \frac{y_{i+1} - y_{i-1}}{2a}, \tag{0.26}$$

$$\frac{\partial^2 y}{\partial x^2}(x) = \frac{y_{i+1} - 2y_i + y_{i-1}}{a^2}. \tag{0.27}$$

Substituting these into the differential equation yields

$$\frac{\partial^2\phi}{\partial x^2} + g(x)\frac{\partial\phi}{\partial x} + h(x)y(x) = f(x), \tag{0.28}$$

$$\implies \frac{y_{i+1} - 2y_i + y_{i-1}}{dx^2} + g_i\frac{y_{i+1} - y_{i-1}}{2dx} + h_i y_i = f_i \tag{0.29}$$

$$\implies \left(1 + \frac{g_i dx}{2}\right) y_{i+1} + (h_i - 2)y_i + \left(1 - \frac{g_i dx}{2}\right) y_{i-1} + = dx^2 f_i \tag{0.30}$$

[10 marks]

The last equation can be written in the form $\mathbf{A} \cdot \mathbf{y} = \mathbf{b}$ where $\mathbf{A}$ is a $N \times N$ tridiagonal matrix where the elements of the main diagonal equal are given by the vector $(h_i - 2)$, the elements of the first sub diagonal are given by the vector $1 - \frac{g_i dx}{2}$ and the elements of the first super diagonal are given by the vector $1 + \frac{g_i dx}{2}$. The elements of the vector $\mathbf{y}$ are y_i. The first and last elements of $\mathbf{b}$ are $dx^2 f_1 - c_1$ and $dx^2 f_N - c_2$ respectively and $dx^2 f_i$ for $i = 2 \cdots N - 1$.

[2 marks]

(d) The forward finite difference equation for the first derivative of a function f is

$$f'(x) = \frac{f(x+a) - f(x)}{a}. \tag{0.31}$$

The centred finite difference equation for the second derivative of a function f is

$$f''(x) = \frac{f(x+a) - 2f(x) + f(x-a)}{a^2}. \tag{0.32}$$

If we discretise the x, t-plane into a lattice with spacing δx in the space direction and Δt in the time direction we can write

$$\phi(x_i, t_n) = \phi(x_0 + i\delta x, t_0 + n\Delta t) = \phi_i^n, \tag{0.33}$$

where (x_i, t_n) is a point on the lattice. Then the Forward Time Centred Space discretisation scheme for this equation is the following finite difference equation.

$$\frac{\partial\phi}{\partial t} = D\frac{\partial^2\phi}{\partial x^2}, \tag{0.34}$$

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = D\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{(\delta x)^2} \tag{0.35}$$

$$\phi_i^{n+1} = \left(1 - \frac{2D\Delta t}{(\delta x)^2}\right)\phi_i^n + \frac{D\Delta t}{(\delta x)^2}\left(\phi_{i+1}^n + \phi_{i-1}^n\right) \tag{0.36}$$

[12 marks]

(e) Considering $\Phi(k)$, the Fourier transform of $\phi(x)$ in the space direction, each Fourier mode evolves independently in time for the diffusion equation. This gives the eigenmode evolution

$$\Phi_K^{n+1} = \xi_k \Phi_K^n \implies \Phi_K^n = \xi_k^n \Phi_K^0. \tag{0.37}$$

Inserting this into the FTCS scheme for the diffusion equation gives

$$\frac{\xi_k^{n+1} e^{ijk\delta x} - \xi_k^n e^{ijk\delta x}}{\Delta t} = D\xi_k^n \frac{e^{i(j-1)k\delta x} - 2e^{ijk\delta x} + e^{i(j+1)k\delta x}}{(\delta x)^2}. \tag{0.38}$$

Letting $n = 0$ and rearranging gives:

$$\xi_k = 1 - \frac{2D\Delta t}{(\delta x)^2}\left(e^{-ik\delta x} - 2 + e^{ik\delta x}\right) = 1 - \frac{4D\Delta t}{(\delta x)^2}\sin^2\left(\frac{k\delta x}{2}\right). \tag{0.39}$$

For stability we need $|\xi_k| \leq 1$ for all k. However, the above equation is always less than one, so we need $\xi_k \geq -1$ for all k. Therefore, we need

$$\frac{4D\Delta t}{(\delta x)^2}\sin^2\left(\frac{k\delta x}{2}\right) \leq 2. \tag{0.40}$$

The worst case is when k is such that $\sin^2(\frac{k\delta x}{2}) = 1$. Hence, to ensure stability, we should choose

$$\frac{4D\Delta t}{(\delta x)^2} \leq 2 \implies \Delta t \leq \frac{(\delta x)^2}{2D}. \tag{0.41}$$

[6 marks]