Maynooth University
National University of Ireland Maynooth

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THE NATIONAL UNIVERSITY OF IRELAND MAYNOOTH

MATHEMATICAL PHYSICS

REPEAT EXAMINATION

2018–2019

Computational Physics 2

MP468C

Prof. D. A. Johnston, Dr. J. Brennan. and Dr. J.-I. Skullerud

Time allowed: 2 hours

Answer ALL questions

1. (a) Use the transformation method to construct a recipe for obtaining pseudo-random numbers with probability distribution

$$p(y) = \frac{3y^2}{y^3+1}, \quad y \in [0, \sqrt[3]{e-1}\,]. \tag{1.1}$$

You may assume a generator of uniform pseudo-random numbers between 0 and 1 is given

[11 marks]

(b) 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 $f(x)$.

[15 marks]

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

$$I_{\mathrm{MC}} = \frac{V}{N}\sum_{i=1}^{N} f(x_i), \tag{1.2}$$

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

$$\langle I_{\mathrm{MC}} \rangle = \int_V f(x)dx. \tag{1.3}$$

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

[12 marks]

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

$$p(x) = e^{-x}, \quad x \in [0, \infty). \tag{1.4}$$

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

$$I = \int_0^\infty 4xe^{(4-x)}dx \tag{1.5}$$

[12 marks]

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

$$A\frac{\partial^2\phi}{\partial x^2} + B\frac{\partial^2\phi}{\partial y^2} + C\frac{\partial\phi}{\partial x} + D\frac{\partial\phi}{\partial y} = \rho(x,y), \qquad 0 \le x, y \le L, \tag{2.1}$$

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.

[13 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.

[10 marks]

(c) Write down the Forward Time Centred Space discretisation scheme for the equation below, assuming equal lattice spacings $\delta x = \delta y = a$ in both space directions, and a spacing Δt in the time direction.

$$\frac{\partial\phi}{\partial t} = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} - \rho(x,y), \tag{2.2}$$

[12 marks]

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

[10 marks]

(e) 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

$$\text{Jacobi: } \rho_J = \cos(\frac{\pi}{N}), \qquad \text{Gauss-Seidel: } \rho_{GS} = \cos^2(\frac{\pi}{N}). \tag{2.3}$$

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.

[5 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 according to

$$p(y) = \frac{3y^2}{y^3 + 1}, \tag{0.4}$$

We know that

$$\text{Probability } X \in [a, b] = \text{Probability } Y \in [f(a), f(b)], \tag{0.5}$$

$$\implies \int_a^b P_X(x)dx = \int_{f(a)}^{f(b)} P_Y(y)dy, \tag{0.6}$$

$$\implies \int_0^x dx' = \int_0^y \frac{3y'^2}{y'^3 + 1}dy', \tag{0.7}$$

$$\implies x = \int_1^{y^3+1} \frac{d\alpha}{\alpha} = \ln(y^3 + 1) \tag{0.8}$$

Inverting this gives

$$y = \sqrt[3]{e^x - 1}. \tag{0.9}$$

Hence, generating a uniformly distributed number X between 0 and 1 and applying the function $f(x) = \sqrt[3]{e^x - 1}$ produces a number Y which is distributed according to (0.4).

[11 marks]

(b) 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 $g(x)$.

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

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

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

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

$$P(Y < x) = \int_{-\infty}^{x} f(\tilde{x})d\tilde{x}. \tag{0.10}$$

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

$$P(Y < x) = P(X < x | u < f(x)/Mg(x)), \tag{0.11}$$

$$= \frac{P(X < x, u < f(x)/Mg(x))}{u < f(x)/Mg(x)}. \tag{0.12}$$

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.

$$(X, u) \sim P(x, y) = g(x) P_{\text{uni}}^{[0,1]}(y). \tag{0.13}$$

Rewriting the probabilities appearing in (0.12) as integrals of the above distribution yields

$$P(Y < x) = \frac{\int_{-\infty}^{x} \left(\int_0^{f(\tilde{x})/Mg(\tilde{x})} g(\tilde{x}) du \right) d\tilde{x}}{\int_{-\infty}^{+\infty} \left(\int_0^{f(\tilde{x})/Mg(\tilde{x})} g(\tilde{x}) du \right) d\tilde{x}} \tag{0.14}$$

$$= \frac{\int_{-\infty}^{x} \left[f(\tilde{x})/Mg(\tilde{x}) \right] g(\tilde{x}) d\tilde{x}}{\int_{-\infty}^{+\infty} \left[f(\tilde{x})/Mg(\tilde{x}) \right] g(\tilde{x}) d\tilde{x}} \tag{0.15}$$

$$= \frac{\int_{-\infty}^{x} f(\tilde{x}) d\tilde{x}}{\int_{-\infty}^{+\infty} f(\tilde{x}) d\tilde{x}} \tag{0.16}$$

$$= \int_{-\infty}^{x} f(\tilde{x}) d\tilde{x} \tag{0.17}$$

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

$$P_Y(y) = \frac{d}{dx} \left(\int_{-\infty}^{x} f(\tilde{x}) d\tilde{x} \right) \Big|_{x=y} = f(y), \tag{0.18}$$

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

[15 marks]

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

$$\langle f \rangle = \int_V f(x) P^V_{\text{uni}}(x) dx = \int_V \frac{f(x)}{V} dx. \tag{0.19}$$

Hence the expectation value of I_{MC} is

$$\langle I_{\text{MC}} \rangle = \frac{V}{N} \sum_{i=1}^{N} \langle f \rangle = \frac{V}{N} \left(N \langle f \rangle \right), \tag{0.20}$$

$$= V \int_V \frac{f(x)}{V} dx = \int_V f(x) dx. \tag{0.21}$$

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.

[12 marks]

(d) Rewritting the integrand yields

$$I = \int_0^\infty 4x e^{(4-x)} dx \tag{0.22}$$

$$= 4e^4 \int_0^\infty x e^{-x} dx \tag{0.23}$$

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

$$I = \frac{4e^4}{N} \sum_{i=1}^{N} x \tag{0.24}$$

[12 marks]

Solutions: Question 2

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

$$f'(x) = \frac{f(x+a) - f(x-a)}{2a}. \tag{0.25}$$

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

$$f''(x) = \frac{f(x+a) - 2f(x) + f(x-a)}{a^2}. \tag{0.26}$$

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

$$\phi(x, y) = \phi(ia, ja) = \phi_{i,j}, \tag{0.27}$$

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

$$\frac{\partial \phi}{\partial x}(x, y) = \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2a}, \tag{0.28}$$

$$\frac{\partial \phi}{\partial x}(x, y) = \frac{\phi_{i,j+1} - \phi_{i,j-1}}{2a}, \tag{0.29}$$

$$\frac{\partial^2 \phi}{\partial x^2}(x, y) = \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{a^2}, \tag{0.30}$$

$$\frac{\partial^2 \phi}{\partial y^2}(x, y) = \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{a^2}. \tag{0.31}$$

Substituting these into the differential equation yields

$$\rho(x, y) = A\frac{\partial^2 \phi}{\partial x^2} + B\frac{\partial^2 \phi}{\partial y^2} + C\frac{\partial \phi}{\partial x} + D\frac{\partial \phi}{\partial y}, \tag{0.32}$$

$$= A\frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{a^2} + B\frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{a^2} \tag{0.33}$$

$$+ C\frac{\phi_{i+1,j} - \phi_{i-1,j}}{2a} + D\frac{\phi_{i,j+1} - \phi_{i,j-1}}{2a}, \tag{0.34}$$

$$= \frac{1}{a^2}\left[\left(A + \frac{Ca}{2}\right)\phi_{i+1,j} + \left(A - \frac{Ca}{2}\right)\phi_{i-1,j}\right. \tag{0.35}$$

$$\left. + \left(B + \frac{Da}{2}\right)\phi_{i,j+1} + \left(B - \frac{Da}{2}\right)\phi_{i,j-1} - 4\phi_{i,j}\right] \tag{0.36}$$

[13 marks]

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

$$\tilde{\rho}_{i,j} = \left(A + \frac{Ca}{2}\right)\phi_{i+1,j} + \left(A - \frac{Ca}{2}\right)\phi_{i-1,j} \tag{0.37}$$

$$+ \left(B + \frac{Da}{2}\right)\phi_{i,j+1} + \left(B - \frac{Da}{2}\right)\phi_{i,j-1} - 4\phi_{i,j}. \tag{0.38}$$

To write this as a matrix equation we number the sites of the $N \times N$ 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

$$M_{m,n} = \left(A + \frac{Ca}{2}\right)\delta_{m,n+1} + \left(A - \frac{Ca}{2}\right)\delta_{m,n-1} \tag{0.39}$$

$$+ \left(B + \frac{Da}{2}\right)\delta_{m,n+N} + \left(B - \frac{Da}{2}\right)\delta_{m,n-N} - 4\delta_{m,n} \tag{0.40}$$

and the vector B is given by

$$B_n = \tilde{\rho}_n = \tilde{\rho}_{i,j}, \tag{0.41}$$

where $n = i + Nj$.

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 0.40 being set to zero for certain values of m (certain row equations). Namely, the following terms in 0.40 are set to zero, (here $i(m)$ and $j(m)$ are the original indices.)

$$\begin{aligned}
&\text{When } i(m) = 1, \quad \delta_{m,n-1} = 0,\\
&\text{When } i(m) = N, \quad \delta_{m,n+1} = 0,\\
&\text{When } j(m) = 1, \quad \delta_{m,n-N} = 0,\\
&\text{When } j(m) = N, \quad \delta_{m,n+N} = 0.
\end{aligned}$$

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 0.41 unaltered.

[10 marks]

(c) If we use a lattice with equal lattice spacings $\delta x = \delta y = a$ 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.

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} - \rho(x, y), \tag{0.42}$$

$$\frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} = \frac{\phi_{i+1,j}^{n} - 2\phi_{i,j}^{n} + \phi_{i-1,j}^{n}}{a^2} + \frac{\phi_{i,j+1}^{n} - 2\phi_{i,j}^{n} + \phi_{i,j-1}^{n}}{a^2} - \rho_{i,j} \tag{0.43}$$

$$\phi_{i,j}^{n+1} = \left(1 - \frac{4\Delta t}{a^2}\right) \phi_{i,j}^{n} + \frac{\Delta t}{a^2} \left(\phi_{i+1,j}^{n} + \phi_{i-1,j}^{n} + \phi_{i,j+1}^{n} + \phi_{i,j-1}^{n}\right) - \Delta t \rho_{i,j} \tag{0.44}$$

[12 marks]

(d) 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.

$$\phi_{i,j}^{n+1} = \frac{1}{4} \left(\phi_{i+1,j}^{n} + \phi_{i-1,j}^{n} + \phi_{i,j+1}^{n} + \phi_{i,j-1}^{n}\right) - \frac{a^2}{4} \rho_{i,j}. \tag{0.45}$$

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

$$\phi_{i,j}^{n+1} = \frac{1}{4} \left(\phi_{i+1,j}^{n} + \phi_{i-1,j}^{n+1} + \phi_{i,j+1}^{n} + \phi_{i,j-1}^{n+1}\right) - \frac{a^2}{4} \rho_{i,j}. \tag{0.46}$$

[10 marks]

(e) 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

$$\rho_s^n = 10^{-p}, \tag{0.47}$$

$$\implies n \ln(\rho_s) = -p \ln(10), \tag{0.48}$$

$$\implies n = \frac{-p \ln(10)}{\ln(\rho_s)}. \tag{0.49}$$

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

$$n_J = \frac{-p\ln(10)}{\ln(\rho_J)} = \frac{-p\ln(10)}{\ln(\cos(\frac{\pi}{N}))}. \tag{0.50}$$

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

$$n_{GS} = \frac{-p\ln(10)}{\ln(\rho_{GS})} = \frac{-p\ln(10)}{\ln(\cos^2(\frac{\pi}{N}))} = \frac{-p\ln(10)}{2\ln(\cos(\frac{\pi}{N}))} = \frac{n_J}{2} \tag{0.51}$$

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

[5 marks]