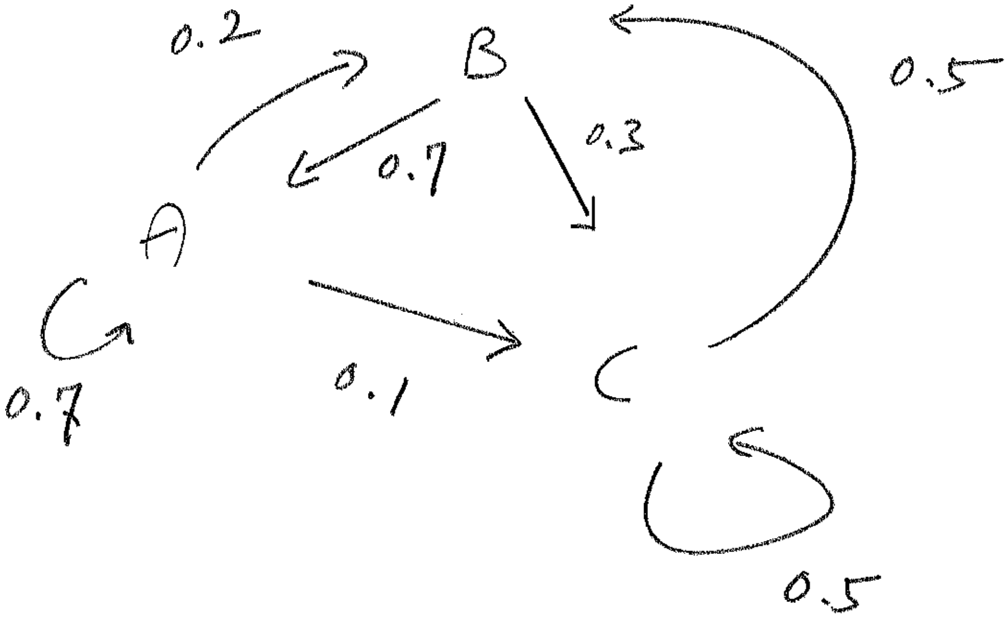
Markov Chain Monte Carlo



$$\underline{P} = \begin{bmatrix} 0.7 & 0.2 & 0.1 \\ 0.7 & 0 & 0.3 \\ 0 & 0.5 & 0.5 \end{bmatrix}$$

$\longrightarrow$ adds to 1

if we start from A

$$\vec{\pi}_1 = [1, 0, 0]$$

$\vec{\pi}_2 \rightarrow \vec{\pi}_1^{\,t} \, \underline{P}$ & keep going.

$$\pi_1 \rightarrow \pi_2 \rightarrow \pi_3 \rightarrow \cdots \underline{\pi_\infty}$$

$\longrightarrow$ Markov chain $\quad \hookrightarrow$ settles in Eq.

$$\vec{\pi}_\infty = \vec{\pi}_\infty \underline{P}$$

$\rightarrow$ (Left) eigenvectors.

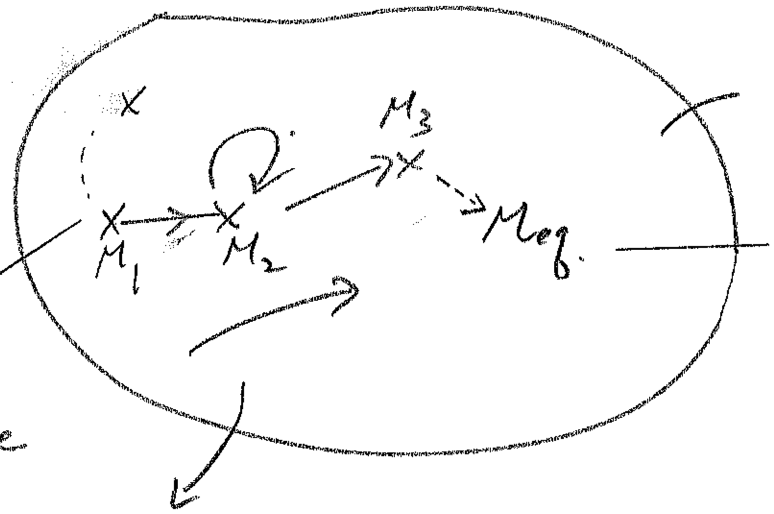
$\vec{\pi}_\infty$ can be obtained

by $\lambda_{\underline{P}^t} = 1$ for $\underline{P}^t$

the eigenvector $\leftrightarrow$ $\vec{\pi}_\infty$.

Generally

config. space.



can't solve for $\underline{P}$

equi prob. density $W(M)$.

start anywhere (ergodic)

Markov Chain : No memory

next step depends only on <u>current</u> state

Metropolis : (Koonin P. 212).

→ criteria to accept a new config :

$$M_1 \xrightarrow{?} M_2$$

W = prob. density

if $W(M_2) > W(M_1)$ → do it

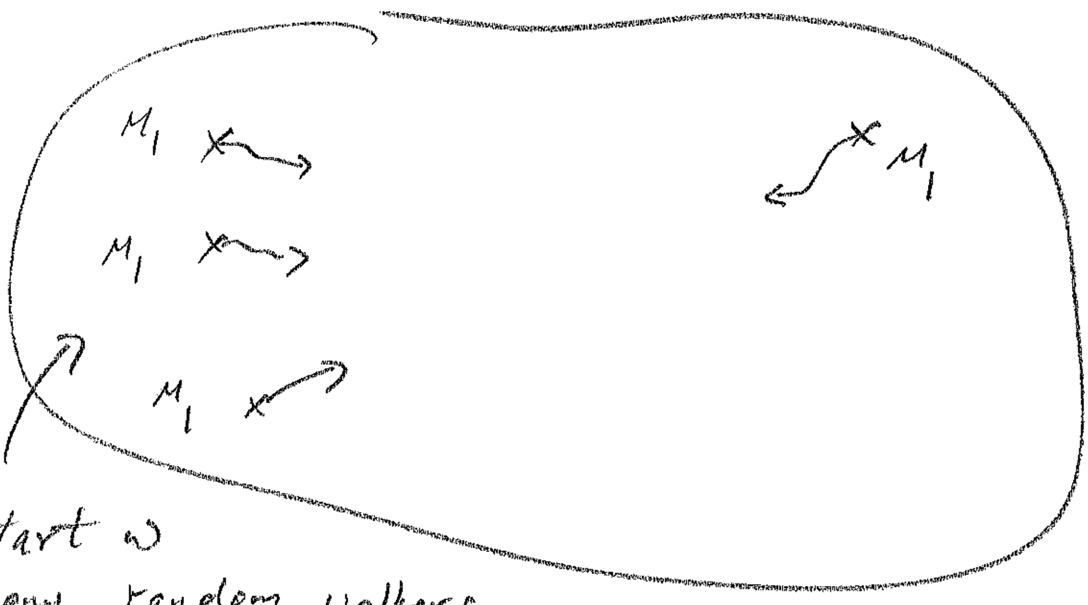
if $W(M_2) < W(M_1)$ → accept with prob. $r = \frac{W(M_2)}{W(M_1)}$

combining :

→ accept w prob

$$\min\left(1, \frac{W(M_2)}{W(M_1)}\right)$$

how this works ?



start w many random walkers

at n-th steps,

$N_n(M)$ = no. of walkers in M-state

$$\Delta N_n(M) = \underbrace{N_n(M') P_{M' \to M}}_{\text{immigrants}} - \underbrace{N_n(M) P_{M \to M'}}_{\text{leaving}}$$

the change in # of states in M at next step.

$$= N_n(M) P_{M' \to M} \times \left\{ \frac{N_n(M')}{N_n(M)} - \frac{P_{M \to M'}}{P_{M' \to M}} \right\}.$$

$\Delta N_n(M) = 0$

if $\dfrac{N_n(M')}{N_n(M)} = \dfrac{N_{eq}(M')}{N_{eq}(M)} = \dfrac{P_{M \to M'}}{P_{M' \to M}}$

if $N_n(M)$ is too large

or $N_n(M')$ too small

$\Delta N_n(M) < 0$ $\quad N_n(M)$ will $\downarrow$

& $N_n(M)$ too small $\rightarrow$ $N_n(M)$ will $\uparrow$

so the system will reach $\Delta N_n(M) = 0$

Now we know

$$N_n(M) \xrightarrow{\text{eventually}} N_{eq}(M)$$

but how do we know the prob. density?

$$N_{eq}(M) \leftrightarrow W(M) \quad ?$$

Metropolis's idea

$$P_{M \to M'} = \underbrace{T_{M \to M'}}_{\text{transition prob.}} \underbrace{A_{M \to M'}}_{\text{acceptance prob.}}$$

if nothing blocking

$$M \leftrightarrow M'$$

e.g. $M' = M + \delta$

$$T_{M \to M'} = T_{M' \to M}$$

$$\frac{P_{M \to M'}}{P_{M' \to M}} = \frac{T_{M \to M'} A_{M \to M'}}{T_{M' \to M} A_{M' \to M}} \to \frac{A_{M \to M'}}{A_{M' \to M}}$$

$$r = \frac{A_{M \to M'}}{A_{M' \to M}}$$

recall

$$A_{M \to M'} = \begin{cases} 1 & \text{if } W_{M'} > W_M \\ \frac{W_{M'}}{W_M} & \text{if } W_{M'} < W_M \end{cases}$$

$$r = \frac{1}{\frac{W_M}{W_{M'}}} \quad \text{if } W_{M'} > W_M$$

$$r = \frac{W_{M'}}{W_M} \quad \text{if } W_{M'} < W_M$$

$$r = \frac{W_{M'}}{W_M} \quad \text{in } \underline{\text{any}} \text{ case}$$

so the Metropolis rule will give

$$\frac{N_n(M')}{N_n(M)} \to r = \frac{W_{M'}}{W_M}$$

$$N_n(M) \propto W(M)$$

as required!

if $M \not\to M'$

e.g. w blocking

generally any T, A s.t.

$$\frac{T_{M\to M'}\, A_{M\to M'}}{T_{M'\to M}\, A_{M'\to M}} = \frac{W_{M'}}{W_M}$$

will work

Metropolis-Hastings

to the extreme:

$$T_{M\to M'} = W_{M'}$$

$A = 1 \longrightarrow$ accept them all

then $\dfrac{T_{M\to M'}}{T_{M'\to M}} = \dfrac{W_{M'}}{W_M}$

$\Rightarrow$ well, if we know $W(M)$ we would not need to do the sampling ...

Metropolis :

to decide whether to accept a change $M \to M'$

$$p = \min(1, r)$$

$$r = w_{M'}/w_M \quad \text{or} \quad r \propto w_{M'}$$

e.g. $w_M = e^{-\beta H[M]}$ in stat. mech.

$$r = \frac{e^{-\beta H[M']}}{e^{-\beta H[M]}}$$

$$\to e^{-\beta(\Delta H)}$$

In Ising Model

M' = flip the spin at site i

$$r = \frac{e^{-\beta H[\sigma_1 \sigma_2 \cdots \sigma_i = s, \cdots]}}{\sum_{s''} e^{-\beta H[\cdots \sigma_i = s'' \cdots]}}$$

nearest neighbor ...

but σ_i only talks to σ_{i-1} & σ_{i+1}

$$\rightarrow \frac{e^{[\beta J (\sigma_{i-1} + \sigma_{i+1}) s]}}{\sum_{s''} e^{\beta J s'' (\sigma_{i-1} + \sigma_{i+1})}}$$

staple

much simpler

$\sigma_{i-1} + \sigma_{i+1}$ can be

$$\left\{ \begin{matrix} -2 \\ 0 \\ 2 \end{matrix} \right\}$$

r :

speed things up.

given the trial s

$\rightarrow$ 3 outcome to decide.