Problem Set 1

Instructions: Aim to earn at least 100 points from the problems below. Subproblems are equally weighted (e.g. Problem 1(a) is worth 48/4 = 12 points), and you can earn credit for later subproblems without solving the previous ones. Points will be cumulative throughout the semester, so you are warmly encouraged to earn more than 100 points on this problem set. You may also submit solutions to *extra problems* (listed on a separate sheet) at the end of any problem sets. Solutions should be written in Latex and submitted in PDF format.

Collaboration with your classmates is encouraged. However you should identify everyone you worked with at the beginning of your solution PDF (e.g. Collaborators: Alice, Bob, and Eve). Your solutions should be <u>written</u> entirely by you, even if you collaborated to <u>solve</u> the problems.

The first person to report each mistake in this problem set (by emailing me and Yufan) will receive up to 5 extra points, depending on the mistake.

Problem 1. Practice with Free Energies (48 points)

Let μ be a probability measure on an arbitrary measurable space Ω , and let $H: \Omega \to [-C, C]$ be a bounded measurable function. The associated partition function, free energy, and Gibbs measure are given by:

$$Z(\beta) = \mathbb{E}^{\omega \sim \Omega}[e^{\beta H(\omega)}], \qquad F(\beta) = \log Z(\beta), \qquad \mu_{\beta}(\mathrm{d}\omega) = \frac{e^{\beta H(\omega)}\mu(\mathrm{d}\omega)}{Z(\beta)}. \tag{1}$$

(a) Show that F is a convex function of β , and

$$\frac{\mathrm{d}F(\beta)}{\mathrm{d}\beta} = \mathbb{E}^{\omega \sim \mu_{\beta}}[H(\omega)].$$

(Hint: Hölder's inequality may be helpful to show convexity.)

(b) Define the super-level set

$$\Omega(\gamma_{+}) = \{ \omega \in \Omega : H(\omega) \ge \gamma \}. \tag{2}$$

Give an integral formula for $F(\beta)$ in terms of the volumes $V(\gamma) = \mu(\Omega(\gamma_+))$.

(c) Let $H_N: \Omega_N \to [-CN, CN]$ be a (non-random) sequence of Hamiltonians on probability spaces (Ω_N, μ_N) , for $N = 1, 2, \ldots$ Let $F_N(\beta) = \frac{1}{N} \log Z_N(\beta)$. Assume that

$$\lim_{N \to \infty} F_N(\beta) = \beta^2 / 2 \tag{3}$$

for each $\beta \in [0, \beta_0]$. Define the super-level set volume $V_N(\gamma)$ as above for each H_N . For each $\beta \in (0, \beta_0)$, show that

$$\limsup_{N \to \infty} \frac{1}{N} \log V_N(\beta) \le -\beta^2/2.$$

(Hint: if $V_N(\beta)$ is too big, $F_N(\beta)$ will be too big.)

(d) Under the conditions of the previous part, show that in fact

$$\lim_{N \to \infty} \frac{1}{N} \log V_N(\beta) = -\beta^2/2.$$

(Hint: suppose that $\frac{1}{N} \log V_N(\beta) \leq -\beta^2/2 - \varepsilon$ is too small. Since $V_N(\cdot)$ is decreasing, the same is true for $\tilde{\beta} = \beta + 2\delta$, where $\delta > 0$ is small depending on (β, ε) . Use the upper bound from the previous part to show that $F_N(\beta + \delta)$ is also too small.)

Problem 2. Random Spherical Perceptron for $\kappa = 0$ (48 points)

In this problem, you will solve the random spherical perceptron in the case $\kappa = 0$. Recall that for $\kappa \in \mathbb{R}$ and $\alpha > 0$, the N-dimensional spherical perceptron is defined by the $M = \alpha N$ constraints

$$\langle \boldsymbol{\sigma}, \mathbf{g}_a \rangle \ge \kappa \sqrt{N}, \quad 1 \le a \le M.$$

Here the vectors $\mathbf{g}_1, \dots, \mathbf{g}_M \in \mathbb{R}^N$ are IID standard Gaussian (i.e. the NM coordinates are IID standard Gaussian). We say the point $\boldsymbol{\sigma} \in \mathcal{S}_N \subseteq \mathbb{R}^N$ with norm $\|\boldsymbol{\sigma}\| = \sqrt{N}$ is a solution if it obeys all of these constraints.

(a) Consider the M hyperplanes

$$U_a = \mathbf{g}_a^{\perp} \subseteq \mathbb{R}^N.$$

Argue that each region in \mathbb{R}^N formed by these hyperplanes corresponds to a different value of the vector

$$\left(\operatorname{sign}(\langle \boldsymbol{\sigma}, \mathbf{g}_1), \operatorname{sign}(\langle \boldsymbol{\sigma}, \mathbf{g}_2), \dots, \operatorname{sign}(\langle \boldsymbol{\sigma}, \mathbf{g}_M)\right) \in \{\pm 1\}^M.$$

In other words, two vectors $\boldsymbol{\sigma}, \boldsymbol{\sigma}' \notin \bigcup_{a=1}^M U_a$ are connected by a continuous path in the complement of $\bigcup_{a=1}^M U_a$ if and only if they have the same sign pattern. (Hint: line segments will suffice as paths.)

(b) Let $R_N(\mathbf{g}_1, \dots, \mathbf{g}_M)$ denote the (random) number of N-dimensional regions formed in this way. Show that if $M \leq N$, then almost surely

$$R_N(\mathbf{g}_1,\ldots,\mathbf{g}_M)=2^M.$$

(Hint: use linear independence and the previous part.)

- (c) Note that R_N does not change if any subset of vectors \mathbf{g}_a are negated. Using symmetry, deduce that for $\kappa = 0$, the probability for a solution $\boldsymbol{\sigma}$ to exist is exactly $\mathbb{E}[R_N(\mathbf{g}_1, \dots, \mathbf{g}_M)]/2^M$.
- (d) Argue that

$$R(N, \mathbf{g}_1, \dots, \mathbf{g}_M) - R(N, \mathbf{g}_1, \dots, \mathbf{g}_{M-1})$$

is equal to the number of regions formed by the (N-2) dimensional subspaces

$$U_1 \cap U_M$$
, $U_2 \cap U_M$,..., $U_{M-1} \cap U_M$

within U_M . Identify this as $R_{N-1}(\boldsymbol{v}_1,\ldots,\boldsymbol{v}_{M-1})$ for some vectors $\boldsymbol{v}_{M-1}\in U_M\simeq\mathbb{R}^{N-1}$, and show the vectors \boldsymbol{v}_a are again IID standard Gaussian.

(e) Show by induction (e.g. on N+M) that $R_N(\mathbf{g}_1,\ldots,\mathbf{g}_M)$ is almost surely constant, and in fact equals

$$2\sum_{k=0}^{N-1} \binom{M-1}{k}.$$

(f) Deduce that for $\kappa = 0$, a spherical perceptron solution $\sigma \in \mathcal{S}_N$ exists with high probability when $\alpha < 2$, but does not exist when $\alpha > 2$.

Problem 3. Concentration and Spin Glass Free Energies (48 points)

This problem concerns p-spin models as in lecture, with Hamiltonian

$$H_N(\boldsymbol{\sigma}) = N^{-(p-1)/2} \sum_{1 \leq i_1, \dots, i_p \leq N} g_{i_1, \dots, i_p} \boldsymbol{\sigma}_{i_1} \dots \boldsymbol{\sigma}_{i_p} = N^{-(p-1)/2} \langle \boldsymbol{G}_N^{(p)}, \boldsymbol{\sigma}^{\otimes p} \rangle.$$

Here $G_N^{(p)} \in \mathbb{R}^{N^p}$ has IID standard Gaussian coordinates $(g_{i_1,\dots,i_p})_{1 \leq i_1,\dots,i_p \leq N}$. The Ising and spherical partition functions are defined by:

$$Z_N^{\mathrm{Is}}(\beta) = Z_N^{\mathrm{Is}}(H_N; \beta) = \beta^{-1} \log \left(2^{-N} \sum_{\boldsymbol{\sigma} \in \{\pm 1\}^N} e^{\beta H_N(\boldsymbol{\sigma})} \right);$$
$$Z_N^{\mathrm{sp}}(\beta) = \beta^{-1} \log \int_{\mathcal{S}_N} e^{\beta H_N(\boldsymbol{\sigma})} d\boldsymbol{\sigma},$$

where the latter integral is with respect to the uniform distribution on the sphere

$$S_N = \{ \boldsymbol{\sigma} \in \mathbb{R}^N : \| \boldsymbol{\sigma} \| = \sqrt{N} \}.$$

We set $F_N^{\mathrm{Is/sp}}(\beta) = \frac{1}{N} \log Z_N^{\mathrm{Is/sp}}(\beta)$. (Note the extra factor of 1/N compared to (1).)

(a) Show that for the Ising p-spin model, one has almost surely

$$\left(\frac{1}{N} \max_{\boldsymbol{\sigma} \in \{\pm 1\}^N} H_N(\boldsymbol{\sigma})\right) - \frac{\log 2}{\beta} \le F_N^{\mathrm{Is}}(\beta)/\beta \le \frac{1}{N} \max_{\boldsymbol{\sigma} \in \{\pm 1\}^N} H_N(\boldsymbol{\sigma}). \tag{4}$$

Explain why this can be interpreted as commutation of $N \to \infty$ and $\beta \to \infty$ limits.

(b) Recall from class that for some C = C(p) > 0 and c > 0 independent of N, we have

$$\max_{\sigma \in \mathcal{S}_N} \|\nabla H_N(\sigma)\| \le C\sqrt{N}$$

with probability $1 - e^{-cN}$. Prove that for any sequence H_1, H_2, \ldots obeying this bound, we have

$$\lim_{\beta \to \infty} \lim_{N \to \infty} \left| \frac{1}{N} \max_{\|\boldsymbol{\sigma}\| = \sqrt{N}} H_N(\boldsymbol{\sigma}) - F_N^{\rm sp}(\beta) / \beta \right| = 0.$$

This qualitatively matches (4). (Hint: consider a ball of radius $\delta\sqrt{N}$ around the maximizer $\sigma \in \mathcal{S}_N$, where δ tends to 0 with β at an appropriate rate.)

(c) Recall from class that both $\max_{\|\boldsymbol{\sigma}\|=\sqrt{N}} H_N(\boldsymbol{\sigma})/N$ and $F_N^{\rm sp}(\beta)$ are $N^{-1/2}$ -Lipschitz functions of $\boldsymbol{G}_N^{(p)}$, hence concentrate sharply around their expectation. Using this and the previous part, prove that

$$\lim_{\beta \to \infty} \lim_{N \to \infty} \mathbb{E} \left| \frac{1}{N} \max_{\|\boldsymbol{\sigma}\| = \sqrt{N}} H_N(\boldsymbol{\sigma}) - F_N^{\mathrm{sp}}(\beta) / \beta \right| = 0.$$

(d) In the famously non-rigorous replica method from physics, one computes free energies using the observation

$$\frac{1}{N}\log Z_N = \lim_{\varepsilon \to 0} \frac{Z_N^{\varepsilon} - 1}{N\varepsilon}.$$
 (5)

The method first finds an asymptotic formula as $N \to \infty$ for $\frac{1}{N} \log \mathbb{E}[Z_N^k]$ for integers $k \ge 1$, and then formally sends $k \downarrow 0$ in this formula. While the latter step seems impossible to justify directly, another potential issue is the inconsistency of the order of limits. Namely the formula (5) sends $\varepsilon \to 0$ for fixed N instead of sending $N \to \infty$ for fixed ε . Using the concentration of the free energy, prove that for any constant β ,

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \left| \frac{1}{N} \mathbb{E} \log Z_N(\beta) - \mathbb{E} \left[\frac{Z_N(\beta)^{\varepsilon/N} - 1}{\varepsilon} \right] \right| = 0.$$

In other words, the interchange of limits is justified if ε is scaled by a factor of N. You may use either the Ising or spherical model here; the proof should not strongly depend on this choice.

(Hint: the main surprise is the upper bound on $\mathbb{E}[Z_N(\beta)^{\varepsilon/N}]$. Here you will really need a sub-Gaussian tail bound for $F_N(\beta)$, not just concentration with exponentially good probability.)

Problem 4: Posterior of Tensor PCA (96 points)

Recall from class that in tensor PCA, one generates $x \in S_N$ uniformly at random, and observes the signal

$$\boldsymbol{T}_N = \boldsymbol{G}^{(p)} + \lambda N^{-(p-1)/2} \boldsymbol{x}^{\otimes p}.$$

Here $G_N^{(p)} \in \mathbb{R}^{N^p}$ is as in the previous problem, and $\lambda > 0$ is a "signal strength" not depending on N. Hence $T_N \in \mathbb{R}^{N^p}$ has entries

$$(T_N)_{i_1,\dots,i_p} = g_{i_1,\dots,i_p} + \lambda N^{-(p-1)/2} x_{i_1} x_{i_2} \dots x_{i_p}.$$

(a) Given T_N , define¹

$$H_N(\boldsymbol{\sigma}) = N^{-(p-1)/2} \langle \boldsymbol{T}_N, \boldsymbol{\sigma}^{\otimes p} \rangle = \langle \boldsymbol{G}_N^{(p)}, \boldsymbol{\sigma}^{\otimes p} \rangle + \lambda N \left(\frac{\langle \boldsymbol{x}, \boldsymbol{\sigma} \rangle}{N} \right)^p.$$

Show that the posterior distribution of x given T_N is the Gibbs measure μ_{λ} for Hamiltonian $H_N: \mathcal{S}_N \to \mathbb{R}$.

(b) Let

$$Band_{\boldsymbol{x}}(q) = \{ \boldsymbol{\sigma} \in \mathcal{S}_N : \langle \boldsymbol{\sigma}, \boldsymbol{x} \rangle / N = q \}$$

and note that $Band_{\boldsymbol{x}}(q)$ has (N-1)-dimensional volume proportional to $(1-q^2)^{N/2}$. Let $\mu_{\boldsymbol{x},q}$ denote the uniform distribution on this band. Explain why, **assuming** that the limit

$$F_{\lambda}(q) = \lim_{N \to \infty} \frac{1}{N} \mathbb{E}^{G_N^{(p)}} \log \int e^{\lambda H_N(\boldsymbol{\sigma})} d\mu_{\boldsymbol{x},q}(\boldsymbol{\sigma})$$
 (6)

exists for each $q \in (-1,1)$ and $\lambda \geq 0$, it is natural to expect the limiting free energy for tensor PCA is

$$\lim_{N \to \infty} \frac{1}{N} \mathbb{E} \log \int_{\mathcal{S}_N} e^{\lambda H_N(\boldsymbol{\sigma})} d\boldsymbol{\sigma} = \max_{q \in (-1,1)} F_{\lambda}(q) + q^p + \frac{\log(1 - q^2)}{2}. \tag{7}$$

(c) Using continuity and concentration properties of H_N , prove that (7) indeed follows rigorously from the assumption that the limit $F_{\lambda}(q)$ exists. (Hint: cover \mathcal{S}_N by a large constant number of thin bands.)

In the next problems, we will find the (Bayes-optimal) minimum mean-squared error in tensor PCA, assuming $F_{\lambda}(q)$ is known. Assume p is odd, and the maximum in (7) is attained uniquely at $q = q_*(\lambda)$.

- (d) Let σ be a sample from the posterior distribution of x given T_N . Show that $\langle \sigma, x \rangle/N$ converges in probability to q_* as $N \to \infty$.
- (e) Let $\sigma^{(1)}, \sigma^{(2)}$ be independent samples from the posterior distribution of \boldsymbol{x} given \boldsymbol{T}_N . Show that averaged over all the randomness (including $\boldsymbol{x} \in \mathcal{S}_N$ and $\boldsymbol{G}_N^{(p)}$), the pair $(\boldsymbol{\sigma}^{(1)}, \boldsymbol{\sigma}^{(2)}) \in \mathcal{S}_N^2$ has the same distribution as $(\boldsymbol{\sigma}^{(1)}, \boldsymbol{x})$.
- (f) Show that

$$\lim_{N \to \infty} \frac{1}{N} \mathbb{E} \big[\| \boldsymbol{x} - \mathbb{E} [\boldsymbol{x} \mid \boldsymbol{T}_N] \|^2 \big] = 1 - q_*^2.$$

The left-hand side is the asymptotic Bayes-optimal mean-squared error in tensor PCA. (Hint: approximate $\mathbb{E}[\boldsymbol{x} \mid \boldsymbol{T}_N]$ by the average of K posterior samples $\boldsymbol{\sigma}^{(j)}$ for a large constant K, and use the previous parts.)

Problem 5. Survey (4 points)

Rate each of the four problems above that you worked on from 1 to 5 based on:

- Interestingness (1 for boring, 5 for exciting)
- Difficulty (1 for too easy, 5 for too hard)
- Learning (1 for almost nothing, 5 if you learned a lot).

Finally (optionally), you are encouraged to share any comments you have regarding this problem set or the recent lectures, especially with potential improvements for future weeks or years of the course.

¹Here the inner product is the usual one in \mathbb{R}^{N^p} , i.e. we ignore the tensor structure that the N^p numbers are arranged into.