

Advanced Machine Learning Summer 2019

Part 8 – Graphical Models II 02.05.2019

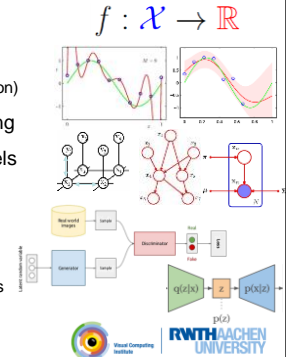
Prof. Dr. Bastian Leibe

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<http://www.vision.rwth-aachen.de>



Course Outline

- Regression Techniques
 - Linear Regression
 - Regularization (Ridge, Lasso)
 - Kernels (Kernel Ridge Regression)
- Deep Reinforcement Learning
- Probabilistic Graphical Models
 - Bayesian Networks
 - Markov Random Fields
 - Inference (exact & approximate)
- Deep Generative Models
 - Generative Adversarial Networks
 - Variational Autoencoders



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Topics of This Lecture

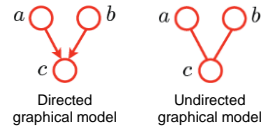
- Recap: Directed Graphical Models
 - Factorization properties
 - Conditional independence
 - Bayes Ball algorithm
- Undirected Graphical Models (Markov Random Fields)
 - Conditional Independence
 - Factorization
 - Converting directed into undirected graphs
- Exact Inference in Graphical Models
 - Marginalization for undirected graphs
 - Inference on a chain
 - Inference on a tree
 - Message passing formalism

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Recap: Graphical Models

- Two basic kinds of graphical models
 - Directed graphical models or Bayesian Networks
 - Undirected graphical models or Markov Random Fields
- Key components
 - Nodes
 - Random variables
 - Edges
 - Directed or undirected



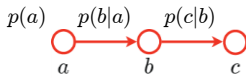
– The value of a random variable may be **known** or **unknown**.

○ unknown ● known

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Recap: Directed Graphical Models

- Chains of nodes:
 
 - Knowledge about a is expressed by the **prior probability**: $p(a)$
 - Dependencies are expressed through **conditional probabilities**: $p(b|a)$, $p(c|b)$
 - **Joint distribution** of all three variables:

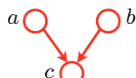
$$p(a, b, c) = p(c|b)p(b|a)p(a)$$

$$= p(c|b)p(b|a)p(a)$$

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Recap: Directed Graphical Models

- Convergent connections:
 
 - Here the value of c depends on both variables a and b.
 - This is modeled with the conditional probability: $p(c|a, b)$
 - Therefore, the joint probability of all three variables is given as:

$$p(a, b, c) = p(c|a, b)p(a, b)$$

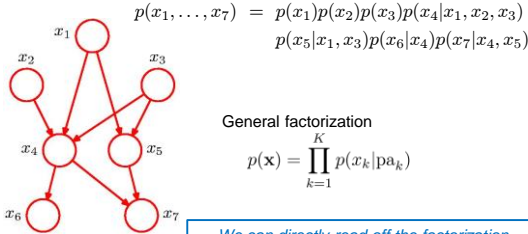
$$= p(c|a, b)p(a)p(b)$$

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Recap: Factorization of the Joint Probability

- Exercise: Computing the joint probability



General factorization

$$p(\mathbf{x}) = \prod_{k=1}^K p(x_k | \text{pa}_k)$$

We can directly read off the factorization of the joint from the network structure!

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Image source: C. Bishop, 2006

Recap: Factorized Representation

- Reduction of complexity

– Joint probability of n binary variables requires us to represent values by brute force

$$\mathcal{O}(2^n) \text{ terms}$$

– The factorized form obtained from the graphical model only requires

$$\mathcal{O}(n \cdot 2^k) \text{ terms}$$

- k : maximum number of parents of a node.

→ It's the edges that are missing in the graph that are important! They encode the simplifying assumptions we make.

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Slide credit: Bernt Schiele, Stefan Roth

Recap: Conditional Independence

- X is **conditionally independent** of Y given V

– Definition: $X \perp\!\!\!\perp Y | V \Leftrightarrow p(X|Y, V) = p(X|V)$

– Also: $X \perp\!\!\!\perp Y | V \Leftrightarrow p(X, Y|V) = p(X|V)p(Y|V)$

– Special case: **Marginal Independence**

$$X \perp\!\!\!\perp Y \Leftrightarrow X \perp\!\!\!\perp Y | \emptyset \Leftrightarrow p(X, Y) = p(X)p(Y)$$

– Often, we are interested in conditional independence between **sets of variables**:

$$\mathcal{X} \perp\!\!\!\perp \mathcal{Y} | \mathcal{V} \Leftrightarrow \{X \perp\!\!\!\perp Y | \mathcal{V}, \forall X \in \mathcal{X} \text{ and } \forall Y \in \mathcal{Y}\}$$

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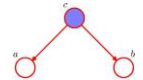


Recap: Conditional Independence

- Three cases

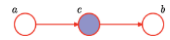
– **Divergent** ("Tail-to-Tail")

- Conditional independence when c is observed.



– **Chain** ("Head-to-Tail")

- Conditional independence when c is observed.



– **Convergent** ("Head-to-Head")

- Conditional independence when **neither c , nor any of its descendants** are observed.



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Image source: C. Bishop, 2006

Recap: D-Separation

- Definition

– Let A , B , and C be non-intersecting subsets of nodes in a directed graph.

– A path from A to B is **blocked** if it contains a node such that either

- The arrows on the path meet either **head-to-tail** or **tail-to-tail** at the node, and the **node is in the set C** , or
- The arrows meet **head-to-head** at the node, and **neither the node, nor any of its descendants, are in the set C** .



– If all paths from A to B are blocked, A is said to be **d-separated** from B by C .

- If A is d-separated from B by C , the joint distribution over all variables in the graph satisfies $A \perp\!\!\!\perp B | C$.

– Read: " A is conditionally independent of B given C ."

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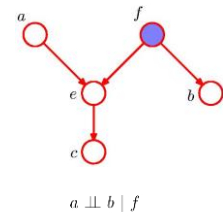
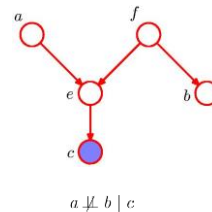
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Slide adapted from Chris Bishop.

D-Separation: Example

- Exercise: What is the relationship between a and b ?



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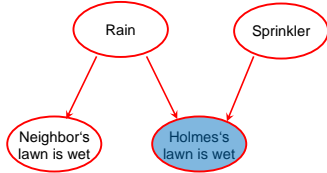
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Image source: C. Bishop, 2006

Explaining Away

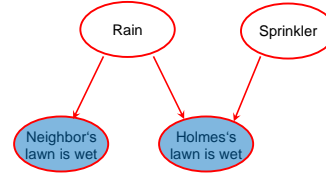
- Let's look at Holmes' example again:



- Observation "Holmes' lawn is wet" increases the probability of both "Rain" and "Sprinkler".

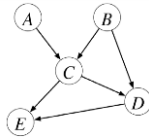
Explaining Away

- Let's look at Holmes' example again:



- Observation "Holmes' lawn is wet" increases the probability of both "Rain" and "Sprinkler".
 - Also observing "Neighbor's lawn is wet" decreases the probability for "Sprinkler". (They're conditionally dependent!)
- ⇒ The "Sprinkler" is **explained away**.

Intuitive View: The "Bayes Ball" Algorithm



- Game
 - Can you get a ball from X to Y without being blocked by V ?
 - Depending on its direction and the previous node, the ball can
 - Pass through (from parent to all children, from child to all parents)
 - Bounce back (from any parent/child to all parents/children)
 - Be blocked

R.D. Shachter, *Bayes-Ball: The Rational Pastime (for Determining Irrelevance and Requisite Information in Belief Networks and Influence Diagrams)*, UAI'98, 1998

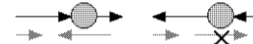
The "Bayes Ball" Algorithm

- Game rules

- An **unobserved** node ($W \notin \mathcal{V}$) passes through balls from parents, but also **bounces back** balls from children.

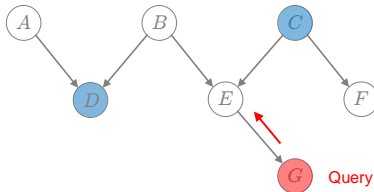


- An **observed** node ($W \in \mathcal{V}$) **bounces back** balls from parents, but **blocks** balls from children.



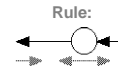
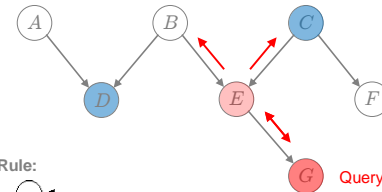
- ⇒ The Bayes Ball algorithm determines those nodes that are **d-separated** from the query node.

Example: Bayes Ball



- Which nodes are d-separated from G given C and D ?

Example: Bayes Ball



- Which nodes are d-separated from G given C and D ?

Example: Bayes Ball

• Which nodes are d-separated from G given C and D ?

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Example: Bayes Ball

• Which nodes are d-separated from G given C and D ?

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Example: Bayes Ball

• Which nodes are d-separated from G given C and D ?

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Example: Bayes Ball

• Which nodes are d-separated from G given C and D ?

$\Rightarrow F$ is d-separated from G given C and D .

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The Markov Blanket

• Markov blanket of a node x_i

- Minimal set of nodes that isolates x_i from the rest of the graph.
- This comprises the set of
 - Parents,
 - Children, and
 - Co-parents of x_i .

← This is what we have to watch out for!

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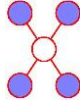
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Undirected Graphical Models

- Undirected graphical models ("Markov Random Fields")
 - Given by undirected graph



- Conditional independence is easier to read off for MRFs.
 - Without arrows, there is only one type of neighbors.
 - Simpler Markov blanket:



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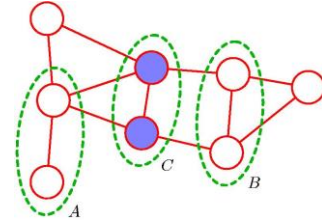
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Undirected Graphical Models



- Conditional independence for undirected graphs
 - If every path from any node in set A to set B passes through at least one node in set C , then $A \perp\!\!\!\perp B \mid C$.

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Factorization in MRFs

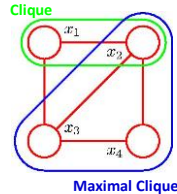
- Factorization
 - Factorization is more complicated in MRFs than in BNs.
 - Important concept: **maximal cliques**

Clique

- Subset of the nodes such that there exists a link between all pairs of nodes in the subset.

Maximal clique

- The biggest possible such clique in a given graph.



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Factorization in MRFs

- Joint distribution
 - Written as product of **potential functions** over **maximal cliques** in the graph:

$$p(\mathbf{x}) = \frac{1}{Z} \prod_C \psi_C(\mathbf{x}_C)$$

- The normalization constant Z is called the **partition function**.

$$Z = \sum_{\mathbf{x}} \prod_C \psi_C(\mathbf{x}_C)$$

Remarks

- BNs are automatically normalized. But for MRFs, we have to explicitly perform the normalization.
- Presence of normalization constant is major limitation!
 - Evaluation of Z involves summing over $\mathcal{O}(K^M)$ terms for M nodes.

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Factorization in MRFs

- Role of the potential functions
 - General interpretation
 - No restriction to potential functions that have a specific probabilistic interpretation as marginals or conditional distributions.

- Convenient to express them as exponential functions ("Boltzmann distribution")

$$\psi_C(\mathbf{x}_C) = \exp\{-E(\mathbf{x}_C)\}$$

with an **energy function** E .

- Why is this convenient?

- Joint distribution is the product of potentials \Rightarrow sum of energies.
- We can take the log and simply work with the sums...

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Comparison: Directed vs. Undirected Graphs

Directed graphs (Bayesian networks)

- Better at expressing causal relationships.
- Interpretation of a link:
 - Conditional probability $p(b|a)$.
- Factorization is simple (and result is automatically normalized).
- Conditional independence is more complicated.



Undirected graphs (Markov Random Fields)

- Better at representing soft constraints between variables.
- Interpretation of a link:
 - "There is *some* relationship between a and b ".
- Factorization is complicated (and result needs normalization).
- Conditional independence is simple.



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Converting Directed to Undirected Graphs

- Simple case: chain

$$p(\mathbf{x}) = p(x_1)p(x_2|x_1)p(x_3|x_2)\cdots p(x_N|x_{N-1})$$

$$p(\mathbf{x}) = \frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \cdots \psi_{N-1,N}(x_{N-1}, x_N)$$

⇒ We can directly replace the directed links by undirected ones.

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Converting Directed to Undirected Graphs

- More difficult case: multiple parents

fully connected, no cond. indep.!

$$p(\mathbf{x}) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$$

Need a clique of x_1, \dots, x_4 to represent this factor!

- Need to introduce additional links (“marry the parents”).
- ⇒ This process is called **moralization**. It results in the **moral graph**.

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Converting Directed to Undirected Graphs

- General procedure to convert directed → undirected
 - Add undirected links to **marry the parents** of each node.
 - Drop the arrows on the original links ⇒ **moral graph**.
 - Find maximal cliques for each node and initialize all clique potentials to 1.
 - Take each conditional distribution factor of the original directed graph and multiply it into one clique potential.
- Restriction
 - Conditional independence properties are often lost!
 - Moralization results in additional connections and larger cliques.

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Example: Graph Conversion

- Step 1) **Marrying the parents.**

$$p(x_1, \dots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

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Example: Graph Conversion

- Step 2) **Dropping the arrows.**

$$p(x_1, \dots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

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Example: Graph Conversion

- Step 3) **Finding maximal cliques for each node.**

$$p(x_1, \dots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

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Example: Graph Conversion

- Step 4) Assigning the probabilities to clique potentials.

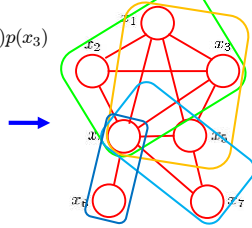
$$\psi_1(x_1, x_2, x_3, x_4) = 1 p(x_4|x_1, x_2, x_3) p(x_2) p(x_3)$$

$$\psi_2(x_1, x_3, x_4, x_5) = 1 p(x_5|x_1, x_3) p(x_1)$$

$$\psi_3(x_4, x_5, x_7) = 1 p(x_7|x_4, x_5)$$

$$\psi_4(x_4, x_6) = 1 p(x_6|x_4)$$

$$p(x_1, \dots, x_7) = p(x_1) p(x_2) p(x_3) p(x_4|x_1, x_2, x_3) p(x_5|x_1, x_3) p(x_6|x_4) p(x_7|x_4, x_5)$$



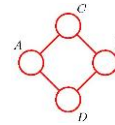
Comparison of Expressive Power

- Both types of graphs have unique configurations.

$$A \not\perp B \mid \emptyset$$

$$A \perp B \mid C \cup D$$

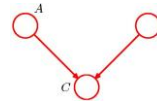
$$C \perp D \mid A \cup B$$



No directed graph can represent these and only these independencies.

$$A \perp B \mid \emptyset$$

$$A \not\perp B \mid C$$



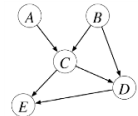
No undirected graph can represent these and only these independencies.

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Inference in Graphical Models

- Inference – General definition
 - Evaluate the probability distribution over some set of variables, given the values of another set of variables (=observations).



- Example:

$$p(A, B, C, D, E) = p(A)p(B)p(C|A, B)p(D|B, C)p(E|C, D)$$

- How can we compute $p(A|C=c)$?

- Idea:

$$p(A|C=c) = \frac{p(A, C=c)}{p(C=c)}$$

Inference in Graphical Models

- Computing $p(A|C=c)$...

- We know

$$p(A, B, C, D, E) = p(A)p(B)p(C|A, B)p(D|B, C)p(E|C, D)$$

- Assume each variable is binary.

- Naïve approach: Two possible values for each $\Rightarrow 2^4$ terms

$$p(A|C=c) = \sum_{B, D, E} p(A, B, C=c, D, E) \quad 16 \text{ operations}$$

$$p(C=c) = \sum_A p(A, C=c) \quad 2 \text{ operations}$$

$$p(A|C=c) = \frac{p(A, C=c)}{p(C=c)} \quad 2 \text{ operations}$$

Total: 16+2+2 = 20 operations

Inference in Graphical Models

- We know

$$p(A, B, C, D, E) = p(A)p(B)p(C|A, B)p(D|B, C)p(E|C, D)$$

- More efficient method for $p(A|C=c)$:

$$p(A, C=c) = \sum_{B, D, E} p(A)p(B)p(C=c|A, B)p(D|B, C=c)p(E|C=c, D)$$

$$= \sum_B p(A)p(B)p(C=c|A, B) \sum_D p(D|B, C=c) \sum_E p(E|C=c, D) = 1$$

$$= \sum_B p(A)p(B)p(C=c|A, B) \quad 4 \text{ operations}$$

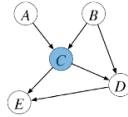
- Rest stays the same:

Total: 4+2+2 = 8 operations

Couldn't we have got this result easier?

Inference in Graphical Models

- Consider the network structure
 - Using what we know about **factorization** and **conditional independence**...



- Factorization properties:**
 - There is no directed path from D or E to either A or C .
 - ⇒ We do not need to consider D and E .
 - Conditional independence properties:**
 - C opens the path from A to B ("head-to-head").
 - ⇒ A is **conditionally dependent** on B given C .
- ⇒ When querying for $p(A, C = c)$, we only need to take into account A , B , and $C = c$.

$$p(A, C = c) = \sum_B p(A)p(B)p(C = c|A, B)$$

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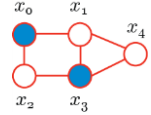


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Computing Marginals

- How do we apply graphical models?

- Given some observed variables, we want to **compute distributions of the unobserved variables**.
- In particular, we want to **compute marginal distributions**, for example $p(x_i)$.



- How can we compute marginals?

- Classical technique: **sum-product algorithm** by Judea Pearl.
- In the context of (loopy) undirected models, this is also called (loopy) **belief propagation** [Weiss, 1997].
- Basic idea: **message-passing**.

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Inference on a Chain

- Chain graph



- Joint probability

$$p(\mathbf{x}) = \frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \cdots \psi_{N-1,N}(x_{N-1}, x_N)$$

- Marginalization

$$p(x_n) = \sum_{x_1} \cdots \sum_{x_{n-1}} \sum_{x_{n+1}} \cdots \sum_{x_N} p(\mathbf{x})$$

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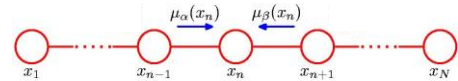


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Slide adapted from Chris Bishop

Image source: C. Bishop, 2006

Inference on a Chain



- Idea: Split the computation into two parts ("messages").

$$p(x_n) = \frac{1}{Z} \underbrace{\left[\sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \cdots \left[\sum_{x_1} \psi_{1,2}(x_1, x_2) \cdots \right] \right]}_{\mu_\alpha(x_n)} \underbrace{\left[\sum_{x_{n+1}} \psi_{n,n+1}(x_n, x_{n+1}) \cdots \left[\sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N) \cdots \right] \right]}_{\mu_\beta(x_n)}$$

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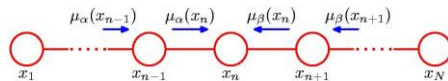


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Inference on a Chain



- We can define the messages recursively...

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

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

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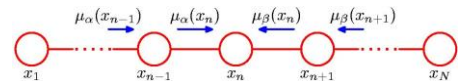


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Inference on a Chain



- Until we reach the leaf nodes...

$$\mu_\alpha(x_2) = \sum_{x_1} \psi_{1,2}(x_1, x_2) \quad \mu_\beta(x_{N-1}) = \sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N)$$

- Interpretation

- We **pass messages** from the two ends towards the query node x_n .

- We still need the normalization constant Z .

- This can be easily obtained from the marginals:

$$Z = \sum_{x_n} \mu_\alpha(x_n) \mu_\beta(x_n)$$

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Summary: Inference on a Chain

- To compute local marginals:
 - Compute and store all forward messages $\mu_\alpha(x_n)$.
 - Compute and store all backward messages $\mu_\beta(x_n)$.
 - Compute Z at any node x_m .
 - Compute

$$p(x_n) = \frac{1}{Z} \mu_\alpha(x_n) \mu_\beta(x_n)$$

for all variables required.

- Inference through message passing
 - We have thus seen a first **message passing** algorithm.
 - How can we generalize this?

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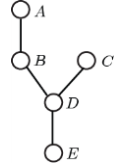
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Inference on Trees

- Let's next assume a **tree graph**.

– Example:



– We are given the following joint distribution:

$$p(A, B, C, D, E) = \frac{1}{Z} f_1(A, B) \cdot f_2(B, D) \cdot f_3(C, D) \cdot f_4(D, E)$$

– Assume we want to know the **marginal** $p(E)$...

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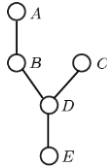
Inference on Trees

- Strategy

– Marginalize out all other variables by summing over them.

– Then rearrange terms:

$$\begin{aligned} p(E) &= \sum_A \sum_B \sum_C \sum_D p(A, B, C, D, E) \\ &= \sum_A \sum_B \sum_C \sum_D \frac{1}{Z} f_1(A, B) \cdot f_2(B, D) \cdot f_3(C, D) \cdot f_4(D, E) \\ &= \frac{1}{Z} \left(\sum_D f_4(D, E) \cdot \left(\sum_C f_3(C, D) \right) \cdot \left(\sum_B f_2(B, D) \cdot \left(\sum_A f_1(A, B) \right) \right) \right) \end{aligned}$$



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Marginalization with Messages

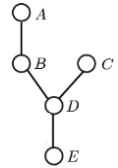
- Use **messages** to express the marginalization:

$$m_{A \rightarrow B} = \sum_A f_1(A, B) \quad m_{C \rightarrow D} = \sum_C f_3(C, D)$$

$$m_{B \rightarrow D} = \sum_B f_2(B, D) m_{A \rightarrow B}(B)$$

$$m_{D \rightarrow E} = \sum_D f_4(D, E) m_{B \rightarrow D}(D) m_{C \rightarrow D}(D)$$

$$\begin{aligned} p(E) &= \frac{1}{Z} \left(\sum_D f_4(D, E) \cdot \left(\sum_C f_3(C, D) \right) \cdot \left(\sum_B f_2(B, D) \cdot \left(\sum_A f_1(A, B) \right) \right) \right) \\ &= \frac{1}{Z} \left(\sum_D f_4(D, E) \cdot \left(\sum_C f_3(C, D) \right) \cdot \left(\sum_B f_2(B, D) \cdot m_{A \rightarrow B}(B) \right) \right) \end{aligned}$$



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Marginalization with Messages

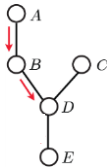
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Marginalization with Messages

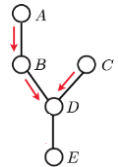
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Marginalization with Messages

- Use **messages** to express the marginalization:

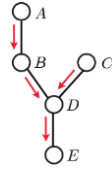
$$m_{A \rightarrow B} = \sum_A f_1(A, B) \quad m_{C \rightarrow D} = \sum_C f_3(C, D)$$

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$$p(E) = \frac{1}{Z} \left(\sum_D f_4(D, E) \cdot \left(\sum_C f_3(C, D) \right) \cdot \left(\sum_B f_2(B, D) \cdot \left(\sum_A f_1(A, B) \right) \right) \right)$$

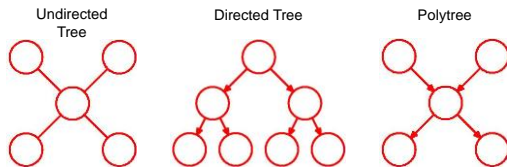
$$= \frac{1}{Z} m_{D \rightarrow E}(E)$$



Inference on Trees

- We can **generalize** this for all tree graphs.
 - Root the tree at the variable that we want to compute the marginal of.
 - Start computing messages at the leaves.
 - Compute the messages for all nodes for which all incoming messages have already been computed.
 - Repeat until we reach the root.
- If we want to compute the marginals for all possible nodes (roots), we can reuse some of the messages.
 - Computational expense linear in the number of nodes.

Trees – How Can We Generalize?



- Next lecture
 - Formalize the message-passing idea \Rightarrow Sum-product algorithm
 - Common representation of the above \Rightarrow Factor graphs
 - Deal with loopy graphs structures \Rightarrow Junction tree algorithm

References and Further Reading

- A thorough introduction to Graphical Models in general and Bayesian Networks in particular can be found in Chapter 8 of Bishop's book.

Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006

