Lecture - 1 (Introductory Class).

AIM :- $\boxed{\text{Random no's}}$

↓

1. $\boxed{\text{Lies b/w 0 - 1 (sequence of numbers)}}$

↓

2. $\boxed{\text{All numbers are independent of each other}}$

↓

3. $\boxed{\text{Equally Probable}}$

↓

4. ~~All~~ $\boxed{\text{Prob. Distribution uniform}}$.

3 main pts —

(A). Independence.

(B). Uniformity

(C). Sample space (All possible conformation) / Microstates.

$\boxed{\text{Sample Space}}$

Set of all possible events {A, B ...}.

Sample space, $S = \{A, B, C ---\}$.

Algebraic Operations

$\overline{A} \rightarrow$ Events doesn't occur.

$A \cup B \rightarrow$ Either A or B will occur.

$A \cap B \rightarrow$ Both A and B occur.

$A/B \rightarrow$ A occurs but B not.

$A \cap \overline{B}$

A, B exclusive event if $A \cap B = \phi$. (Null)

Let, Ω be a set

$B \rightarrow$ Family of subset of Ω.

$\boxed{\text{Borel field}}$

① $\{\phi, \Omega\} \in B$

② A and $\overline{A} \in B$ ($\overline{A}$ is (not A)/A^c)

③ & $A_i \in B$ (where $\forall A_i$, $i = 1, 2 \ldots n$).

④. $\bigcup_{n=1}^{\infty} A_n \in B$.

~~Ast~~ $\boxed{\text{Borel } \sigma\text{- Algebra}}$

Smallest σ- algebra containing all open sets in $\mathbb{R}$

$B_1 \cap B_2 \cap \ldots$

Probability Measure

Let, (Ω, B) be a σ-algebra.

Then $p : B \longrightarrow [0, 1]$ st

$p(\Omega) = 1$ (where $\Omega \rightarrow$ Set).

$p(\phi) = 0$

i.e. ① Positive probability is attached to an event b/w $p \in [0,1]$

② Probability for the entire sample space $= 1$.

*. If $A_1, A_2 \ldots A_n, \ldots \in B$.

st:- $A_i \cap A_j = \phi \;\forall\; i \neq j$ (i.e. A_i & A_j are Mutually Exclusive $\forall\; i \neq j$).

then $P(A_i \cup A_j \ldots) = \sum p(A_i)$.

$p(A \cup \bar{A}) = p(A) + p(\bar{A})$ [since $A \cap \bar{A} = \phi$ & $A \cup \bar{A} = \Omega$ (full sample space).

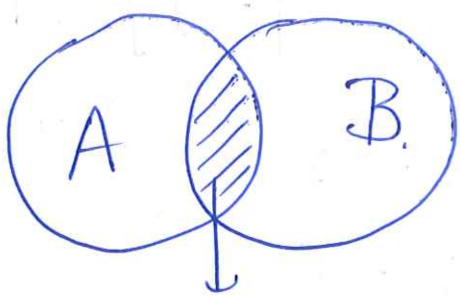
$1 = p(A) + p(\bar{A})$

$\Rightarrow \boxed{p(A) = 1 - P(\bar{A})}$

In General :-

$$p(A \cup B) = p(A) + p(B) - p(A \cap B).$$

Venn's Diagram



$(A \cap B)$.

Conditional Probability

Definition : Let A & B are 2 events in S,
& suppose $p(A) > 0$.
The conditional probability of B given A is —

$$\boxed{p(B|A) = \frac{p(A \cap B)}{p(A)}.}$$

$$p(A \cap B) = p(A)\, p(B|A).$$

Properties :-

① Multiplicative Rule

$$p(A_1 \cap A_2 \cap \ldots A_n) = p(A_1)\, p(A_2|A_1) + p(A_3|A_1 \cap A_2) \ldots p(A_n|A_1 \cap A_2 \ldots A_{n-1})$$

② $p(B) = p(A \cap B) + p(\bar{A} \cap B) = p(B|A)\, p(A) + p(B|\bar{A})\, p(\bar{A})$

(*). Baye's Theorem

Rule to update an initial probability $p(A)$, known as Prior Probability into a revised probability, $p(A|B)$, called as Posterior Probability.

$$p(A|B) = \frac{p(A \cap B)}{p(B)}$$

$$= \frac{p(B|A)\, p(A)}{p(B)}$$

$$= \frac{p(B|A)\, p(A)}{p(B|A)\, p(A) + p(B|\bar{A})\, p(\bar{A})}$$

(using above property ii).

Random Variables

Suppose $A_1, A_2 \ldots A_n$ forms a sample space S, hence $p(A_i) > 0$ & $\sum_{i=1}^{n} p(A_i) = 1$.

We can construct a variable which maps sample space into the integer no's $1, 2, \ldots n$.

Discrete Random Variable

We can associate each event A_i with the value of a discrete variable X, for eg.

$X = i$ if A_i occurs.

Example :-

① During an opinion poll, 2 events yes & no are possible.

Let, E be an event associated with yes.

Event	Random ~~No~~ Variable (X)
Yes	1
NO	0

② Tossing a coin N - times.

Event associated with n(Head) can be provided with a random variable.

6 Even though statement of Probability is an idiotic statement for a single event, yet this has a large precision for very large number of events.

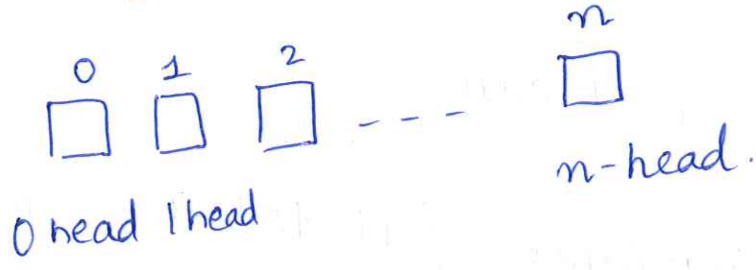
Examples :- ①. N - independent toss

②. N - Gas Molecules in a container.

①. For N- independent toss (independent coins i.e. don't influence each other).

2^N = NO of distinct sequences.

For Example, $N = 2 \Rightarrow 2^2 = 4$ sequence possible $\{HH, HT, TH, TT\}$.

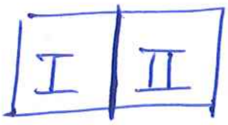


$$\Rightarrow \hat{\Omega}(n) = {}^N C_n \quad \text{(no of configuration for n - heads)}$$

$$= \frac{N!}{n!\,(N-n)!}$$

For $n = N/2$, $\hat{\Omega}(n)$ is maximum.

or, can say,



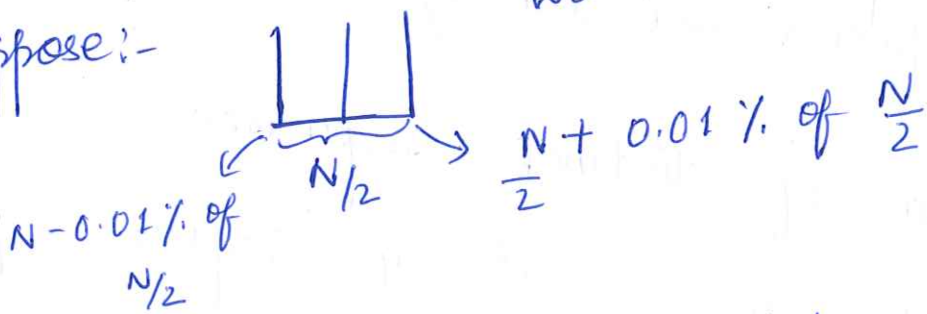
$$\Rightarrow \quad \hat{\Omega}\left(N/2\right) = \frac{N!}{\frac{N}{2}!\,\frac{N}{2}!}$$

i.e. No of Configurations with $\frac{N}{2}$ molecules in 1-part (I) and $N/2$ in 2-part (II)

Mean & Variance

we consider nbd of $N/2$

Suppose:-



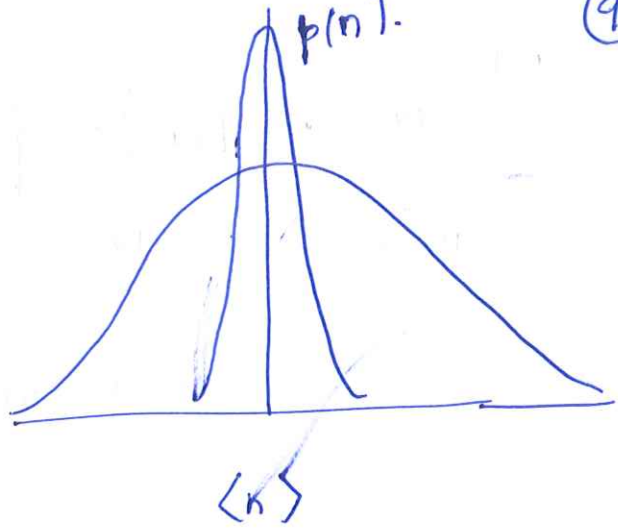
We need to see how much strings lie within this interval ?

$\langle n \rangle = N/2 \rightarrow$ Mean

$\langle n^2 \rangle - \langle n \rangle^2 =$ Variance (It tells how much is the realization of random variable)

$\langle n \rangle = \frac{N}{2}$

$\sigma^2 = \frac{N}{4}.$



Binomial Distribution

$$p(n) = \sum_{n=0}^{N} \frac{1}{2^N} \frac{N!}{n!\,(N-n)!}.$$ (for coin-toss N-times).

In General :-

$$p(n;N,p) = \sum_{n=0}^{N} \frac{N!}{n!\,(N-n)!} p^n (1-p)^{N-n}.$$

$$= (p+q)^N.$$

K^{th} Moment

$$\sum_{n=0} n^k p(n) = \langle n^k \rangle = M_k$$

Let,

$$\sum_{n=0}^{N} z^n P(n) = \phi(z)$$

$$= \sum_{n=0}^{N} \frac{N!}{n!(N-n)!} (zp)^n q^{N-n}$$

$$(\forall p+q=1)$$

$$= (q+zp)^N \quad — (1)$$

(A) Taking derivative w.r.t z & multiply both sides with z, we get —

$$\underline{\underline{LHS}} :- \; z \frac{d\phi}{dz} = \sum_{n=0}^{N} n z^n p(n). \quad — (2)$$

Repeat (A) on (2) —

$$z^2 \frac{d^2\phi}{dz^2} = \sum_{n=0}^{N} n(n-1) z^n p(n) \quad — (3)$$

$\Rightarrow$

$$z \frac{d\phi}{dz}\bigg|_{z=1} = \frac{d\phi}{dz} = \langle n \rangle . \quad — (4a)$$

$$z^2 \frac{d^2\phi}{dz^2}\bigg|_{z=1} = \frac{d^2\phi}{dz^2} = \langle n(n-1) \rangle . \quad — (5a)$$

RHS of 1 —

$$\frac{d}{dz}(q+zp)^N\Big|_{z=1} = Np\underbrace{(p+q)}_{1}^{N-1} = Np. \quad \text{— 4b}$$

$$\frac{d^2}{dz^2}(q+zp)^N\Big|_{z=1} = N(N-1)\,p^2(q+zp)^{N-2}\Big|_{z=1}$$

$$= N(N-1)\,p^2. \quad \text{— 5b}$$

$\Rightarrow$ Equating 4a = 4b & 5a = 5b, we get :-

$\boxed{\langle n\rangle = Np}$. is the Mean — $\circledast$.

$$\langle n(n-1)\rangle = N(N-1)\,p^2$$

$$\langle n^2\rangle - \langle n\rangle = N^2p^2 - Np^2$$

$$\langle n^2\rangle = N^2p^2 - Np^2 + Np$$

Variance $\Rightarrow$ $\sigma^2 = \langle n^2\rangle - \langle n\rangle^2$

$$= \cancel{N^2p^2} - Np^2 + Np - \cancel{N^2p^2}$$

$$= Np(1-p) = Npq$$

Error Estimate

$$\frac{\sigma}{\langle n \rangle} \approx \frac{\sqrt{N}}{N} \sim \frac{1}{\sqrt{N}}$$

For Gas Molecules,

$$N = 6.022 \times 10^{23} \sim 10^{24}$$

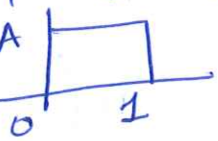
(avagadro number)

$$\sqrt{N} \sim 10^{12}$$

$\Rightarrow$ $\boxed{10^{-12} \text{ error bar.}}$ very small

Example :- Random Number lies b/w [0, 1].

Add pair wise numbers



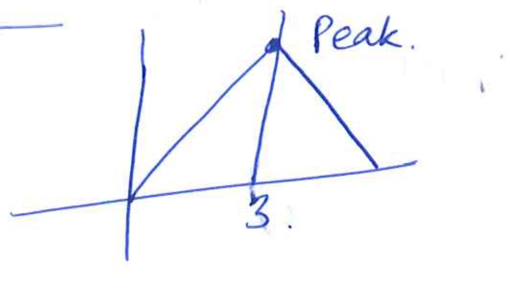
How would the prob. distribution look like ? (Next notes)

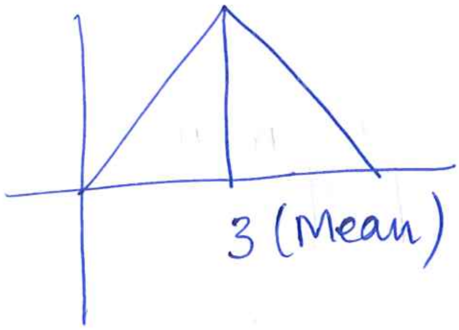
To support this, let consider dice rolled.

$S = \{1, 2, 3, 4, 5, 6\}$.

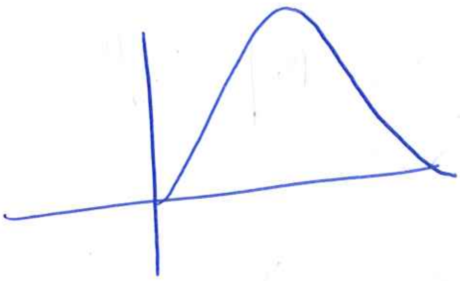
Add pair-wise & divide by 2

	1	2	3	4	5	6
1	2	3	4	5	6	7
2	3	4	5	6	7	8
3	4	5	6	7	8	9
4	5	6	7	8	9	10
5	6	7	8	9	10	11
6	7	8	9	10	11	12





⇓ N large.



$$y = \frac{1}{N} \sum x_i .$$

(Central limit Theorem)

(*) Independence.

(*) Variance associated with each random variable.

Notes ① Individual loose their identity → Central limit theorem.

② Only if the phenomenon has large no. of particles → Statistical Mech.

③ Newtonian or Schrodinger eq^n can't be used for large number of Particles in a room.

22/8/17

Notes 3

Binomial Distribution :-

$$p(n, N) = \frac{N!}{n!(N-n)!} p^n q^{N-n}$$

where $q = 1 - p$.

In the limit $\left.\begin{array}{l} N \to \infty \\ p \to 0 \end{array}\right\} Np = \mu$.

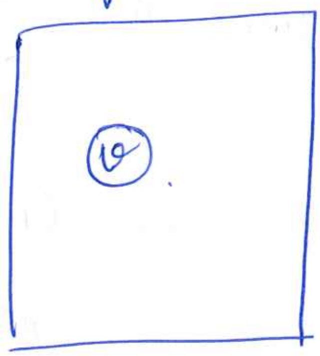
$$p(n, N) \longrightarrow \phi(n, \mu)$$

i.e.

Binomial Distribution reduces to Poisson Distribution :

For Eg. Let's consider a small volume element v in a large container of volume V.

V



then prob. $p = \frac{v}{V}$

$$\underbrace{Np}_{\text{Mean}} = \left(\frac{N}{V}\right) v$$

$$\boxed{\mu = \rho v}$$

represent avg. no. of molecules. (Constant)

(In the limit,
$N \to \infty$, $\rho \to$ Constant density
$V \to \infty$

Thermodynamic Limit

$N \to \infty \qquad \frac{N}{V} = \text{Constant} = \rho.$

$V \to \infty$

where ρ is the no. density

$$p(n, N, p) \xrightarrow[Np \to \mu]{N \to \infty,\ p \to 0} \phi(n, \mu)$$

$$\phi(n, \mu) = \frac{\mu^n e^{-\mu}}{n!}$$ is the Poisson Distribution

B.D : $$p(n, N, p) = \frac{N!}{n!(N-n)!} p^n q^{N-n}.$$

$N \to \infty$ & $Np \to \mu$.
$p \to 0$

Proof 1 :-

Use Stirling's Approx, i.e. in $\lim_{N \to \infty}$,

$$N! = N^N e^{-N} \sqrt{2\pi N}$$

can be proved using Gamma f^n

$$n! = \Gamma(n+1) = \int_0^\infty e^{-x} x^n \, dx$$

$$= \int_0^\infty e^{n \ln x - x} \, dx$$

Put,
$\cancel{n \ln x - x = y}$
$\cancel{\frac{n}{x} - 1 = y}$

$$\cancel{= e^{n \ln n} \, n \int_0^\infty e^{n(\ln y - y)} \, dy}$$

$$I = \int_0^\infty dx\, e^{-n\underbrace{\left(\frac{x}{n} - \ln x\right)}}$$

Saddle pt. Method:-

$$\frac{d}{dx}\left(\frac{x}{n} - \ln(x)\right) = 0 \Rightarrow \frac{1}{n} - \frac{1}{x} = 0$$

$$\Rightarrow \boxed{n = x}.$$

Expand abt $\boxed{x = n}$ —

$$\frac{x}{n} - \ln x = (1 - \ln(n)) + \frac{1}{2}\frac{(x-n)^2}{n^2} + \cdots$$

$$I = \int_0^\infty dx\, e^{-n(1-\ln(n)) - \frac{1}{n}\frac{(x-n)^2}{2}} + \cdots$$

$$= e^{-n+n\ln(n)} \int_0^\infty e^{-\frac{(x-n)^2}{2n}} dx$$

Put,
$x - n = y$
$dx = dy$.

$$= e^{-n+n\ln n} \underbrace{\int_{-\infty}^{\infty} dy\, e^{-y^2/2n}}_{\text{Gaussian Integral}}$$

$\int_0^\infty \to \int_{-n}^\infty$ & $n \to \infty$.

$$\boxed{n! \simeq e^{-n+n\ln(n)}\sqrt{2\pi n}}$$

is the Stirling's approximation

17

$$(1-p)^{N-n} p^n \frac{N^N e^{-N} \sqrt{2\pi N}}{n!\,(N-n)^{(N-n)} e^{-(N-n)} \sqrt{2\pi(N-n)}}$$

$(N-n)^{N-n}$.

Since $N \to \infty$.

$$(1-p)^{N\left(1-\frac{n}{N}\right)} p^n \frac{N^N e^{-N} \cancel{\sqrt{2\pi N}}}{n!\, N^{N\left(1-\frac{n}{N}\right)} \left(1-\frac{n}{N}\right)^{(N-n)} e^{-N\left(1-\frac{n}{N}\right)} \cancel{\sqrt{2\pi N}}}$$

$$\underbrace{(1-p)^N}_{\downarrow\, e^{-pN}} p^n N^n \frac{e^{-N+N\left(1-\frac{n}{N}\right)} \cancel{e^{-N}}}{n!\,.\, \cancel{e^{-N}}}$$

$\frac{n}{N} \to 0$ as $N \to \infty$

$$= \frac{e^{-\mu} \mu^n}{n!} = \phi(\mu; n)$$

Hence in the lim $\left.\begin{matrix} N \to \infty \\ p \to 0 \end{matrix}\right]$ but $Np = \mu$.

$$\boxed{B.D \longrightarrow P.D}.$$

Method 2 :- Method of Generating f^n

$$p(n;N,p) = \frac{N!}{n!\,(N-n)!}\, p^n q^{N-n}$$

$$\tilde{p}(z) = \sum_{n=0} z^n p(z)$$

$$= (q + zp)^N$$

$$= q^N \left(1 + \frac{zp}{q}\right)^N$$

$$= (1-p)^N \left(1 + \frac{zpN}{qN}\right)^N$$

$$= \left(1 - \frac{\mu}{N}\right)^N \left(1 + \frac{z\mu}{qN}\right)^N.$$

$$= e^{-\mu}\, e^{\mu z}.$$

$$e^{\mu z} = \sum_{n=0}^{\infty} \frac{\mu^n z^n}{n!}$$

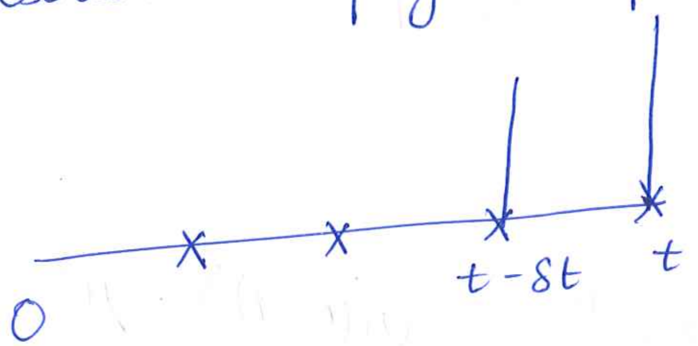
$$\Rightarrow \quad \tilde{p}(z) = \sum_{n=0}^{\infty} \frac{e^{-\mu} \mu^n z^n}{n!}.$$

$\Rightarrow$

$$\phi(n;\mu) = \frac{e^{-\mu}\mu^n}{n!}$$ is the Poisson Distribution.

Poisson Distribution

Describes a physical phenomenon



Poisson Assumption : $\delta t \to 0$.

δt either 0 or 1.

Counting Process : (Eg. Number of Decays in a nucleus reactor)

For Poisson Distribution

$$\boxed{\text{Mean} = \text{Variance}}$$

So, Poisson Distribution is used for counting process.

$$\mu = \sigma^2$$

$$\phi(n) = \frac{\mu^n}{n!} e^{-\mu}.$$

$$\langle n \rangle = \sum n \phi(n)$$

$$\frac{\partial \phi}{\partial z} = e^{-\mu} \mu e^{\mu z} \Big|_{z=1}.$$

$$\boxed{\langle n \rangle = \mu}.$$

$$\frac{\partial^2 \phi}{\partial z^2} = e^{-\mu} \mu^2 e^{\mu z} \Rightarrow \langle n(n-1) \rangle = \mu^2$$

$$\langle n^2 \rangle = \mu^2 + \mu.$$

$$\langle n^2 \rangle - \langle n \rangle^2 = \mu$$

$$\Rightarrow \boxed{\sigma^2 = \mu}$$

i.e. $\boxed{\text{Mean} = \text{Variance} = \mu.}$

Notes - 4

28/8/17

$$p(n) = \sum_{n=0}^{N} \frac{N!}{n!\,(N-n)!}\, p^n q^{N-n} \quad \text{— B D.}$$

In Limit: $N \to \infty,\ p \to 0$

$Np = \mu$.

we get $\quad p = \dfrac{\mu^n e^{-\mu}}{n!}$

Binomial $\to$ Poisson Distribution

$$\phi(n;\mu) = \frac{\mu^n e^{-\mu}}{n!}.$$

Moment Generating f^n:-

$$\tilde{P}(z) = e^{-\mu} e^{\mu z}.$$

$z = e^{-ik}$.

$$P(k) = e^{-\mu} e^{\mu \exp(-ik)}$$

In Lim $k \to 0$,

$$\phi(k) = \sum_n e^{-ikx} p(n) \ \to \text{Gaussian!}$$

Gaussian Distribution

Definitions

Density function $\to$ Let $F_X(x)$ be a continuous function satisfying the conditions —

ⓐ $\lim_{x \to -\infty} F(x) = 0$, $\lim_{x \to \infty} F(x) = 1$.

ⓑ $F(x)$ is a non-decreasing f^n ~~of~~ x.

The associated variable X is then called the ~~Gaussian~~ Continuous random variable.

$$F(x) = \int_{-\infty}^{x} f(t)\,dt$$ is the density f^n (d.f)

& has properties —

① $f(x) \geq 0$ for all $x \in (-\infty, \infty)$

② Normalized $\int_{-\infty}^{\infty} f(x)\,dx = 1$.

So, $X = x$ is the event that X takes value in the range x and $x + dx$ —

and $\int_{x}^{x+dx} f(x)\,dx$ is the probability.

→ Gaussian (Normal) Distribution

A random variable X is said to be normally distributed with mean μ and variance σ^2 if the probability density f^n is :-

$$f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right], \quad -\infty < x < \infty.$$

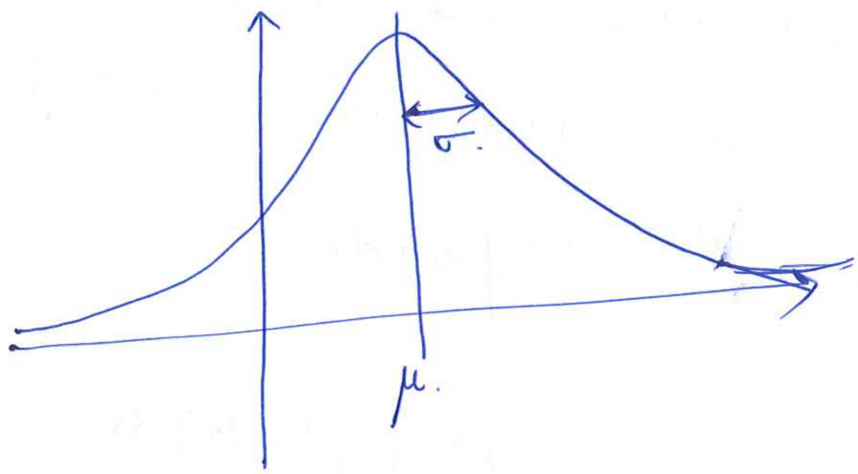
The normal or Gaussian distribution of X is usually represented by :-

$$X \sim N(\mu, \sigma^2)$$

or,

$$X \sim N(x-\mu, \sigma^2).$$

Bell-shaped curve symmetric abt. μ & attains its max. value of $\frac{1}{\sqrt{2\pi}\,\sigma}$ at $x=\mu$.

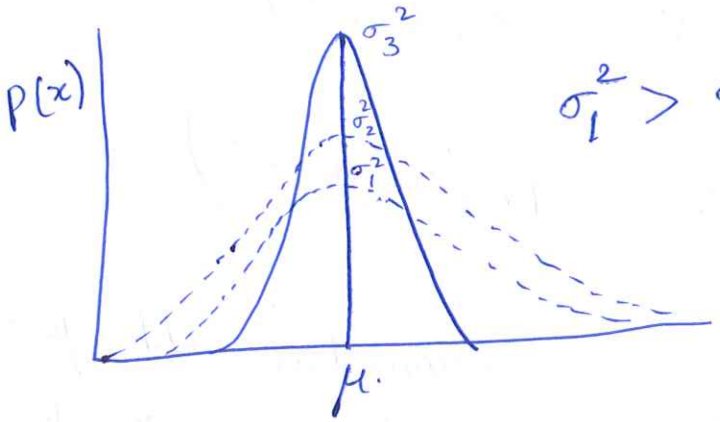


First & second order moments, are μ & σ^2 respectively,

$$\mu = E[X] = \int_{-\infty}^{\infty} x f(x)\, dx$$

$$\sigma^2 = E[(X-\mu)^2] = \int_{-\infty}^{\infty} (x-\mu)^2 f(x)\, dx$$

The variance σ^2 is a measure of the dispersion of random variable around the <u>mean</u>



$\sigma_1^2 > \sigma_2^2 > \sigma_3^2$

σ : Standard Deviation.
is the width of the Gaussian
Area always integrate to 1 (under the bell curve)
For Gaussian, Taking Fourier Transform -

$$\phi(k) = \int_{-\infty}^{\infty} e^{-ikx} f(x)\, dx.$$

$$\phi(k) = \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} \int_{-\infty}^{\infty} x^n f(x)\, dx.$$

$$\log \phi(k) = \psi(k)$$

$$\psi(k) = \sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} \underbrace{\xi_n}_{\text{Cumulants}}.$$

For Gaussian,

$$\phi(k) = e^{-ik\mu + \frac{(-ik)^2}{2!}\sigma^2}$$

$$\phi(k) = \int_{-\infty}^{\infty} e^{-ikx} e^{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}} \frac{1}{\sigma\sqrt{2\pi}} dx.$$

$$= \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx - \frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}} dx$$

Put,

$$\frac{x-\mu}{\sigma} = y$$

$$dx = \sigma dy$$

$e^{-b^2/4a}$.

$$= \frac{\cancel{\sigma}}{\cancel{\sigma}\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik(\sigma y + \mu)} e^{-y^2/2} dy$$

$$= \frac{1}{\cancel{\sqrt{2\pi}}} \cancel{\sqrt{2\pi}} e^{(-ik)^2\sigma^2/2} e^{-ik\mu}.$$

$$= e^{-ik\mu + \frac{(-ik)^2}{2!}\sigma^2}$$

Using formula –

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{-b^2/4a}.$$

$$\log \phi(k) = \psi(k)$$

$$= -ik\mu + \frac{(-ik)^2}{2!}\sigma^2$$

are the remaining cumulants.

(Rest all cumulants are zero).

If $X_1, X_2 \ldots X_n$ are Independent Random Variables.

$y = X_1 + X_2 + \ldots X_n$.

& associated distribution f^n are

$f_1(X_1), f_2(X_2) \ldots f_n(X_n)$.

Density f^n $P(y) = ?$

$$\int_{-\infty}^{\infty} e^{-iky} P(y)\, dy$$

<u>Example</u> :- Let, $y = x_1 + x_2$

Cumulant Density f^n :-

$P(Y \leq y) = P(x_1) P(x_2 < y - x_1)$.

For 2-dice throw,

$P(\text{Sum is } 5)$

$= \sum_{i,j} P(i) P(j)\, \delta(i+j=5)$.

similarly,

$$P(y) = \int dx_1 \int dx_2 \cdots \int dx_n \, f(x_1) f(x_2) \cdots f(x_n) \, \delta\left(\sum_{i=1}^{n} x_i - y\right)$$

$$\int e^{-iky} P(y)\, dy = \int e^{-iky} \int dx_1\, dx_2 \cdots \delta\left(\sum x_i - y\right) \quad \text{— (1)}$$

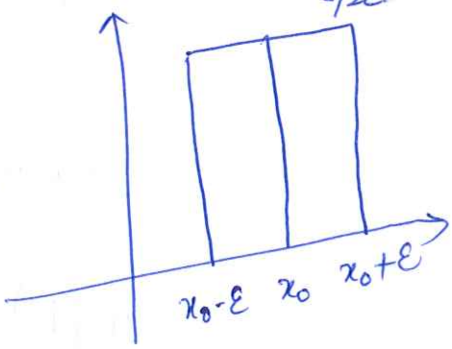
$$= \left[\int e^{-ik(y = x_1 + x_2 \cdots)} f(x_1) f(x_2) \cdots dx_1\, dx_2 \right]$$

$$= \left[\int e^{-ikx} f(x)\, dx \right]^n$$

$$\boxed{\phi_y(k) = [\phi_x(k)]^n}$$

In step (1), we have used the property of Dirac Delta f^n i.e.

$$\text{If} \quad \delta(x - x_0) = \lim_{\epsilon \to 0} \begin{cases} 0 & -\infty < x < x_0 - \epsilon \\ 1/2\epsilon & x_0 - \epsilon < x < x_0 + \epsilon \\ 0 & x_0 + \epsilon < x < \infty \end{cases}$$



$$\frac{1}{2\varepsilon}\int_{x_0-\varepsilon}^{x_0+\varepsilon} f(x)\,dx = \frac{1}{2\varepsilon}\int_{x_0-\varepsilon}^{x_0+\varepsilon} g'(x)\,dx$$

$$= \frac{1}{2\varepsilon}\left[g(x_0+\varepsilon) - g(x_0-\varepsilon)\right]$$

$$= \quad g'(x_0) = f(x_0)$$

$$Y = \sum x_i$$

$$\sum x_i \quad , \quad i = 1, 2 \ldots N$$

$$\Phi_Y(k) = \left[\Phi_X(k)\right]^N$$

Scaling :-

$$Y = \frac{1}{N}(X_1 + X_2 + \ldots X_N)$$

$$\phi_Y(k) = \left[\phi_X\left(k \to \frac{k}{N}\right)\right]^N$$

Cumulant Expansion for $\phi(k)$: -

$$\Phi(k) = e^{\sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} \xi_n}$$

$$\ln \Phi(k) = \sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} \xi_n .$$

$$\phi_Y(k) = e^{N\sum_{n=1}^{\infty} \frac{(-ik)^n}{n!\,N^n} \xi_n} .$$

$$= \exp\left[\underbrace{(-ik)\xi_1 + \frac{(-ik)^2}{2!\,N}\xi_2}_{} + \frac{(-ik)^3}{3!\,N^2}\xi_3 \cdots \right]$$

In limit $N \to \infty$,

Only first 2 terms remains.

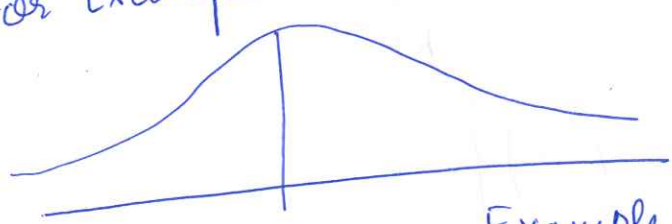
For Gas, $\sqrt{N} \sim 10^{-12}$ (Very small error)

Predictions Based on Probability Theory,

Central limit Theorem works.

Also variance should be finite in $N \to \infty$.

For Example :- For Cauchy Distribution.



Infinite variance.

So, error increase with N.

Example : <u>Fractals</u>

Chebyshev Inequality

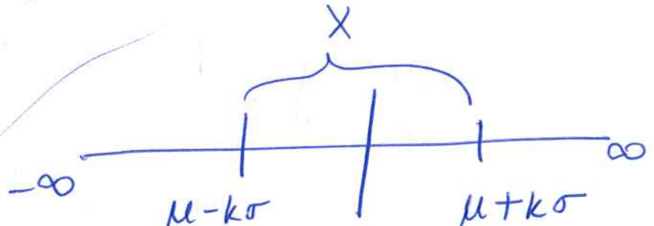
$$P\left(|x-\mu| \geq K\sigma\right) < \frac{1}{K^2}$$

$$\int_{-\infty}^{\infty} f(x)\,dx = 1$$

For the existence of variance, density function goes to zero.

<u>Proof</u> :-

$$\underset{\substack{\downarrow \\ \text{Variance}}}{\sigma^2} = \int_{-\infty}^{\infty} (x' - \mu)^2 f(x')\, dx'$$



$$\sigma^2 \geq \int_{-\infty}^{\mu - k\sigma} (t-\mu)^2 f(t)\, dt + \int_{\mu + k\sigma}^{\infty} (t-\mu)^2 f(t)\, dt$$

Put, $t - \mu = x$

$dt = dx$

$$\geq K^2\sigma^2 \int_{-\infty}^{-k\sigma} f(x)\, dx + K^2\sigma^2 \int_{k\sigma}^{\infty} f(x)\, dx$$

$$\sigma^2 \geq K^2\sigma^2 \left[P\left(|x| \geq K\sigma \right) \right]$$

$$\boxed{P\left(|t-\mu| \geq K\sigma \right) \leq \frac{1}{K^2}} \quad (K > 1)$$

<u>Note</u>

(a) $\displaystyle\int_{-\infty}^{\infty} f(x)\, dx = 1$ (Normalization).

(b). $\sigma = \int x^2 f(x)\, dx < \infty$ (else Chebyshev inequality breaks).

29/8/17

Notes-5

Note :-

1. Random Numbers are used to solve differential equation

2. Monte Carlo is used to find inverse of a very large matrix. Error is linear in number of elements.

3. Large no. of random variables having finite variance $(x_1, x_2 \ldots x_n)$ with any distribution —

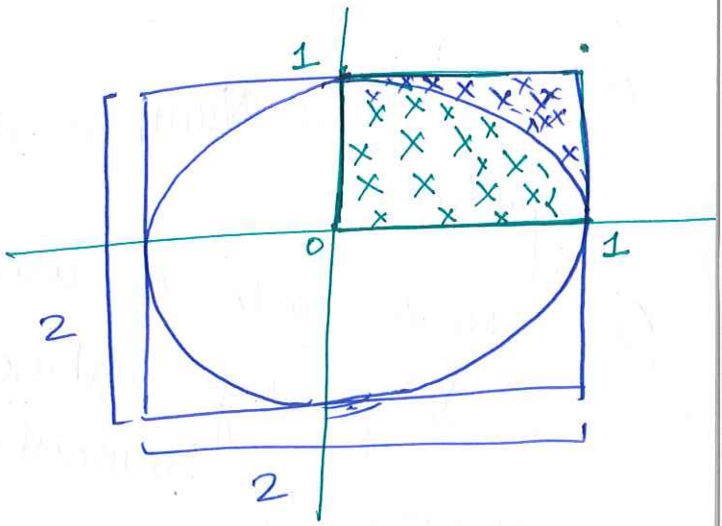
$$Y = \frac{\alpha_1 x_1 + \alpha_2 x_2 + \ldots + \alpha_n x_n}{\sum_i \alpha_i}$$

Distribution for y is Gaussian (in limit $n \to \infty$)

4. All Random number generator are deterministic (predictable).

Monte Carlo Technique - 1

Rejection Technique



If a circle of Radius (say 1 unit) within a square of 2 unit, then the area of the circle is π and square is 4 unit^2.

So Ratio of $\frac{A(\text{Circle})}{A(\text{Square})} = \frac{\pi}{4}$.

So, $\Rightarrow$ Picking N random points inside square, approx $\frac{N\pi}{4}$ pts should fall in circle.

Algorithm :-

Step 1 :- Pick pts random within the square

i.e. Random no. $x \in [0, 1]$

Random no. $y \in [0, 1]$

Step 2 :- $z^2 = x^2 + y^2$

Check if the point is inside the circle

For every x, y Check If.

$$\boxed{x^2 + y^2 \leq 1}$$

↓

Step 3 :- Keep track of how many points fell inside the circle.

Count = Count + 1.

So, π is then approx equal to

$$\boxed{\pi = \frac{4 \times \text{Count}}{N}}$$

where, N = Total points in the square.

As N increases, we get value of π more close to analytic value.

Technique - 2

Inversion Technique

If the desired probability density function is $f(y)$ on the range $-\infty < y < \infty$, its cumulative distribution function (for $y \leq x$), is given by :-

$$F_X(x) = \int_{-\infty}^{x} f_X(y)\, dy.$$

where, X is a random variable with cumulative distribution function F_X. Then, the integrated probability upto pt x is itself a random variable which will occur with uniform probability density on $[0, 1]$.

Let $a \leq x \leq b$.

$$F(x) = \int_{a}^{x} f(y)\, dy.$$

$$F(a) = 0, \quad F(b) = 1.$$

If $F(x) = \xi$, where, ξ is the random number $\in (0,1)$.

$$\boxed{x = F^{-1}(\xi)}$$

$\Rightarrow$ Given a random variable $u \in [0,1]$ & an invertible Cumulative distribution function, the Random variable

$$\boxed{x = F^{-1}(\xi)}$$

has distribution described by F.

Example :-

Choose a random variable —

$u \in [0,1]$

$$f(x) = e^{-x}.$$

$$x = F^{-1}(u).$$

$$F(F^{-1}(u)) = u.$$

$$\exp[-F^{-1}(u)] = u.$$

$$F^{-1}(u) = -\log u.$$

$$x = F^{-1}(u) = -\log u$$

$$\boxed{x = -\log u}$$

Algorithm :-

1. Generate a random number u from the standard uniform distribution in the interval $[0,1]$.
2. Compute the value of x st. $F(x) = u$.
3. Take x to be the random number drawn from the distribution by F.

$$x = -\ln u \quad \text{(for the previous eg.)}$$

$u \in [0,1]$.

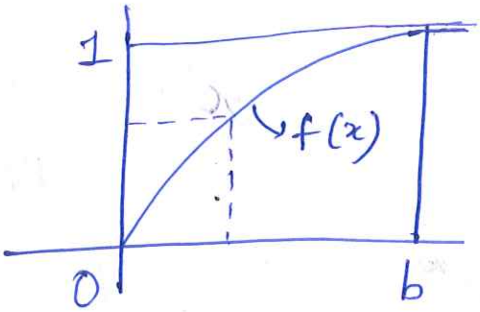
i.e. $\boxed{x = F^{-1}[u]}$.

Inversion Technique

11/9/17

$$x = x(\omega)$$

$$0 \le x \le b.$$



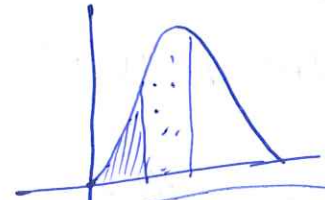
$$F(x) = \int_{-\infty}^{x} f(x')\,dx'.$$

$$0 \le F(x) \le 1$$

↳ Cumulative density function.

$$F(x) = \xi$$

where, $\xi \in [0,1]$.



Frequency distribution Plot

$$\boxed{x = F^{-1}(\xi)}$$

Inversion & Rejection techniques are called sampling.

Ensembles

(*)

$$\langle x^n \rangle = \int x^n f(x)\,dx.$$

$$\langle h \rangle = \int h(x) f(x)\,dx.$$

Boltzmann was the first to use Probability theory for explanation of physical properties

Physicist notion of Average & Variance —

$$\langle x \rangle = \frac{1}{N} \sum x_i$$

$$\sigma^2 = \frac{1}{N-1} \sum_i \left[x_i - \langle x \rangle\right]^2$$

Time Reversal Invariance (in Maxwell Eq^n, Newton's Eq^n, Planet going round the sun etc.)

In Contrast, Thermodynamics phenomenon, there is a clear direction of time (Entropic time).

Individual atoms obey Newton laws.

But, Large no of atoms ($\sim 10^{23}$) don't obey ~~the~~ Newton Laws.

→ What is that, that is giving direction ??

→ At what stage, ~~to~~ disobedience to Newton's equation arise ?

Boltzmann Showed Newton's eq^n can be applied to Large no. of atoms.

Entropy is a dynamical quantity (determine by Newton's eq^n)

Boltzmann Showed using differential equation – (Transport Eqn).

Rate of change of number of particles = No of particles entering – No of Particles exiting.

Guess a solution (Physical intuition). Obeys Thermodynamics.

Maxwell → Interpreted Boltzmann Ideas in Physical terms.

* $\boxed{\text{Ensemble}}$

E	P
H	3/4
T	1/4

Eg. {H H H T}

Ensemble contain information about both sample space & probability.

→ Ensemble Average :

$$\langle h \rangle = \int h(x) f(x)\, dx$$

$$= \frac{1}{N} \sum h(x_i)$$

(*).

Technique - 3

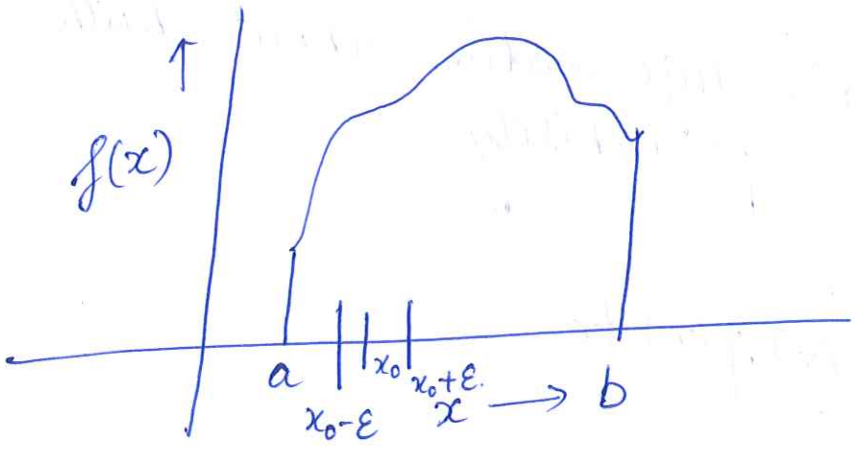
Metropolis Rejection

For a macroscopic system, Probability of Microstate —

$$P(C) \propto e^{-E(C)/k_B T}$$

Partitionfⁿ :- $Q(\beta) = \sum_{C} e^{-\beta E(C)}$ where, $\beta = \frac{1}{k_B T}$ is the Boltzmann Constant.

$$\boxed{P(C) = \frac{e^{-E(C)/k_B T}}{Q}}$$



$\{x_i, i = 1, 2 \ldots N\}$.

Algorithm —

1. Start with arbitrary x_0. Take a small interval around x_0. $x_0 - \varepsilon < x < x_0 + \varepsilon$, where, ε is small (optimally small

2. Random Number

$\xi \in [0, 1]$ uniformly distributed.

$x_t = x_0 - \varepsilon + 2\epsilon\xi$, is also uniformly distributed (linear related).

3. $x_t \rightarrow f(x_t)$ where, $f(x)$ is the given density function.

$x_0 \rightarrow f(x_0)$

$$\boxed{r = \frac{f(x_t)}{f(x_0)}}$$

4. $p = \min(1, r)$ (Probability).

5. When $f(x_t) > f(x_0)$. Accept $f(x_t)$.

$$x_1 = \begin{cases} x_t & p \\ x_0 & 1-p \end{cases}$$

(*) Steps

Given $x = x(w)$ $f(x)$.

a. Select x_0 (arbitrary b/w a and b)

b. Construct an interval $(x_0 - \epsilon, x_0 + \epsilon)$ $\epsilon = ?$

c. Select x_t randomly (uniformly) in the interval.

$$x_t = x_0 - \epsilon + 2\epsilon\xi.$$

(d). $r = \frac{f(x_t)}{f(x_0)}$ $p = \min(1, r)$.

Accept x_t with a probability $p = r$ if $f(x_t) < f(x_0)$.

$$x_1 = \begin{cases} x_t & \text{with prob. } p. \\ x_0 & \text{with prob. } (1-p). \end{cases}$$

$$\boxed{x_0 \longrightarrow x_1 \longrightarrow x_2 - - -}$$

Ensemble Generated

→ Markov Process :-

Present is independent of Past.

Example :- Random walk.

Self-Avoiding Random Walk is an Example of Non-Markovian chain.

→ Choice of ϵ :-

Small ϵ ⇒ Rejection Probability is very large [x_0 will be chosen] → Not evolve

Large ϵ ⇒ Acceptance prob. is very large. (otherwise there is no repitition)

Choose ϵ ~ such that acceptance is b/w 30 - 70 %.

Equilibration →
When the Markov chain become stationary, (Initially Markov chain has memory).
If the algorithm ~~chain~~ generate Markov chain (with certain properties), then Steady state is certain.

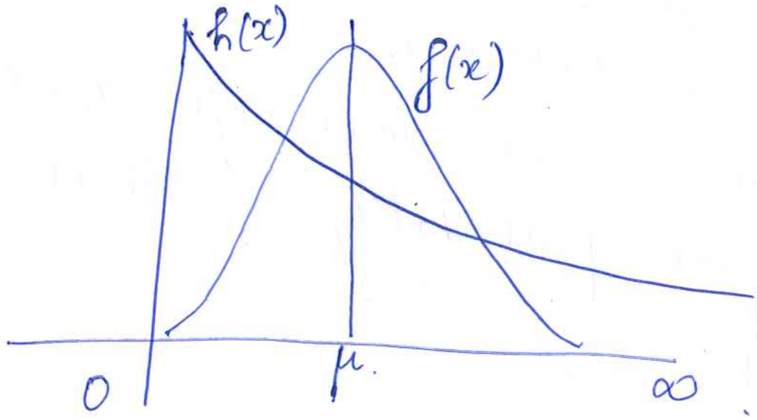
Asymptotic → Microstates in equilibrium.

Notes - 7 12/9/17

$x = x(w)$

Let, $f(x)$ is the Probability density function which is Gaussian

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}}$$



where
$$h(x) = \begin{cases} 0 & x < 0 \\ e^{-x} & 0 \le x \le \infty \end{cases}$$

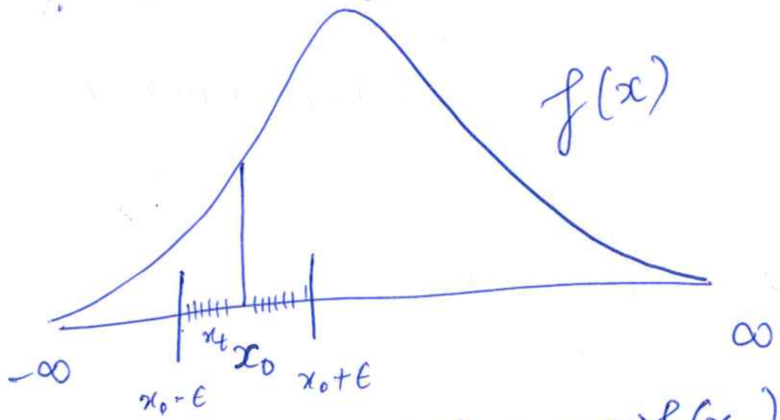
Generate an ensemble of n- realization —

$$\int_{-\infty}^{\infty} h(x) f(x)\, dx = \langle h \rangle \underset{N\to\infty}{=} \frac{1}{N} \sum_i h(x_i)$$

$\{x_i \; ; \; i \in 1, 2 \ldots N\}$. Let, $\mu = 5$, $\sigma = 3$

where, x_i is sampled from a Gaussian.

Metropolis Algorithm



① Choose arbitrary $x_0 \to f(x_0)$

② Take an interval around x_0
Select randomly a real number b/w $x_0 - \epsilon$ & $x_0 + \epsilon$ with equal probability $\to$ (Call it x_t).

③ $x_t = x_0 - \epsilon + 2\epsilon\,\xi$

④ Calculate $f(x_t)$.

⑤ $r = \dfrac{f(x_t)}{f(x_0)}$ Define $p = \min(1, r)$.

[r can be >1 or <1].

⑥ $x_1 = \begin{cases} x_t & \text{with probability } p \\ x_0 & \text{" " } 1-p. \end{cases}$

⑦ Chain of Microstates / Real Number

x_1 can be x_0 or x_t.

$x_0 \longrightarrow x_1 \longrightarrow x_2 \longrightarrow x_3 \longrightarrow \ldots \text{ --- }$

(Ensemble is generated).

How to find ϵ ?

$$\text{Ratio} = \frac{\text{Number of times accepted}}{\text{Total no. of attempts}}$$

(not → too large ~ ∞ or too small ~ 0)

Note : Its very important that Markovian chain is maintained.

Example :- Queing System

Airport → Only 1 Que & many servers.

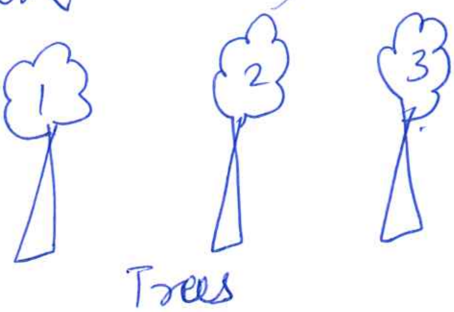
Choose server randomly.

Using Metropolis algorithm find the distribution ?

Markov chain attains a Stationary State asymptotically.

*. Markov Process

Imagine, having a finite no. of microstates (/ markov states).



(Markov) Monkey jumps from 1 tree to other.

2 → 1 → 1 → 3 → 1 → 2 → 2 → 3 → 3 ..

Let, Chain is

$C_n, C_{n-1}, C_{n-2} \text{----} C_2, C_1, C_0.$

C_i is a member of markov state
$C_i = 1, 2, 3.$

$$P(C_n, C_{n-1}, C_{n-2} \text{--} C_2, C_1, C_0) = ?$$

$$\boxed{P(A, B) = P(A|B)\,P(B)}$$ → Conditional Probability definition.

$$P(C_n, C_{n-1}, C_{n-2} \text{--} C_2, C_1, C_0) = P(C_n | C_{n-1}, C_{n-2} \text{--} C_0)$$
$$\times\, P(C_{n-1} | C_{n-2}, C_{n-3} \text{---} C_2, C_1, C_0)$$
$$\times \text{------} \times P(C_1|C_0) \times P(C_0).$$

Markov Assumption :-

$$P(C_{n-1} | C_{n-2} \text{---} C_2, C_1, C_0) = P(C_{n-1} | C_{n-2}).$$

$$P(C_n | C_{n-1} \text{---} C_2, C_1, C_0) = P(C_n | C_{n-1}).$$

Monkey (Eg. $\underbrace{1 \to 2 \to 3 \to 1}_{\text{Irrelevant}} \longrightarrow 2 \longrightarrow =$)

$P(C_n, C_{n-2} \cdots C_2, C_1, C_0)$

$$= P(C_n|C_{n-1})\, P(C_{n-1}|C_{n-2}) \cdots \underbrace{P(C_1|C_0)}_{\text{Transition Probability}}\, \underline{P(C_0)}$$

↓

General Markov Chain

→ Time In-Homogenous Markov chain.

$2 \to 1 \to 1 \to 3 \to 1 \to 2 \to 3$

can go to
1, 2, 3 1, 2, 3

Prob. needn't be same for these 2 cases.

Principle → $\boxed{\text{Entropy Increases}}$ → Gas spread in room
→ Heat flows from higher to lower temp.

whatever is the initial condition, System evolve into a unique equilibrium state.

W_{ij}

$P(1|1)$ $P(2|1)$ $P(3|1)$

$P(1|2)$ $P(2|2)$ $P(3|2)$

$P(1|3)$ $P(2|3)$ $P(3|3)$

$$W = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix}$$

$$W_{ij} = P(i|j)$$

or, $W_{ij} = P(i \to j)$ also valid.

Properties of W —

① Each column adds ~~goes~~ to ~~zero~~ 1.

② Initial Probability vector

$$\boxed{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}}$$

If there are N - identical monkeys,
Initial ensemble comes with probability vector

$$\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}.$$

(3). $\lim_{n\to\infty} W^n = W^*$.

<u>Example</u> :-
Let

$$W = \begin{pmatrix} 0.3 & 0.2 \\ 0.7 & 0.8 \end{pmatrix}.$$

$$W|a_0\rangle = |a_1\rangle$$

$$W|a_1\rangle = |a_2\rangle$$

$$\vdots$$

$$W|a_n\rangle = W|a_{n+1}\rangle = W|a_n\rangle$$

→ Largest eigenvalue has to be **1**.

→. Non-Degenerate.

Non-unique eq^m state $\leftarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

18|9|17

Notes - 8

Properties of W - Matrix

1. Square Matrix.
2. $0 \leq w_{ij} \leq 1 \quad \forall\ i, j$
3. $W_{ij} = P(C_i | C_j)$ & $\sum_i W_{ij} = 1 \ \forall j$

   $= P_{j \to i}$

   (some choose the opposite convention).
4. $W|a\rangle = |a\rangle$ (Largest Eigen value is 1).
5. Non-Degenerate.
6. If $(a_1\ a_2\ a_3) = (a_1\ a_2\ a_3)\begin{pmatrix} W_{11} & W_{21} & W_{31} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix}$

   Left eigenvector is a uniform matrix. All microstates are equally probable.
7. $W|a_1\rangle = |a_2\rangle$

   $W|a_2\rangle = |a_3\rangle$

   $\Rightarrow W^2|a_1\rangle = |a_3\rangle$

   $\vdots$

$W^n|a_1\rangle = |\pi\rangle$.

For some n, Stationary state is obtained.

Additional Properties —

1. Start with i, after some steps (n) reach j
   True for all i & j

   $\Rightarrow$ i communicates with j & vice-versa.

2. Aperiodic. (No periodicity).
3. Markov chain should return to initial state (Transient)

   $\Rightarrow$ Prob (return to initial state) = 1

①, ②, ③ $\Rightarrow$ ERGODICITY

Let, C_1, C_2, C_3 are 3 states

Probability,

$$P(C_1, n) = P(C_1, n-1)\, W_{11} + P(C_2, n-1)\, W_{12} + P(C_3, n-1)\, W_{13}.$$

C_1 → state, n → time

Using $\sum_i W_{ij} = 1 \;\forall\, j$

$$W_{11} = 1 - (W_{21} + W_{31})$$

$$\Rightarrow \; P(C_1, n) = P(C_1, n-1) + P(C_2, n-1) W_{12} + P(C_3, n-1) W_{13} - P(C_1, n-1) W_{21} - P(C_1, n-1) W_{31} \quad \text{--- } (1)$$

Add & subtract $P(C_1, n-1) W_{11}$ in (1)

$$P(C_1, n) = P(C_1, n-1) + \sum_i P(C_i, n-1) W_{1j} - P(C_j, n-1) W_{j1}.$$

In General, we can find the probability for any C_i in time n.

$$P(C_i, n) = \sum_{j \neq i} P(C_j, n-1) W_{ij} - \sum_{j \neq i} P(i, n-1) W_{ji} + P(C_i, n-1).$$

For n - adequately large -

$$P(C_i, n) = P(C_i, n-1) = \pi_i \;(\text{Stationary state})$$

$$\Rightarrow \sum_{j \neq i} \left[P(C_j, n-1) W_{ij} - P(C_i, n-1) W_{ji} \right] = 0$$

We can add & subtract $j=i$ term also.

$$\Rightarrow \sum_{j} \left[P(C_j, n-1) W_{ij} - P(C_i, n-1) W_{ji} \right] = 0.$$

$$\Rightarrow \boxed{\sum_{j} \left[\Pi_j W_{ij} - \Pi_i W_{ji} \right] = 0} \quad \forall j$$

→ Condition for Markov chain becoming stationary.

Additional Constraint

$$\forall j \quad \boxed{\Pi_j W_{ij} = \Pi_i W_{ji}} \rightarrow \text{Detailed Balance.}$$

Metropolis Algorithm :-

Depends only on ratio of Probability.

So, for Physicist, no need of normalization/ Partition function.

$P(C_i) \propto$ Quantity

Note :- Markov chain is suited for system marching towards equilibrium. ③.

If $|\lambda_1\rangle, |\lambda_2\rangle, |\lambda_3\rangle$ are eigenvectors corresponding to C_1, C_2 and C_3.

& $\lambda_1 = 1$

$$|a\rangle = \alpha_1 |\lambda_1\rangle + \alpha_2 |\lambda_2\rangle + \alpha_3 |\lambda_3\rangle$$

$$W^n |a\rangle = \alpha_1 |\lambda_1\rangle + \alpha_2 \lambda_2^n |\lambda_2\rangle + \alpha_3 \lambda_3^n |\lambda_n\rangle$$

Large time n —

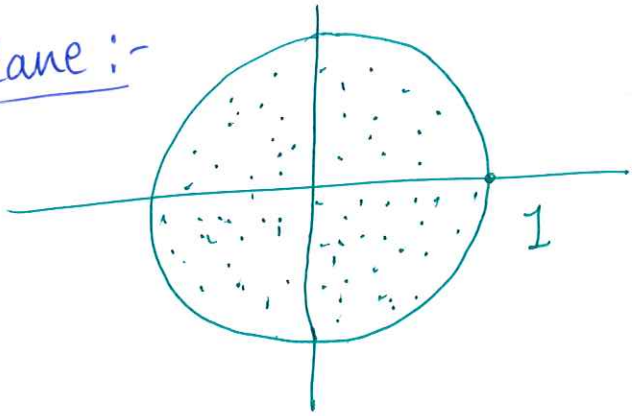
$$W^n |a_1\rangle = \alpha_1 |\lambda_1\rangle$$

Note :-

ⓐ Large eigenvalue $\rightarrow \lambda = 1$, real & non-degenerate.

ⓑ All other eigenvalues can be complex with norm less than 1.

Eigenvalue Plane :-



Example — Transition Matrix

$$W = \begin{pmatrix} 0.1 & 0.3 & 0.5 \\ 0.7 & 0.4 & 0.4 \\ 0.2 & 0.3 & 0.1 \end{pmatrix}.$$

3/10/17

Notes-9

Markov Chain (MC)

1. State space (Microstate space)
   $\{C_1, C_2 - - - C_k\} \rightarrow$ Discrete & finite

2. Time Homogeneous MC.

3. W-Matrix ($k \times k$ Matrix) & Initial state C_0

Properties : W Matrix

a. All elements lies b/w 0 & 1.

b. $W_{ij} = P(C_i | C_j) = P(C_j \rightarrow C_i)$

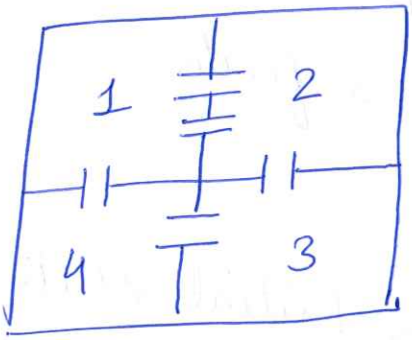
Each Column add to unity

c. Same Probability Distribution.
   Avg properties remain same
   $\Rightarrow$ Stationarity

d. Balanced Condition $\Leftrightarrow$ Stationarity.

Example :-

Rat Problem



Initial Condition — $(P_1 \ P_2 \ P_3 \ P_4)^T = |P_0\rangle$

Either uniform distribution $\begin{pmatrix} 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{pmatrix}$ or $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

Or any other arbitrary I.C.

$$|P_0\rangle = \begin{pmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \end{pmatrix} \quad \text{st} \quad \begin{array}{l} \sum P = 1. \\ W_{ii} = 0 \end{array}$$

$$W = \begin{pmatrix} 0 & 2/3 & 0 & 1/2 \\ 2/3 & 0 & 1/2 & 0 \\ 0 & 1/3 & 0 & 1/2 \\ 1/3 & 0 & 1/2 & 0 \end{pmatrix}$$

$$W|p_0\rangle = |p_1\rangle$$

$$W^2|p_0\rangle = |p_2\rangle$$

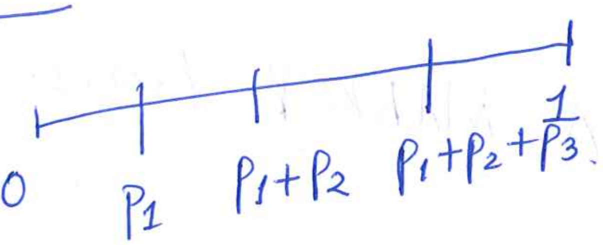
$$\vdots$$

$$W^n|p_{n-1}\rangle = |\pi\rangle$$

$$W|\pi\rangle = |\pi\rangle \quad \text{Stationarity.}$$

$W \rightarrow$ Stochastic / Markov Matrix

Simulation :-

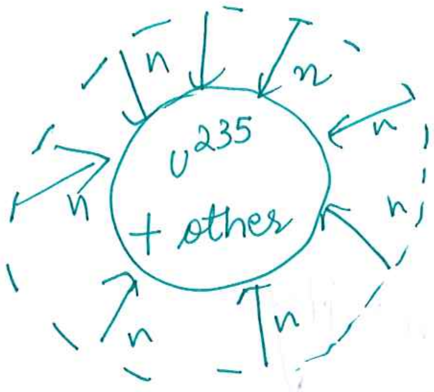


What fraction of rat comes in 1, 2, 3 & 4 ?
(after a long time).

Note :- Time avg. of 1 event = Ensemble avg. of whole system.

2

Fission Process



neutron is reacted with U^{235}. One of the possible reaction is possible :-

1. Fission (Scattering elastic).
2. Non-Fission (like Absorption etc).

Thermal Neutrons (~ 0.05 eV)

→ Stop when reach super-critical fission — 10^{35} fission/sec.

→. Check fission → A MARKOV Process.

9/10/17

Notes - 10

(1).

Time Reversal of Markov Chain is also Markov.

Finite Collection of Markov Chain → Microstate

$\{ C_1, C_2 - - - \}$

$x_0 \Rightarrow x_1 \Rightarrow x_2 \Rightarrow - - - -$

$$P[X_n = C_i] = \sum_{j \neq i} P[X_{n-1} = C_j] W_{ij} + P(X_{n-1} = C_i] W_{ji}$$

$$W_{ii} = 1 - \sum_{j \neq i} W_{ji}$$

$$P(X_n = C_i) = P(X_{n-1} = C_i) + \sum_j \Big[P(X_{n-1} = C_j) W_{ij} + P(X_{n-1} = C_i) W_{ji} \Big]$$

For large time :- $\forall i$

$$0 = \sum_j \pi_j W_{ij} - \pi_i W_{ji} \rightarrow \text{Balanced Condition.}$$

If also true for all j —

i.e. $\boxed{\pi_j W_{ij} = \pi_i W_{ji}}$ → Detailed Balance.

$$C_0 \longrightarrow C_1 \longrightarrow C_2 \longrightarrow - - - C_m$$

Transition Matrix, W

carry out time reversal

$$\boxed{C_m \longrightarrow C_{m-1} - - - \longrightarrow C_0}$$

Time Reversal Markov Chain.

W_R.

$$(W_R)_{ij} = P(X_n = C_i \mid X_{n+j} = C_j)$$

Using Conditional Probability :-

$$P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{P(A,B)}{P(B)}$$

$$= \frac{P(X_n = C_i, X_{n+1} = C_j)}{P(X_n = C_j)}$$

$$(W_R)_{ij} = P(X_{n+1} = C_j \mid X_n = C_i) \frac{\pi_i}{\pi_j}$$

2

Example :- Newtonian trajectory is time reversal invariant.

For time reversal symmetry —

$$(W_{ij})_R = W_{ij}$$

$$\Rightarrow W_{ij} = W_{ji} \frac{\pi_i}{\pi_j}$$

$$\Rightarrow \boxed{W_{ij} \pi_j = W_{ji} \pi_i}$$

So, Markov chain having time Reversal (TR) symmetry i.e. $(W_{ij})_R = W_{ij}$ obey Detailed Balance & vice-versa. (DB)

i.e. TR $\Longleftrightarrow$ DB.

Note :-
Not all thermodynamic phenomenon are time reversal symmetric.

Metropolis & Coworkers →

System has a tendency to go to lower energy.

Boltzmann Weight. $e^{-\beta E}$.

→ Encourage higher probability Region.
→ Markov Chain
→ Time Homogeneous Transition Matrix
→ Detailed Balance.
→ Equilibruim Thermodynamic evolution has time Reversal symmetry.

Extra- Conditions

(1). Every state is reachable from other state in finite time i.e. $W_{ij} > 0 \;\forall\, i, j$.
This is called strong- ergodicity condition.

(2). Glass (Non- Equilibruim)
Ergodicity is broken. But after long-time it become opaque.

or, Glass will have tendency to reach equilibrium in infinite time

→ Metastable state.

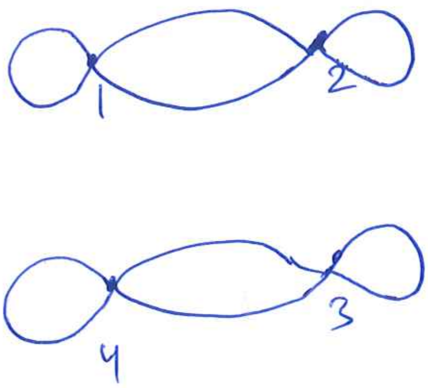
(b). $(W^n)_{ii} > 0$

Periodicity is the property of the state. We want each state to be aperiodic.

(c). Irreducible :-

Eg. If $C = \{C_1, C_2, C_3, C_4\}$

Then,



(Not allowed)

10.10.17

Notes - 11

Random Numbers & Test for Randomness

Consider the two sequence of binary random numbers :-

1 0 1 0 1 0 1 0 1 0 1 0 1 0 — A

1 1 0 1 0 0 1 0 1 1 0 0 1 1 — B

It looks like A is not a random sequence because there is a pattern in it (repetition) and second (B) is perhaps a random sequence as there is no recognizable pattern.

But in General, we can recognize that tossing a fair coin fourteen times can generate both these sequence.

Infact, A & B have the same probability $1/2^{14}$, for an unbiased coin.

→ Test for Randomness

Test, in General sense consists of constructing a function $\varphi(r_1, r_2 - -)$, where $r_1, r_2 - -$ are independent variables.

→ Calculate the value of the function for a sequence of $\underbrace{\text{Pseudo Random}}$, by set $r_i = \xi_i \ \forall i = 1, 2 \ldots$

generated by deterministic algorithm

& are supposed to be destributed independentely & uniformly in the range 0 to 1. → $\{\xi_1, \xi_2 \ldots\}$.

Eg. $$\varphi(r_1, r_2 \ldots) = \frac{1}{N} \sum_{i=1}^{N} r_i$$

defines the average of N - numbers

Run Tests —

Run-up or Run-down Test.

We say run-down length is l if we have a sequence of Random Numbers such that :-

$\xi_{l+1} > \xi_l < \xi_{l-1} \ldots \xi_1$.

Eg. Consider a sequence —

|6 4 1 3| 4 5| 3 2 7| 4 8.

$\downarrow$ 3 $\quad\downarrow$ 1 $\quad\downarrow$ 2 $\quad\downarrow$ 1.

Run-down length → 3

→ Probability distribution of Run-down length —

Let, $P(L \geq l)$ be the probability that the run-down length $L \geq l$.

For. $P(L \geq l)$, consider a sequence of l distinct random numbers.

$l!$ ways of arranging

Only one of these sequences have the correct descending order

$$\Rightarrow P(L \geq l) = 1/l!$$

$$P(L = l) = P(L \geq l) - P(L \geq l+1)$$

$$= \frac{1}{l!} - \frac{1}{(l+1)!}$$

→ Pseudo Random Generators —

Linear Congruential Generator

$$R_{i+1} = aR_i + b \pmod{m}$$

where,

a, b, m are integers.

a is called Generator or Multiplier

b is the increment

m is the modulus.

start with a seed R_i & generate successive R_{i+1}

$\forall\, i = 1, 2 \ldots$

$\{R_1, R_2 \ldots R_m\} \rightarrow$ sequence of integers.

(Random)

Also can be expressed as :-

$$R_{i+1} = (aR_i + b) - \left\lfloor \frac{aR_i + b}{m} \right\rfloor \times m$$

Eg. Let, $a = 5, b = 1, R_1 = 1, m = 100$

$R_1 = 1$

$R_2 = (5 \times 1 + 1) \pmod{100} = 6 \pmod{100} = 6$

$R_3 = 31$

$R_4 = 56$

$R_5 = 81$

$R_6 = 6 = R_2$

$R_7 = R_3$

cycle repeats

So, we just got four random integrals.

Note :-

→ Whatever the ~~sequence of~~ choice of a, b & m, the sequence of randoms numbers generated will repeat after utmost m steps.

→ Periodic

→ Must ensure the no. of Random numbers required for any simulation much less than period

→ Take m very large.

Rules —

1. m & b are relatively prime, i.e. $\gcd(m, b) = 1$

2. $a = 1 \pmod{p}$ for every prime factor p of m

3. $a = 1 \pmod{4}$, if $m = 0 \pmod{4}$

Eg. $a = 7,\ b = 13,\ m = 18,\ R_1 = 1$

$R_{i+1} = (a R_i + b) \pmod m$

$R_1 = 1$

$R_2 = 20 \pmod{18} = 2$

$R_3 = 27 \pmod{18} = 9$

$R_4 = 76 \pmod{18} = 4$

$R_5 = 5,$

$R_6 = 12,\ R_7 = 7,\ R_8 = 8,\ R_9 = 15,$

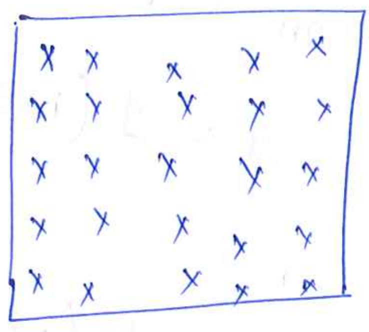
$R_{10} = 10 \ \text{-----}\ R_{18} = 6$

$R_{19} = 1.$

Marsaglia Planes

Marsaglia established the formation of lattice structure is an inherent feature of linear congruential Generator (LCG)

→ serious Defect in (LCG).



17/10/17

Notes-12

Metropolis algorithm fails for collective phenomenon.

$$ds = \frac{dq_{rev}}{T} = \frac{C_v\, dT}{T}$$ → measurable.

Importance Sampling

Importance sampling helps us sample from the important region of the sample space.

Sample $\{x_i \,;\, i = 1, 2 \ldots N\}$

Let, function, $h(x)$ and the associated probabitily density f^n $f(x)$ of the random variable X.

$h(x)$ → called score function

Expectation value, $\langle h \rangle = \int h(x) f(x)\, dx$

$$= \lim_{N\to\infty} \frac{1}{N} \Sigma\, h(x_i)$$

Modified score function $H(x)$ is defined as

$$H(x) = \frac{h(x)\, f(x)}{g(x)}$$

where, we sample $\{x_i\}$ from importance density $g(x)$ instead of $f(x)$.

<u>Steps</u> :-

$$\langle h_f \rangle = \int h(x) f(x)\, dx$$

Divide & Multiply by $g(x)$ —

$$\langle h_f \rangle = \int \boxed{h(x) \frac{1}{g(x)} f(x)} g(x)\, dx$$

$$= \int H(x)\, g(x)\, dx$$

$$\langle h_f \rangle = \frac{1}{N} \sum_{i=1}^{N} H(x_i)$$

$$\boxed{\langle h \rangle_f = \langle H \rangle_g}$$

where, g is some auxiliary distribution

$\{x_i\}$ sample from f

$\{x_i\}$ sample from g

<u>Weight function</u> —

$$W = 1 \text{ (for } f(x) \text{ ensemble)}$$

$$W_i = W \times \frac{1}{g(x_n)} f(x_n)$$

Error bar :- $\frac{\sigma}{\sqrt{N}}$.

$$\bar{H}_N \cancel{\langle hf \rangle} = \frac{1}{N} \sum h(x_i) \underbrace{\frac{f(x_i)}{g(x_i)}}_{\text{Weight } f^n}$$

$\downarrow$

$\lim N \to \infty, \to \langle h \rangle_f$.

→ Also a variance reduction device

Statistical error :-

Second Moment :-

$$M_2^B(H) = \int_{-\infty}^{\infty} H^2(x) g(x)\, dx$$

$$= \int_{-\infty}^{\infty} \frac{h(x) f(x)}{g(x)} \frac{h(x) f(x)}{g(x)} g(x)\, dx$$

$$= \int_{-\infty}^{\infty} \left[\frac{f(x)}{g(x)}\right]^2 h^2(x) g(x)\, dx$$

For, initial sampling $\{x_i\}$ from $h(x)$

$$M_2(h) = \int_{-\infty}^{\infty} h^2(x) \cancel{g}(x)\, dx$$

Thus, choosing properly the importance f^n $g(x)$ & ensure the ratio $\frac{f(x)}{g(x)}$ is less than unity,

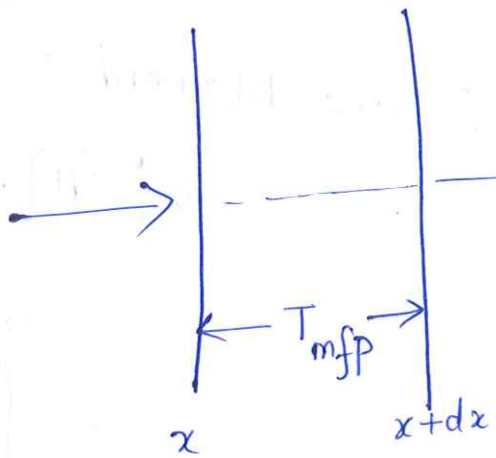
$$M_2^B(H) < M_2(h)$$

So, the importance sampling serve as variance reduction technique.

Example :-

Particle incident normally on the left face of a slab of material of thickness, T

The particle would penetrate a distance x into the shield with prob.



$$p(x) = \Sigma e^{-\Sigma x}$$

$$p(x)\,dx = \Sigma e^{-\Sigma x}\,dx$$

Σ^{-1} = Mean free path (mfp)

Note :- We can measure all distances in units of mfp & hence set $\Sigma = 1$.

→ What fraction of incident photons/particles comes out ?

Monte-Carlo rules — 3

1. Generate x_i for $e^{-x}\,dx$

2. Check $x_i > T$ or $x_i < T$

If $x_i > T$, store unity.

else score zero.

Collect the score from N histories.

3.

$$\int_0^\infty h(x) f(x)\,dx = \int_T^\infty e^{-x}\,dx = \text{small.}$$

Let, $T = 10$ mfp

Auxiliary, $g(x) = b e^{-bx}$

1. In the biased simulation, sample x_i from $b e^{-bx}$.

$b = \tilde{b}$ such that variance is minimum.

2. If $x_i > T$, then score is $w_i = \dfrac{f(x_i)}{g(x_i, \tilde{b})}$

$$= \exp\left[-x_i(1-\tilde{b})\right] / \tilde{b}$$

else score is zero.

$$\mu = \int_0^\infty \exp(-x)\, h(x)\, dx$$

$$= \exp(-T)$$

$$\sigma^2 = (1-\mu)\mu. \quad = \langle h^2 \rangle - \langle h \rangle^2$$

$$= \mu - \mu^2$$

$$\boxed{\sigma^2 = \mu(1-\mu)}$$

Take $T = 5\,mfp,\ 10\ mfp,\ 100\ mfp,$

Calculate μ, σ^2.

→ Importance sampling, $g(x)$.

$$\sigma^2 = \int_{-\infty}^{\infty} H^2(x)\, g(x)\, dx - \left(\int_{-\infty}^{\infty} H(x)\, g(x)\, dx\right)^2$$

$$= \int_M^\infty \frac{\exp(-2x(1-b))}{b^{\cancel{2}}} \cancel{b} e^{-bx}\, dx - e^{-2T}$$

$$= \frac{1}{b}(+)\left.\frac{\exp(-2+b)x}{b(b-2)}\right|_M^\infty - e^{-2T}$$

$$\sigma^2 = \frac{1}{b(2-b)} \exp(-T(2-b)). - e^{-2T}$$

Minimize σ^2 w.r.t b —

$$\left.\frac{\partial \sigma^2}{\partial b}\right|_{b=\tilde{b}} = 0$$ to obtain $\tilde{b}$

$\Rightarrow$ $\tilde{b} = ?$

$$\frac{-1\,(2-2b)}{b^2(2-b)^2}\exp(-T(2-b)) + \frac{T}{b(2-b)}\exp(-T(2-b)) = 0$$

$$\frac{2(b-1)}{b(2-b)} + \frac{T}{1} = 0$$

$$\frac{2b-2}{b(2-b)} = -T$$

$\frac{4}{T^2} - \frac{8}{T^2}$

$$2b-2 = -2bT + Tb^2$$

$\frac{-4}{T^2}$

$$b^2 - 2b\left(1+\frac{1}{T}\right) + \frac{2}{T} = 0$$

$$\tilde{b}_{1,2} = \frac{2\left(1+\frac{1}{T}\right) \pm \sqrt{4\left(1+\frac{1}{T}\right)^2 - \frac{8}{T}}}{2}$$

$$\tilde{b}_{1,2} = \left(1+\frac{1}{T}\right) \pm \sqrt{\cancel{4}\left(1+\frac{1}{T^2}\right)}$$

$$\Rightarrow \tilde{b}_{1,2} = 1 + \frac{1}{T} \pm \sqrt{1 + \frac{1}{T^2}}$$

Choose −ve sign (for minimum variance)

$$\Rightarrow \tilde{b} = 1 + \frac{1}{T} - \sqrt{1 + \frac{1}{T^2}}$$ ✓

So, $\tilde{b}$ depends on thickness.

For $T = 3$, $\tilde{b} = 0.28$

$T = 10$, $\tilde{b} = 0.09$.

Notes-13.

23/10/17

Importance Sampling

Recap :-

Importance sampling helps us sample from the important regions of the sample space.

$x = x(\omega) \rightarrow$ sampled from $f(x)$

$$\langle h \rangle_f = \int h(x) f(x)\, dx$$

$$= \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} h(x_i)$$

In the nbd of avg. of x, let $h(x) = 0$.

Suppose, we want to find probability that person will survive beyond 100 yrs?

For such situations, we can sample $\{x_i : i = 1, 2 - - - N\}$ from an importance density $g(x)$ instead of analogous $f(x)$.

$$\underset{\substack{\downarrow \\ \text{weight function}}}{\langle h\, w \rangle_g} = \langle h \rangle_f$$

$$= \int h(x)\, w(x)\, g(x)\, dx = \frac{1}{N} \sum_i h(x_i) \frac{f(x_i)}{g(x_i)}$$

$$w(x) \rightarrow \frac{f(x_i)}{g(x_i)}$$

$$= \int h(x) f(x)\, dx$$

Error Bar :- $\dfrac{\sigma}{\sqrt{N}}$

Binomial Distribution

N- fair coin

$H \rightarrow p = 1/2$

$T \rightarrow p = 1/2$

$$p(n) = \frac{N!}{n!\,(N-n)!} p^n q^{N-n}$$

1. Toss the coin
2. Generate random no. x.
3. If $x < 0.5 \longrightarrow$ Head.
   else $\longrightarrow$ Tail
4. frequency distribution.

5. 1- Million time tossing 100 coins

6. See the estimate of Binomial distribution

Binomial distribution for 100 heads & 0 tail is very small

$= 2^{-100}$ (very small but non-zero).

*. Pick randomly.

HHHT(H) HHTTH $\rightarrow$ C_0 (Initial Conf.)

$\downarrow$ flip

(T)

$C_0 \longrightarrow C_1 \longrightarrow C_2 \longrightarrow C_3 \longrightarrow - - -$

Eg. $\begin{pmatrix} 5H \\ 5T \end{pmatrix} \xleftarrow{\text{either}} \begin{pmatrix} 6H \\ 4T \end{pmatrix} \xrightarrow{\text{or}} \begin{pmatrix} 7H \\ 3T \end{pmatrix}$

<u>AnOther method</u> —

Let $n_0 = 3$ (denote no. of head (say)

$n_1 = 4$ or $n_1 = 2$

$\downarrow$ $\downarrow$

$p = 0.7$ $p = 0.3$.

$n_0 \longrightarrow n_1 \longrightarrow n_2 \longrightarrow - - .$

If Head $\rightarrow$ 5
Tail $\rightarrow$ 5 $\Big\} \rightarrow$ Equilibrium Configuration

HHHHHTTTTT $\rightarrow$ Ordered Conf.

(Not Equilibrium Microstates)

If $n = 50$, no. of underlying conf. are very large,

i.e. $\dfrac{100!}{50!\,50!} \rightarrow$ Maximum Entropy

Maximum Entropy $\longrightarrow$ Most Probable Configuration

Start	30 H	70 T
p	0.3	0.7

Machinery

50 H, 50 T
$\downarrow$
Equilibrium.

Machinery —

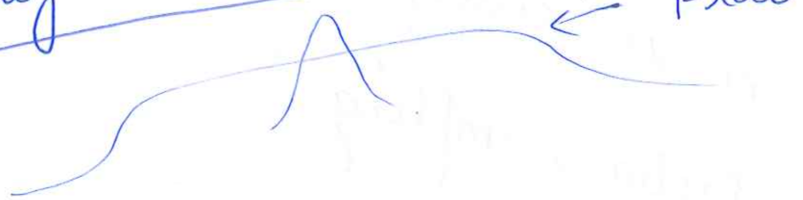
Modify the Markov chain. Reframe the problem to get same Binomial distribution.

Machinery → System away from equilibrium is allowed.

i.e. 30 H → 29 H   70 T → 71 T   is also allowed!

→ Fluctuations are important. Encourage system away from equilibrium.

$\boxed{\text{Flat histogram Technique / Umbrella Tech.}}$



(A) Cheating Way.

Let, C_i → Initial Configiuration

C_t → Trial configiuration

$$g(n_i) \rightarrow \frac{N!}{n!(N-n)!} \quad (\text{for initial})$$

$$g(n_t) \rightarrow \frac{N!}{n_t!(N-n_t)!} \quad (\text{for trial})$$

If $g(n_t) > g(n_i) \rightarrow$ Discourage

$g(n_t) < g(n_i) \rightarrow$ Allow it to go.

→ Follow the histogram

→ $h_i = 0$

→ update the histogram

→ equal no. of configurations in all boxes (umbrella sampling)

30.10.17

Notes - 14

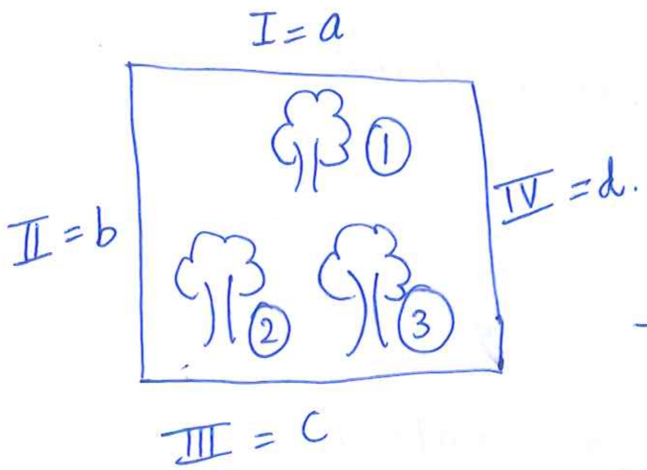
Russian Rolling

→ Statistical Weight

→ Splitting in combination with Russian Rolling (either terminate or continue) ✓

(1) Hidden Markov Model :-

Idea:-



Monkey jumps
→ Start
→ W_{ij} → 3 × 3
→ Inhomogenous Markov chain.

Monkey pick a mango from the picked tree & throw in any of the four direction with some probability.

Observed state → a → a → b → c → d → a → c ...

Hidden state → 1 → 2 → 1 → 3 → 2 → 1 → ...

Eg. (1) Speech (Hear → (a, b, c, d), what person say (1, 2, 3 ...))

(2) Hand Writing Analyses

Observed → Markov process of visible states.

Question:- if Mango is at 'a', what is the prob. that it comes from 1, 2 or 3.

Note:- Vitterbi Algorithm for speech recognition Technique.

(2).

Gillespie Algorithm

Radio-active material, long lived simulate the Geiger Muller Counter and see the tick.

→ No interaction for longer time

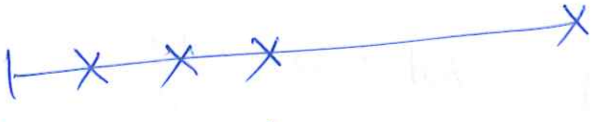
→ Neutrino Oscillation.

Event Based

→ Time at which decay happens.

Generate MC scheme. Time elapses b/w 2 events,

"τ", $f(\tau)$ → Poisson Distribution



0 $P(n, t)$

$P(n, t - \Delta t)$

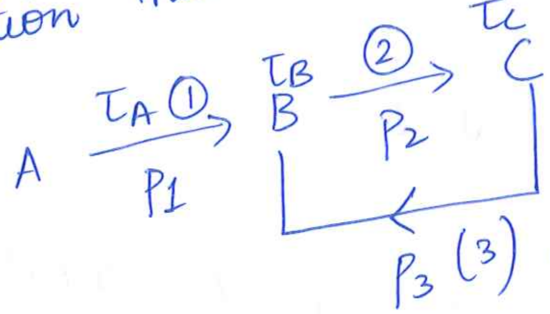
In small interval Δt, either one event occur or no event occur. ②

Poisson Distribution :- $\frac{e^{-\mu} \mu^n}{n!}$

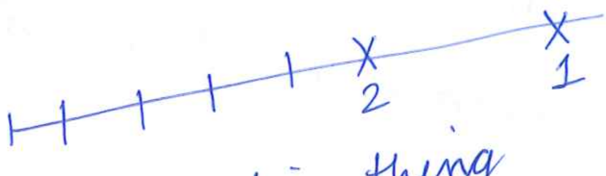
This is event-based Monte Carlo.

<u>Chemical Reaction</u> :- Time Constant, κ

Each Reaction has distinct poisson decay constant.



Rate of decay?



Time is an active thing

③. <u>Voter / Ising Model :-</u>

Things only happen on a local scale.

Array of atoms. Each atom is a spin.

(↑/↓). Each element only interact with neighbouring element.

"Local Interaction" is adequate to change the global property

Eg. Voter Model
Ising Model

$\uparrow \downarrow \uparrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow$

No order.

Only events happening in the nbd decides.

→ Disordering temperature.

→ State of lower energy is preferred.

$i^{\times}$	$j^{\times}$
↑	↑
↑	↓
↓	↑
↓	↓

$\underset{0}{|} \times \times \times \times \times$

$S_i = +1$ ↑

$= -1$ ↓.

$$E_{ij} = -S_i S_j$$

	E
$\uparrow\uparrow$	-1
$\uparrow\downarrow$	$+1$
$\downarrow\uparrow$	$+1$
$\downarrow\downarrow$	-1

$$E = \sum_{\langle ij \rangle} J_{ij} S_i S_j$$

$$H = -\sum_{\langle ij \rangle} J_{ij} S_i S_j$$

$$- B \sum S_l$$

Prevailing influence / Magnetic field for ising model (lift the degeneracy) ✓

Magnetic system :- Whenever there is a loop, magnetic moment ($\vec{B}$) is Generated when current (I) passes through the loop.

→ Magnetic moment associated with spin.

→ Piece of iron → cool

Non Magnetic $\xrightarrow[T\downarrow]{}$ Magnetization.

Paramagnetic (Disordered) → Ferromagnetic (Ordered).

Macroscopic order from Microscopic Interaction.

Local interaction.

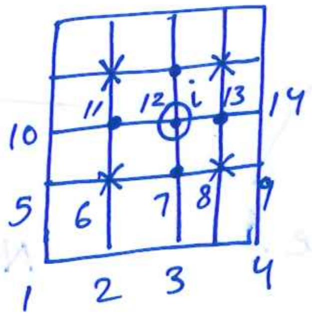
1d - 2 nb

2d - 4 nb.

3d - 6 nb.

⋮

2d Lattice



$S_i \nearrow +1 \uparrow$

$S_i \searrow -1 \downarrow$

For $T < T_c$, there is correlation (co-operation) globally.

Which property of society lead to global behaviour?

Eg. Rumours spread within seconds!

i, j are nearest neighbour state.

$$\epsilon_{ij} = -J_{ij} s_i s_j$$

S_i	S_j	ϵ
+1	+1	$-J$.
+1	-1	$+J$
-1	+1	$+J$
-1	-1	$-J$.

If, $J_{ij} = J$

Alligned spins preferably
(State of low energy)

$$E = -J \sum_{\langle ij \rangle} S_i S_j$$

Low energy state is either all the spins aligned up or aligned down.

System confused!

Note:- In Thermody, this is not eq^m state! (Since fluctuations are always there).

→ Hoff bifurcation

Entropy → Macroscopic Behaviour. Arrow of time.

At microscopic level, there is no preferred direction of time.

Symmetry Breaking → Ising fluctuation ✓

There are 2 organizing principles — (2)

(1). System has tendency to form minimum energy state.

(2). Larger the energy, larger is entropy.

$$\boxed{T\,dS = dU - P\,dV}$$

$$\left(\frac{\partial U}{\partial S}\right) = T.$$

$E(C) =$

$$P(C) \propto e^{-\beta E(C)}.$$

Probability of the Configuration.

In Metropolis alg., we don't need proportionality constant.

→. Problem can be reduced to Binomial distribution

→ Ghost Technique.

Large no. of degrees of freedom. Start with zero energy.

Eg. Bank.

External agent : B.

$$E = -J \sum_{\langle ij \rangle} S_i S_j - B \sum_i S_i$$

$B \uparrow \rightarrow$ Sym. breaking field.

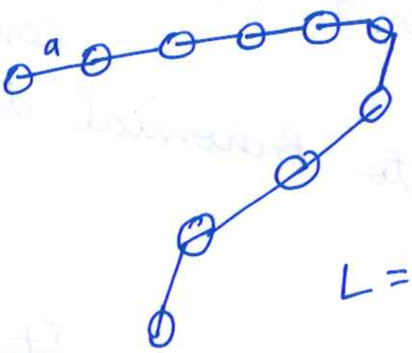
Entropy :-

Suppose, there is no energy interaction at all.

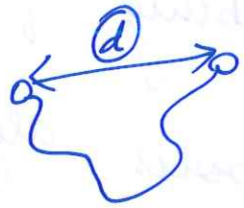
$$E = -J \sum_{\langle ij \rangle} S_i S_j - B \sum S_i$$

$E = -TS$

Maximize entropy



Rubber

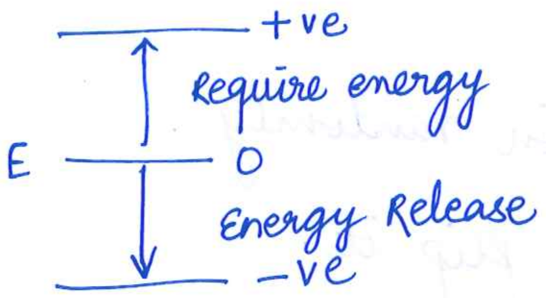


$L = (n-1)a$. $\quad d = L \rightarrow$ Entropy $= 0$

when $d << L$, Entropy max.

When $T \uparrow$es, entropy increases $\Rightarrow$ Shortening of length.

3.



Simulting Soft Material :-

Eg. ~~S~~ Tooth Paste, Gels etc.

Shear Modulus $\simeq 0$

Rigidity & flow like liquid

Entropy dominating

Prediction of property of soft material ✓

$\boxed{\text{Ghost Algorithm.}}$

Boltzmann Weight :- $e^{-\beta E(C)}$.

Metropolis Algo.

Allow entropy to play role in Generating the trial conf.

$$\pi_i W_{ji} = \pi_j W_{ij}$$

- Generate the conformation randomly.
- Pick state randomly & flip it.
- C_0 $P(C_0)$ If, $P(C_0) < P(C_t)$ ✓. (down the energy).

  C_t $P(C_t)$ If, $P(C_0) > P(C_t)$

  Take the ratio & accept the prob.

- 10,000 Microstate.
- Equilibrate
- Canonical Ensemble (T fixed) ✓

Steps —
Fix Temp and get various Macroscopic properties

$$\langle E \rangle = \frac{1}{N} \sum_i E(C_i)$$

$$\langle E^2 \rangle = \frac{1}{N} \sum E^2(C_i)$$

$$\sigma^2 = \langle E^2 \rangle - \langle E \rangle^2.$$

$K_\beta T^2 C_V = \sigma^2$

$\downarrow$

Shots at phase transition .

Net Magnetization

Susceptibility

1

6.11.17

MC. Methods

Notes - 16.

Microscopic → Lowest Energy (order)
Maximum Entropy (disorder).

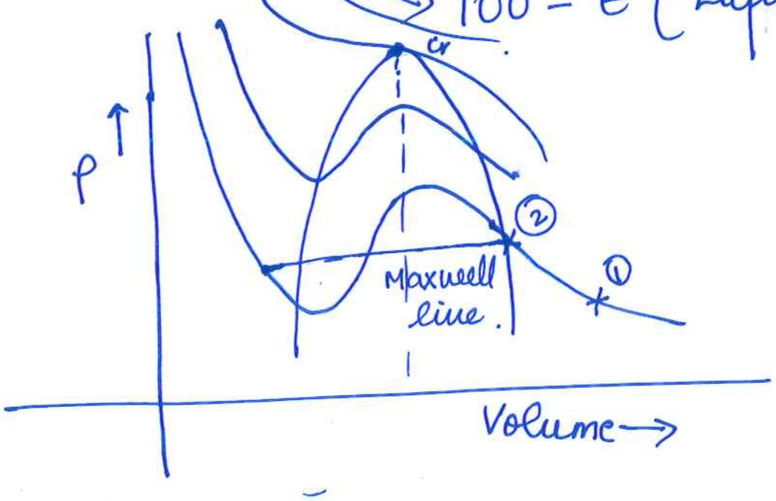
Free energy :- F = Energy - T(entropy)

Energy ↓ Order; T ↓ Temp. (sets the nature of competition); entropy ↓ Disorder.

$$\frac{1}{1+T} \qquad \frac{T}{1+T}$$

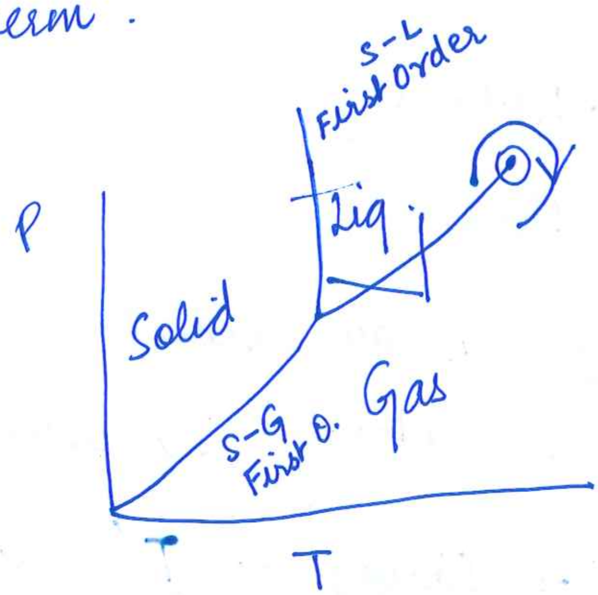
At low temp, energy is given more weight.
high " , entropy " " "

T = 100°C → 100+ε (Gas)
→ 100 − ε (Liquid).



Van der Waals.

Isotherm".



Critical ↳ 2nd order continuous.

Transition :- occurs due to competition b/w entropy and energy.

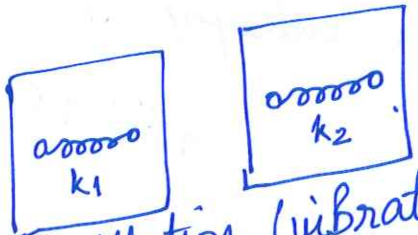
Transition from paramagnetization to ferromag.
→ 2nd order / continuous phase transition.

Temp Induced 2nd order Phase Transition

Heat Capacity :: Amt. of heat required to raise temp. by 1°C

$C_V =$

2 kinds of Solids :-

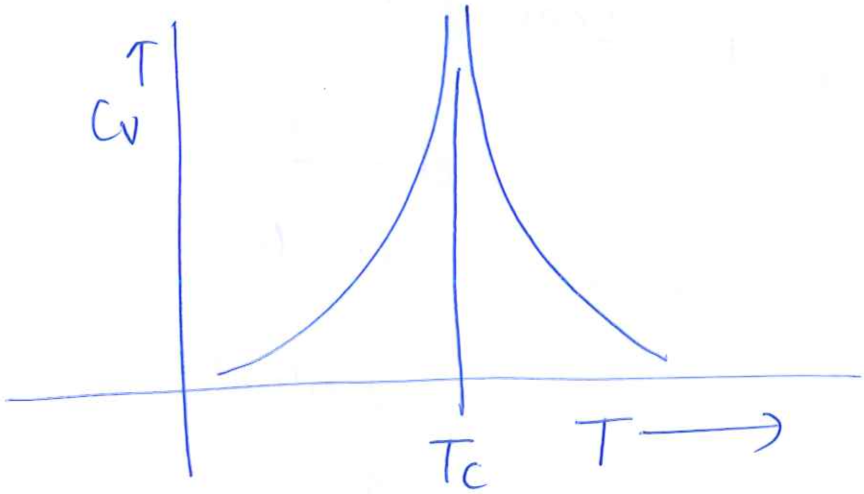


How the incoming energy affect the oscillation (vibration) of spring?

Graphite Carbon atom
↓
Covalent Bonds
↓
Diamond.

Heat capacity depends on Temperature (In principle)
$C_V(T)$ C_V = Material Property.

$$C_V = \frac{\Delta Q}{\Delta T} = \infty \qquad \Delta Q = \text{Latent Heat.}$$



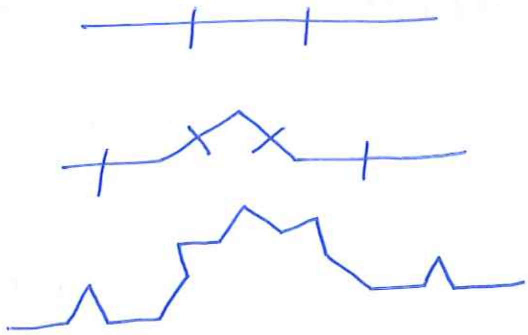
Temperature can be scaled as
K, mK, μK
(Power Law Behaviour)

Self-Similarity → Properly chosen part of a whole looks like "whole".

Scale free objects

→ Fractals

→ Eucledian



→ Scale free

$$C_V \sim (T - T_c)^{\alpha}.$$

(Since divergence to infinity is scale free)

→ Ability of nature

→ Fractal dimension is scale-free.

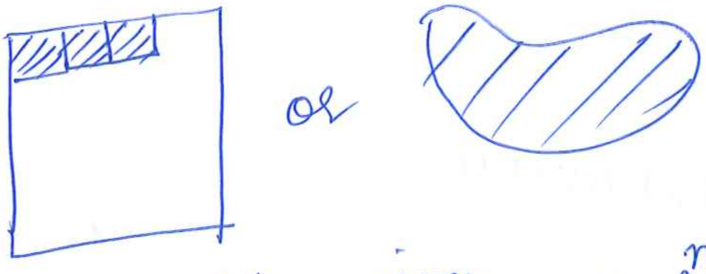
$d = 1$

Line

$$N(\epsilon)\,\epsilon = \lim_{\epsilon \to 0} N(\epsilon)\,\epsilon$$

$= \text{finite no}$

$= 1$

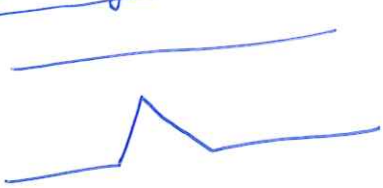


2d.

$N(\epsilon)\,\epsilon^2$

<u>Topological Dimension</u>

$$4^n \left(\frac{1}{3}\right)^n = 4^n \epsilon^d.$$



For what d, this is finite? $d = \log_3 4$ ✓

Phase Transition → Self Similar

Nature's way of affecting infinity !

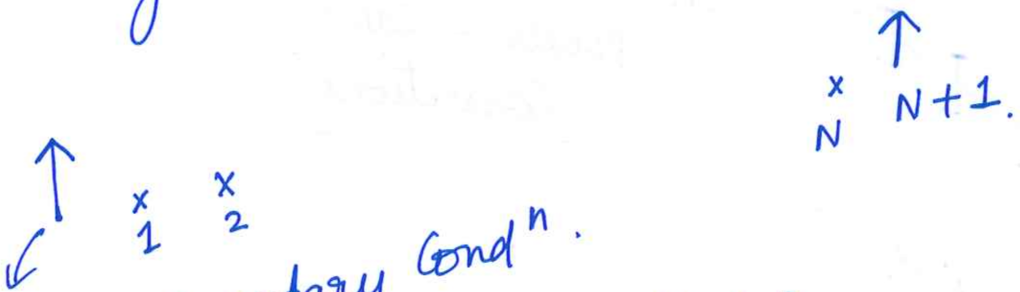
From the part, construct the whole - -

<u>1d</u> :- No Magnetization emerge.

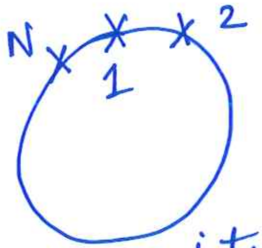
For some co-operate phenomenon to happen, neighbours should be there.

Long-Range behaviour should be emerged from local interaction.

Boundary Cond^n

① 

Rigid Boundary Cond^n.



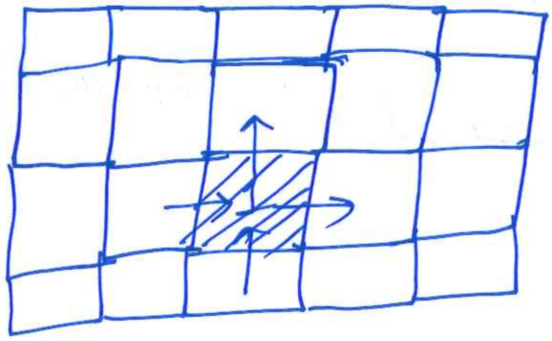
② Periodic B.C

③. Random Boundary Condition.

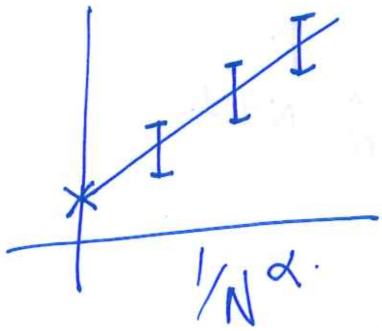
Finite Size affect → Larger the system, small FSE.

FSE are least for periodic B.C.

2-d :-



Finite Size Effects



$1/N^\alpha$

Power - Law Corrections

2-d Ising Model

Plot Energy v/s Temp.

Magnetization v/s Temp.

1 Monte Carlo step

$$\langle E \rangle = \frac{1}{10^6} \sum E(C_i)$$

$$\langle E^2 \rangle = \frac{1}{10^6} \sum E^2(C_i)$$

① **MC Notes - 17** 7/11/17

$E(C)$

$\uparrow \downarrow$
$i \; j$ $\quad \epsilon_{ij} = -J S_i S_j$

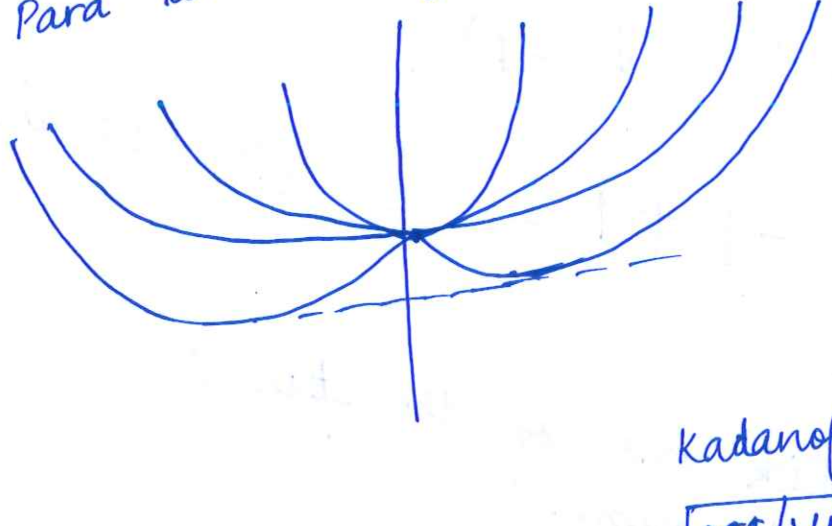
1 2
$\uparrow\uparrow$ × × × × × ... ×
$\downarrow\uparrow$ 1 2 3 4 5 ... N.
$\uparrow\downarrow$
$\downarrow\downarrow$

At the transition pt, → jump in the transition – Ist Order Transition

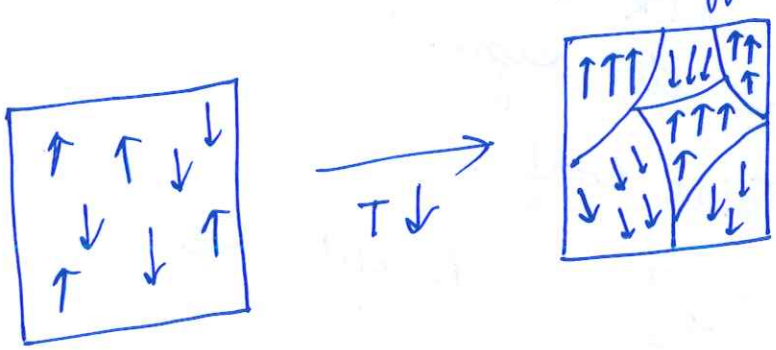
Second Order → Continuous.
Fluctuations grow near the transition point.

Para to Ferromagnetization → 2^{nd} order Transition

$F = U - TS$



Kadanoff Domains.



Microscopic Magnetization

$$E = -J \sum_{\langle ij \rangle} S_i S_j - \overset{\uparrow}{B} \sum S_i$$

B = Symmetry Breaking field

$\underset{1}{\times} \quad \underset{2}{\times} \; - - - - - \; \times_{10,000}$

$$E = -J \sum_{1}^{N-1} S_i S_{i+1} + S_N S_1 - B \sum S_i$$

$\underset{1}{\times} \quad \underset{2}{\times}$

Random No $> 1/2$ $\quad \uparrow (+1)$

$< 1/2$ $\quad \downarrow (-1)$.

$$C_0 = \underbrace{+1 \; -1 \; -1 \; +1 \; - - - - -}_{} \; (10,000 \text{ times})$$

$E[C_0]$

Given T = Temp.

Random No :- Pick one of the spin & change its sign.

$E[C_t]$. $\rightarrow$ Trial conf.

If $E[C_t] < E[C_0] \longrightarrow$ Accept C_t.

$p \propto e^{-\beta E}$

Eg.

C_0 :- $\uparrow \uparrow \downarrow \uparrow \downarrow$ E $\cancel{+0}$ −3

Choose $\underbrace{(\text{Random No} \times 5) + 1}_{\text{lies b/w 1 \& 5}}$,

Truncate.

lies b/w 1 & 5.

Let, we get 3.

C_1 $\uparrow \uparrow \uparrow \uparrow \downarrow$ −2

C_0 $P(C_0)$

C_t $P(C_t)$

If $P(C_t) > P(C_0)$ $C_1 = C_t$.

$P(C_t) < P(C_0)$

$$r = \frac{P(C_t)}{P(C_0)}$$

if $R_n < r$ $C_1 = C_t$,

$R_n > r$ $C_1 = C_0$

$C_0 \longrightarrow C_1$

$$\underbrace{P(C)}_{\text{Higher Prob.}} \propto e^{-\beta \underbrace{E(C)}_{\text{Lower Energy}}}$$

Repeat for 50,000 steps.

Equilibration run ✓ $\boxed{\text{Step 1}}$:

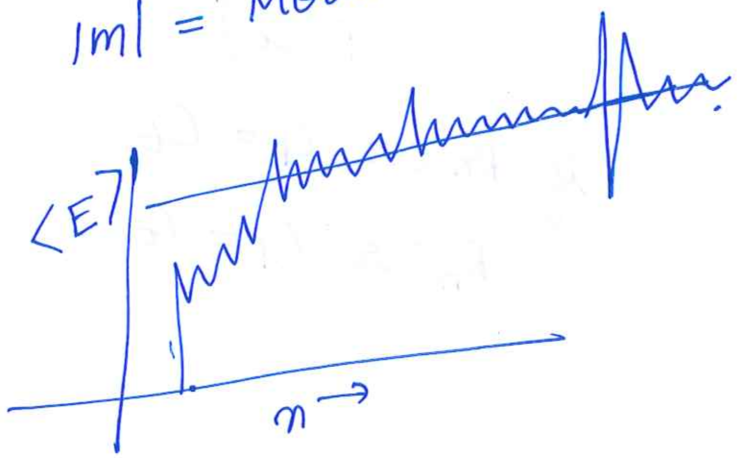
Plot the avg. energy for 100 steps, 1000 steps, and check the fluctuations with steps.

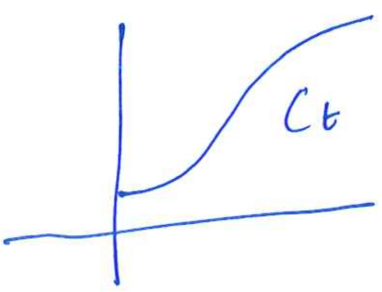
Magnetization → Sum of spins. = S

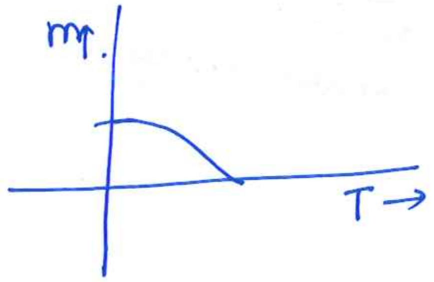
$\langle m \rangle = \frac{S}{N}$, N : Total no. of spins.

$M = \frac{1}{N} \sum_{i=1}^{n} S_i$

|m| = Modulus.

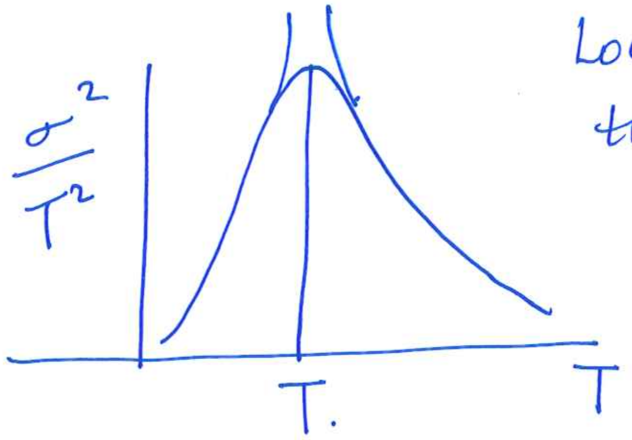






$$\boxed{K_B T^2 C_V = \sigma^2}$$

→ Fluctuation Dissipation Theorem.



Locate the transition temperature:

Finite → sample (Central limit Theorem)

Finite size.

(1) MC Methods 13/11/17

Notes – 18

Ising Model

Summary :- (Boltzmann Algorithm)

1. C_0 (Initial Configuration)
2. $E(C_0) \rightarrow$ Energy of Initial conf. $= E_0$
3. Probability $P(C_0) \propto e^{-E(C_0)/k_B T}$.
4. Construct a trial state C_t.

   $E(C_t) = E_t$

5. $r = \dfrac{E[C_t]}{E[C_0]}$ $\qquad p = \min(1, r)$.

6. Accept the trial state with prob. p.
   (or, in other words, accept the trial state will have lower energy or higher probability).
7. Natural process of picking trial state respects higher entropy.
8. $C_0 \rightarrow C_1 \rightarrow C_2 \rightarrow$ - - -

Any Property —

$$\langle Q(C)\rangle = \frac{1}{N}\sum Q(C_i)$$

Q(C) can be ~~entro~~ energy, Magnetization, specific heat etc.

Such properties are defined by each Microstate (Microstate Property)

→ Mechanical Property.

Non-Boltzmann Algorithm (For Thermal Properties).

Entropy :- $S = -K_B \sum_i p_i \ln p_i$.

(Collective Property)

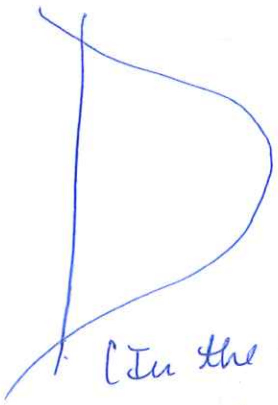
Let, we toss the coin 10 times.

S(n) = Entropy associated with n.

n	S(n)
0	0
1	
2	
3	
4	
$\boxed{5}$	
6	
7	
8	
9	
10	

②

Umbrella sampling



$$g(n) = \frac{N!}{n!\,(N-n)!}$$

(Density of states)

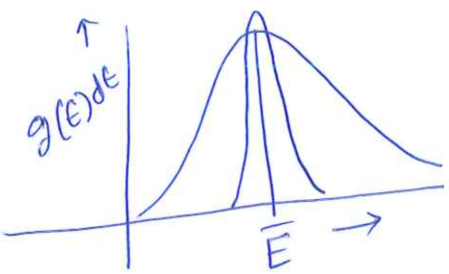
(In the entire parameter space, spreads) ✓

$\boxed{g(E)}\,dE$ = No of microstates having energy $(E, E+dE)$

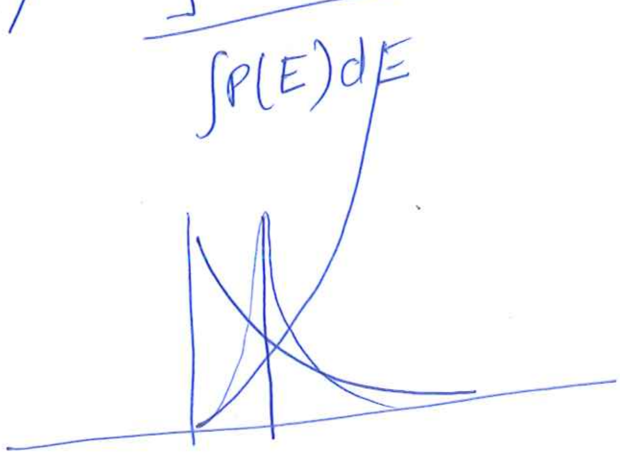
↓

Density of states.

$g(n) \rightarrow$ No of microstates corresponding to n.



$$\langle E\rangle = \frac{\int E\,P(E)\,dE}{\int P(E)\,dE} = \frac{\int E\,e^{-\beta E} g(E)\,dE}{\int e^{-\beta E} g(E)\,dE}$$



Entropy Sampling :-

Non- Boltzmann Algorithm

1. C_0
2. $E(C_0) = E_0$
3. $P(C_0) = \dfrac{1}{g(E(C_0))}$ (Unphysical)

4. C_t
5. $r = \dfrac{P(C_t)}{P(C_0)} = \dfrac{g(E_0)}{g(E_t)}$

   $p = \min(1, r)$

6. No of microstates in each region $\rightarrow$ Flat

Histogram Method.

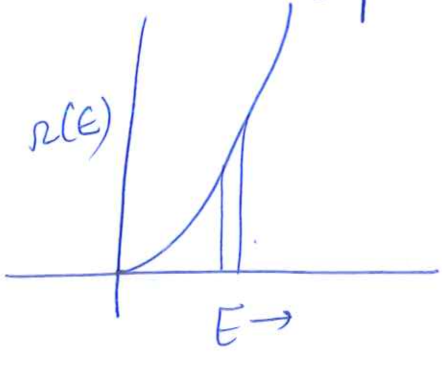
$\text{Prob}_{\text{Low}} > \text{Prob}_{\text{High}}$ $\quad e^{-\beta E}$

E Low $\quad$ High.

$\Downarrow$

10 Mic. $\quad 10^{10}$ Micr.

E low $\quad$ E high



(3)

Number of Microstate . (Exp.)

$10^3 \longrightarrow 10^{20}$

Entropy $3 \longrightarrow 20$. (Log)

$g(E)$ is unknown .

Old Technique.

$\rightarrow$ $C_0 \rightarrow C_t \rightarrow$ - - - 1 Million

$\rightarrow$ Histogram $h(E)$

$\rightarrow$ Take Histogram as $g(E)$

Let, $g(E) = 1 \;\forall\; E$

$g(E) = g(E) \div h(E)$

$= 1$ if $h(E) = 0$

New Technique

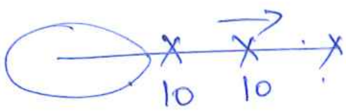
$g(E) = 1 \;\forall$ all E .

C_0 :- $g(E_0) = g(E_0) \times \alpha$.

$\alpha = 10$ (let) or $\alpha = e^1$ ✓

Repeat for $\sqrt{\alpha}$, --

C_t :-



→. If density of state

Concept of Scaling V. Imp.

G I Taylor

End