MATH327: Statistical Physics, Spring 2022

Tutorial problem — Entropy bounds

We met the second law of thermodynamics by considering what happens when two spin (sub)systems are brought into thermal contact with each other — allowed to exchange energy but not particles. Conservation of energy means that if subsystem Ω_1 has energy e_1, the other subsystem Ω_2 must have energy $E - e_1$, where E is the total energy of the micro-canonical combined system Ω. We found (in Eq. 21 on page 34 of the lecture notes) that the total number of micro-states of the overall system is

$$M = \sum_{e_1} M_{e_1}^{(1)} M_{E-e_1}^{(2)}$$

where $M_e^{(S)}$ is the number of micro-states of subsystem $S \in \{1, 2\}$ with energy e.

Because M is a sum of strictly positive terms, we can easily set bounds on it. Say the sum over e_1 has $N_{\text{terms}} \geq 1$ terms $M_{e_1}^{(1)} M_{E-e_1}^{(2)}$, and define $\max$ be the largest of those terms. Then $\max \leq M$, with equality holding when there is only one term in the sum. Similarly, $M \leq N_{\text{terms}} \cdot \max$, with equality holding when every term in the sum is the same. All together, we have

$$\max \leq M \leq N_{\text{terms}} \cdot \max .$$

This can be more powerful than it may initially appear, thanks to the large numbers involved in statistical physics. For illustration, suppose $\max \sim e^N$ and $N_{\text{terms}} \sim N$ for a system with N degrees of freedom. (We have already seen $M = 2^N = e^{N \log 2}$ for a system of N spins with $H = 0$, while $H > 0$ introduces factors of $N!$ that Stirling's formula can recast in terms of $N^N = e^{N \log N}$.) Then we have $e^N \lesssim M \lesssim N e^N$. If we take the logarithm and recall $\log M = S$ is the entropy, this becomes $N \lesssim S \lesssim N + \log N$. With our characteristic $N \sim 10^{23}$, we have $\log N \sim 50$ and $10^{23} \lesssim S \lesssim 10^{23} + 50$, a very tight range in relative terms, with the upper bound only $\sim 10^{-20}\%$ larger than the lower bound. 18 Feb.

To see how this works in practice, let each of Ω_1 and Ω_2 be a spin system with $N_1 = N_2 = 10$ spins and $H = 1$. Fix $E = -10$ for the combined system and numerically compute the bounds on its entropy,

$$\log(\max) \leq S \leq \log(N_{\text{terms}} \cdot \max) .$$

What fraction of the true entropy S is accounted for by $\log(\max)$? How do these answers change for $N_1 = N_2 = 20, 30, 40, \cdots$, still with fixed $E = -10$?

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Tutorial ~~solution~~ Comments — Entropy bounds

As a quick warm-up, let's recall how many micro-states there are for a single micro-canonical spin system with $N_1 = 10$. With $H = 1$, there are 11 distinct energies $E_1 = -(2n_1^+ - N_1)$ evenly spaced between $\pm N_1$, with the following multiplicities:

n_1^+	E_1	Multiplicity		n_1^+	E_1	Multiplicity
10	-10	$\binom{10}{10} = 1$		0	10	$\binom{10}{0} = 1$
9	-8	$\binom{10}{9} = 10$		1	8	$\binom{10}{1} = 10$
8	-6	$\binom{10}{8} = 45$		2	6	$\binom{10}{2} = 45$
7	-4	$\binom{10}{7} = 120$		3	4	$\binom{10}{3} = 120$
6	-2	$\binom{10}{6} = 210$		4	2	$\binom{10}{4} = 210$
5	0	$\binom{10}{5} = 252$				

With $N_1 = N_2 \equiv N = 10$, it's easy enough to exhaustively list the possible ways $-10 \leq E_{1,2} \leq 10$ can add up to the fixed total $E = E_1 + E_2 = -10$:

n_1^+	n_2^+	E_1	E_2	M_1	M_2	$M_1 M_2$
10	5	-10	0	1	252	252
9	6	-8	-2	10	210	2100
8	7	-6	-4	45	120	5400
7	8	-4	-6	120	45	5400
6	9	-2	-8	210	10	2100
5	10	0	-10	252	1	252
					Total:	15,504

We can read off $\max = 5400$ and $N_{\text{terms}} = 6$, so our bound becomes

$$\log(5400) \approx 8.59 \quad \lesssim \quad S = \log(15504) \approx 9.65 \quad \lesssim \quad \log(6 \cdot 5400) \approx 10.39,$$

constraining S at the $\sim 10\%$ level. In particular, considering either one of the two options $(E_1, E_2) = (-4, -6)$ or $(-6, -4)$ would account for about 89% of the total entropy.

We expect these bounds to improve further as N increases. To automate this procedure, we can use computers to do the computations, for instance via the Python code below. Running this with $N = 20$ gives $\max \approx 9.8 \times 10^9$ out of the total $\sum M_1 M_2 \approx 4.0 \times 10^{10}$ from all $N_{\text{terms}} = 16$ possibilities, corresponding to the bounds

$$23.00 \lesssim 24.42 \lesssim 25.77,$$

with approximately 94% of the total entropy accounted for by either of $(E_1, E_2) = (-4, -6)$ or $(-6, -4)$.

Continuing in the same vein produces:

N	$\max$	Total	N_{terms}	Bounds	$\log(\max)/S$
10	5.4×10^{3}	1.6×10^{4}	6	$8.6 \lesssim 9.6 \lesssim 10.4$	0.891
20	9.8×10^{9}	4.0×10^{10}	16	$23.0 \lesssim 24.4 \lesssim 25.8$	0.942
30	1.0×10^{16}	5.2×10^{16}	26	$36.9 \lesssim 38.5 \lesssim 40.1$	0.958
40	1.0×10^{22}	5.8×10^{22}	36	$50.7 \lesssim 52.4 \lesssim 54.3$	0.967
50	9.6×10^{27}	6.1×10^{28}	46	$64.4 \lesssim 66.3 \lesssim 68.3$	0.972
$\vdots$					
80	8.4×10^{45}	6.7×10^{46}	76	$105.7 \lesssim 107.8 \lesssim 110.1$	0.981
$\vdots$					
160	7.2×10^{93}	8.1×10^{94}	156	$216.1 \lesssim 218.5 \lesssim 221.2$	0.989
$\vdots$					

The code below will break down for $N \gtrsim 512$, when M_1M_2 overflows the limit $\sim10^{308}$ that can be represented by 64 bits using the standard format for floating-point (i.e., non-integer) numbers.

In all cases, $\max$ corresponds to energies (and upward-pointing spins) split roughly evenly between the two subsystems: $E_S \in \{-4, -6\}$ which corresponds to $n_s^+ \in \left\{\frac{n}{2}+2, \frac{n}{2}+3\right\}$. This reflects the widespread intuition that the entropy quantifies 'disorder' — there are many more micro-states with the energy evenly divided between the two subsystems, compared to having it all in one subsystem. If we imagine bringing into thermal contact systems that initially have $(E_1, E_2) = (-10, 0)$, after the combined system reaches thermal equilibrium we can expect the energies to be more evenly distributed. On the other hand, it would be rare for evenly distributed energies all to coalesce in a single subsystem, even though all micro-states are equally probable. This illustrates how an "**arrow of time**" can emerge from the statistical physics of a large number of degrees of freedom.

```python
# Entropies for two spin systems in thermal contact
# Set H=1 or equivalently consider E/H
import sys
import numpy as np
from scipy import special

# Parse argument: Number of spins N in each (identical) subsystem
if len(sys.argv) < 2:
  print("Usage:", str(sys.argv[0]), "<spins>")
  sys.exit(1)
N = int(sys.argv[1])

# Quick warm-up: Check entropy for each single-system configuration
for i in range(N+1):        # Number of upward-pointing spins
  E = -(2*i - N)
  M = special.binom(N, i)   # N-choose-i binomial coefficient
  S = np.log(M)
#  print("%2d %3d %4d %.4g" % (i, E, M, S))

# Now two systems in thermal contact
Etot = -10      # Fix total energy E = -10 (could become input arg)
Mtot = []       # Terms in sum(M1*M2)
print("up1 up2  E1  E2        M1        M2     M1*M2")
for i in range(N+1):    # Loop over all possible n_1
  Eone = -(2*i - N)
  Etwo = Etot - Eone
  ntwo = int(0.5 * (N - Etwo))
  if ntwo > N:          # Can't add up to Etot
    continue

  Mone = special.binom(N, i)
  Mtwo = special.binom(N, ntwo)
  Mtot.append(Mone * Mtwo)
  if N < 18:        # Some awkward output formatting...
    print("%3d %3d %3d %3d %9d %9d %9d" \
          % (i, ntwo, Eone, Etwo, Mone, Mtwo, Mtot[-1]))
  else:
    print("%3d %3d %3d %3d %9.3g %9.3g %9.3g" \
          % (i, ntwo, Eone, Etwo, Mone, Mtwo, Mtot[-1]))
print("max=%.4g, total=%.4g, Nterms=%d" \
      % (max(Mtot), sum(Mtot), len(Mtot)))

# True entropy and bounds on it
Smin = np.log(max(Mtot))
Strue = np.log(sum(Mtot))
Smax = np.log(len(Mtot) * max(Mtot))
print("Entropy bounds: %.4g <= %.4g <= %.4g" % (Smin, Strue, Smax))
print("Entropy saturation: %.4g percent" % (100*Smin/Strue))
```

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Tutorial problem — Stirling's formula

We have already made use of Stirling's formula in the following form:

$$\log(N!) = N \log N - N + \mathcal{O}(\log N) \approx N \log N - N \qquad \text{for } N \gg 1,$$

which implies

$$N! \approx \exp\left[N \log N - N\right] = \left(\frac{N}{e}\right)^N.$$

This can be made more precise:

$\sum_h \frac{1}{x^h}$

$$N! \approx \sqrt{2\pi N} \left(\frac{N}{e}\right)^N \left(1 + \frac{A}{N} + \frac{B}{N^2} + \frac{C}{N^3} + \cdots\right) \tag{1}$$

with calculable coefficients A, B, C, etc.[1] By performing a sequence of analyses of increasing complexity, we can build up these results.

First, derive the bounds
(1)

$$N \log N - N < \log(N!) < N \log N \tag{2}$$

for $N \gg 1$. The second bound is the easier one. There are multiple ways to obtain the first bound. One pleasant approach is to consider the series expansion for e^x. Together, these bounds establish

$$1 - \underset{0}{\frac{1}{\log N}} < \frac{\log(N!)}{N \log N} < 1 \qquad \Longrightarrow \qquad \log(N!) \sim N \log N$$

Second, consider the **gamma function**

$$\Gamma(n+1) \equiv \int_0^\infty x^n e^{-x}\, dx.$$

(2) Show that $\Gamma(N+1) = N!$ for integer $N \geq 0$. In other words, derive the Euler integral (of the second kind)

$$N! = \int_0^\infty x^N e^{-x}\, dx. \tag{3}$$

Again, this can be done in multiple ways, including induction with integration by parts or by manipulating

$$\int_0^\infty e^{-ax}\, dx = -a$$

and then setting $a = 1$.

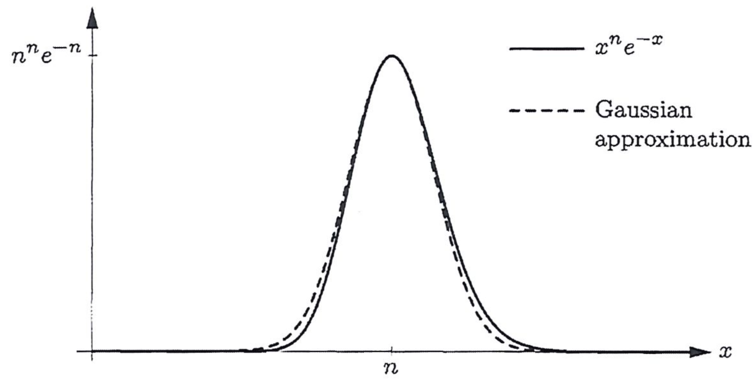
[1] James Stirling computed the $\sqrt{2\pi}$ while Abraham de Moivre derived the expansion in powers of $1/N$. An interesting aspect of this expansion is that it is **asymptotic** — it has a vanishing radius of convergence but can provide precise approximations if truncated at an appropriate power.

The next step in this second analysis is to approximate the gamma function as a gaussian integral. Show that the integrand $x^N e^{-x} = \exp\left[N \log x - x\right]$ is maximized at $x = n$.

Finally, change variables to $y \equiv x - N$ and expand the $\log x$ up to and including terms quadratic in $y \ll N$. You should be left with a factor that can be approximated by a gaussian integral (note the lower bound of integration):

$$\int_{-N}^{\infty} e^{-y^2/(2N)}\, dy \approx \int_{-\infty}^{\infty} e^{-y^2/(2N)} = \sqrt{2\pi N}.$$

Optionally, as a third analysis, you can pursue the $\frac{1}{N^k}$-suppressed corrections in Eq. 1. Again, there are many ways to perform this computation, including higher-order expansions of the $\log x$ considered above. One pleasant approach is to compare $N!$ and $(N+1)!$, now that we have derived the series prefactor $\sqrt{2\pi N}\left(\frac{N}{e}\right)^N$.



$n^n e^{-n}$
$x^n e^{-x}$
Gaussian approximation
n
x