Course: Computer Applications in Physics-II(CAP-II)

Course No.: MPC 43

Semester: M.Sc. SEM-IV (2021)

Topics: Integration, Diff. Eqn. & Roots of Equations

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Write C++ Programmes to implement the tasks as described below.

Integration

1. Integrate: $\int_0^{\frac{\pi}{2}} \frac{x^2 dx}{\sin^2 x}$, Ans. : $\pi ln2$

2. Integrate: $\int_0^\infty \frac{e^{-qx}}{\sqrt{x}} dx$, q > 0, Ans.: $\sqrt{\frac{\pi}{q}}$

3. Integrate: $\int_0^1 \left(\frac{x^{p-1}}{1-x} - \frac{qx^{pq-1}}{1-x^q} \right) dx$, q > 0, Ans.: $\ln q$

4. Integrate: $\int_0^\infty \frac{\sin(x)}{x} dx$, Ans.: $\frac{\pi}{2}$

5. Integrate: $\int_0^{\frac{2}{\pi}} x^2 \sin(1/x) dx$, Ans.: .0585676

6. Integrate: $\int_0^1 \frac{x^p - x^{-p}}{1+x} dx$, $p^2 < 1$, $Ans.: \frac{1}{p} - \frac{\pi}{\sin(p\pi)}$

7. Integrate: $\int_{-1}^{1} dx x^{-\frac{2}{n}}, n > 2$, $Ans.: \frac{2n}{n-2}$

8. Integrate $I = \int_0^1 \frac{dx}{1+x^2}$ by using Trapezoidal as well as Simpson- $\frac{1}{3}$ rules with an accuracy of the order of 10^{-5} . Find the minimum number of subintervals required to achieve the specified accuracy. Ans. $I = \frac{\pi}{4}$.

9. Integrate $I=\int_0^1 dx e^{x^2}$ by using Trapezoidal rule. Choose the total number of subintervals n=1000 and plot error vs. n. (Ans.:I=1.46265)

10. Find $(\triangle x)^2 = \langle x^2 \rangle - (\langle x \rangle)^2$ for the one dimensional simple harmonic oscillator.

11. The integral representation of Beta Function $B(m,n) = \frac{\Gamma(m)\Gamma(n)}{\Gamma(m+n)}$ can be expressed in many different, but, equivalent forms. Some of the expressions are given below. Evaluate the corresponding integrals.

$$B(m,n) = \int_0^1 u^{m-1} (1-u)^{n-1} du,$$

$$B(m+1,n+1) = \int_0^\infty \frac{u^m du}{(1+u)^{m+n+2}},$$

$$B(m+1,n+1) = 2 \int_0^{\frac{\pi}{2}} \cos^{2m+1} \theta \sin^{2n+1} \theta d\theta$$

12. The error function erf(x) is defined as,

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

Evaluate erf(x) by using Simpson's $\frac{1}{3}$ formula for 20 distinct points within the interval $0 \le x \le 2$ and plot it as a function of x.

13. One of the Fresnel integrals is defined as,

$$C(x) = \int_0^x \cos\left(\frac{\pi}{2}t^2\right) dt$$

Evaluate C(x) by using Simpson's $\frac{1}{3}$ formula for 20 distinct points within the interval $0 \le x \le 2$ and plot it as a function of x.

14. One of the Fresnel integrals is defined as,

$$S(x) = \int_0^x \sin\left(\frac{\pi}{2}t^2\right) dt$$

Evaluate S(x) by using Simpson's $\frac{1}{3}$ formula for 20 distinct points within the interval $0 \le x \le 2$ and plot it as a function of x.

15. The Euler's integral is defined as,

$$\Gamma(p) = \int_0^\infty e^{-x} x^{p-1} dx, \ p > 0$$

Evaluate $\Gamma(p)$ by using Simpson's $\frac{1}{3}$ formula for 20 distinct points within the interval $0 \le p \le 2$ and plot it as a function of p.

Monte Carlo Method of Integration

- 1. Use the Monte Carlo Method of integration to find the area of (i) a circle, (ii) an ellipse.
- 2. Use the Monte Carlo Method of integration to find the volume of (i) a sphere, (ii) an ellipsoid, (iii) a tetrahedron, (iv) a spherical shell with inner and outer radii as r_i and r_o , respectively.
- 3. Use the Monte Carlo Method of integration to find the volume of a 10-dimensional sphere (S^9) .
- 4. Evaluate: (i) $I = \int_0^{\frac{3\pi}{2}} \sin(x) dx$, (ii) $I = \int_{x=-5}^5 \int_{y=-3}^7 (x^2 3xy + y^2) dx dy$

Roots of equations, Fractal and Zeroes of functions

- 1. Find the roots of the equation $x^2 3x + 2 = 0$ by using bi-section as well as Newton-Raphson method.
- 2. Find both the roots of the equation $x^2 2$ n x 3 $n^2 = 0$ for all prime numbers between n = 1 to 1000 and write the results in an output file.
- 3. Use 1000 random numbers between 0 and 2n as the guess/initial values for finding the roots of the equation $x^2 2$ n x 3 $n^2 = 0$ for a fixed integer n by using Newton-Raphson(NR) method. Tabulate the random guess values corresponding to each root in an output file.
- 4. Find the values of b and c within the ranges $-20 \le b \le 20, -20 \le c \le 20$ and with the least interval h = .1 so that the equation $x^2 + bx + c = 0$ has only real roots. Plot 'b vs. c' within the specified ranges.
- 5. Find all the roots of the equation: (i) $z^4 + 5z^2 + 4 = 0$, (ii) $\sin z = z$.
- 6. Take the guess/initial values x_0, y_0 , for finding the roots of the equation $z^n 1 = 0, n \in \mathbb{N}$ by using Newton-Raphson method, from the region defined by $-a \leq x \leq a, -b \leq y \leq b, \ a, b \in \mathbb{R}$. Plot $y \ vs. \ x$ for those values of x_0, y_0 for which the root converges to z = 1.

- 7. Find all the roots of the following equations: (i) $x^3 5x = 0$, (ii) $x^3 2x + 2 = 0$, (iii) $x^2 \alpha x + \alpha^2$, $\alpha \neq 0$. State the problem, if any, for the seed values $x_0 = 0, 1$. Give an explanation and a remedy of the problem.
- 8. Show that the roots of the following set of equations correspond to the zeroes of the Nth order Hermite polynomial:

$$x_i + \sum_{j(\neq i)=1}^{N} \frac{1}{x_i - x_j} = 0, \ i = 1, 2, \dots N.$$

Differential equation

1. Solve the following equation by using the Runge-Kutta fourth-order formula:

$$\ddot{y} + b\dot{y} + cy = 0$$
, $y(0) = 1$, $\dot{y}(0) = 0$, $\dot{y} \equiv \frac{dy}{dt}$, $\delta \equiv b^2 - 4c$

for (i) $b > 0, \delta < 0$, (ii) $b < 0, \delta < 0$, (iii) $b > 0, \delta = 0$ and (iv) $b < 0, \delta = 0$.

Plot y(t) vs t for all the cases within a suitable range of t.

2. Solve the following equation by using the Runge-Kutta fourth-order formula:

$$\ddot{y} = y(y^2 - 1), \ \dot{y} \equiv \frac{dy}{dt}$$

for (i) y(0) = 0, $\dot{y}(0) = 0$, (ii) y(0) = 1, $\dot{y}(0) = 1$, (iii) y(0) = 0, $\dot{y}(0) = -1$ and (iv) y(0) = 1, $\dot{y}(0) = 0$.

Plot y(t) vs t for all the cases within a suitable range of t.

3. Solve the following equation by using the Runge-Kutta fourth-order formula:

$$\ddot{y} + \sin y = 0, \ \dot{y} \equiv \frac{dy}{dt}$$

for (i) $y(0) = 1, \dot{y}(0) = 0$, (ii) $y(0) = 0, \dot{y}(0) = 1$, (iii) $y(0) = 0, \dot{y}(0) = -1$ and (iv) $y(0) = 1, \dot{y}(0) = 0$.

Plot y(t) vs t for all the cases within a suitable range of t.

4. Solve the following equation by using the Runge-Kutta fourth-order formula:

$$\ddot{y} + \omega_0^2 y = \cos(\omega t), \quad \dot{y} \equiv \frac{dy}{dt},$$

with $\omega \sim \omega_0$ for (i) $y(0) = 1, \dot{y}(0) = 0$. Plot y(t) vs t for all the cases within a suitable range of t.

5. Driven damped harmonic oscillator:

$$\ddot{y} + b\dot{y} + \omega_0^2 y = a\cos(\omega t), \quad a, b, \omega, \omega_0 \in R$$

Consider different limiting cases of the above equation to study beats, resonances, damping etc.

6. Kepler Problem and its Generalizations:

$$\frac{d^2u}{d\theta^2} + \omega u = \omega_0 + \omega_1 u^2; \quad Q \equiv \frac{1}{2\omega_0} \left[\left(\frac{du}{d\theta} \right)^2 + u^2 \right] - u.$$

Choose Q < 0 and find the orbits(polar plot of $r \equiv \frac{1}{u}$ vs. θ) for the following cases:

- (i) Standard Kepler Problem: $\omega = 1, \omega_1 = 0$,
- (ii) Precession of orbits: $\omega \neq 1, \omega_1 = 0$,
- (iii) Generalized Kepler Problem: $\omega \neq 1, \omega_1 \neq 0$.

Repeat the above computations for Q = 0 and Q > 0.

7. Coupled equations:

$$\dot{x}_a = \sum_{b=1}^{N} M_{ab} x_b, \ M_{ab} \equiv \omega_0 \delta_{ab} + \omega_+ \delta_{a \ a+1} + \omega_- \delta_{a \ a-1}, \ x_{N+1} = x_1$$

8. The following sets of equations exhibit chaos for suitable ranges of the real parameters a, b and c.

Find the time-development of X(t), Y(t) and Z(t) and check sensitivity of the solutions to the initial conditions.

Plot (i) Y vs. X, (ii) Z vs. X and (iii) Z vs. Y.

(a) Damped Driven Non-linear Pendulum(DDNP):

$$\dot{X} = Y, \ \dot{Y} = -bY - \sin X + a \cos Z, \ \dot{Z} = c$$

(Check that the decoupled second order equation in terms of $X=x,Y=\dot{x},Z=ct$ indeed corresponds to a DDNP.)

(b) Lorenz Attractor (Canonical values: a=28, b=8/3, c=10):

$$\dot{X} = -c(X - Y), \ \dot{Y} = aX - Y - XZ, \ \dot{Z} = b(XY - Z)$$

(c) Chua's Circuit:

$$\dot{X} = a(Y-X) - f(X), \ \dot{Y} = b[a(X-Y) + Z], \ \dot{Z} = -c(Y+dZ), \ d \in R,$$

where f(-X) = -f(X) and is defined for positive X as follows:

$$f(X) = -X \text{ for } X < 1,$$

$$f(X) = -1 - .636(X - 1)$$
 for $1 < X < 10$,

$$f(X) = 10(X - 10) - 6.724 \text{ for } X > 10$$