THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

PHYS2020
COMPUTATIONAL PHYSICS

FINAL EXAM

SESSION 1 2008

Answer all questions

Time allowed = 2 hours

Total number of questions = 5

Marks = 40

The questions are NOT of equal value.

This paper may be retained by the candidate.

Candidates may not bring their own calculators.

Calculators will be provided by the Enrolment and Assessment Section.

Answers must be written in ink. Except where they are expressly required, pencils may only be used for drawing, sketching or graphical work.

PPS

Question 1 (8 marks)

(a) From geometric considerations, derive an expression for the Newton-Raphson (Newton's) method for finding the roots of a non-linear equation for which you have the explicit form of the equation,
$y = f(x)$,
and an initial approximation to the root of x_0.

The expression should clearly show how to find the next approximation to the root, x_1, in terms of $f(x)$ and x_0. Illustrate you answer with a clear sketch (or sketches) showing how Newton's method works. Mark on your sketch the position of both x_0 and x_1, and show how they are related.

(b) Briefly state the main differences between the bisection method and Newton's method for finding the roots of an equation in terms of robustness and time taken to converge.

(c) Use pseudocode to write a program which uses the bisection method to find the single root of the equation

$$x^3 - 2x - 2$$

on the interval $1 \le x \le 2$, to a precision of ± 0.1. You should use comments in your program to explain what each section of the code does.

(d) Use the bisection method to find the root of equation in part (c), on the given interval. The precision required is ± 0.1.

Question 2 (6 marks)

(a) With the aid of graphs, qualitatively compare the midpoint, trapezoidal and Simpson's approximation techniques for numerically integrating a function, discussing the order of the approximating function used in each case. You should state which method would give the most accurate approximation to the interval.

(b) You wish to integrate the function $y = x^2$ over the interval 0 to 3. Use the rectangular and trapezoidal techniques to evaluate the integral, using 3 "strips" of width 1 in each case. Compare your answer for both methods to analytical evaluation of the integral. Which method is more accurate in this case? Is this what you expect? Explain your answer.

Question 3 (9 marks)

The first order ordinary differential equation

$$\frac{dy}{dx} = f(x, y)$$

can be solved using Euler's method. Given an initial condition (x_0, y_0), successive points on the solution curve (x, y(x)) can be generated by taking equal steps of size h in the independent variable x, and determining the new y value using $y_{i+1} = y_i + hf(x_i, y_i)$. The numerical solution is then a set of points that approximate the solution curve. A second method of solution is the modified Euler method

$$y_{i+1} = y_i + hf\left[x_i + \frac{h}{2}, y_i + \frac{h}{2} f(x_i, y_i)\right]$$

(a) Explain the operation of the Euler and modified Euler methods in geometrical terms.

(b) Derive an expression for the Euler method using a Taylor series expansion.

(c) Use the simple Euler method to solve the ODE $y' = y$, given that f(0)=1, on the interval $0 \le x \le 2$ for a step size of 0.25. Compare with the exact result at x = 2 (The function is of course $y = e^x$).

(d) The modified Euler method is part of a general class called Runge-Kutta methods. What order Runge-Kutta method is the modified Euler method, and of what order will be the error term associated with this method.

Question 4 (9 marks)

The table below shows experimental measurements displacement, y, at a time x. Fit an approximating polynomial function to the data by following the steps below to make the fit.

(a) Complete the following difference table. Make sure you complete the table in your book, not on this exam paper!

x	y	Δ	Δ^2	Δ^3	Δ^4
1	4				
2	14				
3	36				
4	76				
5	140				
6	234				
7	364				
8	536				
9	756				
10	1030				

(b) What order polynomial would you consider the most appropriate to fit the above data set? Why?

(c) Use the Gregory Newton equation

$$y = f(x) = f(a) + \frac{1}{h}(x-a)\Delta + \frac{1}{2!}\frac{1}{h^2}(x-a)(x-a-1)\Delta^2 + \frac{1}{3!}\frac{1}{h^3}(x-a)(x-a-1)(x-a-2)\Delta^3 + \ldots$$

to approximate the polynomial of whichever order you think is most appropriate. Is the polynomial an exact fit to the measured data? (Hint: use the first and last x values to see if you can reproduce the exact y value.)

Question 5 (8 marks)

When fitting a line of the form

$$y = a + bx$$
$$y = a_0 + a_1 x$$

to a set of data points, the coefficients a_0 and a_1 can be determined via the technique of least squares.

(a) Briefly describe how the least-squares criteria determine an objective "line of best fit" for a data set. You may assume that we are concerned with the uncertainty in the "y" value only. Illustrate your answer with a hypothetical graph with 5 points scattered around a line-of-best-fit by drawing on this graph the geometric quantity to be minimised.

(b) Determine the actual least-squares best-fit straight line to the data points by minimising the error in the coefficients a_0 and a_1. Hence find the matrix equation for the coefficients as functions of the data points.

(c) Assume that for each measurement y(i) in the above problem you have an uncertainty $\sigma(i)$. Describe qualitatively how you would take into account this uncertainty when using the method of least squares to obtain a line-of-best-fit to the data. Explain why this makes the least squares minimisation more robust if a few very noisy measurements (measurements with large uncertainties) are included in the data. Why is it better to include the noisy measurements with weighting rather than just discarding the measurements? Illustrate you answer by drawing a second diagram, this time including error bars.

(d) What is the meaning of the term *robust estimator* when applied to a statistical measure of a distribution of numbers? Why are the average-deviation and the median regarded as *robust estimators* when the standard-deviation and average are not? Illustrate you answer with a sketch which shows the difference between the average and the mean for a Gaussian type distribution with several outliers.