## CS 3750 Machine Learning Lecture 3

## Graphical models: inference

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## Factors

- Factor: is a function that maps value assignments for a subset of random variables to $\mathfrak{R}$ (reals)
- The scope of the factor:
- a set of variables defining the factor
- Example:
- Assume discrete random variables $x$ (with values a1,a2, a3) and y (with values b1 and b2)
- Factor:

$$
\phi(x, y) \longrightarrow
$$

- Scope of the factor:

$$
\{x, y\}
$$

| a 1 | b 1 | 0.5 |
| :---: | :---: | :---: |
| a 1 | b 2 | 0.2 |
| a 2 | b 1 | 0.1 |
| a 2 | b 2 | 0.3 |
| a 3 | b 1 | 0.2 |
| a 3 | b 2 | 0.4 |

## Factor Product

Variables: A,B,C
$\phi(A, B, C)=\phi(B, C) \circ \phi(A, B)$
$\phi(B, C)$
$\phi(A, B)$

| b1 | cl | 0.1 |
| :---: | :---: | :---: |
| b 1 | c 2 | 0.6 |
| b 2 | cl | 0.3 |
| b 2 | c 2 | 0.4 |


| a1 | b1 | 0.5 |
| :---: | :---: | :---: |
| a1 | b2 | 0.2 |
| a2 | b1 | 0.1 |
| a2 | b2 | 0.3 |
| a3 | b1 | 0.2 |
| a3 | b2 | 0.4 |

$$
\phi(A, B, C)
$$

| a1 | b1 | c1 | $0.5^{*} 0.1$ |
| :---: | :---: | :---: | :---: |
| a1 | b1 | c2 | $0.5^{*} 0.6$ |
| a1 | b2 | c1 | $0.2^{*} 0.3$ |
| a1 | b2 | c2 | $0.2^{*} 0.4$ |
| a2 | b1 | c1 | $0.1^{*} 0.1$ |
| a2 | b1 | c2 | $0.1^{*} 0.6$ |
| a2 | b2 | c1 | $0.3^{*} 0.3$ |
| a2 | b2 | c2 | $0.3^{*} 0.4$ |
| a3 | b1 | c1 | $0.2^{*} 0.1$ |
| a3 | b1 | c2 | $0.2^{*} 0.6$ |
| a3 | b2 | c1 | $0.4^{*} 0.3$ |
| a3 | b2 | c2 | $0.4^{*} 0.4$ |

## Factor Marginalization

Variables: A,B,C $\phi(A, C)=\sum_{B} \phi(A, B, C)$

| a1 | b1 | c1 | 0.2 |
| :---: | :---: | :---: | :---: |
| a1 | b1 | c2 | 0.35 |
| a1 | b2 | c1 | 0.4 |
| a1 | b2 | c2 | 0.15 |
| a2 | b1 | c1 | 0.5 |
| a2 | b1 | c2 | 0.1 |
| a2 | b2 | c1 | 0.3 |
| a3 | b2 | c2 | 0.2 |
| a3 | b1 | c1 | 0.25 |
| a3 | b2 | c1 | 0.45 |
| a3 | b2 | c2 | 0.15 |

## Factor division

| $\mathrm{A}=1$ | $\mathrm{~B}=1$ | 0.5 |
| :--- | :--- | :--- |
| $\mathrm{~A}=1$ | $\mathrm{~B}=2$ | 0.4 |
| $\mathrm{~A}=2$ | $\mathrm{~B}=1$ | 0.8 |
| $\mathrm{~A}=2$ | $\mathrm{~B}=2$ | 0.2 |
| $\mathrm{~A}=3$ | $\mathrm{~B}=1$ | 0.6 |
| $\mathrm{~A}=3$ | $\mathrm{~B}=2$ | $\mathrm{~A}=1$ |
| $\mathrm{~A}=2$ | 0.4 |  |
| $\mathrm{~A}=3$ | 0.4 |  |
|  |  |  |


| $\mathrm{A}=1$ | $\mathrm{~B}=1$ | $0.5 / 0.4=1.25$ |
| :--- | :--- | :--- |
| $\mathrm{~A}=1$ | $\mathrm{~B}=2$ | $0.4 / 0.4=1.0$ |
| $\mathrm{~A}=2$ | $\mathrm{~B}=1$ | $0.8 / 0.4=2.0$ |
| $\mathrm{~A}=2$ | $\mathrm{~B}=2$ | $0.2 / 0.4=2.0$ |
| $\mathrm{~A}=3$ | $\mathrm{~B}=1$ | $0.6 / 0.5=1.2$ |
| $\mathrm{~A}=3$ | $\mathrm{~B}=2$ | $0.5 / 0.5=1.0$ |

Inverse of a factor product

## Inferences

We have already seen VE inferences on both BBNs and MRFs

- Inference on chains and trees structures can be often done efficiently in time: linear in the number of nodes in the tree
chain tree




## Inference on a Chain

$$
\begin{gathered}
p(\mathbf{x})=\frac{1}{Z} \psi_{1,2}\left(x_{1}, x_{2}\right) \psi_{2,3}\left(x_{2}, x_{3}\right) \cdots \psi_{N-1, N}\left(x_{N-1}, x_{N}\right) \\
p\left(x_{n}\right)=\sum_{x_{1}} \cdots \sum_{x_{n-1}} \sum_{x_{n+1}} \cdots \sum_{x_{N}} p(\mathbf{x})
\end{gathered}
$$



$$
\begin{aligned}
& p\left(x_{n}\right)= \frac{1}{Z} \underbrace{\left[\sum_{x_{n-1}} \psi_{n-1, n}\left(x_{n-1}, x_{n}\right) \cdots\left[\sum_{x_{1}} \psi_{1,2}\left(x_{1}, x_{2}\right)\right] \cdots\right]}_{\mu_{\alpha}\left(x_{n}\right)} \\
& \underbrace{\left.\left[\sum_{x_{n+1}} \psi_{n, n+1}\left(x_{n}, x_{n+1}\right) \cdots \sum_{x_{N}} \psi_{N-1, N}\left(x_{N-1}, x_{N}\right)\right] \cdots\right]}_{\mu_{\beta}\left(x_{n}\right)}
\end{aligned}
$$

## Inference on a Chain

$$
\begin{aligned}
\mu_{\alpha}\left(x_{n}\right) & =\sum_{x_{n-1}} \psi_{n-1, n}\left(x_{n-1}, x_{n}\right)\left[\sum_{x_{n-2}} \cdots\right] \\
& =\sum_{x_{n-1}} \psi_{n-1, n}\left(x_{n-1}, x_{n}\right) \mu_{\alpha}\left(x_{n-1}\right) \\
\mu_{\beta}\left(x_{n}\right) & =\sum_{x_{n+1}} \psi_{n, n+1}\left(x_{n}, x_{n+1}\right)\left[\sum_{x_{n+1}} \cdots\right] \\
& =\sum_{x_{n+1}} \psi_{n, n+1}\left(x_{n}, x_{n+1}\right)
\end{aligned}
$$

## Inference on a Chain

$$
\begin{gathered}
\mu_{\alpha}\left(x_{2}\right)=\sum_{x_{1}} \psi_{1,2}\left(x_{1}, x_{2}\right) \quad \mu_{\beta}\left(x_{N-1}\right)=\sum_{x_{N}} \psi_{N-1, N}\left(x_{N-1}, x_{N}\right) \\
Z=\sum_{x_{n}} \mu_{\alpha}\left(x_{n}\right) \mu_{\beta}\left(x_{n}\right)
\end{gathered}
$$

## Inference on a Chain

To compute local marginals:

- Compute and store all forward messages, $\mu_{\alpha}\left(x_{n}\right)$.
- Compute and store all backward messages, $\mu_{\beta}\left(x_{n}\right)$.
- Compute $Z$ at any node $x_{m}$
- Compute

$$
p\left(x_{n}\right)=\frac{1}{Z} \mu_{\alpha}\left(x_{n}\right) \mu_{\beta}\left(x_{n}\right)
$$

for all variables required.

## Trees

Undirected Tree


Directed Tree


Polytree


## Factor graph

A graphical representation that lets us express a factorization of a function over a set of variables
A factor graph is bipartite graph where:

- One layer is formed by variables
- Another layer is formed by factors or functions on subsets of variables
Example: a function over variables $x_{1}, x_{2}, \ldots x_{5}$

$$
g\left(x_{1}, x_{2}, \ldots x_{5}\right)=f_{A}\left(x_{1}\right) f_{B}\left(x_{2}\right) f_{C}\left(x_{1}, x_{2}, x_{3}\right) f_{D}\left(x_{3}, x_{4}\right) f_{E}\left(x_{3}, x_{5}\right)
$$



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## Factor Graphs



$$
p(\mathbf{x})=f_{a}\left(x_{1}, x_{2}\right) f_{b}\left(x_{1}, x_{2}\right) f_{c}\left(x_{2}, x_{3}\right) f_{d}\left(x_{3}\right)
$$

$$
p(\mathbf{x})=\prod_{s} f_{s}\left(\mathbf{x}_{s}\right)
$$

## Inferences on factor graphs

- Efficient inference algorithms for factor graphs built for trees [Frey, 1998; Kschischnang et al., 2001] :
- Sum-product algorithm
- Max product algorithm


## The Sum-Product Algorithm (1)

Objective:
i. to obtain an efficient, exact inference algorithm for finding marginals;
ii. in situations where several marginals are required, to allow computations to be shared efficiently.

## Key idea: Distributive Law

$$
a b+a c=a(b+c)
$$

## The Sum-Product Algorithm (2)



## The Sum-Product Algorithm (4)



$$
F_{s}\left(x, X_{s}\right)=f_{s}\left(x, x_{1}, \ldots, x_{M}\right) G_{1}\left(x_{1}, X_{s 1}\right) \ldots G_{M}\left(x_{M}, X_{s M}\right)
$$

## The Sum-Product Algorithm (5)



$$
\begin{aligned}
\mu_{f_{s} \rightarrow x}(x) & =\sum_{x_{1}} \ldots \sum_{x_{M}} f_{s}\left(x, x_{1}, \ldots, x_{M}\right) \prod_{m \in \operatorname{ne}\left(f_{s}\right) \backslash x}\left[\sum_{X_{s m}} G_{m}\left(x_{m}, X_{s m}\right)\right] \\
& =\sum_{x_{1}} \cdots \sum_{x_{M}} f_{s}\left(x, x_{1}, \ldots, x_{M}\right) \prod_{m \in \operatorname{ne}\left(f_{s}\right) \backslash x} \mu_{x_{m} \rightarrow f_{s}}\left(x_{m}\right)
\end{aligned}
$$

## The Sum-Product Algorithm (6)

$$
\begin{array}{ll}
\mu_{x_{m} \rightarrow f_{s}}\left(x_{m}\right) \equiv \sum_{X_{s m}} G_{m}\left(x_{m}, X_{s m}\right) & =\sum_{X_{s m}} \prod_{l \in \operatorname{ne}\left(x_{m}\right) \backslash f_{s}} F_{l}\left(x_{m}, X_{m l}\right) \\
& \prod_{f_{l} \rightarrow x_{m}}\left(x_{m}\right)
\end{array}
$$

## The Sum-Product Algorithm (7)

Initialization


## The Sum-Product Algorithm (8)

To compute local marginals:

- Pick an arbitrary node as root
- Compute and propagate messages from the leaf nodes to the root, storing received messages at every node.
- Compute and propagate messages from the root to the leaf nodes, storing received messages at every node.
- Compute the product of received messages at each node for which the marginal is required, and normalize if necessary.

