Exercises Bayesian Networks (and Logistic Regression): Solutions

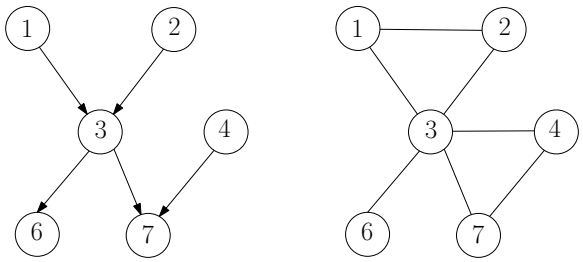
Exercise 1

(a) Factorization:

$$\begin{aligned} P(X) &= \prod_{i=1}^{9} P(X_i \mid X_{pa(i)}) \\ &= P(X_1)P(X_2)P(X_3|X_1,X_2)P(X_4)P(X_5|X_2)P(X_6|X_3) \\ &\quad P(X_7|X_3,X_4)P(X_8|X_6,X_7)P(X_9|X_5,X_7) \end{aligned}$$

(b) $6 \perp\!\!\!\perp 7$
To verify $X \perp\!\!\!\perp Y \mid Z$, take the directed independence graph on $\text{an}^+(X \cup Y \cup Z)$ and moralize this graph. Then you can verify the independence property in the resulting undirected graph using separation.

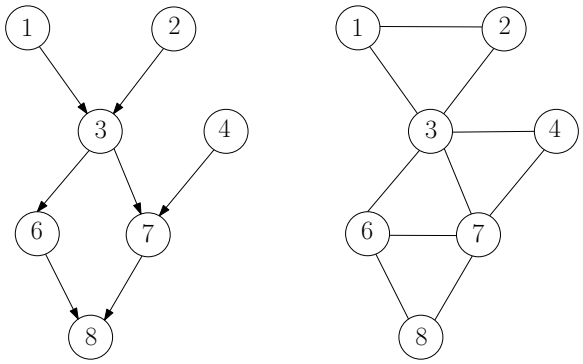
The directed independence graph on $\text{an}^+(\{6,7\})$ is given left, the corresponding moral graph is given right:



Since 6 and 7 are not separated by the empty set (there is a path between 6 and 7), they are not marginally independent.

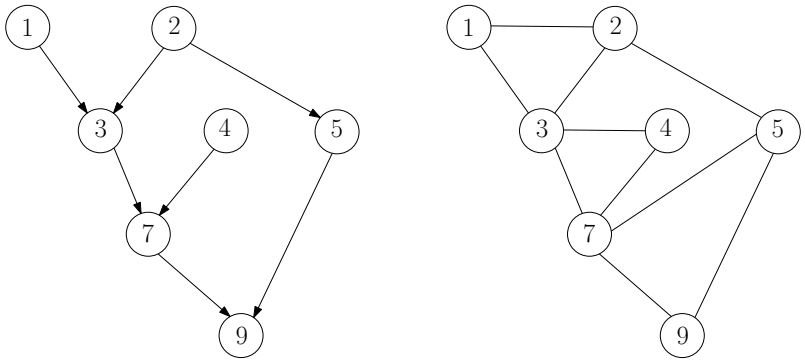
(c) $6 \perp\!\!\!\perp 7 \mid 3$
For the graphs, see (b). Yes, every path between 6 and 7 must pass through 3.

(d) $6 \perp\!\!\!\perp 7 \mid 8$
The directed independence graph on $\mathrm{an}^+(\{6,7,8\})$ is given left, the corresponding moral graph is given right:



No, 8 does not separate 6 and 7 in the moral graph.

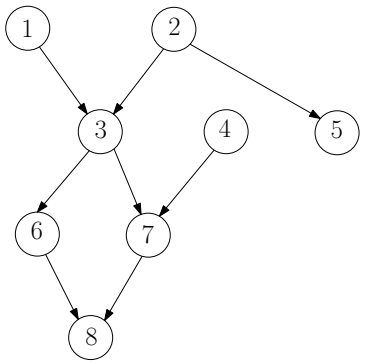
(e) $2 \perp\!\!\!\perp 9 \mid \{5,7\}$
The directed independence graph on $\mathrm{an}^+(\{2,5,7,9\})$ is given left, the corresponding moral graph is given right:

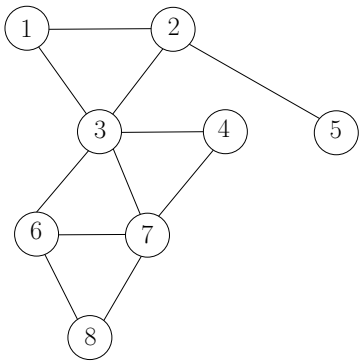


Yes: {5,7} separates 2 from 9, that is, every path from 2 to 9 must pass through a node in the set {5,7}.

(f) $2 \perp\!\!\!\perp 9 \mid \{3,5\}$
For the graphs, see (e). Yes: {3,5} separates 2 from 9.

(g) $5 \perp\!\!\!\perp 8$
The directed independence graph on $\mathrm{an}^+(\{5,8\})$ is given left, the corresponding moral graph is given right:





No, there is a path between 5 and 8.

(h) $5 \perp\!\!\!\perp 8 \mid 3$
For the graphs, see (g). Yes, 3 separates 5 from 8 in the moral graph.

Exercise 2

(a) The maximum likelihood estimates are:

$$\hat{p}_1(0) = \frac{n_1(0)}{n} = \frac{5}{10} \qquad \hat{p}_1(1) = \frac{n_1(1)}{n} = \frac{5}{10}$$
$$\hat{p}_2(0) = \frac{n_2(0)}{n} = \frac{6}{10} \qquad \hat{p}_2(1) = \frac{n_2(1)}{n} = \frac{4}{10}$$
$$\hat{p}_3(0) = \frac{n_3(0)}{n} = \frac{5}{10} \qquad \hat{p}_3(1) = \frac{n_3(1)}{n} = \frac{5}{10}$$

where, for example, $\hat{p}_1(0)$ is shorthand for $\hat{p}(x_1 = 0)$.

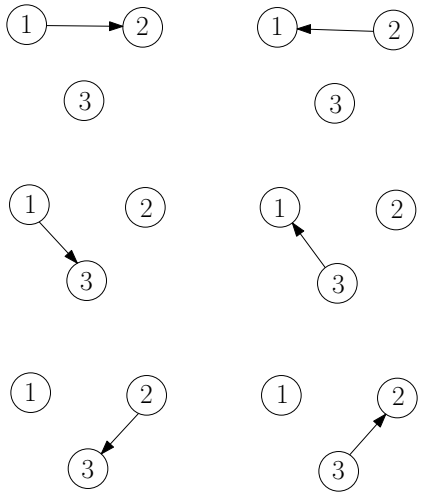
(b) The contribution of each node (variable) to the loglikelihood score is:

Node 1: $5 \log \frac{5}{10} + 5 \log \frac{5}{10}$.
Node 2: $6 \log \frac{6}{10} + 4 \log \frac{4}{10}$.
Node 3: $5 \log \frac{5}{10} + 5 \log \frac{5}{10}$.

Hence, the total loglikelihood score is:

$$\mathcal{L} = 5 \log \frac{5}{10} + 5 \log \frac{5}{10} + 6 \log \frac{6}{10} + 4 \log \frac{4}{10} + 5 \log \frac{5}{10} + 5 \log \frac{5}{10} \approx -20.59$$

(c) The neighbors are:



Pairs of models in the same row are equivalent, because moralisation does not require marrying parents, and the resulting undirected graphs are the same.

(d) No, X_1 and X_2 are independent in the data, that is, for all values x_1 of X_1 and x_2 of X_2: $\hat{P}(x_2) = \hat{P}(x_2|x_1)$. This means that adding an edge from X_1 to X_2 does not improve the loglikelihood score. The BIC-score will go down because of the extra parameter.

(e) We compute

$$\hat{p}_{3|1}(0 \mid 0) = \frac{1}{5} \quad \hat{p}_{3|1}(1 \mid 0) = \frac{4}{5} \quad \hat{p}_{3|1}(0 \mid 1) = \frac{4}{5}, \quad \hat{p}_{3|1}(1 \mid 1) = \frac{1}{5}$$

where $\hat{p}_{3|1}(0 \mid 0)$ is shorthand for $\hat{p}(x_3 = 0 \mid x_1 = 0)$. Hence, the new contribution of node 3 to the loglikelihood score is:

$$\log \frac{1}{5} + 4 \log \frac{4}{5} + 4 \log \frac{4}{5} + \log \frac{1}{5}$$

The change in loglikelihood score is:

$$\Delta\mathcal{L} = \left(\log \frac{1}{5} + 4 \log \frac{4}{5} + 4 \log \frac{4}{5} + \log \frac{1}{5} \right) - \left(5 \log \frac{5}{10} + 5 \log \frac{5}{10} \right) \approx 1.93$$

The loglikelihood score improves by 1.93. This is at the cost of one extra parameter that costs $0.5 \log 10 = 1.15$. All in all adding an edge from X_1 to X_3 improves the BIC score by $1.93 - 1.15 = 0.78$.

Exercise 3

(a) The maximum likelihood estimates are:

$$\hat{p}_1(0) = \frac{n_1(0)}{n} = \frac{4}{10} \qquad \hat{p}_1(1) = \frac{n_1(1)}{n} = \frac{6}{10}$$

$$\hat{p}_2(0) = \frac{n_2(0)}{n} = \frac{5}{10} \qquad \hat{p}_2(1) = \frac{n_2(1)}{n} = \frac{5}{10}$$

$$\hat{p}_{3|12}(0|0,0) = \frac{n_{123}(0,0,0)}{n_{12}(0,0)} = \frac{0}{2} = 0 \qquad \hat{p}_{3|12}(1|0,0) = \frac{n_{123}(0,0,1)}{n_{12}(0,0)} = \frac{2}{2} = 1$$

$$\hat{p}_{3|12}(0|0,1) = \frac{n_{123}(0,1,0)}{n_{12}(0,1)} = \frac{1}{2} \qquad \hat{p}_{3|12}(1|0,1) = \frac{n_{123}(0,1,1)}{n_{12}(0,1)} = \frac{1}{2}$$

$$\hat{p}_{3|12}(0|1,0) = \frac{n_{123}(1,0,0)}{n_{12}(1,0)} = \frac{3}{3} = 1 \qquad \hat{p}_{3|12}(1|1,0) = \frac{n_{123}(1,0,1)}{n_{12}(1,0)} = \frac{0}{3} = 0$$

$$\hat{p}_{3|12}(0|1,1) = \frac{n_{123}(1,1,0)}{n_{12}(1,1)} = \frac{1}{3} \qquad \hat{p}_{3|12}(1|1,1) = \frac{n_{123}(1,1,1)}{n_{12}(1,1)} = \frac{2}{3}$$

$$\hat{p}_{4|3}(0|0) = \frac{n_{34}(0,0)}{n_3(0)} = \frac{2}{5} \qquad \hat{p}_{4|3}(1|0) = \frac{n_{34}(0,1)}{n_3(0)} = \frac{3}{5}$$

$$\hat{p}_{4|3}(0|1) = \frac{n_{34}(1,0)}{n_3(1)} = \frac{4}{5} \qquad \hat{p}_{4|3}(1|1) = \frac{n_{34}(1,1)}{n_3(1)} = \frac{1}{5}$$

where, for example, $\hat{p}_{3|12}(0|0,0)$ is shorthand for $\hat{p}(x_3 = 0|x_1 = 0, x_2 = 0)$.

(b) The loglikelihood score is:

$$\begin{aligned}
\mathcal{L} &= 4\log\frac{4}{10} + 6\log\frac{6}{10} + 5\log\frac{5}{10} + 5\log\frac{5}{10} \\
&\quad + 0\log 0 + 2\log 1 + \log\frac{1}{2} + \log\frac{1}{2} \\
&\quad + 3\log 1 + 0\log 0 + \log\frac{1}{3} + 2\log\frac{2}{3} \\
&\quad + \boxed{2\log\tfrac{2}{5} + 3\log\tfrac{3}{5} + 4\log\tfrac{4}{5} + \log\tfrac{1}{5}} \\
&= -22.82450
\end{aligned}$$

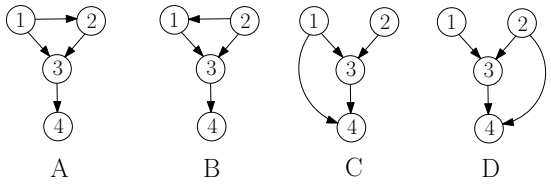
(c) Count the number of parameters per node (variable) as follows. Suppose a node has k different parent configurations (possible value assignments to its parents), and it can take on m different values itself. Then the number of parameters associated with that node is $k(m-1)$ because you have to estimate k different conditional distributions, and each conditional distribution requires the estimation of $m-1$ probabilities. If a node doesn't have any parents, then the number of parameters associated with it is $m-1$. Specified per node, the number of parameters is therefore:

- Node 1: 1.
- Node 2: 1.
- Node 3: $4 \times 1 = 4$.
- Node 4: $2 \times 1 = 2$.

Hence, the BIC score is:

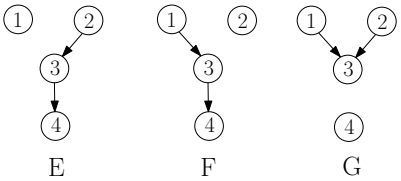
$$-22.82450 - 1.15\,(1 + 1 + 4 + 2) = -32.02450$$

(d) Adding an arc:

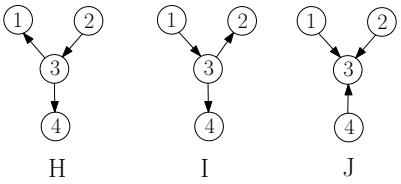


A and B are equivalent.

Removing an arc:



Reversing an arc:



H and I are equivalent.

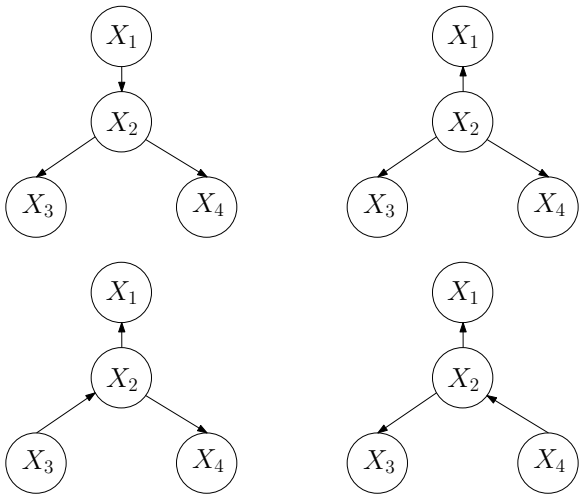
(e) The parent set of X_4 changes so we have to recompute the part of the score corresponding to this node. The boxed part of the loglikelihood under (b) is replaced by

$$2\log\frac{2}{4} + 2\log\frac{2}{4} + \log\frac{1}{2} + \log\frac{1}{2} \approx -4.16,$$

where we left out all the terms that evaluate to zero. The boxed part under (b) evaluates to -5.86 so the loglikelihood increases by 1.7. This is however at the cost of two extra parameters, that cost 1.15 each, so all in all addition of an arc from X_1 to X_4 decreases the BIC score. Hence it is not preferred to the current model.

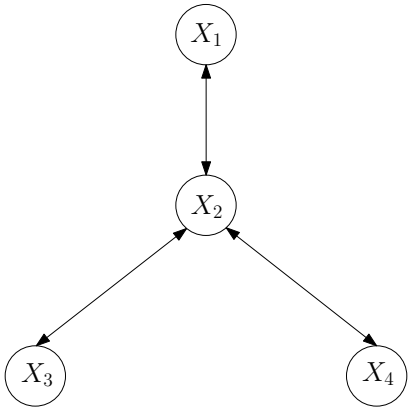
Exercise 4: Essential Graph

The equivalence class is:



These four graphs all have the same skeleton and the same set of v-structures (in this case: none).

The essential graph is:



All edges are bi-directional because each edge occurs in opposite directions in different members of the equivalence class.

Exercise 5: Structure Learning

We need to compute Δ Score (add($B \to D$)), Δ Score (add($C \to D$)),
Δ Score (add($E \to D$)). You may also mention Δ Score (remove($A \to D$)), and
Δ Score (reverse($A \to D$)), although the first returns to the initial model, and the second leads to a model that is equivalent to the current model (and therefore has the same BIC-score).

In general: you need to compute the Δ scores for operations (addition, removal, reversal) that change the parent set of node D, because the parent set of node D has changed in the previous step. The other Δ scores are the same as in the previous step, and can therefore be retrieved from memory.

Exercise 6: Maximum Likelihood Estimation

The loglikelihood function is:

$$\mathcal{L} = \sum_{i=1}^{k} \left\{ \sum_{x_{pa(i)}} n(x_i = 0, x_{pa(i)}) \log p(x_i = 0 \mid x_{pa(i)}) + n(x_i = 1, x_{pa(i)}) \log(1 - p(x_i = 0 \mid x_{pa(i)})) \right\}$$

The partial derivative of $\mathcal{L}$ with respect to $p(x_j = 0 \mid x_{pa(j)})$ is:

$$\frac{\partial \mathcal{L}}{\partial p(x_j = 0 \mid x_{pa(j)})} = \frac{n(x_j = 0, x_{pa(j)})}{p(x_j = 0 \mid x_{pa(j)})} - \frac{n(x_j = 1, x_{pa(j)})}{1 - p(x_j = 0 \mid x_{pa(j)})}$$

Let's introduce some shorthand to simplify notation. Let

- $n_0 = n(x_j = 0, x_{pa(j)})$
- $n_1 = n(x_j = 1, x_{pa(j)})$
- $p_0 = p(x_j = 0 \mid x_{pa(j)})$

The partial derivative of $\mathcal{L}$ with respect to p_0 is:

$$\frac{\partial \mathcal{L}}{\partial p_0} = \frac{n_0}{p_0} - \frac{n_1}{1 - p_0}$$

Equate to zero and solve for p_0 to get

$$p_0 = \frac{n_0}{n_0 + n_1}$$

Exercise 7: Logistic Regression

(a) Recall that:

$$p_i = (1 + e^{-\beta^\top x_i})^{-1},$$

so we have (apply the chain rule)

$$\begin{aligned}\frac{\partial p_i}{\partial \beta_j} &= -(1+e^{-\beta^\top x_i})^{-2} \cdot e^{-\beta^\top x_i} \cdot -x_{ij} \\ &= \frac{e^{-\beta^\top x_i}}{(1+e^{-\beta^\top x_i})^2} \cdot x_{ij} \\ &= \frac{1}{(1+e^{-\beta^\top x_i})} \cdot \frac{e^{-\beta^\top x_i}}{(1+e^{-\beta^\top x_i})} \cdot x_{ij} \\ &= p_i(1-p_i)x_{ij}\end{aligned}$$

(b)

$$\begin{aligned}g(\beta_j) &= \sum_{i=1}^{n} \frac{y_i}{p_i} p_i(1-p_i)x_{ij} - \frac{1-y_i}{1-p_i} p_i(1-p_i)x_{ij} \\ &= \sum_{i=1}^{n} y_i(1-p_i)x_{ij} - (1-y_i)p_i x_{ij} \\ &= \sum_{i=1}^{n} y_i x_{ij} - y_i p_i x_{ij} - p_i x_{ij} + y_i p_i x_{ij} \\ &= \sum_{i=1}^{n} y_i x_{ij} - p_i x_{ij} \\ &= \sum_{i=1}^{n} (y_i - p_i)x_{ij}\end{aligned}$$

(c) We have

$$p_i^{(0)} = \frac{1}{1+e^{3-10\times 0.15}} = \frac{1}{1+e^{1.5}} = 0.182,$$

so $y_i - p_i^{(0)} = 0.818$. Hence,

$$\beta_1^{(1)} = \beta_1^{(0)} + \eta(y_i - p_i^{(0)})x_{i1} = 0.15 + 0.001 \times 0.818 \times 10 = 0.15 + 0.0818 = 0.2318$$

Likewise

$$\beta_0^{(1)} = -3 + 0.001 \times 0.818 \times 1 = -2.99182$$

Using the new coefficient estimates, we obtain

$$p_i^{(1)} = 0.338,$$

so $y_i - p_i^{(1)} = 0.662$.