ETH
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D-BSSE
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Statistical Models in Computational Biology

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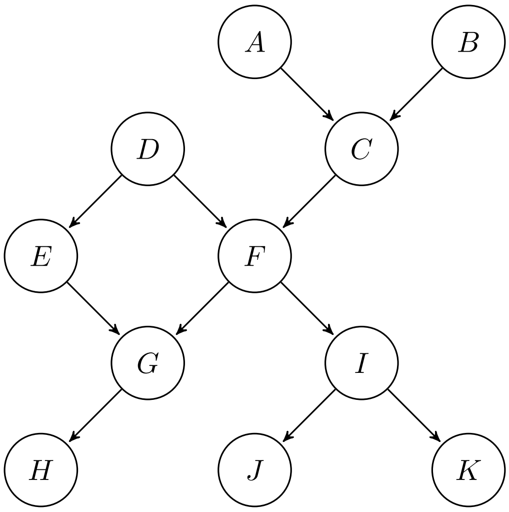
Due 21st of April 2022
Please submit your project with the filename `Lastname(s)_Project7.pdf`.

Problem 17: Junction Tree Algorithm **(2 points)**

Consider the Bayesian network on the variables $U = \{A, \ldots, K\}$ given by the graph:



(a) Build the *Junction Tree* of the network. (1 point)

(b) Write the joint probability $P(U)$ in terms of the cluster and separator potentials. (1 point)

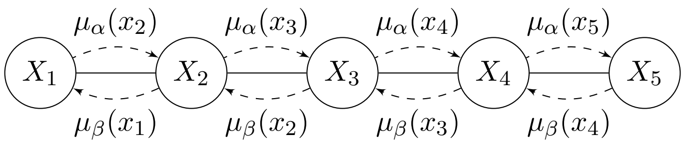


Figure 1: Message passing on the undirected chain.

Problem 18: Benefit of storing messages **(3 points)**

Consider message passing on the undirected chain in Figure 1, in which $\mu_\alpha(x_n)$ and $\mu_\beta(x_n)$ represent the forward and backward messages for $n \in \{2, 3, 4, 5\}$, as seen in the lecture.

(a) Write the formula for recursively computing the forward and backward messages. (1 point)

(b) What is the complexity of computing the marginal probability $P(X_4 = 1)$ using message passing? (1 point)

(c) If you store all the messages, what is the complexity of computing all marginal probability distributions X_1, X_2, X_3, X_4, and X_5? How about the general case, with a chain of length N where each node can assume K values? Assume that storing and multiplying is free, so that only summation counts for the complexity. (1 point)

Problem 19(data analysis): Message passing on a chain **(5 points)**

We will now use R to perform the message passing shown in Figure 1. Suppose that we have the following (conditional) probability distributions:

$$(1) \quad p(X_1 = 1) = 1/3, \quad p(X_2 = 1 \mid X_1) = \begin{cases} 4/5 & \text{if } X_1 = 0 \\ 2/3 & \text{if } X_1 = 1 \end{cases}, \quad p(X_3 = 1 \mid X_2) = \begin{cases} 5/7 & \text{if } X_2 = 0 \\ 1/3 & \text{if } X_2 = 1 \end{cases},$$

$$(2) \quad p(X_4 = 1 \mid X_3) = \begin{cases} 3/5 & \text{if } X_3 = 0 \\ 2/5 & \text{if } X_3 = 1 \end{cases}, \quad p(X_5 = 1 \mid X_4) = \begin{cases} 1/2 & \text{if } X_4 = 0 \\ 7/9 & \text{if } X_4 = 1 \end{cases}.$$

Note that these equations fully determine each (conditional) probability distribution, since $X_i \in \{0, 1\}$ for $i \in \{1, \dots, 5\}$.

(a) **Store clique potentials in an R object** **(2 points)**

Since all $X_i \in \{0, 1\}$, each clique potential $\psi_{n,n+1}$ can be stored as a 2×2 matrix

$$(3) \quad \Psi_{n,n+1} := \begin{pmatrix} \psi_{n,n+1}(0,0) & \psi_{n,n+1}(0,1) \\ \psi_{n,n+1}(1,0) & \psi_{n,n+1}(1,1) \end{pmatrix}.$$

Each $\psi_{n,n+1}(\cdot, \cdot)$ can be computed using the factorisation from conditional probabilities in equations (1) and (2). Compute and store these clique potentials in a three-dimensional array, such that the third dimension holds the clique matrices in equation (3) for $n = 1, \dots, 4$.

Hint: `array(dim = c(2, 2, 4), dimnames = list(c("0", "1"), c("0", "1"), c("Psi12", "Psi23", "Psi34", "Psi45")))`

(b) **Computing forward messages** **(1 point)**

In the problem *Message passing*, you have written the formula for recursively computing the forward messages $\mu_\alpha(x_n)$ for $n \in \{2, 3, 4, 5\}$. How can these be computed for $x_n \in \{0, 1\}$ as the matrix product of the vector $\big(\mu_\alpha(X_{n-1} = 0), \mu_\alpha(X_{n-1} = 1)\big)$ multiplied by $\Psi_{n-1,n}$, with $\Psi_{n-1,n}$ as defined in equation (3)? Initialise $\mu_\alpha(x_1) = 1$ for $x_1 \in \{0, 1\}$, and compute the remaining forward messages.

(c) **Computing backward messages** **(1 point)**

Similarly, how can the backward messages $\mu_\beta(x_n)$ for $n \in \{4, 3, 2, 1\}$ can be computed for $x_n \in \{0, 1\}$ as the matrix product of $\Psi_{n,n+1}$ multiplied by the vector $\big(\mu_\beta(X_{n+1} = 0), \mu_\beta(X_{n+1} = 1)\big)^\top$? Initialise $\mu_\beta(x_5) = 1$ for $x_5 \in \{0, 1\}$, and compute the remaining backward messages.

(d) **Compute the marginal probability distribution for each node** **(1 point)**

Multiply (element-wise) forward and backward messages at each position to obtain the marginal probability distributions for X_1, X_2, X_3, X_4, and X_5. What is the normalising constant Z?