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Tutorial 1

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Instructions

- We encourage you to work in groups on the problems. Groups of 3 will be assigned at random at the beginning of the tutorial
- Unless otherwise specified, you can go through the tutorial in whichever order you prefer
- If you are unable to attend a tutorial, you should work on the tutorial on your own (for about 1.5 hours) and submit your written work

1 Statistical mechanics from coin flips

Consider a biased coin, which flips to Heads (H) with probability p and Tails (T) with probability $1-p$. We will consider the statistics of the outcomes of $N \gg 1$ flips of this coin. There are two situations: (1) I can flip a single coin N times and gather its statistic, or (2) I can flip an *ensemble* of N coins and flip them and gather its statistic. Ergodic hypothesis says that as $N \gg 1$, (certain) time averaged quantities from will converge to the ensemble averaged quantities from (2). The quantity we consider is the fraction of H obtained in N flips, as I increase N.

The ergodic hypothesis can be viewed in this numerical plot of a particular experiment in Fig. 1. We find that the fraction equilibriates to a steady state value. Here we will show that the steady state value is actually the ensemble average.

a) Suppose we have N coin flips, and have found there are m heads and $N-m$ tails. What is the probability that *any specific sequence of H and T* has this property? How

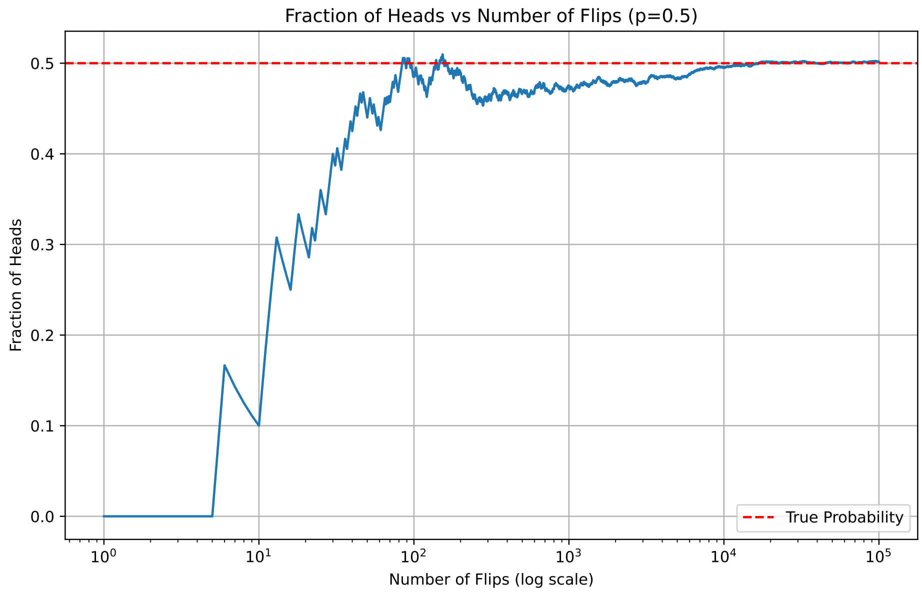

Figure 1: Statistical Mechanics from coin flips: a single experiment of N coin flips. The fraction of H is plotted.

many such sequences are there with this property? What is the probability that in an experiment we obtain m heads, $P(m)$?

Hint: Note the subtle differences in the first and third sub-questions. The answers should remind you of the fundamental assumption of statistical mechanics: all accessible microstates are equally likely for a given macrostate. Here, a microstate is any sequence of coin flip outcomes, while a macrostate is a collection of sequences which all have m Heads.

b) At what value of m is the probability $P(m)$ maximized?

Hint: Consider $\log P(m)$*, and use Stirling's approximation,*

$$Q! \approx \sqrt{2\pi Q}\left(\frac{Q}{e}\right)^Q$$

for $Q \gg 1$*. This approximation will be our friend for the rest of the course!*

c) What is the expected value ('mean') of the number of heads, i.e. $\overline{m} = \sum_{m=0}^{N} mP(m)$? What is the variance of the expected number of heads, defined as $\mathrm{var}_m = \sum_{m=0}^{N}(m -$

$\overline{m})^2 P(m)$? How does the standard deviation (square root of the variance) compare to the mean, $\overline{m}$, at large N?

Comment: You may have seen this in statistics as 'central limit theorem'.

2 Ensembles from information entropy

In this problem we will connect the idea of entropy from information theory with the thermodynamic entropy. For a probability distribution $\{p_i\}$ with $i = 1, 2, \cdots, N$ outcomes, the Shannon entropy is defined as $H(\{p_i\}) = -\sum_i p_i \log p_i$ (with the identification $0 \log 0 = 0$). This captures the amount of uncertainty in the probability distribution: if probability is 1 for a particular outcome (totally certain), the entropy is 0; while if the probability of all outcomes are the same i.e. $p_i = 1/N$ (totally uncertain), the entropy is its maximum $\log N$ (you will show this in the problem). This concept was discovered by Gibbs in the context of thermodynamics, reinterpreted in quantum mechanics by von Neumann, and rediscovered by Shannon in information theory.

a) We want to derive the microcanonical ensemble as the probability distribution that maximizes entropy. Maximize $H(\{p_i\})$ with the constraint that the probabilities must sum to 1, i.e. $\sum_i p_i = 1$. What is the entropy of this probability distribution? Compare this with the microcanonical entropy $S = k_B \log \Omega$, where Ω (number of microstates) and N (number of outcomes) should be analogous.

b) Next, we maximize the entropy with the constraint that the average energy of the distribution is fixed. Assign some energy E_i to every outcome i, and demand that $\sum_i p_i E_i = E$ is fixed, while the entropy is to be maximized. What is the probability distribution $\{p_i\}$ that satisfies this?

3 Quantum harmonic oscillators

Consider N independent quantum oscillators subject to a Hamiltonian

$$\mathcal{H}(\{n_i\}) = \sum_{i=1}^{N} \hbar\omega \left(n_i + \frac{1}{2} \right),$$

where $n_i = 0, 1, 2, \cdots$ is the quantum occupation number for the ith oscillator.

a) Calculate the entropy S, as a function of the total energy E.

b) Calculate the temperature using thermodynamics relation between entropy and energy.

Hint: Use Stirling's approximation to find a simple expression using

$$\frac{1}{T} = \frac{\partial S}{\partial E}.$$

c) Calculate the energy E, and heat capacity C, as functions of temperature T, and N.

Hint: Heat capacity is defined as $C = \frac{\partial E}{\partial T}$*. Invert the previous result (after Stirling's approximation) to obtain this result.*

d) Plot $\frac{C}{Nk_B}$ for a fixed value of ω (choosing $\hbar/k_B$, as a function of T. What is it's behavior at high T? This is exactly the behavior expected for classical harmonic oscillators.

Hint: Heat capacity is defined as $C = \frac{\partial E}{\partial T}$*. Invert the previous result to obtain this result.*

4 Ideal gas - microcanonical ensemble

Consider an isolated system of N non-interacting particles in a box of volume V with energy E. We'll work in the continuous case, where

$$\rho(q,p) = \delta(H(q,p)/E - 1). \tag{1}$$

Here q, p are vectors in $3N$ dimensions, labeled by $i\alpha$ for the $i = 1, 2, \cdots, N$th particle's position/momentum in the $\alpha = x, y, z$ direction.

For non-interacting particles, the Hamiltonian is just the kinetic energy, $H(q,p) = \frac{||p||^2}{2m}$

a) Discussion topic: argue why it makes sense to choose $W_0 = \omega^{3N}$, where ω is a fixed intensive quantity with the dimensions of an action. Recall that the definition of entropy for classical continuous systems is,

$$S = -k_B \int \mathcal{P}(q,p) \log\left(\mathcal{P}(q,p) W_0\right) dq dp, \tag{2}$$

where,

$$\mathcal{P}(q,p) = \frac{\rho(q,p)}{\int \rho(q,p) dq dp}. \tag{3}$$

b) Use the fact that

$$\int_{\mathbb{R}^n} f(\alpha\|x\|^2)d^n x = \frac{2\pi^{n/2}}{\Gamma(n/2)}\int_0^\infty r^{n-1} f(\alpha r^2)dr = \frac{(\pi/\alpha)^{n/2}}{\Gamma(n/2)}\int_0^\infty u^{n/2-1} f(u)du \tag{4}$$

if $\alpha > 0$[1] and the Stirling approximations

$$\ln(N!) \sim N\ln N - N \quad (N \to \infty) \tag{5}$$

$$\ln(\Gamma(x)) \sim x\ln x - x \quad (x \to \infty) \tag{6}$$

to show that the entropy of the system is asymptotically equivalent to

$$S \sim kN \ln\left[\frac{V}{N\omega^3}\left(\frac{4m\pi E}{3N}\right)^{3/2}\right] + \frac{5Nk}{2} \tag{7}$$

as $N \to \infty$.

c) Make sure that S is extensive. What would have happened if you didn't include the correction factor of $1/N!$ (which you remembered, of course)?

d) Now that you have S, show that

$$E = \frac{3kNT}{2}. \tag{8}$$

e) Use the fact that

$$dS = \frac{1}{T}dE + \frac{P}{T}dV \tag{9}$$

to compute P and show that the ideal gas law is recovered.

[1] You don't have to prove this.