later: need to get back to METROPOLIS algorithm.

DRUNKARD'S WALK / RANDOM WALK

simplest MCMC

@ each step, randomly move in one of the allowed directions

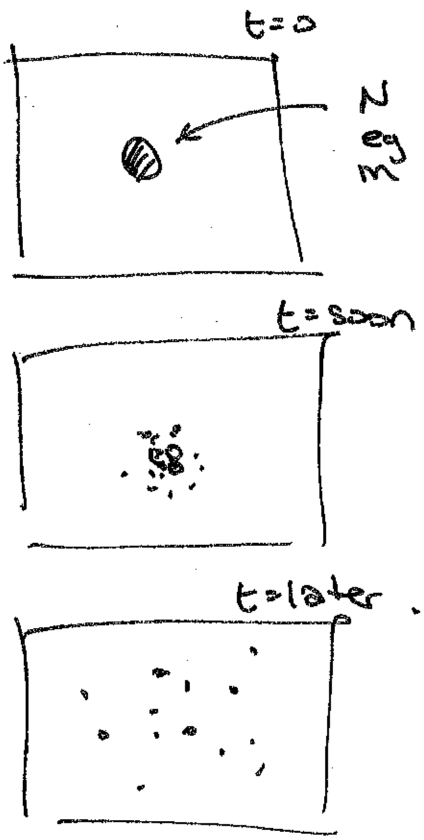
eg. 

or 3D, ...

homework: calculate $\langle x \rangle$, $\langle x^2 \rangle$

ENTROPY: GIORDANO & NAKANISHI 7.3

has to do w/ diffusion



N particles eg creamer in coffee

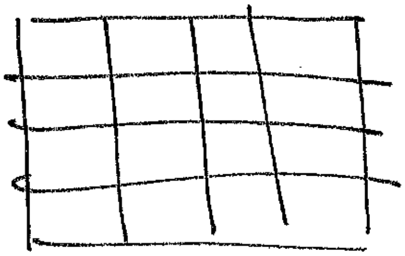
SUBJECT TO "BROWNIAN" MOTION

want to calculate ENTROPY

Shannon Entropy: information entropy.

related to # of microstates contributing to a macrostate.

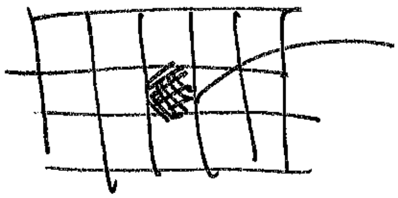
$$S = -\sum_{i}^{\text{states}} P_i \ln_2 P_i$$



BREAK UP SPACE INTO BIG CHUNKS.

nothing to do w/ grid size of discrete particle positions

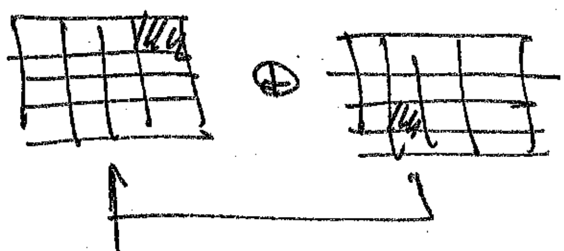
state :



particle in this chunk

if just one particle, then these are all the states.

2 PARTICLES :



independent!

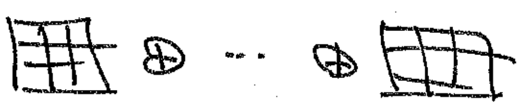
like two subsystems.

RECALL: ENTROPY IS EXTENSIVE, scales w/ system size

$$S_C = S_A + S_B$$

if $C = A \oplus B$ (non interacting)

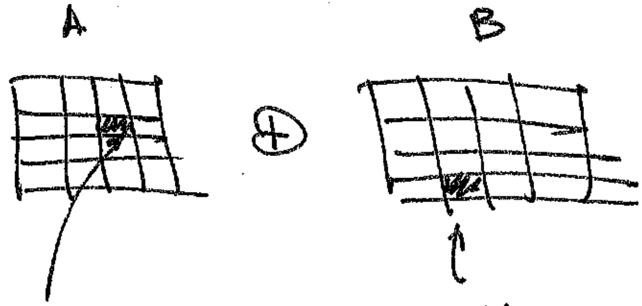
N · PARTICLES :



$$S_N = N S_1$$

so all info is contained in S_1

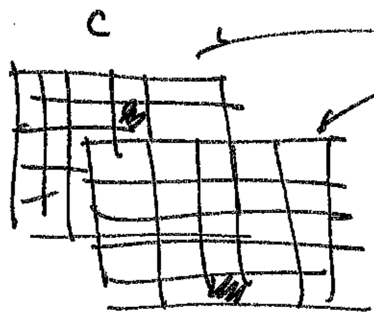
PROOF:



j^{th} runs over all grid positions for A

k^{th} runs over all grid positions for B

=



$i = (j, k)$ runs over all pairs of grid positions

(ignore issue of 2x counting...)

then:
$$S_c = -\sum_i P_c(i) \ln P_c(i)$$
$$= -\sum_{jk} \left(P_A(j) P_B(k)\right)\left[\ln P_A(j) + \ln P_B(k)\right]$$
$$= -\sum_j P_A(j) \ln P_A(j) \times \sum_k P_B(k)$$
$$- \sum_j P_B(k) \ln P_B(k) \times \underbrace{\sum_j P_A(j)}_{=1 \text{ by completeness}}$$
$$= S_A + S_B.$$

ALL WE NEED IS S_1 ← entropy of one particle diffusing.

BUT HOW TO CALCULATE? NEED P_i

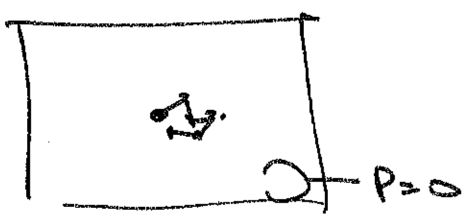
IN FACT, NEED $\boxed{P_i(t)}$

time dependence

in this case, the MCMC is really a simulation of a physical process.

each step is a plausible evolution of the actual system,

eg AREA of CIRCLE → (not only a trick to sample the space of configurations)



for small t, unlikely to populate distant areas of the space.

so: $S(t\ \text{small}) = -P_1 \ln P_1 - P_2 \ln P_2 - \cdots$

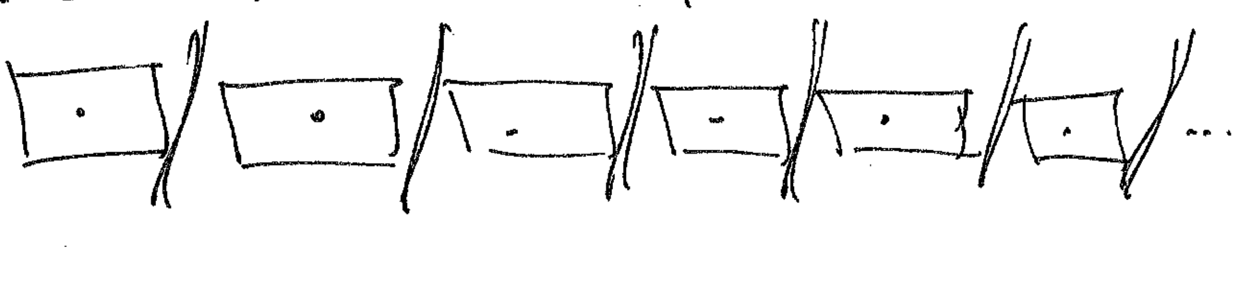
many of these are zero b/c particle has no way to get to outer regions

so $S(t\ \text{small}) = \text{small}$

HOW TO ESTIMATE? DRAW FROM AN ENSEMBLE OF N PARTICLES!

@ t= SMALL, FIXED 1 PARTICLE:

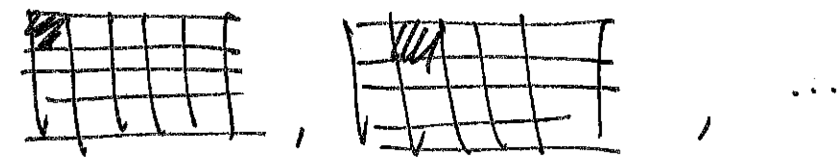
each is unrelated! JUST HAD SAME i.c.



then calculate S from this distribution

$$S = -\sum_i P_i \ln P_i$$

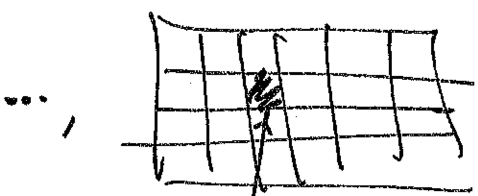
coarse grid



$i=1$ $\qquad$ $i=2$

$P_1(\text{small time}) = 0$ $\qquad$ $P_2(\text{small time}) = 0$

too far.



$$P_{\hat{n}} \neq 0 \leftarrow P_{\hat{n}} = \frac{\#\text{ samples w/ particle in } \hat{n}}{\text{total }\#\text{ samples}}$$

AGAIN: DO NOT GET CONFUSED BY COARSE GRID OF MACRO STATES & SMALL GRID OF μ states

ALSO: DO NOT CONFUSE N PARTICLES IN PHYSICAL SITUATION ($N \sim 10^{23}$) VS. N TIMES WE SIMULATE 1 PARTICLE RANDOM WALK!