Statistical Physics of Computation - Exercises

Emanuele Troiani, Vittorio Erba, Yizhou Xu

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Week 4

4.1 Tools for the replica method

4.1.1 Eigenvalues of the replica symmetric overlap

Consider an $n \times n$ matrix with all entries on the diagonal equal to q and all entries outside of the diagonal equal to r. This is called a replica symmetric (RS) matrix. We want to compute the eigenvalues of the matrix.

1. Map this problem to finding the eigenvalues of a matrix with all entries equal to r.

The eigenvalues λ of a matrix Q the solutions to the equation

$$Qv = \lambda v \tag{1}$$

where v is a certain vector. Let's call 1 the matrix with ones on every entry, and 1 the identity matrix. We have $Q = \mathbf{1}r + \mathbb{1}(q-r)$. If we substitute this in the definition of eigenvalue we get

$$[\mathbf{1}r + \mathbf{1}(q-r)] v = \lambda v \tag{2}$$

$$\mathbf{1}rv = (\lambda + r - q)v \tag{3}$$

2. Recognise that the eigenvalues of such a matrix are either 0 with multiplicity n-1 or nr with multiplicity one.

A matrix with the same value r on each entry is of rank one. The only non zero eigenvalue needs to be equal to the trace, so it equals nr.

3. Find the eigenvalues of the original matrix.

The n-1 degenerate eigenvalues correspond to $\lambda = q-r$, the non-degenerate one to $\lambda = q + (n-1)r$

4.1.2 Entropic piece of the free entropy

A common ingredient of replica computations where the degrees of freedom are constrained on the sphere is given by the integral

$$S_{\text{entropy}}(q^{ab}) = \log \left(\int \prod_{a} d\mathbf{x}^{a} \prod_{a \le b} \delta \left(Nq^{ab} - (\mathbf{x}^{a})^{\top} \mathbf{x}^{b} \right) \right)$$
(4)

for a given symmetric matrix q^{ab} , where $q^{aa}=1$ on the diagonal. Here $a=1,\ldots,n$, and each $x^a\in\mathbb{R}^N$ In the context of the storage problem we saw in the lecture, q^{ab} is the $n\times n$ replica overlap, with $1\leq a,b\leq n$, \mathbf{x}^a and \mathbf{x}^b are two replicas of the perceptron's weights, which means that they are two independent sample both extracted from the uniform distribution on the N-dimensional sphere, and N is taken to be large. This quantity encodes the different ways in which n vectors on the sphere x^a can have a certain overlap structure q^{ab} .

1. Use the Fourier representation of the delta functions to rewrite the integral as

$$S_{\text{entropy}}(q^{ab}) = \log \left(\int d\hat{q} \, e^{N \sum_{a,b} \hat{q}_{ab} q_{ab}} \int \prod_{a} d\mathbf{x}^{a} \exp \left\{ -\sum_{a,b} \hat{q}^{ab} (\mathbf{x}^{a})^{\top} \mathbf{x}^{b} \right\} \right)$$
(5)

$$\int \prod_{a} d\mathbf{x}^{a} \prod_{a \le b} \delta \left(Nq^{ab} - (\mathbf{x}^{a})^{\top} \mathbf{x}^{b} \right) =$$
(6)

$$\int d\hat{q} \int \prod_{a} d\mathbf{x}^{a} \prod_{a \leq b} \exp \left\{ N \hat{q}^{ab} q^{ab} - \hat{q}^{ab} (\mathbf{x}^{a})^{\top} \mathbf{x}^{b} \right\} =$$
 (7)

$$\int d\hat{q} \int \prod_{a} d\mathbf{x}^{a} \exp \left\{ N \sum_{a,b} \hat{q}^{ab} q^{ab} - \sum_{a,b} \hat{q}^{ab} (\mathbf{x}^{a})^{\top} \mathbf{x}^{b} \right\} =$$
(8)

$$\int d\hat{q} \, e^{N \sum_{a,b} \hat{q}_{ab} q_{ab}} \int \prod_{a} d\mathbf{x}^{a} \exp \left\{ -\sum_{a,b} \hat{q}^{ab} (\mathbf{x}^{a})^{\top} \mathbf{x}^{b} \right\}$$
(9)

where in the third line we sent $\hat{q}_{ab} \to \hat{q}_{ab}/2$ for all $a \neq b$ plus used the symmetry in a, b to promote the sums from $a \leq b$ to a, b.

2. Show that one can write

$$S_{\text{entropy}}(q^{ab}) = \log \left(\int d\hat{q} \, e^{N \left[\sum_{a,b} \hat{q}_{ab} q_{ab} + I_{\text{entropy}}(\hat{q}^{ab}) \right]} \right)$$
 (10)

where

$$I_{\text{entropy}}(\hat{q}^{ab}) = \log \left(\int \prod_{a} dx^{a} \exp \left\{ -\sum_{a,b} \hat{q}^{ab} x^{a} x^{b} \right\} \right)$$
 (11)

Notice that here the integral is not anymore over x is not \mathbb{R}^N , but it is just over \mathbb{R} .

$$\int \prod_{a} d\mathbf{x}^{a} \exp \left\{ -\sum_{a,b} \hat{q}^{ab} (\mathbf{x}^{a})^{\top} \mathbf{x}^{b} \right\} =$$
(12)

$$\int \prod_{a,i} \mathrm{d}x_i^a \exp\left\{-\sum_i \sum_{a,b} \hat{q}^{ab} x_i^a x_i^b\right\} = \tag{13}$$

$$\left[\int \prod_{a} \mathrm{d}x^{a} \exp \left\{ -\sum_{a,b} \hat{q}^{ab} x^{a} x^{b} \right\} \right]^{N} \tag{14}$$

3. Now we are reduced to a n-dimensional integral. Using a Gaussian integration, show that

$$I_{\text{entropy}}(\hat{q}^{ab}) = -\frac{1}{2}\log\det 2\hat{q}^{ab} + \frac{n}{2}\log(2\pi)$$
(15)

We first integrate over x. This is a Gaussian integral, so

$$\int \prod_{a} \mathrm{d}x^{a} \exp\left\{-\sum_{a,b} \hat{q}^{ab} x^{a} x^{b}\right\} = \sqrt{\frac{(2\pi)^{n}}{\det(2\hat{q}^{ab})}}$$
 (16)

The result follows from taking the log.

4. Using the saddle point method for $N \gg 1$ conclude that at leading order

$$\frac{1}{N}S_{\text{entropy}}(q^{ab}) = \frac{1}{2}\log\det q^{ab} + 2n + \frac{n}{2}\log(2\pi)$$
(17)

A comment on this formula: it's typical in the physics literature to drop the last two pieces because they are independent of q^{ab} , i.e. they do not alter the state equations. Hint: you can use Jacobi's formula to take the derivative of a determinant.

We take a saddle point. We get the equation (remember to use the chain rule when taking derivatives):

$$q^{ab} = \frac{1}{2} \left(2\hat{q}^{ab} \right)^{-1} 2 = \left(2\hat{q}^{ab} \right)^{-1} \tag{18}$$

where the $(\cdot)^{-1}$ is intended as a matrix inverse. Plugging this in back in our exponent we obtain

$$\sum_{a,b} \left[q^{ab} \hat{q}^{ab} \right] = \sum_{a,b} \left[\hat{q}^{ab} \left(2\hat{q}^{ab} \right)^{-1} \right] = 2 \sum_{a,b} \left[\delta_{ab} \right] = 2n \tag{19}$$

and

$$-\frac{1}{2}\log\det 2\hat{q}^{ab} = -\frac{1}{2}\log\det\left(q^{ab}\right)^{-1} = \frac{1}{2}\log\det q^{ab}$$
 (20)

5. Now let's assume we are replica symmetric, with q^{ab} with entries on the diagonal equal to one and entries out of the diagonal equal to q. Neglecting all q-independent term, show that

$$\lim_{n \to 0} \frac{S_{\text{entropy}}}{nN} = \frac{1}{2} \log(1 - q) + \frac{q}{2(1 - q)}$$
 (21)

The determinant of a matrix is the product of its eigenvalues. Using the previous exercise, we have

$$\det(q^{ab}) = (1-q)^{n-1}[1+(n-1)q]$$
(22)

Or equivalently

$$S_{\text{entropy}}(q) = \frac{N}{2} \log \det(q^{ab}) = \frac{N}{2} \left((n-1) \log(1-q) + \log[1 + (n-1)q] \right)$$
 (23)

We need to be careful in taking the $n \to 0$ limit. We have (expanding in powers of n):

$$\log[1 + (n-1)q] = \log(1-q) + \frac{n}{1-q}(-q) + \mathcal{O}(n) = \log(1-q) + \frac{nq}{1-q} + \mathcal{O}(n)$$
 (24)

So we get

$$\lim_{n \to 0} \frac{S_{\text{entropy}}}{nN} = \frac{1}{2} \log(1 - q) + \frac{q}{2(1 - q)}$$
 (25)

4.2 Zooming in close to the SAT/UNSAT transition in the storage problem

We have seen in class that the overlap q is the solution to the state equation

$$\frac{q}{1-q} = \frac{\alpha}{2\pi} \int \mathcal{D}t \, e^{-\frac{(\kappa - \sqrt{q}t)^2}{1-q}} \left[H\left(\frac{\kappa - \sqrt{q}t}{\sqrt{1-q}}\right) \right]^{-2} \tag{26}$$

where \mathcal{D} is the Normal Gaussian measure and H(x) is the cumulative function of the Gaussian

$$H(x) = \frac{1}{\sqrt{2\pi}} \int_{r}^{+\infty} e^{-\frac{t^2}{2}} dt$$
 (27)

Here κ is the margin and $\alpha = P/N$ is the number of patterns per dimension.

1. Assume that there is a phase transition at $\alpha = \alpha_c(\kappa)$. For which values of α is there a SAT phase and for which an UNSAT one? What is the effect of changing κ on the critical $\alpha_c(\kappa)$?

If there are many patterns it's hard to satisfy our constraints, so for $\alpha > \alpha_C$ is UNSAT, and viceversa $\alpha < \alpha_C$ is SAT. Having a larger κ reduces the space of solutions, as the contraints are more difficult to satisfy, so increasing κ raises $\alpha_c(\kappa)$.

2. What is the overlap at small α ? Answer intuitively and then check with the equation.

If there are very little constraints then basically all vectors J on the sphere solve the constraints. Then q is the projection of a random vector on the sphere on another one, which in the high dimensional limit is zero (there are $N-1\gg 1$ orthogonal direction to each vector, so a random vector will have overlap zero with a given vector with very high probability).

We can see that $\alpha = 0$ in the state equation immediately implies that q = 0.

3. What is the overlap as α approaches α_c from the SAT phase, i.e. $\alpha \to \alpha_c^-$?

In the SAT phase there is an non-empty space of solutions by definition, which shrinks as $\alpha \to \alpha_C^-$. This means that if we take two solutions they are going to be extremely similar in this limit, so $q \to 1^-$.

4. We now use point 3 to compute $\alpha_c(\kappa)$. It is often the case that even if we cannot solve analytically the state equations, we can at least characterise the phase transition points to some extent. Show that in the limit $q \to 1^-$, the cumulative function H has the following limit

$$H\left(\frac{\kappa - \sqrt{qt}}{\sqrt{1-q}}\right) = \theta(t-\kappa) + \theta(\kappa - t)e^{-\frac{(\kappa - t)^2}{2(1-q)}}\sqrt{\frac{1-q}{2\pi}}\frac{1}{\kappa - t}$$
 (28)

Hint: recall that for very large arguments $x \to +\infty$, H(x) has the following asymptotics

$$H(x) \approx \frac{1}{\sqrt{2\pi}x} e^{-\frac{x^2}{2}} \tag{29}$$

We have two cases.

(a) Case $t < \kappa$: here $\kappa - \sqrt{q}t \approx \kappa - t > 0$ will be positive and the argument of the H function will diverge to plus infinity, where $H(x) \approx 1$.

- (b) Case $t > \kappa$: here $\kappa \sqrt{q}t \approx \kappa t < 0$ will be negative and the argument of the H function will diverge to minus infinity, where H(x) vanishes. At leading order, H(x) behaves as the hint suggests, giving the answer.
- 5. The decomposition of the H function strongly suggests us to split the integral in two regions, namely $t \in (-\infty, \kappa)$ and $t \in (\kappa, +\infty)$. Using the expansion for the H function, show that the contribution from the integral $t \in (\kappa, +\infty)$ goes to zero as $q \to 1^-$.

We consider the integral

$$\int_{\kappa}^{+\infty} \mathcal{D}t \, e^{-\frac{(\kappa - \sqrt{q}t)^2}{1 - q}} \left[H\left(\frac{\kappa - \sqrt{q}t}{\sqrt{1 - q}}\right) \right]^{-2} \,. \tag{30}$$

The H function converges to 1 as $q \to 1^-$ as we saw in the previous point, so we have

$$\int_{\kappa}^{+\infty} \mathcal{D}t \, e^{-\frac{(\kappa - \sqrt{q}t)^2}{1 - q}} \left[H\left(\frac{\kappa - \sqrt{q}t}{\sqrt{1 - q}}\right) \right]^{-2} \approx \int_{\kappa}^{+\infty} \mathcal{D}t \, e^{-\frac{(\kappa - \sqrt{q}t)^2}{1 - q}} = \int_{\kappa}^{+\infty} \frac{dt}{\sqrt{2\pi}} \, e^{-\frac{t^2}{2} - \frac{(\kappa - \sqrt{q}t)^2}{1 - q}} \,. \tag{31}$$

Now change variable to $z = (\kappa - \sqrt{q}t)/\sqrt{1-q}$ to get

$$\int_{\kappa}^{+\infty} \mathcal{D}t \, e^{-\frac{(\kappa - \sqrt{q}t)^2}{1 - q}} \left[H\left(\frac{\kappa - \sqrt{q}t}{\sqrt{1 - q}}\right) \right]^{-2} \approx \sqrt{\frac{1 - q}{q}} \int_{\kappa}^{+\infty} \frac{dz}{\sqrt{2\pi}} \, e^{-\frac{(\kappa - z\sqrt{1 - q})^2}{2q} - z^2} \,. \tag{32}$$

This, at leading order in 1-q equals

$$\int_{\kappa}^{+\infty} \mathcal{D}t \, e^{-\frac{(\kappa - \sqrt{q}t)^2}{1 - q}} \left[H\left(\frac{\kappa - \sqrt{q}t}{\sqrt{1 - q}}\right) \right]^{-2} \approx \sqrt{1 - q} \int_{\kappa}^{+\infty} \frac{dz}{\sqrt{2\pi}} \, e^{-\frac{\kappa^2}{2} - z^2} \,, \tag{33}$$

and the remaining integral is independent on q, so that the overall expression vanishes.

6. Thus, in the $q \to 1^-$ limit we can approximate

$$\int \mathcal{D}t \, e^{-\frac{(\kappa - \sqrt{q}t)^2}{1-q}} \left[H\left(\frac{\kappa - \sqrt{q}t}{\sqrt{1-q}}\right) \right]^{-2} \approx \int_{-\infty}^{\kappa} \mathcal{D}t \, e^{-\frac{(\kappa - \sqrt{q}t)^2}{1-q}} \left[H\left(\frac{\kappa - \sqrt{q}t}{\sqrt{1-q}}\right) \right]^{-2} \,. \tag{34}$$

Now use again the expansion for H to show that the state equation can be written as

$$\alpha = \left[\int_{-\infty}^{\kappa} \mathcal{D}t \left(\kappa - t \right)^2 \right]^{-1} \tag{35}$$

We start by using the expansion of H

$$\frac{q}{1-q} = \frac{\alpha}{2\pi} \int_{-\infty}^{\kappa} \mathcal{D}t \, e^{-\frac{(k-t)^2}{1-q}} \left[\frac{2\pi(\kappa-t)^2}{1-q} e^{\frac{(k-t)^2}{1-q}} \right]$$
(36)

Doing some simplifications we get

$$1 = \alpha \int_{-\infty}^{\kappa} \mathcal{D}t \left(\kappa - t\right)^2 \tag{37}$$

which is equivalent to the result

7. Conclude that for $\kappa = 0, \, \alpha = 2$

The result follows from the fact that

$$\int_{-\infty}^{0} \mathcal{D}t \, t^2 = \frac{1}{2} \tag{38}$$

To be precise, one should also consider a possible contribution to the integral $t \in (\kappa - \epsilon \sqrt{1-q}, \kappa + \epsilon \sqrt{1-q})$ where the expansion in point 4 breaks down, but one can show that in this problem this contribution also vanishes. This part of the computation is outside of the scope (and level of mathematical rigour) of the course, so we do not pursue it.