

(26)

Chem 220b

2023-01-17

Tu Th 2-3:30 (1a)

INTRODUCTION TO STOCHASTIC THERMODYNAMICS

"STATISTICAL MECHANICS"

Dr. GAVIN CROOKS
gavin.crooks@gmail.com

ADITYA SINGH

what makes now

→ Dynamics

→ Small systems

80% of talk!

1 Information Theory

2 Thermodynamics - Reversible, physics of information
work, heat, energy, entropy, free energy, thermo equilibrium
physics of information.

3 Fluctuation Theorems

4 Linear Response

5 Dynamics. OTMC, CTMC, Classical, Langevin, MD, Quantum

6 Advanced Topics

7 Guest Lectures - Contemporary Stat Mech.

(2a)

ADITYA SINGH

→ Discussion sections
Office Hours

~~2:00-2:30~~
~~2:30-3:00~~

Prerequisites

- Equilibrium Thermodynamics / stat. Mech
- Quantum
- Linear Algebra
- Code (elementary school level)

OFFICE HOURS

319A Gilman

Tu 11-12
Th 3:30 - 4:30

Discussion Sections

GRADERS

~78 Homeworks

~65%

35% - Final report

on a topic of your choice

Due in recitation week

Coin Flip

- Coin
- flip heads or tails
- what's the probability heads or tails?

what assumptions are you making
→ flip & hide

→ what the probability

Digression a frequentist

→ peek at coin

what's your probability? what's mine.

I tell you heads? what's your probability

→ information

E. T. Jaynes - Great proponent of Bayesian reasoning.
subjective, versus objective

Probabilities are not a property of the system but of what we know. Contextual
How we know

$$2^{30} \approx \frac{1}{\ln 10^{30}}$$

$$\ln 10^{30} \approx \ln e^{70} \\ \approx 70$$

$$\sum_i P(a_i) \leq 1$$

(Probabilities are numbers
represent degrees of possibility)

$$P(\text{coin is heads}) \neq$$

$$P(\text{true}) = 1$$

$$P(\text{false}) = 0$$

$$P(\text{heads}) = 1/2$$

$$P(\text{tails}) = 1/2$$

$$\sum_c P(c) = 1$$

$$c = \{\text{heads}, \text{tails}\}$$

$$\left(\text{Why } 1/2? \text{ Permutational symmetry } P(x) = \frac{1}{N} \right)$$

Probabilities represent logical statements.

~~Ensemble (Probability space)~~

5

Ensemble (Probability Space) A set of propositions $\Omega_A = \{a, b, c, \dots\}$ Sample space a_1, a_2, a_3, \dots

This Dice is $\frac{1}{6}$ $P_A(a)$ $P(A=a)$ $P(a)$ Dice = 1 2 3 4 ...

\uparrow Random Variable

	B		
	C	\bar{C}	
A	?	?	$\rightarrow A$
	?	?	
Cont			
	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$ Probabilities
	$\frac{1}{2}$	0	$\frac{1}{2} P(a) = (\frac{1}{2}, \frac{1}{2})$

$$P(b) = \{3/4, 1/4\}$$

Joint ensemble
Joint Prob.

A, B
 $P_{AB}(a, b)$ $P(a \text{ and } b)$

	<u>Bool</u>			<u>* logical or</u>
a and b	ab	$a \vee b$	a, b	
a or * b	$a+b$	$a \wedge b$		
not a	\bar{a}	$\neg a$		

$$P(a \text{ or } b) = P(a) + P(b) - P(a \text{ and } b)$$

$$P(a=0 \text{ or } b=1) = \frac{1}{2} + \frac{1}{4} - \frac{1}{4} = \frac{1}{2}$$

Independent

$$P(a, b) = P(a) P(b)$$

$$\begin{pmatrix} \frac{3}{8} & \frac{1}{8} \\ \frac{3}{8} & \frac{1}{8} \end{pmatrix}$$

BayesConditional Probability : ~~$P(b|a) =$~~

$$P(a|b) =$$

chain rule / product Rule.

$$P(a, b) = P(a|b) P(b) = P(b|a) P(a)$$

$$P(a|b) = \frac{P(b|a) P(a)}{P(b)}$$

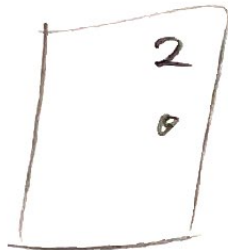
Bayes' Rule

Probabilities depend on what you know.

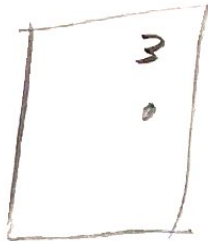
Monty Hall Problem



Pick #1



Monty opens

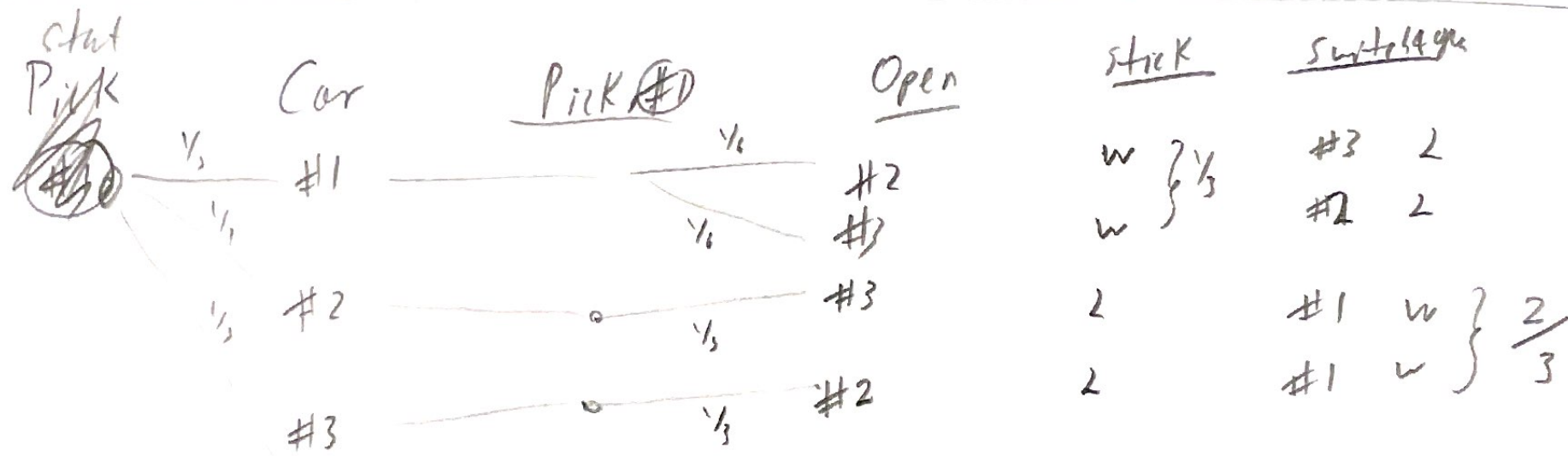


- 1) stick
- 2) switch
- 3) Doesn't Matter.

Vote!

Prize behind one door.

1, 2, or 3?



why do people not think wrong?

The car does not move? So how does Monty ever make a difference?

$$P(\text{car loc.} \mid \text{monty opened door, I pick car a})$$

Probabilities are contextual

Reading → Monty Hall problem (e.g. wikipedia)

Information Theory (ch 20 + Thomas & Cover)

Extra (or) problem

Probability a 30 digit number is prime?

$$P(\text{prime } N \text{ is prime}) \approx \frac{1}{\ln N} = \frac{1}{\ln 10^{30}} = \frac{1}{\ln e^{70}} \approx \frac{1}{70}$$

Prime number Theorem

→ Probabilistic Tests

24 8 219538998414003318890440248291

402587