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THE NATIONAL UNIVERSITY OF IRELAND MAYNOOTH

MATHEMATICAL PHYSICS

Third Year

AUTUMN REPEAT EXAMINATION
2009-2010

Computational Physics I
MP354

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Time allowed: 1.5 hours

Answer two questions

All questions carry equal marks

1. The following MatLab function is meant to calculate the Bessel function $J_0(x)$ using the series representation

$$J_0(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n!)^2} \left(\frac{x}{2}\right)^{2n}$$

by computing each term from the previous one. It should return an error if $x < 0$, and also if x is a vector or matrix rather than a single number. The code contains 10 mistakes (errors or highly inefficient ways of calculating). Find these mistakes, and write out the correct and improved code.

```
function J = bessel(z)
% evaluate the bessel function J0(x) using the representation
%                 _oo_     n      2n
%                 \     (-1) (x/2)
%    J0(x) =      /    -----------
%                 ----     (n!)
%                 n=0
% to a given precision.  x must be a non-negative number

prec = 1e-8; % Set the precision

% check for valid arguments
if ( numel(x) == 1 ) % numel(x) = number of elements of x
    error('Argument must be a scalar, not a vector or matrix')
end
while (x < 0)
    error('Bessel function undefined for negative numbers')
end

term = 0; % the leading (n=0) term of the sum
J0 = term; % initialise sum

for ( abs(term) > prec)
  % compute the n-th term of the sum
  term = -term*(x/2^2)*(factorial(n)/factorial(n-1))^2;
  J = J*term;
  n = n + 1;
end
```

2. The integral

$$I = \int_a^b f(x)dx$$

may be computed numerically using the trapezium formula,

$$I_T = \sum_{k=1}^{N} \Big[\frac{1}{2} f\big(a + (k-1)\Delta\big) + \frac{1}{2} f\big(a + k\Delta\big) \Big] \Delta \,,$$

with $\Delta = (b - a)/N$. By subdividing the integral into a sum of N sub-integrals and Taylor expanding each term of the sum, determine the accuracy of this method.

3. The formula for *Heun's method* for solving a general first-order ODE,

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

is given by

$$y(x + \varepsilon) = y(x) + \frac{\varepsilon}{2} \Big(F(x, y(x)) + F(x + \varepsilon, \tilde{y}(x + \varepsilon)) \Big)$$

with

$$\tilde{y}(x + \varepsilon) = y(x) + \varepsilon F(x, y(x)) \,.$$

By means of appropriate Taylor expansions obtain the order of accuracy of this formula.

4. (a) What is meant by *bracketing a root* of a function $f(x)$? Describe some of the difficulties you may encounter in attempting to bracket a root.

   (b) Describe how the solution of the equation

$$f(x) = 0 \,,$$

   where $f(x)$ is some computable function of x, can be found using the *bisection method*, assuming the root has been bracketed. Write out the key steps of the numerical procedure. What are the main strengths and weaknesses of this method?