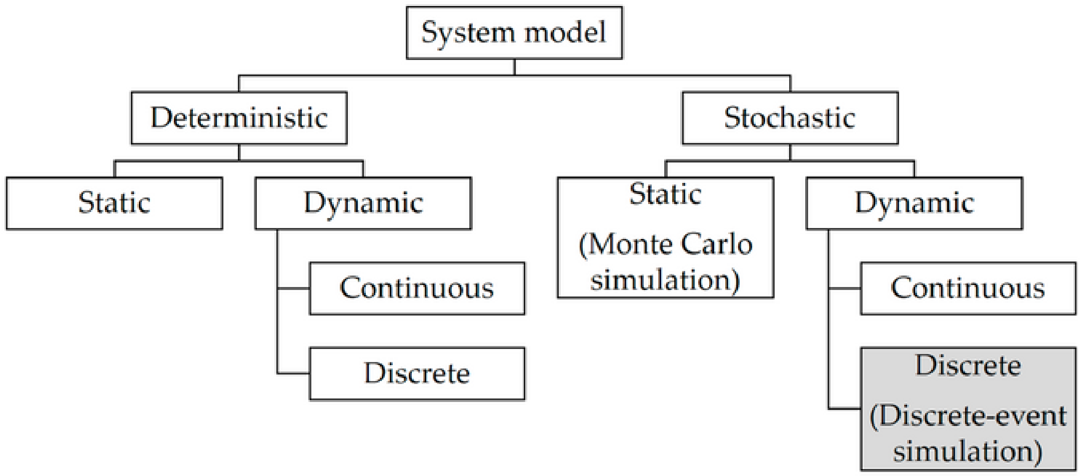
Simulation and modeling 412
notebook

by mishari

Model :A Representation of an object, a system, or an idea in some form other than that of the entity itself.
•It is the abstraction or a representation or a conceptual framework that describes the system.

Types of Models:**Physical** (Scale models, prototype plants,…) , **Mathematical** (Analytical queueing models, linear programs, simulation)

•A **Simulation of a system** is the operation of a model, which is a representation of that system.
System: A collection of entities that act and interact together toward the achievement of some logical end. E.g. computer system



a. Model: An abstraction of reality, representing physical or non-physical systems, phenomena, or processes
b. Environment: A virtual created setting that mimics real world systems or processes for simulation
c. System: A representation in simulations, encompassing selected elements and boundaries to depict a simplified version of reality.
e. Computer Simulation: The use of computer-based mathematical models to emulate the behavior or outcomes of real-world systems.
f. Continuous Model: A simulation approach using continuously changing variables, typically governed by differential equations.
g. Discrete Event Model: A simulation technique that models system changes as a sequence of distinct, individual events.
h. Model Accuracy: The extent to which a simulation model accurately reflects the real world scenario it is designed to represent.
i. Model Performance: The efficiency and effectiveness with which a simulation model operates and produces results.
j. Quality of a Random Number: An assessment of how well a random number generation process simulates true randomness in simulations.

Simulation traffic

Types Of Simulation In Transportation

Time	State	Space		
		Continuous	Discrete	N/A
Continuous	Disc.	Real Transportation Systems * Traffic flow, pedestrians Dynamic traffic assignment		Discrete Event Systems * queueing inventory manufacturing
	Cont.	PDE Traffic flow models Pedestrian models		ODE vehicle motion car suspension queueing (fluid approx)
Discrete	Disc.		Cellular Automata * Traffic, pedestrians Land use Urban sprawl Random Number Generation	Discrete Event Simulation * queueing inventory manufacturing
	Cont.	Car-following models * Microscopic traffic flow models *	Numerical PDE methods Godunov, Variational	Numerical ODE methods Euler, Runga-Kutta time-series * ARIMA
N/A	Disc. or Cont.	Monte Carlo method * : use of pseudo-random number Simulation of static probabilistic problems Integration, Optimization		Econometric models trip generation, distribution, modal split Optimization static traffic assignment

Simulation population

continuous

Exponential Growth/Decay

$$P = P_0 e^{rt}$$

P = total population after time t
P_0 = starting population
r = % rate of growth/decay
t = time
e = Euler's number

discrete

$$P(t) = P_0 (1+r)^t$$

Where:

- $P(t)$: The total population after time t.
- P_0: The starting population or initial population size at time $t = 0$.
- r: The per-period rate of growth (or decay if the rate is negative), expressed as a decimal. For example, a 5% growth rate per period would be written as 0.05.
- t: The number of time periods over which the population is growing. Depending on the context, this could be years, months, days, etc.
- The base of the exponent is $(1+r)$, which accounts for the original population plus the growth each period. This model assumes that growth occurs in discrete steps at the end of each period.

- exponential decay
  - $N(t) = N_0\, e^{-rt}$
- exponential growth
  - $N(t) = N_0\, e^{rt}$

$$\boxed{N(t+\Delta t) = \left(1 + \lambda \frac{\Delta t}{\sigma}\right) N(t)}$$

In the case of bacteria:

- duplication happens every 20 minutes, then $\sigma = 1/3$ (in hours)
- the number of children is 1, then $\lambda = 1$

Assume that at time $t = 0$ there is only 1 bacterium, after 20 minutes (1/3 hours) we have 2 bacteria:

$$N(0 + 1/3) = \left(1 + 1\frac{1/3}{1/3}\right) 1 = 2$$

with $r_d = 1 + \lambda \frac{\Delta t}{\sigma}$ representing the (constant) birth rate.

Queue

Customer	Arrival time	service time	time service begin	time service ends (departure)	time customer waits	time spent on system	time of system idle
1	1	2	1	3	0	2	1
2 last served in 20s	4	5	4	9	0	5	-
3 service not done	8	15	9	24	1	16	-
4	17	2	24	26	7	9	-

System Throughput (X) -> λ :

- Equation and Calculation: $X = \frac{\text{Total number of customers served}}{\text{Total time period}} = \frac{4}{26} \approx 0.15$ customers/second

Total Busy Time (B):

- Equation and Calculation: $B = \sum \text{Service Times} = 2+5+15+2 = 24$

Mean Service Time (Ts):

- Equation and Calculation: $Ts = \frac{\sum X}{N} = \frac{24}{4} = 6$ = aveарge service time

Utilization (U):

- Equation and Calculation: $U = \frac{\text{Total Busy Time}}{\text{Total time period}} = \frac{24}{26} \approx 0.923 \approx 92.3\%$

Mean System Time (W):

- Equation and Calculation: $W = \frac{\sum(\text{Departure Time} - \text{Arrival Time})}{\text{Total Number Of Customers}} = \frac{2+5+16+9}{4} = 8$

Mean Time in Queue:

- Equation and Calculation: Mean t in q $= \frac{\text{Total Time in Queue}}{\text{Total Number Of Customers}} = \frac{7+1}{4} = 2$

Mean Number in the System (L):

- Equation and Calculation: L= Little's law = $L = \lambda \times W = .154 * 8 \approx 1.232$ Customers

- Throughput (X): **Number of customers served / Total time.**
- Total Busy Time (B): **Sum of service times.**
- Mean Service Time (Ts): **Total Busy Time / Number of customers served.**
- Utilization (U): **Total Busy Time / Total time.**
- Mean System Time (W): **Total time each customer spent in the system / Total number of customers.**
- Mean Number in the System (L): **Using Little's Law: L=λW, where λ is the arrival rate.**

Queue-2

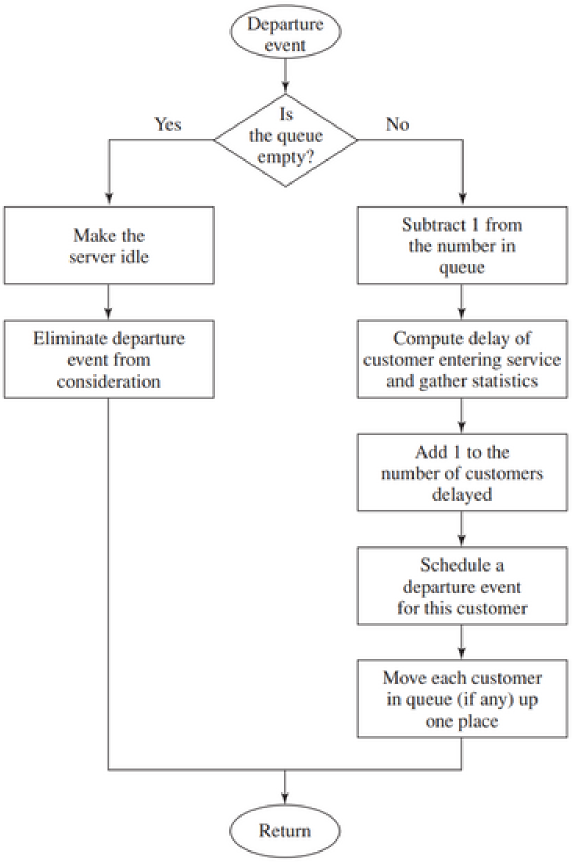


FIGURE 1.9
Flowchart for departure routine, queueing model.

```
Single-server queueing system

Mean interarrival time       1.000 minutes

Mean service time            0.500 minutes

Number of customers           1000


Average delay in queue       0.430 minutes

Average number in queue      0.418

Server utilization           0.460

Time simulation ended     1027.915 minutes
```

FIGURE 1.19
Output report, queueing model.

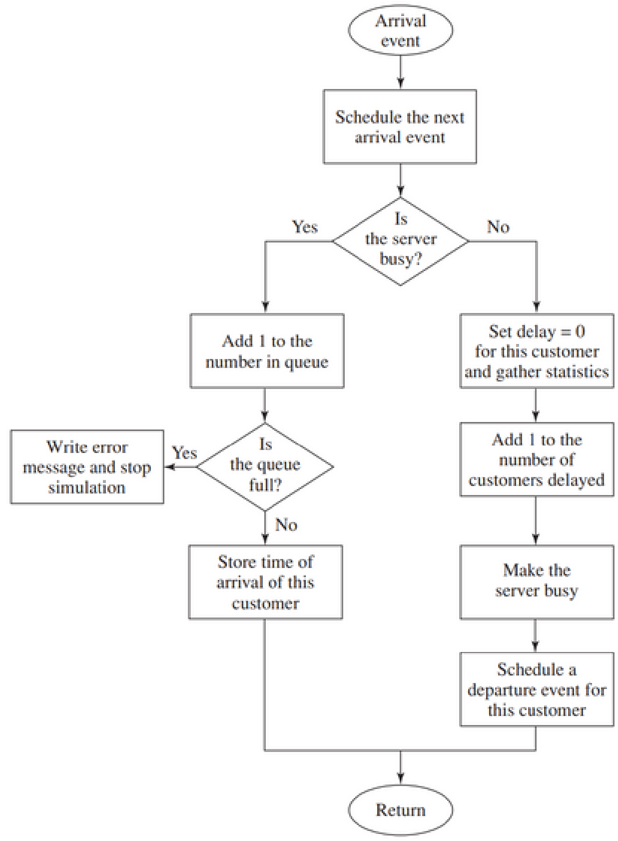


FIGURE 1.8
Flowchart for arrival routine, queueing model.

1. **Arrival Rate (λ):**
   $\lambda = \frac{1}{\text{Mean Interarrival Time}}$
2. **Service Rate (μ):**
   $\mu = \frac{1}{\text{Mean Service Time}}$
3. **Utilization (ρ):**
   $\rho = \frac{\lambda}{\mu}$
4. **Average Number in Queue (Lq):**
   $L_q = \frac{\lambda^2}{\mu(\mu-\lambda)}$
   (For M/M/1 queue only)
5. **Average Time in Queue (Wq):**
   $W_q = \frac{L_q}{\lambda}$
   (Using Little's Law)
6. **Average Number in System (L):**
   $L = \lambda W$
   (Using Little's Law)
7. **Average Time in System (W):**
   $W = \frac{L}{\lambda}$
   (Using Little's Law)
8. **Throughput (X):**
   $X = \frac{\text{Number of Customers Served}}{\text{Total Time}}$
9. **Total Busy Time (B):**
   $B = \text{Number of Customers Served} \times \text{Mean Service Time}$
10. **Server Utilization (U):**
   $U = \frac{B}{\text{Total Time}}$

CFD

kinematic viscosity $\nu = \frac{\mu}{\rho}$ — μ: velocity of the fluid; ρ: Pressure

velocity profile

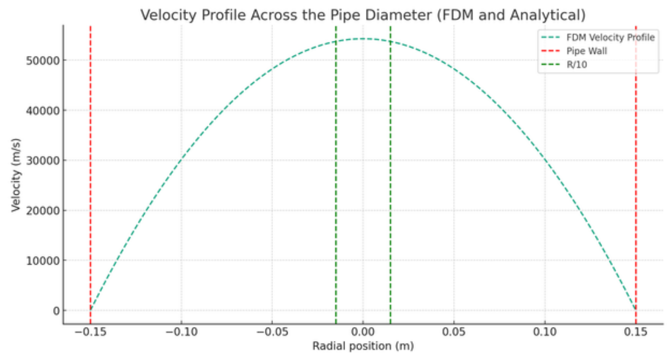
max at position 0

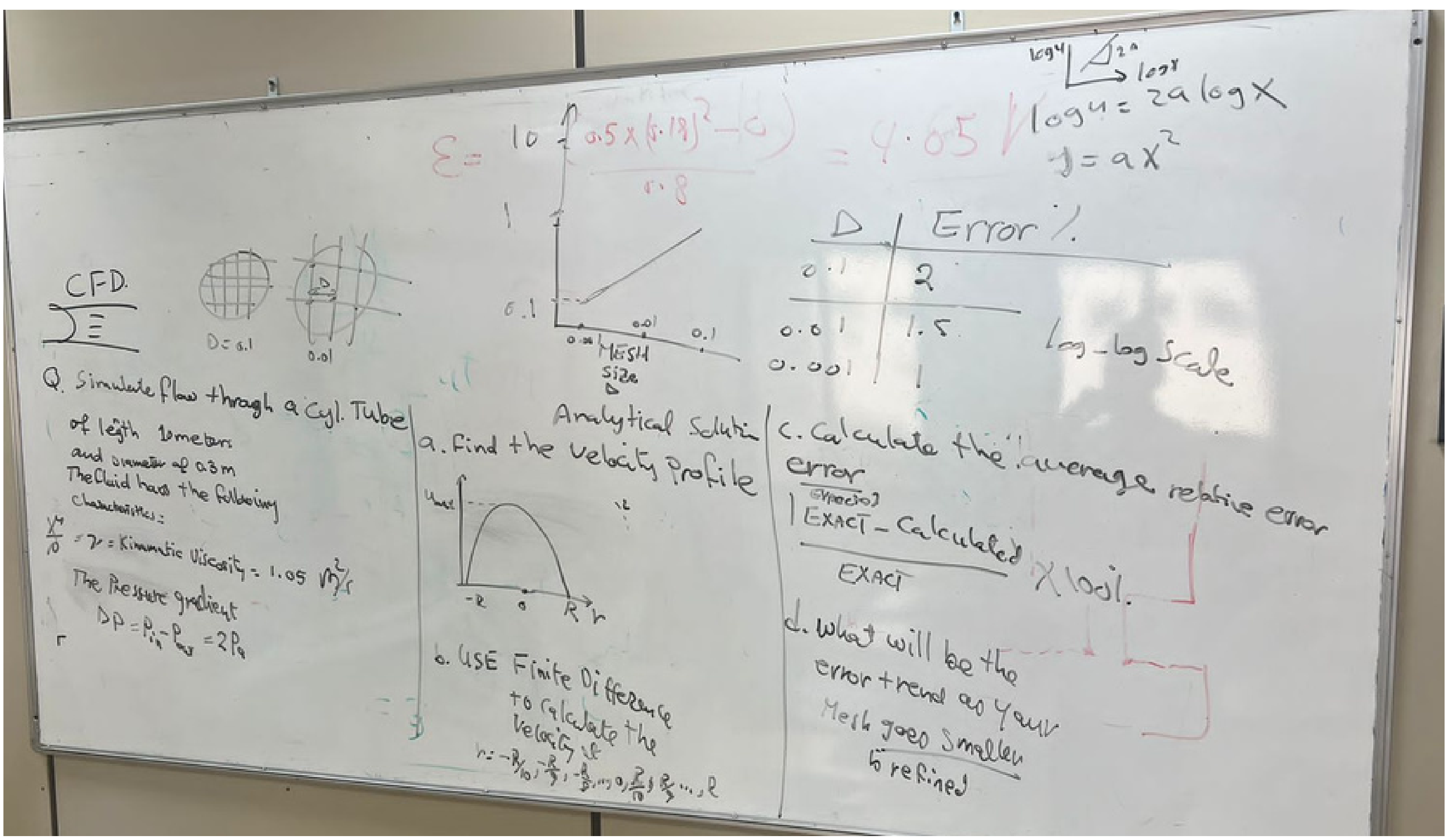
$$u = u_0\left(1 - \frac{1}{r}\right)^2$$

idk? maybe for any point in the pipe

$$u = u_0\left(1 - \frac{4r^2}{D^2}\right)$$

- u represents the velocity at a given point within a flow field.
- r is the radial position from a central point (like the center of a tube or pipe in fluid dynamics).
- u0 is a reference or maximum velocity, typically at the center or another specific point in the flow field.

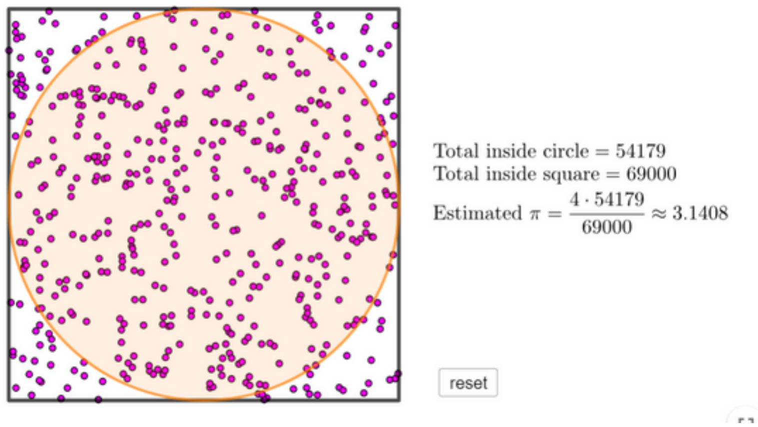


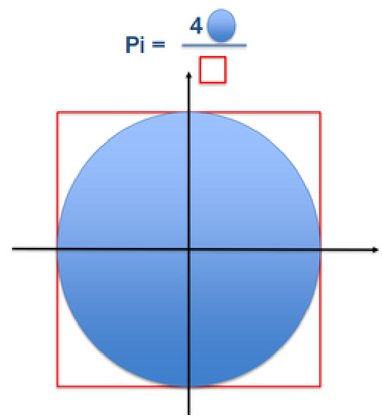


error

- **Average Relative Error Calculation:** Used to assess the accuracy of the simulation against analytical or empirical data.
- $$\text{Error} = \frac{\sum |y_{exact} - y_{calculated}|}{\sum y_{exact}} \times 100\%$$

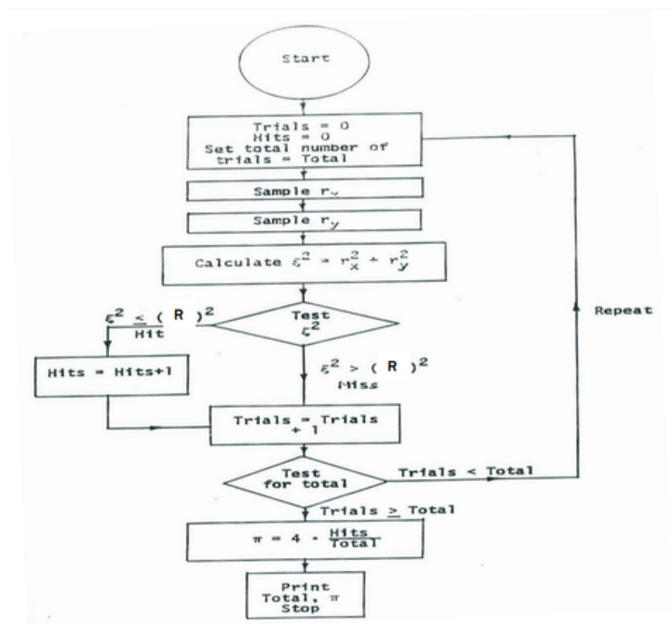
Monte carlo





1. **Estimating Pi**:
   $\pi \approx \frac{4 \times \text{number of points inside the circle}}{\text{total number of points sampled}}$
2. **Integral Estimation**:
   $I \approx \frac{1}{N} \sum_{i=1}^{N} f(x_i)$
   where I is the estimated value of the integral, $f(x)$ is the function being integrated, and x_i are the random samples within the domain of f.
3. **Expectation Value**:
   $E[X] \approx \frac{1}{N} \sum_{i=1}^{N} x_i$
   where $E[X]$ is the expected value of the random variable X, and x_i are the random samples.
4. **Variance Estimation**:
   $\text{Var}(X) \approx \frac{1}{N-1} \sum_{i=1}^{N} (x_i - E[X])^2$

6. **Error Estimation**:
   The error in a Monte Carlo estimation typically decreases at a rate of $1/\sqrt{N}$, where N is the number of samples. The standard error is:
   $\text{SE} \approx \frac{\sigma}{\sqrt{N}}$
   where σ is the standard deviation of the sample.

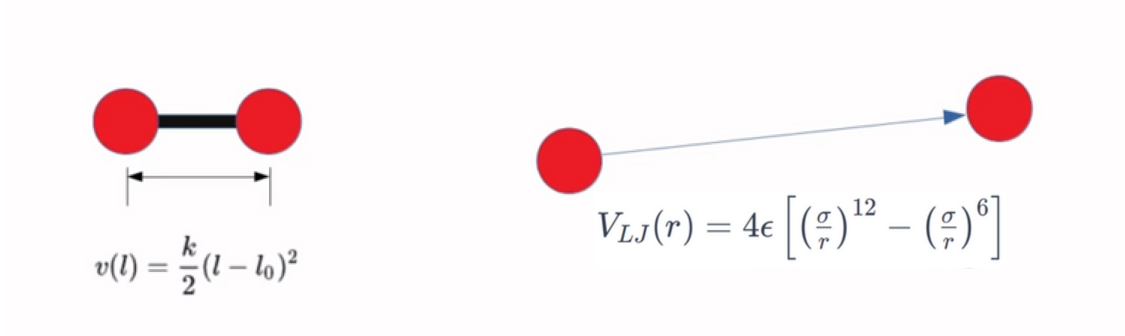


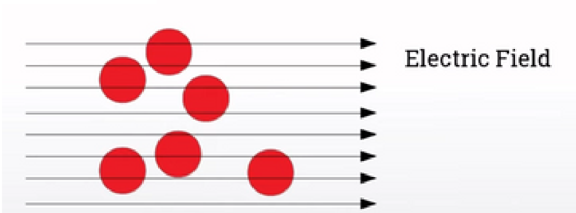

```python
import random

# Define the number of trials
total_trials = 1_000_000  # 1 million trials for a good approximation

# Initialize count of hits inside the circle
hits = 0

# Conduct the trials
for _ in range(total_trials):
    # Sample random x, y points in the range [-1, 1]
    rx = random.uniform(-1, 1)
    ry = random.uniform(-1, 1)
    # Calculate the square of the distance from the origin (0,0)
    distance_squared = rx*2 + ry*2
    # If the point is inside the unit circle, count it as a hit
    if distance_squared <= 1:
        hits += 1

# Calculate the approximation of Pi
pi_estimate = 4 * hits / total_trials

# Print the results
print(f"Total trials: {total_trials}")
print(f"Pi approximation: {pi_estimate}")
```

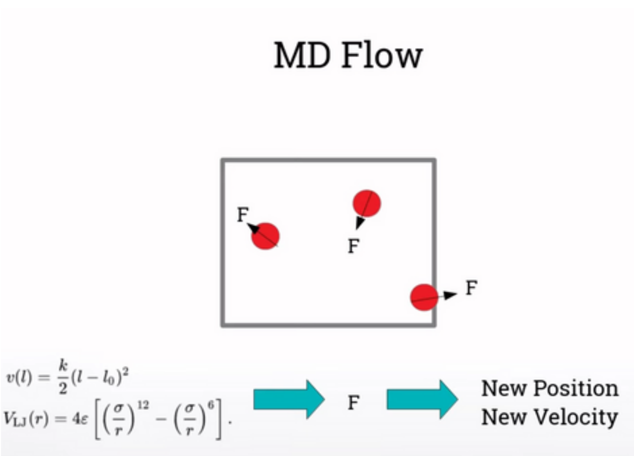
psudocode:

```
import library for random numbers

set total_trials to 1000000
set hits to 0

for each trial from 1 to total_trials do
    set rx to random number between -1 and 1
    set ry to random number between -1 and 1

    set distance_squared to rx squared plus ry squared

    if distance_squared is less than or equal to 1 then
        increment hits by 1
    end if
end for

set pi_estimate to 4 times (hits divided by total_trials)

output "Total trials: ", total_trials
output "Pi approximation: ", pi_estimate
```

Molecular dynamics







In the Lennard-Jones potential equation:

- σ is the distance at which the intermolecular potential between two particles is zero. It represents the point at which the attraction and repulsion between particles balance each other out.
- ϵ represents the depth of the potential well, corresponding to the strength of the attraction at the equilibrium intermolecular distance.
- r is the distance between the two particles.
- $V_{LJ}(r)$ is the potential energy between the particles as a function of the distance r.

The Lennard-Jones potential is used to model interactions between a pair of neutral atoms or molecules, especially in simulations of molecular dynamics. The r^{-12} term represents the repulsive forces (short-range), while the r^{-6} term models the attractive forces (long-range).

Assume $\epsilon = 1.65 \times 10^{-21}$ J and $\sigma = 3.4 \times 10^{-10}$ m, which are typical values for argon. Calculate the force experienced by one argon atom when it is 3.4×10^{-10} m (σ), 6.8×10^{-10} m (2σ), and 1.02×10^{-9} m (3σ) away from the other argon atom.

Using the given $\epsilon = 1.65 \times 10^{-21}$ J and $\sigma = 3.4 \times 10^{-10}$ m:

For $r = \sigma$:

$$V_{LJ}(\sigma) = 4 \times 1.65 \times 10^{-21}\left[\left(\frac{3.4\times10^{-10}}{3.4\times10^{-10}}\right)^{12} - \left(\frac{3.4\times10^{-10}}{3.4\times10^{-10}}\right)^{6}\right]$$

For $r = 2\sigma$:

$$V_{LJ}(2\sigma) = 4 \times 1.65 \times 10^{-21}\left[\left(\frac{3.4\times10^{-10}}{2\times3.4\times10^{-10}}\right)^{12} - \left(\frac{3.4\times10^{-10}}{2\times3.4\times10^{-10}}\right)^{6}\right]$$

For $r = 3\sigma$:

$$V_{LJ}(3\sigma) = 4 \times 1.65 \times 10^{-21}\left[\left(\frac{3.4\times10^{-10}}{3\times3.4\times10^{-10}}\right)^{12} - \left(\frac{3.4\times10^{-10}}{3\times3.4\times10^{-10}}\right)^{6}\right]$$

from stat101

$\bar{X}$ Mean (المتوسط)

Mean for Raw
(المتوسط العادي)

$\bar{X} = \frac{\sum_{i=1}^{n} X_i}{n}$ مجموعهم / عددهم

مثال : 4, 6, 9, 1

$\frac{4+6+9+1}{4} = 5$ $\bar{X} = 5$

Weighted Mean
(المتوسط المرجح)

حساب المعدل

		X_i الدرجة	W_i الساعات	W_iX_i
تقن	A	5	3	15
ريد	B	4	1	4
انجل	B	4	6	24
ريض	C	3	4	12
TOTAL			14	55

$\bar{X} = \frac{\sum_{i=1}^{z} W_i X_i}{\sum W_i}$

$\frac{55}{14}$

$\bar{X} = 3.93$

Mean for continuous frequency table
(البيانات المجدولة التكرارية)

$\bar{X} = \frac{\sum_{i=1}^{k} F_i M_i}{\sum F_i}$

mid point m_i	f_i	fm
12.5	8	100
14.5	2	29
16.5	5	82.5
43.5	15	

$\frac{211.5}{15}$

$\bar{X} = 14.1$

Mean for discrete frequency table
(البيانات المجدولة المنفصلة)

$\bar{X} = \frac{\sum_{i=1}^{m} F_i x_i}{\sum F_i}$

x_i	f_i	f_ix_i
0	7	0
1	4	4
2	9	18

$\frac{22}{20}$

$\bar{X} = 1.1$

Variance (التباين)

Variance for frequency distribution
(التباين للبيانات المجدولة)

$S^2 = \frac{\sum F_i (X_i - \bar{X})^2}{\sum F_i - 1}$

MID POINT	F
1	1
2	2
3	1
4	4
5	2
	10

$\bar{X} = 3.4$

$S^2 = \frac{1(1-3.4)^2+2(2-3.4)^2+1(3-3.4)^2+4(4-3.4)^2+2(5-3.4)^2}{10-1}$

$S^2 = 1.822$

Variance for Raw Data
(التباين العادي)

$S^2 = \frac{\sum (X_i - \bar{X})^2}{n-1}$

EX : 2, 3, 5, 6, 9

$S^2 = \frac{(2-5)^2+(3-5)^2+(5-5)^2+(6-5)^2+(9-5)^2}{5-1} = 7.5$

- $S^2 \geq 0$ Always

Standard Deviation
(الأنحراف المعياري) :

$S = +\sqrt{S^2}$

$S = +\sqrt{1.82} = 1.349$

$S = +\sqrt{7.5} = 2.738$

- $S \geq 0$ Always

الجذر الموجب للتباين

Positive square root of the variance

- The **BEST** measure of disperion in general
- The standard deviation is sensitive to extreme values

PERCENTILES , DECILES , QUARTILES

خطوات الحل :

1- نرتب البيانات تصاعدياً

2- نحسب الحرف الصغير q , p ,d

3- نحسب الحرف الكبير Q , P , D

الحرف الصغير q , p , d = $\frac{r\,(n+1)}{4,\ 100,\ 10}$ = K , S

المطلوب بالسؤال *عدد البيانات*

الحرف الكبير Q , P , D = $X_k + S(X_{k+1} - X_k)$

Calculate for the given data 0 , 1 , 3 , 7 , 8 , 10 , 11 : ($X_1, X_2, X_3, X_4, X_5, X_6, X_7$)

Q_2

$q_r = \frac{r(n+1)}{4}$

$q_2 = \frac{2\,(7+1)}{4} = 4.0$ K.S

$Q_r = X_k + S(X_{k+1} - X_k)$

$Q_2 = 7 + 0\,(8 - 7)$

$Q_2 = 7$

P_{75}

$p_r = \frac{r(n+1)}{100}$

$p_{75} = \frac{75\,(7+1)}{100} = 6.0$ K.S

$P_r = X_k + S(X_{k+1} - X_k)$

$P_{75} = 10 + 0\,(11 - 10)$

$P_{75} = 10$

D_5

$d_r = \frac{r(n+1)}{10}$

$d_5 = \frac{5\,(7+1)}{10} = 4.0$ K.S

$D_r = X_k + S(X_{k+1} - X_k)$

$D_5 = 7 + 0\,(8 - 7)$

$D_5 = 7$

Coefficient of Variation
(معامل الأختلاف)

Useful measure to compare between sets of data with different Units (measures)

$CV = \frac{S}{\bar{X}} \times 100$

Z-score
(الدرجة المعيارية)

Converts data to make its mean = 0 and S = 1

$Z_{x_i} = \frac{X_i - \bar{X}}{S}$

Range (المدى) is sensitive to extreme values

Range for raw data = $X_L - X_S$

Range for distribution table (continuos) = $X_k - X_1$

Range for frequency table (Discrete) = $X_m - X_1$

IQR = Q3 - Q1 • also called as mid-spread

In the context of probability

Expected Value (Mean, $E(X)$):

- $E(X) = \mu = \sum xP(x)$

x is an outcome in the distribution (values)
P(X) is the probability

Variance (σ^2):

- $\sigma^2 = \sum(x-\mu)^2P(x)$

x is an outcome in the distribution (values)
μ is mean

example:
E(X) = μ =**∑xP(x)** = 0×0.4+1×0.6 = 0.6
σ2 = **∑(x−μ)2P(x)** = (0−0.6)2×0.4+(1−0.6)2×0.6 = 0.24