STAT260 Mean Field Asymptotics in Statistical Learning	Lecture 2 - 01/25/2021

Lecture 2: Basic concepts in statistical physics

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In this lecture, we introduce some basic concepts in statistical physics. We start with introducing the Gibbs distribution on a given configuration space with an energy function (or the Hamiltonian). Then we introduce the thermodynamic potentials, and derive their connections. The free energy function (one of the thermodynamical potential) is the most important quantity to be calculated in studying the mean field asymptotics.

> *"The free energy function is the most important quantity to be calculated in statistical physics. It can be used to derive most of the properties of a given physical system."*

1 Configuration space and Gibbs distribution

We denote by Ω the **configuration space**, which is the set of **configurations** $\sigma \in \Omega$. An **observables** is a mapping $f : \Omega \to \mathbb{R}$ from the configuration space to real numbers. The **energy function** (or **Hamiltonian**) $H : \Omega \to \mathbb{R}$ is a special observable. For better understanding of these concepts, here we use an example of the Ising model, which is a mathematical model of ferromagnetism in statistical mechanics.

Concept	Example (Ising model)
Configuration space : Ω	$\Omega = \{\pm 1\}^n$ (possible state of n-spins)
Configuration : $\sigma \in \Omega$	$\sigma = (+1, -1, +1, +1, \ldots, -1)$
Observable : $f : \Omega \to \mathbb{R}$	$f(\sigma) = \sum_{i=1}^n \sigma_i$
Energy function : $H : \Omega \to \mathbb{R}$ (Hamiltonian)	$H(\sigma) = \sum_{i \neq j, i,j \in [n]} J_{ij}\sigma_i\sigma_j$ Ferromagnetic model : $J_{ij} = -1$ Spin glass model : $J_{ij} \overset{i.i.d}{\sim} N(0, \sigma^2)$

1.1 Gibbs/Boltzman distribution and Ensemble average of an observable

From now on, we will disregard measure-theoretic niceties throughout this course. (Configuration space Ω will be a measurable set and functions will be measurable functions). Now fix our configuration space Ω and the Hamiltonian H, and fix a given reference measure ν_0 on Ω. Then for $\beta \geq 0$, we define the **Gibbs distribution** on Ω by

$$P_\beta(\mathrm{d}\sigma) := \frac{1}{Z(\beta)} \exp\{-\beta H(\sigma)\}\nu_0(\mathrm{d}\sigma). \tag{1}$$

Here $Z(\beta)$, named the **partition function**, is defined by

$$Z(\beta) := \int_\Omega \exp\{-\beta H(\sigma)\}\nu_0(\mathrm{d}\sigma), \tag{2}$$

which works as a normalizing factor to make the Gibbs distribution a probability density on Ω. The parameter β is called the inverse temperature ($\beta = 1/T$) of the system.

For a given observable $f : \Omega \to \mathbb{R}$, the **ensemble average** of the observable f, denoted by $\langle f \rangle_\beta$, is defined as the expectation of f under the Gibbs distribution:

$$\langle f \rangle_\beta := \int_\Omega f(\sigma) P_\beta(\mathrm{d}\sigma). \tag{3}$$

Remark 1. *We consider the high temperature limit $\beta \to 0$ and the low temperature limit $\beta \to \infty$ of the Gibbs distribution. One can easily check that when $\beta \to 0$ or $T \to \infty$, then $P_\beta \to \nu_0$ (the high temperature limit) when ν_0 is a probability measure. When $\beta \to \infty$ or $T \to 0$, then P_β concentrates on $\Omega_0 := \arg\min_\sigma H(\sigma)$ (the low temperature limit), i.e., we have $\lim_{\beta\to\infty} \mathbb{P}_\beta(\Omega_0) = 1$.*

2 Thermodynamic potentials

2.1 Thermodynamic potentials and properties

We define 4 thermodynamic potentials in statistical physics. Now we fix a configuration space Ω, a Hamiltonian H, and a reference measure ν_0 (and thus the Gibbs distribution P_β can be defined). The thermodynamics potentials are as functions of β defined as below:

$$\text{Free energy}: \ F(\beta) := -\frac{1}{\beta}\log Z(\beta), \tag{4}$$

$$\text{Free entropy}: \ \Phi(\beta) := \log Z(\beta), \tag{5}$$

$$\text{Internal energy}: \ U(\beta) := \langle H \rangle_\beta, \tag{6}$$

$$\text{Canonical entropy}: \ S(\beta) := -\int_\Omega P_\beta(\sigma)\log P_\beta(\mathrm{d}\sigma). \tag{7}$$

Then we have following identities.

Proposition 2. *The following identities hold:*

$$\Phi'(\beta) = -\langle H\rangle_\beta = -U(\beta) \tag{8}$$

$$\Phi''(\beta) = \langle H^2\rangle_\beta - \langle H\rangle_\beta^2 \geq 0 \tag{9}$$

$$S(\beta) = \beta U(\beta) + \Phi(\beta) \tag{10}$$

Sketch of proof. Here we drop a little bit of rigorousness where we assume the functions are smooth enough so that we can change the order of differentiation and integration without justifying them (this is why we call the "sketch" of proof). Further justification will be made on individual examples. To prove Eq. (8), we start with

$$Z'(\beta) = \frac{d}{d\beta}\int_\Omega \exp\{-\beta H(\sigma)\}\nu_0(\mathrm{d}\sigma) = \int_\Omega (-H(\sigma))\exp\{-\beta H(\sigma)\}\nu_0(\mathrm{d}\sigma), \tag{11}$$

and thus we have

$$\Phi'(\beta) = \frac{d}{d\beta}\log Z(\beta) = \frac{Z'(\beta)}{Z(\beta)} = \int_\Omega (-H(\sigma))P_\beta(\mathrm{d}\sigma) = -\langle H\rangle_\beta. \tag{12}$$

To prove Eq. 9, we take second derivative of the partition function, so we have

$$Z''(\beta) = \frac{d}{d\beta}\int_\Omega (-H(\sigma))\exp\{-\beta H(\sigma)\}\nu_0(\mathrm{d}\sigma) = \int_\Omega (H(\sigma))^2\exp\{-\beta H(\sigma)\}\nu_0(\mathrm{d}\sigma), \tag{13}$$

and thus,

$$\Phi''(\beta) = \frac{d}{d\beta}\frac{Z'(\beta)}{Z(\beta)} = \frac{Z''(\beta)}{Z(\beta)} - \Big(\frac{Z'(\beta)}{Z(\beta)}\Big)^2 = \int_\Omega (H(\sigma))^2 P_\beta(\mathrm{d}\sigma) - (-\langle H\rangle_\beta)^2 = \langle H^2\rangle_\beta - \langle H\rangle_\beta^2, \tag{14}$$

where the third equality comes from Eq. (8). FInally, Eq. (10), we prove the case where the configuration space is discrete and our reference measure is the counting measure.

$$\begin{aligned}
S(\beta) &= -\sum_{\sigma\in\Omega} P_\beta(\sigma)\log P_\beta(\sigma) \\
&= -\sum_{\sigma\in\Omega} P_\beta(\sigma)(-\beta H(\sigma) - \log Z(\beta)) \\
&= \beta\langle H\rangle_\beta + \log Z(\beta) \\
&= \beta U(\beta) + \Phi(\beta).
\end{aligned}$$

Where the third equality uses the fact that $\sum_{\sigma\in\Omega} P_\beta(\sigma) = 1$.

2.2 Thermodynamic limit and phase transition

Throughout most of the remaining lectures, we will work with a sequence of configuration spaces $\{\Omega_n\}$ and Hamiltonians $\{H_n\}$, so that we can define a sequence of potentials $F_n(\beta)$, $\Phi_n(\beta)$, $U_n(\beta)$ and $S_n(\beta)$. In many systems, for large n, these potentials are often proportional to n, and thus it is natural to define the **free energy density** as below

$$f(\beta) := \lim_{n\to\infty} F_n(\beta)/n. \tag{15}$$

Now let's assume that $f(\beta)$ can be well defined (the limit exists for each β). Then we can similarly define $\phi(\beta)$, $u(\beta)$ and $s(\beta)$. Since Eq. (9) guarantees that each $\Phi_n(\beta)/n$ is convex, the limit is also convex. Thus $\phi(\beta)$ is continuous, so that $f(\beta)$ is also continuous.

In many examples in statistical physics, $f(\beta)$ is often analytic in some region of β. However, at some critical temperature $\beta = \beta_c$, $f(\beta)$ can be non-analytic. In that case, we say that there is a **phase transition** of the system at critical temperature β_c. We will go through actual examples in next lectures where the phase transition occurs. □

3 Ensemble average/variance of an observable using perturbed systems

In this section, we introduce a method to calculate the ensemble average/variance of given observables. Let's say we have an observable $M(\sigma)$ and we want to calculate $\lim_{n\to\infty}\langle M\rangle_\beta/n$. (In this section, we drop the subscript n in (H_n, F_n, M_n, ...) for notational simplicity). We assume that we have some oracles: given any Hamiltonian H_λ, we are able to calculate its free energy function

$$F(\beta,\lambda) := -\frac{1}{\beta}\log\int_\Omega \exp\{-\beta H_\lambda(\sigma)\}\nu_0(\mathrm{d}\sigma). \tag{16}$$

To calculate $\langle M\rangle_\beta$, the idea is to introduce a perturbed Hamiltonian

$$H_\lambda(\sigma) := H(\sigma) + \lambda M(\sigma), \tag{17}$$

and define the associated Gibbs measure $P_{\beta,\lambda}(\mathrm{d}\sigma) \propto \exp\{-\beta H_\lambda(\sigma)\}\nu_0(\mathrm{d}\sigma)$. We can also define $Z_{\beta,\lambda}$, $\Phi_{\beta,\lambda}$ and $F_{\beta,\lambda}$ for each β,λ. Finally, for an observable $g:\Omega\to\mathbb{R}$, we define

$$\langle g\rangle_{\beta,\lambda} := \int_\Omega g(\sigma)P_{\beta,\lambda}(\mathrm{d}\sigma). \tag{18}$$

The following proposition enables us to calculate the ensemble average and variance of M.

Proposition 3. *Given a perturbed system from Eq. (17), the following identities hold:*

$$\partial_\lambda F(\beta,\lambda) = \langle M\rangle_{\beta,\lambda}, \tag{19}$$

$$\partial_\lambda^2 \Phi(\beta,\lambda) = \beta^2\Big(\langle M^2\rangle_{\beta,\lambda} - \langle M\rangle_{\beta,\lambda}^2\Big). \tag{20}$$

So with $\lambda = 0$, we have

$$\partial_\lambda F(\beta,\lambda)|_{\lambda=0} = \langle M\rangle_{\beta} \tag{21}$$

$$\partial_\lambda^2 \Phi(\beta,\lambda)|_{\lambda=0} = \beta^2\Big(\langle M^2\rangle_{\beta} - \langle M\rangle_{\beta}^2\Big) \tag{22}$$

where the ensemble averages are from original Hamiltonian H (note that $H_0(\sigma) = H(\sigma)$).

Sketch of proof. Again, we assume that functions are nice enough so that we are free to change the orders of derivatives and integrals. With similar arguments from the proof of Proposition 2, we have

$$\begin{aligned}
\partial_\lambda F(\beta,\lambda) &= \frac{\partial}{\partial\lambda}\Big(-\frac{1}{\beta}\log\int_\Omega \exp\{-\beta H_\lambda(\sigma)\}\nu_0(\mathrm{d}\sigma)\Big)\\
&= -\frac{1}{\beta}\frac{\partial}{\partial\lambda}\Big(\int_\Omega \exp\{-\beta H(\sigma) - \beta\lambda M(\sigma)\}\nu_0(\mathrm{d}\sigma)\Big)/Z(\beta,\lambda)\\
&= -\frac{1}{\beta}\int_\Omega (-\beta M(\sigma))\frac{1}{Z(\beta,\lambda)}\exp\{-\beta H_\lambda(\sigma)\}\nu_0(\mathrm{d}\sigma)\\
&= \langle M\rangle_{\beta,\lambda},
\end{aligned}$$

which proves Eq. (19). Similarly,

$$\begin{aligned}
\partial_\lambda^2\Phi(\beta,\lambda) &= (\partial_\lambda^2 Z(\beta,\lambda))/Z(\beta,\lambda) - ((\partial_\lambda Z(\beta,\lambda))/Z(\beta,\lambda))^2\\
&= \int_\Omega (-\beta M(\sigma))^2\frac{1}{Z(\beta,\lambda)}\exp\{-\beta H_\lambda(\sigma)\}\nu_0(\mathrm{d}\sigma) - (\int_\Omega (-\beta M(\sigma))\frac{1}{Z(\beta,\lambda)}\exp\{-\beta H_\lambda(\sigma)\}\nu_0(\mathrm{d}\sigma))^2\\
&= \langle(-\beta M)^2\rangle_{\beta,\lambda} - \langle(-\beta M)\rangle_{\beta,\lambda}^2\\
&= \beta^2\Big(\langle M^2\rangle_{\beta,\lambda} - \langle M\rangle_{\beta,\lambda}^2\Big)
\end{aligned}$$

which proves Eq. (20). □

Remark 4. *Define*

$$f(\beta,\lambda) := \lim_{n\to\infty} F_n(\beta,\lambda)/n, \qquad m_\star(\beta,\lambda) := \lim_{n\to\infty}\langle M\rangle_{\beta,\lambda}/n. \tag{23}$$

If we drop a little bit of rigorousness again and assume that we can change the order of derivatives and limits, we have the following identity:

$$\partial_\lambda f(\beta,\lambda) = m_\star(\beta,\lambda) \tag{24}$$

So that $m_\star(\beta,0)$, which was our original interest, can be calculated from the free energy density of the perturbed system.