Lecture #7 Dynamics

[redacted]

(1)

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(1) Discrete - time Markov chain

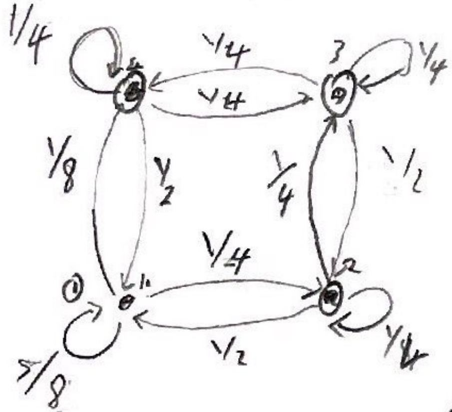
- Discrete time
- Discrete state
- Stochastic
- Markov

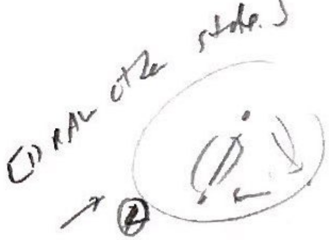
[Why - dynamics matter for Modern stat. Mech.]

[Reality complicated, QM, CM

- standard trick → use simplest model
- But have to check correct physics / biology / chem]

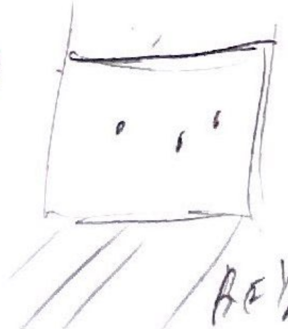
(3)





(4) Ergodic - [connected get anywhere from anywhere

(2)



Homogenious

$BE\, 1/k_BT$

[examples
MCMC
Ising Model
Random walk]

(5)

$$
M = \begin{array}{c|cccc}
\text{"out"} \backslash \text{"in"} & 1 & 2 & 3 & 4 \\
\hline
1 & 5/8 & 1/2 & 0 & 1/2 \\
2 & 1/4 & 1/4 & 1/2 & 0 \\
3 & 0 & 1/4 & 1/4 & 1/4 \\
4 & 1/8 & 0 & 1/4 & 1/4
\end{array}
$$

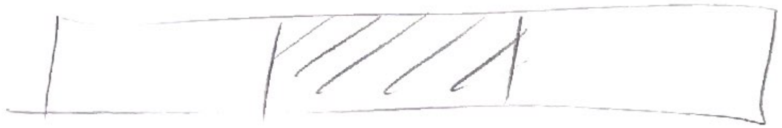
$P(i \to j) = M_{ji}$

Stochastic Matrix

$$P_{t+1}(x) = M\, P_t(x)$$

$$\sum_j M_{ji} = 1 \qquad \mathbb{1}^T M = \mathbb{1}^T$$

Complication



physics $\rho_{t+1}(x) = M \rho_t(x)$ column vector $\begin{pmatrix}\rho(1)\\ \rho(2)\\ \rho(3)\end{pmatrix}$

[But not all the time]

[But elsewhere] $\rho_t^T M^T = \rho_{t+1}^T$ Row vector $(\quad)$

[Why]? $|x'\rangle = U|x\rangle$

$\rho' = S\rho$

time $\longleftarrow$

$|x'\rangle = U_3 U_2 U_1 |x\rangle$

Could have Bras instead.

$\langle x| U_1^\dagger U_2^\dagger U_3^\dagger = \langle x'|$

But we didn't

[Last time] Data Processing Inequality

$X_t \to X_{t+1} \to X_{t+2}$ $\qquad S(X_t) \geq I(X_t : X_{t+1}) \geq I(X_t : X_{t+2})$

IT 2nd Law

$A_t \to A_{t+1} \to A_{t+2}$

$B_t \to B_{t+1} \to B_{t+2}$

[Same dynamics, M, different initial conditions]

$$D(A_t, A_{t+1} \| B_t, B_{t+1}) = D(A_t \| B_t) + \overbrace{D(A_{t+1} | A_t \| B_{t+1} | B_t)}^{0}$$

$$= D(A_{t+1} \| B_{t+1}) + \underbrace{D(A_t | A_{t+1} \| B_t | B_{t+1})}_{\geq 0}$$

Chain Rule
$S(A,B) = S(A) + S(B|A)$

Cottle Born

$$\sum_{x,y} P_A(x_{t+1}, x_t) \ln \frac{P_A(x_{t+1} | x_t)}{P_B(x_{t+1} | x_t)}$$

$$D(A_t \| B_t) \geq D(A_{t+1} \| B_{t+1})$$

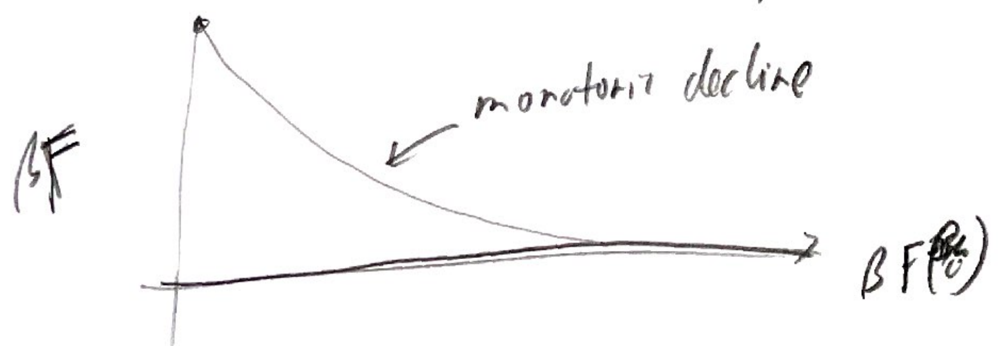
[Distribution converge] $M\pi = \pi$ $\quad \pi = \frac{e^{-\beta E}}{Z}$

$$\underline{\beta F^{ex}} = D(A_t \,\|\, \pi) \geq D(A_{t+1} \,\|\, \pi)$$

[Difference in F.E between $\beta(F^{neq} - F^{eq})$]

[All distribution converge monotonically to stationary distribution]

[If π is canonical, excess Free energy monotonically non-increasing]



3 representation

state
Ensemble
trajectory

MR & Detailed balance $\Longleftrightarrow$ Time Reversal Symmetric

5

state $x_t \to x_{t+1}$

Ensemble $P_{t+1}(x) = M P_t(x)$

Time Reversal

$X \to$

X $\quad x_1 \quad x_2 \quad x_3 \quad x_4 \quad \dots \quad x_t$

$\leftarrow \tilde{X}$ time reversed

start in π, stay in π

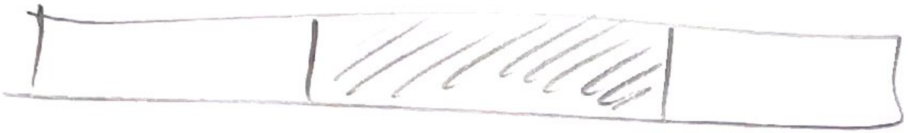
$M\pi = \pi \qquad \tilde{M}\pi = \pi$

$\pi_i \, m(i \to j) = \pi_j \, \tilde{m}(j \to i)$

$\tilde{M} = \mathrm{diag}(\pi) \, M^T \, \mathrm{diag}(\pi^{-1})$

Detailed Balance
Microscopic Reversibility
$\tilde{M} = M$ T.R.S

ornal Matrix
Detailed Balanced.



Is

$$\frac{\pi(2)}{\pi(1)} = \frac{P(1\to 2)}{P(2\to 1)} = \frac{1/4}{1/2} = 1/2$$

$$\frac{\pi(3)}{\pi(2)} = \frac{P(2\to 3)}{P(3\to 2)} = \frac{1/4}{1/2} = 1/2$$

$$\frac{\pi(4)}{\pi(3)} = \frac{P(3\to 4)}{P(4\to 3)} = \frac{1/4}{1/4} = 1$$

$$\frac{\pi(4)}{\pi(1)} = \frac{P(1\to 4)}{P(4\to 1)} = \frac{1/8}{1/2} = 1/4$$

$P(x) = (1/2,\ 1/4,\ 1/8,\ 1/8)$ ✓

Detailed Balanced

$\beta E(x) = x \ln 2$ $\quad P(x) \propto e^{-x\ln 2}$

$\propto 2^{-x}$

Markov Chain Monte Carlo

⑦

Slide

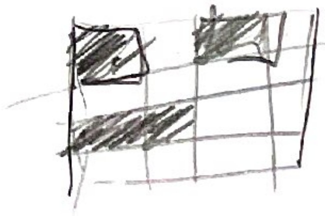
Metropolis came up with MC
room

Detailed balance $\Longrightarrow$ stationary distribution

$$M = \mathrm{diag}(p)\, M^T\, \mathrm{diag}(p^{-1})$$

$$M p = \underbrace{\mathrm{diag}(p)\, \underbrace{M^T\, \underbrace{\mathrm{diag}(p^{-1})\, p}_{\mathbb{1}}}_{\mathbb{1}}}_{p}$$

Markov Chain Monte Carlo

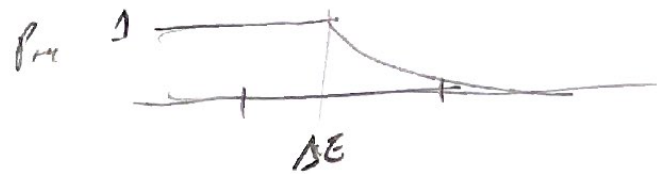


$\sigma = \pm 1$

$$E = -\sum_{\substack{\langle i j \rangle \\ \text{pairs } ij}} J_{ij}\, \sigma_i \sigma_j - \sum_j h_j \sigma_j$$

so (long as Move is D.B. w.r.t. to canonical distribution)

$$P_{acc} = \min\left(1, \frac{p(\sigma')}{p(\sigma)} = e^{-\beta \Delta E}\right)^{\sigma \to \sigma'}$$



"Heat Bath"

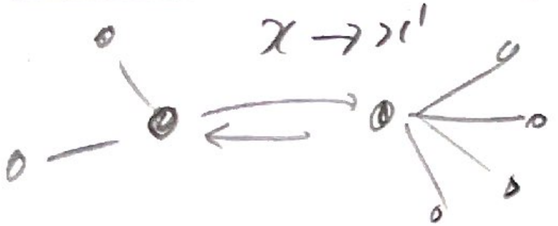
Gibbs/Glauber $$P(\sigma_i = +1) = \frac{e^{-\beta E(\sigma_i = +1)}}{e^{-\beta E(\sigma_i = +1)} + e^{-\beta E(\sigma_i = -1)}}$$

(Partition function cancels out!)

Complications

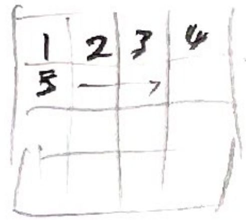
Metropolis-Hastings

$x \to x'$



$$P_{acc} = \min\left(1, \frac{P(x')}{P(x)} \frac{g(x|x')}{g(x'|x)}\right)$$

Ising

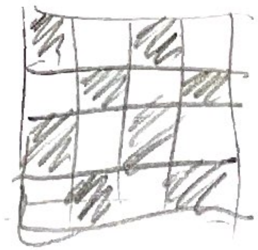


Typewriter update

[Detailed balance? No]

$\pi = M\pi$ Balanced

[Do I care? Maybe]



Checkerboard

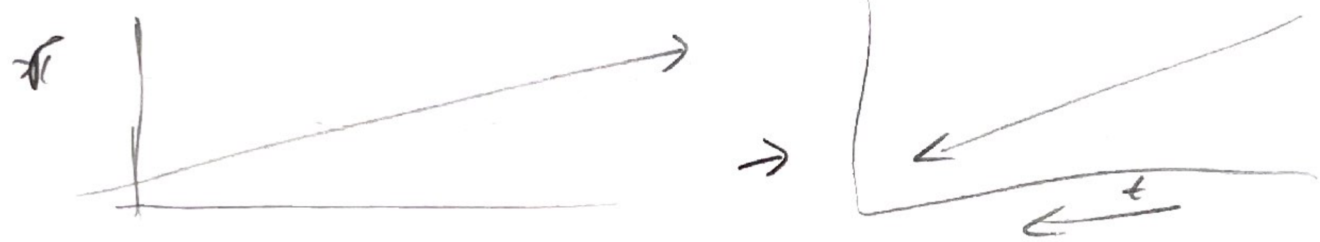
$\Rightarrow$ B W B W B W

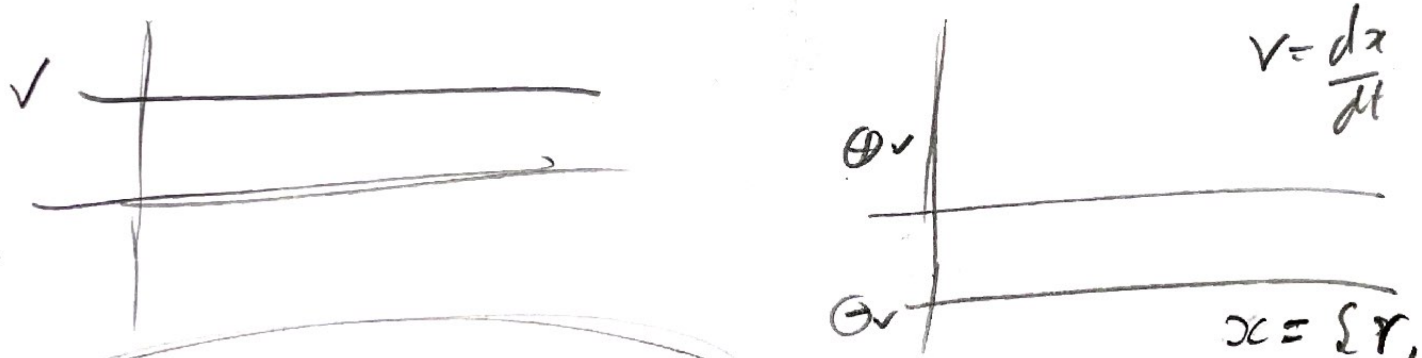
[Not DB]

$\rightarrow \underbrace{BWWB}_{t=1} \; \underbrace{BWWB}_{2} \; \underbrace{BWWB}_{3}$

Palindromic substeps

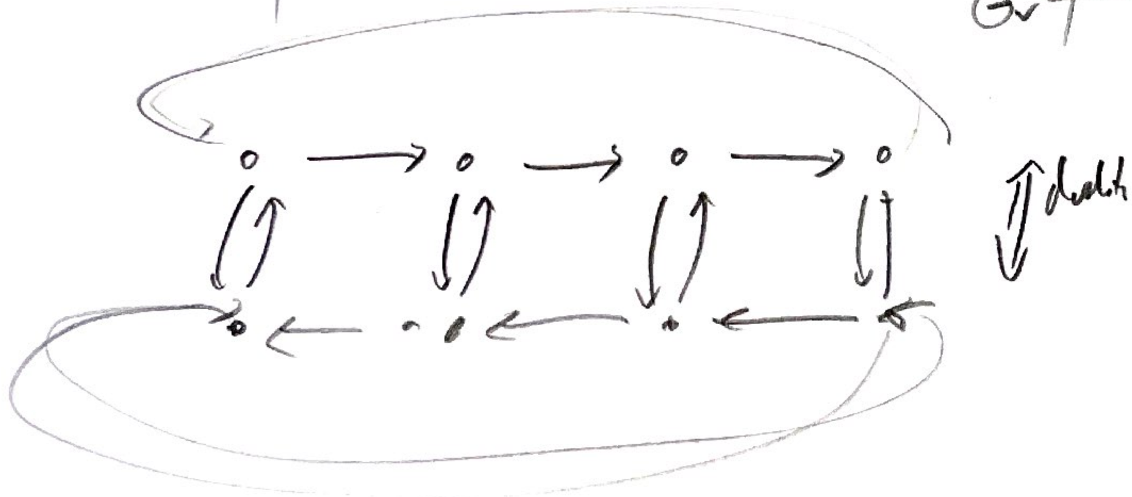
Velocity





$v = \frac{dx}{dt}$ (positive time)

$x = \{r, v\}$



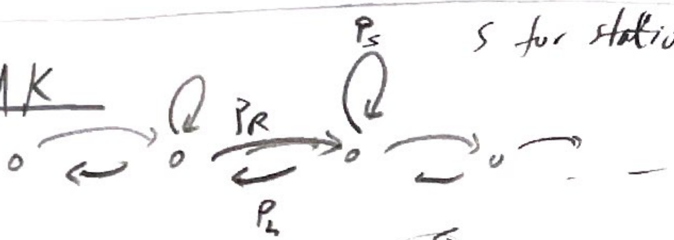
$x \to r$

$v \to -v$

$\hat{x} = \{r, -v\}$

~~Biased~~ A/L

Biased Random Walk



s for stationary

$$P_L + P_s + P_R = 1$$

t steps, $t = n_L + n_s + n_R$

(number of steps)

$$\begin{pmatrix} P_L & 0 & 0 & 0 \\ P_s & P_L & 0 & \\ P_R & P_s & P_L & \\ 0 & P_R & P_s & \\ & & P_R & \ddots \end{pmatrix}$$

or

$$P(n_R, n_c, n_L) = \binom{t}{n_L\, n_s\, n_R} P_L^{n_L} P_s^{n_s} P_R^{n_R}$$

trinomial coefficient

$$\binom{t}{n} = \frac{t!}{n!\,(t-n)!} \qquad \binom{t}{n_1, n_2, n_3} = \frac{(n_1+n_2+n_3)!}{n_1!\, n_2!\, n_3!}$$

Exact

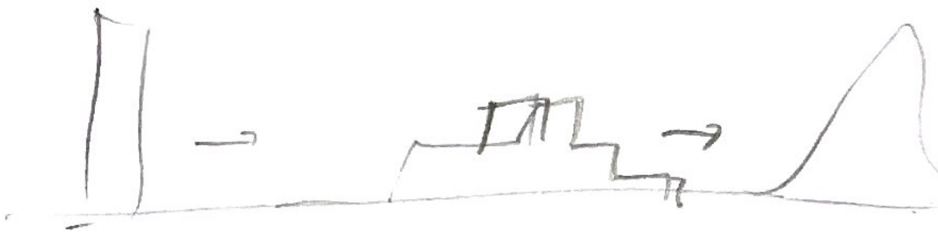
$$P(\Delta x) = \sum_{n_R=0}^{t} \sum_{n_L=0}^{t} \delta(n_R - n_L = \Delta x)\, P(n_R, \underbrace{n_s}_{t-n_R-n_L}, n_L)$$

A2

$$\langle n_R \rangle = t\, P_R$$

$$\mathrm{Var}[n_R] = t\, P_R (1 - P_R)$$

$$\mathrm{CoVar}[n_R, n_L) = t\, P_R P_L$$

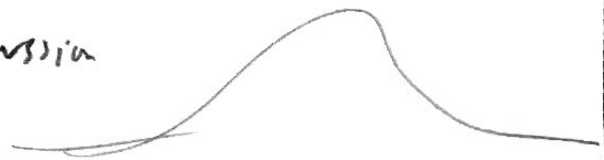


$$\langle \Delta x \rangle = \langle n_R \rangle - \langle n_L \rangle = t(P_R - P_L)$$

[look it up]

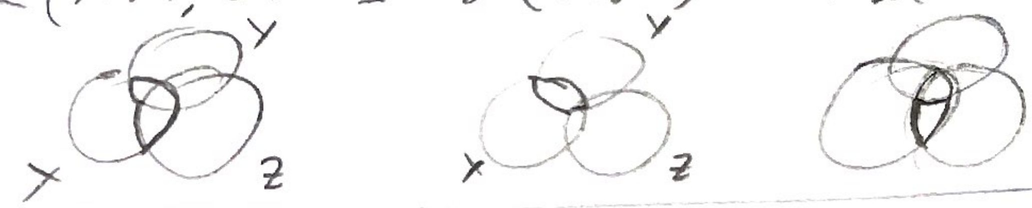
$$\mathrm{Var}(\Delta x) = \mathrm{Var}(n_R) + \mathrm{Var}(n_L) - 2\,\mathrm{CoVar}(n_R, n_L)$$

$$= t\left(P_R(1-P_R) + P_L(1-P_L) - 2 P_R P_L\right) \rightarrow \text{Gaussian}$$



$I(X:Y,Z) = I(X:Y) + I(X:Z|Y)$

Data Processing Inequality



extra

A3

Markov chain $X \to Y \to Z$

$p(x,y,z) = p(x)\,p(y|x)\,p(z|y)$ ← not $p(z|x,y) = p(z|y)$

$S(X) \geq I(X:Y) \geq I(X:Z)$

$I(X:Y,Z) = I(X:Z) + I(X:Y|Z)^{\geq 0}$

$= I(X:Y) + I(X:Z|Y) \to 0$ conditionally independent

Self information $I(X:X) = \sum \overset{P(x)}{P(x,x)} \ln \frac{P(x \text{ and } x)}{P(x)\,P(x)} \leftarrow P(x) = -\sum P(x) \log P(x)$