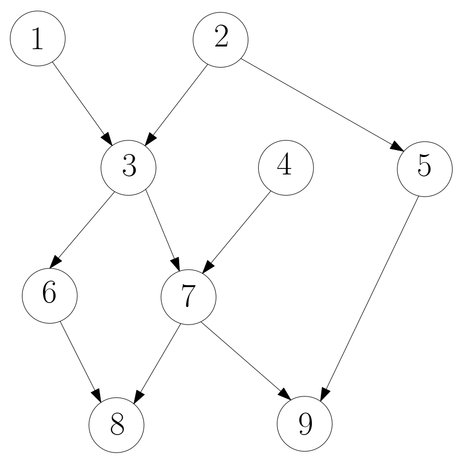
Data Mining 2018
Exercises Bayesian Networks (and Logistic Regression)

Exercise 1: Independence Properties of Bayesian Networks

Consider the following directed independence graph.



(a) Give the factorization of $P(X_1, X_2, \ldots, X_9)$ corresponding to this independence graph.

Construct the appropriate moral graphs to check whether the following conditional independencies hold:

(b) $6 \perp\!\!\!\perp 7$

(c) $6 \perp\!\!\!\perp 7 \mid 3$

(d) $6 \perp\!\!\!\perp 7 \mid 8$

(e) $2 \perp\!\!\!\perp 9 \mid \{5, 7\}$

(f) $2 \perp\!\!\!\perp 9 \mid \{3, 5\}$

(g) $5 \perp\!\!\!\perp 8$

(h) $5 \perp\!\!\!\perp 8 \mid 3$

Exercise 2: Learning Bayesian Networks

In structure learning of Bayesian networks one often uses a score function to determine the quality of a network structure, in combination with a hill-climbing local search strategy. One popular score function is BIC (Bayesian Information Criterion):

$$\mathrm{BIC}(M) = \mathcal{L}(M) - \frac{\ln n}{2}\dim(M),$$

where $\mathcal{L}(M)$ denotes the value of the loglikelihood function of model M evaluated at the maximum (also called the loglikelihood score), $\dim(M)$ denotes the number of parameters of model M, and n denotes the number of observations in the data set.
We want to construct a model on the following data set on 3 binary variables:

	X_1	X_2	X_3
1	1	1	0
2	1	0	0
3	1	0	0
4	1	0	0
5	0	0	0
6	0	1	1
7	1	1	1
8	0	1	1
9	0	0	1
10	0	0	1

The initial model in the search is the mutual independence model (corresponding to the empty graph).

(a) Give the maximum likelihood estimates of the parameters of the mutual independence model.

(b) Compute the loglikelihood score of the mutual independence model. The loglikelihood score is the value of the loglikehood function evaluated in the maximum. Use the *natural* logarithm in your computations.

(c) Give all neighbours of the current model, assuming a neighbour can be obtained by either: adding an edge, removing an edge, or reversing an edge. Which of these neighbour models are equivalent? **Note:** Define the skeleton of a directed graph as the undirected graph obtained by dropping the directions of the edges. Two models are equivalent if and only if they have the same skeleton and the same v-structures.

(d) Would adding an edge from X_1 to X_2 (or vice versa) improve the BIC score? Explain.

(e) Consider the neighbour model obtained by adding an edge from X_1 to X_3. Is this model preferred to the initial model on the basis of the BIC-score? Explain.

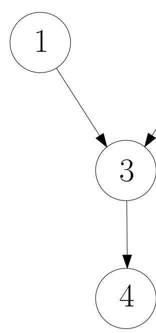
Exercise 3: Learning Bayesian Networks

This exercise is similar to exercise 2; it just gives you more practice.

We are constructing a model on the following data set on 4 binary variables:

	X_1	X_2	X_3	X_4
1	1	1	0	0
2	1	0	0	1
3	1	0	0	0
4	1	0	0	1
5	0	1	0	1
6	1	1	1	1
7	1	1	1	0
8	0	1	1	0
9	0	0	1	0
10	0	0	1	0

Suppose the current model in the search has the following structure:



(a) Give the maximum likelihood estimates of the model parameters.

(b) Compute the loglikelihood score for the given model and data set. Use the *natural* logarithm in your computations.

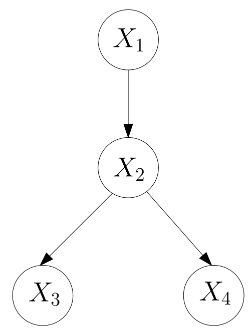
(c) Compute the BIC score of this model on the given data set.

(d) Give all neighbours of the current model, assuming a neighbour can be obtained by either: adding an edge, removing an edge, or reversing an edge. Which of these neighbour models are equivalent?

(e) Consider the neighbour model obtained by adding an edge from X_1 to X_4. Is this model preferred to the current model? Explain.

Exercise 4: Essential Graph

Construct a graph from the DAG below as follows: orient all edges whose direction is fixed in the equivalence class that the DAG belongs to, and make edges bi-directional if there are two members in the equivalence class which have edges in opposite directions. The resulting graph is called the *essential* graph. Recall that two DAGs belong to the same equivalence class iff they have the same skeleton and the same immoralities (v-structures). Hint: it doesn't suffice to check if you remain in the same equivalence class if you turn a single edge around!



Exercise 5: Structure Learning

We perform a greedy hill-climbing search to find a good Bayesian network structure on 5 variables denoted A, B, C, D, and E. Neighbour models are obtained by adding, deleting, or reversing an edge. We start our search from the empty graph. In step 1 of the search we find that adding the edge $A \to D$ gives the biggest improvement in the BIC score. Which Δ scores do we need to compute in step 2?

Exercise 6: Maximum Likelihood Estimation

The loglikelihood function of a Bayesian network is given by:

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

To simplify matters somewhat, we assume all variables are binary, so that we can write:

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

(a) Determine

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

that is, the partial derivative of the loglikelihood function with respect to $p(x_j = 0 \mid x_{pa(j)})$ for arbitrary $j \in \{1, \ldots, k\}$ and arbitrary parent configuration $x_{pa(j)} \in \{0,1\}^{|pa(j)|}$.
Verify that this partial derivative doesn't depend on any unknown parameter, except for $p(x_j = 0 \mid x_{pa(j)})$ itself.

(b) Equate the answer you obtained under (a) to zero, and solve for $p(x_j = 0 \mid x_{pa(j)})$. You should get the solution

$$p(x_j = 0 \mid x_{pa(j)}) = \frac{n(x_j = 0, x_{pa(j)})}{n(x_j = 0, x_{pa(j)}) + n(x_j = 1, x_{pa(j)})} = \frac{n(x_j = 0, x_{pa(j)})}{n(x_{pa(j)})}$$

Verify that this solution coincides with the general formula given for the maximum likelihood parameter estimates of a Bayesian network.

Exercise 7: Logistic Regression

The log-likelihood function for a sample of n independent Bernoulli random variables Y_i, with probability of success on the i-th outcome denoted by p_i is given by:

$$\ell = \sum_{i=1}^{n} \{y_i \ln p_i + (1 - y_i) \ln(1 - p_i)\}$$

Since, by assumption, for the logistic regression model:

$$\begin{aligned} p_i &= (1 + e^{-\beta^\top x_i})^{-1} \\ 1 - p_i &= (1 + e^{\beta^\top x_i})^{-1} \end{aligned}$$

the log-likelihood function for logistic regression becomes:

$$\ell(\beta) = \sum_{i=1}^{n} \left\{ y_i \ln \left(\frac{1}{1 + e^{-\beta^\top x_i}} \right) + (1 - y_i) \ln \left(\frac{1}{1 + e^{\beta^\top x_i}} \right) \right\}$$

The partial derivative of the log-likelihood function with respect to β_j, $j = 0, \ldots, m$, is given by:

$$g(\beta_j) = \frac{\partial \ell(\beta)}{\partial \beta_j} = \sum_{i=1}^{n} \frac{y_i}{p_i} \cdot \frac{\partial p_i}{\partial \beta_j} + \frac{1 - y_i}{1 - p_i} \cdot \frac{\partial(1 - p_i)}{\partial \beta_j} \tag{1}$$

where

$$\frac{\partial p_i}{\partial \beta_j} = p_i(1 - p_i)x_{ij} \tag{2}$$

Substituting equation (2) into equation (1) gives:

$$g(\beta_j) = \sum_{i=1}^{n} (y_i - p_i) x_{ij} \tag{3}$$

Questions:

(a) Show that

$$\frac{\partial p_i}{\partial \beta_j} = p_i(1 - p_i) x_{ij}$$

(b) Show that

$$g(\beta_j) = \sum_{i=1}^{n} (y_i - p_i) x_{ij}$$

(c) Suppose we try to maximize the log-likelihood function using the method of gradient ascent. Consider a single training observation of someone with 10 months of programming experience ($x_{i1} = 10$) who has completed the programming assignment in time ($y_i = 1$). Update the initial guesses $\beta_0^{(0)} = -3$ and $\beta_1^{(0)} = 0.15$ using the method of gradient ascent with step size $\eta = 0.001$. Compute the probability of success for this person using the updated coefficient estimates. Has the error $y_i - p_i$ gone down?