Week 3: Tutorial

The intuition for how the Hammersley-Clifford theorem works

Consider a simple chain $X - Y - Z$. The corresponding graphical model is given by all distributions that factorize

$$f(x, y, z) = \alpha(x, y)\beta(y, z).$$

We want to show that this is equivalent to $X \perp Z | Y$ as long as $\alpha(x, y) > 0$ and $\beta(y, z) > 0$ for all x, y, z.

We will use the characterization that $X \perp Z | Y$ if and only if $f(x|y, z) = f(x|y)$ does not depend on z.

For the left implication note that

$$f(x, y, z) = f(y, z)f(x|y, z) = f(x|y)f(y, z).$$

So the statement works with $\alpha(x, y) = f(x|y)$ and $\beta(y, z) = f(y, z)$.

For the right implication note that

$$f(y, z) = (\sum_x \alpha(x, y))\beta(y, z).$$

and so

$$f(x|y, z) = \frac{\alpha(x, y)\beta(y, z)}{(\sum_x \alpha(x, y))\beta(y, z)} = \frac{\alpha(x, y)}{\sum_x \alpha(x, y)}$$

which does not depend on z proving the conditional independence.

Gaussian log-likelihood

Suppose we observe some data from the m-variate Gaussian distribution $\mathbf{x}_{1:n} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$. For this calculation we will assume that the underlying mean is 0. This is something that can be assumed without loss of generality by centering the data. Denote $K = \Sigma^{-1}$. Recall that the logarithm of the Gaussian density is

$$log f(\mathbf{x}; K) = -\frac{m}{2}\log(2\pi) + \frac{1}{2}\log\det K - \frac{1}{2}\mathbf{x}^\top K\mathbf{x}.$$

Up to the obvious constants that do not depend on K, the log-likelihood is

$$\ell_n(K; \mathbf{x}_{1:n}) = \frac{n}{2}\log\det(K) - \frac{1}{2}\sum_{i=1}^{n}\mathbf{x}_i^\top K\mathbf{x}_i.$$

Note that

$$\sum_{i=1}^{n}\mathbf{x}_i^\top K\mathbf{x}_i = \sum_{i=1}^{n}\mathrm{tr}(\mathbf{x}_i^\top K\mathbf{x}_i) = \sum_{i=1}^{n}\mathrm{tr}(K\mathbf{x}_i\mathbf{x}_i^\top) = n\mathrm{tr}(KS_n),$$

where

$$S_n = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}\mathbf{x}^\top.$$

With this new notation

$$\ell_n(K; \mathbf{x}_{1:n}) = \frac{n}{2}(\log\det(K) - \mathrm{tr}(KS_n)).$$

Some useful facts:

- $\log\det(K)$ is a strictly concave function of K.
- $\mathrm{tr}(KS_n)$ is linear in K.
- The gradients are $\nabla\log\det(K) = K^{-1}$ and $\nabla\mathrm{tr}(KS_n) = S_n$.

MRFs as exponential families

Consider a simple undirected graph $X_1 - X_2 - X_3$ where each variable is binary. Consider the following graphical model

$$p(x_1, x_2, x_3|\theta) \;=\; \frac{1}{Z(\theta)}\psi_{1,2}(x_1, x_2|\theta_{1,2})\psi_{2,3}(x_2, x_3|\theta_{2,3})$$

or equivalently

$$p(x_1, x_2, x_3|\theta) \;=\; \exp\Big\{\log\psi_{1,2}(x_1, x_2|\theta_{1,2}) + \log\psi_{2,3}(x_2, x_3|\theta_{2,3}) - \log Z(\theta)\Big\}$$

The vector (x_1, x_2) takes four values $(0,0), (0,1), (1,0), (1,1)$. Take

$$\theta_{1,2} \;:=\; \begin{bmatrix}\log\psi_{1,2}(0,0)\\ \log\psi_{1,2}(0,1)\\ \log\psi_{1,2}(1,0)\\ \log\psi_{1,2}(1,1)\end{bmatrix} \;\in\; \mathbb{R}^4.$$

and let $\psi_{1,2}(x_1, x_2)$ be the function that satisfies

$$\phi_{1,2}(0,0) = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}, \;\; \phi_{1,2}(0,1) = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}, \;\; \phi_{1,2}(1,0) = \begin{bmatrix}0\\0\\1\\0\end{bmatrix}, \;\; \phi_{1,2}(1,1) = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}.$$

With these definitions $\log \psi_{1,2}(x_1, x_2|\theta_{1,2}) = \theta_{1,2}^\top \phi_{1,2}(x_1, x_2)$. We define $\theta_{2,3}$ and $\phi_{2,3}(x_2, x_3)$ in a similar way obtaining that

$$p(x_1, x_2, x_3|\theta) \;=\; \exp\left\{\theta_{1,2}^\top \phi_{1,2}(x_1, x_2) + \theta_{2,3}^\top \phi_{2,3}(x_2, x_3) - \log Z(\theta)\right\},$$

which forms an exponential family with sufficient statistics

$$\phi_{1,2}(x_1, x_2) = \begin{bmatrix}(1-x_1)(1-x_2)\\(1-x_1)x_2\\x_1(1-x_2)\\x_1x_2\end{bmatrix}, \qquad \phi_{2,3}(x_2, x_3) = \begin{bmatrix}(1-x_2)(1-x_3)\\(1-x_2)x_3\\x_2(1-x_3)\\x_2x_3\end{bmatrix}$$

and with $Z(\theta) = 1$.

As a side comment we note that this exponential family is not minimal in the sense that the values of $\phi_{1,2}(x_1, x_2)$ and $\phi_{2,3}(x_2, x_3)$ lie in a hyperplane in the sense that

$$\phi_{1,2}(x_1, x_2)^\top \begin{bmatrix}1\\1\\1\\1\end{bmatrix} \;=\; 1 \qquad \text{for all } (x_1, x_2) \in \{0,1\}^2.$$

Non-minimal exponential families do not satisfy the gradient equation $\nabla A(\theta) = \mathbb{E}_\theta T(X)$ -- indeed, here $A(\theta) = 0$. An easy solution is to get rid of the first coordinate in $\phi_{1,2}(x_1, x_2)$ and replace it with the corresponding functions of the remaining entries of $\phi_{1,2}(x_1, x_2)$. This defines new natural parameters

$$\bar{\theta}_{1,2} \;=\; \begin{bmatrix}\log\psi_{1,2}(0,1) - \log\psi_{1,2}(0,0)\\\log\psi_{1,2}(1,0) - \log\psi_{1,2}(0,0)\\\log\psi_{1,2}(1,1) - \log\psi_{1,2}(0,0)\end{bmatrix}, \qquad \bar{\theta}_{2,3} \;=\; \begin{bmatrix}\log\psi_{2,3}(0,1) - \log\psi_{2,3}(0,0)\\\log\psi_{2,3}(1,0) - \log\psi_{2,3}(0,0)\\\log\psi_{2,3}(1,1) - \log\psi_{2,3}(0,0)\end{bmatrix}$$

and new sufficient statistics

$$\bar{\phi}_{1,2}(x_1, x_2) = \begin{bmatrix}(1-x_1)x_2\\x_1(1-x_2)\\x_1x_2\end{bmatrix}, \qquad \bar{\phi}_{2,3}(x_2, x_3) = \begin{bmatrix}(1-x_2)x_3\\x_2(1-x_3)\\x_2x_3\end{bmatrix}$$

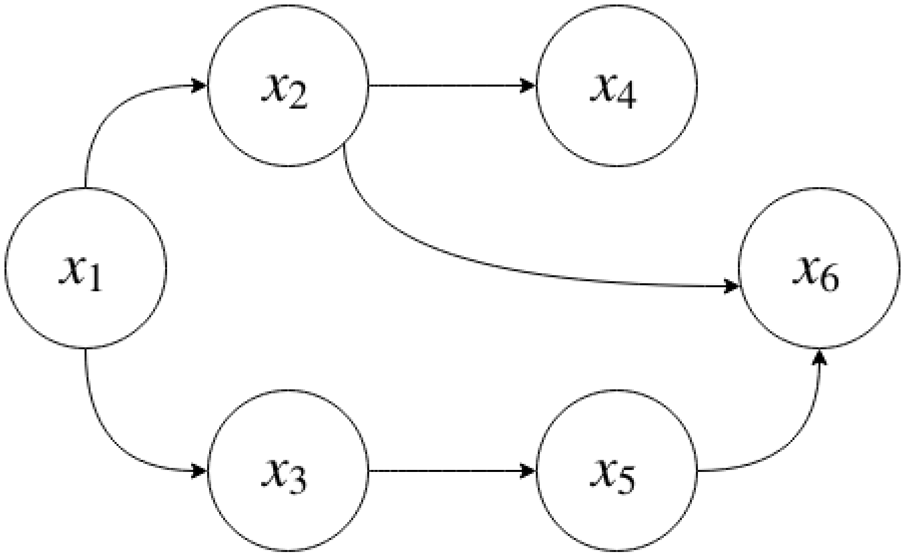
Moreover,

$$A(\bar{\theta}) \;=\; \log \psi_{1,2}(0,0)\psi_{2,3}(0,0),$$

which should be now be explicitly expressed in terms of $\bar{\theta}_{1,2}$ and $\bar{\theta}_{2,3}$.

Simple variable elimination example

Consider the following DAG



Suppose that we observe the variable $X_6 = \bar{x}_6$. What is $p(X_1|\bar{x}_6)$?

The corresponding dAG model implies the factorization:

$$p(x_1, \ldots, x_6) = p(x_1)p(x_2|x_1)p(x_3|x_1)p(x_4|x_2)p(x_5|x_3)p(x_6|x_2, x_5)$$

We have

$$x_F = \{x_1\}, x_E = \{x_6\},\ x_R = \{x_2, x_3, x_4, x_5\}$$

$$\begin{aligned} p(x_F|x_E) &= \frac{\sum_{x_R} p(x_F, x_E, x_R)}{\sum_{x_F, x_R} p(x_F, x_E, x_R)} \\ \Rightarrow p(x_1|\bar{x}_6) &= \frac{p(x_1, \bar{x}_6)}{p(\bar{x}_6)} = \frac{p(x_1, \bar{x}_6)}{\sum_{x \in x_F, x_R} p(x, \bar{x}_6)} \end{aligned}$$

To compute $p(x_1, \bar{x}_6)$, we use variable elimination in the order $2, 3, 4, 5$

$$\begin{aligned} p(x_1, \bar{x}_6) &= p(x_1) \sum_{x_2} \sum_{x_3} \sum_{x_4} \sum_{x_5} p(x_2|x_1)p(x_3|x_1)p(x_4|x_2)p(x_5|x_3)p(\bar{x}_6|x_2, x_5) \\ &= p(x_1) \sum_{x_2} p(x_2|x_1) \sum_{x_3} p(x_3|x_1) \sum_{x_4} p(x_4|x_2) \sum_{x_5} p(x_5|x_3)p(\bar{x}_6|x_2, x_5) \\ &= p(x_1) \sum_{x_2} p(x_2|x_1) \sum_{x_3} p(x_3|x_1) \sum_{x_4} p(x_4|x_2)p(\bar{x}_6|x_2, x_3) \end{aligned}$$

Note that $p(\bar{x}_6|x_2, x_3)$ does not need to participate in $\sum_{x_4}$.

$$
\begin{aligned}
&= p(x_1)\sum_{x_2} p(x_2|x_1)\sum_{x_3} p(x_3|x_1)p(\bar{x}_6|x_2,x_3)\sum_{x_4} p(x_4|x_2)\\
&= p(x_1)\sum_{x_2} p(x_2|x_1)\sum_{x_3} p(x_3|x_1)p(\bar{x}_6|x_2,x_3)\\
&= p(x_1)\sum_{x_2} p(x_2|x_1)p(\bar{x}_6|x_1,x_2)\\
&= p(x_1)p(\bar{x}_6|x_1)
\end{aligned}
$$

Finally,

$$p(x_1|\bar{x}_6) = \frac{p(x_1)p(\bar{x}_6|x_1)}{\sum_{x_1} p(x_1)p(\bar{x}_6|x_1)}.$$

Restricted Boltzmann machines

A restricted Boltzmann machine (RBM) is a simple generative stochastic artificial neural network model. In the language of todays lecture, it is obtained from a special form of the Ising model with variables $(X_1, \dots, X_k, H_1, \dots, H_l) \in \{-1,1\}^{k+1}$. The underlying graph is the bipartite graph with all pairs $H_i - X_j$ connected but with no other edges. The Ising model is then given by all distributions

$$p(x_1,\dots,x_k,h_1,\dots,h_l) \;\propto\; \exp\{\sum_i \alpha_i x_i + \sum_i \beta_i h_i + \sum_{i=1}^{k}\sum_{j=1}^{l} J_{ij}x_i h_j\}.$$

We can write it in terms of factors

$$\psi_{X_i,H_j}(x_i,h_j) = \exp\{\frac{1}{l}\alpha_i x_i + \frac{1}{k}\beta_j h_j + J_{ij}x_i h_j\}$$

so that

$$p(x_1,\dots,x_k,h_1,\dots,h_l) \;=\; \frac{1}{Z}\prod_{i=1}^{k}\prod_{j=1}^{l}\psi_{X_i,H_j}(x_i,h_j).$$

Note that computing Z may be computationally expensive but we will see that many quantities can be efficiently computed without knowing Z.

The corresponding RBM is given as the marginal distribution

$$p(x) = \sum_{h\in\{-1,1\}^l} p(x,h).$$

Note that both

$$\sum_{h\in\{-1,1\}^l}\prod_{i=1}^{k}\prod_{j=1}^{l}\psi_{X_i,H_j}(x_i,h_j) \quad \text{and} \quad \sum_{x\in\{-1,1\}^k}\prod_{i=1}^{k}\prod_{j=1}^{l}\psi_{X_i,H_j}(x_i,h_j)$$

can be computed very efficiently. This shows that both $p(x|h)$ and $p(h|x)$ are easy to obtain and this computation does not even require any knowledge of the normalizing constant Z.

This computation confirms what we know from the Hammersley-Clifford theorem that all H_i's are mutually independent given the vector X. The individual activation functions are given by

$$p(h_j|x) = \frac{\prod_{i=1}^{k} \psi_{ij}(x_i, h_j)}{\prod_{i=1}^{k} \psi_{ij}(x_i, -1) + \prod_{i=1}^{k} \psi_{ij}(x_i, 1)} = \sigma(\beta_j + \sum_i J_{ij} x_i)$$

with

$$\sigma(y) = \frac{e^y}{e^{-y} + e^y} = \frac{1}{1 + e^{-2y}}$$

called the sigmoid function.