{Lecture 2}

Gibbs variational approach

Introduce Kullback-Leibler (KL) divergence:

$$D_{KL}(P\|Q) = \int d\vec{x}\, P(\vec{x}) \log \frac{P(\vec{x})}{Q(\vec{x})}$$

Using $\log x \leq x-1$, $x \geq 0$,

[$\log x = x-1$ iff $x = 1$]

we obtain:

$$-D_{KL}(P\|Q) = \int d\vec{x}\, P(\vec{x}) \log \frac{Q(\vec{x})}{P(\vec{x})} \leq$$

$$\leq \int d\vec{x}\, P(\vec{x}) \left(\frac{Q(\vec{x})}{P(\vec{x})} - 1 \right) = \int d\vec{x}\, Q(\vec{x}) - \int d\vec{x}\, P(\vec{x}) =$$

$=0$, so that

$$D_{KL}(P\|Q) \geq 0 \quad \text{and} \quad D_{KL}(P\|Q) = 0$$

iff $P(\vec{x}) = Q(\vec{x})$.

Next, consider $P(\vec{x}) = \dfrac{e^{-\beta H(\vec{x})}}{Z_N}$:

$$\langle \log P(\vec{x}) \rangle_Q = -\beta \langle H \rangle_Q - \underbrace{\log Z_N}_{= N\Phi_N} , \text{ or}$$

$\langle \ldots \rangle_Q$ = expectation wrt $Q(\vec{x})$

$$\underbrace{\langle \log P \rangle_Q - \langle \log Q \rangle_Q}_{-D_{KL}(Q\|P)} = -\beta \langle H \rangle_Q - N\varphi_N - $$
$$- \langle \log Q \rangle_Q .$$

Define $N\varphi^{\text{gibbs}} = \underbrace{\overset{\text{entropy}}{S[Q]}}_{-\langle \log Q \rangle_Q} - \beta \langle H \rangle_Q$, then

$$-D_{KL}(Q\|P) = N\varphi^{\text{gibbs}} - N\varphi_N \quad , \text{ or}$$

$$N\varphi_N = N\varphi^{\text{gibbs}} + \underbrace{D_{KL}(Q\|P)}_{\geq 0} .$$

Thus, $\varphi_N \geq \varphi^{\text{gibbs}}$

$[\ \varphi_N = \varphi^{\text{gibbs}}$ iff $Q = P\ ]$

Now, consider Curie-Weiss model again:
(CW)

recall that
$$\begin{cases} p = \dfrac{N_+}{N} = \dfrac{1+m}{2}, \\ 1-p = \dfrac{N_-}{N} = \dfrac{1-m}{2} . \end{cases}$$

Consider a system of N <u>independent</u> spins:

$$\underbrace{Q(\vec{S})}_{\text{prob. of } \vec{S}} = \prod_{i=1}^{N} \underbrace{Q(S_i)}_{p\,\delta_{S_i,+1} + (1-p)\,\delta_{S_i,-1}} .$$

For each spin,

$$m_s = p(+1) + (1-p)(-1) = 2p - 1 = m,$$

as expected

Here, $$-\langle \log Q \rangle_Q = -N[\underbrace{p\log p + (1-p)\log(1-p)}_{-\underbrace{H(m)}_{\text{one-spin entropy}}}] \ominus$$

$\ominus$ $NH(m)$.

For example, $$\sum_{\{\vec{s}\}} \frac{\sum_{i=1}^{N} s_i}{N} \prod_{j=1}^{N} Q(s_i) = \frac{Nm}{N} = m$$

Next, $$-\beta\langle H \rangle_Q = \beta N \left[\frac{m^2}{2} + hm\right].$$

Then $$\varphi^{gibbs}(m) = \beta\left[\frac{m^2}{2} + hm\right] + \underline{\underline{H(m)}}.$$

Recall that

$$\varphi(\beta, h) = \lim_{N\to\infty} \varphi_N(\beta, h) = \varphi(m^*) =$$

$$= H(m^*) + \frac{\beta m^{*2}}{2} + \beta h m^*.$$

m^* maximizes $\varphi(m)$.

If we maximize $\varphi^{gibbs}(m)$ as a function of m, we'll get $\varphi(\beta, h)$ <u>exactly</u>.

The cavity method

What happens if we add one more variable to the system: $N \to N+1$?

Consider
$$-\beta' H_{N+1} = \frac{\beta'}{2}(N+1)\left(\frac{\overset{\text{extra spin}}{S_0} + \sum_{i=1}^{N} S_i}{N+1}\right)^2 +$$
$$+ \underbrace{\beta' h'}_{\text{new prms}}\left(S_0 + \sum_{i=1}^{N} S_i\right) = \frac{\beta'}{2(N+1)} + \frac{\beta'}{2}\frac{N^2}{N+1}\left(\frac{\sum_i S_i}{N}\right)^2 +$$
$$+ \beta' S_0 \frac{N}{N+1}\left(\frac{\sum_i S_i}{N}\right) + \beta' h' \sum_i S_i + \beta' h' S_0 \,.$$

Define
$$\begin{cases} \beta' = \beta \dfrac{N+1}{N}, & \to \beta' h' = \beta h \\ h' = h \dfrac{N}{N+1}, & \text{then} \end{cases}$$

$$-\beta' H_{N+1}(h') = \frac{\beta}{2} N \left(\frac{\sum_i S_i}{N}\right)^2 + \beta S_0 \left(\frac{\sum_i S_i}{N}\right) +$$
$$+ \beta h \sum_i S_i + \beta h S_0 + \text{const}(\vec{S}, S_0) =$$
$$= -\beta H_N + \beta S_0 \underbrace{\left(\frac{\sum_i S_i}{N}\right)}_{\equiv \bar{S}\text{, average value in the old system}} + \beta h S_0 + \text{const}(\vec{S}, S_0) \,.$$

Now, consider
$$\langle S_0 \rangle_{N+1,\beta'} = \frac{\sum_{S_0,\vec{S}} S_0\, e^{-\beta' H'_{N+1}}}{\sum_{S_0,\vec{S}} e^{-\beta' H'_{N+1}}} \boxed{=}$$

$$\Leftrightarrow \frac{\sum_{\vec{s}} \sum_{s_0} s_0 \, e^{-\beta H_N + \beta s_0 \bar{s} + \beta h s_0}}{\sum_{\vec{s}} \sum_{s_0} e^{-\beta H_N + \beta s_0 \bar{s} + \beta h s_0}} =$$

$$= \frac{\langle \sinh(\beta(\bar{s}+h)) \rangle_{N,\beta}}{\langle \cosh(\beta(\bar{s}+h)) \rangle_{N,\beta}} .$$

as $N \to \infty$, $\beta' \to \beta$ & $h' \to h$.

Moreover, $\bar{s} \to m^*$ (single max of $\varphi(m)$ assumed here)

Then $\langle s_0 \rangle_{N+1,\beta'} \to m^*$ as well, and

$$m^* \underset{N\to\infty}{=} \frac{\sinh(\beta(m^*+h))}{\cosh(\beta(m^*+h))} = \underline{\underline{\tanh(\beta(m^*+h))}} .$$

[We recovered the mean-field equation from before (!)]

Next, we focus on

$$\frac{1}{N} \log Z_N = \frac{1}{N} \log\left(\frac{Z_N}{Z_{N-1}} Z_{N-1} \right) =$$

$$= \frac{1}{N} \log\left(\frac{Z_N}{Z_{N-1}} \frac{Z_{N-1}}{Z_{N-2}} \cdots \frac{Z_1}{\underset{\underset{1}{\parallel}}{Z_0}} \right) = \underbrace{\frac{1}{N} \sum_{n=0}^{N-1} \log \frac{Z_{n+1}}{Z_n}}_{\log \frac{Z_{\tilde{n}+1}}{Z_{\tilde{n}}} \text{ for some } \tilde{n}}$$

In the $N \to \infty$ limit, $\tilde{n} \to \infty$ as well.

Thus, $\Phi(\beta, h) = \lim_{N\to\infty} \log \dfrac{Z_{N+1}(\beta,h)}{Z_N(\beta,h)}$.

rename $\tilde{n} \to N$

We can compute

$$-\beta H_{N+1} = \frac{\beta}{2}(N-1+o(1))\,\bar{s}^2 + \beta s_0 (1+o(1))\,\bar{s} + \beta h (s_0 + \sum_i s_i) + \underbrace{o(1)}_{\frac{\beta}{2(N+1)}} =$$

$$\begin{cases} \dfrac{N}{N+1} = 1 - \underbrace{\dfrac{1}{N+1}}_{o(1)}, & \text{'little o'} \\[2ex] \dfrac{N^2}{N+1} = \dfrac{N(N+1)-N}{N+1} = N - 1 + \underbrace{\dfrac{1}{N+1}}_{o(1)} \end{cases}$$

$$= -\beta H_N - \frac{\beta}{2}\bar{s}^2 + \underbrace{\beta s_0 \bar{s} + \beta h s_0}_{= \beta s_0 (\bar{s}+h)} + o(1).$$

Finally, $\dfrac{Z_{N+1}}{Z_N} = \left\langle e^{-\frac{\beta}{2}\bar{s}^2}\, 2\cosh(\beta(\bar{s}+h)) \right\rangle_{N,\beta}$.

Since $\bar{s} \to m^*$ in the $N \to \infty$ limit,

$$\Phi(\beta,h) = \underbrace{-\frac{\beta}{2} m^{*2} + \log[2\cosh(\beta(m^*+h))]}_{= \tilde{\varphi}(m^*)}.$$

Now, $\Phi(\beta,h) = \max_m \tilde{\varphi}(m)$

$\tilde{\varphi}(m) \neq \varphi(m)$ from before, but

$\tilde{\varphi}(m)$ & $\varphi(m)$ coincide at all fixed points.

First, note that

$$\left.\frac{d\tilde{\varphi}}{dm}\right|_{m^*} = -\beta m^* + \beta \tanh(\beta(m^*+h)) = 0, \text{ or}$$

$$m^* = \tanh(\beta(m^*+h)), \text{ the correct}$$

mean-field equation.

One can use the identity:

$$\log\left[2\cosh(\operatorname{atan}(x))\right] = x \operatorname{atanh}(x) +$$

$$+ \underbrace{H(x)}_{-\left(\frac{1+x}{2}\log\frac{1+x}{2} + \frac{1-x}{2}\log\frac{1-x}{2}\right)}$$

entropy function

to obtain: $\tilde{\varphi}(m^*) = -\frac{\beta}{2}m^{*2} + \log[2\cosh(\underbrace{\beta(m^*+h)}_{\operatorname{atanh}(m^*)})] =$

$$= -\frac{\beta}{2}m^{*2} + m^* \underbrace{\operatorname{atanh}(m^*)}_{\beta(m^*+h)} + H(m^*) =$$

$$= \frac{\beta}{2}m^{*2} + \beta h m^* + H(m^*) = \varphi(m^*).$$