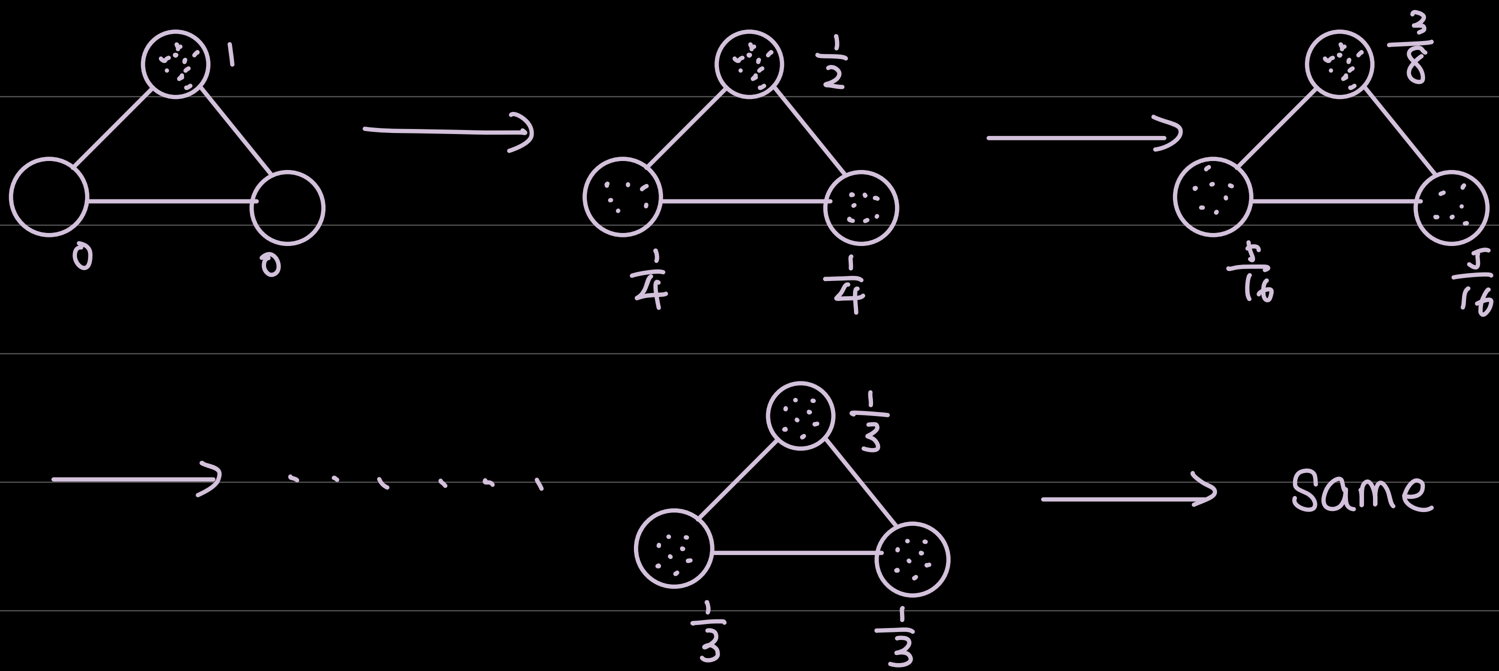
Markov Chain

random walk in state space

1 million people



Population migration

probability $\frac{1}{2}$, Stay. probability $\frac{1}{4}$ to one other state.

arrow of time, coverage to stationary distribution

Entropy (randomness) increases

Notation :

X_t : State at time t

$p^{(t)}$: distribution of X_t (population distribution)

$p^{(t)}$	$p_1^{(t)}$	$p_2^{(t)}$	$p_3^{(t)}$
$t=0$	1	0	0
$t=1$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$
$t=2$	$\frac{3}{8}$	$\frac{5}{16}$	$\frac{5}{16}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$t\to\infty$ π	$\frac{1}{3}\pi_1$	$\frac{1}{3}\pi_2$	$\frac{1}{3}\pi_3$

$$p^{(t)} \xrightarrow[\infty]{t} \pi$$

"arrow of time"

Key / driving force :

Transition Probability

$$k_{ij} = P(X_{t+1} = j \mid X_t = i)$$

or $[k(x,y) = P(X_{i+1} = y \mid X_i = x)]$

transition matrix:

$$\begin{array}{c|ccc} i \backslash j & 1 & 2 & 3 \\ \hline 1 & \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ 2 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ 3 & \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \end{array}$$

Master Equation

→ # of ppl in j at t-1

$$P_j^{(t+1)} = P(X_{t+1} = j)$$

→ # in j at t+1 and in i at t

$$= \sum_i P(X_{t+1} = j \;\&\; X_t = i)$$

→ # in i at t

$$= \sum_i P(X_t = i)\, P(X_{t+1} = j \mid X_t = i)$$

↓ fraction of these in i who will go to j

$$= \sum_i P_i^{(t)} K_{ij}$$

So the master equation is:

$$\underline{P_j^{(t+1)} = \sum_i P_i^{(t)} K_{ij}}$$

eigen-analysis

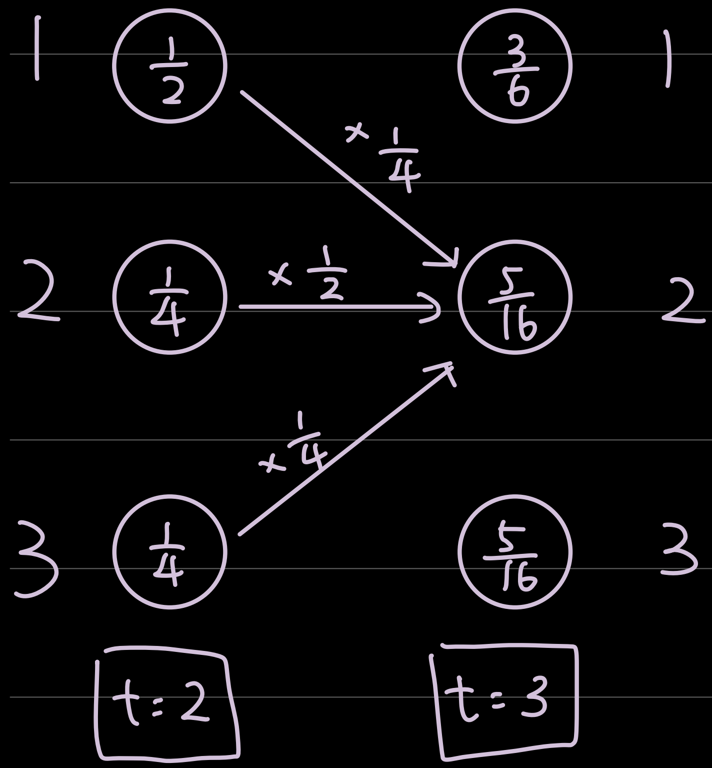
$$P^{(t)} \xrightarrow{\quad K \quad} P^{(t+1)}$$

converge ↗ π

$$P^{(t+1)} = P^{(t)} K \implies P^{(t)} = P^{(0)} \boxed{K^t}$$

$$\begin{bmatrix} \frac{3}{8} & \frac{5}{16} & \frac{5}{16} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \end{bmatrix}$$

Interpret the master equation



$P_i^{(t)}$ = # of people in i at t

K_{ij} = fraction of people in i who will go to j

$P_i^{(t)} K_{ij}$ = # of people in i at t who will go to j

$\sum P_i^{(t)} K_{ij}$ = # of people who will end up in j at t+1

≈ equillibrium

Stationary π

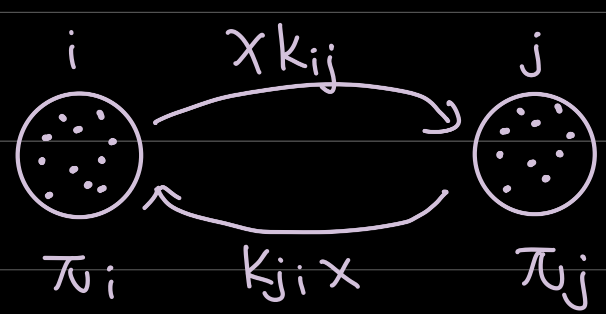
$$\pi = \pi K$$

$$\pi_j = \sum_i \pi_i K_{ij} \longrightarrow$$ ① condition Overall balance

② Detailed balance $\forall i,j$

stronger condition : satisfies overall balance when it's satisfied.

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



Page Rank : know K, want π

Start from $p^{(0)}$ (e.g. uniform)

$p^{(0)} \xrightarrow{K} p^{(1)} \xrightarrow{K} p^{(2)} \xrightarrow{K} \cdots\cdots \xrightarrow{K}$

$p^{(T)} \approx \pi$

K is a stochastic matrix, the sum of each row $=1$

Why recursive : more stable, accurate measure of popularity

MCMC : know π (target distribution), want K (iterative algorithm)

to implement

so that $\pi = \pi K$ (design principle)

Start from $X_0 \sim p^{(i)}$

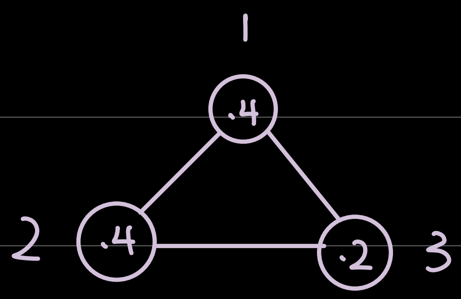
$X_0 \to X_1 \to X_2 \to \cdots \to X_t \to X_{t+1} \to \cdots \to X_T$

Approx: $X_T \sim \pi$

Metropolis algorithm

1950s Metropolis, Roseblatt², Teller²

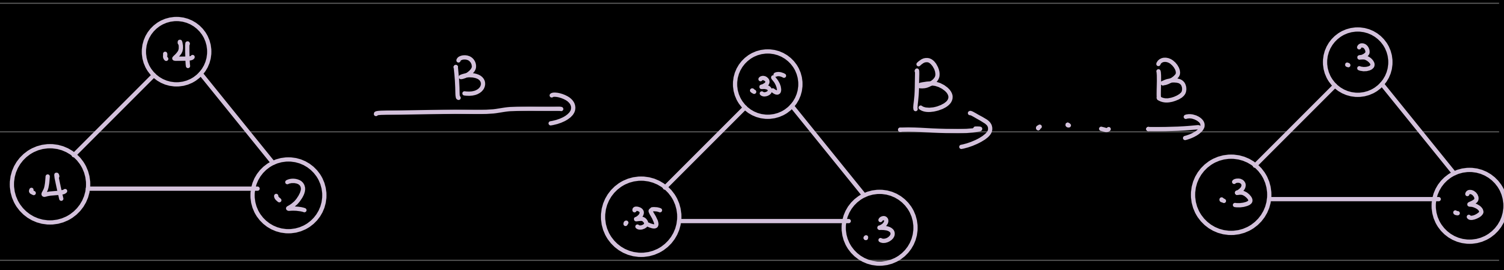
Basic idea



π

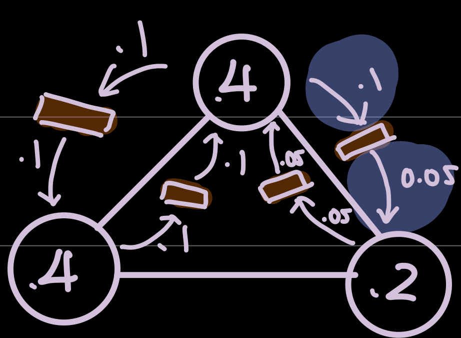
Base Chain: B

$$
\begin{array}{c|ccc}
i \backslash j & 1 & 2 & 3 \\
\hline
1 & \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\
2 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\
3 & \frac{1}{4} & \frac{1}{4} & \frac{1}{2}
\end{array}
$$



π

good, balanced



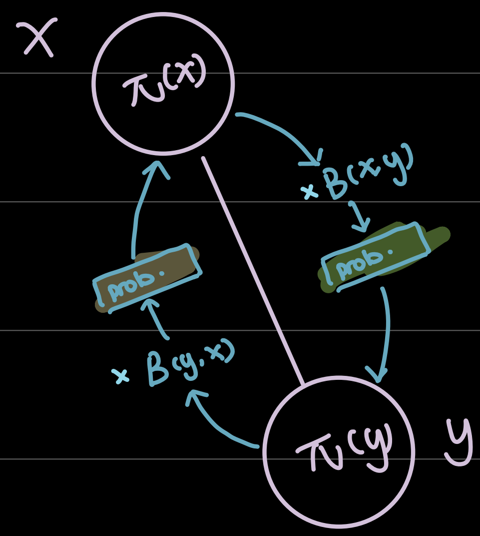
π

bad, unbalanced

Think of ▬ as a visa approval/rejection office

Extra-rejection probability

General:



Algorithm:

(1) If $\pi(x)B(x,y) > \pi(y)B(y,x)$

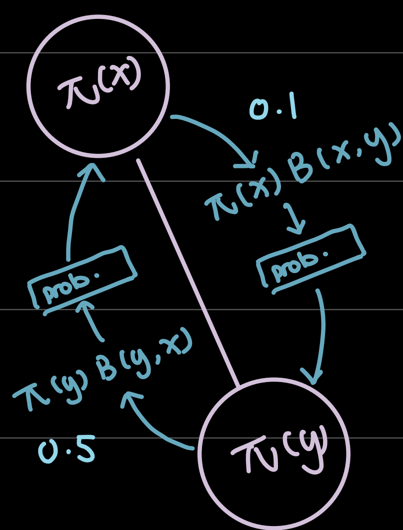
$$\text{prob(accept } x \to y) = \frac{\pi(y)B(y,x)}{\pi(x)B(x,y)}$$

(2) If $\pi(x)B(x,y) \leq \pi(y)B(y,x)$

$$\text{prob(accept } x \to y) = 1$$

(3) Combine (1), (2):

$$\text{prob(accept } x \to y) = \min\left(1, \frac{\pi(y)B(y,x)}{\pi(x)B(x,y)}\right)$$ *



$$X_t = x$$

$$X_{propose} \sim B(x,y) = P(X_{propose} = y \mid X_t = x)$$

let $X_{t+1} = \begin{cases} X_{propose} & \text{with } P = \min\left(1, \dfrac{\pi(y)B(y,x)}{\pi(x)B(x,y)}\right) \\ X_t = x & \text{with } 1-P \end{cases}$

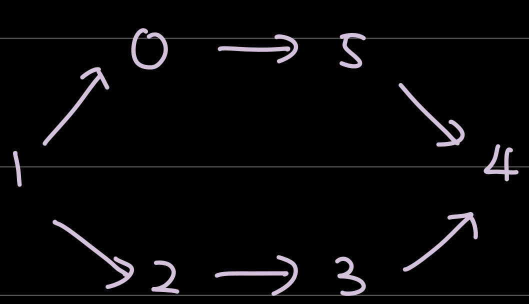
Special Case :

Metropolis algorithm : $B(x,y) = B(y,x)$

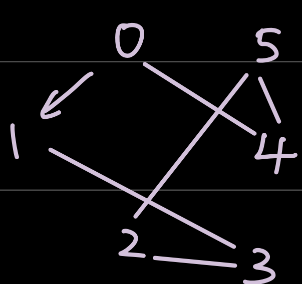
$$P = \min\left(1, \frac{\pi(y)}{\pi(x)}\right)$$

Hastings Extension : general B

Traveling Salesman Problem



X: path $0 \to 1 \to 2 \to 3 \to 4 \to 5 \to 0$



another X : $0 \to 1\,3\,2\,5\,4 \to 0$

$\mathcal{E}(x)$ = total length of path x.

$$\pi(x) = \frac{1}{Z} e^{-\mathcal{E}(x)}$$

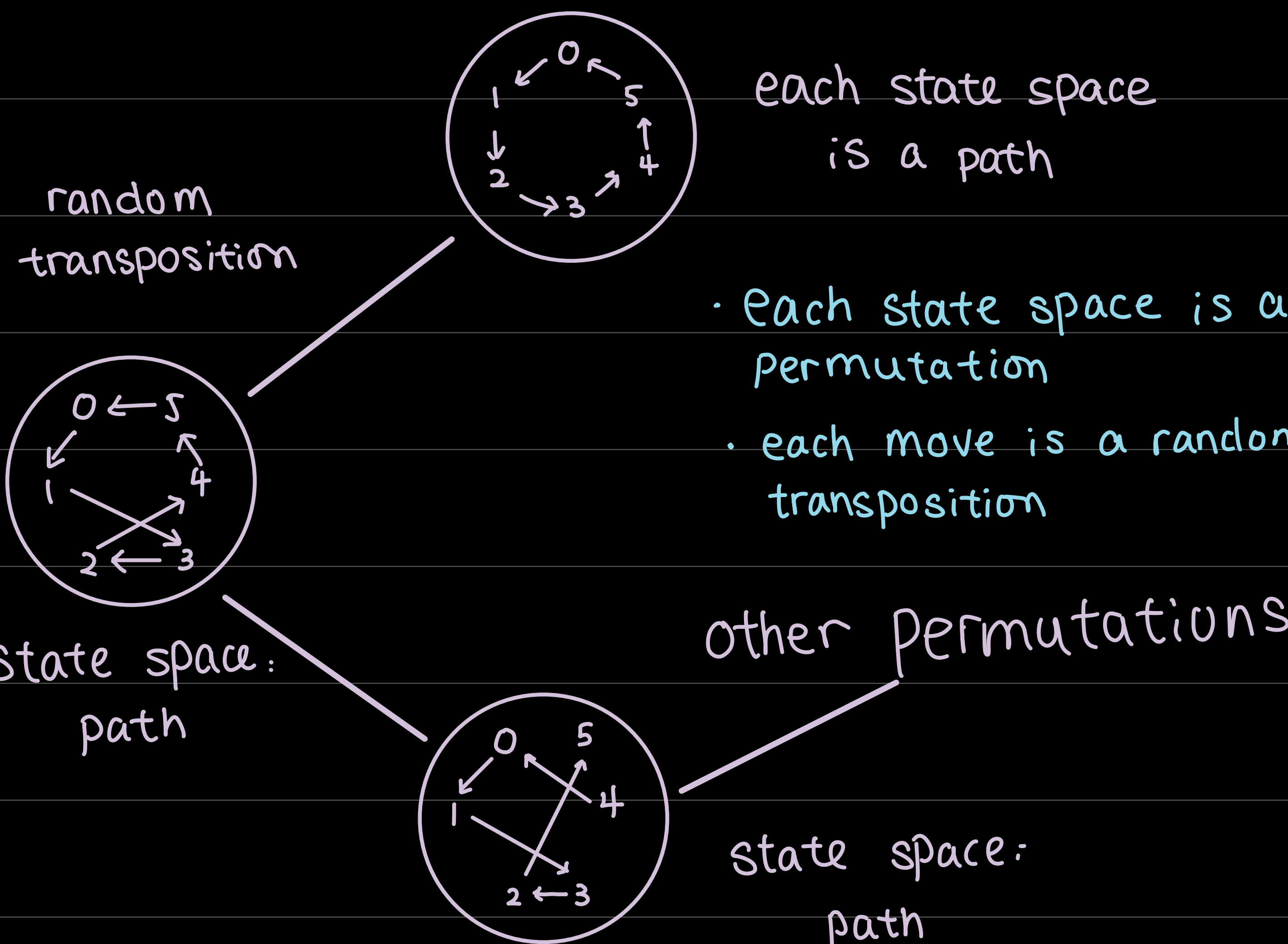
$$Z = \sum_x e^{-\mathcal{E}(x)}$$

Gibbs distribution / Boltzman distribution

Searching thru such huge space is extremely difficult

Sampling and optimization are related here

State space (n factorial)



- each state space is a permutation
- each move is a random transposition

Base Chain

x 1 2 3 4 5

$\downarrow$

y 1 4 3 2 5

1 4 2 3 5

⋮

Randomly pick 2 cities & exchange their positions, Propose change by random transposition.

accept change with

$$p = \min\left(1, \frac{\pi(y)}{\pi(x)}\right)$$

$$= \min\left(1, e^{\mathcal{E}(x) - \mathcal{E}(y)}\right)$$

here $\frac{1}{Z}$ gets cancelled

recall

$$\pi(-) = \frac{1}{Z} e^{-\mathcal{E}(\cdot)}$$

$$X_0 \longrightarrow X_1 \longrightarrow X_2 \longrightarrow X_3 \longrightarrow \cdots$$

(12345) (14325) (14235) (14235)

$\rightarrow X_{1000}$ we end up w/ a good permution

Approx: $X_{1000} \sim \pi(x)$