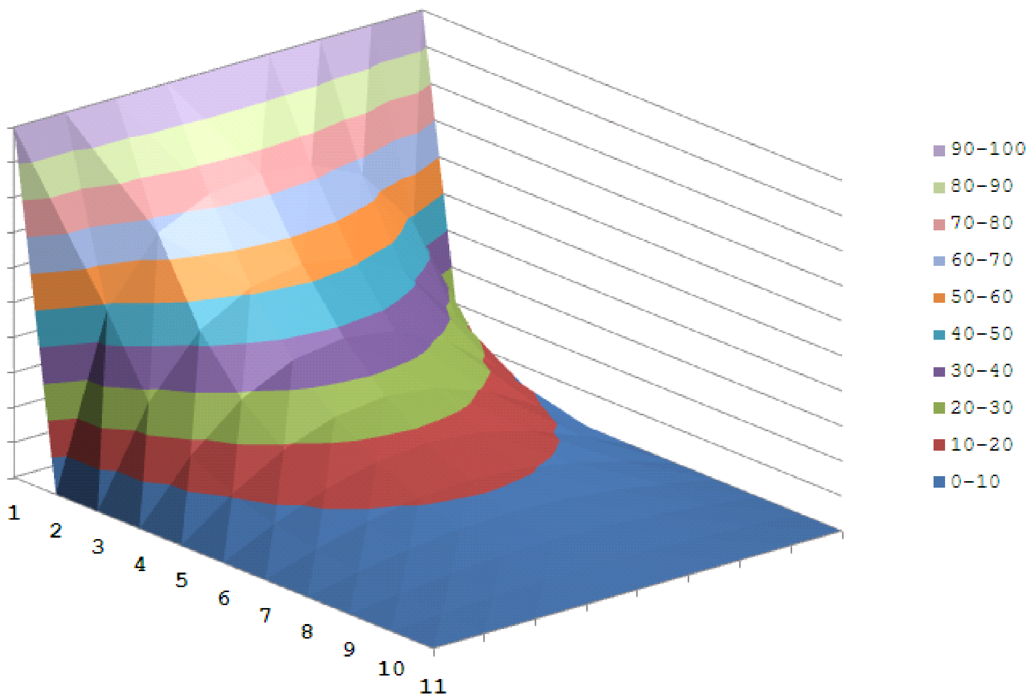


EP 208

Computational Methods in Physics
Examples of Exam Questions

May 2010

SOURCES OF ERRORS

Question 1

a) Explain the term 'truncation error', and give an example.
How can truncation errors be reduced?

b) Explain the term 'round-off error'.
How can round-off errors be reduced?

c) Explain the terms 'overflow' and 'underflow'.
How can overflow and underflow be avoided.

Question 2

Using only 8 binary digits, write down the closest representations in binary of the decimal numbers: 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, and 0.9. Write down the round-off error for each value. Which numbers are represented exactly?

Hint: You can write a computer program that calculates all binary states in the form $(0.00000000)_2$ to $(0.11111111)_2$ and find the ones that are closest to your decimal values.

Question 3

a) An integer variable x of 4 bytes (32 bit) is stored in the computer memory as follows:

```
00000000 00000000 00000000 01100101
```

Evaluate the value of x in base-10 and in base-16?

b) A real (float) variable y of 4 bytes (32 bit) is stored in the computer memory as follows:

```
01000000 01100110 01100110 01100110
```

Evaluate the value of y in base-10. What is the approximate value of y?

NUMERICAL DIFFERENTIATION

Question 1

a) Write a computer program to evaluate the first derivative of a function $f(x) = x^2 + e^{-2x}$ using the Central Difference Approximation method: CDA = (f(x+h) - f(x-h)) / 2h

b) Using Taylor's expansion show that the truncation error in this approximation is given by: error = $(h^2/6).f'''(x) + O(h^4)$

c) Theoretically, how can the error in the CDA be minimised? In practice, what other type of error exists in this method?

d) i. Using the CDA with h = 0.1, evaluate the first derivative of $f(x) = x^4$ at x = 3.2
   ii. Using calculus, determine the value for the error in your result and show that it equals $(h^2/6).f'''(x)$

Question 2

a) Write a computer program to evaluate the first derivative of a function $f(x) = x^2 + e^{-2x}$ using the Richardson Extrapolation Approximation method:
   REA = (f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)) / 12h

b) Using Taylor's expansion show that the truncation error in this approximation is given by: error = $-(h^4/30).f'''''(x) + O(h^6)$

c) Theoretically, how can the error in the REA be minimised? In practice, what other type of error exists in this method?

d) i. Using the REA with h=0.1, evaluate the first derivative of $f(x) = x^6$ at x = 3.2
   ii. Using calculus, determine the value for the error in your result and show that it equals $-(h^4/30).f'''''(x)$

Question 3

a) Write a computer program to evaluate the second derivative of a function $f(x) = x^2 + e^{-2x}$ using the Central Difference Approximation method: CDA2 = (f(x-h) - 2f(x) + f(x+h)) / h^2

b) Using Taylor's expansion show that the truncation error in this approximation is given by: error = $(h^2/12).f''''(x) + O(h^4)$

c) Theoretically, how can the error in the CDA2 be minimised? In practice, what other type of error exists in this method.

d) i. Using the CDA2 with h=0.1, evaluate the second derivative of $f(x) = x^5$ at x = 3.2
   ii. Using calculus, determine the value for the error in your result and show that it equals $(h^2/12).f''''(x)$

Question 4

a) Write a computer program to evaluate the second derivative of a function $f(x) = x^2 + e^{-2x}$ using the Richardson Extrapolation Approximation method: REA2 = $(-f(x-2h)+16f(x-h)-30f(x)+16f(x+h)-f(x+2h))/(12h^2)$

b) Using Taylor's expansion show that the truncation error in this approximation is given by: error = $-(h^4/90).f''''''(x) + O(h^6)$

c) i. Using the REA2 with h = 0.1, evaluate the second derivative of $f(x) = x^7$ at x = 1.5
   ii. Using calculus, determine the value for the error in your result and show that it equals $-(h^4/90).f''''''(x)$

ROOTS

Question 1

a) Show that, for the bisection root-finding method, the number of iterations, n, required to reduce the error from an initial value of e_i to a final value of e_f is given by: n = log(e_i / e_f) / log(2)

b) Given that a root of the function f(x) = $e^x - 3x^2$ is near 1.0, estimate the number of iterations required to achieve an accuracy of at least 6 decimal places.

Question 2

a) Using Taylor's expansion derive the following Newton-Raphson iterative formula for finding the root of a function f(x):
x[i+1] = x[i] - f(x[i]) / f'(x[i])

b) Using the Newton-Raphson method evaluate the root of the function f(x) = $e^x - 3x^2$, which is near 1.0, to an accuracy of at least 6 decimal places. Show the result of each iteration.

c) Write a computer program to implement the Newton-Raphson method for the evaluation of the root of f(x) = $e^x - 3x^2$. Your program should include a tolerance as an input.

Question 3

a) Using Taylor's expansion derive the following Secant iterative formula for finding the root of a function f(x):
x[i+1] = x[i] - f(x[i]) (x[i] - x[i-1]) / (f(x[i]) - f(x[i-1]))

b) Using the Secant method evaluate the root of the function f(x) = $e^x - 3x^2$, which is near 1.0, to an accuracy of at least 6 decimal places. Show the result of each iteration.

c) Write a computer program to implement the Secant method for the evaluation of the root of f(x) = $e^x - 3x^2$. Your program should include a tolerance as an input.

Question 4

a) Using the Newton-Raphson iterative formula for the root of a function f(x):
x[i+1] = x[i] - f(x[i]) / f'(x[i])
show that the iterative formula:
x[i+1] = x[i] - (x[i]-p/x[i])/2
converges to the square-root of p.

b) Write a computer program to implement the above formula. Your program should include a tolerance as an input.

c) Using the above formula evaluate the square-root of 45.6 to an accuracy of at least 6 decimal places. Show the result of each iteration.

d) Generalise Newton's Square root to compute the n'th root of a number p.

Question 5

Given the function f(x) = 2x – sin(x) – 2. Determine the root of f(x) to an accuracy of at least 3 decimal places,

a) by using the fixed-point-iteration method. (Take initial guess x0 = 3)
b) by using the bisection method. (Take initial bracket [0, 3])
c) by using the Newton-Raphson method. (Take initial guess x0 = 3)
d) by using the Secant method. (Take initial guess x0 = 3)

OPTIMIZATION

Question 1

a) Using Taylor's expansion, derive Newton's iterative formula for finding the extremum of a function f(x):

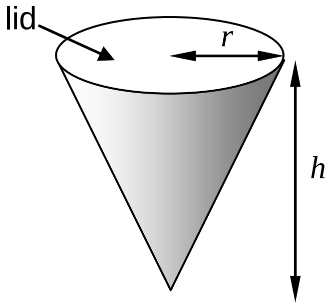
```
x[i+1] = x[i] - f'(x[i]) / f''(x[i])
```

b) Using the Newton's iterative formula, find the maximum of the function $f(x) = e^x - 3x^2$, which is near 0.2, to an accuracy of at least 6 decimal places. Show the result of each iteration.

c) Write a computer program to implement Newton's method. Your program should include a tolerance as an input.

Question 2

Design an optimum conical container that has a cover and walls of negligible thickness. The container is to hold 0.2 m^3 waste water.



a) Find the analytical result of the values of r and h that minimize the area of its top and sides.

b) Write a program that minimizes the area of its top and sides.

NUMERICAL INTEGRATION

Question 1

Show that the integration of f(x), $\int_a^b f(x)\,dx$, can be is approximated by Trapezoidal method as follows:

```
It = h [ (f0 + fn)/2 + f1  + f2  + ... + fn-1 ]
   = h [ (f(a) + f(b))/2 + f1  + f2  + ... + fn-1 ]
```

where fi = f(xi) and xi = a + i*h and h = (b-a)/n.

Question 2

Given the function f(x) = $6x^2 - e^x$

a) Find the analytical solution of the integral $\int_1^5 f(x)\,dx$

b) Using the Trapezoidal method, evaluate the integral $\int_1^5 f(x)\,dx$ by dividing the region of integration n = 10 equally spaced intervals.

c) Using the Simpson's method, evaluate the integral $\int_1^5 f(x)\,dx$ by dividing the region of integration n = 10 equally spaced intervals.

Question 3

Given the function f(x) = $6x^2 - e^x$

a) Write a computer program to implement Trapezoidal method for n = 100 intervals.
b) Write a computer program to implement Simpson's method for n = 100 intervals.

Question 4

Many engineering problems involve the calculation of work. Here is an example of a variable force acting on a block. For this case the angle and as well as magnitude of force varies as a function of x as shown below.

Data for force F(x) and angle θ(x) as a function of position x

x (m)	F (N)	θ (deg)	F*cos(θ)
0.0	1.0	28.6	0.878
5.0	9.0	80.2	1.532
10.0	13.0	43.0	9.508
15.0	14.0	51.6	8.696
20.0	10.5	74.5	2.806
25.0	12.0	84.8	1.088
30.0	5.0	66.6	1.986

Note that the general formula to calculate for the one dimension is given by

$$\int_{x0}^{x1} F(x)\cos[\theta(x)]dx$$

For the given data, using Trapezoidal method, evaluate the work done by F(x) between [0 m, 30 m]

SOLUTIONS OF DIFFERENTIAL EQUATIONS I

Question 1
Consider the initial value problem

$$y' = \frac{dy}{dx} = f(x, y) \quad ; \quad y(x_0) = y_0$$

Show that the Simple-Euler solution steps for y(x) is given by

yi+1 = yi + h*f(xi,yi) ; for i = 0,1,2,...

where yi+1 = y(xi+h) and yi = y(xi).

Question 2
Given the initial value problem

$$y' = \frac{dy}{dx} = \frac{y}{x} + x \quad ; \quad y(1) = 0$$

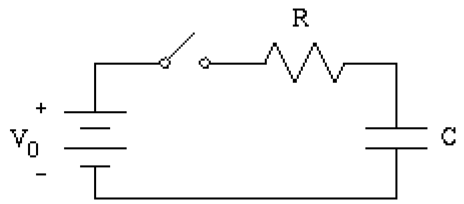
a) Use Euler method with h = 0.4 to solve the D.E. for the range $1 \leq x \leq 5$. Write down the result of each iteration.

b) Write computer program to implement Simple Euler method.

c) Write computer program to implement second order Runge-Kutta method.

Iter	X	Y
0	1.000	0.000
1		
2		
.		
.		

Question 3
A charging R-C circuit is governed by the 1st order D.E.



$$\frac{dq}{dt} = \frac{V_0 C - q}{RC} \quad ; \quad q(0) = 0$$

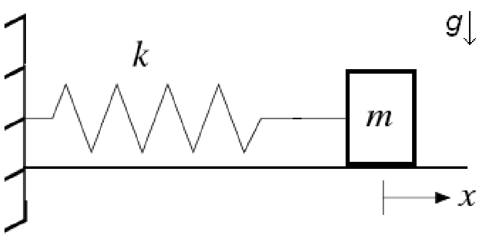
where R = 50 kΩ, C = 10.0 μF, charging voltage V_o is 12 Volts.

a) Use simple Euler method with the time step of $h = dt$ = 0.1 seconds and evolve the system for 1.0 seconds. Write down the solution of each iteration.

b) Write computer program to implement second order Runge-Kutta method.

Iter	t	q
0	0.000	0.000
1		
2		
.		
.		

Question 4
A spring-mass system is governed by the 2nd order D.E.



$$m\frac{d^2x}{dt^2} + kx = 0 \quad ; \quad v(0) = 0, x(0) = \ 0.2\ m$$

where the mass is m = 1.01 kg, the spring constant is k = 10 N/m, $v = dx/dt$ is the velocity in m/s and x is the displacement in m. Using a time step of $h = dt$ = 0.05 s, evolve the system for 10 seconds. Write a computer program to solve the position x and velocity v of the mass via forth order Runge-Kutta method.

SOLUTIONS OF DIFFERENTIAL EQUATIONS II

Question 1

Using the central-difference approximation to the second derivative of a function F(x)

$$CDA2 = (F(x-h) - 2F(x) + F(x+h)) / h^2$$

show that for a region of space that does not contain any electric charge the following expression satisfies Laplace equation:

```
V(i,j,k) = [ V(i-1,j,k) + V(i+1,j,k) +
             V(i,j-1,k) + V(i,j+1,k) +
             V(i,j,k-1) + V(i,j,k+1) ] / 6
```

where the matrix V represents the potential at discrete points i, j, k in a three-dimensional lattice. Your answer should include an explanation of the mapping of x, y, and z space onto i, j, and k points in the lattice (e.g x = i*h etc).

Hint: In cartesian coordinate system, Laplace's equation for chargeless region of space is given by

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0$$

Question 2

The temperature in a thin rod (length a) can be described by the one-dimensional heat equation:

$$\frac{\partial T}{\partial t} = c\frac{\partial^2 T}{\partial x^2}$$

where T=T(x,t) is the temperature of the rod at various positions (x) and times (t).
Using CDA2 = $(F(x-dx)-2F(x)+F(x+dx))/dx^2$ and FDA = (F(t+dt)-F(t))/dt, show that the finite difference solution to the heat equation is given by

```
T(i,j+1) = r*T(i-1,j) + (1-2r)*T(i,j) + r*T(i+1,j)
```

where
T(i,j) represents temperature at discrete points i,j in a two-dimensional lattice.
$r = c*dt/dx^2$.

Question 3

In a region of space, the electric potential distribution in Volts is given by

$$V(x,y,z) = x^3 - 2xy^2 + \exp(-x-y-z)$$

where x, y and z are measured in meters.
Using CDA with $\Delta x = \Delta y = \Delta z = 10$ mm, determine the magnitude of electric field at point (1 m, 2 m, 3 m).

PROBABILITY, RANDOM VARIABLES AND FREQUENCY EXPERIMENTS

Question 1

Given the random variable and corresponding probability mass function (PMF)

$$X = \{1, 2, 3, 4, 5\}$$
$$f(x) = \{0.1, 0.3, 0.4, 0.1, 0.1\}$$

Calculate

a) $\sum f(x_i)$ c) $E[x]$ e) RMS g) standard deviation

b) $P(1<x<5)$ d) $E[x^2]$ f) Variance

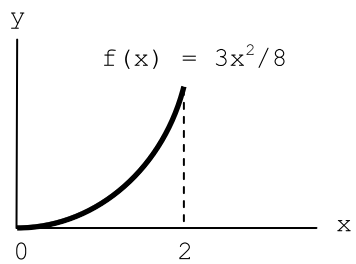
Question 2

Given the probability density function $f(x) = 3x^2/8$

Calculate

a) First moment c) Second Central moment

b) second moment d) $P(x>0.5)$ e) RMS



Question 3

Given the pdf $f(x) = N*\sin(x)$ for $0<x<\pi$.

a) Compute the normalization constant N.

b) Compute the expectation value and variance.

Question 4

Suppose that a sample consists of the weights of 100 students. The data is given right.

a) Draw the histogram of the data

b) Draw the relative frequency distribution

c) Calculate mean, variance and standard dev.

d) Calculate the probability of a randomly selected student whose weight is less than 75.

Weight (kg)	Number of students
50-55	5
55-60	15
60-65	25
65-70	30
70-75	10
75-80	5
85-90	3
90-100	2

Question 5

a) A fair coin is tossed 6 times.

i) Find the probability that exactly 3 heads occur. (i.e. k=3)

ii) Find the probability that at least three heads occur. (i.e. k=3,4,5,6)

iii) Draw the probability mass function (for k = 0, 1, 2, 3, 4, 5, 6).

b) Suppose that 1% of the people on average is left-handed. Find the probability of 3 left-handed among 200 people.

Question 6

a) Write a computer program to simulate tossing four coins at a time and output probability of getting at least two heads.

b) Write a computer program to simulate tossing four dice at a time and output probability of getting at least two six.

c) Suppose the diameters of screws manufactured by a company are normally distributed with mean 2.5 mm and standard deviation 0.2 mm. For a sample of 1000 screws, write a program to find the number N of screws with diameters between 2.1 mm and 2.8 mm. Use Simpson method for the integration of Gaussian function.

MONTE CARLO METHODS

Question 1

A nucleus of an atom has a probability of decaying that is described by the pdf $f(t) = 0.1 \exp(-0.1t)$ where $t \geq 0$ is the time in seconds.

a) Determine the probability that the nucleus survives 20 seconds.
b) Write a program to perform a stochastic experiment for case (a).

Question 2

The following Fortran and C++ programs estimates the area of a circle of unit radius

```fortran
implicit none
  integer :: i, m=0, n=10000000
  real    :: x, y
  do i = 1, n
    call random_number(x)
    call random_number(y)
    if ( x**2+y**2 < 1.0 ) m=m+1
  end do
  print *, 4.0*m/n
  end
```

```cpp
#include <iostream>
int main(){
  int i, m=0, n=10000000;
  double  x, y;
  for (i = 1; i<=n; i++){
    x = double(rand())/(RAND_MAX+1);
    y = double(rand())/(RAND_MAX+1);
    if ( x*x+y*y < 1.0 ) m++;
  }
  cout << 4.0*m/n << endl;
}
```

Modify the program to estimate the volume of a sphere of unit radius.

Question 3

a) Write a Monte Carlo integration program to integrate the function $f(x) = (1-x^2)^{1/2}$ over the range $x = -1$ to $x = 1$.
b) Write a program to compute the transcendental number $e = 2.7182818...$
   (Hint: Consider the Monte Carlo integral of $1/x$ from $x=1$ to $x=10$)

Question 4

For each the following target distribution functions, Py(y):

a) $Py = 2y^2$
b) $Py = \ln(y)$
c) $Py = \sin(y)$

- Determine the transformation functions $y = f(x)$
- Sketch the distribution Py(y) and f(x)
- Write a program to view function Py

Question 5

For each the following target distribution functions, Py(y), (for given ranges in the square brakets) :

a) $Py = \pi+\cos(y)$ $[-\pi, 3\pi]$
b) $Py = \exp(-y^2)$ $[-10, 10]$
c) $Py = 1-x^2$ $[-1, 1]$

- Sketch the distribution Py(y).
- Write a program to view function Py.

LEAST SQUARE FITTING

Question 1

a) Fit the data given right into function y = a*x + b
b) Calculate the regression coefficient.

x	y
1	12
2	9
3	8
4	5
5	3

Question 2

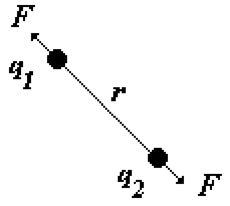
Table shows experimental results of a freely falling body.

t(s)	0.000	0.200	0.400	0.600	0.800	1.000
y(m)	0.000	1.960	0.785	1.767	3.141	4.908

where t is the time measured in seconds and y is the distance measured in meter.
Using linear Least square method,
a) determine gravitational acceleration, g
b) calculate the regression coefficient.

Question 3

The table shows the experimental results of the measured Coulomb Force , F, between two charges, (q_1 and q_2) corresponding to distance r. Experimental set up is shown in Figure.



r	F
40	2.5
30	4.5
20	10.1
10	40.5
5	162.0

r is measured in cm
F is measured in Newton
q1 = 5 μC
q2 = 9 μC

The form of the Coulomb Force is:

$$F(r) = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r^2}$$

Using the results, determine value of the constant ε_0 (permittivity of free space) via least-square fitting method.

Question 4

a) Write a computer program for the Question 1
b) Write a computer program for the Question 2
c) Write a computer program for the Question 3