

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 \bar{x}
 - ii. Variance σ_x^2
 - iii. Standard deviation σ_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 approaches better the uniform distribution and why?
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:

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

- i. Inverse transformation method
- ii. Hit or Miss method

[Solution](#)

[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 needed to have error $\frac{10^{-6}}{2}$;

[Solution](#)

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

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

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

[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 method
- 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:

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

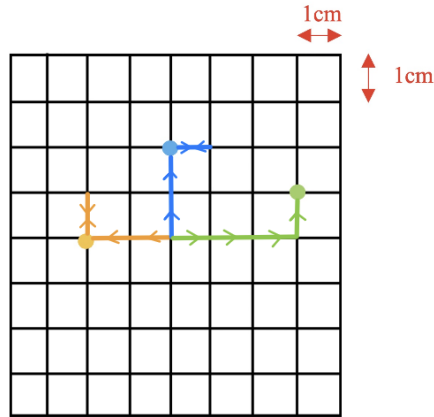


Figure 1: Example of Brownian motion of three particles after $t=4\text{sec}$

- i. Hist 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 them. How many dice it takes to win the game?

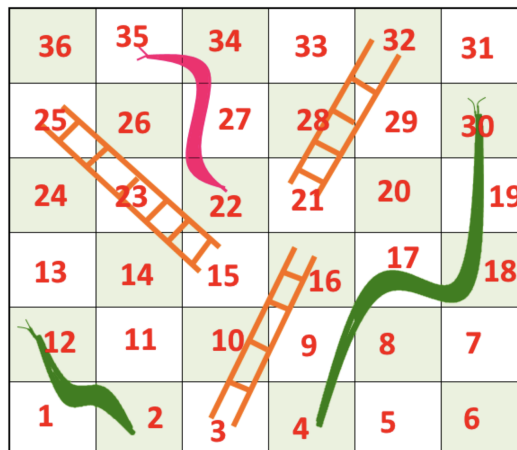


Figure 2: Snakes and Ladders game!

[Solution](#)

3. **Monty Hall problem!** Suppose you're on a game show, and you're 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 .. hahaha! 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

- Hir or Miss
- Crude 1D

[Solution](#)

2. Calculate the $I = \int_1^5 x^2 e^x dx$ with

- Hir or Miss
- Crude 1D

[Solution](#)

3. Calculate the $I = \int_0^1 \int_0^5 \frac{20}{13} (x + y) dx dy$ with

- Hir or Miss
- Crude 2D

[Solution](#)

4. Calculate the $I = \int_{-1}^4 \int_{-2}^3 (9x^2 - 1)(1 + 4y) dx dy$ with

- i. Hir or Miss
- ii. Crude 2D

[Solution](#)

5. Calculate the $I = \int_0^{2\pi} \int_0^1 r e^{r^2} dr d\theta$ 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 Squared method.
Use

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

#	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 above.

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 above.

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 $R = 5 \text{ k}\Omega$ and inductance $L = 4 \text{ mH}$ connected in parallel, with the resistance grounded, a current $I(t) = I_o \sin(\omega t)$ is applied with $I_o = 25 \text{ mA}$. 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: $[\Omega] = [\text{Hz}][\text{H}] = [\text{H}]/[\text{s}]$

- i. Calculate the values of voltage U for $\omega = 0.1(0.2)1.9 \text{ MHz}$ and $t = 0.1, 1, 10 \text{ }\mu\text{s}$.
- 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

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

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

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

Solution

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

Solution

- 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

- 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:

$$E(z) = \frac{Q}{4\pi\epsilon_0} \left(\frac{z}{(r^2 + z^2)^{3/2}} + \frac{h-z}{(r^2 + (h-z)^2)^{3/2}} \right)$$

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:

$$\frac{d^2 E}{dz^2} = \frac{Q}{4\pi\epsilon_0} \left(\frac{15z^3}{(r^2 + z^2)^{7/2}} - \frac{9z}{(r^2 + z^2)^{5/2}} + \frac{15(h-z)^3}{[r^2 + (h-z)^2]^{7/2}} - \frac{9(h-z)}{[r^2 + (h-z)^2]^{5/2}} \right)$$

- 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 $Q/(4\pi\epsilon_0 h^2)$, 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](#)