Lecture 17

Recall from last lecture...

- Integrals can be evaluated using Monte Carlo algorithms ...

$$\langle |m| \rangle = \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \cdots \sum_{S_N=\pm 1} \frac{e^{-\beta E(S_1, S_2, \ldots S_N)}}{Q(\beta, h)} \left| \frac{1}{N} \sum_i S_i \right|$$

Sum/integrate out 1st spin

- Randomly pick ± 1 for each S_i (Uniformly)
- Compute a weighted average of the samples, giving each spin configuration a weight of:

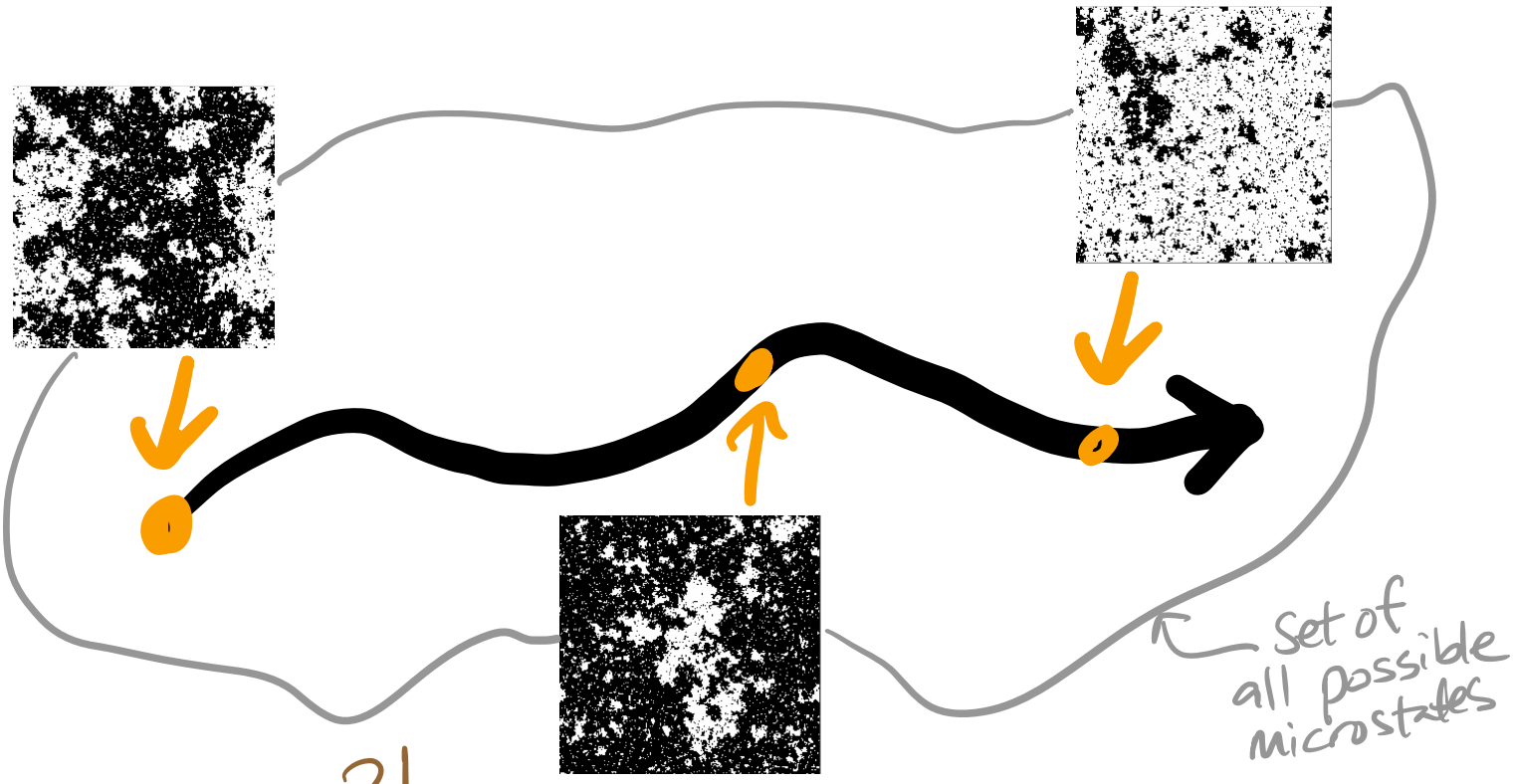
$$\frac{e^{-\beta E(S_1, S_2, \ldots S_N)} \left| \frac{1}{N} \sum_i S_i \right|}{Q(\beta, h)}$$

Unfortunately this scheme requires that we already know $Q(\beta, h)$ if we want to give the proper weight to each sample.

Viewed differently, we could think of drawing samples from the canonical (rather than uniform) distribution and giving them a simpler weight.

How should we sample spin configurations from the canonical ensemble?

Use Dynamics!

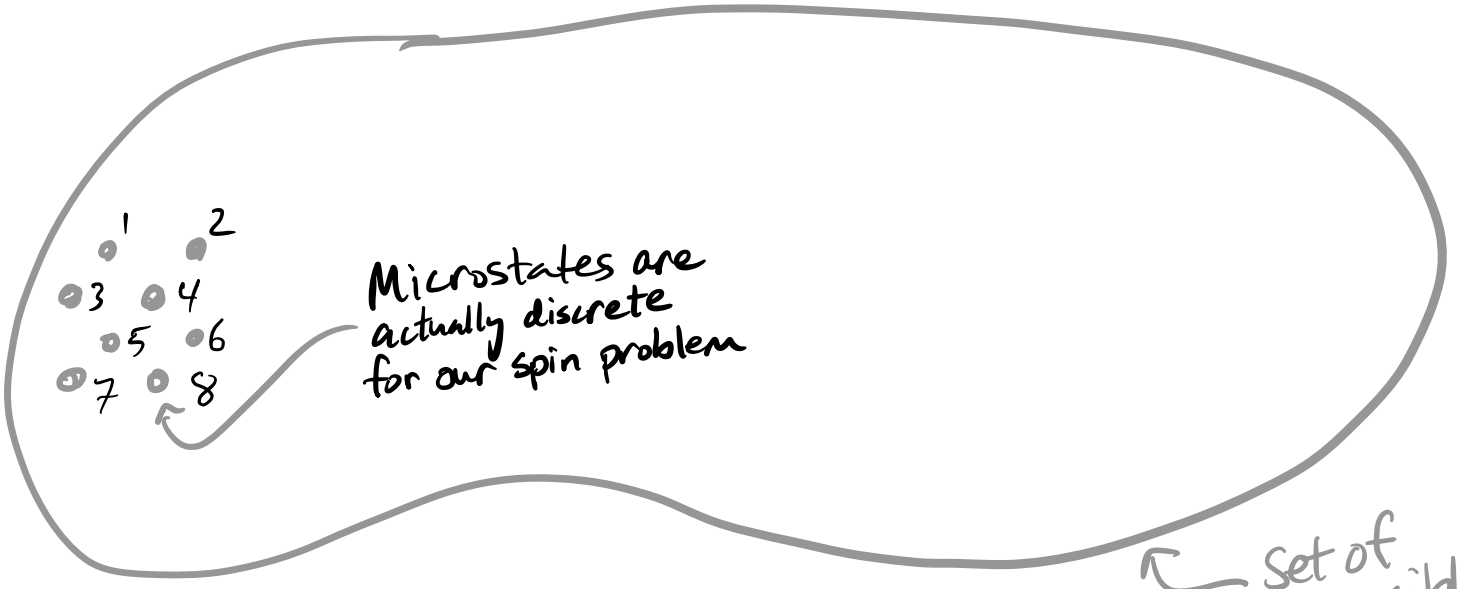


?!

We will make up a dynamics (a set of rules for how to transition from one configuration to another), constructed for the sole purpose of visiting the various microstates with probability $e^{-\beta E}/Q$

Even though the number of possible microstates is HUGE, I can still define a time-dependent vector which records the probability of each ν at time t.

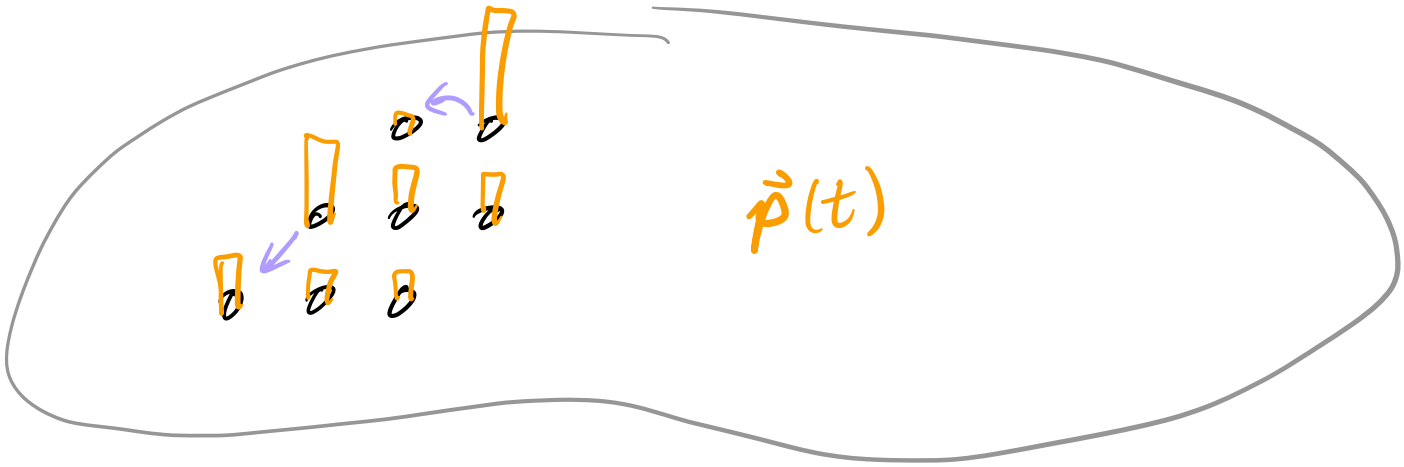
(I could never practically write down the whole vector)

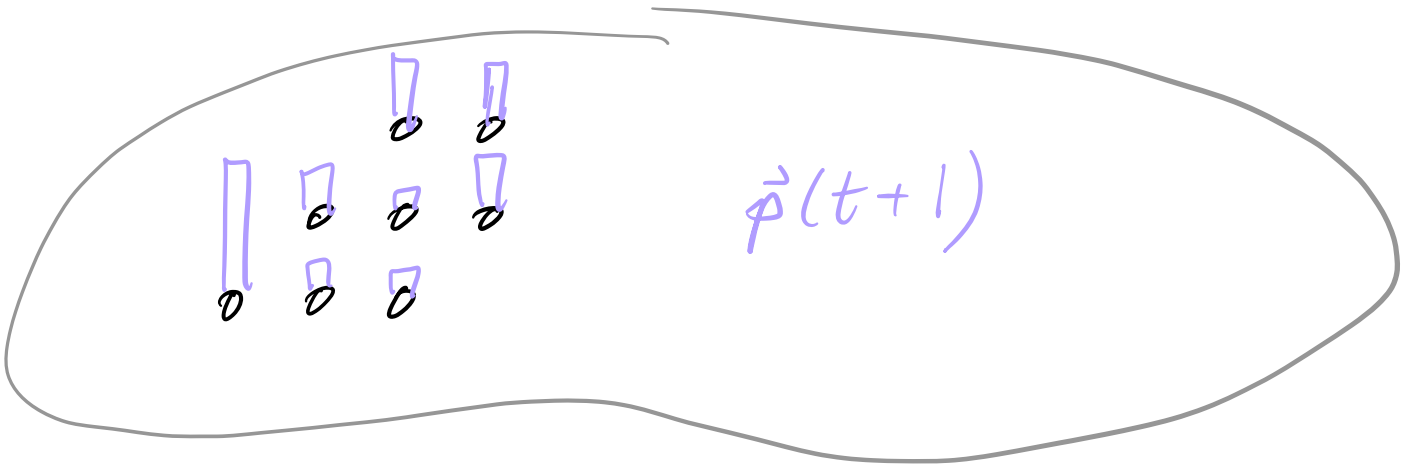


$$\vec{p}(t) = \begin{pmatrix} p(1,t) \\ p(2,t) \\ p(3,t) \\ \vdots \\ p(L^2,t) \end{pmatrix}$$

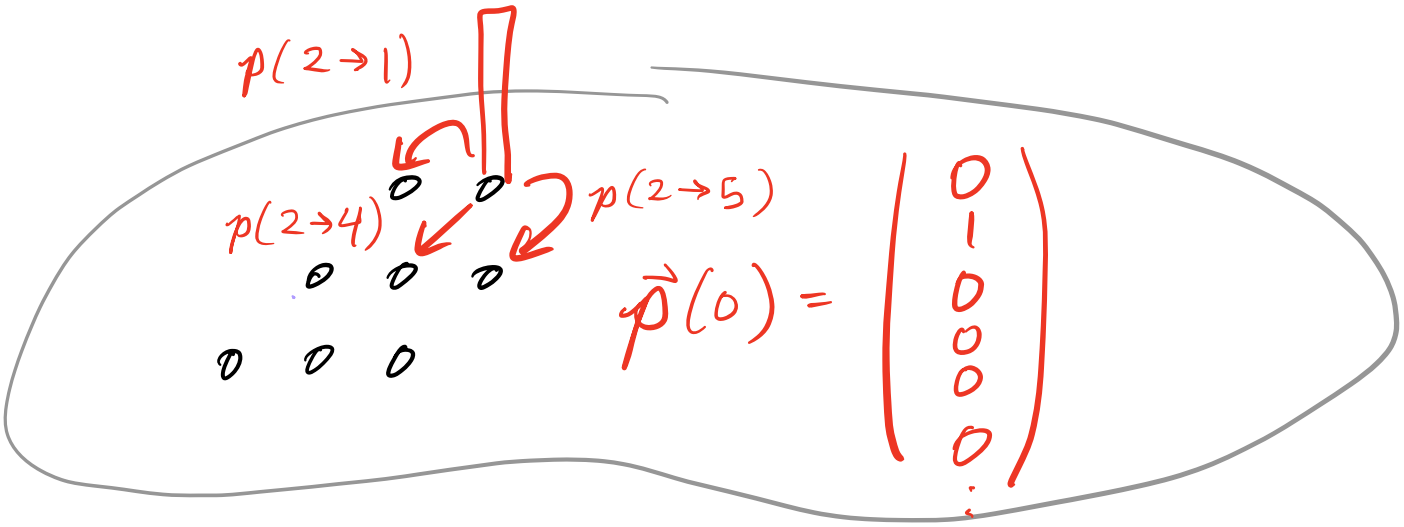
Probability of microstate #1 @ time t.

After one step of dynamics, what is $\vec{p}(t+1)$?


$\vec{p}(t)$


$\vec{p}(t+1)$

Easier to think through if we had started in a specific state.

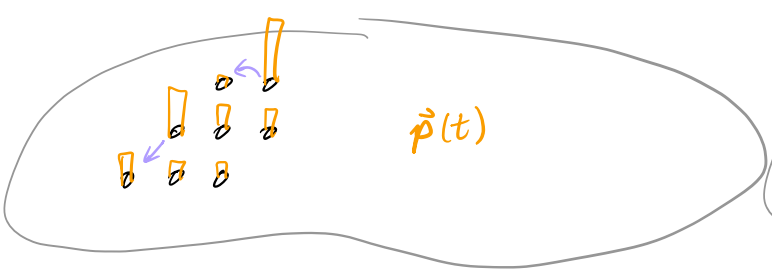


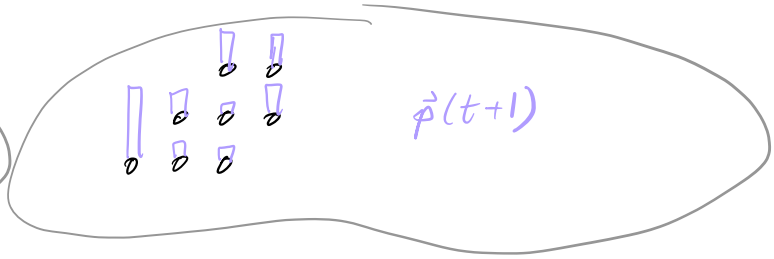
a coordinate vector with a 1 in the row corresponding to the initial microstate

$$\vec{p}(1) = \begin{pmatrix} p(2\to 1) \\ p(2\to 2) \\ p(2\to 3) \\ \vdots \end{pmatrix}$$

Can you go from any state to any state?

[In principle yes, for our Ising MC, we will choose $p(i\to j) = 0$ unless $i \neq j$ differ by a single spin flip.]





$$\vec{p}(t+1) = p(1,t)\begin{pmatrix} p(1\to 1) \\ p(1\to 2) \\ p(1\to 3) \\ \vdots \end{pmatrix} + p(2,t)\begin{pmatrix} p(2\to 1) \\ p(2\to 2) \\ p(2\to 3) \\ \vdots \end{pmatrix} + \dots$$

$$= \begin{pmatrix} p(1\to 1) & p(2\to 1) & \dots \\ p(1\to 2) & p(2\to 2) & \\ \vdots & & \ddots \end{pmatrix} \vec{p}(t)$$

Call this matrix of all transition probabilities the "transition matrix" T.

T defines the dynamics. It tells how probability evolves in time.

$$\vec{p}(t+1) = T\,\vec{p}(t)$$

$$\vec{p}(t+n) = T^n\,\vec{p}(t)$$

(n steps)

Our goal was to design a dynamics such that

$$\lim_{t\to\infty} \vec{p}(t) = \frac{1}{Q}\begin{pmatrix} e^{-\beta E(v_1)} \\ e^{-\beta E(v_2)} \\ \vdots \end{pmatrix} \equiv \vec{\pi}$$

$\vec{\pi}$ is a stationary distribution (not a function of time).
Once you reach $\vec{\pi}$, more time steps don't change the probability distribution.

$\Rightarrow$ Our dynamics must satisfy

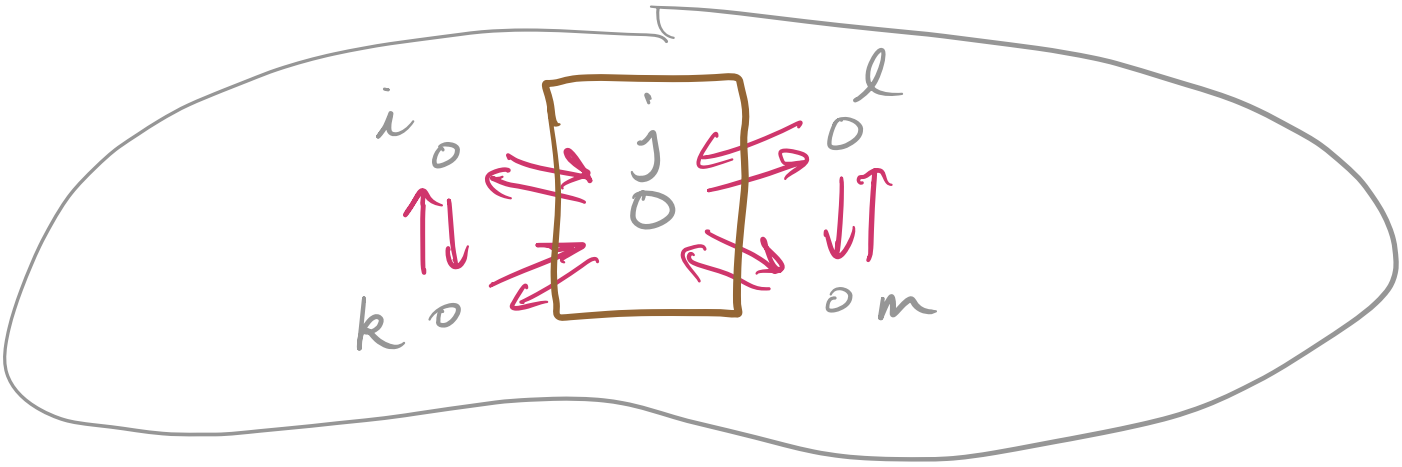
$$T\vec{\pi} = \vec{\pi}$$

Balance Condition

Result of another step of dynamics

Exactly the same distribution we started with

Why must T satisfy that balance condition?



The total probability of leaving site j:

$$\pi(j)\left(p(j\to l)+p(j\to m)+\dots\right)$$

out flows

must balance with the total probability entering j:

$$\pi(l)\,p(l\to j)+\pi(m)\,p(m\to j)+\dots$$

in flows

If the in-flows + out-flows did not balance then the probability of j would change from one time to the next.

$$\vec{p}(0) = \vec{\pi} + \vec{\Delta}$$ ← deviation from steady state

$$\vec{p}(1) = T\left(\vec{\pi} + \vec{\Delta}\right) = \vec{\pi} + T\vec{\Delta}$$

$$\vec{p}(n) = T^n\left(\vec{\pi} + \vec{\Delta}\right) = \vec{\pi} + T^n\vec{\Delta}$$

One way (not the only way) to ensure balance is to require that every pair of states is balanced

$\Longrightarrow$ Right flow $= \pi(i)\,p(i \to j)$ prob. site i is losing to go into j

$\Longleftarrow$ Left flow $= \pi(j)\,p(j \to i)$

Forcing every pair to be balanced is called "detailed balance". It is a stronger condition that implies "global balance" ($T\vec{\pi} = \vec{\pi}$)

For every pair of configurations $i \neq j$, we need a rule for picking $p(i \to j)$ & $p(j \to i)$ such that...

$$\pi(i)\, p(i \to j) = \pi(j)\, p(j \to i)$$

$$\Rightarrow \quad \frac{p(j \to i)}{p(i \to j)} = \frac{\pi(i)}{\pi(j)} = \frac{e^{-\beta E(i)} / \cancel{Q}}{e^{-\beta E(j)} / \cancel{Q}}$$

$$= e^{-\beta [E(i) - E(j)]}$$

The partition function has dropped out!

An obvious choice...

$$p(j \to i) = e^{-\beta E(i)} \quad \& \quad p(i \to j) = e^{-\beta E(j)} \qquad (*)$$

This would satisfy $\dfrac{p(j \to i)}{p(i \to j)} = e^{-\beta [E(i) - E(j)]}$

but there is a problem.

Problem? We require that

$$\sum_j p(i \to j) = 1 \qquad \text{(Normalization)}$$

Given you start in i, you must go to some new configuration

But, there is another way!

Conceptually, we split $p(i \to j)$ into two:

1. Propose a new j with some probability you pick

$$p_{gen}(i \to j): \text{ generation probability}$$

2. Decide to accept or reject that proposal with probability $p_{acc}(i \to j)$. If you reject, stay in i.

To transition from $i \to j$, you must <u>both</u> generate $i \to j$ <u>and</u> accept that $i \to j$, so

$$p(i \to j) = p_{gen}(i \to j)\, p_{acc}(i \to j)$$

$P_{gen}(i \to j)$ can be almost anything you want,
but then $P_{acc}(i \to j)$ must be constructed accordingly
so detailed balance will hold:

$$\pi(i)\, P_{gen}(i \to j)\, P_{acc}(i \to j) = \pi(j)\, P_{gen}(j \to i)\, P_{acc}(j \to i)$$

$$\Rightarrow \frac{P_{acc}(i \to j)}{P_{acc}(j \to i)} = \frac{\pi(j)\, P_{gen}(j \to i)}{\pi(i)\, P_{gen}(i \to j)}$$

There are many ways to choose such a P_{acc}.
The Metropolis and Glauber criteria are the most popular.

Metropolis:

$$P_{acc}(i \to j) = \min\left[1, \frac{\pi(j)\, P_{gen}(j \to i)}{\pi(i)\, P_{gen}(i \to j)}\right]$$

$$P_{acc}(j \to i) = \min\left[1, \frac{\pi(i)\, P_{gen}(i \to j)}{\pi(j)\, P_{gen}(j \to i)}\right]$$

To confirm that Metropolis satisfies detailed balance, it is useful to split into 3 cases.

$$\frac{\min\left[1, \frac{\pi(j)\, P_{gen}(j \to i)}{\pi(i)\, P_{gen}(i \to j)}\right]}{\min\left[1, \frac{\pi(i)\, P_{gen}(i \to j)}{\pi(j)\, P_{gen}(j \to i)}\right]} \stackrel{?}{=} \frac{\pi(j)\, P_{gen}(j \to i)}{\pi(i)\, P_{gen}(i \to j)}$$

$$\pi(i)\, P_{gen}(i \to j)\, P_{acc}(i \to j) \boxed{\stackrel{?}{=}} \pi(j)\, P_{gen}(j \to i)\, P_{acc}(j \to i)$$

↑ Check this for metropolis

$$\Downarrow$$

$$\pi(i)\, P_{gen}(i \to j) \min\left[1, \frac{\pi(j)\, P_{gen}(j \to i)}{\pi(i)\, P_{gen}(i \to j)}\right] =$$

$$\pi(j)\, P_{gen}(j \to i) \min\left[1, \frac{\pi(i)\, P_{gen}(i \to j)}{\pi(j)\, P_{gen}(j \to i)}\right]$$

Case 1: $\pi(i)\, P_{gen}(i \to j) < \pi(j)\, P_{gen}(j \to i)$

$$\pi(i)\, P_{gen}(i \to j)\ 1 = \pi(j)\, P_{gen}(j \to i)\, \frac{\pi(i)\, P_{gen}(i \to j)}{\pi(j)\, P_{gen}(j \to i)}$$

Case 2: $\pi(i) p_{gen}(i \to j) > \pi(j) p_{gen}(j \to i)$ ✓

Case 3: $\pi(i) p_{gen}(i \to j) = \pi(j) p_{gen}(j \to i)$ ✓