Graphical models and the Ising model

Representing problems by graphical models

Write the following problems (a) in terms of a probability distribution and (b) in terms of a graphical model by drawing an example of the corresponding factor graph.

(1) **p-spin model**

One model that is commonly studied in physics is the so-called Ising 3-spin model. The Hamiltonian of this model is written as

$$\mathcal{H}(\{S_i\}_{i=1}^N) = -\sum_{(ijk)\in E} J_{ijk} S_i S_j S_k - \sum_{i=1}^N h_i S_i \tag{1}$$

where E is a given set of (unordered) triplets $i \neq j \neq k$, J_{ijk} is the interaction strength for the triplet $(ijk) \in E$, and h_i is a magnetic field on spin i. The spins are Ising, which in physics means $S_i \in \{+1, -1\}$.

Solution.

(a) The corresponding Boltzmann distribution of the given model is

$$\begin{aligned} P(\{S_i\}_{i=1}^N) &= \frac{1}{Z(\beta)} \exp\left(-\beta \mathcal{H}(\{S_i\}_{i=1}^N)\right) \\ &= \frac{1}{Z(\beta)} \left[\prod_{(ijk)\in E} \mathrm{e}^{\beta J_{ijk} S_i S_j S_k}\right] \left[\prod_{i=1}^N \mathrm{e}^{\beta h_i S_i}\right], \end{aligned} \tag{2}$$

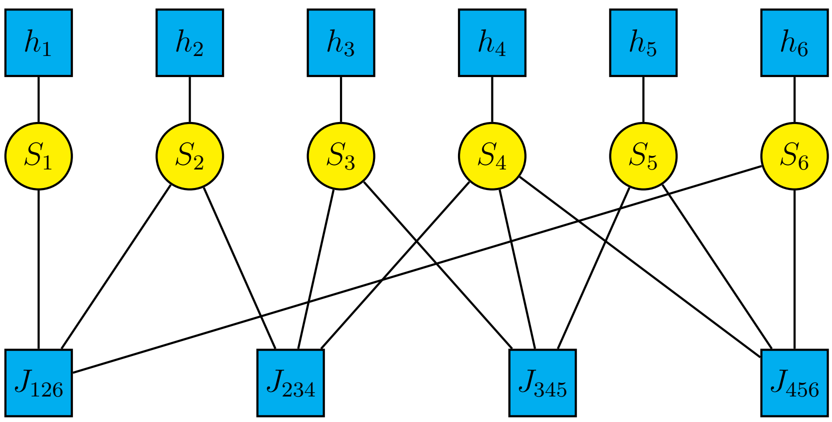
where β is the inverse temperature and

$$Z(\beta) = \sum_{\{S_i\}_{i=1}^N} \exp\left(-\beta \mathcal{H}(\{S_i\}_{i=1}^N)\right),$$

is the partition function under inverse temperature β to guarantee that $P(\{S_i\}_{i=1}^N)$ sum to one for all possible configurations.

(b) From eqn 2 we can see the probability distribution (without normalization) is the product of $|E|$ interaction terms and N local magnetic field terms.

For example, consider a 3-spin model with $N = 6$ spins and triplet set $E = \{(123), (245), (356), (456)\}$, the corresponding factor graph looks like



$\square$

(2) **Independent set problem**

Independent set is a problem defined and studied in combinatorics and graph theory. Given a (unweighted, undirected) graph $G(V, E)$, an independent set $S \subseteq V$ is defined as a subset of nodes such that if $i \in S$ then for all $j \in \partial i$ we have $j \notin S$. In other words in for all $(ij) \in E$ only i or j can belong to the independent set.

(a) Write a probability distribution that is uniform over all independent sets on a given graph. (b) Write a probability distribution that gives a larger weight to larger independent sets, where the size of an independent set is simply $|S|$.

Solution.

(a) First let's construct the factor graph for this problem. Denote $N = |V|$ as the number of nodes in the graph, we can use a length-N spin configuration $\underline{\sigma}^S$ to represent any set $S \subseteq V$ by

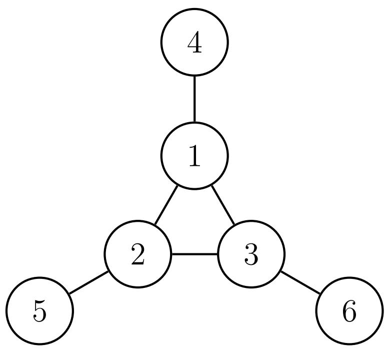
$$\sigma_i^S = \begin{cases} +1, & \text{if node } i \text{ is in } S \\ -1, & \text{if node } i \text{ is not in } S \end{cases}$$

Besides, for any edge $(ij) \in E$, we associated it with a function node e_{ij} whose compatibility function is $\psi_{ij}(\sigma_i, \sigma_j) = \mathbb{I}(\sigma_i + \sigma_j < 2)$, which equals to 1 whenever $i, j \in S$ and $(ij) \in E$

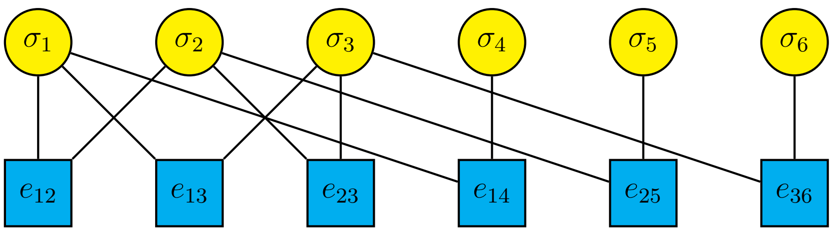
A node set $S \subseteq V$ is an independent set if and only if $\psi_{ij}(\sigma_i^S, \sigma_j^S) = 1$ for all distinct $i, j \in S$. The probability distribution that is uniform over all independent sets

$$P(\underline{\sigma}) = \frac{1}{Z} \prod_{(ij)\in E} \psi_{ij}(\sigma_i, \sigma_j) = \frac{1}{Z} \prod_{(ij)\in E} \mathbb{I}(\sigma_i + \sigma_j < 2). \tag{3}$$

For example, suppose we have the following graph



The corresponding factor graph looks like



(b) Note that $|S| = (N + \sum_{i=1}^{N} \sigma_i^S)/2$. If we want a probability distribution that gives a larger weight to larger independent sets, we can simply introduce a positive increasing function $g(\cdot)$ and multiply $g(|S|)$ to the probability distribution in part (a), i.e.

$$P(\underline{\sigma}) = g\left(\frac{N + \sum_{i=1}^{N} \sigma_i}{2}\right) \times \frac{1}{Z} \prod_{(ij)\in E} \mathbb{I}(\sigma_i + \sigma_j < 2). \tag{4}$$

For example, we can choose $g(x) = \exp(\mu x)$ for some $\mu > 0$. The last thing to notice is that the normalizing constant Z is different in eqn 3 and eqn 4.

□

(3) **Matching problem**

Matching is another classical problem of graph theory. It is related to a dimer problem in statistical physics. Given a (unweighted, undirected) graph $G(V, E)$ a matching $M \subseteq E$ is defined as a subset of edges such that if $(ij) \in M$ then no other edge that contains node i or j can be in M. In other words a matching is a subset of edges such that no two edges of the set share a node.

(a) Write a probability distribution that is uniform over all matchings on a given graph.
(b) Write a probability distribution that that gives a larger weight to larger matchings, where the size of a matching is simply $|M|$.

Solution.

(a) First let's construct the factor graph for this problem. We can use a length-$|E|$ spin configuration $\underline{\sigma}^M$ to represent any set $M \subseteq E$ by

$$\sigma_{ij}^M = \begin{cases} +1, & \text{if edge } (ij) \text{ is in } M \\ -1, & \text{if edge } (ij) \text{ is not in } M \end{cases}.$$

Besides, for any node $i \in V$, we associated it with a function node f_i whose compatibility function is

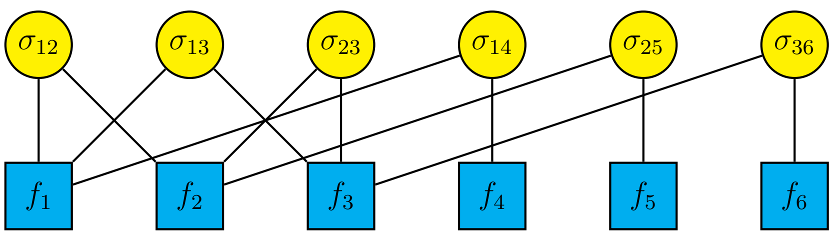
$$\psi_i(\{\sigma_{ij}\}_{j\in\partial i}) = \mathbb{I}\left(\frac{1}{2}\sum_{j\in\partial i}(\sigma_{ij}+1) \le 1\right),$$

which equals to 1 whenever there is at most one edge in M that is incident to node i.

An edge set $M \subseteq E$ is a matching if and only if $\psi_i(\{\sigma_{ij}^M\}_{j\in\partial i}) = 1$ for all $i \in S$. The probability distribution that is uniform over all matchings on a given graph

$$P(\underline{\sigma}) = \frac{1}{Z}\prod_{i\in V}\psi_i(\{\sigma_{ij}\}_{j\in\partial i}) = \frac{1}{Z}\prod_{i\in V}\mathbb{I}\left(\sum_{j\in\partial i}(\sigma_{ij}+1) \le 2\right). \tag{5}$$

For example, suppose we have the same graph as last independent set problem. The corresponding factor graph looks like



(b) Note that $|M| = (|E| + \sum_{(ij)\in E} \sigma_{ij}^M)/2$. If we want a probability distribution that gives a larger weight to larger matchings, we can simply introduce a positive increasing function $g(\cdot)$ and multiply $g(|M|)$ to the probability distribution in part (a), i.e.

$$P(\underline{\sigma}) = g\left(\frac{|E| + \sum_{(ij)\in E} \sigma_{ij}}{2}\right) \times \frac{1}{Z} \prod_{i\in V} \mathbb{I}\left(\sum_{j\in\partial i} (\sigma_{ij} + 1) \leq 2\right). \tag{6}$$

For example, we can choose $g(x) = \exp(\mu x)$ for some $\mu > 0$. The last thing to notice is that the normalizing constant Z is different in eqn 5 and eqn 6.

$\square$