Homework 6
(due Friday, April 21, 2006)

April 26, 2006

1. **Mean field theory:** Consider the objective function

$$E(s) = -\left[\frac{1}{2}\sum_{m=0}^{N-1}\sum_{n=0}^{N-1} J_{mn} s_m s_n + \sum_{n=0}^{N-1} h_n s_n\right] \tag{1}$$

with $s_m \in \{-1, 1\}, \forall m$. In (1). (In the above, $m \oplus 1 = 0$ when $m = N-1$ and $m \ominus 1 = N-1$ when $m = 0$.) $J_{mn} = 0$ when $n \neq m \oplus 1$ or $n \neq m \ominus 1$. The corresponding probability distribution is

$$\Pr(S = s) = \frac{\exp\{-\beta E(s)\}}{Z(\beta)}. \tag{2}$$

- If the free energy $F \stackrel{\text{def}}{=} -T \log Z$ where $T = \frac{1}{\beta}$, evaluate $\frac{\partial F}{\partial T}$ and show its relationship to the entropy. What does this relationship mean conceptually?

The free energy $F = -T \log\, Z = -T \log(\sum_s \exp\{-\frac{E(s)}{T}\})$. From this we get

$$\begin{aligned}\frac{\partial F}{\partial T} &= -\log(\sum_s \exp\{-\frac{E(s)}{T}\}) - \frac{1}{T}\frac{\sum_s E(s)\exp\{-\frac{E(s)}{T}\})}{\sum_s \exp\{-\frac{E(s)}{T}\})} \\ &= -\log\, Z - \frac{1}{T} < E > \\ &= -S. \end{aligned} \tag{3}$$

This relationship indicates that the rate of change of the free energy with temperature is equal to the negative of the entropy. It gives us an alternative way of computing the entropy.

- Relate $\frac{\partial \log Z}{\partial h_i}$ and $\frac{\partial^2 \log Z}{\partial h_i^2}$ to the mean and variance of s_m. Construct corresponding derivatives to express the mean and variance of the product $s_m s_n$. What do these relationships mean conceptually?

The partial derivative

$$\frac{\partial \log Z}{\partial h_i} = \frac{\partial \log(\sum_s \exp\{-\frac{E(s)}{T}\})}{\partial h_i} = \frac{1}{T}\frac{\sum_s s_i \exp\{-\frac{E(s)}{T}\})}{\sum_s \exp\{-\frac{E(s)}{T}\})} = \frac{1}{T} < s_i > .$$

The second derivative

$$\frac{\partial^2 \log Z}{\partial h_i^2} = \frac{1}{T^2}\frac{\sum_s s_i^2 \exp\{-\frac{E(s)}{T}\})}{\sum_s \exp\{-\frac{E(s)}{T}\})} - \frac{1}{T^2}\left(\frac{\sum_s s_i \exp\{-\frac{E(s)}{T}\})}{\sum_s \exp\{-\frac{E(s)}{T}\})}\right)^2 = \frac{1}{T^2}(< s_i^2 > - < s_i >^2).$$

Similarly,

$$\begin{aligned}\frac{\partial \log Z}{\partial J_{ij}} &= \frac{1}{T} < s_i s_j > \\ \frac{\partial^2 \log Z}{\partial J_{ij}^2} &= \frac{1}{T^2}(< s_i s_j >^2 - < s_i s_j >^2).\end{aligned}$$

- Assume a mean field approximation wherein we construct a second distribution $Q(s) = \frac{\exp\{-\beta \sum_{m=0}^{N-1} r_m s_m\}}{\prod_{m=0}^{N-1}(\exp\{\beta r_m\}+\exp\{-\beta r_m\})}$ and determine the best $\{r_m\}$ that minimizes the Kullback-Leibler (KL) divergence $D(Q||P) = \sum_{\{s\}} Q(s) \log \frac{Q(s)}{P(s)}$. What is the optimized value of $D(Q||P)$ in terms of the optimal value of $\{r_m\}$?