p-spin model and belief propagation

1. The "3-spin" Curie-Weiss model

The 3-spin ferromagnetic model is a generalization of the Curie-Weiss model that reads

$$\mathcal{H}\left(\{S_i\}_{i=1}^N\right) = -\frac{1}{N^2}\sum_{i,j,k} S_iS_jS_k - h\sum_i S_i = -N\left[\left(\frac{\sum_i S_i}{N}\right)^3 + h\frac{\sum_i S_i}{N}\right]$$

(a) Using the method we developed in the lecture, by computing the number of configuration with a given magnetization m and then using the Stirling formula, show that the free energy per spin of the 3-spin model $f(\beta,h) = -\frac{1}{N\beta}\lim_{N\to\infty}\log Z_N(\beta,h)$ can be written (asymptotically) as $f(\beta,h) = \min_{m\in[-1,1]}\mathcal{F}_m(\beta,h,m)$, with the free energy at fixed magnetization $\mathcal{F}_m(\beta,h,m)$ being given by:

$$\mathcal{F}_m(\beta,h,m) = -m^3 - hm + \frac{1}{\beta}\left[\frac{1+m}{2}\log\left(\frac{1+m}{2}\right) + \frac{1-m}{2}\log\left(\frac{1-m}{2}\right)\right]$$

and the equilibrium value of the magnetization is given by the minimizer m^*:

$$\left\langle\frac{\sum_i S_i}{N}\right\rangle = m^*$$

(b) Consider the case $h = 0$ (also in part (c) and (d)) and plot the function $\mathcal{F}_m(\beta, h = 0, m)$ as a function of m for different values of the inverse temperature β. Compute the value of m^* for many temperatures to show that it has a *first order transition* (that is: there is a discontinuity).

(c) Show (numerically) that there is are three regions: for $\beta < \beta_s$ there is a unique minima in $m = 0$. For $\beta_s < \beta < \beta_c$ a second local minima appears. For $\beta_c < \beta$ the second minima is now the global one. Find the values of β_s and β_c.

(d) Describe your expectation about the long-time (but not exponentially in N long) behavior of the Monte Carlo Markov Chain designed to sample the Boltzmann distribution. When initialized at magnetization $m = 0$, and when initialized at $m = 1$. You can modify your code from the previous homework to support your intuition.

Solution.

(a) First for notation simplicity, define the natural-based entropy function

$$H_e(x) = -x\log(x) - (1-x)\log(1-x)$$

Denote $\mathcal{N}(m)$ to be the number of configurations with magnetization m, it is easy to see

$$\mathcal{N}(m) = \binom{N}{\frac{N+Nm}{2}} = \frac{N!}{\left(\frac{1+m}{2}N\right)!\left(\frac{1-m}{2}N\right)!}$$

When $N \to \infty$, use Stirling formula

$$\begin{aligned}
\mathcal{N}(m) &\approx \frac{\sqrt{2\pi N}\left(\frac{N}{\mathrm{e}}\right)^N}{\sqrt{2\pi\frac{1+m}{2}N}\left(\frac{(1+m)N}{2\mathrm{e}}\right)^{\frac{1+m}{2}N}\cdot\sqrt{2\pi\frac{1-m}{2}N}\left(\frac{(1-m)N}{2\mathrm{e}}\right)^{\frac{1-m}{2}N}} \\
&= \sqrt{\frac{2}{(1-m^2)\pi N}}\exp\left(-N\left[\frac{1+m}{2}\log\left(\frac{1+m}{2}\right)+\frac{1-m}{2}\log\left(\frac{1-m}{2}\right)\right]\right) \\
&= \exp\left(-N\left[\frac{1+m}{2}\log\left(\frac{1+m}{2}\right)+\frac{1-m}{2}\log\left(\frac{1-m}{2}\right)+\mathrm{o}(1)\right]\right) \\
&= \exp\left(N\left[H_{\mathrm{e}}\left(\frac{1+m}{2}\right)+\mathrm{o}(1)\right]\right) \qquad (1)
\end{aligned}$$

Given the Hamiltonian $\mathcal{H}$, we can write down the partition function

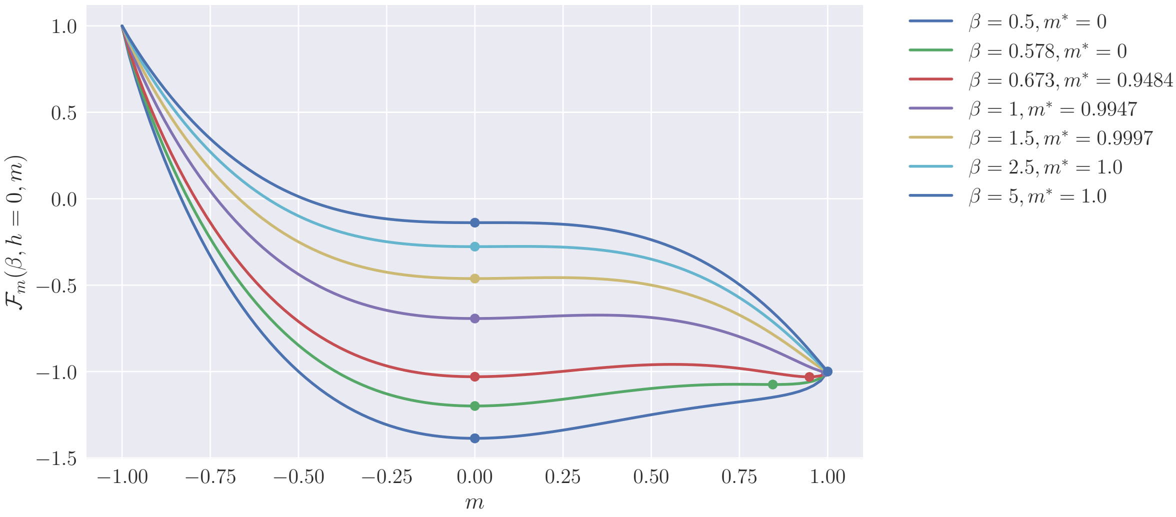
$$\begin{aligned}
Z_N(\beta,h) &= \sum_{\{S_i\}_{i=1}^N}\exp\left(-\beta\mathcal{H}\left(\{S_i\}_{i=1}^N\right)\right) \\
&= \sum_{\{S_i\}_{i=1}^N}\exp\left(N\beta\left[\left(\frac{\sum_i S_i}{N}\right)^3+h\frac{\sum_i S_i}{N}\right]\right) \\
&= \sum_{\substack{m=-1\\ \text{step }\frac{2}{N}}}^{+1}\sum_{\{S_i\}_{i=1}^N}\mathbb{I}\left(\frac{\sum_i S_i}{N}=m\right)\exp\left(N\beta\left[\left(\frac{\sum_i S_i}{N}\right)^3+h\frac{\sum_i S_i}{N}\right]\right) \\
&= \sum_{\substack{m=-1\\ \text{step }\frac{2}{N}}}^{+1}\mathcal{N}(m)\exp\left(N\beta\left(m^3+hm\right)\right) \qquad (2)
\end{aligned}$$

As $N \to \infty$, by plugging eqn 1 to eqn 2 and notice that the o(1) term is negligible, the free energy per spin can be computed as

$$\begin{aligned}
f(\beta,h) &= -\lim_{N\to\infty}\frac{1}{N\beta}\log\left(Z_N(\beta,h)\right) \\
&= -\lim_{N\to\infty}\frac{1}{N\beta}\log\left\{\sum_{\substack{m=-1\\ \text{step }\frac{2}{N}}}^{+1}\mathcal{N}(m)\exp\left(N\beta\left(m^3+hm\right)\right)\right\} \\
&= -\lim_{N\to\infty}\frac{1}{N\beta}\log\left\{\int_{-1}^{+1}\mathrm{d}m\,\exp\left(N\beta\left(m^3+hm-\frac{1}{\beta}H_{\mathrm{e}}\left(\frac{1+m}{2}\right)+\mathrm{o}(1)\right)\right)\right\} \\
&\overset{\text{Laplace}}{=\!=} -\frac{1}{\beta}\max_{m\in[-1,1]}\left[\beta\left(m^3+hm-\frac{1}{\beta}H_{\mathrm{e}}\left(\frac{1+m}{2}\right)\right)\right] \\
&= \min_{m\in[-1,1]}\left[-m^3-hm+\frac{1}{\beta}H_{\mathrm{e}}\left(\frac{1+m}{2}\right)\right] \\
&= \min_{m\in[-1,1]}\mathcal{F}_m(\beta,h,m)
\end{aligned}$$

When N is large, the Boltzmann distribution is dominated by the 'typical' configurations $\{S_i\}_{i=1}^N$ such that $\sum_i S_i/N = m^*$, where m^* is the minimizer of $\mathcal{F}_m(\beta,h,m)$. Therefore, when we compute the Boltzmann average $\langle\sum_i S_i/N\rangle$, in the large N limit it is just the magnetization of 'typical' configurations, which is m^*.

(b) The plot of function $\mathcal{F}_m(\beta,h,m)$ under $h=0$ and $\beta = 0.5, 0.578, 0.673, 1, 1.5, 2.5, 5$, the local minima are marked at dot.



It can be seen when $m = 0$ is always a local minima, as β increases to some value, the second local minima emerges at right side but the global minima is still at $m = 0$. If β keeps on increasing to a higher value, the global minima suddenly jumps to the right local minima, causing a discontinuity on $m^*(\beta, h)$.

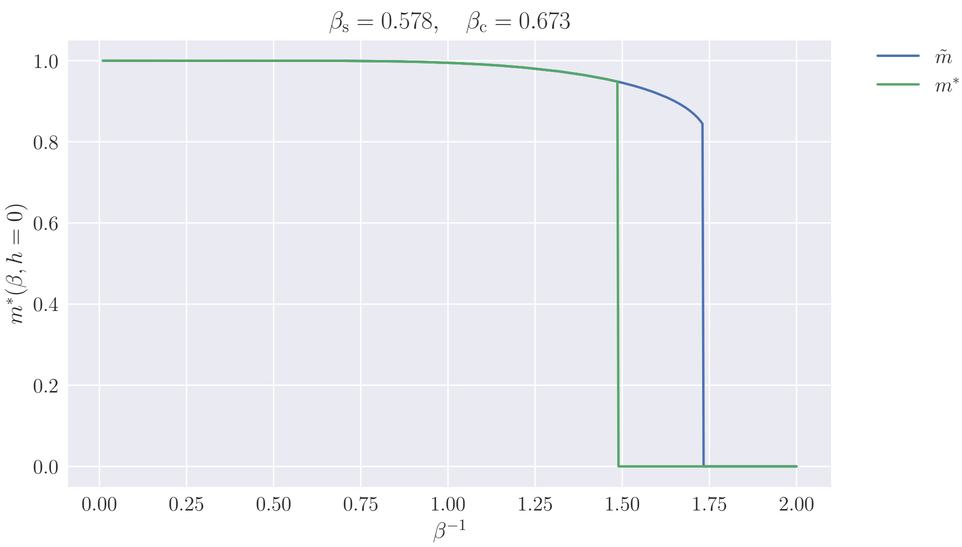
(c) To prove $m = 0$ is always a local minima

$$\frac{\partial}{\partial m}\mathcal{F}_m(\beta, h, m)\bigg|_{\substack{h=0\\m=0}} = -3m^2 - h + \frac{\operatorname{atanh}(m)}{\beta}\bigg|_{\substack{h=0\\m=0}} = 0$$
$$\frac{\partial^2}{\partial m^2}\mathcal{F}_m(\beta, h, m)\bigg|_{\substack{h=0\\m=0}} = -6m + \frac{1}{(1-m^2)\beta}\bigg|_{\substack{h=0\\m=0}} = \frac{1}{\beta} > 0$$

Define the right-most local minima to be

$$\tilde{m}(\beta, h) = \max\left\{m \,\middle|\, \frac{\partial}{\partial m}\mathcal{F}_m(\beta, h, m) = 0\right\}$$

The plot of $m^*(\beta, h)$ and $\tilde{m}(\beta, h)$ under $h = 0$ and $\beta^{-1} \in (0, 2]$ is



It is easy to see both curves have jumps, the second local minima emerges when the blue curve jumps, the second local minima becomes global minima when the green curve jumps.

(d) Using the δ function and Fourier trick,

$$
\begin{aligned}
Z_N(\beta, h) &= \sum_{\{S_i\}_{i=1}^N} \exp\left(N\beta\left[\left(\frac{\sum_i S_i}{N}\right)^3 + h\frac{\sum_i S_i}{N}\right]\right) \\
&= \sum_{\{S_i\}_{i=1}^N} \int \mathrm{d}m\, \delta\left(\frac{\sum_i S_i}{N}, m\right) \exp\left(N\beta\left(m^3 + hm\right)\right) \\
&= \sum_{\{S_i\}_{i=1}^N} \int \mathrm{d}m \int \mathrm{d}\lambda \exp\left(2\pi\mathbb{i}\lambda\left[Nm - \sum_i S_i\right]\right) \exp\left(N\beta\left(m^3 + hm\right)\right) \\
&\overset{\hat{m}=2\pi\mathbb{i}\lambda}{=\!=} \sum_{\{S_i\}_{i=1}^N} \int_{\mathbb{R}} \mathrm{d}m \int_{-2\pi\mathbb{i}\infty}^{2\pi\mathbb{i}\infty} \mathrm{d}\hat{m} \exp\left(\hat{m}\left[Nm - \sum_i S_i\right]\right) \exp\left(N\beta(m^3 + hm)\right) \\
&= \int_{\mathbb{R}} \mathrm{d}m \int_{-2\pi\mathbb{i}\infty}^{2\pi\mathbb{i}\infty} \mathrm{d}\hat{m} \underbrace{\left[\sum_{\{S_i\}_{i=1}^N} \exp\left(-\hat{m}\sum_i S_i\right)\right]}_{=[2\cosh(\hat{m})]^N} \exp\left(N\beta(m^3 + hm) + N\hat{m}m\right) \\
&= \iint \mathrm{d}m\, \mathrm{d}\hat{m} \exp\left\{N\beta\left[m^3 + hm + \frac{1}{\beta}\hat{m}m + \frac{1}{\beta}\log\left(2\cosh(\hat{m})\right)\right]\right\}
\end{aligned}
$$

Apply the saddle-point method, take partial derivative w.r.t. $\hat{m}$ gives

$$
\begin{aligned}
0 &= \frac{\partial}{\partial m}\left[m^3 + hm + \frac{1}{\beta}\hat{m}m + \frac{1}{\beta}\log\left(2\cosh(\hat{m})\right)\right] = 3m^3 + h + \frac{1}{\beta}\hat{m} \\
0 &= \frac{\partial}{\partial \hat{m}}\left[m^3 + hm + \frac{1}{\beta}\hat{m}m + \frac{1}{\beta}\log\left(2\cosh(\hat{m})\right)\right] = \frac{1}{\beta}m + \frac{1}{\beta}\tanh(\hat{m}) \\
\Rightarrow &\quad \begin{cases} m = -\tanh(\hat{m}) \\ \hat{m} = -\beta\left(3m^2 + h\right) \end{cases} \\
f(\beta, h) &= -\lim_{N\to\infty} \frac{1}{N\beta}\log\left(Z_N(\beta)\right) \\
&\overset{\hat{m}=-\beta\left(3m^2+h\right)}{=\!=} -\max_{m\in[-1,1]}\left[-2m^3 + \frac{1}{\beta}\log\left[2\cosh\left(3\beta m^2 + \beta h\right)\right]\right] \\
&= \min_{m\in[-1,1]}\left[2m^3 - \frac{1}{\beta}\log\left[2\cosh\left(3\beta m^2 + \beta h\right)\right]\right]
\end{aligned}
$$

(e) To describe the long-time (but not exponentially in N long) behavior of the Monte Carlo Markov Chain, we need to consider cases according to β

- $\beta < \beta_{\mathrm{s}}$: There is only one local minima at $m = 0$, so no matter where the chain is initialed, the trace plot of $m(t)$ will first go to $m = 0$ and stuck there.
- $\beta > \beta_{\mathrm{s}}$: There are two local minima $m = 0$ and $m = \tilde{m}$. Since the chain does not run exponentially in N long, it is hard for the chain to traverse from one local minima to another. If the chain starts at $m = 0$ it will just stay there; if the chain starts at $m = 1$, it will first go to $\tilde{m}$ and then stuck there.

  But if the chain runs long enough, the chain will stay at the global minima for exponentially longer time.

□

B. Bethe free entropy

(a) Show from the generic formula for Bethe free entropy per spin that we derived in the lecture

$$f_{\text{Bethe}}^{\text{general}} = \frac{1}{N}\sum_{i=1}^{N}\log(Z^i) + \frac{1}{N}\sum_{a=1}^{M}\log(Z^a) - \frac{1}{N}\sum_{ia}\log(Z^{ia}) \tag{†}$$

where

$$\begin{aligned} Z^i &= \sum_s g_i(s) \prod_{a\in\partial i} \psi_s^{a\to i} \\ Z^a &= \sum_{\{s_i\}_{i\in\partial a}} f_a\left(\{s_i\}_{i\in\partial a}\right) \prod_{i\in\partial a} \chi_{s_i}^{i\to a} \\ Z^{ia} &= \sum_s \psi_s^{a\to i}\chi_s^{i\to a} \end{aligned}$$

that the Bethe free entropy for graph coloring can be written as

$$f_{\text{Bethe}}^{\text{coloring}} = \frac{1}{N}\sum_{i=1}^{N}\log\left(Z^{(i)}\right) - \frac{1}{N}\sum_{(ij)\in E}\log\left(Z^{(ij)}\right)$$

where

$$\begin{aligned} Z^{(i)} &= \sum_s \prod_{k\in\partial i}\left[1-\left(1-\mathrm{e}^{-\beta}\right)\chi_s^{k\to i}\right] \\ Z^{(ij)} &= 1-\left(1-\mathrm{e}^{-\beta}\right)\sum_s \chi_s^{i\to(ij)}\chi_s^{j\to(ij)} \end{aligned}$$

(b) **A key connection between Belief Propagation and the Bethe free entropy**: Show that the BP equations we derived in the lecture

$$\begin{aligned} \chi_{s_j}^{j\to a} &= \frac{1}{Z^{j\to a}} g_j(s_j) \prod_{b\in\partial j\backslash a} \psi_{s_j}^{b\to j} \\ \psi_{s_i}^{a\to i} &= \frac{1}{Z^{a\to i}} \sum_{\{s_j\}_{j\in\partial a\backslash i}} f_a\left(\{s_j\}_{j\in\partial a}\right) \prod_{j\in\partial a\backslash i} \chi_{s_j}^{j\to a} \end{aligned}$$

are stationarity conditions of the Bethe free entropy (†) under the constraint that both $\sum_s \psi_s^{a\to i} = 1$ and $\sum_s \chi_s^{i\to a} = 1$ for all $(ia)\in E$.

Solution.

(a) Given graph $G(V,E)$, let's define its associated factor graph $\mathsf{FG}(\tilde{V},\tilde{F},\tilde{E})$, where

- $\tilde{V} = V$ is the set of variable nodes in factor graph, the value is the color of the corresponding node
- $\tilde{F} = E$ is the set of factor nodes in factor graph, the constraint function is $f_{ij}(s_i,s_j) = \mathbb{I}(s_i \neq s_j)$. However, since the indicator constraint function is hard to deal with, usually we soften the constraint as $f_{ij}(s_i,s_j) = \mathrm{e}^{-\beta\,\mathbb{I}(s_i=s_j)}$ and let $\beta\to\infty$.
- $\tilde{E} = \bigcup_{(ij)\in E}\{(i,ij),(j,ij)\}$ is the set of edges in factor graph

The Boltzmann distribution of the factor graph is

$$P\left(\{s_i\}_{i=1}^N\right) = \frac{1}{Z}\prod_{(ij)\in\tilde{F}} f_{ij}(s_i,s_j) = \frac{1}{Z}\prod_{(ij)\in E} \mathrm{e}^{-\beta\,\mathbb{I}(s_i=s_j)}$$

Notice that in this factor graph, every factor node has exactly degree 2, this type of model is called *pair-wise model*. According to BP rule we have

$$\begin{aligned}
\psi_{s_i}^{(ij)\to i} &= \frac{1}{\tilde{Z}^{(ij)\to i}}\sum_{s_j} f_{ij}(s_i,s_j)\chi_{s_j}^{j\to(ij)} = \frac{1}{\tilde{Z}^{(ij)\to i}}\left[f_{ij}(s_i,s_i)\chi_{s_i}^{j\to(ij)} + \sum_{s_j\neq s_j} f_{ij}(s_i,s_j)\chi_{s_j}^{j\to(ij)}\right] \\
&= \frac{\mathrm{e}^{-\beta}\chi_{s_i}^{j\to(ij)} + \sum_{s_j\neq s_i}\chi_{s_j}^{j\to(ij)}}{\tilde{Z}^{(ij)\to i}} = \frac{1-(1-\mathrm{e}^{-\beta})\chi_{s_i}^{j\to(ij)}}{\tilde{Z}^{(ij)\to i}} \qquad (2)
\end{aligned}$$

where $\tilde{Z}^{(ij)\to i}$ is the normalization constant of $\psi_{s_i}^{(ij)\to i}$.

Hence, it is sufficient to only use one set of BP messages, here we choose χ's.

Besides, to distinguish the neighborhood of node i in $G(V,E)$ and the neighborhood of variable node i in $\mathsf{FG}(\tilde{V},\tilde{F},\tilde{E})$, I will use $\partial^* i$ to denote the neighborhood in $G(V,E)$, i.e.

$$\partial^* i = \{j\,|\,(ij)\in E\}\,, \qquad \partial i = \left\{(ij)\,\middle|\,(i,ij)\in\tilde{E}\right\}$$

Therefore, start from (†) we have

$$\begin{aligned}
f_{\text{Bethe}}^{\text{coloring}} &= \frac{1}{N}\sum_{i\in\tilde{V}}\log(\tilde{Z}^{(i)}) + \frac{1}{N}\sum_{(ij)\in\tilde{F}}\log(\tilde{Z}^{(ij)}) - \frac{1}{N}\sum_{(i,ij)\in\tilde{E}}\log(\tilde{Z}^{(i,ij)}) \\
&= \frac{1}{N}\sum_{i=1}^{N}\log(\tilde{Z}^{(i)}) + \frac{1}{N}\sum_{(ij)\in E}\log(\tilde{Z}^{(ij)}) - \frac{1}{N}\sum_{(ij)\in E}\left[\log(\tilde{Z}^{(i,ij)}) + \log(\tilde{Z}^{(j,ij)})\right] \quad (\ddagger)
\end{aligned}$$

where

$$\begin{aligned}
\tilde{Z}^{(i)} &= \sum_s \prod_{(ik)\in\partial i}\psi_s^{(ik)\to i} \overset{\text{by }(*)}{=\!=} \sum_s\prod_{k\in\partial^* i}\frac{1-\left(1-\mathrm{e}^{-\beta}\right)\chi_s^{(ik)\to i}}{\tilde{Z}^{(ik)\to i}} = \frac{Z^{(i)}}{\prod_{k\in\partial^* i}\tilde{Z}^{(ik)\to i}} \\
\tilde{Z}^{(ij)} &= \sum_{s_i,s_j} f_{ij}(s_i,s_j)\,\chi_{s_i}^{i\to(ij)}\chi_{s_j}^{j\to(ij)} = \mathrm{e}^{-\beta}\sum_s\chi_s^{i\to(ij)}\chi_s^{j\to(ij)} + \sum_{s_i\neq s_j}\chi_{s_i}^{i\to(ij)}\chi_{s_j}^{j\to(ij)} \\
&= \left(\mathrm{e}^{-\beta}-1\right)\sum_s\chi_s^{i\to(ij)}\chi_s^{j\to(ij)} + \sum_{s_i}\chi_{s_i}^{i\to(ij)}\cdot\sum_{s_j}\chi_{s_j}^{j\to(ij)} \\
&= 1-\left(1-\mathrm{e}^{-\beta}\right)\sum_s\chi_s^{i\to(ij)}\chi_s^{j\to(ij)} = Z^{(ij)} \\
\tilde{Z}^{(i,ij)} &= \sum_s\psi_s^{(ij)\to i}\chi_s^{i\to(ij)} = \frac{1}{\tilde{Z}^{(ij)\to i}}\sum_s\left[1-\left(1-\mathrm{e}^{-\beta}\right)\chi_s^{(ij)\to i}\right]\chi_s^{i\to(ij)} \\
&= \frac{1}{\tilde{Z}^{(ij)\to i}}\left[1-\left(1-\mathrm{e}^{-\beta}\right)\sum_s\chi_s^{i\to(ij)}\chi_s^{j\to(ij)}\right] = \frac{Z^{(ij)}}{\tilde{Z}^{(ij)\to i}}
\end{aligned}$$

Finally, substituting equations above back to (‡) yields

$$\begin{aligned}
f_{\text{Bethe}}^{\text{coloring}} &= \frac{1}{N}\sum_{i=1}^{N}\left[\log(Z^{(i)}) - \sum_{k\in\partial^* i}\log\left(\tilde{Z}^{(ik)\to i}\right)\right] + \frac{1}{N}\sum_{(ij)\in E}\log(Z^{(ij)}) \\
&\quad -\frac{1}{N}\sum_{(ij)\in E}\left[\log(Z^{(ij)}) - \log(\tilde{Z}^{(ij)\to i}) + \log(Z^{(ij)}) - \log(\tilde{Z}^{(ij)\to j})\right] \\
&= \frac{1}{N}\log\left(Z^{(i)}\right) - \frac{1}{N}\sum_{(ij)\in E}\log\left(Z^{(ij)}\right)
\end{aligned}$$

since the sum $\sum_{i=1}^{N}\sum_{k\in\partial^* i}$ counts each edge twice ((ij) and (ji)).

The proof is finished by simplify the notation $\chi_s^{i\to(ij)}$ to $\chi_s^{i\to j}$.

(b) To compute the stationarity conditions of Bethe free entropy, we start from taking partial derivative w.r.t. every BP message components $\chi_{s_i}^{i\to a}$ and $\psi_{s_i}^{a\to i}$ for all $i\in[N]$, $a\in[M]$ and $s_i\in\mathcal{X}$, where $\mathcal{X}$ is the alphabet of spin.

$$
\begin{aligned}
N\frac{\partial}{\partial\chi_{s_i}^{i\to a}} f_{\text{Bethe}}^{\text{general}} &= \frac{\partial}{\partial\chi_{s_i}^{i\to a}}\log\left(Z^a\right) - \frac{\partial}{\partial\chi_{s_i}^{i\to a}}\log\left(Z^{ia}\right)\\
&= \frac{\sum_{\{s_k\}_{k\in\partial a\backslash i}} f_a\left(s_i,\{s_k\}_{k\in\partial a\backslash i}\right)\prod_{k\in\partial a\backslash i}\chi_{s_k}^{k\to a}}{\sum_{\{s_k\}_{k\in\partial a}} f_a\left(\{s_k\}_{k\in\partial a}\right)\prod_{k\in\partial a}\chi_{s_k}^{k\to a}} - \frac{\psi_{s_i}^{a\to i}}{\sum_s\psi_s^{a\to i}\chi_s^{i\to a}}\\
N\frac{\partial}{\partial\psi_{s_i}^{a\to i}} f_{\text{Bethe}}^{\text{general}} &= \frac{\partial}{\partial\psi_{s_i}^{a\to i}}\log\left(Z^i\right) - \frac{\partial}{\partial\psi_{s_i}^{a\to i}}\log\left(Z^{ia}\right)\\
&= \frac{g_i(s_i)\prod_{c\in\partial i\backslash a}\psi_{s_i}^{c\to i}}{\sum_s g_i(s)\prod_{a\in\partial i}\psi_s^{a\to i}} - \frac{\chi_{s_i}^{i\to a}}{\sum_s\psi_s^{a\to i}\chi_s^{i\to a}}
\end{aligned}
$$

Setting these partial derivatives to zero and using the normalization constraints gives

$$
\begin{aligned}
\psi_{s_i}^{a\to i} &= \underbrace{\frac{\sum_s\psi_s^{a\to i}\chi_s^{i\to a}}{\sum_{\{s_k\}_{k\in\partial a}} f_a\left(\{s_k\}_{k\in\partial a}\right)\prod_{k\in\partial a}\chi_{s_k}^{k\to a}}}_{\text{independent of } s_i}\sum_{\{s_k\}_{k\in\partial a\backslash i}} f_a\left(\{s_k\}_{k\in\partial a}\right)\prod_{k\in\partial a\backslash i}\chi_{s_k}^{k\to a}\\
\psi_{s_i}^{a\to i} &= \frac{\psi_{s_i}^{a\to i}}{\sum_s\psi_s^{a\to i}} = \frac{\sum_{\{s_k\}_{k\in\partial a\backslash i}} f_a\left(\{s_k\}_{k\in\partial a}\right)\prod_{k\in\partial a\backslash i}\chi_{s_k}^{k\to a}}{\underbrace{\sum_{\{s_k\}_{k\in\partial a}} f_a\left(\{s_k\}_{k\in\partial a}\right)\prod_{k\in\partial a\backslash i}\chi_{s_k}^{k\to a}}_{=Z^{a\to i}}}\\
\chi_{s_i}^{i\to a} &= \underbrace{\frac{\sum_s\psi_s^{a\to i}\chi_s^{i\to a}}{\sum_s g_i(s)\prod_{c\in\partial i}\psi_s^{c\to i}}}_{\text{independent of } s_i} g_i(s_i)\prod_{c\in\partial i\backslash a}\psi_{s_i}^{c\to i}\\
\chi_{s_i}^{i\to a} &= \frac{\chi_{s_i}^{i\to a}}{\sum_s\chi_s^{i\to a}} = \frac{g_i(s_i)\prod_{c\in\partial i\backslash a}\psi_{s_i}^{c\to i}}{\underbrace{\sum_s g_i(s)\prod_{c\in\partial i\backslash a}\psi_s^{c\to i}}_{=Z^{i\to a}}}
\end{aligned}
$$

Finally we have the stationarity conditions for Bethe free entropy, for all $i\in[N], a\in[M]$ and $s_i\in\mathcal{X}$

$$
\begin{aligned}
\psi_{s_i}^{a\to i} &= \frac{1}{Z^{a\to i}}\sum_{\{s_k\}_{k\in\partial a\backslash i}} f_a\left(\{s_k\}_{k\in\partial a}\right)\prod_{k\in\partial a\backslash i}\chi_{s_k}^{k\to a}\\
\chi_{s_i}^{i\to a} &= \frac{1}{Z^{i\to a}} g_i(s_i)\prod_{c\in\partial i\backslash a}\psi_{s_i}^{c\to i}
\end{aligned}
$$

which is exactly identical to BP equations.

□

C. Belief propagation for the k-factor problem on random graphs

Consider now the k-factor problem on random Erdős-Rényi graphs of average degree $c=\mathrm{O}(1)$. Use the graphical model representation from the previous homeworks.

(a) Write belief propagation equations able to estimate the marginals of the probability distribution

$$P\left(\left\{S_{(ij)}\right\}_{(ij)\in E}\right) = \frac{1}{Z(\beta)} \prod_{(ij)\in E} e^{\beta S_{(ij)}} \prod_{i=1}^{N} \mathbb{I}\left(\sum_{j\in\partial i} S_{(ij)} \leq k\right)$$

Be careful that in the k-factor model the nodes of the graph play the role of factor nodes in the graphical model and edges in the graph carry the variables nodes in the graphical model.

(b) Write the corresponding Bethe free entropy in order to estimate $\log(Z(\beta))$. Use results of the previous homework to suggest how to estimate the number of k-factors of a given size $s(e)$ on a given randomly generated large graph G.

(c) Consider now d-regular random graphs and express the plot $s(e)$ for $k = 1, 2, 3$, for several values of d. Comment on what you obtained, does it correspond to your expectation from the previous homework? If now, explain the differences.

(d) **BONUS** Implement the BP equations and compute the $s(e)$ for the k-factor model on a given random Erdős-Rényi graph. Plot $s(e)$ for several values of the average degree c and $k = 1$ and 2.

Solution.

(a) Given graph $G(V, E)$, let's define its associated factor graph $\mathsf{FG}(\tilde{V}, \tilde{F}, \tilde{E})$, where

- $\tilde{V} = E$ is the set of variable nodes in factor graph. Given any $\mathsf{M} \subseteq E$, the values $S_{(ij)} \in \{0, 1\}$ represent whether edge $(ij) \in \mathsf{M}$ or not.
- $\tilde{F} = V$ is the set of factor nodes in factor graph. The constraint function is

$$f_i\left(\left\{S_{(ij)}\right\}_{j\in\partial^* i}\right) = \mathbb{I}\left(\sum_{j\in\partial^* i} S_{(ij)} \leq k\right)$$

- $\tilde{E} = \bigcup_{(ij)\in E} \{(ij, i), (ij, j)\}$ is the set of edges in factor graph.

Therefore, the BP equations

$$\begin{aligned}
\psi^{i\to(ij)}_{S_{(ij)}} &= \frac{1}{Z^{i\to(ij)}} \sum_{\left\{S_{(il)}\right\}_{(il)\in\partial i\setminus(ij)}} f_i\left(\left\{S_{(il)}\right\}_{(il)\in\partial i}\right) \prod_{(il)\in\partial i\setminus(ij)} \chi^{(il)\to i}_{S_{(il)}} \\
&= \frac{1}{Z^{i\to(ij)}} \sum_{\left\{S_{(il)}\right\}_{l\in\partial^* i\setminus j}} \mathbb{I}\left(\sum_{l\in\partial^* i} S_{(il)} \leq k\right) \prod_{l\in\partial^* i\setminus j} \chi^{(il)\to i}_{S_{(il)}} \\
\chi^{(ij)\to i}_{S_{(ij)}} &= \frac{1}{Z^{(ij)\to i}} g_{ij}(S_{(ij)}) \prod_{c\in\partial(ij)\setminus i} \psi^{c\to(ij)}_{S_{(ij)}} = \frac{1}{Z^{(ij)\to i}} e^{\beta S_{(ij)}} \psi^{j\to(ij)}_{S_{(ij)}}
\end{aligned}$$

where $Z^{i\to(ij)}$ and $Z^{(ij)\to i}$ are normalization constants to ensure

$$\sum_s \psi^{i\to(ij)}_s = 1, \qquad \sum_s \chi^{(ij)\to i}_s = 1$$

(b) Before we write the Bethe free entropy, let's first write down each component separately

$$\text{For variable nodes} \quad Z^{(ij)} = \sum_s g_{ij}(s) \prod_{c\in\partial(ij)} \psi_s^{c\to(ij)} = \sum_s \mathrm{e}^{\beta s}\psi_s^{i\to(ij)}\psi_s^{j\to(ij)}$$

$$\begin{aligned}\text{For factor nodes} \quad Z^i &= \sum_{\{s_{(ij)}\}_{j\in\partial^* i}} f_i\left(\{s_{(ij)}\}_{j\in\partial^* i}\right) \prod_{j\in\partial^* i} \chi_{s_{(ij)}}^{(ij)\to i} \\ &= \sum_{\{s_{(ij)}\}_{j\in\partial^* i}} \mathbb{I}\left(\sum_{j\in\partial^* i} S_{(ij)} \le k\right) \prod_{j\in\partial^* i} \chi_{s_{(ij)}}^{(ij)\to i}\end{aligned}$$

$$\text{For edges} \quad Z^{(ij),i} = \sum_s \psi_s^{i\to(ij)}\chi_s^{(ij)\to i}$$

Hence, the Bethe free entropy for k-factor problem at inverse temperature β is

$$f_{\text{Bethe}}^{k\text{-factor}}(\beta) = \frac{1}{N}\left\{\sum_{(ij)\in E}\log\left(Z^{(ij)}\right) + \sum_{i=1}^{N}\log\left(Z^i\right) - \sum_{(ij)\in E}\left[\log\left(Z^{(ij),i}\right) + \log\left(Z^{(ij),j}\right)\right]\right\}$$

According to HW1, what we want to compute is the free entropy density

$$f(\beta) = \lim_{N\to\infty}\frac{\log(Z(\beta))}{N}$$

Since as $N\to\infty$, the Erdős-Rényi graphs are locally tree-like, the Bethe free entropy per spin is asymptotically close to the true free entropy density, i.e.

$$f(\beta) \approx f_{\text{Bethe}}^{k\text{-factor}}(\beta)$$

Therefore, to compute $s(e)$, we need to do the following steps

1) Run BP long enough to reach equilibrium to get BP messages χ's and ψ's.
2) Use the BP messages to compute Bethe free entropy per spin $f_{\text{Bethe}}^{k\text{-factor}}(\beta)$ as an approximation of the free entropy density $f(\beta)$
3) Use conclusion of HW1, compute $s(e) = \inf_{\beta\in\mathbb{R}}\left[f(\beta) - \beta e\right]$

(c) For a d-regular graph, in its associated factor graph, every variable node has degree 2, every factor node has degree d. The local structure of each variable node and factor node are same thus we do need to distinguish them. Hence, denote $\chi_s^{(ij)\to i} \equiv \chi_s$ and $\psi_s^{i\to(ij)} \equiv \psi_s$ for all $(ij)\in E$ and $s\in\{\pm1\}$. The BP equations becomes

$$\begin{aligned}\psi_s &\propto \sum_{\{s_l\}_{l=1}^{d-1}} \mathbb{I}\left(s + \sum_{l=1}^{d-1} s_l \le k\right)\prod_{l=1}^{d-1}\chi_{s_l} \\ &= \sum_{\kappa=0}^{k-s}\sum_{\{s_l\}_{l=1}^{d-1}} \mathbb{I}\left(\sum_{l=1}^{d-1} s_l = \kappa\right)\prod_{l=1}^{d-1}\chi_1^{s_l}\chi_0^{1-s_l} = \sum_{\kappa=0}^{k-s}\binom{d-1}{\kappa}\chi_1^\kappa\chi_0^{d-1-\kappa} \\ \psi_s &= \frac{\sum_{\kappa=0}^{k-s}\binom{d-1}{\kappa}\chi_1^\kappa\chi_0^{d-1-\kappa}}{\binom{d-1}{k}\chi_1^k\chi_0^{d-1-k} + 2\sum_{\kappa=0}^{k-1}\binom{d-1}{\kappa}\chi_1^\kappa\chi_0^{d-1-\kappa}} \\ \chi_s &= \frac{\mathrm{e}^{\beta s}\psi_s}{\psi_0 + \mathrm{e}^{\beta}\psi_1} = \frac{\mathrm{e}^{\beta s}\psi_s}{1 + (\mathrm{e}^{\beta}-1)\psi_1}\end{aligned}$$

Or, we can use a more compact parameterization: likelihood-ratio (LR), define

$$h = \frac{\chi_1}{\chi_0}, \qquad \hat{h} = \frac{\psi_1}{\psi_0}$$

The BP equations become

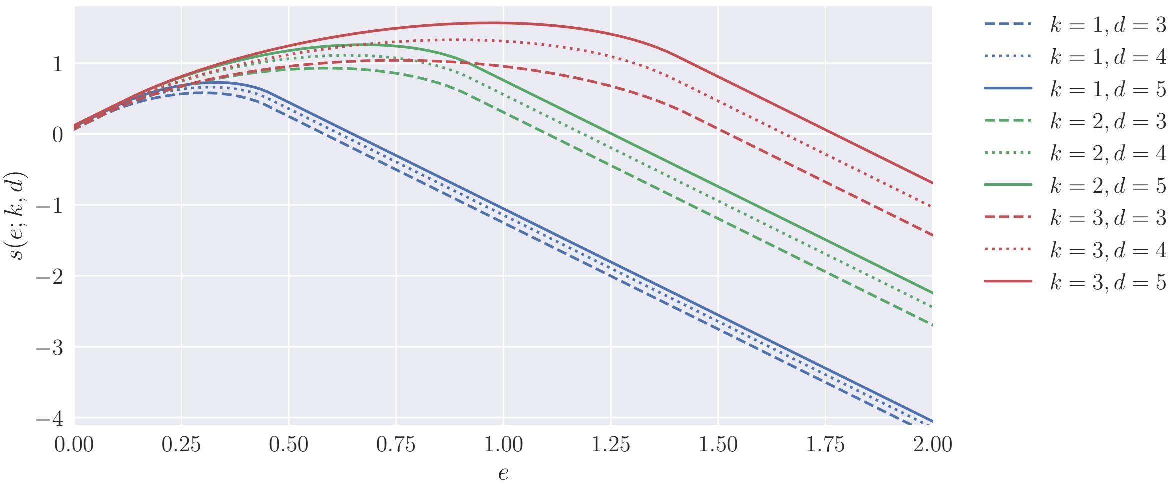
$$\hat{h} = \frac{\sum_{\kappa=0}^{k-1} \binom{d-1}{\kappa} h^\kappa}{\sum_{\kappa=0}^{k} \binom{d-1}{\kappa} h^\kappa}, \quad h = \mathbb{e}^\beta \hat{h} \quad \Rightarrow \quad h = \mathbb{e}^\beta \left[1 - \frac{\binom{d-1}{k} h^k}{\sum_{\kappa=0}^{k} \binom{d-1}{\kappa} h^\kappa}\right]$$

Therefore, once we found the fixed point of h under certain β, we can rewrite the Bethe free entropy of k-factor problem on a random d-regular graph at inverse temperature β can be computed as

$$\begin{aligned} f_{\text{Bethe}}^{k\text{-factor}}(\beta; d) &= \frac{d}{2} \log\left(\psi_0^2 + \mathbb{e}^\beta \psi_1^2\right) + \log\left(\sum_{\kappa=0}^{k} \binom{d}{\kappa} \chi_1^\kappa \chi_0^{d-\kappa}\right) - d \log\left(\psi_0 \chi_0 + \psi_1 \chi_1\right) \\ &= \frac{d}{2}\beta - \frac{d}{2} \log\left(\mathbb{e}^\beta + h^2\right) + \log\left(\sum_{\kappa=0}^{d} \binom{d}{\kappa} h^\kappa\right) \end{aligned}$$

Then, to obtain the curve $s(e)$, we can just use the procedure in part (b).

The curve $s(e)$ under $k \in \{1, 2, 3\}$ and $d \in \{3, 4, 5\}$ are given below



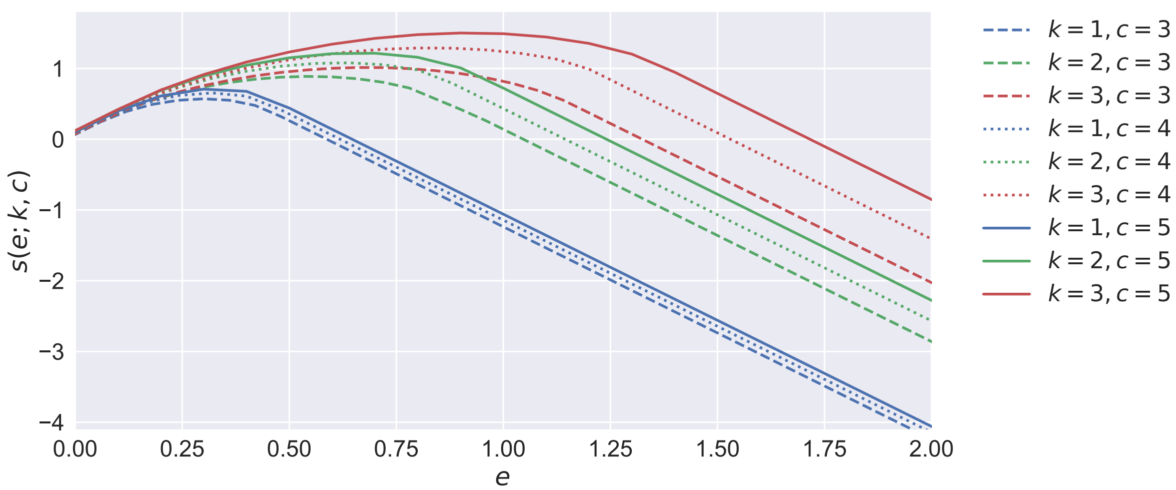
- Fix k, the larger d is, the higher $s(e; k, d)$ is.
- Fix d, the larger k is, the higher $s(e; k, d)$ is. When $k \geq d$, every subset of edges is a valid k-factor, and $s(e; k, d) = H_{\mathbb{e}}\left(\frac{2e}{d}\right)$, where $H_{\mathbb{e}}(\cdot)$ is the binary entropy function under natural base.
- As long as $k < d$, there exists a e_{lin} such that $s(e; k, d)$ becomes linear when $e > e_{\text{lin}}$.
- As long as $k < d$, there exists a e_{sup} such that $s(e; k, d) < 0$ for all $e > e_{\text{sup}}$, which means when $N \to \infty$ there is no k-factor with size e w.h.p. if $e > e_{\text{sup}}$.

(d) Again, we use the same LR parameterization as part (c), the BP equation and Bethe free entropy can be written as

$$h^{(ij)\to i} = \mathrm{e}^{\beta}\frac{\sum_{\kappa=0}^{k-1}\sum_{\substack{I\subseteq\partial^* i\setminus j\\|I|=\kappa}}\prod_{\ell\in I}h^{(i\ell)\to i}}{\sum_{\kappa=0}^{k}\sum_{\substack{I\subseteq\partial^* i\setminus j\\|I|=\kappa}}\prod_{\ell\in I}h^{(i\ell)\to i}} = \mathrm{e}^{\beta}\left[1-\frac{\sum_{\substack{I\subseteq\partial^* i\setminus j\\|I|=k}}\prod_{\ell\in I}h^{(i\ell)\to i}}{\sum_{\substack{I\subseteq\partial^* i\setminus j\\|I|\le k}}\prod_{\ell\in I}h^{(i\ell)\to i}}\right]$$

$$\begin{aligned}
N f_{\text{Bethe}}^{k\text{-factor}}(\beta;k,G) = &\sum_{(ij)\in E}\log\left\{\frac{\mathrm{e}^{2\beta}+\mathrm{e}^{\beta}h^{(ij)\to i}h^{(ij)\to j}}{\left(\mathrm{e}^{\beta}+h^{(ij)\to i}\right)\left(\mathrm{e}^{\beta}+h^{(ij)\to j}\right)}\right\}\\
&+\sum_{i=1}^{N}\log\left\{\sum_{\substack{I\subseteq\partial^* i\\|I|\le k}}\prod_{j\in I}\frac{h^{(ij)\to i}}{1+h^{(ij)\to i}}\prod_{j\in\partial^* i\setminus I}\frac{1}{1+h^{(ij)\to i}}\right\}\\
&-\sum_{(ij)\in E}\left[\log\left\{\frac{\mathrm{e}^{\beta}+h^{(ij)\to i}h^{(ij)\to j}}{\left(1+h^{(ij)\to i}\right)\left(\mathrm{e}^{\beta}+h^{(ij)\to j}\right)}\right\}+\log\left\{\frac{\mathrm{e}^{\beta}+h^{(ij)\to j}h^{(ij)\to i}}{\left(1+h^{(ij)\to j}\right)\left(\mathrm{e}^{\beta}+h^{(ij)\to i}\right)}\right\}\right]\\
= &\ \beta\,|E| - \sum_{(ij)\in E}\log\left(\mathrm{e}^{\beta}+h^{(ij)\to i}h^{(ij)\to j}\right)+\sum_{i=1}^{N}\log\left(\sum_{\substack{I\subseteq\partial^* i\\|I|\le k}}\prod_{j\in I}h^{(ij)\to i}\right)
\end{aligned}$$

The figure below gives the $s(e)$ for three Erdős-Rényi drawn from ensemble $\mathbb{G}_{\text{ER}}(N,c)$ with $N = 1000$ and $c \in \{3,4,5\}$. For each sampled random graph, I ran BP for the k-factor problem for $k \in \{1,2,3\}$ and $\beta \in [-3,3]$ to compute $f_{\text{Bethe}}^{k\text{-factor}}(\beta;k,G)$. Finally, I apply Legendre transformation to get the $s(e;k,c)$ curve for a (k,c) pair.



It can be seen that the result is very similar to the random regular graph in part (c). One reasonable explanation is that the self-averaging property and the fact that random d-regular graph ensemble $\mathbb{G}_{\text{reg}}(N,d)$ and Erdős-Rényi ensemble $\mathbb{G}_{\text{ER}}(N,d)$ are asymptotically equivalent when $N \to \infty$. The difference between these two random graph ensemble does not affect the leading exponential order of the partition function.

□