Advanced Machine Learning
Summer 2019

Part 7 – Graphical Models I
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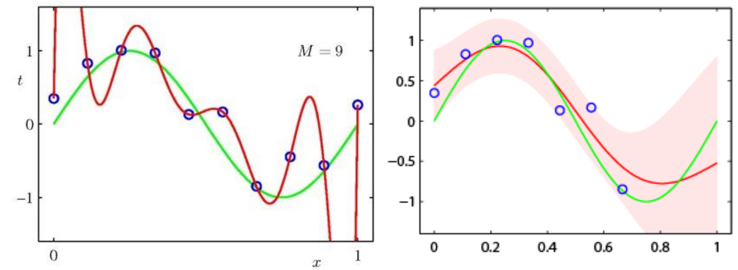
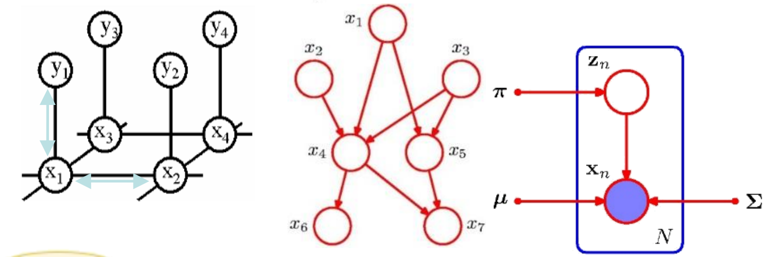
Many slides adapted from B. Schiele, S. Roth

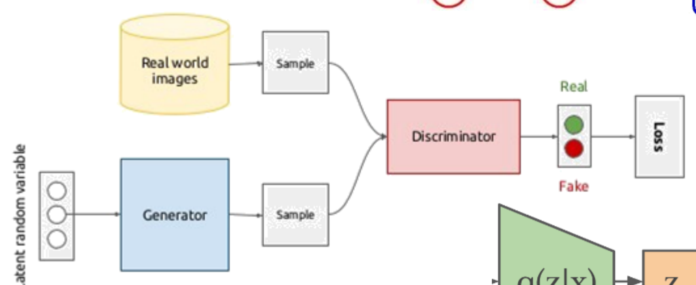
Course Outline

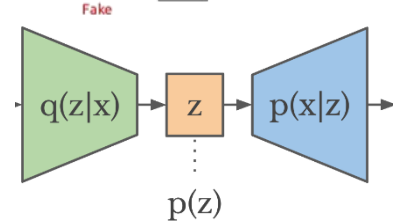
- Regression Techniques
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
- Deep Reinforcement Learning
- Probabilistic Graphical Models
  - Bayesian Networks
  - Markov Random Fields
  - Inference (exact & approximate)
- Deep Generative Models
  - Generative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

$$f : \mathcal{X} \rightarrow \mathbb{R}$$









Topics of This Lecture

- Probabilistic Graphical Models
  - Introduction
- Directed Graphical Models (Bayesian Networks)
  - Notation
  - Conditional probabilities
  - Computing the joint probability
  - Factorization
  - Conditional Independence
  - D-Separation
  - Explaining away

Graphical Models – What and Why?

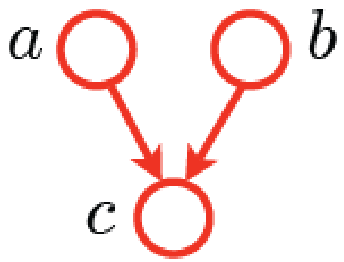
- *It's got nothing to do with graphics!*
- Probabilistic graphical models
  - Marriage between probability theory and graph theory.
    - Formalize and visualize the structure of a probabilistic model through a graph.
    - Give insights into the structure of a probabilistic model.
    - Find efficient solutions using methods from graph theory.
  - Natural tool for dealing with uncertainty and complexity.
  - Has become an important way of designing and analyzing machine learning algorithms.

Slide credit: Bernt Schiele

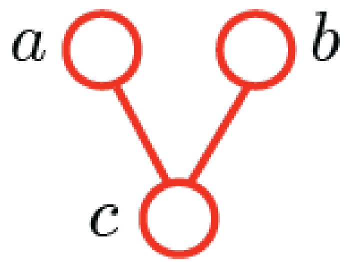
Graphical Models

- There are two basic kinds of graphical models
  - Directed graphical models or Bayesian Networks
  - Undirected graphical models or Markov Random Fields

- Key components
  - Nodes
  - Edges
    - Directed or undirected



Directed graphical model



Undirected graphical model

Slide credit: Bernt Schiele

Topics of This Lecture

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  - Introduction
- Directed Graphical Models (Bayesian Networks)
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Example: Wet Lawn

- Mr. Holmes leaves his house.
  - He sees that the lawn in front of his house is wet.
  - This can have several reasons: Either it rained, or Holmes forgot to shut the sprinkler off.
  - Without any further information, the probability of both events (rain, sprinkler) increases (knowing that the lawn is wet).

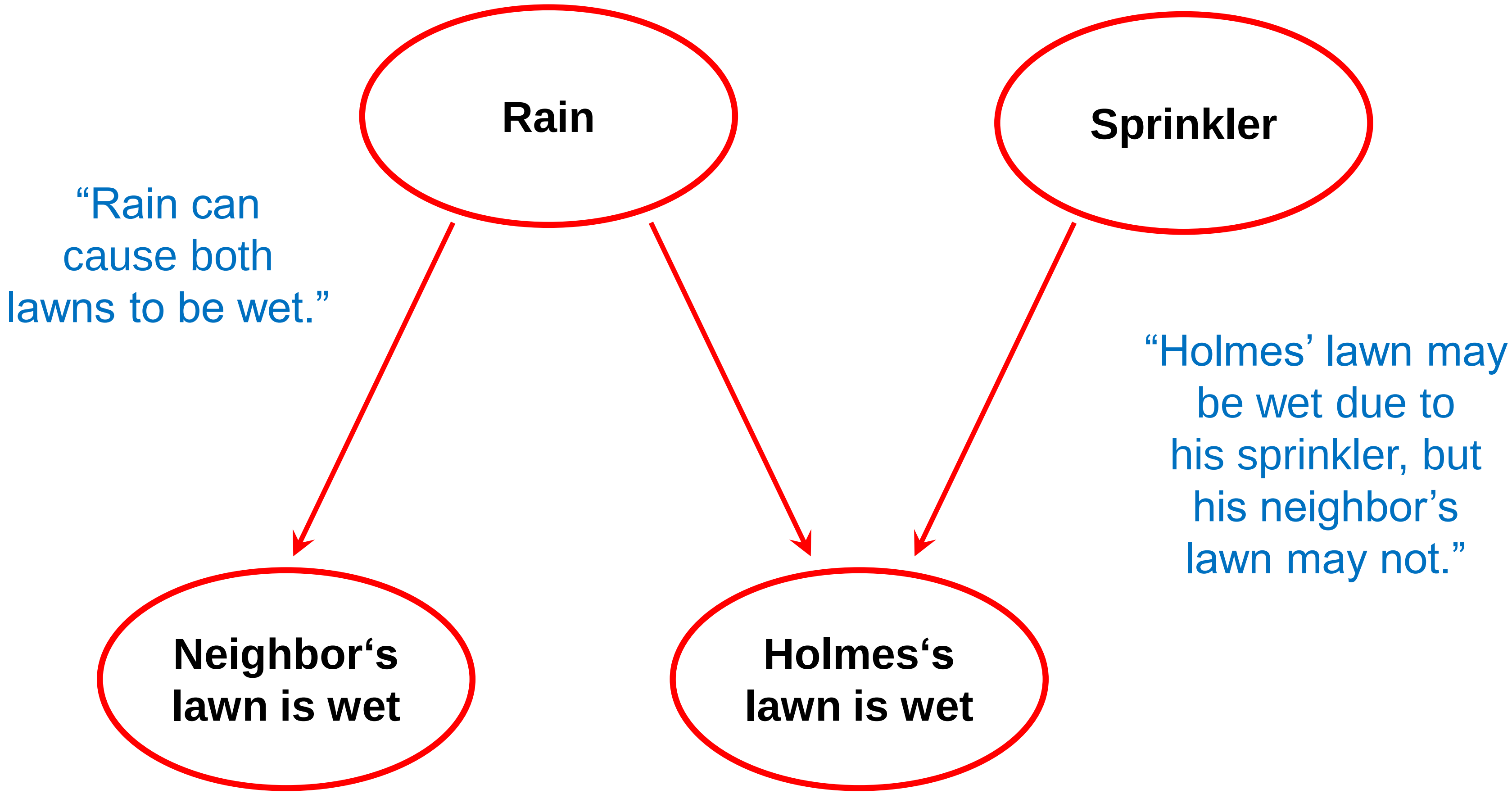
- Now Holmes looks at his neighbor’s lawn
  - The neighbor’s lawn is also wet.
  - This information increases the probability that it rained. And it lowers the probability for the sprinkler.

$\Rightarrow$ How can we encode such probabilistic relationships?

Slide credit: Bernt Schiele, Stefan Roth

Example: Wet Lawn

- Directed graphical model / Bayesian network:



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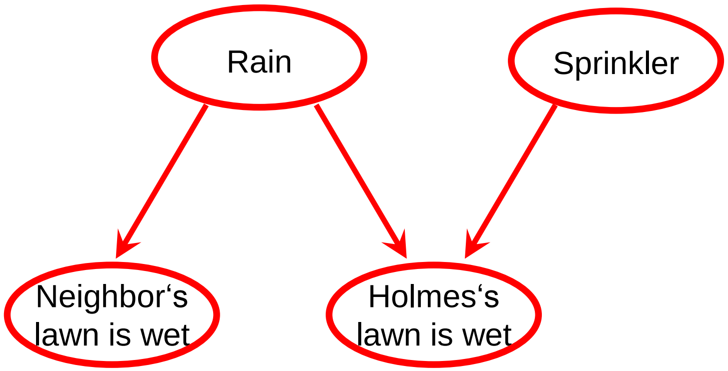
Directed Graphical Models



- or Bayesian networks
  - Are based on a directed graph.
  - The nodes correspond to the random variables.
  - The directed edges correspond to the (causal) dependencies among the variables.
    - The notion of a causal nature of the dependencies is somewhat hard to grasp.
    - We will typically ignore the notion of causality here…
  - The structure of the network qualitatively describes the dependencies of the random variables.

Slide credit: Bernt Schiele, Stefan Roth

Directed Graphical Models

- Nodes or random variables
  - We usually know the range of the random variables.
  - The value of a variable may be known or unknown.
  - If they are known (observed), we usually shade the node:

- Examples of variable nodes
  - Binary events: Rain (yes / no), sprinkler (yes / no)
  - Discrete variables: Ball is red, green, blue, …
  - Continuous variables: Age of a person, …

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Directed Graphical Models

- Most often, we are interested in quantitative statements
  - i.e. the probabilities (or densities) of the variables.
    - Example: What is the probability that it rained? …
  - These probabilities change if we have
    - more knowledge,
    - less knowledge, or
    - different knowledge

    about the other variables in the network.

Slide credit: Bernt Schiele, Stefan Roth

Directed Graphical Models

- Simplest case:

- This model encodes
  - The value of b depends on the value of a.
  - This dependency is expressed through the conditional probability:
  $$p(b|a)$$
  - Knowledge about a is expressed through the prior probability:
  $$p(a)$$
  - The whole graphical model describes the joint probability of a and b:
  $$p(a, b) = p(b|a)p(a)$$

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Directed Graphical Models

- If we have such a representation, we can derive all other interesting probabilities from the joint.
  - E.g., marginalization

$$p(a) = \sum_b p(a,b) = \sum_b p(b|a)p(a)$$

$$p(b) = \sum_a p(a,b) = \sum_a p(b|a)p(a)$$

  - With the marginals, we can also compute other conditional probabilities:

$$p(a|b) = \frac{p(a,b)}{p(b)}$$

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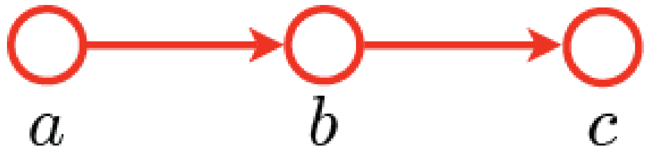
Directed Graphical Models

- Chains of nodes:



  – As before, we can compute

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

  – But we can also compute the joint distribution of all three variables:

$$\begin{aligned} p(a,b,c) &= p(c|\cancel{a},b)p(a,b) \\ &= p(c|b)p(b|a)p(a) \end{aligned}$$

  – We can read off from the graphical representation that variable c does not depend on a, if b is known.
    - How? What does this mean?

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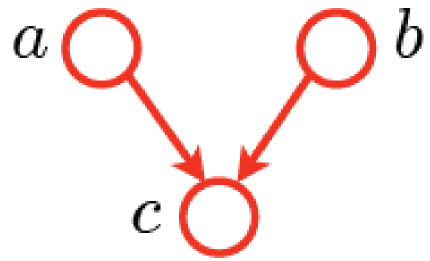
Directed Graphical Models

- 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:

$$\begin{aligned} p(a,b,c) &= p(c|a,b)p(a,b) \\ &= p(c|a,b)p(a)p(b) \end{aligned}$$

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Example

$$p(C)$$

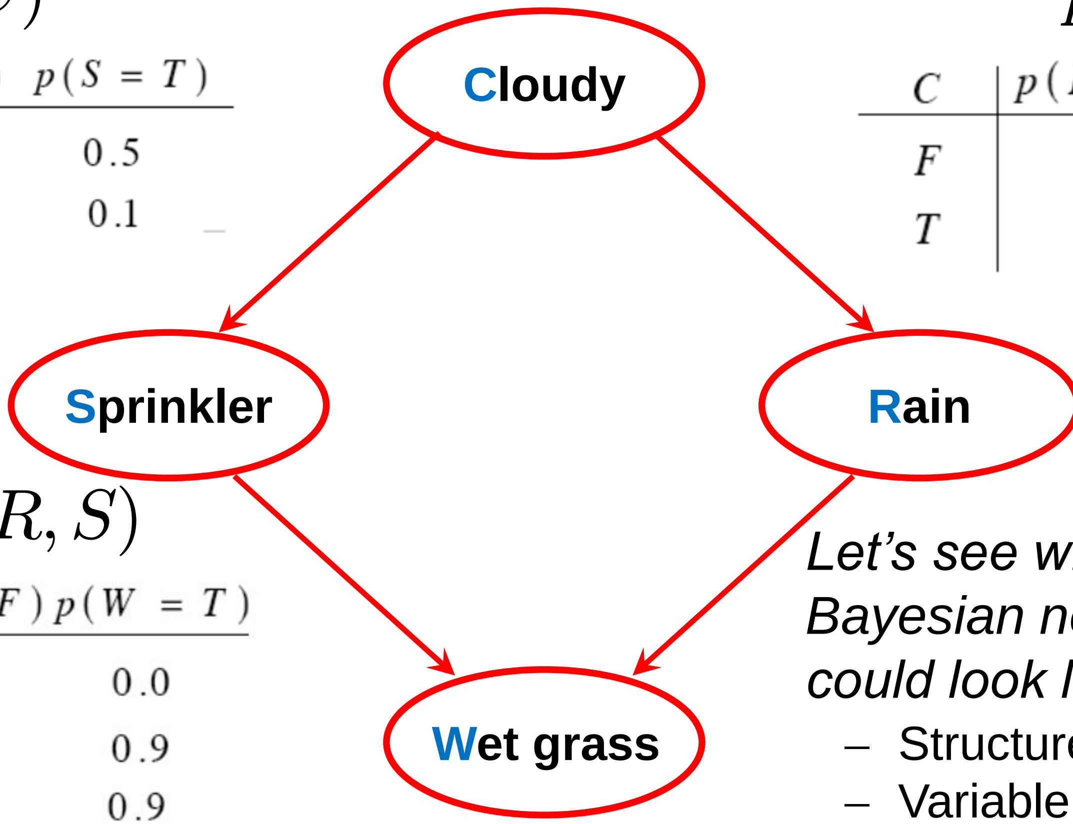
$p(C=F)$	$p(C=T)$
0.5	0.5

$$p(S|C)$$

C	$p(S=F)$	$p(S=T)$
F	0.5	0.5
T	0.9	0.1

$$p(R|C)$$

C	$p(R=F)$	$p(R=T)$
F	0.8	0.2
T	0.2	0.8



$$p(W|R,S)$$

SR	$p(W=F)$	$p(W=T)$
FF	1.0	0.0
TF	0.1	0.9
FT	0.1	0.9
TT	0.01	0.99

Let's see what such a Bayesian network could look like…

- Structure?
- Variable types? Binary.
- Conditional probabilities?

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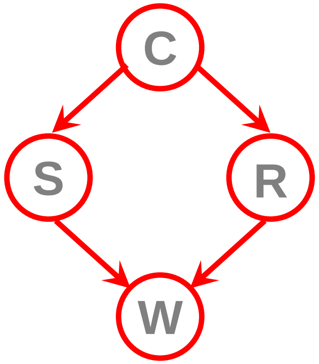
Example

- Evaluating the Bayesian network…
  - We start with the simple product rule:

$$\begin{aligned} p(a,b,c) &= p(a|b,c)p(b,c) \\ &= p(a|b,c)p(b|c)p(c) \end{aligned}$$



  - This means that we can rewrite the joint probability of the variables as

$$p(C,S,R,W) = p(C)p(S|C)p(R|C,\cancel{S})p(W|\cancel{C},S,R)$$

  - But the Bayesian network tells us that

$$p(C,S,R,W) = p(C)p(S|C)p(R|C)p(W|S,R)$$

    - I.e. rain is independent of sprinkler (given the cloudyness).
    - Wet grass is independent of the cloudiness (given the state of the sprinkler and the rain).

  $\Rightarrow$ This is a factorized representation of the joint probability.

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Directed Graphical Models

- A general directed graphical model (Bayesian network) consists of
  - A set of variables: $U = \{x_1, \ldots, x_n\}$
  - A set of directed edges between the variable nodes.
  - The variables and the directed edges define an acyclic graph.
    - Acyclic means that there is no directed cycle in the graph.
  - For each variable x_i with parent nodes pa_i in the graph, we require knowledge of a conditional probability:

$$p(x_i | \{x_j | j \in \mathrm{pa}_i\})$$

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Directed Graphical Models

- Given
  - Variables: $U = \{x_1, \ldots, x_n\}$
  - Directed acyclic graph: $G = (V, E)$
    - V: nodes = variables, E: directed edges
  - We can express / compute the joint probability as

$$p(x_1, \ldots, x_n) = \prod_{i=1}^{n} p\left(x_i | \{x_j | j \in \mathrm{pa}_i\}\right)$$

    where pa_i denotes the parent nodes of x_i.
  - We can express the joint as a product of all the conditional distributions from the parent-child relations in the graph.
  - We obtain a factorized representation of the joint.

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Directed Graphical Models

- Exercise: Computing the joint probability

$$p(x_1, \ldots, x_7) \;=\; ?$$

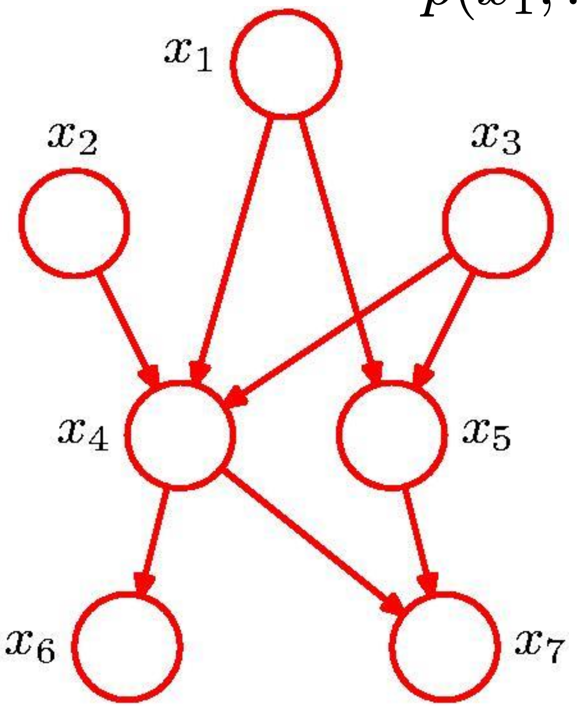
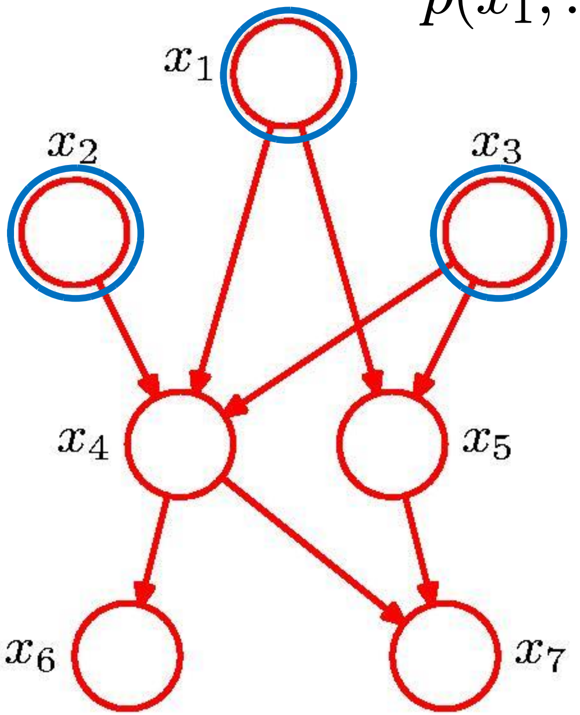


Image source: C. Bishop, 2006

Directed Graphical Models

- Exercise: Computing the joint probability

$$p(x_1, \ldots, x_7) = p(x_1)p(x_2)p(x_3)\ldots$$



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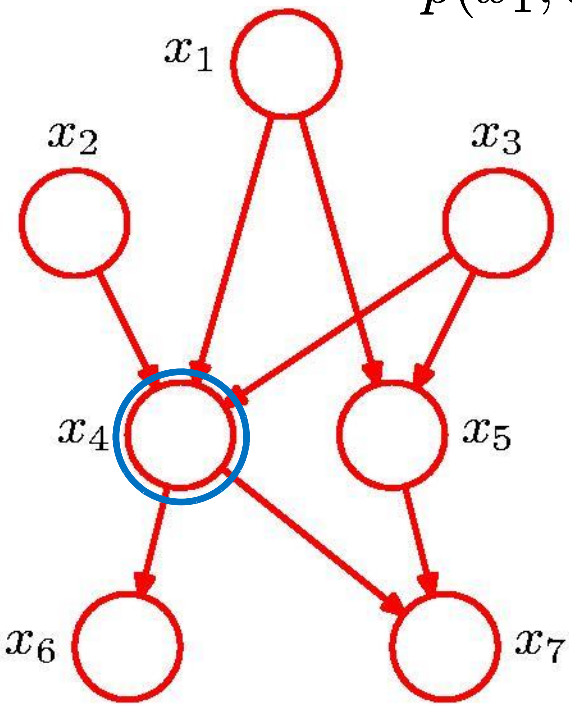
Directed Graphical Models

- Exercise: Computing the joint probability

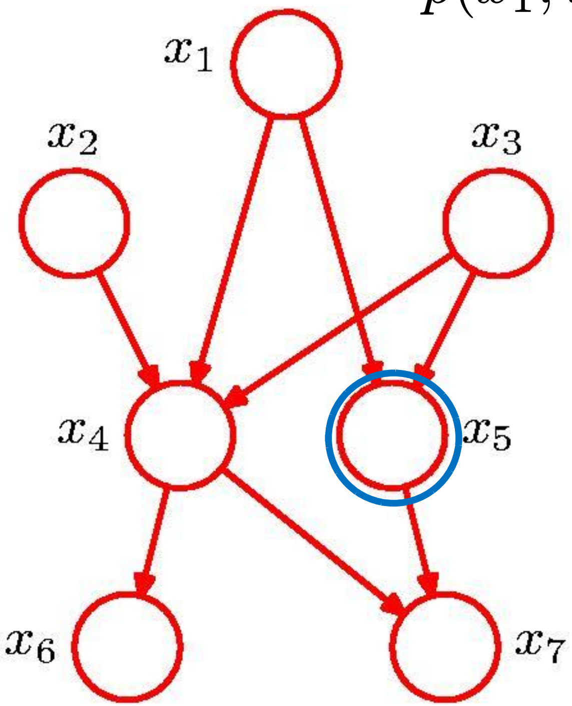


$$p(x_1,\ldots,x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1,x_2,x_3)$$
$$\ldots$$

Image source: C. Bishop, 2006

Directed Graphical Models

- Exercise: Computing the joint probability

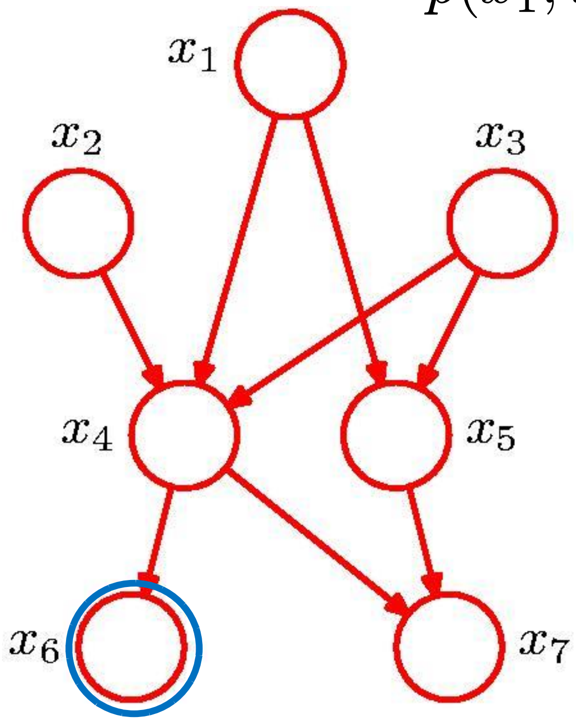


$$
\begin{aligned}
p(x_1, \ldots, x_7) \; &= \; p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) \\
&\quad\; p(x_5|x_1, x_3) \ldots
\end{aligned}
$$

Image source: C. Bishop, 2006

Directed Graphical Models

- Exercise: Computing the joint probability

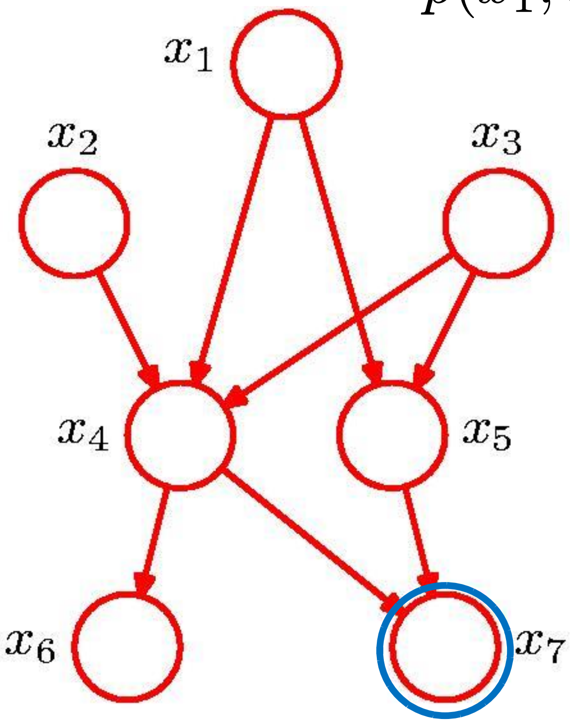


$$
\begin{aligned}
p(x_1, \ldots, x_7) \; &= \; p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) \\
&\quad\; p(x_5|x_1, x_3)p(x_6|x_4) \ldots
\end{aligned}
$$

Image source: C. Bishop, 2006

Directed Graphical Models

- Exercise: Computing the joint probability



$$\begin{aligned} p(x_1, \ldots, x_7) &= p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) \\ &\quad p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5) \end{aligned}$$

General factorization

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

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

Image source: C. Bishop, 2006

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.

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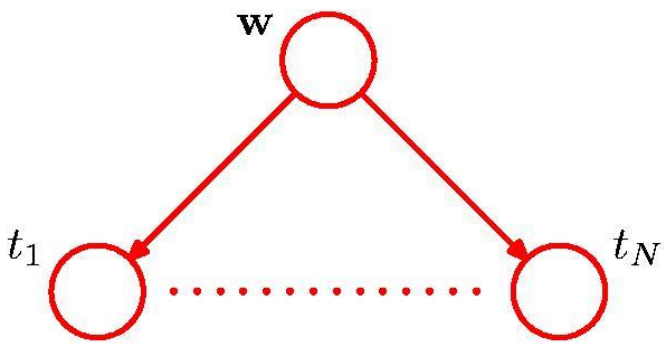
Example: Classifier Learning

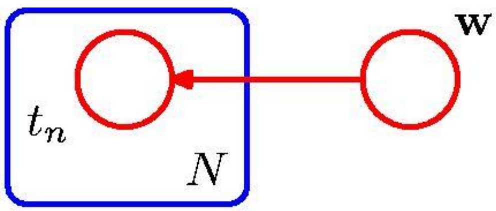
- Bayesian classifier learning
  - Given N training examples $\mathbf{x} = \{x_1,\ldots,x_N\}$ with target values $\mathbf{t}$
  - We want to optimize the classifier y with parameters $\mathbf{w}$.
  - We can express the joint probability of $\mathbf{t}$ and $\mathbf{w}$:

$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{w}) \prod_{n=1}^{N} p(t_n | y(\mathbf{w}, x_n))$$

  - Corresponding Bayesian network:



Short notation:



"Plate"
(short notation for N copies)

Conditional Independence

- Suppose we have a joint density with 4 variables.

$$p(x_0, x_1, x_2, x_3)$$

  – For example, 4 subsequent words in a sentence:

  x_0 = "Machine", x_1 = "learning", x_2 = "is", x_3 = "fun"

- The product rule tells us that we can rewrite the joint density:

$$\begin{aligned} p(x_0, x_1, x_2, x_3) &= p(x_3 | x_0, x_1, x_2) p(x_0, x_1, x_2) \\ &= p(x_3 | x_0, x_1, x_2) p(x_2 | x_0, x_1) p(x_0, x_1) \\ &= p(x_3 | x_0, x_1, x_2) p(x_2 | x_0, x_1) p(x_1 | x_0) p(x_0) \end{aligned}$$

Slide credit: Bernt Schiele, Stefan Roth

Conditional Independence

$$p(x_0, x_1, x_2, x_3) = p(x_3|x_0, x_1, x_2)p(x_2|x_0, x_1)p(x_1|x_0)p(x_0)$$

- Now, suppose we make a simplifying assumption
  - Only the previous word is what matters, i.e. given the previous word we can forget about every word *before* the previous one.
  - E.g. $p(x_3|x_0,x_1,x_2) = p(x_3|x_2)$ or $p(x_2|x_0,x_1) = p(x_2|x_1)$
  - Such assumptions are called conditional independence assumptions.
  - They are directly reflected in the structure of the graphical model.

$\Rightarrow$ *It's the edges that are missing in the graph that are important! They encode the simplifying assumptions we make.*

Slide credit: Bernt Schiele, Stefan Roth

Conditional Independence

- The notion of conditional independence means that
  - Given a certain variable, other variables become independent.
  - More concretely here:

$$p(x_3|x_0,x_1,x_2) = p(x_3|x_2)$$

    - This means that x_3 ist conditionally independent from x_0 and x_1 given x_2.

$$p(x_2|x_0,x_1) = p(x_2|x_1)$$

    - This means that x_2 is conditionally independent from x_0 given x_1.
  - Why is this?

$$\begin{aligned} p(x_0,x_2|x_1) &= p(x_2|\cancel{x_0},x_1)p(x_0|x_1) \\ &= p(x_2|x_1)p(x_0|x_1) \end{aligned}$$

independent given x_1

Slide credit: Bernt Schiele, Stefan Roth

Conditional Independence – Notation

- X is conditionally independent of Y given V
  - Equivalence: $$X \perp\!\!\!\perp Y | V \quad \Leftrightarrow \quad p(X|Y,V) = p(X|V)$$
  - Also: $$X \perp\!\!\!\perp Y | V \quad \Leftrightarrow \quad p(X,Y|V) = p(X|V)\, p(Y|V)$$
  - Special case: Marginal Independence

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

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

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

Conditional Independence

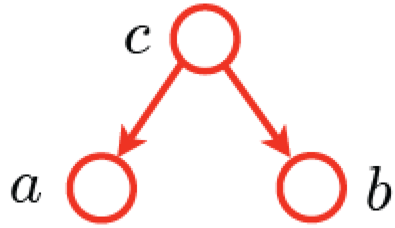
- Directed graphical models are not only useful…
  - Because the joint probability is factorized into a product of simpler conditional distributions.
  - But also, because we can read off the conditional independence of variables.

- Let's discuss this in more detail…

Slide credit: Bernt Schiele, Stefan Roth

First Case: Divergent ("Tail-to-Tail")

- Divergent model



  - Are a and b independent?
  - Marginalize out c:

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

  - In general, this is not equal to $p(a)p(b)$.
    $\Rightarrow$ The variables are not independent.

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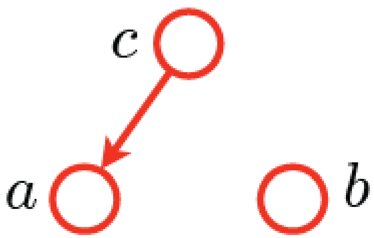
First Case: Divergent (“Tail-to-Tail”)

- What about now?



  - Are a and b independent?
  - Marginalize out c:

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

$\Rightarrow$ If there is no undirected connection between two variables, then they are independent.

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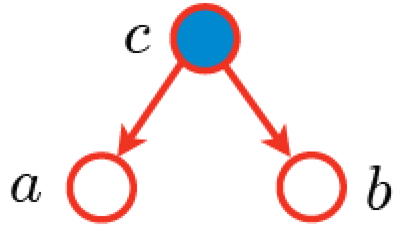
First Case: Divergent ("Tail-to-Tail")

- Let's return to the original graph, but now assume that we observe the value of c:



  – The conditional probability is given by:

$$p(a, b|c) = \frac{p(a, b, c)}{p(c)} = \frac{p(a|c)p(b|c)p(c)}{p(c)} = p(a|c)p(b|c)$$

$\Rightarrow$ If c becomes known, the variables a and b become conditionally independent.

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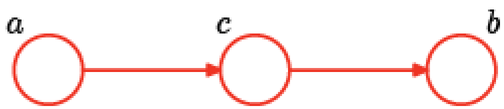
Second Case: Chain ("Head-to-Tail")

- Let us consider a slightly different graphical model:

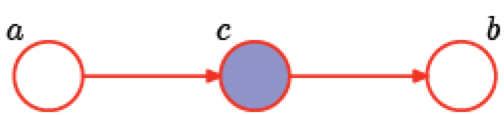


Chain graph

  – Are a and b independent? No!

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

  – If c becomes known, are a and b conditionally independent? Yes!



$$p(a,b|c) = \frac{p(a,b,c)}{p(c)} = \frac{p(a)p(c|a)p(b|c)}{p(c)} = p(a|c)p(b|c)$$

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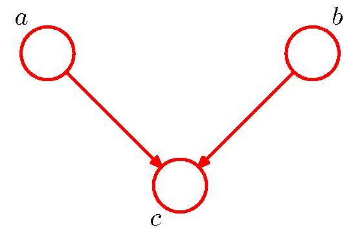
Third Case: Convergent (“Head-to-Head”)

- Let’s look at a final case: Convergent graph



  - Are a and b independent? YES!

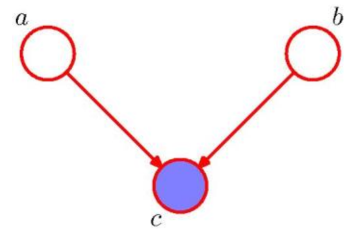
$$p(a,b) = \sum_c p(a,b,c) = \sum_c p(c|a,b)p(a)p(b) = p(a)p(b)$$

  - This is very different from the previous cases.
  - Even though a and b are connected, they are independent.

Slide credit: Bernt Schiele, Stefan Roth
Image source: C. Bishop, 2006

Third Case: Convergent ("Head-to-Head")

- Now we assume that c is observed



  - Are a and b independent? NO!

$$p(a,b|c) = \frac{p(a,b,c)}{p(c)} = \frac{p(a)p(b)p(c|a,b)}{p(c)}$$

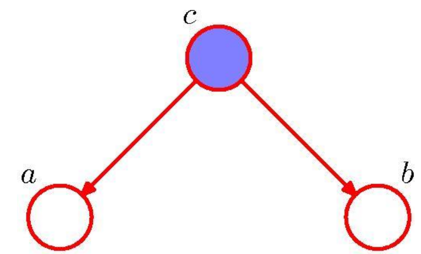
  - In general, they are not conditionally independent.
    - This also holds when any of c's descendants is observed.
  - This case is the opposite of the previous cases!

Slide credit: Bernt Schiele, Stefan Roth

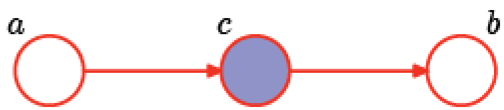
Image source: C. Bishop, 2006

Summary: 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.

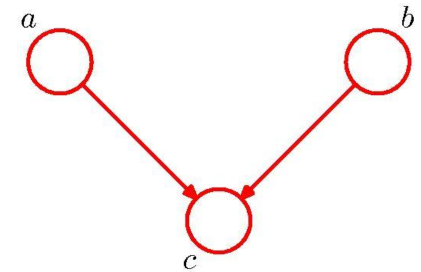
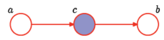
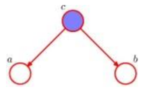


Image source: C. Bishop, 2006

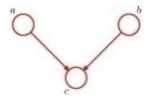
D-Separation

- 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.



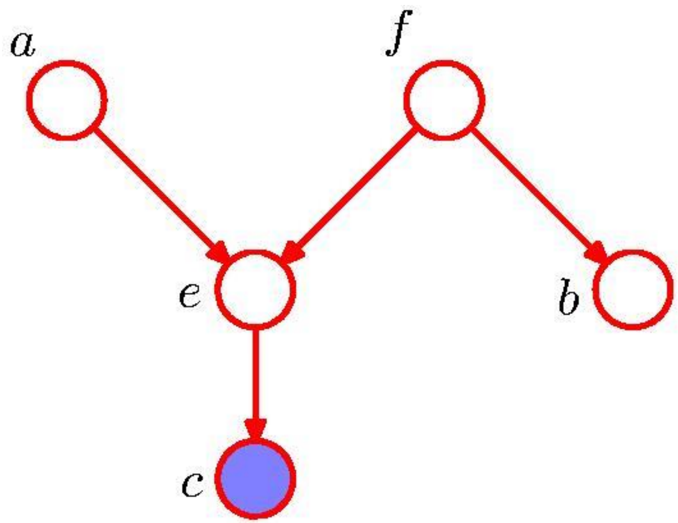
  - If all paths from A to B are blocked, A is said to be d-separated from B by C.

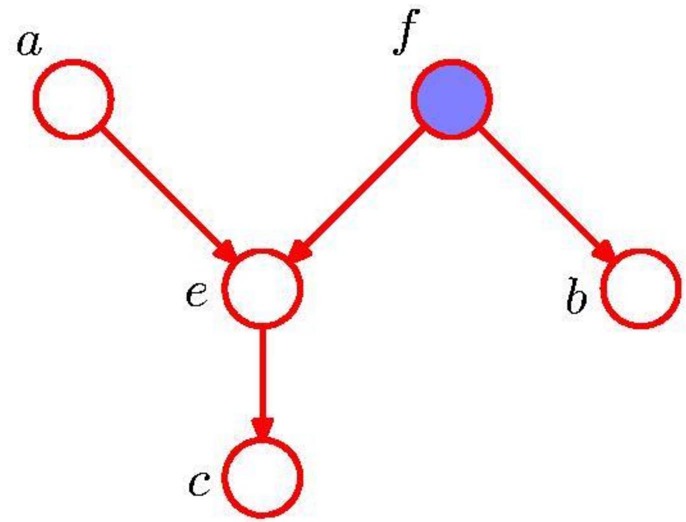
- If A is d-separated from B by C, the joint distribution over all variables in the graph satisfies $A \perp\!\!\!\perp B \mid C$.
  - Read: "A is conditionally independent of B given C."

Slide adapted from Chris Bishop

D-Separation: Example

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





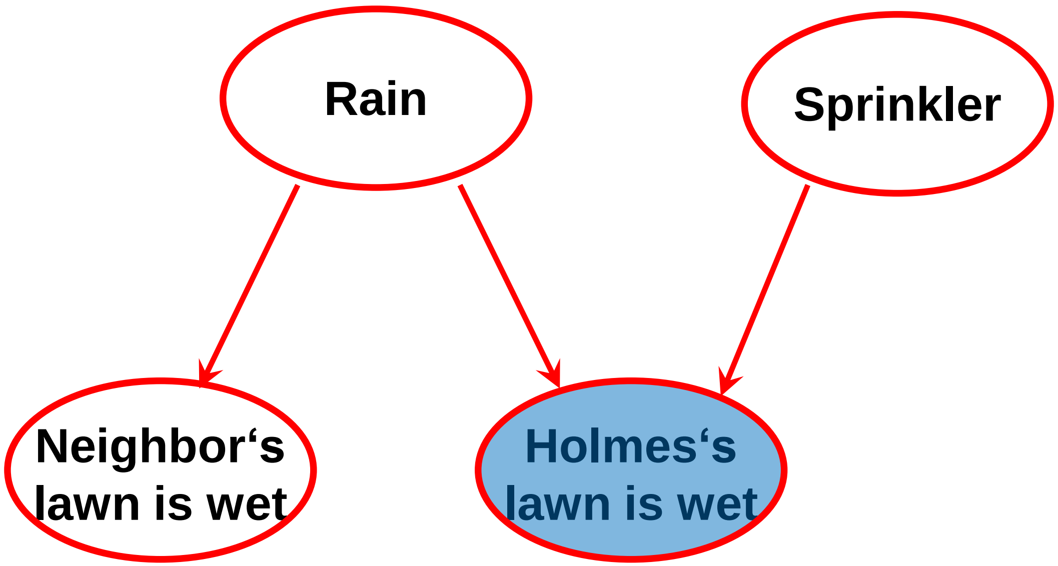
$a \not\perp\!\!\!\perp b \mid c$

$a \perp\!\!\!\perp b \mid f$

Image source: C. Bishop, 2006

Explaining Away

- Let's look at Holmes' example again:

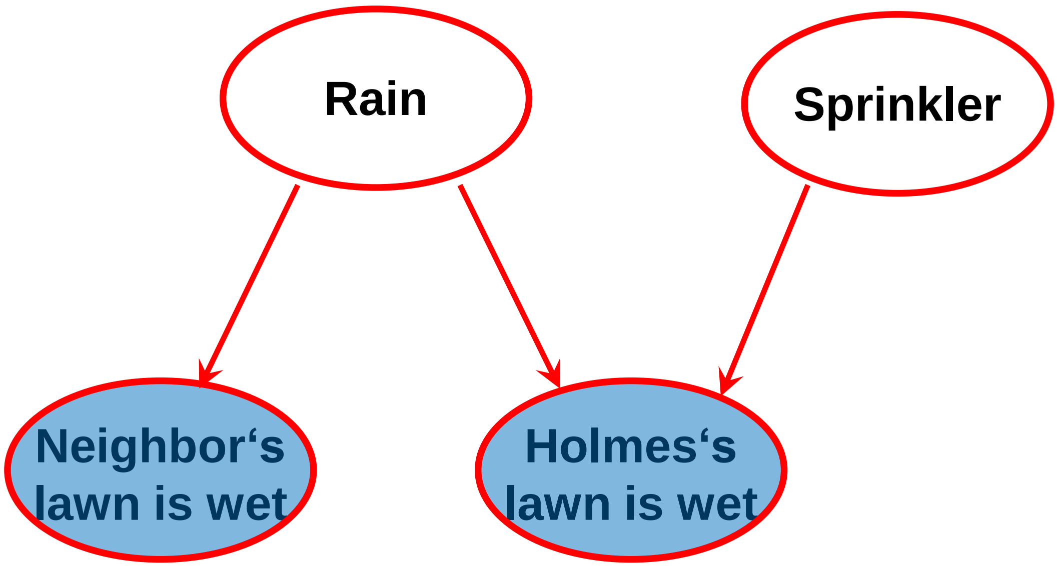


  – Observation "Holmes' lawn is wet" increases the probability of both "Rain" and "Sprinkler".

Slide adapted from Bernt Schiele, Stefan Roth

Explaining Away

- Let's look at Holmes' example again:

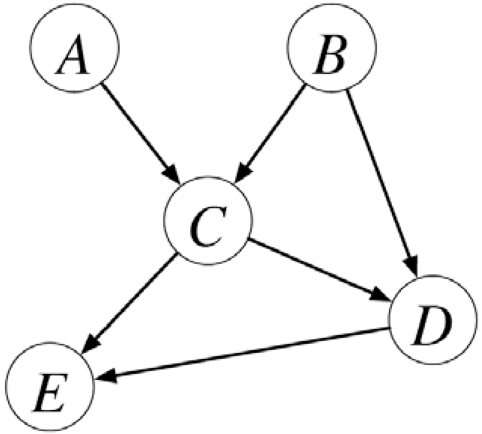


  – Observation "Holmes' lawn is wet" increases the probability of both "Rain" and "Sprinkler".
  – Also observing "Neighbor's lawn is wet" decreases the probability for "Sprinkler". (They're conditionally dependent!)

$\Rightarrow$The "Sprinkler" is explained away.

Slide adapted from Bernt Schiele, Stefan Roth

Intuitive View: The "Bayes Ball" Algorithm



- Game
  - *Can you get a ball from X to Y without being blocked by $\mathcal{V}$?*
  - 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

Slide adapted from Zoubin Gharahmani

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.

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

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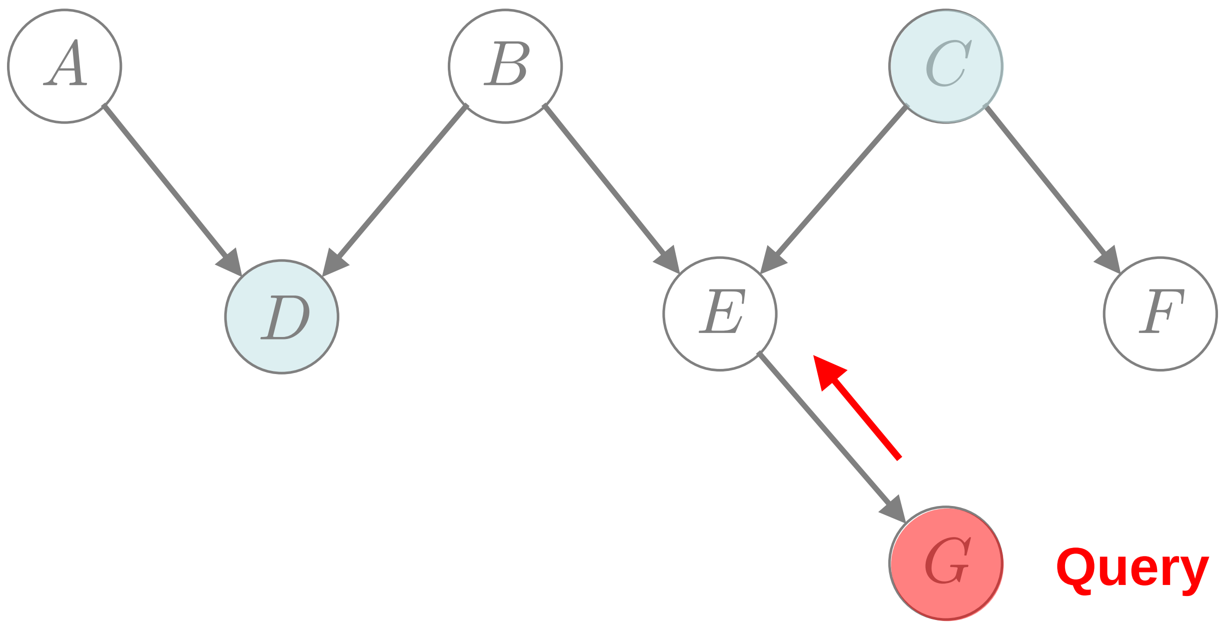
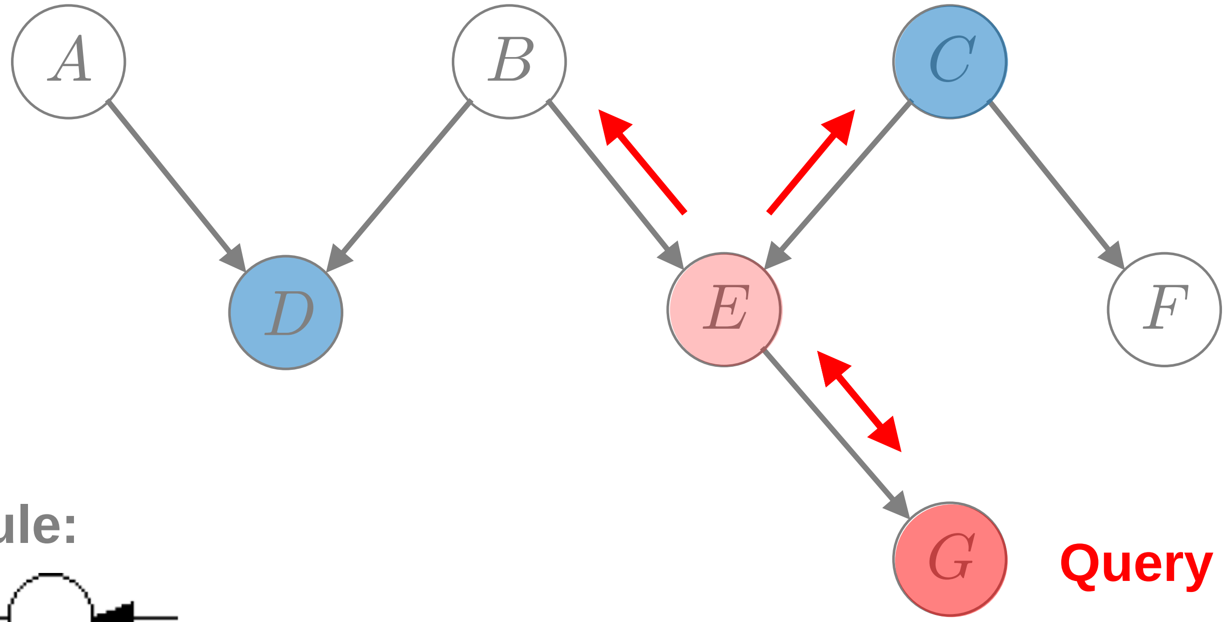
Image source: R. Shachter, 1998

Example: Bayes Ball

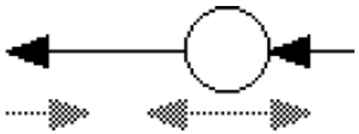


- Which nodes are d-separated from G given C and D?

Example: Bayes Ball



Rule:



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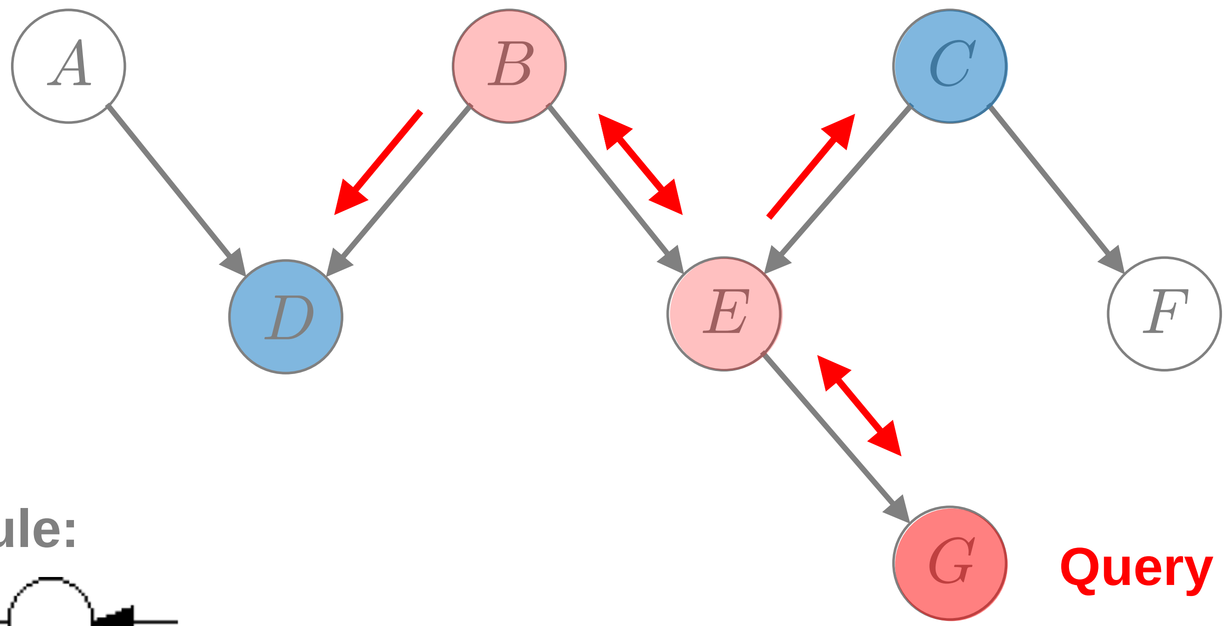
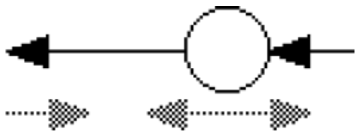
Example: Bayes Ball



Rule:



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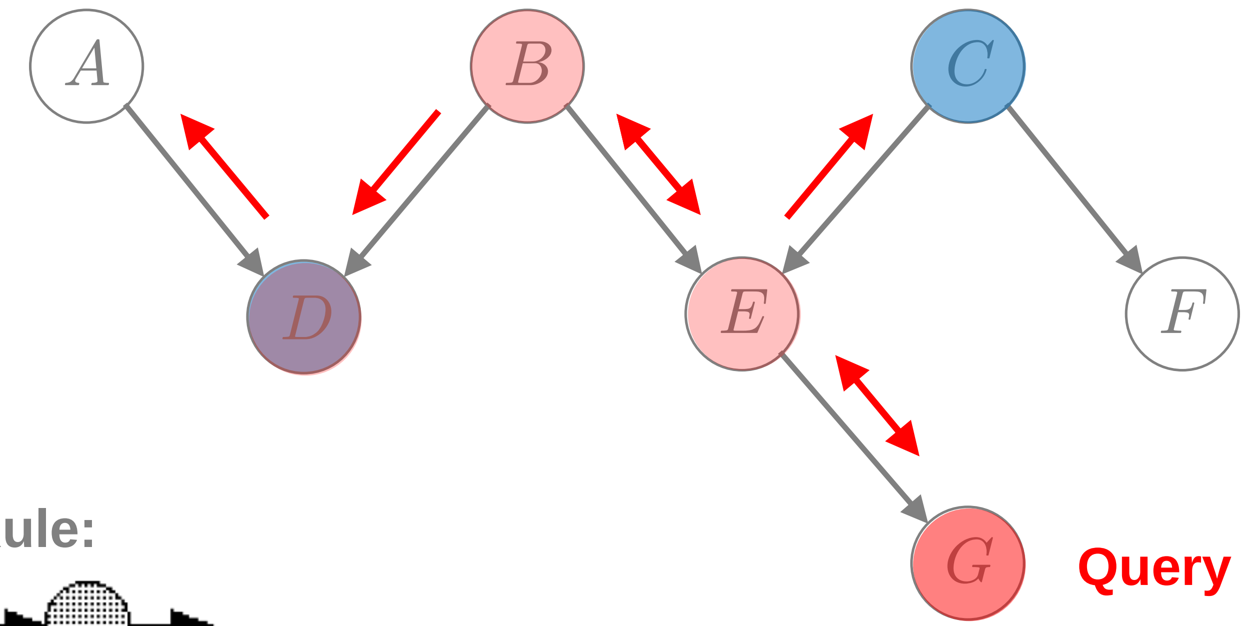
Example: Bayes Ball



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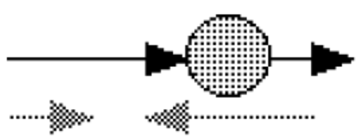
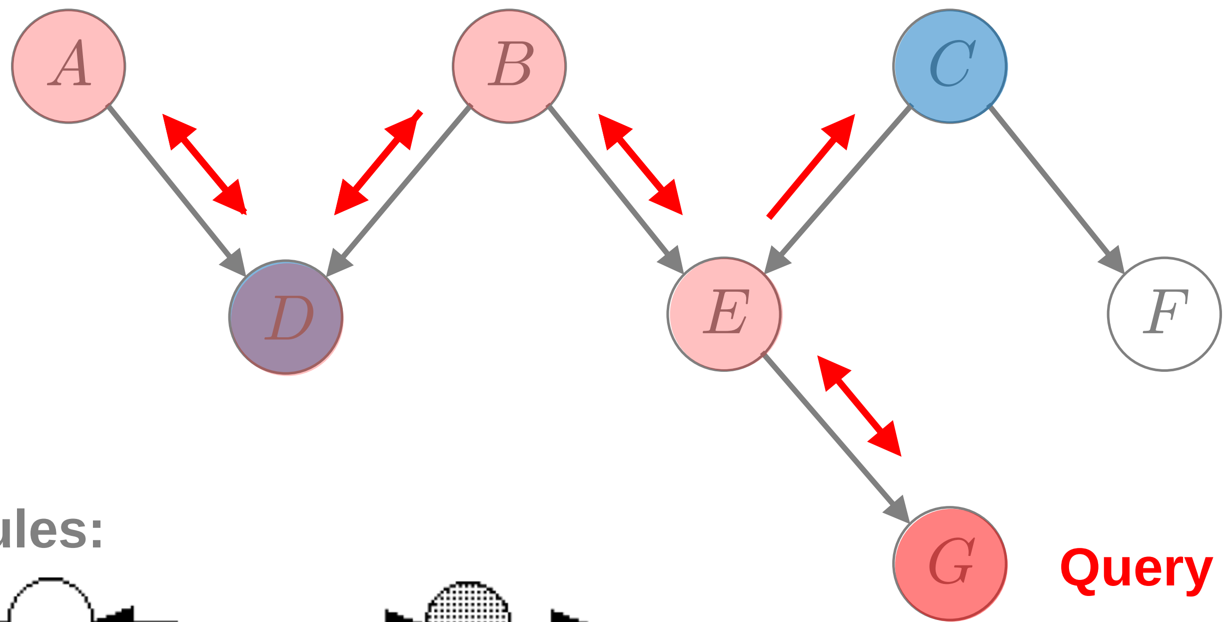
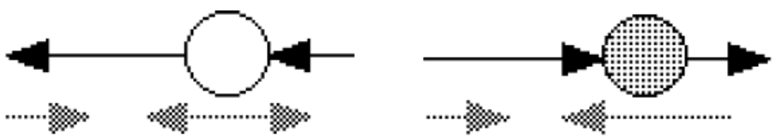


- Which nodes are d-separated from G given C and D?

Example: Bayes Ball

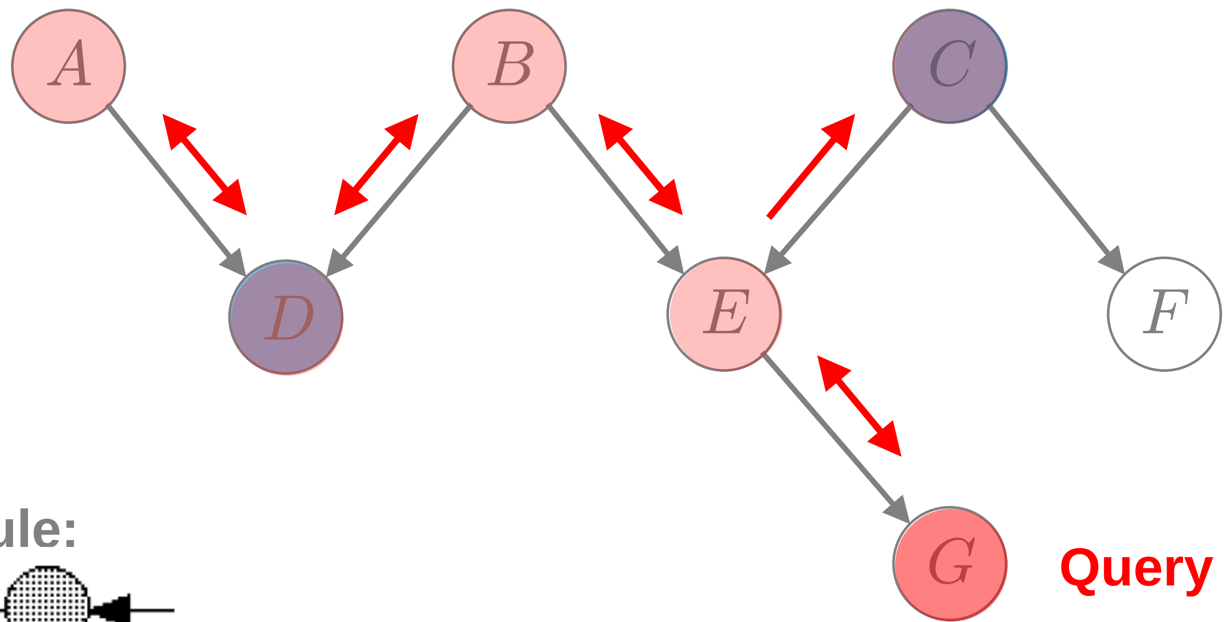


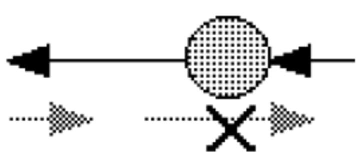
Rules:



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

Example: Bayes Ball

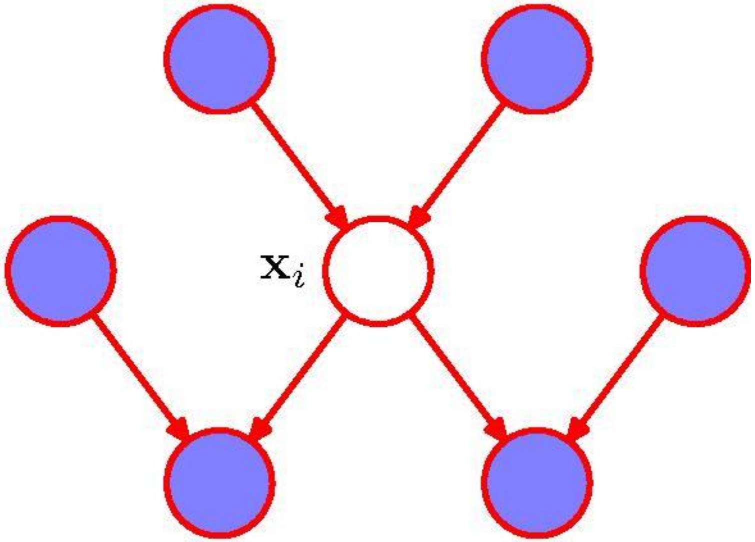




- Which nodes are d-separated from G given C and D?

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

The Markov Blanket

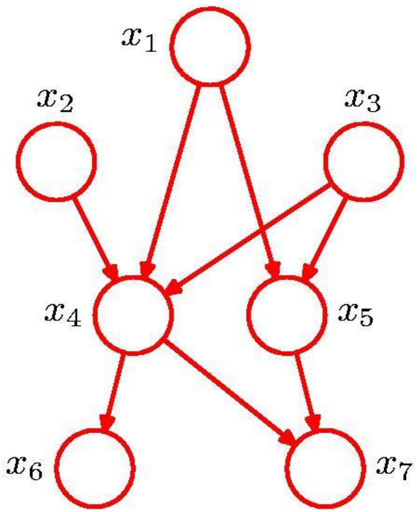


- Markov blanket of a node $\mathbf{x}_i$
  - Minimal set of nodes that isolates $\mathbf{x}_i$ from the rest of the graph.
  - This comprises the set of
    - Parents,
    - Children, and
    - Co-parents of $\mathbf{x}_i$. ← This is what we have to watch out for!

Image source: C. Bishop, 2006

Summary

- Graphical models
  - Marriage between probability theory and graph theory.
  - Give insights into the structure of a probabilistic model.
    - Direct dependencies between variables.
    - Conditional independence
  - Allow for efficient factorization of the joint.
    - Factorization can be read off directly from the graph.
    - We will use this for efficient inference algorithms!
  - Capability to explain away hypotheses by new evidence.



- Next lecture
  - Undirected graphical models (Markov Random Fields)
  - Efficient methods for performing exact inference.

Image source: C. Bishop, 2006

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