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THE NATIONAL UNIVERSITY OF IRELAND MAYNOOTH

THEORETICAL PHYSICS

Fourth Year

SEMESTER 1

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Computational Physics II
MP468
Solutions

Exam

1. (a) If X is uniformly distributed between 0 and 1 ($p(x) = 1, x \in [0, 1]$) and f is a function, How is the random variable $Y = f(X)$ distributed?

   [15 marks]

   (b) Use the transformation method to construct a recipe for obtaining pseudo-random numbers in the interval $[0, \sqrt{e-1}\,]$, with probability distribution

   $$p(y) = \frac{2y}{y^2+1}, \tag{1}$$

   given a generator of uniform pseudo-random numbers between 0 and 1

   [40 marks]

   (c) List the main steps of the rejection method for generating a pseudo-random number distributed according to $f(x)$, given a constant $M \in \mathbb{R}$ and generators for uniform pseudo-random numbers between 0 and 1 and pseudo-random numbers distributed according to $g(x)$ such that $f(x) < Mg(x)$, for all $x \in \mathbb{R}$. Prove that the rejection method produces a variable Y distributed according to $f(x)$.

   [45 marks]

2. (a) If x_i are N independent uniformly distributed random points within a d-dimensional volume V , and

   $$I_{\mathrm{MC}} = \frac{V}{N}\sum_{i=1}^{N} f(x_i), \tag{2}$$

   show that the expectation value of I_{MC} is equal to the integral of the function f over the volume V,

   $$\langle I_{\mathrm{MC}} \rangle = \int_V f(x)dx. \tag{3}$$

   Explain how this relation can be used to compute the integral I using Monte Carlo integration.

   [20 marks]

   (b) Show that the variance of I_{MC} is given by

   $$\mathrm{var}(I_{\mathrm{MC}}) = \langle (I_{\mathrm{MC}} - \langle I_{\mathrm{MC}} \rangle)^2 \rangle = \frac{V^2}{N}[\langle f^2 \rangle - \langle f \rangle^2] \tag{4}$$

   [40 marks]

   (c) Assuming you have a random number generator to generate pseudo-random numbers $x \in [0, \infty)$ with distribution $p(x) = \lambda \sin^2(x)\exp(-x)$ (where λ is a normalising constant), explain how you would compute the integral

   $$I = \int_0^\infty \sin(x)\sin(2x)e^{-x}dx \tag{5}$$

   using Monte Carlo integration with importance sampling.

[40 marks]

3. (a) Using symmetric first and second derivatives, write down the discretised version of the equation

$$A\frac{\partial^2 \phi}{\partial x^2} + B\frac{\partial^2 \phi}{\partial y^2} + C\frac{\partial \phi}{\partial x} + D\frac{\partial \phi}{\partial y} = \rho(x, y), \qquad 0 \le x, y \le L, \tag{6}$$

where A, B, C and D are known constants and $\rho(x, y)$ is a known function of x and y, on a square symmetric grid of $N \times N$ points with zero Dirichlet boundary conditions.

[25 marks]

(b) Explain how the resulting equation can be written as a matrix equation, $M\Phi = B$, where M is a sparse $N^2 \times N^2$ matrix and B is a known vector of length N^2. Write down expressions for M and B, taking the boundary conditions into account.

[25 marks]

(c) Consider the matrix equation

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b}, \tag{7}$$

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.

[25 marks]

(d) 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.

[25 marks]

4. (a) Consider the 2-dimensional Poisson equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = \rho(x, y). \tag{8}$$

Explain how the solution of this equation can be obtained by solving the diffusion equation

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} - \rho(x, y), \tag{9}$$

with an arbitrary initial condition for $\phi(x, y)$.

[15 marks]

(b) Write down the Forward Time Centred Space discretisation scheme for this equation, assuming equal lattice spacings $ax = ay = a$ in both space directions, and a spacing Δt in the time direction.

[35 marks]

(c) Using the von Neumann stability criterion for this scheme, $\Delta t \leq a^2/4$, derive the *Jacobi* method for solving the Poisson equation, and explain how it may be modified to obtain the *Gauss-Seidel* method.

[25 marks]

(d) Assuming that each iteration reduces the difference between your estimate and the true solution by a factor ρ_s (called the spectral radius), find how many iterations are required to reduce this difference by a factor 10^{-p}.

For the Poisson equation on a square $N \times N$ grid with homogeneous Dirichlet boundary conditions, the spectral radii for the Jacobi and Gauss-Seidel methods are given by

$$\text{Jacobi: } \rho_J = \cos\left(\frac{\pi}{N}\right), \qquad \text{Gauss-Seidel: } \rho_{GS} = \cos^2\left(\frac{\pi}{N}\right). \tag{10}$$

Use this to show that the Gauss-Seidel method converges twice as fast as the Jacobi method, and that the number of iterations required for both to converge increases as N^2 in the limit of large N.

[25 marks]

Solutions: Question 1

(a) If X is uniformly distributed between 0 and 1, f is a function and we define the random variable $Y = f(X)$, we must have

$$\text{Probability } X \in [a,b] = \text{Probability } Y \in [f(a), f(b)], \tag{11}$$

$$\implies \int_a^b P_X(x)dx = \int_{f(a)}^{f(b)} P_Y(y)dy, \tag{12}$$

$$= \int_a^b P_Y(f(x))|f'(x)|dx. \tag{13}$$

As this must be true for every interval $[a,b] \subset [0,1]$, we have

$$P_Y(y) = P_Y(f(x)) = \frac{P_X(x)}{|f'(x)|} = \frac{1}{|f'(x)|}. \tag{14}$$

[15 marks]

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

$$p(y) = \frac{2y}{y^2+1}, \tag{15}$$

We know that

$$
\begin{aligned}
\text{Probability } X \in [a, b] &= \text{Probability } Y \in [f(a), f(b)], && (16)\\
\implies \int_a^b P_X(x)dx &= \int_{f(a)}^{f(b)} P_Y(y)dy, && (17)\\
\implies \int_0^x dx' &= \int_0^y \frac{2y'}{y'^2+1}dy', && (18)\\
\implies x &= \int_1^{y^2+1} \frac{d\alpha}{\alpha}, && (19)\\
&= [\ln(\alpha)]_1^{y^2+1} = \ln(y^2+1) && (20)
\end{aligned}
$$

Inverting this gives

$$
y = \sqrt{e^x - 1}. \tag{21}
$$

[20 marks]

Hence, generating a uniformly distributed number X between 0 and 1 and applying the function $f(x) = \sqrt{e^x - 1}$ produces a number Y which is distributed according to (15).

[20 marks]

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

(i) Generate a random number X according to $f(x)$.

(ii) Generate a uniformly distributed random number u between 0 and 1.

(iii) If $u < f(X)/Mg(X)$, accept $Y = X$. Other wise reject X and execute these three steps again.

[20 marks]

To prove Y is distributed according to $f(x)$, we first show that the probability of Y being less than x is given by

$$
P(Y < x) = \int_{-\infty}^{x} f(\tilde{x})d\tilde{x}. \tag{22}
$$

We note, for Y to be less than x, two things must be true. Firstly, the random number u must be less than $f(X)/Mg(X)$. Then, provided that's true, X must be less than x. Hence, we have

$$
\begin{aligned}
P(Y < x) &= P(X < x | u < f(X)/Mg(X)), && (23)\\
&= \frac{P(X < x, u < f(X)/Mg(X))}{P(u < f(X)/Mg(X))}. && (24)
\end{aligned}
$$

We now note, that since X and u are independent random variables, the tuple (X, u) is distributed in the plane according to the product of distributions for X and u.

$$(X, u) \sim P(x, y) = g(x) P_{\text{uni}}^{[0,1]}(y). \tag{25}$$

Rewriting the probabilities appearing in (24) as integrals of the above distribution yields

$$P(Y < x) = \frac{\int_{-\infty}^{x} \left(\int_0^{f(\tilde{x})/Mg(\tilde{x})} g(\tilde{x}) dy \right) d\tilde{x}}{\int_{-\infty}^{+\infty} \left(\int_0^{f(\tilde{x})/Mg(\tilde{x})} g(\tilde{x}) dy \right) d\tilde{x}} \tag{26}$$

$$= \frac{\int_{-\infty}^{x} \left[f(\tilde{x})/Mg(\tilde{x}) \right] g(\tilde{x}) d\tilde{x}}{\int_{-\infty}^{+\infty} \left[f(\tilde{x})/Mg(\tilde{x}) \right] g(\tilde{x}) d\tilde{x}} \tag{27}$$

$$= \frac{\int_{-\infty}^{x} f(\tilde{x}) d\tilde{x}}{\int_{-\infty}^{+\infty} f(\tilde{x}) d\tilde{x}} \tag{28}$$

$$= \int_{-\infty}^{x} f(\tilde{x}) d\tilde{x} \tag{29}$$

The probability density of Y is given by the derivative of its cumulative distribution. So the distribution of Y must be

$$P_Y(y) = \frac{d}{dx} \left(\int_{-\infty}^{x} f(\tilde{x}) d\tilde{x} \right) \Big|_{x=y} = f(y), \tag{30}$$

proving that Y is distributed according to $f(x)$.

[25 marks]

Solutions: Question 2

(a) If X is uniformly distributed inside the d-dimensional volume V, then the expectation value of the quantity $f(X)$ is

$$\langle f \rangle = \int_V f(x) P_{\text{uni}}^V(x) dx = \int_V \frac{f(x)}{V} dx. \tag{31}$$

Hence the expectation value of I_{MC} is

$$\langle I_{\text{MC}} \rangle = \frac{V}{N} \sum_{i=1}^{N} \langle f \rangle = \frac{V}{N} \left(N \langle f \rangle \right), \tag{32}$$

$$= V \int_V \frac{f(x)}{V} dx = \int_V f(x) dx. \tag{33}$$

For the first equality we used the fact that the x_is are independent. Hence the expectation value of I_{MC} is the integral of f over the region V.

[20 marks]

(b)

$$
\begin{aligned}
\mathrm{var}(I_{\mathrm{MC}}) &= \langle (I_{\mathrm{MC}} - \langle I_{\mathrm{MC}} \rangle)^2 \rangle, && (34)\\
&= \langle (I_{\mathrm{MC}})^2 \rangle - \langle I_{\mathrm{MC}} \rangle^2, && (35)\\
&= \left\langle \left(\frac{V}{N} \sum_{i=1}^{N} f(x_i) \right)^2 \right\rangle - \left\langle \frac{V}{N} \sum_{i=1}^{N} f(x_i) \right\rangle^2, && (36)\\
&= \frac{V^2}{N^2} \left[\left\langle \left(\sum_{i=1}^{N} f(x_i) \right)^2 \right\rangle - \left\langle \sum_{i=1}^{N} f(x_i) \right\rangle^2 \right], && (37)\\
&= \frac{V^2}{N^2} \left[\left\langle \sum_{i=1}^{N} f(x_i)^2 + \sum_{\substack{i,j=1\\ i\neq j}}^{N} f(x_i) f(x_j) \right\rangle - (N\langle f \rangle)^2 \right], && (38)\\
&= \frac{V^2}{N^2} \left[N\langle f^2 \rangle + \sum_{\substack{i,j=1\\ i\neq j}}^{N} \langle f \rangle \langle f \rangle - N^2 \langle f \rangle^2 \right], && (39)\\
&= \frac{V^2}{N^2} \left[N\langle f^2 \rangle + \frac{N(N-1)}{N} \langle f \rangle^2 - N^2 \langle f \rangle^2 \right], && (40)\\
&= \frac{V^2}{N} \left[\langle f^2 \rangle - \langle f \rangle^2 \right]. && (41)
\end{aligned}
$$

[40 marks]

(c) Multiplying and dividing the integrand by $p(x)$ yields

$$
\begin{aligned}
I &= \int_0^\infty \sin(x)\sin(2x) e^{-x} dx && (42)\\
&= \int_0^\infty \sin(x)\sin(2x) e^{-x} \frac{p(x)}{p(x)} dx && (43)\\
&= \int_0^\infty \frac{\sin(x)\sin(2x)e^{-x}}{\lambda \sin^2(x) e^{-x}} p(x) dx && (44)\\
&= \int_0^\infty \frac{2\sin^2(x)\cos(x)}{\lambda \sin^2(x)} p(x) dx && (45)\\
&= \int_0^\infty \frac{2\cos(x)}{\lambda} p(x) dx && (46)
\end{aligned}
$$

[25 marks]

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

$$
I = \sum_{i=1}^{N} \frac{2\cos(x_i)}{\lambda} \tag{47}
$$

[15 marks]

Solutions: Question 3

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

$$f'(x) \to \frac{f(x+a) - f(x-a)}{2a}. \tag{48}$$

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

$$f''(x) \to \frac{f(x+a) - 2f(x) + f(x-a)}{a^2}. \tag{49}$$

We discretise the defined square region of the x, y-plane into a symmetric $(N+2) \times (N+2)$ grid, with lattice spacing $a = \frac{L}{N+1}$. For a function $\phi(x, y)$ on the interior points of the lattice we write

$$\phi(x, y) = \phi(ia, ja) = \phi_{i,j}, \tag{50}$$

where $i, j = 1 \cdots N$. The first and second derivatives, at interior points of the lattice, are then given by

$$\frac{\partial \phi}{\partial x}(x, y) \to \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2a}, \tag{51}$$

$$\frac{\partial \phi}{\partial x}(x, y) \to \frac{\phi_{i,j+1} - \phi_{i,j-1}}{2a}, \tag{52}$$

$$\frac{\partial^2 \phi}{\partial x^2}(x, y) \to \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{a^2}, \tag{53}$$

$$\frac{\partial^2 \phi}{\partial y^2}(x, y) \to \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{a^2}. \tag{54}$$

[10 marks]

Substituting these into the differential equation yields

$$\rho(x, y) = A\frac{\partial^2 \phi}{\partial x^2} + B\frac{\partial^2 \phi}{\partial y^2} + C\frac{\partial \phi}{\partial x} + D\frac{\partial \phi}{\partial y}, \tag{55}$$

$$\to A\frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{a^2} + B\frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{a^2} \tag{56}$$

$$+ C\frac{\phi_{i+1,j} - \phi_{i-1,j}}{2a} + D\frac{\phi_{i,j+1} - \phi_{i,j-1}}{2a}, \tag{57}$$

$$= \frac{1}{a^2}\left[\left(A + \frac{Ca}{2}\right)\phi_{i+1,j} + \left(A - \frac{Ca}{2}\right)\phi_{i-1,j}\right. \tag{58}$$

$$\left. + \left(B + \frac{Da}{2}\right)\phi_{i,j+1} + \left(B - \frac{Da}{2}\right)\phi_{i,j-1} - 4\phi_{i,j}\right] \tag{59}$$

[15 marks]

(b) We first define $\tilde{\rho}_{i,j} = a^2\rho(x, y)$ so we can write

$$\tilde{\rho}_{i,j} = \left(A + \frac{Ca}{2}\right)\phi_{i+1,j} + \left(A - \frac{Ca}{2}\right)\phi_{i-1,j} \tag{60}$$
$$+ \left(B + \frac{Da}{2}\right)\phi_{i,j+1} + \left(B - \frac{Da}{2}\right)\phi_{i,j-1} - 4\phi_{i,j}. \tag{61}$$

To write this as a matrix equation we number the sites of the $N \times N$ interior lattice 1 to N^2. The number we assign to the site (i, j) is $n = i + Nj$. Then we can list the values of $\phi_{i,j}$ and $\tilde{\rho}_{i,j}$, from 1 to N^2, in column vectors Φ and B respectively. The above equation then turns into the matrix equation $M\Phi = B$, where M is a $N^2 \times N^2$ matrix whose components are given by

$$\begin{aligned} M_{m,n} = &\left(A + \frac{Ca}{2}\right)\delta_{m,n+1} + \left(A - \frac{Ca}{2}\right)\delta_{m,n-1} \\ &+ \left(B + \frac{Da}{2}\right)\delta_{m,n+N} + \left(B - \frac{Da}{2}\right)\delta_{m,n-N} - 4\delta_{m,n} \end{aligned} \tag{62}$$

and the vector B is given by

$$B_n = \tilde{\rho}_n = \tilde{\rho}_{i,j}, \tag{63}$$

where $n = i + Nj$.

[20 marks]

Equations involving boundary terms, in the set of linear equations $M\Phi = B$, are treated differently since $\phi_{0,j} = \phi_{N+1,j} = \phi_{i,0} = \phi_{i,N+1} = 0$ (zero Dirichlet boundary conditions). This amounts to terms appearing in (62) being set to zero for certain values of m (certain row equations). Namely, the following terms in (62) are set to zero, (here $i(m)$ and $j(m)$ are the original indices.)

$$\text{When } i(m) = 1, \quad \delta_{m,n-1} = 0. \tag{64}$$
$$\text{When } i(m) = N, \quad \delta_{m,n+1} = 0. \tag{65}$$
$$\text{When } j(m) = 1, \quad \delta_{m,n-N} = 0. \tag{66}$$
$$\text{When } j(m) = N, \quad \delta_{m,n+N} = 0. \tag{67}$$

In general, to implement Dirichlet boundary conditions, one must subtract the boundary values from $\tilde{\rho}_n$ appropriately to form the vector B. However, since we want to implement zero Dirichlet boundary conditions, this amounts to subtracting zero, leaving the equation (63) unaltered.

[5 marks]

(c) 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.

(i) First divide the first row by its first element so that the top left element is 1.

(ii) Subtract the first row from the remaining $N-1$ rows so that the first element in each is 0.

(iii) repeat (i) and (ii) on the remaining $(N-1)\times(N-1)$ sub-matrix.

(iv) Continue until the matrix $\mathbf{A}$ is in upper triangular form.

(v) the vector $\mathbf{x}$ can then be found by back substitution.

[25 marks]

(d) 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

$$\sum_{n=1}^{N} n(2n-1) \approx N^3. \tag{68}$$

[25 marks]

Solutions: Question 4

(a) If we let an arbitrary state $\phi(x,y)$ evolve under the equation

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} - \rho(x,y), \tag{69}$$

for a long enough time, it will generally converge to a stationary solution Φ. For a stationary solution the left hand side of the above equation is zero and so $\Phi(x,y)$ satisfies

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = \rho(x,y). \tag{70}$$

[15 marks]

(b) If we use a lattice with equal lattice spacings $ax = ay = a$ in both space directions, and a spacing Δt in the time direction, the Forward Time Centred Space discretisation scheme for this equation is the following finite difference equation.

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} - \rho(x,y), \tag{71}$$

$$\frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} = \frac{\phi_{i+1,j}^{n} - 2\phi_{i,j}^{n} + \phi_{i-1,j}^{n}}{a^2} + \frac{\phi_{i,j+1}^{n} - 2\phi_{i,j}^{n} + \phi_{i,j-1}^{n}}{a^2} - \rho_{i,j} \tag{72}$$

$$\phi_{i,j}^{n+1} = \left(1 - \frac{4\Delta t}{a^2}\right)\phi_{i,j}^{n} + \frac{\Delta t}{a^2}\left(\phi_{i+1,j}^{n} + \phi_{i-1,j}^{n} + \phi_{i,j+1}^{n} + \phi_{i,j-1}^{n}\right) - \Delta t \rho_{i,j} \tag{73}$$

[35 marks]

(c) The von Neumann stability criterion for this scheme is $\Delta t \leq a^2/4$. The Jacobi method for solving the Poisson equation is to use the largest possible time step size $\Delta t = a^2/4$. This amounts to iterating the following equation to evolve an arbitrary initial state ϕ until it converges to a stationary state.

$$\phi_{i,j}^{n+1} = \frac{1}{4}\left(\phi_{i+1,j}^{n} + \phi_{i-1,j}^{n} + \phi_{i,j+1}^{n} + \phi_{i,j-1}^{n}\right) - \frac{a^2}{4}\rho_{i,j}. \tag{74}$$

[10 marks]

The above procedure can be modified to obtain the GaussSeidel method by using values of $\phi(n+1)$ that have already been computed to calculate each $\phi_{i,j}^{n+1}$. This amounts to using the following equation

$$\phi_{i,j}^{n+1} = \frac{1}{4}\left(\phi_{i+1,j}^{n} + \phi_{i-1,j}^{n+1} + \phi_{i,j+1}^{n} + \phi_{i,j-1}^{n+1}\right) - \frac{a^2}{4}\rho_{i,j}. \tag{75}$$

[15 marks]

(d) Assuming that each iteration reduces the difference between the estimate and the true solution by a factor ρ_s, the number of iterations n required to reduce this difference by a factor 10^{-p} is given by

$$\rho_s^n = 10^{-p}, \tag{76}$$

$$\implies n\ln(\rho_s) = -p\ln(10), \tag{77}$$

$$\implies n = \frac{-p\ln(10)}{\ln(\rho_s)}. \tag{78}$$

[15 marks]

For the Jacobi method we have $\rho_s = \rho_J = \cos(\frac{\pi}{N})$. So the number of iterations of the Jacobi method needed to reduce the difference by a factor of 10^{-p} is

$$n_J = \frac{-p\ln(10)}{\ln(\rho_J)} = \frac{-p\ln(10)}{\ln(\cos(\frac{\pi}{N}))}. \tag{79}$$

For the GaussSeidel method we have $\rho_s = \rho_{GS} = \cos^2(\frac{\pi}{N})$. So the number of iterations of the GaussSeidel method needed to reduce the difference by a factor of 10^{-p} is

$$n_{GS} = \frac{-p\ln(10)}{\ln(\rho_{GS})} = \frac{-p\ln(10)}{\ln(\cos^2(\frac{\pi}{N}))} = \frac{-p\ln(10)}{2\ln(\cos(\frac{\pi}{N}))} = \frac{n_J}{2} \tag{80}$$

Hence the GaussSeidel converges twice as fast as the Jacobi method.

[10 marks]