732A96/TDDE15 Advanced Machine Learning

Graphical Models

Jose M. Peña
IDA, Linköping University, Sweden

Lecture 2: Probabilistic Inference

Contents

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.

Probabilistic Inference for BNs: Naive Solution

- What is the state of a random variable X_k if a random variable X_i is observed to be in the state x_i ?

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

- 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 $A \to B \to C \to D$.

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

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.

Probabilistic Inference for BNs: Naive Solution

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

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

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.

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

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

Figure 9.3 The first transformation on the sum of figure 9.2

Probabilistic Inference for BNs: Naive Solution

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

Figure 9.3 The first transformation on the sum of figure 9.2

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

Figure 9.4 The second transformation on the sum of figure 9.2

Probabilistic Inference for BNs: Naive Solution

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

Figure 9.4 **The second transformation on the sum of figure 9.2**

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

Figure 9.5 **The third transformation on the sum of figure 9.2**

Probabilistic Inference for BNs: Naive Solution

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

Figure 9.5 The third transformation on the sum of figure 9.2

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

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

$$
\begin{aligned}
p(d) &= \sum_c p(d|c)\tau_2(c) \\
&= \sum_c p(d|c) \sum_b p(c|b)\tau_1(b) \\
&= \sum_c p(d|c) \sum_b p(c|b) \sum_a p(a)p(b|a)
\end{aligned}
$$

- Do we gain anything ? **Yes**, the former case implies 62 operations (multiplications and additions) and the latter only 18.

Probabilistic Inference for BNs: Variable Elimination

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

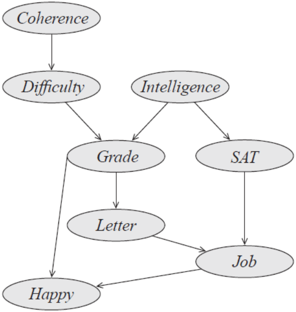

Figure 9.8 **The** Extended-Student **Bayesian network**

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

Probabilistic Inference for BNs: Variable Elimination

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

Algorithm 9.1 Sum-product variable elimination algorithm

Procedure Sum-Product-VE (
  Φ, // Set of factors
  $\boldsymbol{Z}$, // Set of variables to be eliminated
  $\prec$ // Ordering on $\boldsymbol{Z}$
)
  Let $Z_1, \ldots, Z_k$ be an ordering of $\boldsymbol{Z}$ such that
    $Z_i \prec Z_j$ if and only if $i < j$
  for $i = 1, \ldots, k$
    $\Phi \leftarrow$ Sum-Product-Eliminate-Var(Φ, Z_i)
  $\phi^* \leftarrow \prod_{\phi \in \Phi} \phi$
  return ϕ^*

Procedure Sum-Product-Eliminate-Var (
  Φ, // Set of factors
  Z // Variable to be eliminated
)
  $\Phi' \leftarrow \{\phi \in \Phi \ : \ Z \in Scope[\phi]\}$
  $\Phi'' \leftarrow \Phi - \Phi'$
  $\psi \leftarrow \prod_{\phi \in \Phi'} \phi$
  $\tau \leftarrow \sum_Z \psi$
  return $\Phi'' \cup \{\tau\}$

Probabilistic Inference for BNs: Variable Elimination

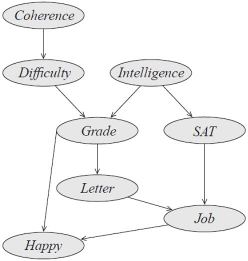

Figure 9.8 **The** Extended-Student **Bayesian network**

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

Step	Variable eliminated	Factors used	Variables involved	New 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	$\tau_7(J)$

Table 9.1 **A run of variable elimination for the query** $P(J)$

Probabilistic Inference for BNs: Variable Elimination

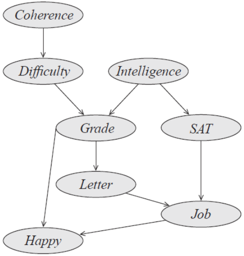

Figure 9.8 The Extended-Student **Bayesian network**

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

Step	Variable eliminated	Factors used	Variables involved	New 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	$\tau_7(J)$

Table 9.2 A different run of variable elimination for the query $P(J)$

Probabilistic Inference for BNs: Variable Elimination

- What is the state of a random variable X_k if a random variable X_i is observed to be in the state x_i ?

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

- E.g., $p(d|a) = \frac{\sum_c p(d|c) \sum_b p(d|b) p(a) p(b|a)}{\sum_{a,c} p(d|c) \sum_b p(d|b) p(a) p(b|a)}$ 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 $\phi(U)$, let us define the reduced factor $\phi[E = e](Y)$ as a factor with scope $Y = U \setminus E$ such that $\phi[E = e](y) = \phi(y, z)$ where $Z = U \cap E$.

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

Procedure Cond-Prob-VE (
$\mathcal{K}$, // A network over $\mathcal{X}$
$\boldsymbol{Y}$, // Set of query variables
$\boldsymbol{E} = \boldsymbol{e}$ // Evidence
)
$\Phi \leftarrow$ Factors parameterizing $\mathcal{K}$
Replace each $\phi \in \Phi$ by $\phi[\boldsymbol{E} = \boldsymbol{e}]$
Select an elimination ordering $\prec$
$\boldsymbol{Z} \leftarrow \; = \mathcal{X} - \boldsymbol{Y} - \boldsymbol{E}$
$\phi^* \leftarrow$ Sum-Product-VE($\Phi, \prec, \boldsymbol{Z}$)
$\alpha \leftarrow \sum_{\boldsymbol{y} \in Val(\boldsymbol{Y})} \phi^*(\boldsymbol{y})$
return α, ϕ^*

Probabilistic Inference for BNs: Variable Elimination

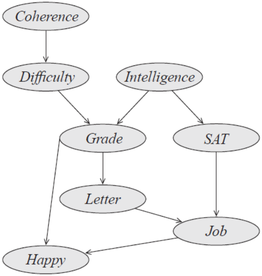

Figure 9.8 **The** Extended-Student **Bayesian network**

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

Step	Variable eliminated	Factors used	Variables involved	New 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** $P(J, i^1, h^0)$

Probabilistic Inference for MNs

- The VE algorithm can also be used for probabilistic inference in MNs. Simply,
  - initialize the set of factors Φ 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.

Beyond Variable Elimination

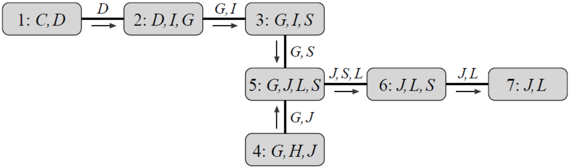

Figure 10.1 **Cluster tree for the VE execution in table 9.1**

- 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 $Scope(\psi_i)$.
  - The tree has an edge annotated with an arrow from C_i to C_j if the factor (a.k.a. message) τ_i is used in the computation of τ_j.
- Now, consider passing messages towards the cluster C_6 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.

Contents

- Probabilistic Inference for BNs
  - Naive Solution
  - Variable Elimination
- Probabilistic Inference for MNs
- Beyond Variable Elimination

Thank you