

ANNOUNCE

→ MIDTERMS

- today {
1. Julián : Binary Search
 2. Gus : Stacks
 3. Nick : + + conquer
 4. BRE : QUICKSORT
 5. Steven : HASH TABLE

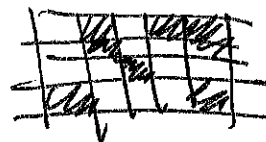
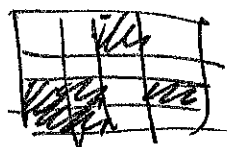
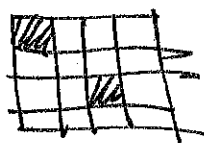
Thu : next 4

INDEX CARD

- QUESTIONS/ Feedback re: class
- SUGGESTION for future midterm talks

REVIEW

- Stat Mech is hard : $N \sim 10^{23}$ eg 2 state system is 2^N dim. space!!
 - many M states that we have to average over
 - "microstate" this is a WEIGHTED average
- care about macro properties

eg Magnetization is an average over spins

etc.

if we just averaged over all config.
of 2^N M states $\rightarrow M = 0$
no magnetism.

but: what we're missing:

DIFF - ENERGY CONFIGURATIONS ... weighting:

$$P_i = e^{-\beta E_i} / Z$$

↑
indep of i , but impossible to calculate

So: let's throw computers @ this problem.

alternative: fancy math... leave that to a proper stat mech course $\#$

• Monte Carlo / Can'to Right

- use random # generator to sample
 $N \ll 10^{23}$ μ states.

- since the macro-observables are averages, we just need enough samples to get a good average.

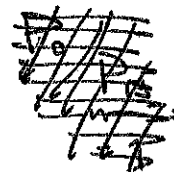
eg:



$S_i = 1$ in circ.
 $S_i = 0$ outside circ.

small circle marble game

$$A_o / A_{\square} =$$




$\pi/4$
 analytic.

as a statmech problem:

assuming uniform probability across square

can ask: $\langle s \rangle = \sum_i S_i P_i$

\uparrow
 0 or 1 \uparrow $= \frac{1}{\# \text{ grid points}}$
 if 

eg: $r_i = 1$ in square

\rightarrow or: $1/N$ some unknown BUT CAN DIVIDE OUT

$$\langle r \rangle = \sum_i r_i P_i$$

$$= \sum_i \frac{1}{P}$$

$$\sim e^{-BE_i/2}$$

then calc: $\langle s \rangle' = \frac{\langle s \rangle}{\langle r \rangle} = \sum_i S_i \left(\frac{P_i}{\sum_j P_j} \right) = \sum_i S_i$

so that's easy - direct sampling

↳ we know P_i & it's trivial.

ANALOGY: each marble position $\sim \mu$ state.

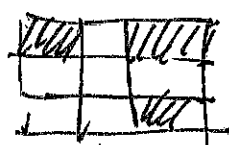
$S_i \sim$ observable to avg over.



BUT

REAL STAT MECH: $P_i \sim e^{-\beta E_i} / Z$ is hard to calc.

WE NEED: A SAMPLE OF μ STATES THAT ARE REPRESENTATIVE OF THE BOLTZMANN DISTRIBUTION

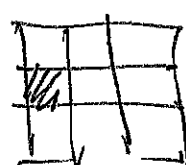
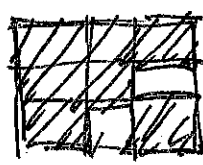
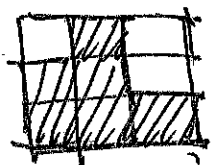
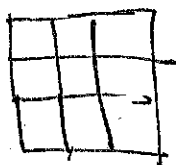
so:



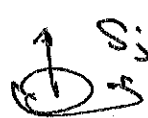
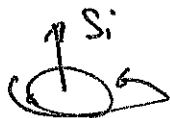
 $S_i = +1$
 $S_i = -1$

not really a great sample of SPINS

expect (@ low temp)



clumpy!



neighboring spins affect each others' energy configs!

BTW: BOTH SAMPLES HAVE $M = \langle S \rangle = 0$

~~but second has~~ ↓

~~M =~~

but imagine a small eg \vec{B} field...

SO

NEED WAY TO SAMPLE Faithfully

MARKOV CHAIN:

generate sample sequentially

given M_{state_i} , RULES $\rightarrow M_{state_{i+1}}$

↑
we have to
choose these
(MCMC algorithm choice)

Markov chain Monte Carlo



then take this as our ENSEMBLE.

Markov: probability to go to a given state dep. only on current state
(locality in time, analog of why our ~~PDE~~ EOM are always PDEs)

REMEMBER: $P(\text{state})$: unknown (Boltzmann)
prob to ~~for~~ sample a state


PhysicsALGORITHM

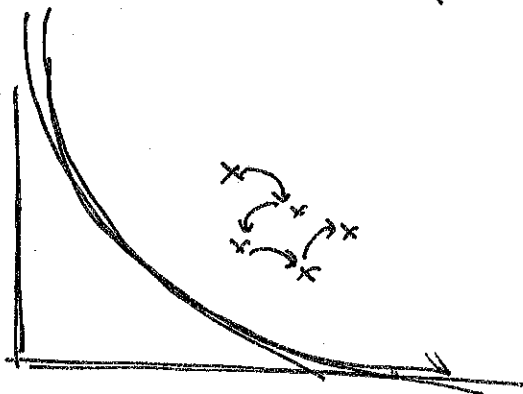
$p(\text{state}_i \rightarrow \text{state}_j)$: transfer probability
of our MCMC algo

BIG MARBLE GAME : MCMC, Drunkard's walk
(RANDOM WALK)

Random walk is an eg of a MCMC algo.

↳ each step: uniform ^{TRANSITION} probability
to a neighboring site

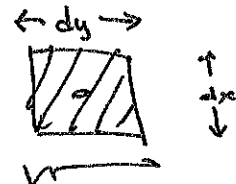
eg.  $P(i \rightarrow \text{nbr}) = 1/4$



or



or



what we did in
sample code

last time : how to pick a MCMC algo?

↳ DETAILED BALANCE, -

we will return to this : Metropolis's algo
for ISING model