Statistical Physics of Computation 2025 - Exercises

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Week 11

11.1 Matching

Consider the matching problem on graphs. Use the factor graph model representation from the previous homework.

1. Write belief propagation equations for the probability distribution

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

where $S_{(ij)} \in \{0,1\}$ denotes whether a link (ij) is selected for the given matching or not, and E is the edge set of the given graph. Be careful that in the matching problem the nodes of the graph play the role of factor nodes in the factor graph model and edges in the graph carry the variable nodes in the factor graph model.

Let $G(V,E)$ be the graph of interest, and denote $\mathsf{FG}(\tilde{V},\tilde{F},\tilde{E})$ the factor graph associated to $G(V,E)$ for the matching problem. Recall from last week exercise's that we have:

- $\tilde{V} = E$ 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.
- $\tilde{F}$ is the set of factor nodes in factor graph. Note that we have two kinds of factor nodes in the distribution eq. (1): one living in the nodes V corresponding to the constraint function

$$f_i\left(\{S_{(ij)}\}_{j\in\partial i}\right) = \mathbb{I}\left(\sum_{j\in\partial i} S_{(ij)} \leq 1\right)$$

and one living on the edges corresponding to:

$$g_{(ij)}(S_{(ij)}) = e^{\beta S_{(ij)}}. \tag{2}$$

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

The BP equations are therefore given by:

$$\psi^{i\to(ij)}_{S_{(ij)}} = \frac{1}{Z^{i\to(ij)}} \sum_{\{S_{(il)}\}_{(il)\in\partial i\setminus(ij)}} f_i\left(\{S_{(il)}\}_{(il)\in\partial i}\right) \prod_{(il)\in\partial i\setminus(ij)} \chi^{(il)\to i}_{S_{(il)}}$$
$$= \frac{1}{Z^{i\to(ij)}} \sum_{\{S_{(il)}\}_{l\in\partial i\setminus j}} \mathbb{I}\left(\sum_{l\in\partial i} S_{(il)} \le 1\right) \prod_{l\in\partial i\setminus j} \chi^{(il)\to i}_{S_{(il)}}$$
$$\chi^{(ij)\to i}_{S_{(ij)}} = \frac{1}{Z^{(ij)\to i}} g_{ij}(S_{(ij)}) \prod_{c\in\partial(ij)\setminus i} \psi^{c\to(ij)}_{S_{(ij)}} = \frac{1}{Z^{(ij)\to i}} e^{\beta S_{(ij)}} \psi^{j\to(ij)}_{S_{(ij)}} \tag{3}$$

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

$$\sum_s \psi^{i\to(ij)}_s = 1, \qquad \sum_s \chi^{(ij)\to i}_s = 1 \tag{4}$$

2. Write the corresponding Bethe free entropy in order to estimate $\log Z(\beta)$.

We can write the Bethe free energy for the matching problem as:

$$N\Phi_{\text{Bethe}} = \sum_{i\in\tilde{V}} \log Z^i + \sum_{a\in\tilde{F}} \log Z^a - \sum_{(i,a)\in\tilde{E}} \log Z^{i,a}$$
$$= \sum_{(ij)\in E}^{N} \log Z^{(ij)} + \sum_{i=1}^{N} \log Z^i - \sum_{(ij)\in E} \left(\log Z^{(ij),i} + \log Z^{(ij),j}\right) \tag{5}$$

We can use the BP equations above to compute each of these terms separately. First, for the variable nodes:

$$Z^{(ij)} = \sum_S g_{ij}(S) \prod_{c\in\partial(ij)} \psi^{c\to(ij)}_s = \sum_S e^{\beta S} \psi^{i\to(ij)}_S \psi^{j\to(ij)}_S \tag{6}$$

Next, for the factor nodes:

$$Z^i = \sum_{\{S_{(ij)}\}_{j\in\partial^* i}} f_i\left(\{S_{(ij)}\}_{j\in\partial^* i}\right) \prod_{j\in\partial^* i} \chi^{(ij)\to i}_{S_{(ij)}} = \sum_{\{S_{(ij)}\}_{j\in\partial^* i}} \mathbb{I}\left(\sum_{j\in\partial^* i} S_{(ij)} \le 1\right) \prod_{j\in\partial^* i} \chi^{(ij)\to i}_{S_{(ij)}} \tag{7}$$

Finally, for the factor graph edges:

$$Z^{(ij),i} = \sum_S \psi^{i\to(ij)}_S \chi^{(ij)\to i}_S \tag{8}$$

3. Describe how to estimate the number of matchings of a given size on a given randomly generated large graph G.

The Bethe free energy contains all the information we need to estimate the total number of matchings of a given size $|M| = \sum_{(ij)\in E} S_{(ij)}$. Indeed, defining the energy:

$$e = \frac{1}{N}|M| = \frac{1}{N} \sum_{(ij)\in E} S_{(ij)} \tag{9}$$

The total number of matchings of a given size is related to the entropy at a given energy:

$$\mathcal{N}(e) = e^{Ns(e)} \tag{10}$$

which can be obtained from the free entropy $\Phi(\beta)$ through a Legendre transform:

$$s(e) = \inf_{\beta} \{\Phi(\beta) - \beta e\} \tag{11}$$

As we have seen in the lectures, on a random graph the loops are of size $\log N$, and therefore in the thermodynamic limit $N \to \infty$ the Bethe free entropy is a good approximation to the free entropy:

$$\Phi_{\text{Bethe}} \underset{N\to\infty}{=} \Phi(\beta). \tag{12}$$

Therefore, an algorithm to compute $\mathcal{N}(e)$ is given by:

(a) Run BP until convergence to get fixed point messages χ, ψ.

(b) Use the messages to compute the Bethe free entropy.

(c) Solve $s(e) = \inf_{\beta} \{\Phi_{\text{Bethe}}(\beta) - \beta e\}$ to get the entropy for a matching size.

(d) Estimate $\mathcal{N}(e) = e^{Ns(e)}$.

4. Consider now that the graph is a uniformly distributed d-regular random graph. Write the Replica Symmetric BP equations (i.e. the BP equations under the uniform neighborhood ansatz), and obtain the single scalar equation

$$\frac{1-a}{a} = 1 + (d-1)\frac{a}{1-a}e^{\beta} \tag{13}$$

where $a = \psi_1$.

In a d-regular graph G, every variable node (recall these are the edges of G) has degree 2, and every factor node has degree d (recall these are the nodes of G). The local structure of every variable and factor node are identical, and therefore we do not need to distinguish them. This motivates the following ansatz for the messages:

$$\chi_S^{(ij)\to i} = \chi_S, \qquad \psi_S^{i\to(ij)} = \psi_S. \tag{14}$$

The BP equations therefore simplify considerably:

$$\psi_S \propto \sum_{\{S_l\}_{l=1}^{d-1}} \mathbb{I}\left(S + \sum_{l=1}^{d-1} S_l \leq 1\right) \prod_{l=1}^{d-1} \chi_{S_l}, \qquad \chi_S = e^{\beta S}\psi_S \tag{15}$$

Therefore, under the parametrization $\psi_1 = a$, $\psi_0 = 1-a$, we get the following set of two equations:

$$\psi_1 \equiv a = \frac{1}{Z}(1-a)^{d-1}, \quad \psi_0 \equiv 1-a = \frac{1}{Z}\left((1-a)^{d-1} + (d-1)e^{\beta}a(1-a)^{d-2}\right) \tag{16}$$

where the first expression accounts for $S = 1$ (so all neighbors $S_l = 0$ to satisfy the matching constraint) and the second term for $S = 0$, where any of the other $d-1$ neighbors can take $S_l = 1$. Note moreover that the normalization are the same, and therefore we can close the equations on a:

$$\frac{1-a}{a} = 1 + (d-1)\frac{a}{1-a}e^{\beta} \tag{17}$$

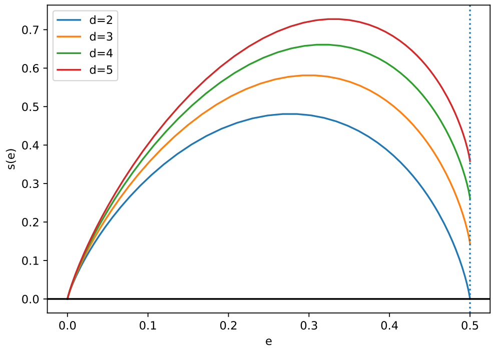

Figure 1: Entropy as a function of the size of the matching set.

5. Solve the equation found in the previous point, and compute the Bethe free entropy and the matching size (energy) as functions of β.

   This is a simple quadratic equation on $x = \frac{1-a}{a}$, and can be solved exactly to give:

$$a^\star = \frac{2}{3 + \sqrt{1 + 4e^\beta(d-1)}} \tag{18}$$

   On the homogeneous ansatz, the Bethe free entropy can also be simplified:

$$\Phi_{\text{Bethe}} = \log\left((1-a)^d + de^\beta a(1-a)^{d-1}\right) - \frac{d}{2}\log\left(e^\beta a^2 + (1-a)^2\right) \tag{19}$$

   Similarly, we can also compute the energy as a function of a by taking the derivative of Φ_{Bethe} and remembering that the BP are stationary points of the Bethe free energy (so that we need only to take the derivative of Φ w.r.t. the explicit β dependence, and not also on the implicit β dependence through the messages at the solution of the BP equations):

$$e^* = \partial_\beta \Phi_{\text{Bethe}}|_{a=a^\star} = \frac{da^\star(1-a^\star)^{d-1}e^\beta}{(1-a^\star)^d + de^\beta a^\star(1-a^\star)^{d-1}} - \frac{d}{2}\frac{a^{\star 2}e^\beta}{e^\beta a^{\star 2} + (1-a^\star)^2} \tag{20}$$

6. Plot the entropy as a function of the energy for different degrees d, and comment the curves.

   The entropy (and therefore the total number of matchings at fixed matching size) is given by: $s(e^\star) = \Phi_{\text{Bethe}}(\beta) - \beta e^\star$. Although we don't have a closed form expression for the entropy, it can be easily plotted parametrically in β for a fixed d, see Fig. 1. As we expect:

   - $s(0) = 0$, i.e. there is only 1 matching of size zero.
   - $s(e)$ is only defined in the interval $e \in [0, 1/2]$. This makes sense since each edge in a matching M connect 2 nodes. So $|M| \leq N/2$ (at most $N/2$ matchings).
   - The $d = 2$ regular graph is just a chain of nodes. In this case, there are only 2 ways of matching all the nodes available, and therefore $s(1/2) = 0$.
   - As the figure suggests, the larger the degree d, the easier it is to find a matching - which is quite intuitive.

7. Consider now the measure

$$P\left(\{S_{(ij)}\}_{(ij)\in E}\right) = \frac{1}{Z}\prod_{i=1}^{N} \mathbb{I}\left(\sum_{j\in\partial i} S_{(ij)} \leq 1\right) \tag{21}$$

i.e. the $\beta = 0$ case of the previous measure, still for random d-regular graphs. What is the size of a matching extracted randomly from this measure at leading order in the $N \to \infty$ limit, and how many matchings of that size are there at leading order?

This is just the previous measure for $\beta = 0$, so we have

$$a^\star = \frac{2}{3 + \sqrt{1 + 4(d-1)}} \tag{22}$$

and

$$s = \Phi_{\mathrm{Bethe}}(\beta = 0) = \log\left((1-a)^d + da(1-a)^{d-1}\right) - \frac{d}{2}\log\left(a^2 + (1-a)^2\right) \tag{23}$$

and

$$e^* = \frac{da^\star(1-a^\star)^{d-1}}{(1-a^\star)^d + da^\star(1-a^\star)^{d-1}} - \frac{d}{2}\frac{a^{\star 2}}{a^{\star 2} + (1-a^\star)^2} \tag{24}$$

Referring to the previous plots, the energy and entropy above correspond to the point at which the curve $s(e)$ reaches its stationary point, as

$$\partial_e s(e) = -\beta \tag{25}$$

and $\beta = 0$.