ANNOUNCEMENTS

- 5 min midterm demo
- CLASS AS USUAL — TUE + THU
- MAKE UP CLASS next wk : WED

- questions?
  - ↳ perhaps on the HW due tomorrow?

LAST TIME & BIG PICTURE

Stat Mech is annoying.

$N \sim 10^{28}$ particles → intractable using "ORDINARY" PHYSICS

so over the last 100 years, we developed clever ways to understand the MACROSCOPIC PROPERTIES of such systems

→ leads to some impressive math (PATH INTEGRALS, PARTITION FUNCTIONS, ...)

but this often obscures the physics!

Monte Carlo
(carlo bright)

Strategy: USE computer simulations w/ $N \ll 10^{23}$ particles, expect MACROSCOPIC BEHAVIOR to be the same.

tricky: have to draw from Boltzmann probability distribution

we can write as an "∞" sum ... have to find a way to estimate by sampling

what we've been doing all this time w/ integration!

- IF WE'RE $\boxed{\text{SAMPLING}}$ TO FIND THE PROBABILITY DISTRIBUTION, *from what do we sample?*

  how do we generate a sample?

  Krauth (SMAC): DIRECT SAMPLING IS LIKE HAVING AN ANALYTICAL, EXACT SOLUTION.

Physical guiding principle:

ERGODIC HYPOTHESIS ← not proved from microphysics (CONFIRMED FOR MANY SYSTEMS)

all states of a closed system in equilibrium will be occupied w/ equal probabilities

$\boxed{\text{MARKOV CHAIN}}$: alternative to direct sampling

one marble, huge area.

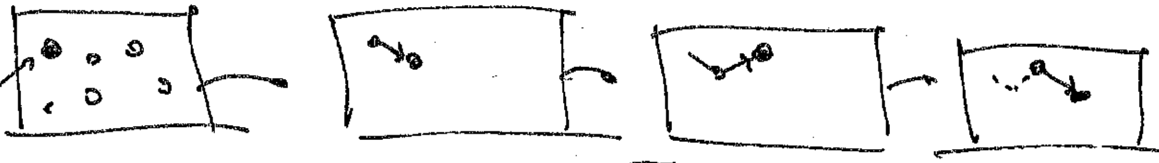
throwing marbles

technically: MC (or MCMC for "markov-chain Monte Carlo")

is when you generate the sample "one at a time" where $(i+1)^{th}$ sample is created from i^{th} sample.

Depends only on current config to get next config.

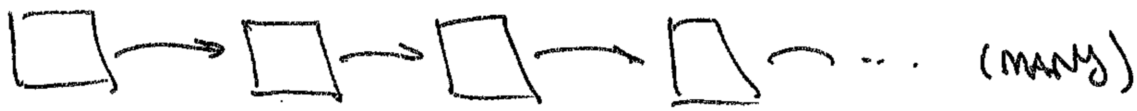
eg.



focus on one molecule

these are the samples.

eventually sample whole space



X_1 X_2 X_3 X_4 ← some physical macroscopic quantity we want to measure

eg. P_y for THIS CONFIG.

want to estimate $\langle X \rangle = \sum_i X_i P_i$

PROB of i^{th} μ state

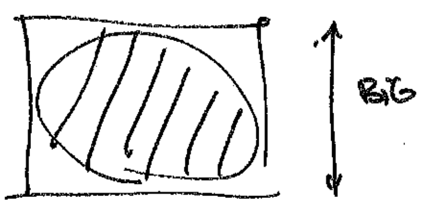
micro states → config. (states)

value of X for i^{th} μ state

<u>claim</u> : in our MCMC, each sampled state appears w/ probability P_i.

this is completely analogous to area of big circle w/ <u>one</u> marble + a stick.

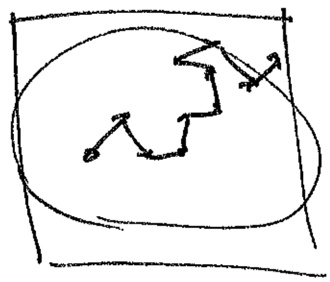
to mark spots.



PROB (in circle)

$$\frac{A_\circ}{A_\square} = \frac{\langle N_{HITS} \rangle}{N_{TOT}} = \sum_I P_I \quad \leftarrow \quad X_I = 1$$

- CAN SEE ("proof" by intuition ... not really a proof) THAT A MARBLE WILL EVENTUALLY SAMPLE WHOLE SPACE



RANDOM WALK

→ MCMC : P_{i+1} (some position) depends only on prev. position

strategy: mark the ground @ every place the marble lands.

pick up marble & throw again from where it last landed.

⊗ impossible to reach this in one step

- then we get to the problem of:

WHAT TO DO W/ OUT OF BOUNDS?

many plausible options...
but give different answers!
(ie most are WRONG)

- do over?
- throw it from outside?
- count, but do over? ⟵ winner. why?
- etc.

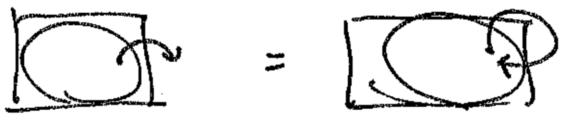
π demo 1 — from kato

Answer: Metropolis Algorithm (will give full alg later)

if MCMC generates an invalid state,

eg 

then count the throw as landing in same spot



why? DETAILED BALANCE.

BIG PICTURE: there's really one choice to be made when doing MCMC → how to assign probabilities for each step.

WARNING: do not confuse the different probabilities!

P_i PROB of being in state i IN THE PHYSICAL SYSTEM

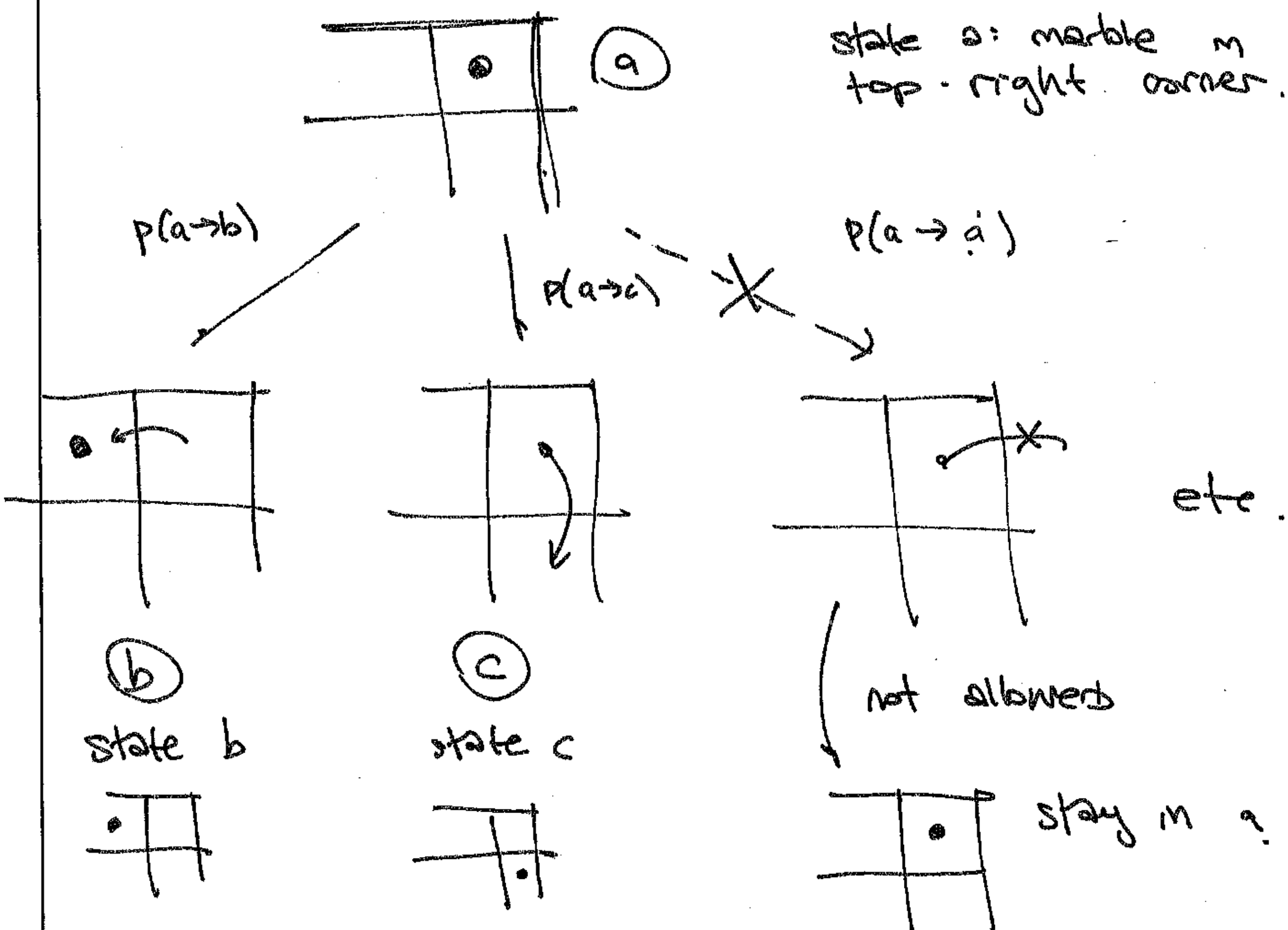
WE DON'T KNOW THIS, WOULD LIKE TO USE MCMC TO SAMPLE IT.

$p(i \to i+1)$ PROB OF EVOLVING SYSTEM FROM CURRENT STATE TO NEXT STATE

nothing inherently physical about this we get to choose it ... we only need this so that over many steps, we sample the entire state space faithfully.

~~Rules / constraints of probability~~

Related, simpler system



RULES : 1. cons. of probability ("unitarity")

$$\boxed{p(a \to a) + p(a \to b) + p(a \to c) = 1}$$

2. "FLOW"

$$\boxed{P(a) = P(a)\,p(a \to a) + P(b)\,p(b \to a) + P(c)\,p(c \to a)}$$

PROB to be in a now

eg. PROB in B last step × PROB OF GOING FROM b to a.

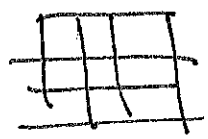
<u>then</u>

$$P(a)\,[\underbrace{1 - p(a\to a)}_{= p(a\to b) + p(a\to c)}] = P(b)\,p(b\to a) + P(c)\,p(c\to a)$$

← note: diff. directions!

$$\Rightarrow \boxed{P(a)\,p(a\to b)} + P(a)\,p(a\to c) = \boxed{P(b)\,p(b\to a)} + P(c)\,p(c\to a)$$

detailed balance ansatz:
these are separately equal.

for our simple example:  ← $P(\text{any state}) = 1/9$

 ← $p(x\to y) = 1/4$ in "BULK" (away from edge)

satisfies detailed balance.

BUT THEN EDGE STATES:

 need this to be $P(a\to b) = 1/4$

so let the unallowed moves count as $p(a\to a)$.