MATH327: Statistical Physics, Spring 2022
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:

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

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

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

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

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

Second, consider the **gamma function**

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

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

$$\frac{d}{da}\left(\int_0^\infty e^{-ax}\,dx = a^{-1}\right)$$

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 $x^N e^{-x} = \exp[N \log x - x]$ 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):

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

The error introduced by extending the integration from $(-N, \infty)$ to $(-\infty, \infty)$ is exponentially small and could be captured by computing the series of corrections suppressed by powers of $\frac{1}{N}$ in Eq. 1.

This leads us to the third and final analysis, which is to compute some of the leading power-suppressed corrections in Eq. 1. Again, there are many ways to achieve this, 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 $\sqrt{2\pi N}\left(\frac{N}{e}\right)^N$.

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Tutorial comments — Stirling's formula

For the first analysis, deriving bounds related to Stirling's formula, we can begin by noting

$$N! = \prod_{k=0}^{N-1} (N-k) < \prod_{k=0}^{N-1} N = N^N$$

for $N > 1$, implying $\log(N!) < N \log N$. For the other bound, we can consider the Nth term in the power series

$$e^N = \sum_{k=0}^{\infty} \frac{N^k}{k!} > \frac{N^N}{N!}$$

because every term in the series is positive. Rearranging, this is

$$N! > \left(\frac{N}{e}\right)^N \qquad \Longrightarrow \qquad \log(N!) > N \log N - N.$$

Putting these together gives the desired result

$$N \log N - N < \log(N!) < N \log N \tag{1}$$

that establishes $\log(N!) \sim N \log N$ for $N \gg 1$.

Moving on to the second analysis, we can consider what happens when we take the derivative of both sides of the equation

$$\int_0^\infty e^{-ax}\,dx = a^{-1}$$

with respect to a. The first derivative gives

$$\frac{d}{da}\left(\int_0^\infty \cancel{-}xe^{-ax}\,dx = \cancel{-}a^{-2},\right)$$

with negative signs that we can cancel out. Repeating, we have

$$\int_0^\infty x^2 e^{-ax}\,dx = 2a^{-3}$$
$$\int_0^\infty -x^3 e^{-ax}\,dx = -6a^{-4}$$
$$\vdots$$
$$\frac{d^N}{da^N} \longrightarrow \qquad \int_0^\infty x^N e^{-ax}\,dx = N!\,\cancel{a}^{-(N+1)}.$$

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Setting $a = 1$, we obtain the desired result,

$$N! = \int_0^\infty x^N e^{-x}\,dx. \tag{2}$$

Of course, this is just the first step in the full derivation of Stirling's formula. The next task is to show that the integrand $x^N e^{-x} = \exp\left[N \log x - x\right]$ is maximized at $x = N$. Demanding that its derivative with respect to x vanishes, we have

$$\frac{d}{dx}x^N e^{-x} = Nx^{N-1}\cancel{e^{-x}} - x^N \cancel{e^{-x}} = 0 \qquad \Longrightarrow \qquad Nx^{N-1} = x^N,$$

or in other words $x = N$. Considering the second derivative at $x = N$,

$$\begin{aligned}\frac{d^2}{dx^2}x^N e^{-x} &= N(N-1)x^{N-2}e^{-x} - Nx^{N-1}e^{-x} - Nx^{N-1}e^{-x} + x^N e^{-x}\Big|_{x=N} \\ &= e^{-N}\left[(\cancel{N}-1)N^{N-1} - \cancel{2}N^N + \cancel{N^N}\right] = -\frac{N^{N-1}}{e^N} < 0,\end{aligned}$$

confirming a maximum.

Changing variables to $y \equiv x - N$, we have

$$N! = \int_{-N}^{\infty} \exp\left[N\log(y+N) - (y+N)\right]\,dy.$$

Expanding the argument of this exponential for $\left|\frac{y}{N}\right| \ll 1$ around this maximum identified above gives

$\log(1+x) \approx x - \frac{x^2}{2} + \ldots$

$$\begin{aligned}N\log(y+N) - (y+N) &= N\log N + N\left(\cancel{\frac{y}{N}} - \frac{y^2}{2N^2}\right) - \cancel{y} - N + \mathcal{O}\left(\frac{y^3}{N^3}\right) \\ &= N\log N - N - \frac{y^2}{2N} + \mathcal{O}\left(\frac{y^3}{N^3}\right)\end{aligned}$$

Reinserting this into the integral above, we obtain the advertised result,

$$N! \approx N^N e^{-N}\int_{-N}^{\infty} e^{-y^2/(2N)}\,dy \approx \sqrt{2\pi N}\left(\frac{N}{e}\right)^N. \tag{3}$$

Finally turning to the third analysis, we start with Eq. 3 and assume that the approximations leading to it can be captured by a power series in $\frac{1}{N} \ll 1$,

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

The defining property of the factorial means $(N+1)! = (N+1)N!$, so that

$$\begin{aligned}&\sqrt{\cancel{2\pi}(N+1)}\left(\frac{N+1}{e}\right)^{N+1}\left[1 + \frac{A}{N+1} + \frac{B}{(N+1)^2} + \frac{C}{(N+1)^3} + \mathcal{O}\left(\frac{1}{N^4}\right)\right] \\ &\quad = (N+1)N! = (N+1)\sqrt{\cancel{2\pi}N}\left(\frac{N}{e}\right)^N\left[1 + \frac{A}{N} + \frac{B}{N^2} + \frac{C}{N^3} + \mathcal{O}\left(\frac{1}{N^4}\right)\right].\end{aligned}$$

Rearranging,

$$\begin{aligned}\underbrace{\left(\sqrt{\frac{N+1}{N}}\left(\frac{N+1}{N}\right)^N\right)}_{\left(1+\frac{1}{N}\right)^{N+1/2}} e^{-1}&\left[1 + \frac{A}{N+1} + \frac{B}{(N+1)^2} + \frac{C}{(N+1)^3} + \mathcal{O}\left(\frac{1}{N^4}\right)\right] \\ &= 1 + \frac{A}{N} + \frac{B}{N^2} + \frac{C}{N^3} + \mathcal{O}\left(\frac{1}{N^4}\right).\end{aligned}$$

$e = \lim_{N\to\infty}\left(1+\frac{1}{N}\right)^N$

We need to reorganize the left-hand side of this equation in terms of $\frac{1}{N^k}$, which we can do in two stages. First, for the terms in the square brackets we can apply the geometric series $\frac{1}{1+x} = \sum_{k=0}^{\infty}(-x)^k$ to find

$$\begin{aligned}
\frac{A}{N+1} &= \frac{A}{N}\left(1 - \frac{1}{N} + \frac{1}{N^2}\right) + \mathcal{O}\left(\frac{1}{N^4}\right) = \frac{A}{N} - \frac{A}{N^2} + \frac{A}{N^3} + \mathcal{O}\left(\frac{1}{N^4}\right) \\
\frac{B}{N^2+2N+1} &= \frac{B}{N^2}\left(1 - \frac{2}{N}\right) + \mathcal{O}\left(\frac{1}{N^4}\right) = \frac{B}{N^2} - \frac{2B}{N^3} + \mathcal{O}\left(\frac{1}{N^4}\right) \\
\frac{C}{N^3+3N^2+3N+1} &= \frac{C}{N^3} + \mathcal{O}\left(\frac{1}{N^4}\right),
\end{aligned}$$

and all together

$$\begin{aligned}
1 + \frac{A}{N+1} &+ \frac{B}{(N+1)^2} + \frac{C}{(N+1)^3} + \mathcal{O}\left(\frac{1}{N^4}\right) \\
&= 1 + \frac{A}{N} + \frac{B-A}{N^2} + \frac{C-2B+A}{N^3} + \mathcal{O}\left(\frac{1}{N^4}\right)
\end{aligned}$$

Second, the overall factor can be handled by exponentiation,

$$\begin{aligned}
\left(1+\frac{1}{N}\right)^{N+1/2} e^{-1} &= e^{-1}\exp\left[\left(N+\frac{1}{2}\right)\log\left(1+\frac{1}{N}\right)\right] \\
&= e^{-1}\exp\left[\left(N+\frac{1}{2}\right)\left(\frac{1}{N} - \frac{1}{2N^2} + \frac{1}{3N^3} - \frac{1}{4N^4}\right) + \mathcal{O}\left(\frac{1}{N^4}\right)\right] \\
&= \exp\left[\frac{1}{12N^2} - \frac{1}{12N^3} + \mathcal{O}\left(\frac{1}{N^4}\right)\right] \\
&= 1 + \frac{1}{12N^2} - \frac{1}{12N^3} + \mathcal{O}\left(\frac{1}{N^4}\right).
\end{aligned}$$

$e^x = 1 + x + \frac{1}{2}x^2$

Bringing things back together,

$$\begin{aligned}
\left(1+\frac{1}{12N^2} - \frac{1}{12N^3}\right)\left(1 + \frac{A}{N} + \frac{B-A}{N^2} + \frac{C-2B+A}{N^3}\right) &+ \mathcal{O}\left(\frac{1}{N^4}\right) \\
&= 1 + \frac{A}{N} + \frac{B}{N^2} + \frac{C}{N^3} + \mathcal{O}\left(\frac{1}{N^4}\right)
\end{aligned}$$

$(N+1)! = (N+1)N!$

The terms proportional to $\frac{1}{N^0}$ require $1 = 1$ while those proportional to $\frac{1}{N}$ indicate $A = A$, both of which are self-consistent but not useful. Interesting things happen when we equate the $\frac{1}{N^2}$ terms:

$$\frac{1}{12} + \cancel{B} - A = \cancel{B} \qquad \Longrightarrow \qquad A = \frac{1}{12}.$$

Similarly, from the $\frac{1}{N^3}$ terms we can determine B,

$$-\cancel{\frac{1}{12}} + \frac{A}{12} + \cancel{C} - 2B + \cancel{A} = \cancel{C} \qquad \Longrightarrow \qquad B = \frac{A}{24} = \frac{1}{288}.$$

So in the end we find

$$N! = \sqrt{2\pi N}\left(\frac{N}{e}\right)^N\left(1 + \frac{1}{12N} + \frac{1}{288N^2} + \cdots\right), \tag{4}$$

with a clear procedure to compute higher-order terms.

$\log(N!) = N\log N - N + \frac{1}{2}\log(2\pi N) + \log\left(1 + \frac{1}{12N} + \frac{1}{288N^2} + \cdots\right)$

How much should we care about these corrections? You can check that although our usual approximation $\log(N!) \approx N \log N - N$ deviates from the exact result by $\sim 36\%$ for $N = 5$, it quickly becomes more accurate as N increases. Already for $N = 100$ (still tiny compared to the typical $N \sim 10^{23}$ of statistical physics), it brings us within 1% of the exact value. In addition, even for minuscule $N = 5$, adding in Stirling's $\sqrt{2\pi N}$ factor recovers the true $\log(N!)$ to better than percent-level precision.

The main challenge in the table below is to include enough significant figures to observe any discrepancy between the direct result and the approximations we computed above!

	$N = 5$	$N = 10$	$N = 50$	$N = 100$
$N \log N - N$	3.04719	13.025851	145.60115027	360.517018599
Add $\log(\sqrt{2\pi N})$	4.77085	15.096082	148.47610031	363.738542225
Add $\frac{1}{N}$	4.78738	15.104381	148.47776559	363.739375211
Add $\frac{1}{N^2}$	4.78751	15.104415	148.47776697	363.739375558
Direct $\log(N!)$	4.78749	15.104413	148.47776695	363.739375556

In addition to providing continuous functions that are easier to integrate, differentiate, or manipulate in other ways, these approximations can also improve upon the capabilities of computers we might try to use to compute $\log(N!)$ directly. The numbers above were produced by the Python code below, which determines $\log(N!)$ by first calculating $N!$ and then taking its logarithm. For $N > 170$, however, $N! \gtrsim 10^{308}$ overflows the standard floating-point precision of modern computers, and this part of the code breaks down. However, the logarithm itself is ~ 700, and remains easy to compute through the simple expression we have derived, which remains usable for far larger N.

As another application of Stirling's formula, we can revisit our consideration of the micro-canonical entropy for a spin system in Section 2.2. Specifically, on page 30, we computed the entropy $S = 2N \log 2$ for $2N$ spins with vanishing magnetic field $H = 0$, which reduced to $\log \binom{2N}{N}$ when $H > 0$ and we considered the zero-energy micro-states that remained, with N spins aligned up and the other N down. We can now apply Stirling's formula to simplify

$$\begin{aligned}
S = \log \binom{2N}{N} &= \log\left[(2N)!\right] - 2\log\left[N!\right] \\
&\approx 2N \log(2\cancel{N}) - 2\cancel{N} + \frac{1}{2}\log\left[2\pi(2N)\right] - 2N \cancel{\log N} + 2\cancel{N} - \log(2\pi N) \\
&= 2N \log 2 - \log\left(\frac{\cancel{2}\pi N}{\sqrt{\cancel{4}\pi N}}\right) = 2N \log 2 - \frac{1}{2}\log(\pi N).
\end{aligned}$$

Considering $2N = 8$, we found $S = \log(70) \approx 4.25$, which is indeed well approximated by $8 \log 2 - \log(\sqrt{4\pi}) \approx 4.28$. More generally, this result confirms our expectation that the entropy should decrease when not all 2^{2N} micro-states are accessible, and specifies the particular amount $\log(\sqrt{\pi N})$ by which it decreases.

Some other fun things you can explore with Stirling's formula include checking how it compares to the result

$$\binom{N}{k} = \frac{2^N}{\sqrt{2\pi N}} \exp\left[-\frac{(2k-N)^2}{2N}\right]$$

that we derived using the central limit theorem in Section 2.3 (pages 36–37). In addition, for the special case $p = q = \frac{1}{2}$ of the one-dimensional random walk with fixed step lengths that we analyzed in Section 1.5, you can prove that as the number of steps $N \to \infty$, the walk will return to its starting point infinitely many times, with 100% probability. This result also holds for two-dimensional random walks, where the fixed step length corresponds to walking on a square 'lattice' of points — stepping either up, down, left or right with equal probability. In the case of three (or more) dimensions, however, this probability decreases all the way down to 0%.

```
# Approximations to N!
import sys
import numpy as np
from scipy import special

# Parse argument: N
if len(sys.argv) < 2:
  print("Usage:", str(sys.argv[0]), "<spins>")
  sys.exit(1)
N = float(sys.argv[1])
print("N = %d" % N)

direct = np.log(special.factorial(N))
approx = N * np.log(N) - N
rel = 100.0 * np.abs(1 - approx/direct)
print("Nlog(N) - N = %.12g (%.2g percent off)" % (approx, rel))

approx += 0.5 * np.log(2.0 * np.pi * N)
rel = 100.0 * np.abs(1 - approx/direct)
print("Include log(N): %.12g (%.2g percent off)" % (approx, rel))

A = approx + np.log(1.0 + 1.0 / (12.0 * N))
rel = 100.0 * np.abs(1 - A/direct)
print("Include 1/N: %.12g (%.2g percent off)" % (A, rel))

B = approx + np.log(1.0 + 1.0 / (12.0 * N) + 1.0 / (288.0 * N * N))
rel = 100.0 * np.abs(1 - B/direct)
print("Include 1/N^2: %.12g (%.2g percent off)" % (B, rel))

print("Direct log(N!) = %.12g" % direct)
```

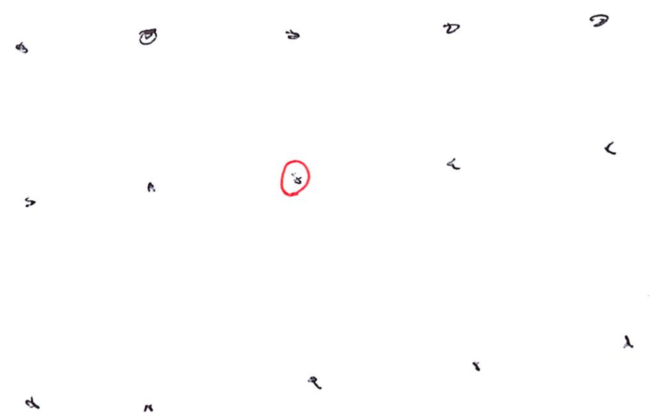
$H > 0 \quad E = 0$

$$\log\binom{2N}{N} = \log((2N)!) - 2\log(N!)$$

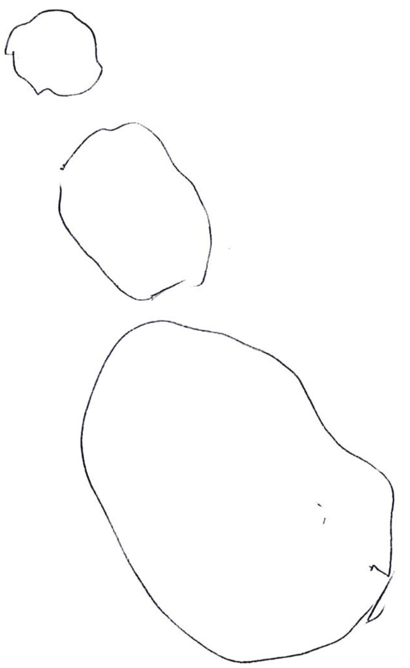
$$\simeq 2N\log(2\cancel{N}) - \cancel{2N} - 2(N\cancel{\log}N - \cancel{N})$$

$$= 2N\log 2$$

Same as $H=0$



$t\downarrow$



$* \longrightarrow$