Statistical Physics of Computation 2025 - Exercises

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Week 1

1.1 Introduction to the saddle point method

1.1.1 Basic idea

This exercise will introduce a very useful tool to compute the asymptotics of a certain type of integrals, and will allow you to practice using a toy example. Suppose we want to compute the leading order of the integral I_β for $\beta \gg 1$:

$$I_\beta = \int_{\mathbb{R}} e^{-\beta f(t)}\, dt$$

for a reasonably regular function $f(t)$ on $\mathbb{R}$, say at least twice differentiable and bounded from below.

1. Intuitively, what portion of the integration domain will dominate the leading behavior of the integral for $\beta \gg 1$?

   The portion around the values of t that minimize $f(t)$, as the integrand is very peaked around such value due to $\beta \gg 1$. More precisely, for any t that is not a minimizer of f, $e^{-\beta f(t)}$ is exponentially smaller than $e^{-\beta f(t_0)}$ if t_0 is one of the minimizer of $f(t)$.

Call $T_0 = \arg\min_t f(t) \subset \mathbb{R}$ the set of points for which $f(t)$ is (globally) minimized. Notice that as f is bounded from below, $T_0 \neq \emptyset$. Consider first the case $T_0 = \{t_0\}$, i.e. that is there is a unique global minimum.

2. Taylor expand $f(t)$ around t_0. Argue that if $f''(t_0) > 0$, then

   $$I_\beta \approx e^{-\beta f(t_0)} \int_{\mathbb{R}} e^{-\beta f''(t_0) t^2/2}\, dt\,.$$

   Write

   $$f(t) = f(t_0) + \frac{1}{2} f''(t_0) t^2 + \mathcal{O}(t^2)$$

   where we used that $f'(t_0) = 0$ because f is stationary in t_0. We obtain the result by truncating this expression at second order and plugging it into the integral. It is intuitive that far from t_0, the integrand is exponentially suppressed, so that all reminder terms are exponentially small.
   If we were to be rigorous we would need to follow these steps:

   (a) Split the integral over $\mathbb{R}$ into an integral over a small interval I_0 around t_0, and one integral over the complement $\mathbb{R} \setminus I_0$.

   (b) Show that the integral over $\mathbb{R} \setminus I_0$ is asymptotically subleading.
   (c) Show that the integral over I_0 of the original function is the same (at leading order) as the one of the function expanded to the second order around t_0, as I_0 is a small interval around t_0 (this step actually makes it possible to formalize what "small" should mean in this context).
   (d) Show that the integral of the approximated function on I_0 is the same as the one on $\mathbb{R}$ at leading order (basically redoing the first step in reverse with the approximated integrand).

3. Conclude that

$$I_\beta \approx \sqrt{\frac{2\pi}{\beta f''(t_0)}} e^{-\beta f(t_0)}$$

   Recall that $f''(t_0) > 0$ as t_0 is a minimum, so the integral is a simple Gaussian integral. The result follows from the well known formula valid for $a > 0$:

$$\int_{\mathbb{R}} e^{-at^2}\, dt = \sqrt{\frac{\pi}{a}}$$

4. Suppose $T_0 = \{t_0, t_1\}$ with $t_0 \neq t_1$. Show that

$$I_\beta \approx \sqrt{\frac{2\pi}{\beta f''(t_0)}} e^{-\beta f(t_0)} + \sqrt{\frac{2\pi}{\beta f''(t_1)}} e^{-\beta f(t_1)}$$

   Since exponential functions are rapidly decreasing we can apply the expansion trick as above independently around each of the minimizers, giving the result.

1.1.2 Concentration though the saddle point

In the class we will typically study systems with characteristic size $N \gg 1$, and study quantities of the form $\langle f(x) \rangle$

$$\langle f(x) \rangle = \frac{\int \mathrm{d}x\, f(x) e^{N\phi(x)}}{\int \mathrm{d}x\, e^{N\phi(x)}}\,. \tag{1}$$

Here you should interpret

$$p(x) = \frac{e^{N\phi(x)}}{\int \mathrm{d}x\, e^{N\phi(x)}} \tag{2}$$

as a (properly normalized) probability measure describing the statistical behavior of a macroscopic quantity $x \in \mathbb{R}$ in a complicated system of N interacting particles. We will often call x an "order parameter", a low-dimensional quantity that describes the macroscopic behavior of the system. In a magnetic system of N spins for example, x could be the magnetization of the system, i.e. the average direction in which the spins point towards. $f(x)$ is then an observable, a quantity that we want to measure in a thermodynamic system, that depends only on the order parameter, and $\langle f(x) \rangle$ is the average value of the observable in the system.

1. Assume that ϕ has a unique global maximizer x_0. Show that if N is large enough, then $\langle f(x)\rangle = f(x_0)$.

   We use the saddle point method. We can compute the denominator, which will simply be

$$\int \mathrm{d}x\, e^{N\phi(x)} = Ce^{N\phi(x_0)} \tag{3}$$

   for some constant C that we can leave unspecified in this context. For the numerator, multiplying the integrand by $f(x)$ does not change the saddle point derivation of the previous exercise, as it's independent of N. In fact:

$$\int \mathrm{d}x\, f(x)e^{N\phi(x)} = \int \mathrm{d}x\, e^{N[\phi(x)+\log f(x)/N]} \tag{4}$$

   So the integral is still dominated by the value of the integral around x_0, giving

$$\int \mathrm{d}x\, f(x)e^{N\phi(x)} = Cf(x_0)e^{N\phi(x_0)} \tag{5}$$

   with the same constant C as for the denominator. This gives the result.

2. What happens if $\phi(x)$ has two global maxima $\{x_1, x_2\}$?

   We first notice that having two global maxima means $\phi(x_1) = \phi(x_2)$, but the curvature ϕ'' near these points can look be different. Using again the saddle point method for the denominator we have

$$\sqrt{\frac{2\pi}{N}}e^{N\phi(x_1)}\left(\frac{1}{\sqrt{\phi''(x_1)}} + \frac{1}{\sqrt{\phi''(x_2)}}\right) \tag{6}$$

   while for the numerator

$$\sqrt{\frac{2\pi}{N}}e^{N\phi(x_1)}\left(\frac{f(x_1)}{\sqrt{\phi''(x_1)}} + \frac{f(x_2)}{\sqrt{\phi''(x_2)}}\right) \tag{7}$$

   A compact way to write the result is to introduce the ratio of the curvatures γ

$$\gamma = \sqrt{\frac{\phi''(x_1)}{\phi''(x_2)}} \tag{8}$$

   giving

$$\langle f(x)\rangle = \frac{f(x_1) + f(x_2)\gamma}{1+\gamma}\,. \tag{9}$$

   This is just the weighted average of f over the maxima of ϕ, with relative weighting ratio γ determined by the ratio of the curvatures.

1.1.3 Stirling's formula

Let's use the saddle point method to derive an asymptotic approximation of the factorial $n!$ for $n \gg 1$.

1. Show that for $n \in \mathbb{N}$, $n! = \int_0^\infty x^n e^{-x}\, dx$

   We do it by induction: first notice that:

   $$0! = \int_0^\infty e^{-x}\, dx = e^0 = 1$$

   then with integration by parts :

   $$n!(n+1) = (n+1)\int_0^\infty x^n e^{-x}\, dx = \int_0^\infty x^{n+1} e^{-x}\, dx = (n+1)!$$

2. Write $n! = n^{n+1}\int_0^\infty e^{-nf(x)}\, dx$ for a certain function $f(x)$

   We first do some manipulations:

   $$\int_0^\infty x^n e^{-x}\, dx = \int_0^\infty e^{n\log x - x}\, dx$$

   Now we want all the terms in the exponent to scale with the same power of n, so we do a change of variable $x \to nx$:

   $$n\int_0^\infty e^{n\log x - nx + n\log n}\, dx = n^{n+1}\int_0^\infty e^{-nf(x)}\, dx$$

   where $f(x) = x - \log x$

3. Use the saddle point method to show that for $n \gg 1$ we have:

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

   Let's study $f(t)$:

   $$f'(t) = 1 - \frac{1}{x}$$

   $$f''(t) = \frac{1}{x^2}$$

   $$f'(t) = 0 \implies x = 1$$

   $$f(1) = f''(1) = 1$$

   So with using the saddle point method we get:

   $$n! \approx \sqrt{\frac{2\pi}{n}} n^{n+1} e^{-n}$$

   We get the final formula using some algebraic manipulation

2 Entropy and free entropy

In this exercise, we review some useful relationship between entropy and free entropy. Recall that, given a system with degrees of freedom (also called microscopic variables) s and Hamiltonian (energy function) $\mathcal{H}[s]$, the free entropy is defined as

$$\Phi = \log \mathcal{Z} = \log \int ds\, e^{-\beta \mathcal{H}[s]}\,, \tag{10}$$

where we also defined the partition function $\mathcal{Z}$. The partition function $\mathcal{Z}$ is the normalization of the Gibbs distribution

$$p(s) = \frac{e^{-\beta \mathcal{H}[s]}}{\mathcal{Z}} \tag{11}$$

describing the behavior at equilibrium of the system at inverse temperature $1/\beta$.

Here we think of s as a collection of N identical variables, either continuous (then $s \in \mathbb{R}^N$) or discrete (then $s = D^N$ for some discrete set D, e.g. $D = \{+1, -1\}$, and all integrals should be though of as sums). Recall that the Hamiltonian is normalized to be extensive in the thermodynamic limit, i.e. $\mathcal{H}[s] = \mathcal{O}(N)$ for $N \gg 1$, as the energy of the system should be roughly proportional to the number of its microscopic components.

1. Show that for any model with free entropy Φ we have:

   $$\langle \mathcal{H} \rangle = -\frac{\partial \Phi}{\partial \beta}\,, \tag{12}$$

   where the angular average is w.r.t. the Gibbs distribution

   $$\langle f \rangle = \frac{\int ds\, e^{-\beta \mathcal{H}[s]} f(s)}{\int ds\, e^{-\beta \mathcal{H}[s]}}\,. \tag{13}$$

   Is this relationship true for all N, or only in the thermodynamic limit $N \to \infty$?

   We have the following identity:

   $$\frac{\partial}{\partial \beta}\mathcal{Z} = \int \frac{\partial}{\partial \beta} e^{-\beta \mathcal{H}[s]}\, ds = -\int \mathcal{H}[s] e^{-\beta \mathcal{H}[s]}\, ds = -\mathcal{Z}\langle \mathcal{H} \rangle$$

   So we have:

   $$\langle \mathcal{H} \rangle = -\frac{1}{\mathcal{Z}}\frac{\partial \mathcal{Z}}{\partial \beta} = -\frac{\partial \log \mathcal{Z}}{\partial \beta} = -\frac{\partial \Phi}{\partial \beta}$$

   This is true for any N.

2. Defining the entropy at fixed energy $S(E)$ as the logarithm of the number of configurations s at energy $\mathcal{H}[s] = E$, show that you can write the partition function as:

   $$\mathcal{Z} = \int e^{-\beta E + S(E)}\, dE \tag{14}$$

   Is this relationship true for all N, or only in the thermodynamic limit $N \to \infty$?

   We have:

   $$\mathcal{Z} = \int e^{-\beta \mathcal{H}[s]}\, ds = \int e^{-\beta E} \delta(\mathcal{H}[s] - E)\, dE ds = \int e^{-\beta E}\, dE \int \delta(\mathcal{H}[s] - E)\, ds$$

The result follows from the definition of $S(E)$:

$$S(E) = \log\left[\int \delta(\mathcal{H}[s] - E)\, ds\right]$$

3. Combine the last two results to argue that in the large N limit:

$$S(E_{\text{eq}}) = \Phi(E_{\text{eq}}) + \beta E_{\text{eq}}\,. \tag{15}$$

What is the condition that determines E_{eq}? (Hint: both E and $S(E)$ are extensive, meaning that they are proportional to N).

Notice that both E and $S(E)$ scale linearly with N, so in the large N limit e and $s(e)$ are finite (and can take non-zero values):

$$e = \frac{E}{N} \qquad s(e) = \frac{S(e)}{N}$$

We can now apply the saddle point method on equation (14) to obtain that up to a constant independent from N we have:

$$\Phi = -\beta E_{\text{eq}} + S(E_{\text{eq}})$$

where

$$E_{\text{eq}} = \arg\min_E (S(E) - \beta E)\,, \tag{16}$$

which gives the condition for E_{eq}

$$\beta = \frac{\partial S(E_{\text{eq}})}{\partial E_{\text{eq}}}\,. \tag{17}$$

Similarly in this limit $\langle E\rangle = E_{\text{eq}}$ and $\Phi = \Phi(E_{\text{eq}})$.