**Computational Physics - Solved Problems**
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# 1 Statistics

1. If X={1,2,2,3,3,3,4,4,5,6} calculate the following:

   i. Mean value $\overline{x}$

   ii. Variance $\sigma_x^2$

   iii. Standard deviation $\sigma_x$

   iv. Plot histogram

Solution

# 2 Random numbers

1. Generate a uniform distribution with the following domain using the build-in function np.random.rand() :

   i. X $\sim$ [0,5] , N=100

   ii. X $\sim$ [1,5] , N=10000

   iii. Which of the above is closer to the uniform distribution and why?

Solution

2. Generate random numbers with the following distributions using the inverse transformation method :

   i. X $\sim$ x , x $[0, 1]$

   ii. X $\sim$ x , x $[1, 2]$

   iii. X $\sim$ $x^2$ , x $[1, 2]$

Solution

3. Generate random numbers with the following distribution:

$$X \sim e^x \;\; , \;\; x\,[0, 5]$$

   i. Inverse transformation method

   ii. Hit or Miss method

Solution

# 3 Root Finding

1. Find the root of $f(x) = x^3 - x - 1 \in (0, 2)$ using the following methods:

   i. Bisection

   ii. Regula Falsi

   iii. Newton Raphson

   iv. Secant

   v. Fixed Point

Solution

2. Let $f(x) = x^2 + 4x + 3 \in (-2, 0)$.

   i. Find the root using the Fixed Point method.

   ii. How many iterations are needed to have an error of $\frac{10^{-6}}{2}$.

Solution

3. Given the potential

$$V(x) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

   For $\varepsilon = 1$ and $\sigma = 1$, find the root of V(r)=3, r $\in$ (1,10) using the Newton Raphson method with precision $10^{-6}$.

Solution

# 4 Linear Systems

1. For the linear system,

$$2x + y + z = 7$$

$$2x - y + 2z = 6$$

$$x - 2y + z = 0$$

   Find the solution using the following methods.

   i. Gauss Elimination method.

   ii. LU (Doolittle) method.
   *To find the solution with LU method (Doolittle), use the Gauss Elimination method to solve the following system:*

$$L \cdot y = b \quad , \quad U \cdot x = y$$

Solution

2. Solve the system $A \cdot x = \mathrm{b}$ with LU (Doolittle) method analytically. The LU matrices are given. First, determine the numerical values of elements $L_{31}$ and $U_{15}$.

$$\mathrm{A}= \begin{bmatrix} 1 & 1 & 1 & 2 & 3 \\ 2 & 4 & 4 & 7 & 7 \\ 3 & 1 & 4 & 6 & 10 \\ 1 & 5 & 8 & 12 & 9 \\ 2 & 4 & 1 & 2 & -1 \end{bmatrix}, \mathrm{L}= \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 & 0 \\ \mathrm{L}_{31} & -1 & 1 & 0 & 0 \\ 1 & 2 & 1 & 1 & 0 \\ 2 & 1 & -1 & -2 & 1 \end{bmatrix}, \mathrm{U}= \begin{bmatrix} 1 & 1 & 1 & 2 & \mathrm{U}_{15} \\ 0 & 2 & 2 & 3 & 1 \\ 0 & 0 & 3 & 3 & 2 \\ 0 & 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 0 & -2 \end{bmatrix}$$

$$\mathrm{b}= \begin{bmatrix} 4 \\ 12 \\ 7 \\ 14 \\ 5 \end{bmatrix}$$

Solution

3. Solve the following system with

$$\left[\begin{array}{ccc|c} 3 & -1 & 0 & 10 \\ -1 & 3 & -1 & 5 \\ 0 & -2 & 4 & 10 \end{array}\right]$$

   i. Gauss - Siedel methos
   ii. Jacobi method

Solution

# 5 Monte Carlo

1. **Random Walk!** Brownian motion refers to the random movement displayed by small particles that are suspended in fluids. Consider 10000 Brownian particles, diffusing in a two-dimensional infinite plane. The starting point is the origin of the x-y axes and the particles are moving with a random step on a square grid of one centimeter edge with speed 1cm/s. Find the average distance of the particles after t=100 sec:

$$\bar{d} = \frac{1}{1000} \sum_{i=1}^{1000} \sqrt{x_i^2 + y_i^2}$$

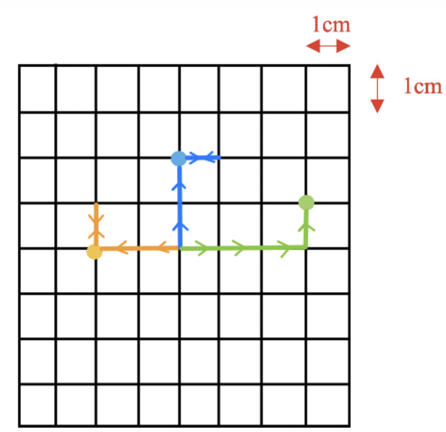


Figure 1: Example of Brownian motion of three particles after t=4sec

i. Plot a histogram with the average final position (x,y) of particles (Plot both x and y in one histogram).

ii. Plot an example of final gas state.

Solution

2. **Snakes and Ladders game!** The object of the game is to be the first player to reach the end by moving across the board from square one to the final square. The rules are simple. Roll the dice and move forward that number of spaces. The ladders on the game board allow you to move upwards and get ahead faster. However, snakes move you back on the board because you must slide down. How many rolls does it takes to win the game?

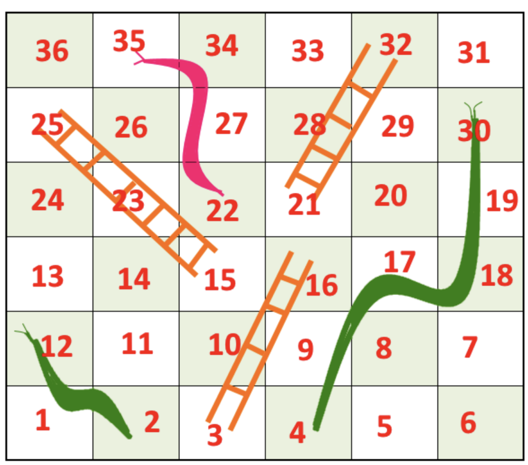


Figure 2: Snakes and Ladders game!

Solution

3. **Monty Hall problem!** Suppose you are on a game show, and you are given the choice of three doors: Behind one door is a car; behind the others, goats. You pick a door, say No. 1, and the host, who knows what's behind the doors, opens another door, say No. 3, which has a goat. He then says to you, "Do you want to pick door No. 2?" Is it to your advantage to switch your choice?

   – **Standard assumptions:** Consider the car as the prize ... you wish!!! The host must always open a door that was not picked by the contestant to reveal a goat and always offer the chance to switch between the originally chosen door and the remaining closed door.


Figure 3: Monty Hall problem!

Solution

# 6 Monte Carlo Integrals

1. Calculate the I=$\int_{0.5}^{10.5} \frac{1}{x} dx$ with

   i. Hir or Miss

   ii. Crude 1D

Solution

2. Calculate the I=$\int_{1}^{5} x^2 e^x dx$ with:

   i. Hir or Miss

   ii. Crude 1D

Solution

3. Calculate the I=$\int_{0}^{1} \int_{0}^{5} \frac{20}{13}(x+y) dx dy$ with:

   i. Hir or Miss

   ii. Crude 2D

Solution

4. Calculate the I=$\int_{-1}^{4}\int_{-2}^{3}(9x^2-1)(1+4y)dxdy$ with:
   i. Hir or Miss
   ii. Crude 2D

Solution

5. Calculate the I=$\int_{0}^{2\pi}\int_{0}^{1} re^{r^2}drd\theta$ with:
   i. Hir or Miss
   ii. Crude 2D

Solution

# 7 Fitting - Least Square Method

1. Find the y=bx+a of best fit for the following data using the Least Squered method. *Use*

$$S_k = \sum \frac{x_i^k}{\sigma_i^2} \quad , \quad M_k = \sum \frac{x_i^k \cdot y_i}{\sigma_i^2}$$

| # | x | y |
|---|---|---|
| 1 | 1.0 | 2.9 |
| 2 | 2.0 | 4.1 |
| 3 | 3.0 | 5.1 |
| 4 | 4.0 | 5.8 |
| 5 | 5.0 | 7.2 |

Table 1: Experimental Data

Solution

2. The theoretical curve of the following experimental data is:

$$f(x) = k(x - x_o)^2 + y_o$$

Find the $k, x_o$ and $y_o$.

| # | x | y |
|---|---|---|
| 1 | 0.0 | 1.0 |
| 2 | 1.0 | 0.0 |
| 3 | 2.0 | 1.1 |

Table 2: Experimental Data

Solution

# 8 Interpolation

1. Calculate the f(1) and plot the interpolation curve, using the Lagrange - Interpolation method from the data set below.

| **x** | -1.6 | -1.0 | -0.4 | 0.2 | 0.8 | 1.4 |
|---|---|---|---|---|---|---|
| **y** | 0.28 | 0.61 | 0.92 | 0.98 | 0.73 | 0.38 |

Table 3: Data Set

Solution

2. Calculate the f(1) and plot the interpolation curve, using the Neville - Interpolation method from the data set below.

| **x** | -1.6 | -1.0 | -0.4 | 0.2 | 0.8 | 1.4 |
|---|---|---|---|---|---|---|
| **y** | 0.28 | 0.61 | 0.92 | 0.98 | 0.73 | 0.38 |

Table 4: Data Set

Solution

3. In a circuit of resistance R = 5 kΩ and inductance L = 4 mH connected in parallel, with the resistance grounded, a current I(t)= $I_o sin(\omega t)$ is applied with $I_o$ = 25 mA. The voltage developed across the circuit after equilibrium is restored is:

$$U(t) = \frac{\omega R L I_o}{\sqrt{R^2 + \omega^2 L^2}} \cdot sin\left(\omega t + tan^{-1}\frac{R}{\omega L}\right)$$

*Units:* [Ω]=[Hz][H]=[H]/[s]

   i. Calculate the values of voltage U for ω=0.1(0.2)1.9 MHz and t = 0.1, 1, 10 μs.

   ii. Using the values you calculated, approximate the voltage V by first-order Lagrange interpolation. Compare the results with the exact values from the analytical relationship of voltage V.

Solution

# 9 Differentiation

1. Find the derivative of the following functions using the definition of the derivative for $h = 10^{-8}$.

$$lim_{h\to 0}\frac{f(x+h)-f(x)}{h}$$

   i. f(x)=$3x^5 \cdot e^x$ at x=1
   ii. f(x)=$ln(x) \cdot e^{x^2}$ x=2
   iii. f(x)=$sin(3x) \cdot cos(x)$ x=1

Solution

2. Find the equation of the line tangent to the function $f(x) = x^2 + 4$ at x=4.

Solution

3. Find the derivative and the error of the following functions using the definition of the derivative for $h = 10^{-8}$ at x=1.
*To find the Error, us the following fomula*

$$Error = -\frac{h}{2}\frac{d^2 f(\xi)}{d\xi^2}$$

Solution

4. Two horizontal thin rings of the same radius r are placed with their centers on the same vertical z-axis, at the positions z = 0 and z = h, and carry total charges Q and -Q, respectively. The electric field on the z-axis is parallel to the axis, with direction from the positive to the negative ring, and has magnitude:

$$E(z) = \frac{Q}{4\pi\varepsilon_o}\left(\frac{z}{(r^2+z^2)^{3/2}} + \frac{h-z}{(r^2+(h-z)^2)^{3/2}}\right)$$

This field is symmetric around z = h /2 , between the centers of the two rings. So the point z = h/2 is a local extremum of the field. This means that the field is homogeneous around this point, or, in other words, there is no variation of the field with distance from the center z = h /2 to a first-order approximation. The next order of approximation in which changes of the field with distance from the center will appear will be the fourth and not the third, since the field is symmetric with respect to z = h/2 (an even function of z") and therefore all odd-order generators of the measure zero at this point. The second derivative has the form:

$$\frac{d^2E}{dz^2} = \frac{Q}{4\pi\varepsilon_o}\left(\frac{15z^3}{(r^2+z^2)^{7/2}} - \frac{9z}{(r^2+z^2)^{5/2}} + \frac{15(h-z)^3}{[r^2+(h-z)^2]^{7/2}} - \frac{9(h-z)}{[r^2+(h-z)^2]^{5/2}}\right)$$

i. Plot the field as a function of z, in a unit system where the unit of z is h and the unit of E(z) is Q $/(4\pi\varepsilon_o h^2)$, for r = 0.1h, 0.3h, h $\sqrt{6}$, h. Characterize the extremity of the field at the midpoint z = h /2 for each value of r and give the physical meaning of the E(z) curves for each value of r.

ii. For the same values of r, calculate the second derivative $d^2E/dz^2$ with Newton-Gregory method at the points z = 0.1(0.05)0.8

iii. For the same values of r, calculate the third-order derivative $d^3E/dz^3$ with Newton-Gregory method at the points z = 0.1(0.05)0.75

Solution

# 10 Integrals

1. Calculate the following integrals using the definition of the Integrals ($n = 10^8$):

*Definition of Integrals*

$$I = \sum_{i}^{n} f(x) \cdot \left(\frac{b-a}{n}\right)$$

i. $\int_1^5 e^x \sqrt{x}$ dx

ii. $\int_0^1 cos(3x)\sqrt{sin(x)}$ dx

Solution

2. Calculate the following integrals using the Trapezium method:

i. $\int_0^4 e^x + 5x$ dx

ii. $\int_5^{89} e^x log^2(x)$ dx

Solution

3. Calculate the following integrals using the Simpson method:

i. $\int_0^4 e^x + 5x^3$ dx

ii. $\int_5^{89} \frac{\sqrt{x^3}}{x^2}$ dx

Solution

4. Calculate the following integral using,

$$I = \int_2^{10} e^x \sqrt{x} dx$$

i. General Trapezium method:

i. General Simpson method:

Solution