

# Statistical Physics of Computation 2025 - Exercises

Vittorio Erba, Emanuele Troiani

## 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  $I_\beta$  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  $\beta \gg 1$ ?

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 there is a unique global minimum.

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

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

3. Conclude that

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

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

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

### 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  $\langle f(x) \rangle$

$$\langle f(x) \rangle = \frac{\int dx f(x) e^{N\phi(x)}}{\int dx e^{N\phi(x)}}. \quad (1)$$

Here you should interpret

$$p(x) = \frac{e^{N\phi(x)}}{\int dx e^{N\phi(x)}} \quad (2)$$

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  $\phi$  has a unique global maximizer  $x_0$ . Show that if  $N$  is large enough, then  $\langle f(x) \rangle = f(x_0)$ .
2. What happens if  $\phi(x)$  has two global maxima  $\{x_1, x_2\}$ ?

### 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  $n \in \mathbb{N}$ ,  $n! = \int_0^\infty x^n e^{-x} dx$
2. Write  $n! = n^{n+1} \int_0^\infty e^{-nf(x)} dx$  for a certain function  $f(x)$
3. Use the saddle point method to show that for  $n \gg 1$  we have:

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

## 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

$$\Phi = \log \mathcal{Z} = \log \int ds e^{-\beta \mathcal{H}[s]}, \quad (3)$$

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

$$p(s) = \frac{e^{-\beta \mathcal{H}[s]}}{\mathcal{Z}} \quad (4)$$

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 thought 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  $\Phi$  we have:

$$\langle \mathcal{H} \rangle = -\frac{\partial \Phi}{\partial \beta}, \quad (5)$$

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

$$\langle f \rangle = \frac{\int ds e^{-\beta \mathcal{H}[s]} f(s)}{\int ds e^{-\beta \mathcal{H}[s]}}. \quad (6)$$

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

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:

$$\mathcal{Z} = \int e^{-\beta E + S(E)} dE \quad (7)$$

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

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

$$S(E_{\text{eq}}) = \Phi(E_{\text{eq}}) + \beta E_{\text{eq}}. \quad (8)$$

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