# 732A96/TDDE15 Advanced Machine Learning Graphical Models

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Lecture 2: Probabilistic Inference

#### Contents

- Probabilistic Inference for BNs
  - ▶ Naive Solution
  - Variable Elimination
- Probabilistic Inference for MNs
- ▶ Most Probable Configuration

#### Literature

- Main source
  - Koller, D. and Friedman, N. Probabilistic Graphical Models: Principles and Techniques. MIT Press, 2009. Chapter 9.2-9.4.
- Additional source
  - Bishop, C. M. Pattern Recognition and Machine Learning. Springer, 2006. Chapter 8.

What is the state of a random variable X<sub>k</sub> if a random variable X<sub>i</sub> is observed to be in the state x<sub>i</sub>?

$$p(x_k|x_i) = \frac{p(x_k, x_i)}{p(x_i)} = \frac{\sum_{x \setminus \{x_i, x_k\}} p(x)}{\sum_{x \setminus x_i} p(x)}$$

▶ For instance,  $p(d) = \sum_{a,b,c} p(a,b,c,d) = \sum_{a,b,c} p(a)p(b|a)p(c|b)p(d|c)$  for the DAG  $A \to B \to C \to D$ .

Figure 9.2 Computing P(D) by summing over the joint distribution for a chain  $A \to B \to C \to D$ ; all of the variables are binary valued.

Figure 9.2 Computing P(D) by summing over the joint distribution for a chain  $A \to B \to C \to D$ ; all of the variables are binary valued.

Figure 9.3 The first transformation on the sum of figure 9.2

$$\begin{array}{c} (P(a^1)P(b^1\mid a^1) + P(a^2)P(b^1\mid a^2)) \quad P(c^1\mid b^1) \quad P(d^1\mid c^1) \\ + \ (P(a^1)P(b^2\mid a^1) + P(a^2)P(b^2\mid a^2)) \quad P(c^1\mid b^2) \quad P(d^1\mid c^1) \\ + \ (P(a^1)P(b^1\mid a^1) + P(a^2)P(b^1\mid a^2)) \quad P(c^2\mid b^1) \quad P(d^1\mid c^2) \\ + \ (P(a^1)P(b^2\mid a^1) + P(a^2)P(b^2\mid a^2)) \quad P(c^2\mid b^2) \quad P(d^1\mid c^2) \\ + \ (P(a^1)P(b^1\mid a^1) + P(a^2)P(b^1\mid a^2) \quad P(c^1\mid b^1) \quad P(d^2\mid c^1) \\ + \ (P(a^1)P(b^2\mid a^1) + P(a^2)P(b^2\mid a^2)) \quad P(c^1\mid b^1) \quad P(d^2\mid c^1) \\ + \ (P(a^1)P(b^1\mid a^1) + P(a^2)P(b^1\mid a^2)) \quad P(c^2\mid b^1) \quad P(d^2\mid c^2) \\ + \ (P(a^1)P(b^2\mid a^1) + P(a^2)P(b^2\mid a^2)) \quad P(c^2\mid b^2) \quad P(d^2\mid c^2) \end{array}$$

Figure 9.3 The first transformation on the sum of figure 9.2  $\,$ 

Figure 9.4 The second transformation on the sum of figure 9.2

Figure 9.4 The second transformation on the sum of figure 9.2

$$\begin{array}{ll} (\tau_1(b^1)P(c^1\mid b^1) + \tau_1(b^2)P(c^1\mid b^2)) & P(d^1\mid c^1) \\ + & (\tau_1(b^1)P(c^2\mid b^1) + \tau_1(b^2)P(c^2\mid b^2)) & P(d^1\mid c^2) \\ \\ & (\tau_1(b^1)P(c^1\mid b^1) + \tau_1(b^2)P(c^1\mid b^2)) & P(d^2\mid c^1) \\ + & (\tau_1(b^1)P(c^2\mid b^1) + \tau_1(b^2)P(c^2\mid b^2)) & P(d^2\mid c^2) \end{array}$$

Figure 9.5 The third transformation on the sum of figure 9.2

$$\begin{array}{c} (\tau_1(b^1)P(c^1\mid b^1)+\tau_1(b^2)P(c^1\mid b^2)) & P(d^1\mid c^1) \\ + & (\tau_1(b^1)P(c^2\mid b^1)+\tau_1(b^2)P(c^2\mid b^2)) & P(d^1\mid c^2) \\ \\ (\tau_1(b^1)P(c^1\mid b^1)+\tau_1(b^2)P(c^1\mid b^2)) & P(d^2\mid c^1) \\ + & (\tau_1(b^1)P(c^2\mid b^1)+\tau_1(b^2)P(c^2\mid b^2)) & P(d^2\mid c^2) \\ \end{array}$$

Figure 9.5 The third transformation on the sum of figure 9.2

$$\begin{array}{ccc} \tau_2(c^1) & P(d^1 \mid c^1) \\ + & \tau_2(c^2) & P(d^1 \mid c^2) \\ \\ & \tau_2(c^1) & P(d^2 \mid c^1) \\ + & \tau_2(c^2) & P(d^2 \mid c^2) \end{array}$$

Figure 9.6 The fourth transformation on the sum of figure 9.2

- Then, instead of  $p(d) = \sum_{a,b,c} p(a)p(b|a)p(c|b)p(d|c)$ , we can do  $p(d) = \sum_{c} p(d|c)\tau_{2}(c)$  $= \sum_{c} p(d|c) \sum_{b} p(c|b)\tau_{1}(b)$  $= \sum_{c} p(d|c) \sum_{c} p(c|b) \sum_{c} p(a)p(b|a)$
- Do we gain anything? Yes, the former case implies 48 operations (multiplications and additions) and the latter only 18. Moreover, the former case requires more storage space.

Let us define a factor  $\phi(U)$  as a function  $\phi: Values(U) \to \mathbb{R}$ . Let us also define  $Scope(\phi) = U$ .

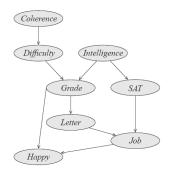


Figure 9.8 The Extended-Student Bayesian network

$$\begin{array}{ll} P(C,D,I,G,S,L,J,H) & = & P(C)P(D\mid C)P(I)P(G\mid I,D)P(S\mid I) \\ & & P(L\mid G)P(J\mid L,S)P(H\mid G,J) \\ & = & \phi_C(C)\phi_D(D,C)\phi_I(I)\phi_G(G,I,D)\phi_S(S,I) \\ & & \phi_L(L,G)\phi_J(J,L,S)\phi_H(H,G,J). \end{array}$$

▶ The following algorithm returns p(y) where  $Y = X \setminus Z$ .

### Algorithm 9.1 Sum-product variable elimination algorithm

```
Procedure Sum-Product-VE (
          \Phi, // Set of factors
         Z. // Set of variables to be eliminated
         \prec // Ordering on Z
         Let Z_1, \ldots, Z_k be an ordering of Z such that
          Z_i \prec Z_i if and only if i < j
         for i = 1, ..., k
            \Phi \leftarrow \text{Sum-Product-Eliminate-Var}(\Phi, Z_i)
5
         \phi^* \leftarrow \prod_{\phi \in \Phi} \phi
         return \phi^*
      Procedure Sum-Product-Eliminate-Var (
          \Phi, // Set of factors
               // Variable to be eliminated
         \Phi' \leftarrow \{ \phi \in \Phi : Z \in Scope[\phi] \}
       \Phi'' \leftarrow \Phi - \Phi'
      \psi \leftarrow \prod_{\phi \in \Phi'} \phi
         \tau \leftarrow \sum_{z} \psi
         return \Phi'' \cup \{\tau\}
```



Figure 9.8 The Extended-Student Bayesian network

$$\begin{split} P(C, D, I, G, S, L, J, H) &= P(C)P(D \mid C)P(I)P(G \mid I, D)P(S \mid I) \\ &\quad P(L \mid G)P(J \mid L, S)P(H \mid G, J) \\ &= \phi_{G}(C)\phi_{D}(D, C)\phi_{I}(I)\phi_{G}(G, I, D)\phi_{S}(S, I) \\ &\phi_{L}(L, G)\phi_{I}(J, L, S)\phi_{H}(H, G, J). \end{split}$$

Step	Variable	Factors	Variables	New
	eliminated	used	involved	factor
1	C	$\phi_C(C)$ , $\phi_D(D,C)$	C, D	$\tau_1(D)$
2	D	$\phi_G(G, I, D), \tau_1(D)$	G, I, D	$\tau_2(G, I)$
3	I	$\phi_I(I)$ , $\phi_S(S, I)$ , $\tau_2(G, I)$	G, S, I	$\tau_3(G, S)$
4	H	$\phi_H(H, G, J)$	H, G, J	$\tau_4(G, J)$
5	G	$\tau_4(G, J), \tau_3(G, S), \phi_L(L, G)$	G, J, L, S	$\tau_5(J, L, S)$
6	S	$\tau_5(J, L, S)$ , $\phi_J(J, L, S)$	J, L, S	$\tau_6(J, L)$
7	L	$\tau_6(J, L)$	J, L	$\tau_7(J)$

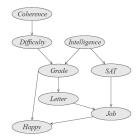


Figure 9.8 The Extended-Student Bayesian network

$$\begin{split} P(C,D,I,G,S,L,J,H) &= & P(C)P(D \mid C)P(I)P(G \mid I,D)P(S \mid I) \\ & & P(L \mid G)P(J \mid L,S)P(H \mid G,J) \\ &= & \phi_G(C)\phi_D(D,C)\phi_I(I)\phi_G(G,I,D)\phi_S(S,I) \\ & \phi_t(L,G)\phi_I(J,L,S)\phi_H(H,G,J). \end{split}$$

Step	Variable	Factors	Variables	New
_	eliminated	used	involved	factor
1	G	$\phi_G(G, I, D), \phi_L(L, G), \phi_H(H, G, J)$	G, I, D, L, J, H	$\tau_1(I, D, L, J, H)$
2	I	$\phi_I(I)$ , $\phi_S(S, I)$ , $\tau_1(I, D, L, S, J, H)$	S, I, D, L, J, H	$\tau_2(D, L, S, J, H)$
3	S	$\phi_J(J, L, S), \tau_2(D, L, S, J, H)$	D, L, S, J, H	$\tau_3(D, L, J, H)$
4	L	$\tau_3(D, L, J, H)$	D, L, J, H	$\tau_4(D, J, H)$
5	H	$\tau_4(D, J, H)$	D, J, H	$\tau_5(D, J)$
6	C	$\phi_C(C)$ , $\phi_D(D,C)$	D, J, C	$\tau_6(D)$
7	D	$\tau_5(D, J),  \tau_6(D)$	D, J	$\tau_7(J)$

What is the state of a random variable X<sub>k</sub> if a random variable X<sub>i</sub> is observed to be in the state x<sub>i</sub>?

$$p(x_k|x_i) = \frac{p(x_k, x_i)}{p(x_i)} = \frac{\sum_{x \setminus \{x_i, x_k\}} p(x)}{\sum_{x \setminus x_i} p(x)}$$

- ► E.g.,  $p(d|a) = \sum_{c} p(d|c) \sum_{b} p(d|b) p(a) p(b|a)$  for  $A \rightarrow B \rightarrow C \rightarrow D$ .
- ► The following algorithm returns  $p(y|e) = \frac{p(y,e)}{p(e)} = \frac{\phi^*}{\alpha}$  where  $Y \subseteq X \setminus E$ .
- Given a factor φ(U), let us define the reduced factor φ[E = e](Y) as a factor with scope Y = U \ E such that φ[E = e](y) = φ(y, z) where Z = U ∩ E.

# Algorithm 9.2 Using Sum-Product-VE for computing conditional probabilities

```
Procedure Cond-Prob-VE ( \mathcal{K},  // A network over \mathcal{X} Y,  // Set of query variables E=e  // Evidence ) 1 \Phi \leftarrow Factors parameterizing \mathcal{K} Replace each \phi \in \Phi by \phi[E=e] 3 Select an elimination ordering \prec 2 \mathcal{K} \leftarrow \mathcal{K} = \mathcal{K} - \mathcal{K} - \mathcal{K} = \mathcal{K} - \mathcal{K} - \mathcal{K} = \mathcal{K} = \mathcal{K} - \mathcal{K} = \mathcal{
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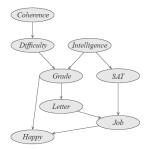


Figure 9.8 The Extended-Student Bayesian network

$$\begin{array}{lcl} P(C,D,I,G,S,L,J,H) & = & P(C)P(D\mid C)P(I)P(G\mid I,D)P(S\mid I) \\ & & P(L\mid G)P(J\mid L,S)P(H\mid G,J) \\ & = & \phi_C(C)\phi_D(D,C)\phi_I(I)\phi_G(G,I,D)\phi_S(S,I) \\ & & \phi_L(L,G)\phi_J(J,L,S)\phi_H(H,G,J). \end{array}$$

Step	Variable	Factors	Variables	New
	eliminated	used	involved	factor
1'	C	$\phi_C(C), \phi_D(D, C)$	C, D	$\tau'_1(D)$
2'	D	$\phi_G[I = i^1](G, D), \phi_I[I = i^1](), \tau'_1(D)$	G, D	$\tau'_2(G)$
5'	G	$\tau'_{2}(G), \phi_{L}(L, G), \phi_{H}[H = h^{0}](G, J)$	G, L, J	$\tau'_5(L, J)$
6'	S	$\phi_S[I = i^1](S), \phi_J(J, L, S)$	J, L, S	$\tau'_6(J, L)$
7'	L	$\tau'_{6}(J, L),  \tau'_{5}(J, L)$	J, L	$\tau_7'(J)$

Table 9.3 A run of sum-product variable elimination for  $P(J, i^1, h^0)$ 

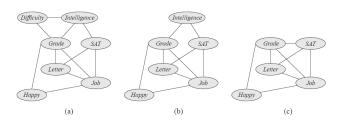


Figure 9.10 Variable elimination as graph transformation in the Student example, using the elimination order of table 9.1: (a) after eliminating C; (b) after eliminating D; (c) after eliminating I.

- VE can be seen as a graph transformation.
- Given a set of factors Φ such that X = ∪<sub>φ∈Φ</sub> Scope(φ), let us define H<sub>Φ</sub> as the undirected graph over X that contains an edge X<sub>i</sub> X<sub>j</sub> if and only X<sub>i</sub>, X<sub>j</sub> ∈ Scope(φ) for some φ ∈ Φ.
- ▶ When the variable Z is eliminated,  $H_{\Phi}$  changes as follows:
  - ▶ The edge  $X_i X_j$  is added to  $H_{\Phi}$  for all  $X_i Z X_j$  in  $H_{\Phi}$ . If this edge was not already in  $H_{\Phi}$ , then it is called a fill edge.
  - ▶ The variable Z is removed from  $H_{\Phi}$ .

- Note that every clique (i.e., maximal complete sets of nodes) in the sequence of graphs H<sub>Φ</sub> is the scope of some factor in the VE process.
- Note also that the size of the largest clique is indicative of the computational cost of the VE process.
- Finally, note that the cliques in the sequence of graphs H<sub>Φ</sub> depends on the elimination ordering.
- Unfortunately, finding the optimal elimination ordering is NP-hard. So, we must resort to heuristics.

# where the evaluation metric $s(\mathcal{H}, X)$ may be

- the number of neighbors X has in  $\mathcal{H}$ ,
- the product of the domain cardinality of the neighbors of X in  $\mathcal{H}$ , or
- the number of fill edges to add to  $\mathcal{H}$  when eliminating X.

#### Probabilistic Inference for MNs

- The VE algorithm can also be used for probabilistic inference in MNs. Simply,
  - initialize the set of factors  $\Phi$  to the MN's clique potentials  $\{\varphi(k)\}$ ,
  - run the VE algorithm, and
  - normalize the returned unnormalized probability distribution by dividing with the MN's normalization constant Z.

# Most Probable Configuration

▶ The following algorithm returns  $\arg \max_{x} p(x)$ .

Algorithm 13.1 Variable elimination algorithm for MAP. The algorithm can be used both in its max-product form, as shown, or in its max-sum form, replacing factor product with factor addition.

```
Procedure Max-Product-VE (
          \Phi. // Set of factors over X

✓ // Ordering on X

        Let X_1, \ldots, X_k be an ordering of X such that
           X_i \prec X_i iff i < j
           for i = 1, ..., k
           (\Phi, \phi_{X_i}) \leftarrow \text{Max-Product-Eliminate-Var}(\Phi, X_i)
           x^* \leftarrow \text{Traceback-MAP}(\{\phi_{X_i} : i = 1, ..., k\})
           return x^*, \Phi // \Phi contains the probability of the MAP
        Procedure Max-Product-Eliminate-Var (
            Φ. // Set of factors
           Z // Variable to be eliminated
           \Phi' \leftarrow \{ \phi \in \Phi : Z \in Scope[\phi] \}
           \Phi'' \leftarrow \Phi - \Phi'
           \psi \leftarrow \prod_{\phi \in \Phi'} \phi
           \tau \leftarrow \max_{Z} \psi
           return (\Phi'' \cup \{\tau\}, \psi)
         Procedure Traceback-MAP (
            \{\phi_{X_i} : i = 1, ..., k\}
           for i = k, \dots, 1
              u_i \leftarrow (x_{i+1}^*, \dots, x_k^*) \langle Scope[\phi_{X_i}] - \{X_i\} \rangle
3
                 // The maximizing assignment to the variables eliminated after
4
              x_i^* \leftarrow \arg \max_{x_i} \phi_{X_i}(x_i, u_i)
                 // x_i^* is chosen so as to maximize the corresponding entry in
                    the factor, relative to the previous choices u_i
6
           return x*
```

## Beyond Variable Elimination

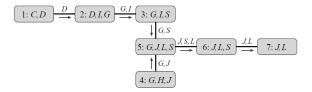


Figure 10.1 Cluster tree for the VE execution in table 9.1

- The execution of VE defines a cluster tree, a graphical flowchart of the factor-manipulation process:
  - Each node  $C_i$  in the tree is called a cluster and it contains the variables in  $Scope(\omega_i)$ .
  - The tree has an edge annotated with an arrow from C<sub>i</sub> to C<sub>j</sub> if the factor (a.k.a. message) \( \tau\_i \) is used in the computation of \( \tau\_j \).
- Now, consider passing messages towards the cluster C<sub>6</sub> in order to compute p(s). Notice the reusing of previously computed messages.
- Therefore, a clique tree is a data structure to perform repeated probabilistic inference efficiently.
- The process of building the cluster tree from a given DAG is known as compilation. You will learn more about cluster trees in the lab.

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Thank you