Lecture 18

Recall from last lecture...

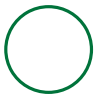
Counting by sampling?!

Claim: $\langle |m| \rangle$ is really a high-dimensional sum/integral

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

sum/integrate out 1st spin

Let's first think about a lower dimensional integral. What is the area of a circle with diameter one?



$$\text{Area} = \frac{\pi}{4}$$

Why is that an integral?

$$\text{Area} = \int_{-\frac{1}{2}}^{\frac{1}{2}} dx \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} dy \; 1$$

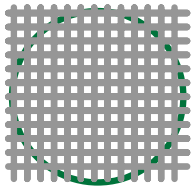
These integrals are summing over all the possible points in the circle

Hm... This is a lot like our microcanonical calculations in that every possible state (x,y) gets equal weight. Then Area is like a microcanonical partition function.

As continuous variables, you can never list out all of the possible values of x & y.
To get the value of the integral, we need either:

(A) to count with more complicated mathematical tools
calculus, geometry

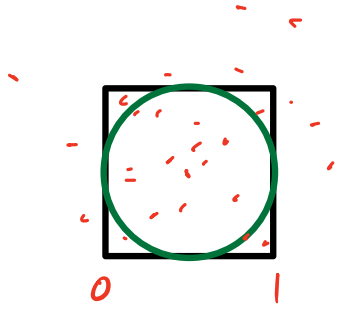
(B) to count by numerically approximating the integral



Break it up into boxes and count the boxes — a Reimann sum. Answer gets more correct as grid size $\to 0$.

But there is another way...

Throw darts. Monte Carlo



Throw darts in the square and count the fraction that land in the circle.

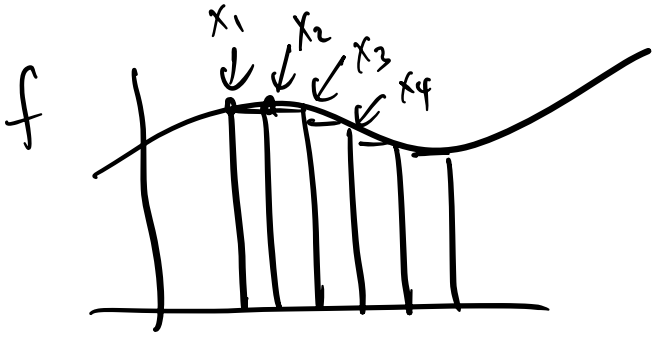
- Randomly draw x coordinate from $U[0,1)$
- Randomly draw y coordinate from $U[0,1)$
- Check if $x^2+y^2 \leq 1$.

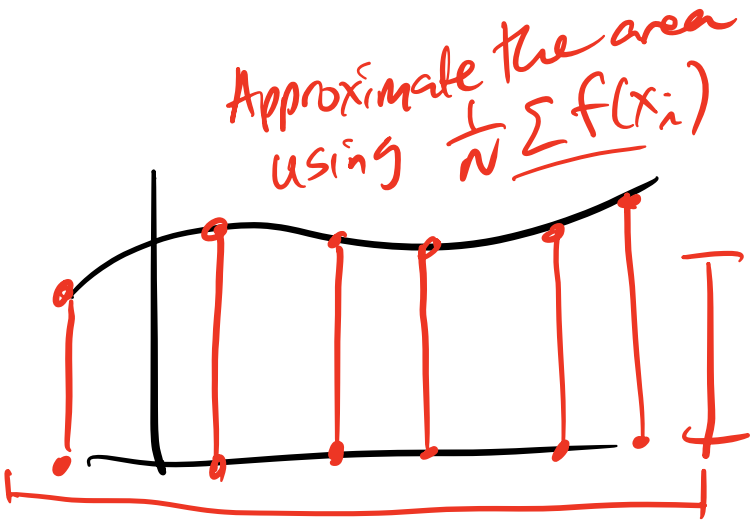
$$\lim_{\#\text{ of darts}\to\infty}(\text{fraction in circle}) = \frac{\pi}{4}$$

Reliance on random numbers ⇒ "Monte Carlo" (MC)

Why use MC in lieu of a grid?

Scaling with dimensionality.
Beyond 2 or 3 dimensions, grids get very expensive





MC is easily adaptable if we want to compute some other integral.

$$\text{Area} = \int_{-\frac{1}{2}}^{\frac{1}{2}} dx \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} dy \; 1$$

$$\langle x^2 \rangle = \int_{-\frac{1}{2}}^{\frac{1}{2}} dx \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} dy \; x^2 \Big/ \text{Area}$$

Throw darts

- Randomly draw x coordinate from $U[0,1)$
- Randomly draw y coordinate from $U[0,1)$
- If $x^2+y^2 \leq 1$, add (x,y) to a list

Weighted Average

- $\langle x^2 \rangle = \frac{1}{N}\sum x_i^2$ from that list

- 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:

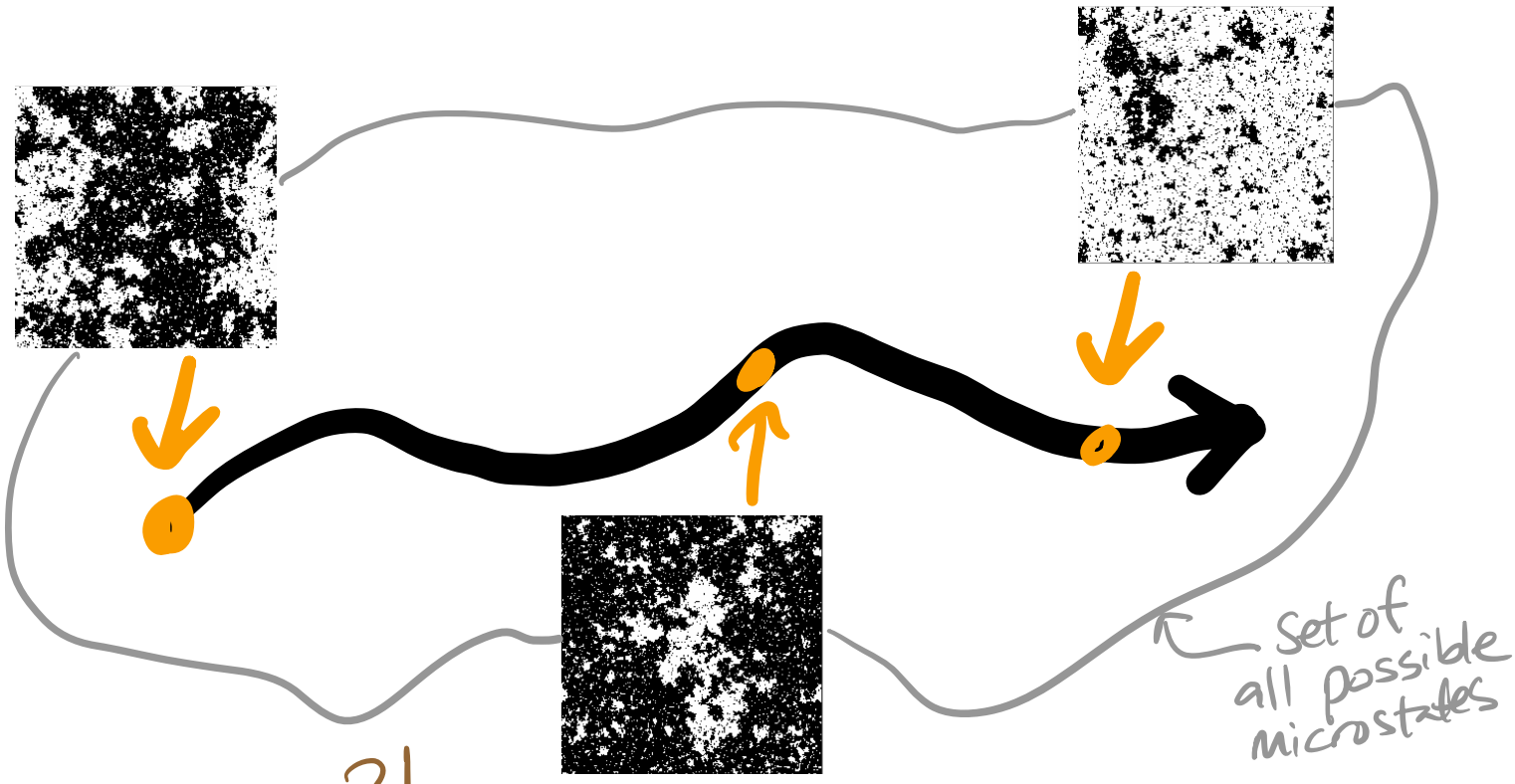
$$\frac{e^{-\beta E(S_1, S_2, \ldots S_N)} \left| \frac{1}{N} \sum_i S_i \right|}{Q(\beta, h)}$$

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!

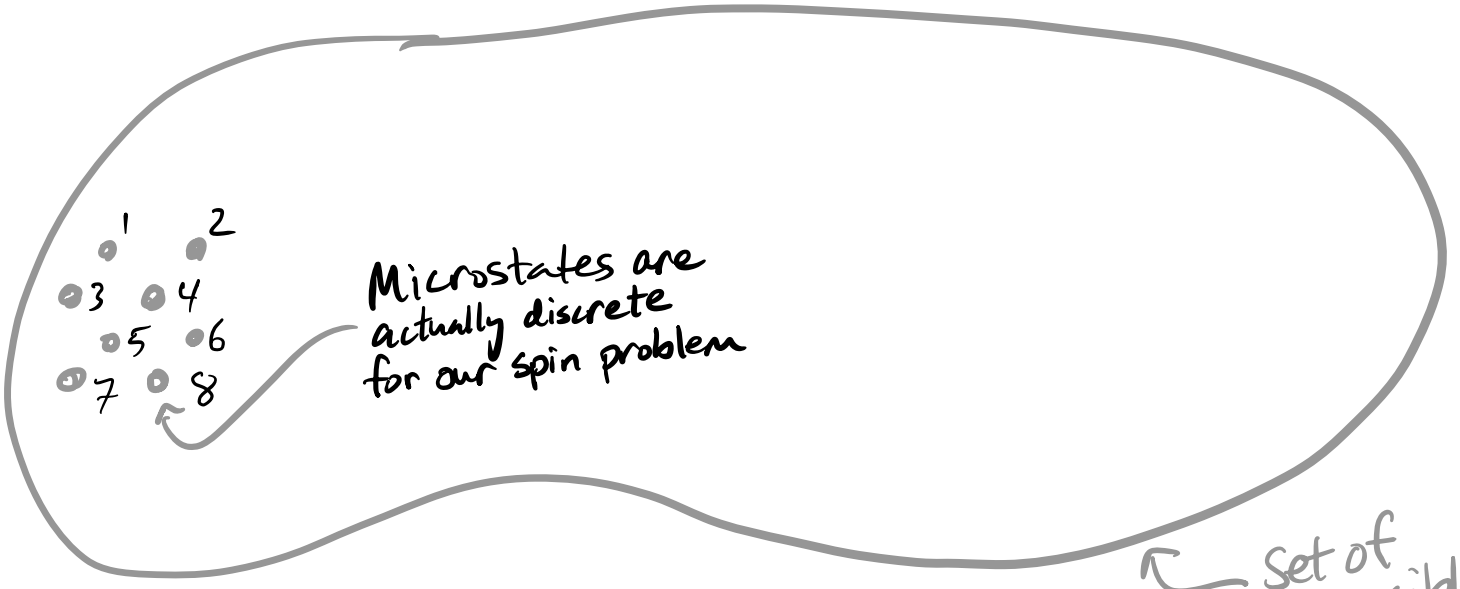


?!

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.

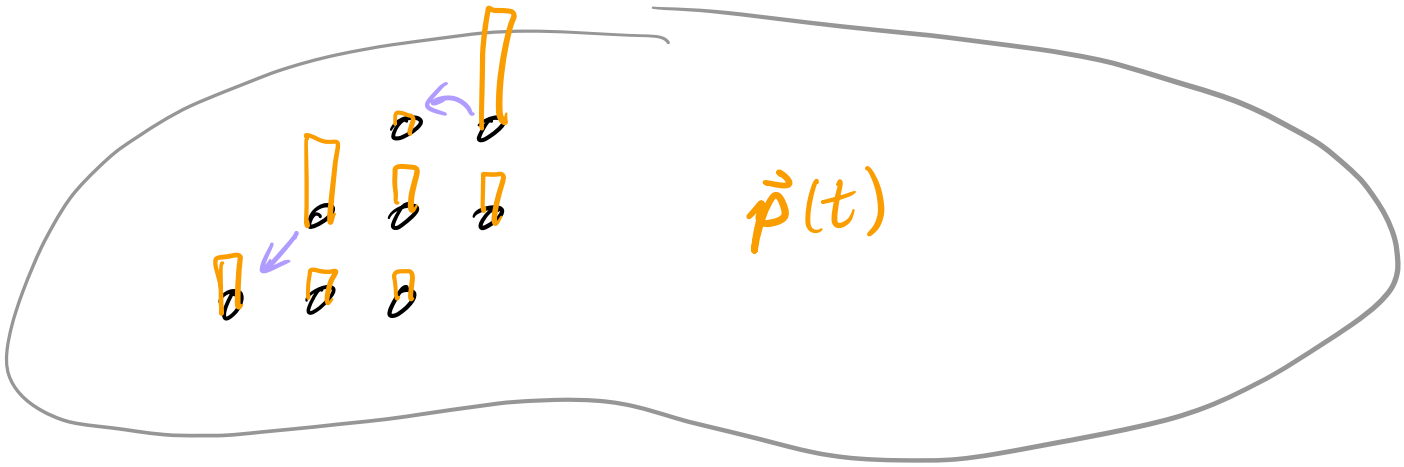
(I could never practically write down the whole vector)

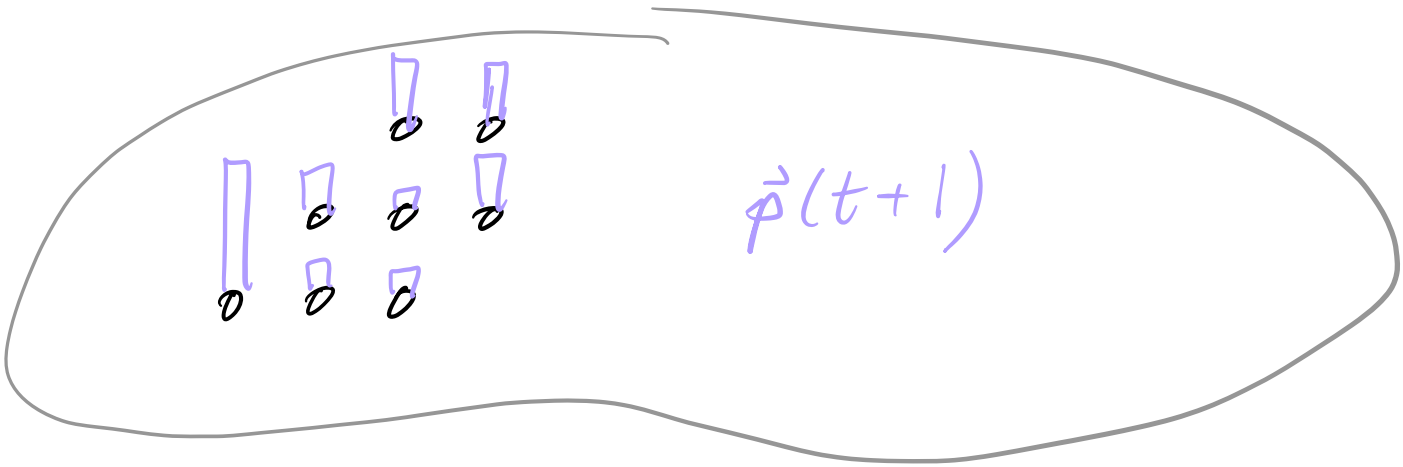


$$\vec{p}(t) = \begin{pmatrix} p(1,t) \\ p(2,t) \\ p(3,t) \\ \vdots \\ p(L^2,t) \end{pmatrix}$$

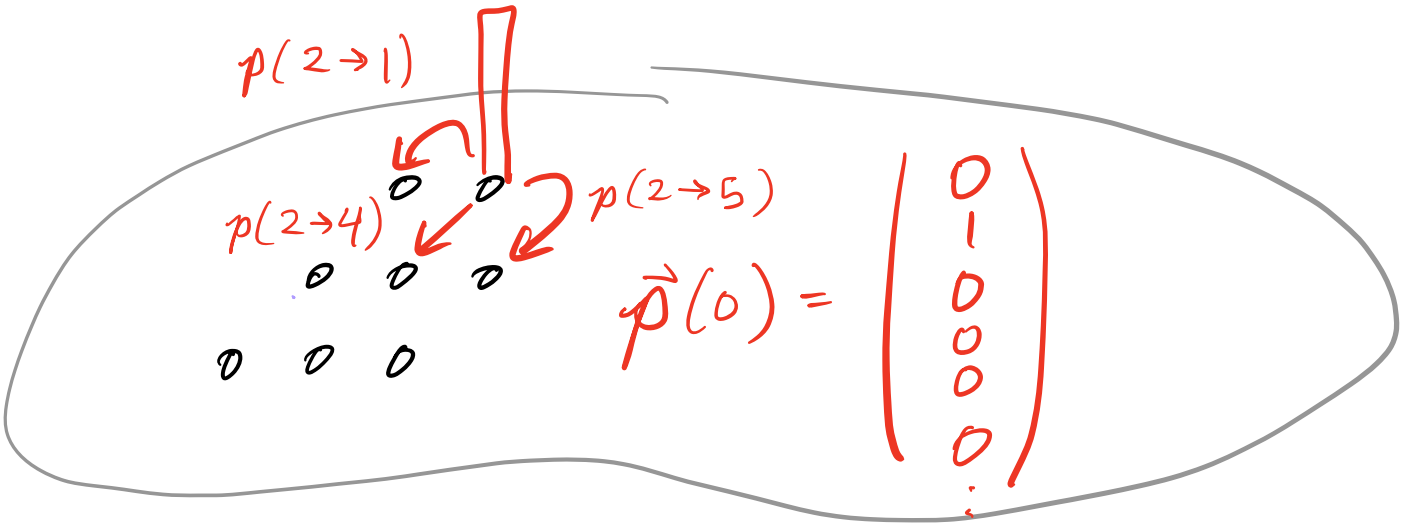
Probability of microstate #1 @ time t.

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.

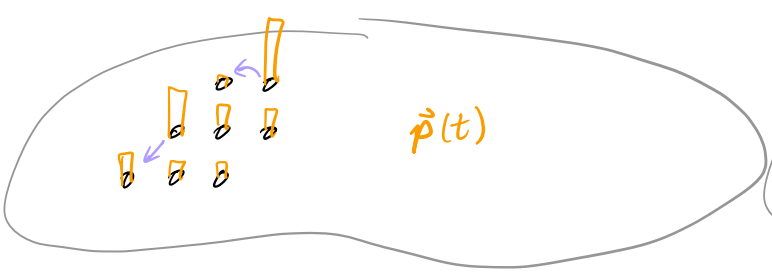


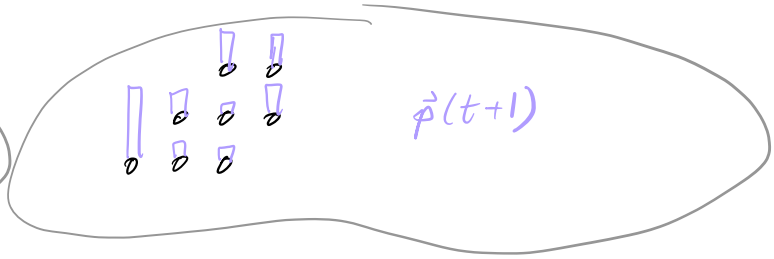
a coordinate vector with a 1 in the row corresponding to the initial microstate

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

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

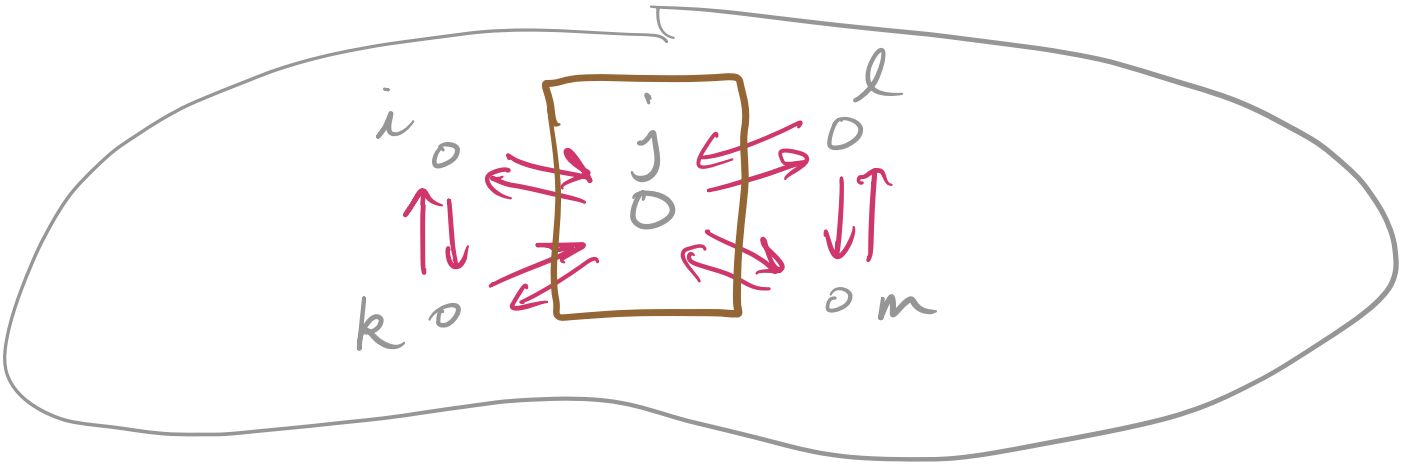
$$T\vec{\pi} = \vec{\pi}$$

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