CIS II

Lecture 1. Coin Toss Statistics

if probability p for heads and $1-p$ for tails then prob. of seeing M heads in n trials $n > M$.

$$P(M:n) = {}^{n}C_{M} \cdot p^{M} \cdot q^{n-M}$$

$$p(X=x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad x \in \mathbb{R}$$

Gaussian Distributⁿ

$$\int_{-\infty}^{\infty} p_x \, dx = 1$$

Q / Error Functⁿ.

Fraction of heads in n coin tosses $= M_n = \frac{M}{n} \Rightarrow 0 \leq M_n \leq 1$

$$\lim_{n \to \infty} M_n = p$$

$$\text{Prob}(x < M_n < y) = \sum_{r \in \mathbb{Z} \wedge x < r/n < y} P(r:n)$$

Cramer's Theorem

Bernoulli Random Variable - 0 or 1.

X_i iid $\rightarrow$ independent identical distributⁿ

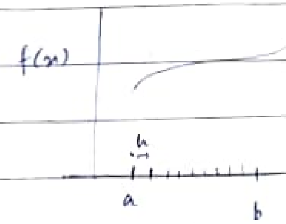
$E[e^{tX_i}] < \infty \quad \forall t \in \mathbb{R}$. $\quad E[X^N] = \sum p(x) x^n$

$\forall a > E[X_i]$.

$$\lim_{n \to a} \frac{1}{n} \log P(S_n \geq a_n) \sim e^{-n I(a)}.$$

Lecture 2 : 18th May

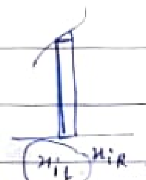
Riemann Integral -



$h = \frac{b-a}{N}$

$$I = \sum_{i=1}^{N} I_i$$

$I_i = h \cdot f(x_{iL})$



Rectangular Approximations for I_i

① Left Integral
Assume height of rectangle = Left side

② $I_i = h \cdot f(x_{iR})$
Right Integral - height is right side

as $h \to 0$ and $N \to \infty$, left and right sum converge

③ Trapezoidal Approximatn for I_i : $\frac{h}{2}\left[f(x_{iL}) + f(x_{iR}) \right]$
Fitting function to straight line

~~④ Simpson's Rule~~ i.e linear Approxn to function by left height and right height

④ Simpson's Rule - Fitting functn to parabola
i.e Quadratic Approxn to functn by left height, right height and one value in the middle.

$f(x) = c + ax + bx^2$ $\quad [f(x_{iL}), f(x_{iR}), f(x_{im})]$ middle

$$\int_{x_{iL}}^{x_{iR}} dx\, f(x) = \left[cx + \frac{ax^2}{2} + \frac{bx^3}{3} \right]_{x_{iL}}^{x_{iR}}$$

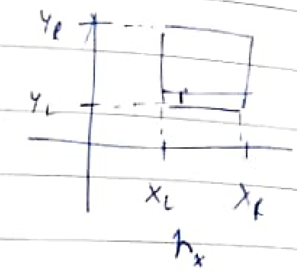
continuous and differentiable at every pt. except finite no. of pts

$\Rightarrow$ Riemann - Stieltjes converges

Cost of computation → need to compute value of funct^n at each ~~de~~ interval.

Extendable to 2D.

$$\int_{x_L}^{x_R} dx \int_{y_L}^{y_R} dy\, f(x, y).$$



$$\approx \sum_{i,j} h_x h_y\, f(x^*, y^*) \qquad x^*, y^* \in A_{ij}$$

$h_x h_y$ → Pixel

Cost of computat^n $O(N^2)$

Voxels → 3D pixels
$h_x h_y h_z$.

For d-dimensional. N^d computat^n required for
Brute force integrat^n only possible for small dimensional

$|I_t - I_u| < \varepsilon$ arbitrary & depending on precision of grid, ~~a~~ usually $1 \sim 2\%$..

∴ Tricks used, for minimizing time.
Equal sized voxels or pixels ~~must be~~ are being used here.
These are for 0 D.

Comp Fluid Dynamics other 3 & 4 D computations

* Adaptive Mesh ~~Met~~ Methods

Error in funct^n is less when funct^n is changing less.
i.e. ~~cabros de~~ error proportional to derivative

What we do here is we make the width of rectangle larger when its changing fast and small ~~width~~ when changing slow

c) h_i is inversely proportional to $|f'(x)|$. $h_i = \dfrac{a}{b+|f'(x)|}$
for first order schemes of integratn.

don't want $f(x)$ to blow up when derivative goes to zero

h_i is inversely proportional to $|f''(x)|$.
for ~~first~~ second order scheme of integratn
(Quadrature schemes) ~~of~~ e.g. Simpson's

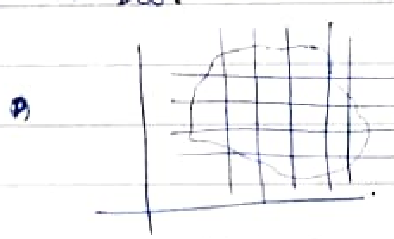
Look at how error scales as width of integral and scale it so that error is approximately same for each width
Because in first order schemes, error comes from ignoring curvature
in OD schemes it comes from slope.

In 2D, we look at the ~~width of~~ magnitude of the gradient.
we look at triangular meshes instead of rectangles and in 3D at pyramid like figures

* HIGHER DIMENSION INTEGRALS

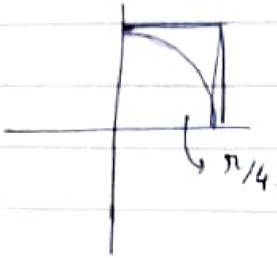
No of evaluatns large.
Monte Carlo Methods have become popular:
① Intuitive
② Implementatn not too difficult
Gambling city
Random numbers used in this ~~SD~~ scheme.

e.g. Inkblot Area - make a grid, ~~pa~~ count no of full squares



A = N × area of grid square

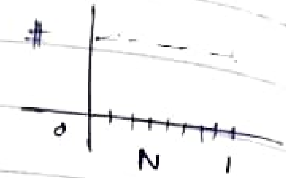
e.g. Area of ~~a~~ Unit Circle



$$I = \int_0^1 dx\,\sqrt{1-x^2} = \frac{\pi}{4}$$

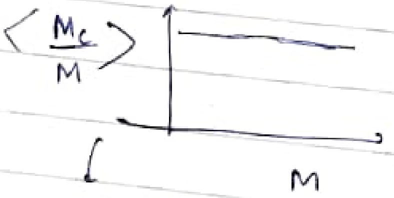
Select random pt. inside unit square
$(x,y) = (\text{rand}[0,1], \text{rand}[0,1])$.

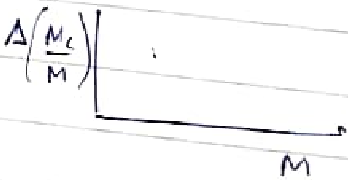
rand → uniform random no.
If you call this funct^n m times, ~~and~~ histogram is almost flat



~~Let~~ $\lim_{M\to\infty} \frac{M_c}{M} = \frac{A\,(\text{Quadrant})}{A.(\text{Rectangle})} = \frac{\pi/4}{1.}$

As $m \to \infty$, $\frac{\text{no. of pts. falling in circle}}{\text{no. of pts falling in square}} = \frac{A_c}{A_B}$.





This is Average we want variance. ~~$\langle A^2\rangle \langle A\rangle$~~

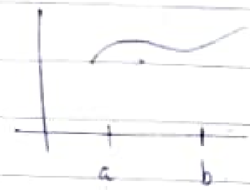
$$\Delta(x) = \sqrt{\sum_{\text{expt},i} (x_i - \bar{x})^2} \times \frac{1}{N}$$

will calculate & show on next page.

$$I = \int_a^b dx\, f(x) = \frac{1}{(b-a)} \int_a^b dx\; \rho_u(x;[a,b]) \cdot f(x).$$

Prob density & prob. of ~~voltage~~ uniform random variable is a const.

$= \frac{1}{(b-a)} \underset{x\sim\rho_u}{\mathbb{E}} f(x) = J_m$ ~~and~~ definite integral interpreted as statistical expectation of pts. b/w a & b
~~a~~ as $m\to\infty$ this equals I_m



$p(x)\,dx = \text{prob}(x \in [x, x+dx])$

For improper integrals you need to modify it otherwise $\frac{1}{(b-a)} = 0$

because 

$\int_0^1 p_u(x)\,dx = 1$. is not satisfied

define $p_u(x) = c \quad 0 \leq x \leq 1$

$= 0 \quad$ otherwise

$$I = \int_{-\infty}^{\infty} dx\, f(x)$$

$p_u(x)\; dx = \text{Prob}(x \in [x, x+dx])$. $\qquad p_u(x) \geq 0$.

$p_u(x : [a, b]) = c \quad a \leq x \leq b$.

$= 0 \quad$ otherwise

$$\int_{-\infty}^{\infty} dx\; p_u(x; [a, b]) = 1.$$

$$\|$$

$$\int_a^b dx\, p_u = c(b - a)$$

$$\boxed{\lim_{M \to \infty} I_m = I}$$

* Important Sampling

Non uniform RNG is used consider any $p(x)$

$$I = \int_a^b dx\, f(x) = \int_a^b dx\; p(x) \cdot \frac{f(x)}{p(x)}$$

1. $p(x) \neq 0 \quad \forall x \in [a, b]$
2. $p(x) \cancel{x f(x)} = +ve$ (if not calculate -ve of integral)
3. $\int_a^b dx\; p(x) = 1$.

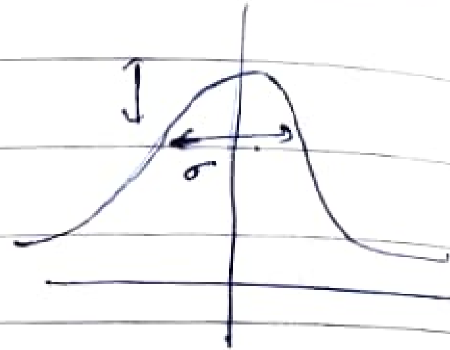
$$\boxed{I = \underset{x \sim p(x)}{\mathbb{E}} \frac{f(x)}{p(x)}.}$$

$\Rightarrow$ $p(x)$ can be interpreted as a probability ~~dis~~ density function.

~~e.g. The Gaussian Distribution~~

e.g. - we Gaussian Distribution

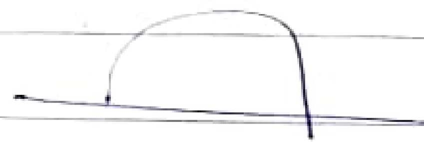
$$\boxed{\rho_g(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-x_0)^2}{2\sigma^2}}}$$



why useful?

consider semicircle

$$f(x) = \begin{cases} \sqrt{1-x^2} & -1 \le x \le 1 \\ 0 & \text{otherwise} \end{cases}$$



Lecture 3 · 22nd May

ODEs

Have seen eqn of the form

$\frac{dx}{dt} = f(x)$, solve for $x(t)$

e.g. - $\frac{dx}{dt} = \alpha x$ decay rate for nuclear process

$\frac{dx}{x} = \alpha dt \Rightarrow \ln x = \alpha t + c$

$\underline{x = x_0 e^{\alpha t}}$

depending on range to which α belongs, we see diff. behaviour

① $\alpha > 0$ $x(t) \to \infty$ $\forall x \in \mathbb{R}^+$

~~$\alpha < 1 \Rightarrow x(t) \to 0$~~

② $\alpha = 0$ $x(t) = X_0$

③ $\alpha < 0$ $\lim_{t\to\infty} x(t) \to 0$ ← Stable Asymptotically

Let $\alpha = a + ib \in \mathbb{C}$

i.e. $x(t) = x_0 e^{(a+ib)t} = (x_0 e^{a}t)e^{ib}$

~~$a > 0$, $b > 0$ $x = \alpha x_0 e^{(a+ib)t}$~~

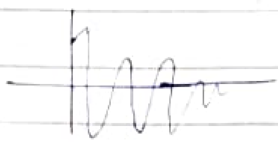
① $a > 0$ oscillatory unstable

② $a = 0$ $e^{ib} \to$ rotatn

③ $a < 0$ same $b > 0$

① $a > 0, b \neq 0 \Rightarrow x(t)$ oscillatory unstable

② $a < 0, b \neq 0 \Rightarrow x(t)$ oscillatory stable



2D

$\frac{dx}{dt} = f_1(x, y, t)$ $\frac{dy}{dt} = f_2(x, y, t)$.

returns scalar, takes input x, y, t

To solve → $\frac{d\vec{r}}{dt} = \vec{f}(\vec{R}, t)$ $\vec{R} = \begin{pmatrix} x \\ y \end{pmatrix}$ Takes input ~~column~~ vector & time

Dependence can be explicit or implicit

explicit e.g. $f(x,t) = \alpha t^2 + ax$

solve pos. fn w.r.t time can solve anything

$$\frac{d\vec{R}}{dt} = \begin{pmatrix} dx/dt \\ dy/dt \end{pmatrix}$$

What we want to solve for are usually steady states / fixed pts.

$\frac{d\vec{R}}{dt} = 0 \Rightarrow \frac{dx}{dt} = 0$ & $\frac{dy}{dt} = 0$

- System behaviour / config doesn't change after this because determined by rate laws
- we analyse behaviour near steady states.
- TAYLOR ~~EXPAN~~ EXPANSION → $\frac{d\vec{R}(t)}{dt} = f(R)$

1D → $f(x) = f(x_0) + \frac{df}{dx_0}(x - x_0) + \dots$

$$= f(x_0) + \sum_{n=1}^{\infty} \frac{d^n f}{dx^n} \frac{(x-x_0)^n}{n!}$$

Linear Analysis take only 1 Degree terms.

$f(x_0) + f'(x_0) f(x - x_0)$.

Harmonic Analysis take till 2 degree terms

$f(x_0) + f'(x_0) \cdot f(x - x_0) + \frac{1}{2} f''(x_0) \cdot f(x - x_0)$

usually if $\Delta x = x - x_0 \ll 1$ i.e 1D analysis is sufficient

then $(\Delta x)^2 \ll x$

If we have fixed pt $\cdot f'(x_0) = 0$ then need to do Harmonic Analysis

2D Taylor series

$$f(x,y) = \underbrace{f(x_0,y_0)}_{0^{th}\text{ order Approx}} + \underbrace{\frac{\partial f}{\partial x}\Big|(x-x_0) + \frac{\partial f}{\partial y}\Big|(y-y_0)}_{1^{st}\text{ order Approx}}$$

$$+ \underbrace{\frac{1}{2}\frac{\partial^2 f}{\partial x^2}\Big|_0 (x-x_0)^2 + \frac{1}{2}\frac{\partial^2 f}{\partial y^2}\Big|_0 (y-y_0)^2 + \overbrace{\frac{1}{2}\frac{\partial^2 f}{\partial x \partial y}\Big|_0 (y-y_0)(x-x_0)}^{\text{Bilinear}}}_{2^{nd}\text{ order Approx}}$$

Linear Analysis

$$f(\vec{R}) = f(\vec{R_0}) + J(\vec{R_0})\cdot(\vec{R}-\vec{R_0})$$

$$\begin{pmatrix} \frac{\partial f}{\partial x}\Big|_0 & \frac{\partial f}{\partial y}\Big|_0 \end{pmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix}$$

$$\frac{d\vec{R}}{dt} = \begin{pmatrix} f_1(R) \\ f_2(R) \end{pmatrix}$$

Linear Analysis $\rightarrow$ $\begin{pmatrix} f_1(R_0) \\ f_2(R_0) \end{pmatrix} + \begin{pmatrix} f_{1x}(0) & f_{1y}(0) \\ f_{2x}(0) & f_{2y}(0) \end{pmatrix}$

$$= f(R_0) + \underbrace{\dot{J_0}}_{\text{Jacobian}}\cdot(\vec{R}-\vec{R_0}).$$

For second order analysis we will have the Hessian

All this is important for stability analysis of the system.

$\frac{d\vec{R}}{dt} = f(R_0) + J_0(R-R_0)$ $\quad$ R_0 in steady state

$\Rightarrow f(R_0) = 0$

$\Rightarrow \frac{d\vec{R}}{dt} = J_0(\vec{R_0})$

$\Rightarrow$ for this pt

$$\frac{d(\vec{R}-\vec{R_0})}{dt} = J_0(R-R_0)$$

$$\frac{d\vec{r}}{dt} = J_0\vec{r}$$

This is of the form $\frac{dx}{dt} = \alpha x$

Standard Trick $\rightarrow$

Solve : $J\cdot\vec{r} = \lambda\vec{r}$ Eigenvalue system

If J is an $N\times N$ matrix, there are N eigenvalues and n eigenvectors
As long as there aren't ~~non~~-degenerate eigenvalues.

Theorem $\rightarrow$ any $\vec{r}(t)$ can then be written as sum of eigenvectors.

$$\sum_{i=1}^{N} c_i(t)\,\vec{v_i}$$

$$\frac{d\vec{r}}{dt} = J\cdot\vec{r} = J_0\left(\sum c_i(t)\vec{v_i}\right)$$

$$= \sum_i c_i(t)\, J_0 v_i = \sum_i c_i(t)\,\lambda_i\vec{v_i}$$

$$\frac{dr}{dt} = \underbrace{\sum_i \frac{dc_i(t)}{dt}\vec{v_i}}_{LHS}$$

$\Rightarrow$ coefficient of each eigenvector has to be equal. (since the basis for eigenspace $\rightarrow$ all v_i must be linearly independent)

$$\Rightarrow \frac{dc_i(t)}{dt} = \lambda_i c_i(t)$$

$$\Rightarrow c_i(t) = c_i e^{\lambda_i t}$$

$$\vec{r}(t) = \vec{R}(t) - \vec{R_0} = \sum_i c_i(0)\, e^{\lambda_i t}\, v_i$$

$\lambda_i < 0 \Rightarrow c_i(t) \rightarrow 0 \quad t\rightarrow\infty$

$\lambda_i > 0 \Rightarrow c_i(t) \rightarrow \infty \quad t\rightarrow\infty$

$\lambda_i = a + b_i \longrightarrow$ analysed earlier

* Prey Predator Model

Prey, Predator Let no of predators X, ~~predators~~ prey $\to Y$

we have to analyse $\frac{dX}{dt}$, $\frac{dY}{dt}$.

Fibonacci model of Birth & death rate

~~For~~ When no predation: should reduce to ~~pr~~ ~~normal~~ natural model.

$$\frac{dX}{dt} = \underbrace{\alpha X}_{\text{Natural Birth rate}} \underbrace{- \alpha_0 X}_{\text{Natural Death Rate}} - \overbrace{\beta X Y}^{\text{Death rate due to predat}^n}$$

~~eq~~ Can be combined to $\alpha X - \beta X Y$

$\beta X Y \to$ ~~[illegible]~~ Modelled as no of collisions b/w X Y which lead to death with certain probability

$\to \alpha$ is a measure of many things e.g how many

$$\frac{dY}{dt} = \gamma X Y - \delta Y$$

$$\vec{R}(t) = \begin{bmatrix} X(t) \\ Y(t) \end{bmatrix}$$

$$\frac{d\vec{R}(t)}{dt} = \begin{bmatrix} f_1(R) \\ f_2(R) \end{bmatrix}$$

Steady State $\to \frac{dX}{dt} = \frac{dy}{dt} = 0$

~~$\alpha - \beta y = 0$~~ ~~$\gamma y = 0$~~.

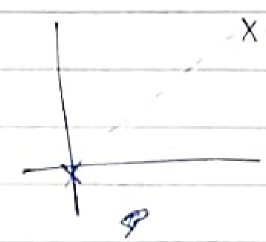
$\frac{dx}{dt} = x(\alpha - \beta y)$ $\frac{dy}{dt} =$ ~~$\gamma\delta$~~ $y(\gamma - \delta x)$

$x = 0,\ y = \frac{\alpha}{\beta}$ $y = 0,\ x = \frac{\gamma}{\delta}$.

So $(0,0)$ is a sol^n

also, ~~α~~ $\left(\frac{\gamma}{\delta}, \frac{\alpha}{\beta}\right)$ is also a sol^n

we want to analyse behaviour. Find Jacobian at $0,0$) and $\left(\frac{\gamma}{\delta}, \frac{\alpha}{\beta}\right)$



Find Jacobian, eigenvectors & eigenvalues at both fixed pts.

$$J(x,y) = \begin{bmatrix} (\alpha - \beta y) & -x\beta \\ \gamma y & (\gamma x - \delta) \end{bmatrix} = \begin{bmatrix} \alpha & 0 \\ 0 & -\delta \end{bmatrix}$$

Find at other stationary pt. and solve for it

Eigenvalues & Eigenvectors

$\vec{R}(t)$ at 0 $\quad \dfrac{d\vec{R}}{dt} \sim \begin{pmatrix} \alpha & 0 \\ 0 & -\delta \end{pmatrix} \vec{R}$

$\vec{\alpha}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

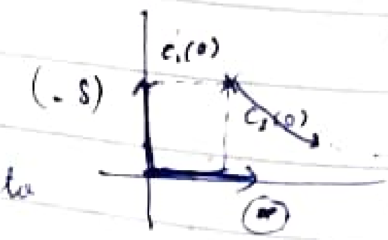
$-\delta \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

solut^{ns} $\rightarrow$ $\vec{R} = c_1(0)\, e^{\alpha t} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2(0)\, e^{-\delta t} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

c_1 & c_2 we find from initial condit^{ns}.

let $R(0) = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$ $\qquad \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = c_1(t) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2(t) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

because $(-\delta)$ term so keeps decreasing monotonically stable w.r.t ~~exp~~ eigenvector $(-\delta)$



Repeat this analysis for 2nd term.

Lecture 4 : 26th May

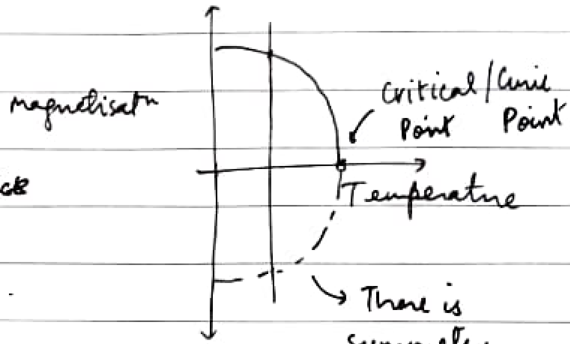
Ising Model → order - Disorder Transition

Computationally straightforward (coding / understanding)

(imp. in statistical Phy)

~~...~~ Model for spin systems - originally created to study Paramagnetic properties.

Magnets lose magnetism slowly on heating.

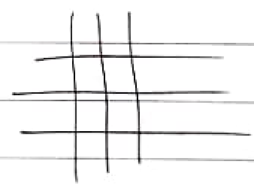


→ There is symmetry actually, system can take +ve or -ve magnetisatn depending on convention

Model

- ~~Asso~~ In 2D, Assume a 2D square lattice (shape can be anything depending on crystalline structure) can be 3D also.
- At every lattice pt. There is a spin. For simplicity quantized to up & down

$\sigma_i = \pm 1$



System has magnets arranged on infinite lattice

Assume: All interactns correspond to nearest neighbour interactns only. Under these Assumptns.

$$E = \left(-J \sum_{\langle ij \rangle} \sigma_i \sigma_j\right) + \left(-\sum h \sigma_i\right)$$

↳ nearest neighbour interactn terms

↳ magnetism term

h → externally imposed magnetic field

-ve sign if both have same spin then should become more stable so energy lower.

σ_i → depending on orientatn w.r.t external field

∴ σ_i tend to align with external field so as to minimize energy.

J, h constants to convert interactn to energy term.

Assume that system is in eq. with a Bath at temperature T

state C of the system = $\{\sigma_1, \sigma_2 --- \sigma_N\}$
(i.e specifying state of each lattice pt. i.e assignment of value to all σ_i variables)

$|C| = 2^N$ where N is no. of particles in the system
even small system can have very large configurat^n space

Boltzmann's law → $p_{eq}(c) \propto \exp\left(\frac{-1}{kT} E(c)\right)$

Probability of seeing any configurat^n is depending on energy of the configurat^n
with Boltzmann's law & First law of Thermodynamics you can derive other thermodynamics
Given this distributn, should be able to calc any property

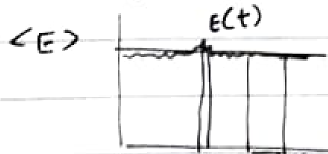
e.g - Average Magnetizat^n for this system:

$$\bar{m}(T) = \sum_c m(c) \cdot p(c).$$ — sum over config. space of magnetisat^n of certain config, weighted by probability

$$\langle A \rangle = \int_c A \cdot e^{-\beta E(x)}.$$ — config. space does not have to be discrete like $\{\sigma_1, \sigma_2 \sim \sigma_N\}$

Q. If system is ~~eq~~ at eq. what is the measured value
Probability of seeing certain configurat^n is given by Boltzman law.
~~[illegible]~~ Expected Value calculated but in measurement you will ~~[illegible]~~ observe only one configurat^n (depending on time of observat^n). Because even while observing system is

exchanging energy w/ environment & changing configuratⁿ. If time of experiment is ~~very~~ vanishingly small, only one config observed



At any single pt there is one value of E(t) corresponding to config at that time

o/w you just measure $\int_{t_1}^{t_2} E(t)dt$

$t_2 - t_1 \to 0$

Because configuratⁿ space is high-dimensional you can't ~~avoid~~ use brute forcing.

what's usually used is IMPORTANCE SAMPLING

Imp. Method → ~~Markov cha~~ Metropolis Markov Chain Monte Carlo

use Importance sampling from config space.

$$\vec{m}(T) = \sum_c m(c) \cdot P_{eq}(c) := \mathbb{E}_{c \sim P_{eq}(c)} m(c).$$

Assuming that c is iid
independent and identical

Metropolis Markov Chain Monte Carlo

- Idea → Select any configuratⁿ of system and do a random perturbatⁿ to it.

e.g → choose any σ_i from $\{\sigma_1, \sigma_2, \ldots \sigma_N\}$ & flip it.

let I & J be the configuratⁿ. E(I) & E(J) are energies of ~~the~~ these configuratⁿs.

from I generate J

E(I) E(J).

$$P_{Acceptance} = \min\left(1, \exp\left(\frac{-\Delta E}{kT}\right)\right)$$

$$\Delta E = E(J) - E(I)$$

$$P_{Acceptance} \in [0,1]$$

Markov Chain I add a new ~~chain~~ member w/ the probability $P_{Acceptance}$

$$I \to J \to P_{Acc.}$$

$$I \to I \to 1 - P_{Acc.}$$

P_{Acc} probability

$1-P_{Acc}$ probability to remain at same pt.

A → A → B → B → B → C → .. ⟼

Equilibriatⁿ
(Discard initial values)

Productⁿ Phase
(These will be sampled from P_{eq})

Problems :-

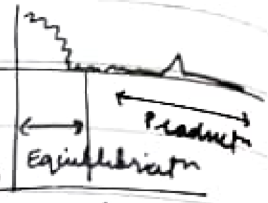
① Don't know what should be the length of the Equilibratn Phase

Even if you chose value σ

e.g $\rightarrow \{\sigma_1, \sigma_2 -- \sigma_N\} \rightarrow \{1, 1, 1 --\}$

As chain length goes to ∞ we will settle close to the expected value

$\langle m \rangle$



$L \rightarrow$ length of Markov Chain

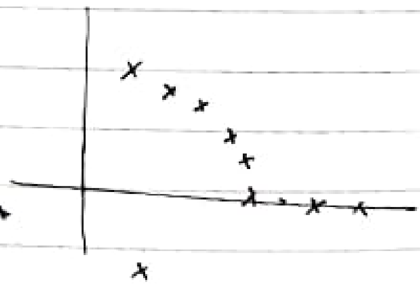
② ~~At~~ I^{th} & J^{th} configuratn are highly correlated because perturbating only one spin. So we cannot assume that there are iids ~~(?)~~ (in Expected value formula e.g).

Solutn : skip N consecutive members in the Markov Chain. ~~—~~ This allows ~~—~~ for each ~~— to~~ spin in configuratn to be flipped so we ~~—~~ can now Assume that the I^{th} and J^{th} config. are sufficiently decorrelated to be iid.

Markov chain $\rightarrow$ J is independent of history of I and only depends on value of I. $(P_{x+1} | P_x) = (P_{x+1} | P_x, P_{x-1}, P_{x-2} \cdots P_1)$

$m(c) = \frac{1}{N} \sum_i \sigma_i$

Can get -ve value also for magnetizatn



Correlatn length $\xi(T)$

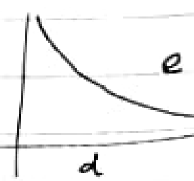
Correlatn Functn $\rightarrow$ $|r_i - r_j| \cdot \sigma_i \sigma_j$

Calculate value of $\sigma_i \sigma_j$ for ~~all distances~~ a certain distance

you get value = $c(d)$

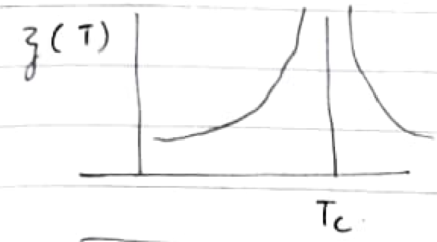
$c(d) = \sum_{i,j} |(r_i - r_j)| \cdot \sigma_i \sigma_j$

such that $|(r_i - r_j)| = d$



$e^{-d/\xi(T)}$

At large distance correlatn curve goes like $e^{-d/\xi(T)}$. Show this by e.g fitting log to straight line



Correlatn ~~factor~~ length goes to ∞ at T_c. This is important ~~part~~ result of classical ~~stat~~ mech.

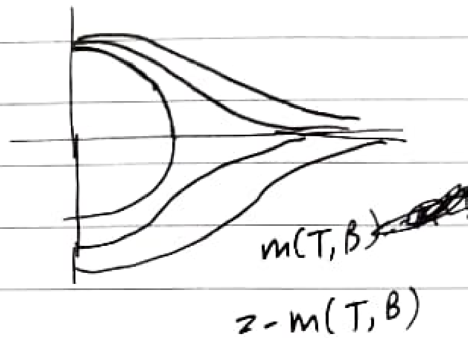
$$\boxed{E = -B \sum_i \sigma_i - \frac{1}{2} J \sum_{i,j} \sigma_i \sigma_j}$$

usually J ~~is~~ taken as 1, then calculate $m(T,B)$

Calculate

① $m(T,B)$

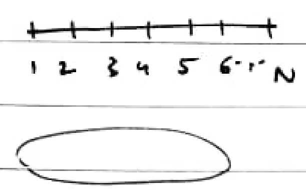
② $\langle E(T) \rangle$; $\left(\langle E^2 \rangle - \langle E \rangle^2\right)$



* <u>Periodic Boundary Conditions</u>

Mathematical Trick to simulate infinite system.

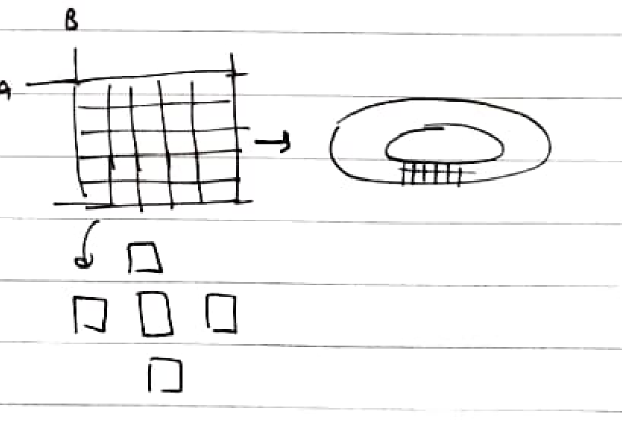
① In 1D, wrap around sides, so N^{th} spin is the 1st spin ~~for~~ $\lim n \to \infty$.
ds on a circle



In 2D,

② Toroidal Geometry

wrap the



$$\rho \propto e^{-\frac{E}{KT}}.$$

$$\rho(N) = \frac{1}{Z} \cdot e^{-\beta E_N}$$

$$\beta = \frac{1}{KT.}$$

$$Z = \sum e^{-\beta E_N}.$$

$$\vec{E} = \sum \rho(n) \cdot E_n.$$

$$E = \frac{-1}{Z} \frac{\partial Z}{\partial \beta}.$$

$$C = \frac{\partial E}{\partial T} = \frac{\beta}{T} (\langle E^2 \rangle - \langle$$

Lecture 5 1st June

Iterative Maps: repeated applicatⁿ of a functⁿ

$f(x_0) = x_1$
$f(x_1) = x_2 = f^2(x_0)$
$\vdots$
$f^n(x_0) = x_n$.

We want to analyse the long term behaviour i.e $\lim_{n\to\infty} f^n(x_0)$

Range & domain should usually be same ~~exactly~~ usually.

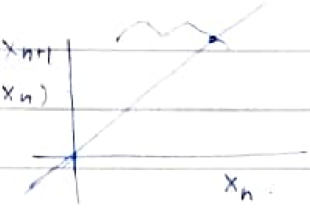
① $f(x) = \text{const.} \to$ not interesting

① $f(x) = mx \to f^n(x) = m^n x$ $|m|<1$ 0
$|m|>1$ $\pm\infty$
converging, diverging, oscillatory, monotonic $m<0 \to$ oscillatory

③ $f(x) = mx+c \to$ Exactly the same behaviour (Prove)

→ This has a stationary pt. if $x_n = f(x_{n-1}) = x_{n-1}$

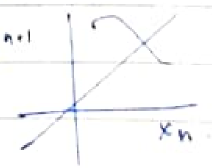
Consider arbitrary functⁿ → $f(x)$



whenever the curve intersects the $x=y$ line it is ~~true~~ a candidate for a fixed pt. in 1D.

We want to understand behaviour of function ~~to~~ in neighbourhood of stationary pt. ~~[illegible]~~ Nice enough functⁿ can be taylor expanded.
linear approx.; $f(x) = f'(x_0)(x-x_0) + f(x_0)$
$y = x^* + f'(x^*)(x-x^*)$.

This problem is ~~similar~~ same as $y = mx+c$ whose ~~behaviour~~ behaviour is same as iterative map $y = mx$.



→ If x_1 is still

if $|f'(x^*)| > 1 \Rightarrow |x_1 - x^*| > |x_0 - x^*|$.

so in neighborhood of fixed pt. If slope > 1, you will continuously move away from the fixed pt. Can continue Taylor expansion if this is still in neighborhood and it will keep moving away ⇒ unstable fixed pt.

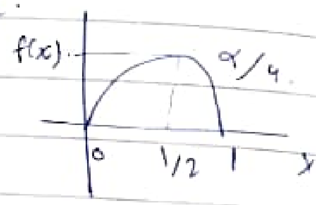
Simplest quadratic map will have 3 free parameters

$ax^2 + bx + c$ $\qquad \alpha(x)(1-x) = \alpha x - \alpha x^2 \rightarrow -D/4a = \frac{\alpha^2 - 4\cdot 0}{4\alpha} = \frac{\alpha}{4}$

~~[illegible]~~ Logistic map only 2 free parameters

$x = 0$ is fixed pt. $\qquad x = 0 \Rightarrow f(x) = 0 \; \forall \alpha$.

Max value $= \frac{\alpha}{4}$. $\qquad$ Range.



$x \in [0, 1]$, $f(x) \in [0, \frac{\alpha}{4}]$.

So choose $0 \le \alpha \le 4$.

Behaviour of f p $x^* = 0$, for various α.

$f(x) \rightarrow \alpha(x)(1-x)$

Linearize about $x = 0$

$-\alpha x^2 + \alpha x$

$f(x) + f'(x^*) \cdot (x - x^*)$

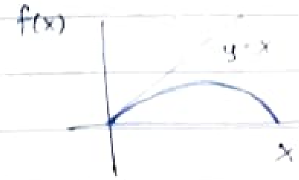
$= 0 + (\alpha - 2\alpha x)\big|_{x=0} (x)$

$= \alpha x$

So approx is αx at $x = 0$

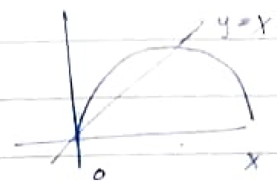
when $\alpha \in [0, 1] \rightarrow x^* = 0 \rightarrow$ stable pt

when $\alpha > 1 \rightarrow x^*$ unstable when $\alpha < 1$, slope < 1



when $\alpha > 1$, slope > 1.

This becomes unstable, but a new fixed pt. has appeared $\Rightarrow$



$x^* = 1 - \frac{1}{\alpha}$

$f(x) = \alpha x (1-x)$

$x = \alpha x (1-x)$

$x = 0$ is trivial fixed pt.

$1 = \alpha(1-x) \Rightarrow \frac{x}{1-x} = \alpha \Rightarrow \frac{x-1}{1-x} + \frac{1}{1-x} = \alpha$

$\Rightarrow \frac{1}{1-x} - 1 = \alpha$ $\quad \alpha + 1 = \frac{1}{1-x}$

$1 - x = \frac{1}{\alpha+1}$

$\Rightarrow x = 1 - \frac{1}{\alpha+1} = \alpha$

for other fixed pt $x = \alpha x(1-x)$. $\Rightarrow 1 = \alpha(1-x)$

$\Rightarrow \boxed{x = 1 - \frac{1}{\alpha}}$

linearise about $x = 1 - \frac{1}{\alpha}$.

$f(x) = f(x^*) + f'(x) \cdot (x - x^*)$

$f(x^*) = \alpha \cdot \left(1 - \frac{1}{\alpha}\right)\left(\cancel{1} - \cancel{1} + \frac{1}{\alpha}\right) = 1 - \frac{1}{\alpha}$

$f'(x) = \alpha - 2\alpha \cdot \left(1 - \frac{1}{\alpha}\right) = \alpha - 2(\alpha - 1) = 2 - \alpha$

$(x - x^*) = \left(x - 1 + \frac{1}{\alpha}\right)$

$$\boxed{f(x) = \left(1 - \frac{1}{\alpha}\right) + (2-\alpha)\left[x - 1 + \frac{1}{\alpha}\right]}$$

$$= 1 - \frac{1}{\alpha} + (2-\alpha)\left[x - 1 + \frac{1}{\alpha}\right]$$

$$= \left[2x - 2 + \frac{2}{\alpha} - \alpha x + \alpha \cancel{x}\right] \quad \cancel{x} = \frac{1}{\alpha}$$

$$\boxed{f(x)_{x^*} = \cancel{\alpha x}\,(2-\alpha)x + \left(\frac{1}{\alpha} - 2\right)}$$

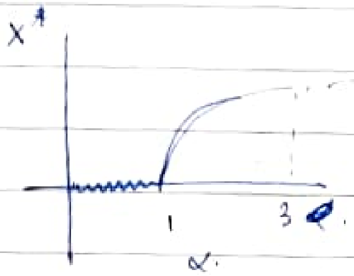
$m = 2 - \alpha$

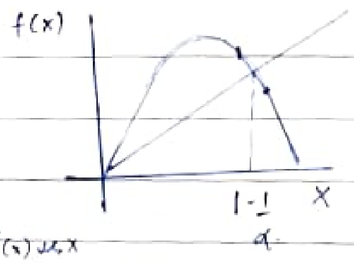
$|m| < 1 \Rightarrow$ stable fixed point

$\alpha \in [1, 3]$

$|m| > 1 \Rightarrow$ unstable fixed pt

$\alpha > 3$





f(x) vs x
for $\alpha > 1$.

for $\alpha > 3$,

$x_0 = 3 + \delta \qquad x_1 = 3 + \varepsilon$

$|\varepsilon| > |\delta|$

it is going farther away from fixed pt.

when x is a little larger than fixed pt., you will ~~only~~ return ~~a value~~ something slightly lower than fixed pt.

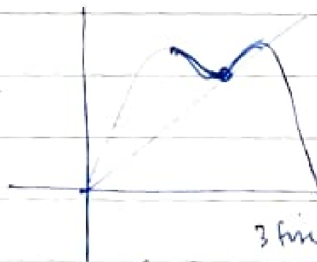
We need to analyse the behaviour of $f(f(x))$

$f(f(x))$

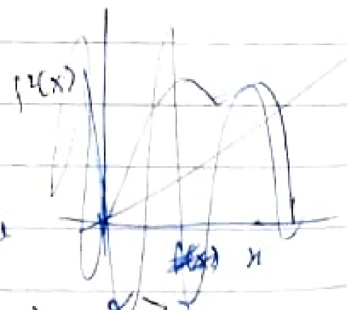
$= \alpha f(x) - \alpha (f(x))^2$

we are trying to solve

$\sim f(f(x)) =$



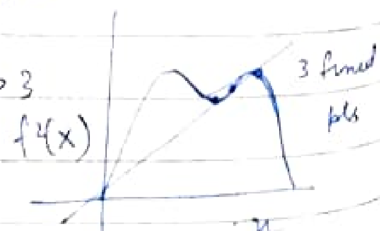
3 fixed pts come to one pt and slope of curve - tangent here



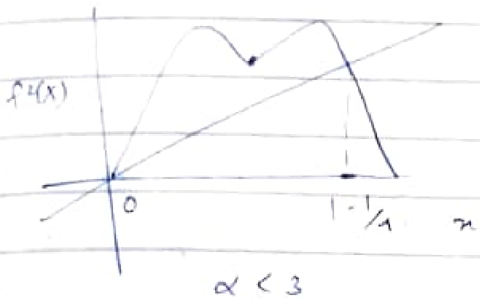
4th order polynomial $\Rightarrow$ 0, 2, 4 solⁿ possible

0 not possible because 0 is trivial solⁿ to original eqⁿ

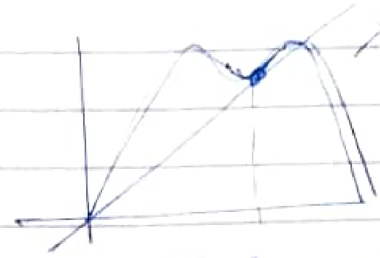
$\alpha > 3$



3 fixed pts



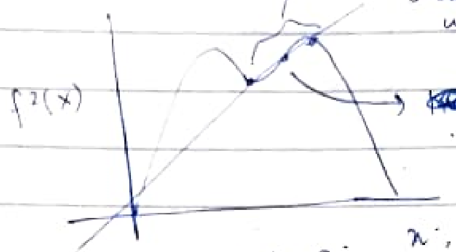
$\alpha < 3$



$\rightarrow$ 4 sol^{n}s exist
$x = 0$,
$\left(1-\frac{1}{\alpha}\right) \rightarrow$ triply degenerate
one sol^n will move higher & lower

$\alpha = 3$

$|m| < 1 \rightarrow$ stable fixed pts
it can be shown that they become unstable at same pt of α.
$|m| > 1$



$\rightarrow$ unstable fixed pt

$\alpha > 3$

$\alpha > 3 \begin{cases} \Rightarrow \text{f.p is unstable for } f(x) \\ \text{f.p is stable for } f(f(x)) \end{cases}$

$f(x)$ because x_0 is f.p of $f(x)$ by def^n of cleanth

$\underbrace{x_0, x_1, x_0, x_1}_{2\text{-cycle}}$

If $f^3(x)$ stable pts $\rightarrow$ 8 degree polynomial
gives you a 4 cycle.
when 4 cycle unstable $f^4(x) \rightarrow$ 8 cycle
Therefore you start making exponentially more stable pts.
this goes faster than power of 2. by $\alpha = 3.7$ you have an infinite cycle. $\alpha = 3.7$ is critical α.

$\alpha > \alpha_c \Rightarrow$ DETERMINISTIC CHAOS

Lecture 6. 5th June

- Logistic map $\quad f(x) = \alpha x(1-x) \qquad \alpha \in [0,4]$.
  $x \in [0,1]$.
- Behaviour near fixed pts $\qquad f(x^*) = x^*$.

① $0 < \alpha \leq 1 \qquad x^* = 0 \qquad$ stable

② $1 < \alpha \leq 3 \qquad x_1^* = 0 \qquad$ unstable

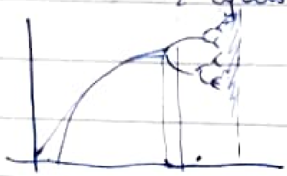
$x_2^* = \left(1 - \frac{1}{\alpha}\right) \qquad$ stable

(3) $\alpha > 3$ $\quad x_2^* = 1 - \frac{1}{\alpha}$ becomes unstable

need to analyse behaviour of $f^2(x)$.

Quartic polynomial $\quad f^2(x) \to \alpha = 3 \to$ $0, (1 - 1/\alpha)$ repeat with multiplicity: 0 and one copy of $(1 - 1/\alpha)$ is stable

<u>period doubling bifurcation</u>



$3.69 \to$

$k \to \infty$ cycle

After this it is chaotic

Deterministic chaos

$x_0 \longrightarrow x_n$

$x_0' = x_0 + \delta \longrightarrow x_n'$

$|x_0' - x_0| = \delta \quad |x_n' - x_n| = \varepsilon.$

$$\varepsilon_n \sim \delta^{\lambda n} \sim e^{(\lambda \ln)\alpha}$$

$$\varepsilon_n \sim \delta^{\lambda(\alpha) n}$$

λ is a function of α.

<u>Lyapunov Exponent</u> $\lambda(\alpha) < 0$

$\lambda(\alpha) > 0$ diverges $\to$ DETERMINISTIC CHAOS.

if $\delta << 1 \Rightarrow \lambda(\alpha) > 0 \to$ DETERMINISTIC CHAOS.

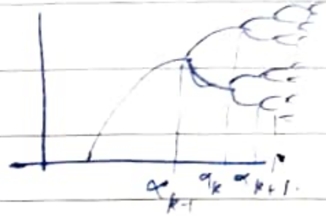
$\lambda(\alpha) < 0$.

Many physical systems have this chaotic behaviour, period doubling cascades etc.

e.g. tap turning on slowly becomes laminar then turbulent then laminar again.

No randomness / stochasticity involved.

→ Universal scaling properties
(Renormalizatⁿ Group).



FEIGENBAUHM NUMBER. $4.2261 = \frac{|\alpha_{k+1}-\alpha_k|}{|\alpha_k-\alpha_{k-1}|}$

* ~~Molecular Me~~

Lecture 7 8th June

Molecular Mechanics

liq. solid phase → . ndist. n-n dist

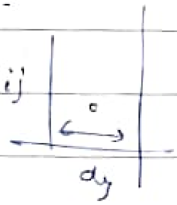
Energy of a system of particles $E = \sum_{i,j} E_{ij}$

e.g.→ Argon at triple pt.

We can assume argon to be a sphere of diameter σ to a good approximatn.

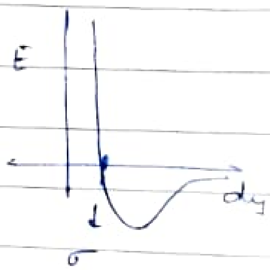
① One approxn that can be used but not very good is Hard sphere approxn

$$E_{ij}^{HS} = \sum\left[\frac{1}{\Theta(d-r)} - 1\right] = \begin{cases} \infty & \text{if } d_{ij} < \sigma \\ 0 & \text{if } d_{ij} \geq \sigma \end{cases}$$



② Better Approxn is Leonard Jones Interactn.

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



Minima happens at $(2^{1/6}\sigma)$.

Argon System now is like $U = \sum_{ij} E_{ij}^{LJ}((\sigma_{ij}), \sigma, \varepsilon)$

This gives Potential Energy Only

$u(\vec{r}_1, \vec{r}_2 \ldots \vec{r}_n)$

Molecular Dynamics

① use PE to calc net force on each atom f_i.

② Use Newton's second Law Find $\frac{dp_i}{dt} = F_i$; $m \frac{d\vec{v_i}}{dt} = P_i$

$$p(t) \longrightarrow p(t + \Delta t)$$

↳ time step of integratⁿ

$$m \cdot \frac{d\vec{r_i}}{dt} = p_i \Rightarrow \cancel{r(t)}\ r(t) \rightarrow r(t + \Delta t)$$

↳ time step of integratⁿ.

$$\cancel{F_i = -\left(\frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \frac{\partial u}{\partial x_3}, \ldots \frac{\partial u}{\partial x_i}\right)} \qquad F_i = -\left(\frac{\partial u}{\partial x_i}, \frac{\partial u}{\partial y_i}, \frac{\partial u}{\partial z_i}\right)$$

$$\cancel{\boxed{= -\nabla u}}$$

$$\boxed{F_i = -\nabla_i u} \qquad F_{ij} = -\vec{\nabla_i} \cdot (u(i,j))$$

$$F_{ij} = -\vec{\nabla_i} \cdot u(i,j)$$

$$= 4\varepsilon \cdot \left(\frac{\sigma^{12}}{\left(\sqrt{x^2+y^2+z^2}\right)^6} - \frac{\sigma^6}{\left(\sqrt{x^2+y^2+z^2}\right)^3}\right)$$

$$* \quad \frac{1}{(x^2+y^2+z^2)^6} = \frac{12x \cdot}{(x^2+y^2+z^2)^{-7}}.$$

$$\sum_{i,j,k} 4\varepsilon\left(\frac{\sigma^{12} \cdot 12x}{(x^2+y^2+z^2)^7} - \frac{\sigma^6 \cdot 6x}{(x^2+y^2+z^2)^4}\right)\hat{i}$$

Calculatⁿ → $\frac{\partial u(i,j)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(4\varepsilon\left(\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^6}{r^6}\right)\right)$

$$= \frac{\partial}{\partial r_{ij}} \cdot u_{ij} \cdot \frac{\partial r_{ij}}{\partial x_i}$$

$$u(i,j) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right) \Rightarrow \frac{\partial u}{\partial r_{ij}} = -\frac{24\varepsilon}{r_{ij}}\left(2\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^6\right)$$

$$-\vec{\nabla}_{i \neq j} \cdot u(i,j) = \frac{-\partial u(i,j)}{\partial r_{ij}} \left[\frac{\partial r_{ij}}{\partial x_i}, \frac{\partial r_{ij}}{\partial y_i}, \frac{\partial r_{ij}}{\partial z_i} \right]$$

$$\frac{\partial r_{ij}}{\partial x_i} = \frac{1}{2 r_{ij}} 2(x_i - x_j) = \frac{x_i - x_j}{r_{ij}} = \frac{\partial r_{ij}}{\partial x_i}$$

$$r_{ij} = |r_i - r_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

$$\vec{F}_{i \leftarrow j} = \frac{-24\varepsilon}{r_{ij}} \left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \cdot \frac{1}{r_{ij}} (x_i - x_j, y_i - y_j, z_i - z_j)$$

$$\vec{F}_i = \sum_{i \neq j} F_{i \leftarrow j}$$

① Get $\vec{r_i}(t), \vec{p_i}(t) \quad \forall i \in [1, N]$

② $\vec{F}_i(t) \quad \forall i \in [1, N]$

③ $\vec{r_i}(t + \Delta t), \vec{p_i}(t + \Delta t)$

$$\frac{d\vec{r_i}}{dt} = \frac{1}{m_i} \cdot \vec{p_i}(t) \qquad \frac{d\vec{p_i}}{dt} = \vec{F_i}$$

Use Euler's Formula → $\dfrac{\vec{r_i}(t+\Delta t) - \vec{r_i}(t)}{\Delta t} = \dfrac{1}{m_i} P_i(t)$

④ Goto step 1 $t = t + \Delta t$.

M steps → $t \rightarrow t + \Delta t$

$\Delta t \sim 10^{-15} s$ femtosecond