Numerical Methods
Natural Sciences Tripos 1B
Lent Term 1999

Problem Sheet 1

1. ROOT FINDING

1.1 Roots of a cubic

Consider the solution to $f(x) = 0.5$ where $f(x) = x^3$. Choosing initial guesses of $x_a = 0$ and $x_b = 1$,

(a) Write down an expression to show how the error ε_n in the bisection method decreases with subsequent iterations.

(b) Using the bisection method, determine the solution to four decimal places. Does the number of iterations this took agree with the predicted number?

(c) Repeat this calculation using the Linear interpolation and secant methods. How do the results compare after each iteration?

(d) Repeat the calculations using the Newton-Raphson method, starting from (i) $x_0 = 1$, (ii) $x_0 = 0$ and (iii) $x_0 = 3$. Comment on your results.

1.2 Direct iteration

(a) Illustrate graphically the direct iteration method and show cases of monotonic convergence, oscillatory convergence and divergence.

(b) Derive the convergence criteria for the direct iteration method for any arbitrary function.

(c) Using only the four basic operations (+–*/), write down a scheme which will solve $f(x)=0.5$, where $f(x)=\sin x$. Starting with $x=90\text{degrees}=\pi/2$ radians, use this scheme to compute the solution to six decimal places. Compare the convergence of your calculation with your analysis of the convergence.

1.3 Direct iteration

Consider the roots of $f(x) = 0$ for some continuous function $f(x)$.

(a) By rerranging and adding iteration labels (*i.e.* change x into x_n or x_{n+1}), derive a direct iteration equation in the form $x_{n+1} = g(x_n)$ from $(x–x)h(x) + f(x) = 0$.

(b) Prove that the quadratic convergence can be obtained with a particular choice of $h(x)$ and explain how this is related to the Newton-Raphson method.

2. LINEAR EQUATIONS

2.1 Gaussian elimination

(a) Use Gaussian elimination to solve

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 5 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 9 \\ 12 \end{pmatrix}$$

(b) Explain what is meant by pivoting. Why are these techniques used? Outline the differences between partial pivoting and full pivoting.

(c) Evaluate the solution of

$$\begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 4 \\ 2 & 2 & 5 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 7 \\ 9 \end{pmatrix}$$

using both partial and full pivoting. Why is pivoting necessary?

2.2 Banded matrices

Prove that if a matrix contains only zeroes outside some band centred around the leading diagonal, then performing Gaussian elimination (without pivoting) will maintain these zeros.

2.3 Tridiagonal matrices

Develop an algorithm for solving a tridiagonal system of equations.

2.4 Over determined systems*

(a) Explain what is meant by the term “over determined system”.

(b) What is meant by the “least squares solution”?

(c) Derive the least squares solution to a system of equations $\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$, and explain why Gaussian elimination should not normally be used to solve the resulting equations.

2.5 LU Factorisation

Compute the LU factorisation (without pivoting) of the matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 2 & 3 \\ 1 & 4 & 4 \end{bmatrix}$$

and use this factorised matrix to solve $\mathbf{A}\boldsymbol{x}=\boldsymbol{b}$ where

$$\boldsymbol{b} = \begin{pmatrix} 6 \\ 7 \\ 9 \end{pmatrix}$$

2.6 LU Factorisation and pivoting

Let

$$\mathbf{A} = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} \\ \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} \end{bmatrix}$$

Find the LU factorisation of $\mathbf{A}$

(a) Using exact arithmetic

(b) Under the assumption that each computer operation is accurate only up to four digits.

(c) Repeat this analysis using pivoting. In each case compare the values of the determinant of **A** as obtained in (a) and (b). Discuss the implications of this “computer” experiment to the applicability of Gaussian elimination.

3. NUMERICAL INTEGRATION

3.1 Trapezium rule

(a) Derive the one-step trapezium rule and the leading order error term.

(b) Use this rule to compute

$$\int_0^1 x^2 + 1 \, \mathrm{d}x$$

and compare with the analytical solution.

(c) Using 2, 4, 8 and 16 steps, show how the error in evaluating this integral is reduced.

(d) Explain how Romberg Integration may be used to improve the accuracy of an estimate evaluated from the Trapezium rule. Compute the solution using one level of Romberg Integration using the results from your 4 and 8 step calculations. How does the convergence compare with your result using 16 steps and with theoretical predictions?

(e) Develop a Romberg Integration scheme which will allow you to combine your results from your 4 and 16 step calculations. How does the result obtained in this way compare with your earlier results and theoretical predictions?

3.2 Midpoint rule

(a) Explain the differences between the midpoint and trapezium rules.
(b) Why is the midpoint rule more useful than the trapezium rule for integrals such as

$$\int_0^1 \frac{1}{\sqrt{x}} \, \mathrm{d}x \, .$$

(c) Discuss the character of this integral and how it influences the method chosen to approximate it.

(d) Compute an estimate for this integral using 1, 2, 4, 8 and 16 steps. Compare these results with an estimate based on Gauss quadrature.

3.3 Simpson’s rule

(a) Derive the one step and compound Simpson’s rules and analyse the errors of each.

(b) Use the one step Simpson’s rule to determine

$$\int_0^1 x^a \, \mathrm{d}x$$

for a=1, 2, 3, 4 and 5. Compare these estimates with the exact solutions.

(c) Compute the solution with a=5 using the compound Simpson’s rule with 2, 4 and 8 applications. Compare the size of the error in these computations with the expected error.

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Problem Sheet 2

4. ORDINARY DIFFERENTIAL EQUATIONS

4.1 Finite difference approximations

Derive a second order approximation to $f'_i \equiv df/dx$ at $x = x_i$ using the function values f_i, f_{i+1}, and f_{i+2}

(a) Assuming $x_{i+1}-x_i=x_{i+2}-x_{i+1}=\Delta x$

(b) For general x (where $x_{i+1}-x_i \neq x_{i+2}-x_{i+1}$).

Derive a third order approximation to $f''_i=d^2f(x_i)/dx^2$ using f_{i-1}, f_i, f_{i+1} and f_{i+2} assuming constant spacing of x_i. Discuss how this approximation may be utilised for an explicit solution of $d^2f/dx^2=g(x,f)$ for some function g subject to initial conditions on f and f' at $x=0$.

4.2 First order equations

(a) Derive the Euler scheme and the error term. Determine the stability condition for this method.

(b) Consider the equation $y' = x - y$ subject to $y=1$ at $x=0$. Utilising the Euler method, compute the approximate value of y at $x=1$ using 1, 2, 4, 8 and 16 steps. Compare this with the exact solution and discuss the convergence, comparing it with theoretical estimates.

(c) Apply Richardson extrapolation to your results from 8 and 16 steps to compute an improved estimate for $y(x=1)$.

(d) Compare your result from (c) with a calculation using 16 steps with the Improved Euler method.

(e) Compare your results above with a calculation using 16 steps with the Crank-Nicholson method.

(f) Discuss the benefits of the various schemes used above.

4.3 Second order equations

(a) Describe how explicit time stepping schemes method may be used to solve second order equations with two boundary conditions rather than two initial conditions.

(b) Using the Euler method in combination with the bisection method, compute the first five iterations with $\Delta x=0.2$ to find the solution to $y''=-2$ subject to $y(x=0)=1/2$ and $y(x=1)=0$. Start with $y'(x=0)=+/-1$.

(c) Why is this method difficult to use for higher order equations with boundary conditions at both ends?

5. PARTIAL DIFFERENTIAL EQUATIONS

5.1 Poisson's equation

Consider Poisson's equation in two dimensions

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)u = f\left(x,y\right).$$

(a) Derive a first order finite difference approximation for the Laplacian operator.

(b) Describe how this may be used in a matrix formulation to obtain the solution. Outline the structure of the matrix and how a knowledge of this can aid rapid solution.

(c) How can the number of computer operations (required to setup this system) be reduced if the step size in the x and y directions are equal?

(d) Taking $f(x,y)=-4$ and $u(x=0,y)=u(x=1,y)=u(x,y=0)=u(x,y=1)=0$, compute the solution using $\Delta x=\Delta y=1/4$. Compare this with the exact solution. How would you expect the size of the error to change if we reduce the step size to $\Delta x=\Delta y=1/8$? How would the number of computer operations required to reach this solution increase?

5.2 Relaxation methods

(a) Outline the differences between Jacobi Iteration, Gauss-Seidel Iteration and Successive Over Relaxation (SOR). Describe strategies for determining when to stop the iterative process.

(b) Utilise five iterations of each of these to compute the solution to Poisson's equation with $f(x,y)=-4$ and $u(x=0,y) = u(x=1,y) = u(x,y=0) = u(x,y=1) = 0$ using $\Delta x=\Delta y=1/4$. Take $u(x,y)=0$ as the initial *guess* and $\sigma = 1.4$ in the SOR method. Comment on the relative rates of convergence and on the effect of different relaxation coefficients for SOR.

(c) Outline what is meant by "Red-Black Ordering". Explain why this may be computationally more efficient.

5.4 Diffusion equation

Consider the diffusion equation

$$\frac{\partial C}{\partial t} = \nabla^2 C$$

in one dimension.

(a) Show how this may be approximated by a system of ordinary differential equations in time. Determine the truncation error in these equations.

(b) Show how this system of equations may be used in combination with the Euler method to determine the evolution of the scalar C.

(c) Derive the stability criterion for the time step. How is this altered by changing to three dimensions? Changing to n dimensions?

6. MORE INTERESTING QUESTIONS

Model answers to these questions are available on the web.

6.1 Roots of an integrated quantity

Consider the integral

$$F(x) = \int_a^x f(\xi)\, \mathrm{d}\xi ,$$

where $f(x)$ is an easily evaluated function.

(a) Show how $F(x)$ may be calculated from $f(x)$ for some arbitrary value of x using the Trapezium Rule with the interval $[a,x]$ subdivided into $n-1$ subintervals.

(b) Derive the error term in this approximation and show how Romberg Integration may be used to improve the accuracy of the solution given estimates of $F(x)$ obtained from $n-1$ and $2n-1$ subintervals. Show that this estimate is equivalent to calculating the integral using Simpson's Rule.

(c) Suppose we wish to find the value of x such that $F(x) = 1$. Using the Newton-Raphson method, predict the location of the root using a single iteration. You may assume $F(x)$ is a monotonically increasing function of x from $x = a$ to the neighbourhood of the root $x = x^*$. Why is this assumption important?

(d) Describe how the second and subsequent iterations may be calculated. Discuss how precisely the integral $F(x)$ should be evaluated for each iteration and suggest an appropriate method for achieving this.

6.2 Shooting

Consider the second order ordinary differential equation

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = f\left(x, y, \frac{\mathrm{d}y}{\mathrm{d}x}\right)$$

with boundary conditions $y = y_a$ at $x = x_a$ and $y = y_b$ at $x = x_b$.

(a) Show how this equation may be rewritten as a system of two first order ordinary differential equations.

(b) Show how the Euler method may be used to step this system from $x = x_a$ to $x = x_b$, using n steps, if we assume a knowledge of $\mathrm{d}y/\mathrm{d}x$ at $x = x_a$. Derive an expression for the truncation error for each step in this process.

(c) Describe how the Euler method may be combined with a root finding algorithm to determine the value of $\mathrm{d}y/\mathrm{d}x$ at $x = x_a$ required to satisfy our boundary condition at $x = x_b$.

(d) Taking $f(x,y,\mathrm{d}y/\mathrm{d}x) = y$, $(x_a,y_a) = (0,1)$ and using initial guesses of $\mathrm{d}y/\mathrm{d}x = 0$ and $\mathrm{d}y/\mathrm{d}x = -1$ at $x = x_a$, use the Linear Interpolation method to calculate an improved estimate for $\mathrm{d}y/\mathrm{d}x$ at $x = x_a$ given the other boundary condition $(x_a,y_a) = (1,1/2)$. Formulate your solution using two steps between x_0 and x_1 (*i.e.* $\Delta x = 1/2$).