Statistical Physics of Computation - Exercises

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Week 1

Introduction to the saddle point method

Basic idea

This exercise will introduce a very useful tool to compute asymptotics of integral and show it in practice in an example. Suppose we want to compute 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 $\mathbb{R}$.

1. Intuitively, what values of $f(t)$ will affect the integral the most?

Call $T_0 = \arg\min_t f(t) \subset \mathbb{R}$ the set of points for which $f(t)$ is (globally) minimized. If $f(t)$ is not bounded from below, i.e. $T_0 = \emptyset$, the integral is infinite. We assume $T_0 = \{t_0\}$, that is there is a unique global minimum.

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

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

   where the corrections to this integral are exponentially small in β.

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 $t_0 \neq t_1$. As a consequence of the previous question, why do we have that?

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

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 $\langle f(x) \rangle$:

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

1. Show that if N is large enough, then $\langle f(x) \rangle = f(x_0)$, where x_0 is the global maximum of $\phi(x)$
2. What would happen if $\phi(x)$ has two global maxima $\{x_1, x_2\}$?

Stirling's formula

Let's use the saddle point method to derive a famous approximation of the factorial.

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:

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

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 s and Hamiltonian $\mathcal{H}[s]$, the free entropy is defined as

$$\Phi = \log \mathcal{Z} = \log \int ds\, e^{-\beta \mathcal{H}[s]}\,, \tag{2}$$

where we also defined the partition function $\mathcal{Z}$. Recall that the Hamiltonian is extensive in the thermodynamic limit, i.e. $\mathcal{H}[s] = \mathcal{O}(N)$.

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

$$\langle \mathcal{H} \rangle = -\frac{\partial \Phi}{\partial \beta}\,, \tag{3}$$

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

$$\langle f \rangle = \frac{\int ds\, e^{-\beta \mathcal{H}[s]} f(s)}{\int ds\, e^{-\beta \mathcal{H}[s]}}\,. \tag{4}$$

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

2. Defining the entropy at fixed energy $S(E)$ as the logarithm of the number of configurations at energy E, show that you can write the partition function as:

$$\mathcal{Z} = \int e^{-\beta E + S(E)}\, dE \tag{5}$$

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

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

$$S(E_{\text{eq}}) = \Phi(E_{\text{eq}}) + \beta E_{\text{eq}} \tag{6}$$

where E_{eq} is the energy given from the saddle point approximation maximisation condition. What is the condition that determines E_{eq}? (Hint: both E and $S(E)$ are extensive, meaning that they are proportional to N).

Central Limit Theorem using field theory

Consider N independent samples x_1, ... x_N of a random variable $x \sim p(x)$, where p has mean μ and variance σ^2. We define the random variable y_N as the average of the N samples:

$$y_N = \frac{1}{N}\sum_n x_n \,, \tag{7}$$

then in the large N limit y_N converges in distribution to $y \sim q(y) = \mathcal{N}(\mu, \sigma^2/N)$. This basic fact of probability theory is called the Central Limit Theorem. As an exercise we will derive it using field theory techniques.

Recall the definition of the Dirac's delta distribution δ

$$\int dx \delta(x - x_0) f(x) = f(x_0) \,, \tag{8}$$

and its Fourier representation

$$\delta(x) = \int \frac{d\hat{x}}{2\pi} \exp^{i\hat{x}x} \,. \tag{9}$$

1. Write the distribution of y_n, which we want to show it converges to $q(y)$, as a function of $p(x)$ by using the delta function to impose the definition of y.

2. Rewrite the delta in Fourier representation (also called informally exponential form).

3. We start with a weaker form of the result (the law of large numbers): let's show that at the zeroth order in N, $\hat{y}_N$ converges in distribution to $q(y) = \delta(y - \mu)$. Do it by expanding the exponential in power series, keep the zeroth order terms in N, then resum.

4. (Bonus) As we saw from the previous computation, $y = \mu$ at leading order in N. Thus, in the previous computation, we could have avoided enforcing the definition of y using the δ distribution, as y naturally respects the constraint enforced by the delta in the large N limit (recall that $\sum_i x_i/N \to \mu$ for large N). Whenever this is the case, i.e. whenever we enforce a "vacuous" constraint using a delta function, we can take $\hat{y} \approx 0$. Intuitively, $\hat{y}$ is an external field that enforces the constraint (very much like a magnetic field used to induce a magnetisation in a magnetic system), and if the system satisfies already the constraint, no external field is needed.

   Thus, it's reasonable to expand around $\hat{y} = 0$. Expand the exponential in power series and keep only the leading order terms up to second order in $\hat{y}$, then "resum" the exponential to show that the fluctuations are Gaussian