Recap:

We have a very high-dimensional space

ex: $\vec{S} = \{S_1, S_2, \ldots, S_N\}$

S_1: state of spin 1 (± 1)

So the number of microstates is HUGE — we could never practically enumerate them all.

We are interested in the mean value of an order parameter, which is a function of $\vec{S}$, in this case $|M|(\vec{S})$

For any sample of possible spin configurations, $\vec{S}^{(1)} = \{S_1^{(1)}, S_2^{(1)}, S_3^{(1)}, \ldots S_N^{(1)}\}$ (sample #1.),
it is trivial to compute $M^{(1)} = \sum_i S_i^{(1)}$, but it is not trivial to compute

$\langle |M| \rangle$, the average over all possible spin configurations.

If we could generate p independent samples $\vec{S}^{(1)}, \vec{S}^{(2)}, \ldots \vec{S}^{(p)}$, we could approximate the expectation value by

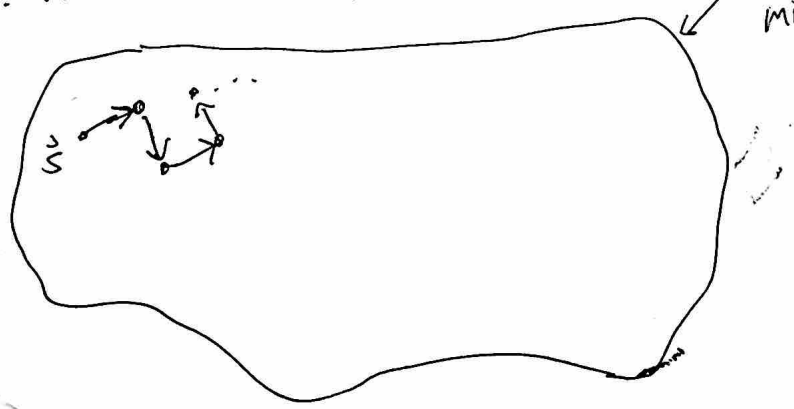
$$\langle |M| \rangle \approx \left[|M|(\vec{S}^{(1)}) + |M|(\vec{S}^{(2)}) + \ldots + |M|(\vec{S}^{(p)}) \right] \frac{1}{p}$$

provided the samples come from the canonical distribution

$$P(\vec{S}) \propto e^{-\beta E(\vec{S})} \xrightarrow{\text{After normalization}} P(\vec{S}) = \frac{e^{-\beta E(\vec{S})}}{Q}$$

How do we sample a configuration $\vec{S}$ from this distribution when we have no hope of computing Q?

Answer: We cook up a dynamics



Goal of the dynamics: No matter where we start, if you run the movie long enough and pick out a frame, it will have probability $P(\vec{S}) = \frac{e^{-\beta E(\vec{S})}}{Q}$.

Imagine for a moment that we could list all the possible microstates
And we make a vector of the probability of being in each microstate at time t.

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

After one step of our dynamics we are at time $t+\Delta t$ with

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

$$= \underbrace{\begin{pmatrix} p(1\to 1) & p(2\to 1) \\ p(1\to 2) & p(2\to 2) & \cdots \\ & \vdots \end{pmatrix}}_{\text{Call this matrix of all the transition probabilities the "transition matrix" } T.} \vec{p}\,(t)$$

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

T defines the "dynamics" – it tells us how to transform from one microstate to another.

What is $\vec{p}(0)$? (For a simulation)
We'll start in one particular configuration, so

$$\vec{p}(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

The index of this spot is the state we start in with probability 1

Pictorally

After n steps,

$$\vec{p}(n\Delta t) = T^n \vec{p}(0).$$

We want

$$\lim_{n\to\infty} \vec{p}(n\Delta t) = \lim_{n\to\infty} T^n \vec{p}(0) = \frac{1}{Q}\begin{pmatrix} e^{-\beta E(\vec{s}_1)} \\ e^{-\beta E(\vec{s}_2)} \\ \vdots \end{pmatrix} \equiv \vec{\pi}$$

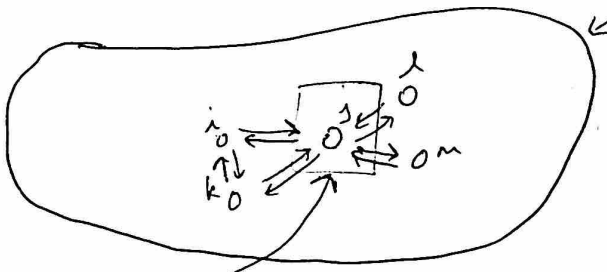
↑ A stationary distribution (not a function of time). Once you reach this distribution the prob. dist. stops changing.

That means our dynamics must satisfy

$$\underbrace{T\vec{\pi}}_{\text{Result of another step of dynamics}} = \underbrace{\vec{\pi}}_{\text{Exactly the same dist. we started with}}$$

Balance Condition

Why?



The total probability leaving site j: $\pi(j)\left[p(j\to l) + p(j\to m) + \dots\right]$ must balance with the total probability ~~flow~~ entering site j: $\pi(i)p(i\to j) + \pi(k)p(k\to j) + \dots$

If the out flows did not balance the in flows, then the prob. of being in site j would change from one step to the next.

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

$$i \rightleftharpoons j \qquad \pi(i)p(i\to j) = \pi(j)p(j\to i)$$

Forcing all pairs to be balanced is called detailed balance — it is a stronger condition that ensures $T\vec{\pi} = \vec{\pi}$.

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

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

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

↑ The partition function has dropped out!

One choice you could make is

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

~~but~~ This choice would satisfy $\frac{p(j \to i)}{p(i \to j)} = e^{-\beta(E(i) - E(j))}$, but there is a problem. We require that

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

Why? Given that you start in i, you must go to some ~~of~~ new config's with probability 1. The new config. could be any j (including $i = j$), but normalization must be imposed for the random walker.

Our choice above $(*)$ could be adapted to make that normalization work out:

$$p(j \to i) = C e^{-\beta E(i)} \quad \text{and} \quad p(i \to j) = C e^{-\beta E(j)} \quad \text{for } i \neq j$$

(C: a constant)

$$p(i \to i) = 1 - \sum_{i \neq j} C e^{-\beta E(i)}, \text{ with } C \text{ chosen such that } 0 \leq p(i \to i) \leq 1.$$

But computing C & $p(i \to i)$ requires me to sum over $i \neq j$, a huge # of microstates.

Not looking great!

But there is another way

Conceptually we could split $p(i \to j)$ into two steps.

1. Propose a new j with some probability that you choose

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

2. Decide whether to accept or reject that proposal with probability

   $P_{acc}(i \to j)$

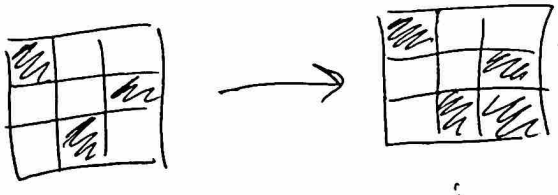
   If you reject, stay in i.

The total probability of going from i to j is

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

$P_{gen}(i \to j)$ can be (almost) anything you want as long as you compute an appropriate P_{acc}. We'll see how to do that.

Ex:



i $\qquad$ j

1. Pick a spin at random. We pick the spin w/ probability $1/N$.
2. Flip that spin to produce config. j.

Hence this "MC move" has $P_{gen}(i \to j) = \frac{1}{N}$.

Can $P_{acc}(i \to j)$ be anything I want like $P_{gen}(i \to j)$ could? NO!

We choose $P_{acc}(i \to j)$ & $P_{acc}(j \to i)$ in such a way to ensure the detailed balance condition holds:

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

There are many choices of p_{acc} that work. The most popular are the Metropolis choice + the Glauber choice

Metropolis:

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

Next class we'll confirm that this works.