Probabilistic Graphical Models

Fall 2019

Instructor: Shandian Zhe
zhe@cs.utah.edu
School of Computing

THE UNIVERSITY OF UTAH

Overview

- A marriage between the graph theory and probability theory: it uses graphs to represent probabilistic models and facilitate inference
- The graphical structures reflect the conditional independency of the model (intuitive, convenient and expressive for modeling)
- The inference relies on the graphical structures (easy to implement, apply, analyze and improve)
- Neural networks are instances of graphical models

Outline

- Bayesian networks
  - Graphical representation
  - Conditional independence
  - D-separation, Bayes ball algorithm
  - Markov blanket
- Markov random field
  - Conditional independence
  - Relation to directed graphs
- Inference
  - Factor-graphs
  - Sum-product algorithm
  - Max-product, max-sum algorithms

Outline

- Bayesian networks
- Markov random fields
- Inference

Bayesian networks

- Bayes' Rule (theorem) revisited

$$p(\mathbf{x}_2|\mathbf{x}_1) = \frac{p(\mathbf{x}_1, \mathbf{x}_2)}{p(\mathbf{x}_1)}$$

↓

$$p(\mathbf{x}_1, \dots, \mathbf{x}_n) = p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1)p(\mathbf{x}_3|\mathbf{x}_1, \mathbf{x}_2) \dots p(\mathbf{x}_n|\mathbf{x}_1, \dots, \mathbf{x}_{n-1})$$

Why?

This can also be seen as a sampling procedure. We sequentially sample each variable given the previously sampled ones

Bayesian networks

- Consider a probabilistic model over 3 random variables: *a,b,c*

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

Bayesian networks

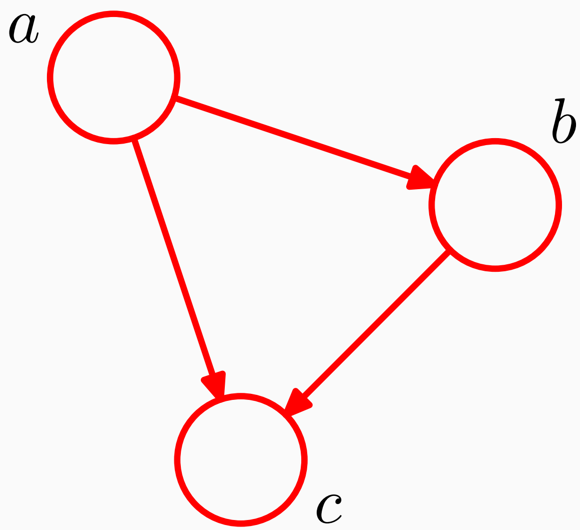
- Question: can we use a graph to represent their joint probability?

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

Bayesian networks

- Question: can we use a graph to represent their joint probability?

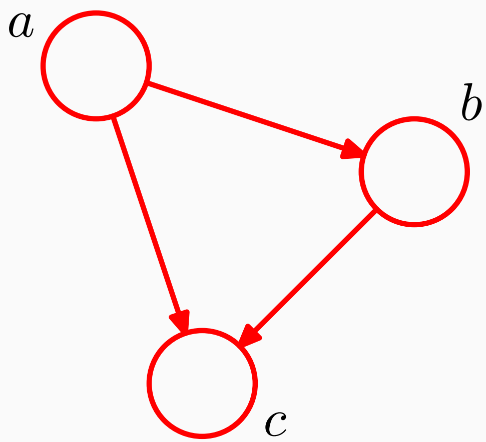
$$p(a, b, c) = p(c|a, b)p(b|a)p(a)$$



Bayesian networks - representation

- Given the joint probability,
  - Use a node to represent each random variable (RV)
  - For each conditional distribution in the joint probability, $p(a|b_1,\ldots, b_m)$, add an edge from each b_i to a ($1 \leq i \leq m$). The RVs in the condition parts are represented as the parents
  - If no condition parts, the node has no parents

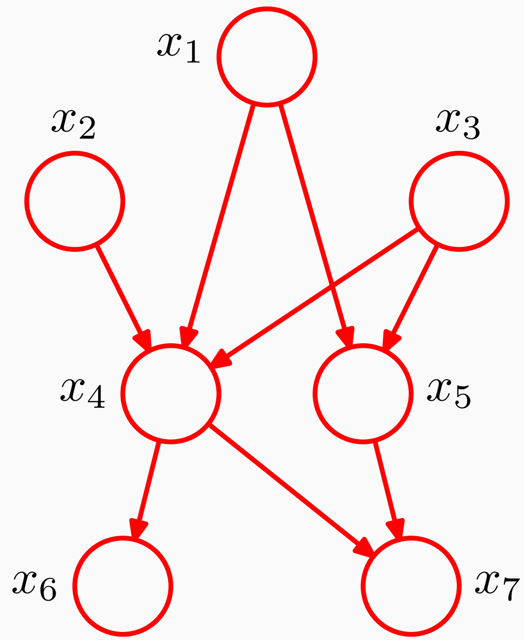
$$p(a, b, c) = p(c|a, b)p(b|a)p(a)$$



Bayesian networks - representation

- Another example

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



Bayesian networks

- We name this representation as a Bayesian network
- Bayesian networks must be a Directed Acyclic Graphs (DAG)! Why?

Bayesian networks

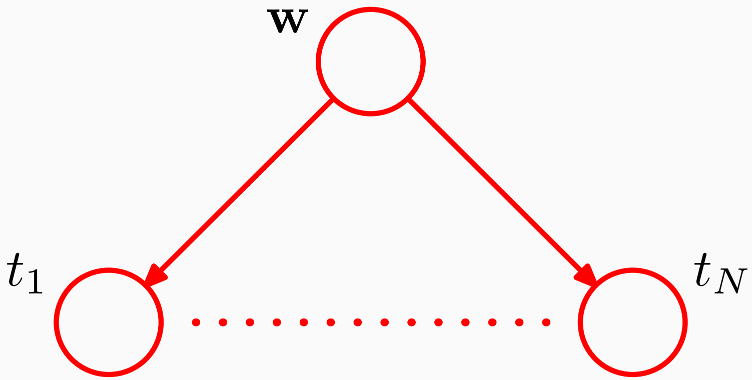
- We name this representation as a Bayesian network
- Bayesian networks must be a Directed Acyclic Graphs (DAG)! Why?

A cycle means one variable is sampled, appears in the conditional part to sample other variables, and then is sampled again. This violates Bayes' Rule!

Bayesian networks

- Polynomial regression

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



Bayesian networks

- How to be more specific and succinct?

$$\mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha\mathbf{I})$$

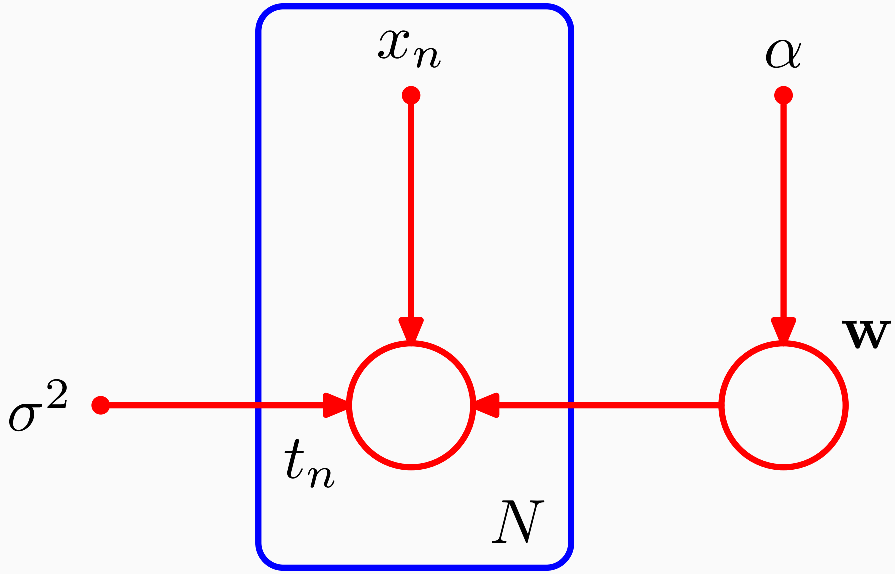
$$\mathcal{N}(t_n|\sum_{j=0}^{d-1} w_j x_n^j, \sigma^2)$$

$$p(\mathbf{t}, \mathbf{w}|\mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w}|\alpha) \prod_{n=1}^{\boxed{N}} p(t_n|\mathbf{w}, x_n, \sigma^2)$$

parameters

observations

Bayesian networks



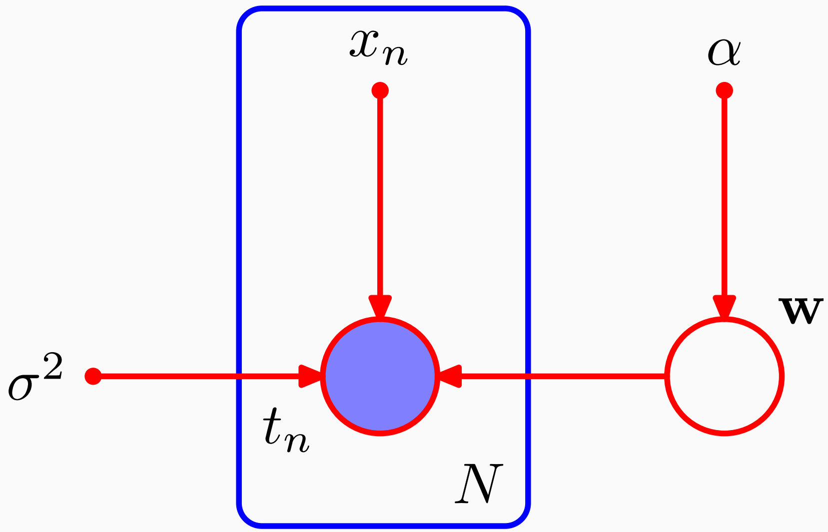
Small solid nodes: deterministic parameters, uninterested observations

Big empty nodes: latent variables

Plate with label *N*: *N* replicates

Bayesian networks

- In the training data, the outputs have been observed



Shaded nodes: observed latent variables

Bayesian networks - notes

- The network structure is determined by the factorization of the joint probability; different factorization leads to different structures

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

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

What are the networks?

So, equivalent models may have different structures

Bayesian networks - notes

- How to design the factorization of the joint probability is the key of the probabilistic modeling.
- Using the full Bayes formula will lead to a fully connected network, which represents the most general modelling (without any assumptions). But this is not what we want.
- For probabilistic modeling, we nearly always use domain knowledge to simplify the joint probability, which can be reflected by the network structure. The simplification is called conditional independence.

Bayesian networks

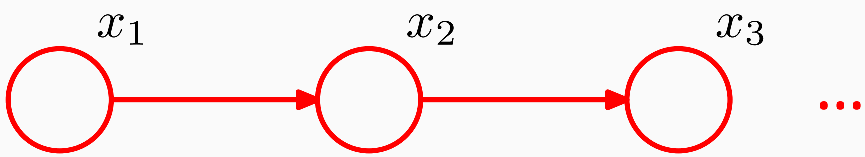
- Linear Gaussian model
- For multivariate Gaussian variables $x_1, \ldots, x_N$

Question1: what is the network structure if we do not make any assumption? Fully connected

Question2: How many parameters do we need to estimate? $O(N^2)$

Bayesian networks

- Linear Gaussian model: Let us choose a chain structure



$$p(x_i|\mathrm{pa}_i) = \mathcal{N}\left(x_i \middle| \sum_{j \in \mathrm{pa}_i} w_{ij} x_j + b_i, v_i\right)$$

Question2: How many parameters do we need to estimate? O(N)

Bayesian networks

- In general, the simplification of the Bayes‘ Rule reflects our ideas, tricks and knowledge in probabilistic modeling

- How is the simplification reflected?

Conditional independence!

Conditional Independence

- Consider a probabilistic model over 3 random variables: *a,b,c*

a is conditional independent of b given c if

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

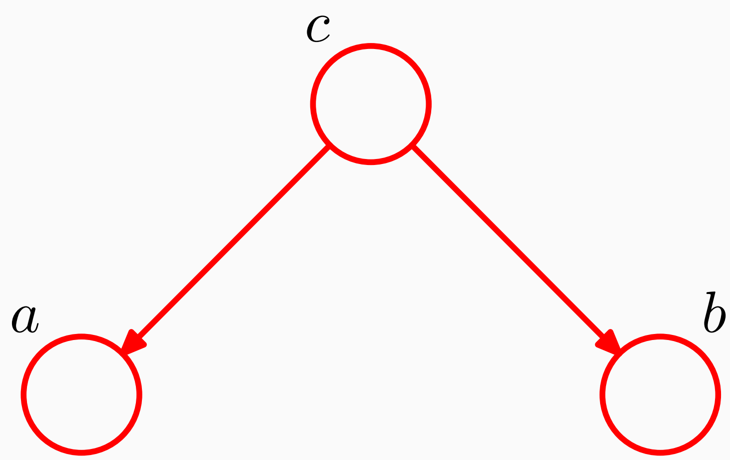
Why?

$$a \perp\!\!\!\perp b \mid c$$

Conditional Independence

- What is the Bayesian network?

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

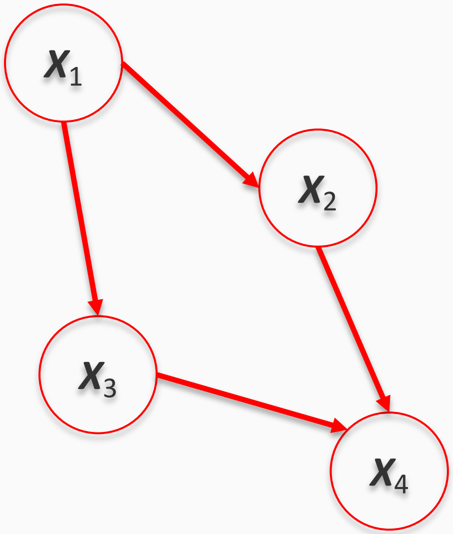


The network structure is simplified as well

Conditional Independence

- Practically , how do we design a Bayesian network?

Consider a sampling (generative) process



We usually do not explicitly consider all possible conditional independences!

…

Conditional Independence

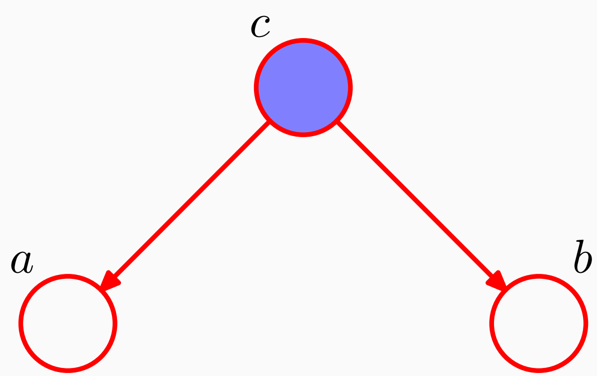
- Question: For a (complex) Bayesian network, given arbitrary nonintersecting sets of nodes *A, B, C*, how do we test the conditional independency?

$$A \perp\!\!\!\perp B \mid C$$

- This is important to analyze our model

D-separation

- Basic case I: *tail-to-tail*



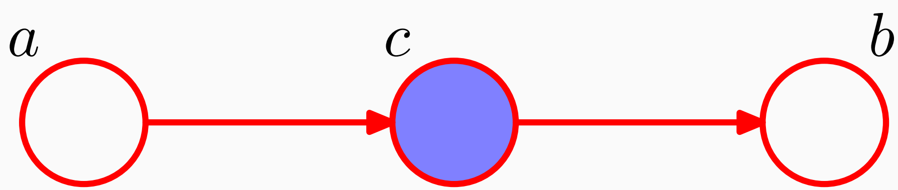
$$a \not\perp\!\!\!\perp b \mid \emptyset$$

$$a \perp\!\!\!\perp b \mid c$$

Why?

D-separation

- Basic case II: *head-to-tail*



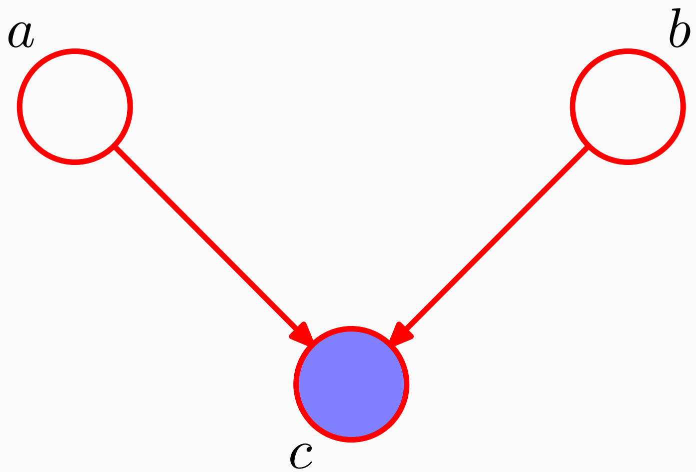
$$a \not\perp\!\!\!\perp b \mid \emptyset$$

$$a \perp\!\!\!\perp b \mid c$$

Why?

D-separation

- Basic case III (a little odd): *head-to-head*



$$a \perp\!\!\!\perp b \mid \emptyset$$

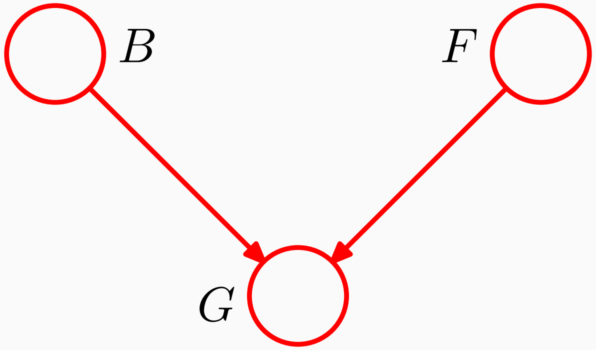
$$a \not\perp\!\!\!\perp b \mid c$$

Why?

D-separation

B: battery
F: fuel tank
G: gauge

- *head-to-head:* explain away effect



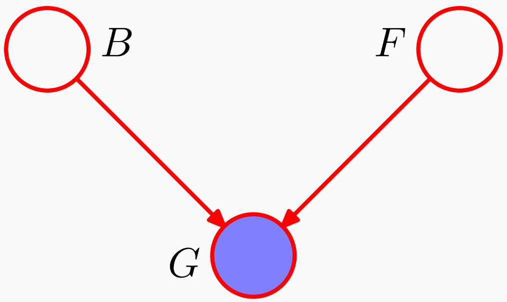
$$
\begin{aligned}
p(B=1) &= 0.9 \\
p(F=1) &= 0.9.
\end{aligned}
$$

$$
\begin{aligned}
p(G=1|B=1,F=1) &= 0.8 \\
p(G=1|B=1,F=0) &= 0.2 \\
p(G=1|B=0,F=1) &= 0.2 \\
p(G=1|B=0,F=0) &= 0.1
\end{aligned}
$$

D-separation

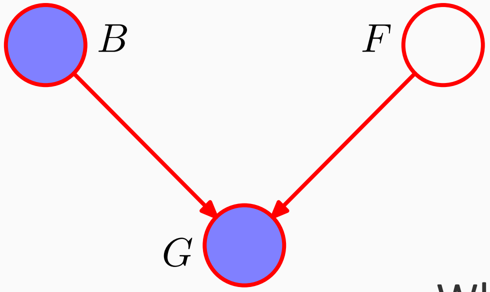
B: battery
F: fuel tank
G: gauge

- *head-to-head:* explain away effect



$$p(F=0|G=0) = \frac{p(G=0|F=0)p(F=0)}{p(G=0)} \simeq 0.257$$

>

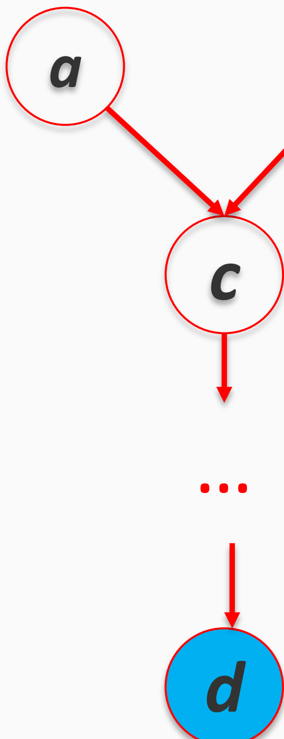


$$p(F=0|G=0,B=0) = \frac{p(G=0|B=0,F=0)p(F=0)}{\sum_{F\in\{0,1\}} p(G=0|B=0,F)p(F)} \simeq 0.111$$

Why? Batter being dead partly takes away the effect of zero Gauge

D-separation

- *head-to-head: more general case*



$a \not\perp\!\!\!\perp b \mid$ c or any descendent(*c*)

D-separation

- In general, for a (complex) Bayesian network, given arbitrary nonintersecting sets of nodes *A, B, C*, how to test the conditional independency?

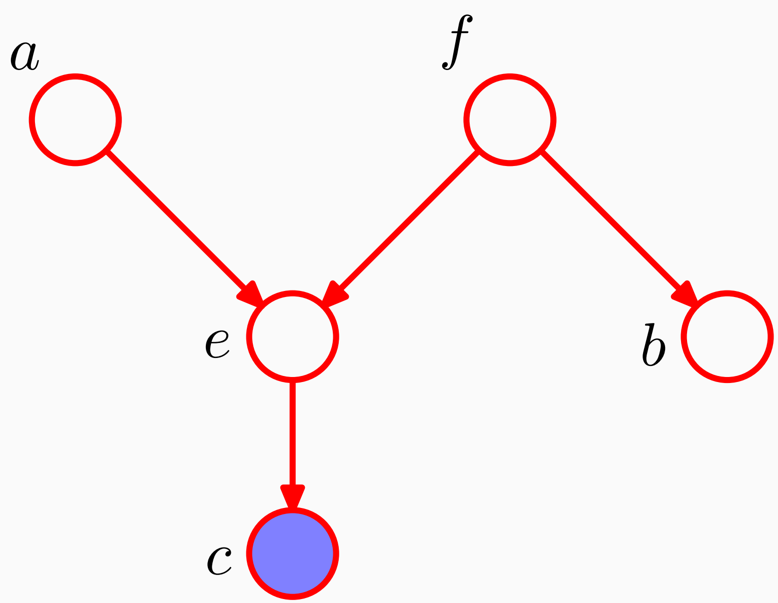
$$A \perp\!\!\!\perp B \mid C$$

D-separation (Bayes ball algo.) $A \perp\!\!\!\perp B \mid C$

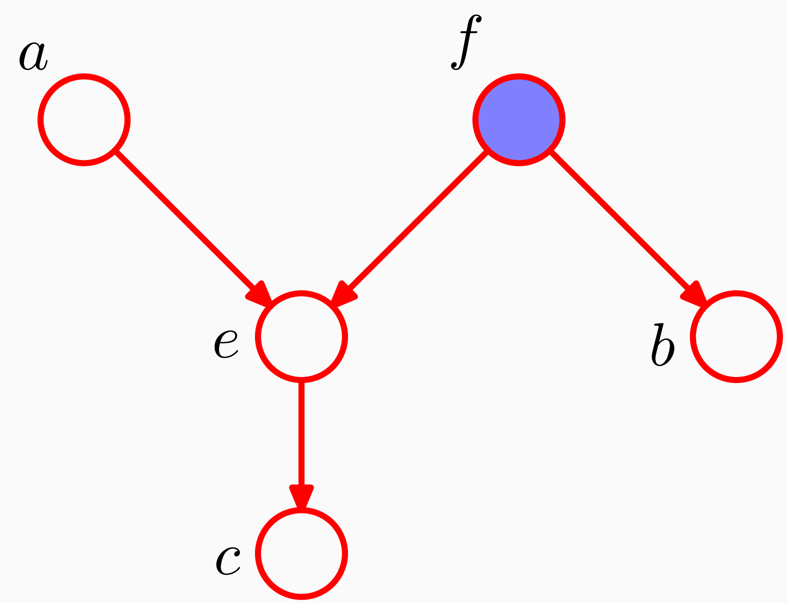
- Step 1: Shade all the nodes in *C*
- Step 2: For every path from any node in A to any node in B
  - If the path contains a node, such that
    - the arrows on the path meet *head-to-tail* or *tail-to-tail* at a node in C, the path is blocked and continue, OR
    - the arrows on the path meet head-to-head at a node, and neither the node or any of its descendent is in C,

    the path is blocked and continue
  - Otherwise, return $A \perp\!\!\!\perp B \mid C$ does not hold
- Step 3: if every path is blocked, return $A \perp\!\!\!\perp B \mid C$ holds

D-separation - examples



A = {a}, B = {b}, C = {c}



A = {a}, B = {b}, C = {f}

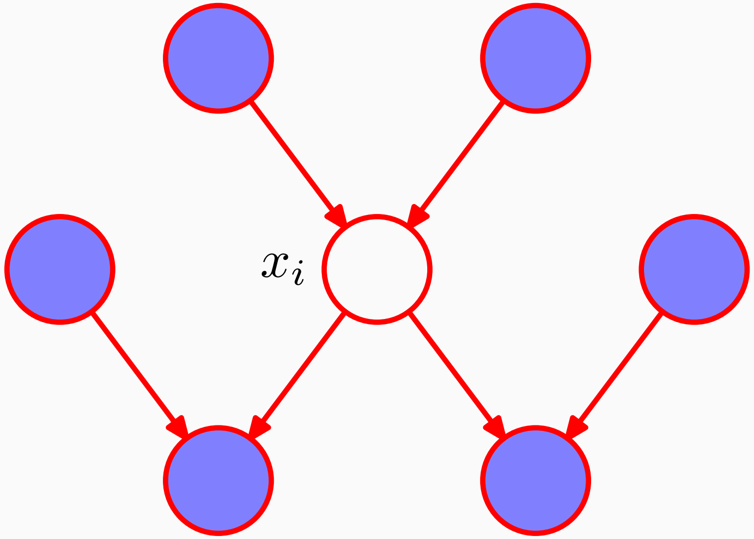
Markov-blanket

- Consider a Bayesian network with *D* nodes, $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_D$
- For a particular node $\boldsymbol{x}_i$, conditioned on what set of variables, $\boldsymbol{x}_i$ are independent to the remaining variables?

$$
\begin{aligned}
p(\mathbf{x}_i|\mathbf{x}_{\{j\neq i\}}) &= \frac{p(\mathbf{x}_1,\ldots,\mathbf{x}_D)}{\displaystyle\int p(\mathbf{x}_1,\ldots,\mathbf{x}_D)\,\mathrm{d}\mathbf{x}_i} \\
&= \frac{\displaystyle\prod_k p(\mathbf{x}_k|\mathrm{pa}_k)}{\displaystyle\int \prod_k p(\mathbf{x}_k|\mathrm{pa}_k)\,\mathrm{d}\mathbf{x}_i}
\end{aligned}
$$

Markov-blanket

- Answer: $\boldsymbol{x}_i$'s parents, $\boldsymbol{x}_i$'s children and the children's co-parents
- These variables are called the Markov-blanket of $\boldsymbol{x}_i$

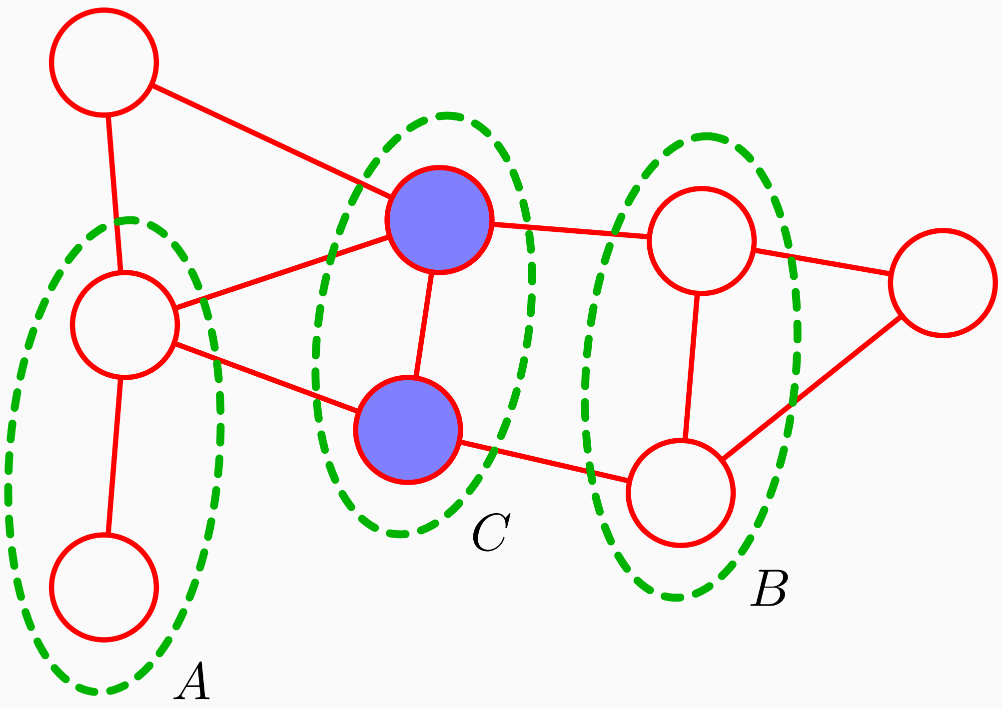


Some thoughts

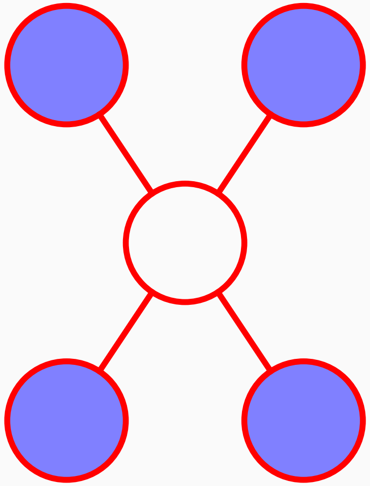
- D-separation is a bit subtle to test the conditional independency

- Can we have easier graphical representations that allow more natural tests? e.g., only based on paths without considering arrow directions?

Markov random fields

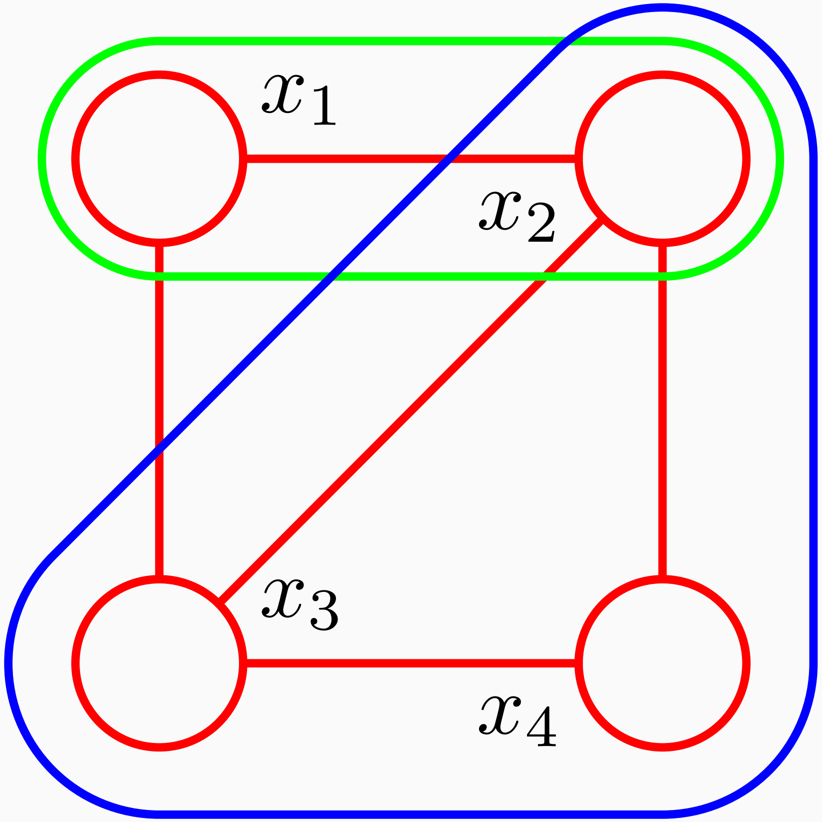


$$A \perp\!\!\!\perp B \mid C$$



Markov blanket

Cliques and maximum cliques



Joint distribution

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

Where $\psi_C(\mathbf{x}_C) \geqslant 0$ is the *potential function* over maximum clique C

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

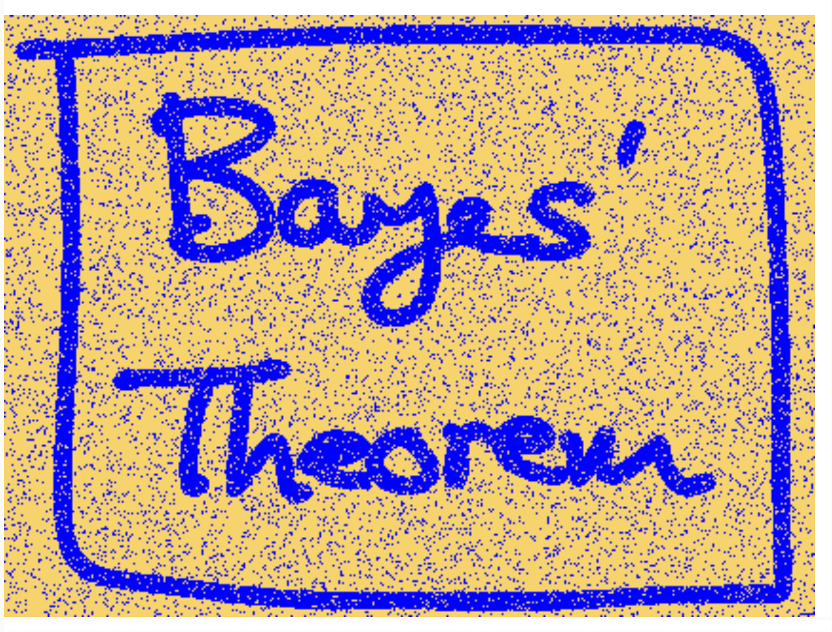
is the normalization constant, also called *partition* function

Energy and the Boltzmann distribution

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

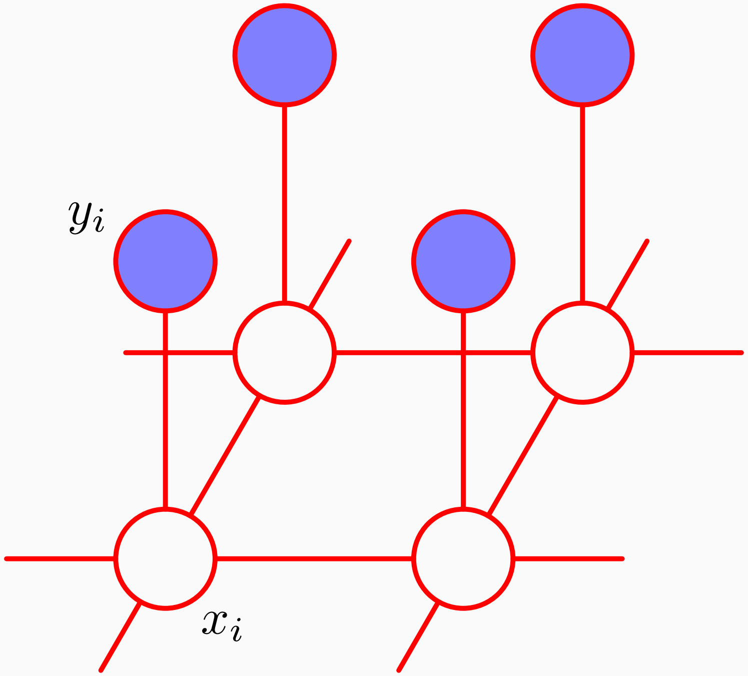
Illustration: Image Denoise

Ground-truth



noisy observation

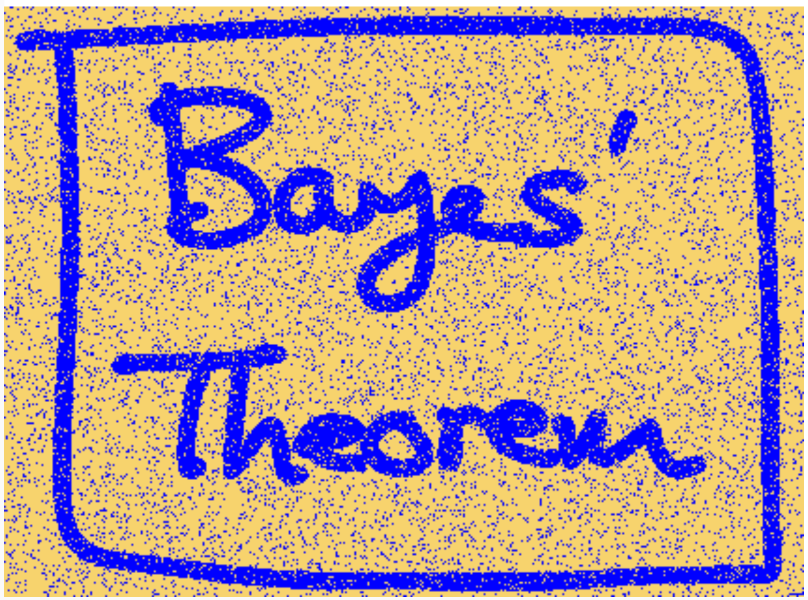
Illustration: Image Denoise



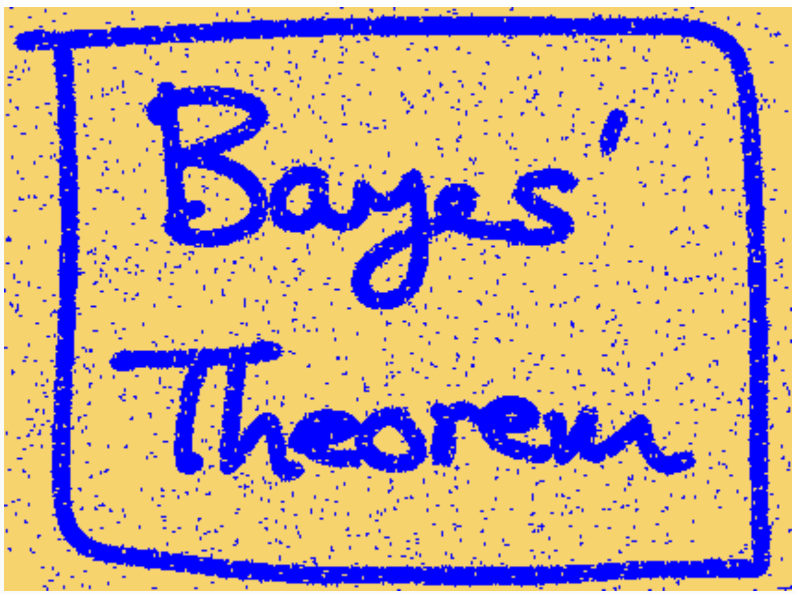
$$E(\mathbf{x}, \mathbf{y}) = h \sum_i x_i - \beta \sum_{\{i,j\}} x_i x_j - \eta \sum_i x_i y_i$$

$$p(\mathbf{x}, \mathbf{y}) = \frac{1}{Z} \exp\{-E(\mathbf{x}, \mathbf{y})\}$$

Illustration: Image Denoise

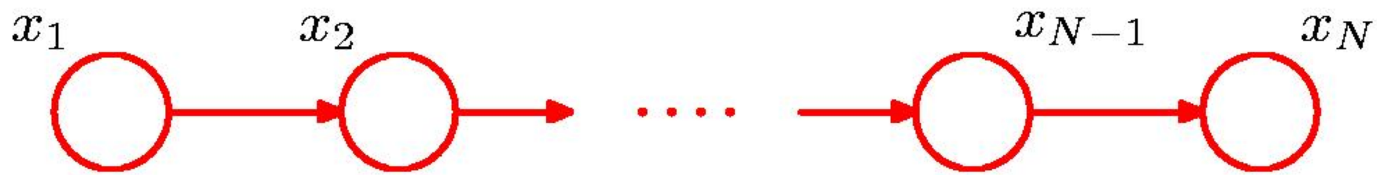


noisy observation



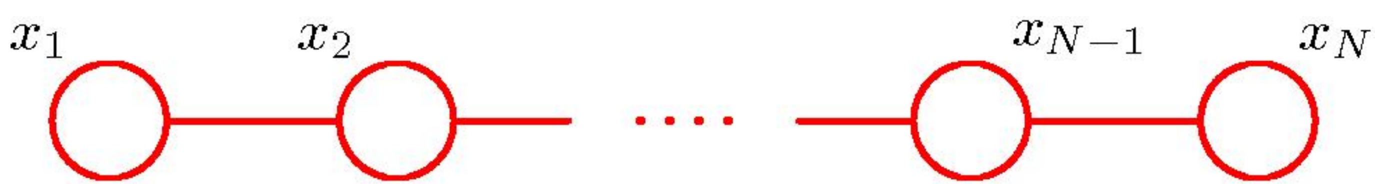
restored version (ICM)

How to convert directed to undirected graphs



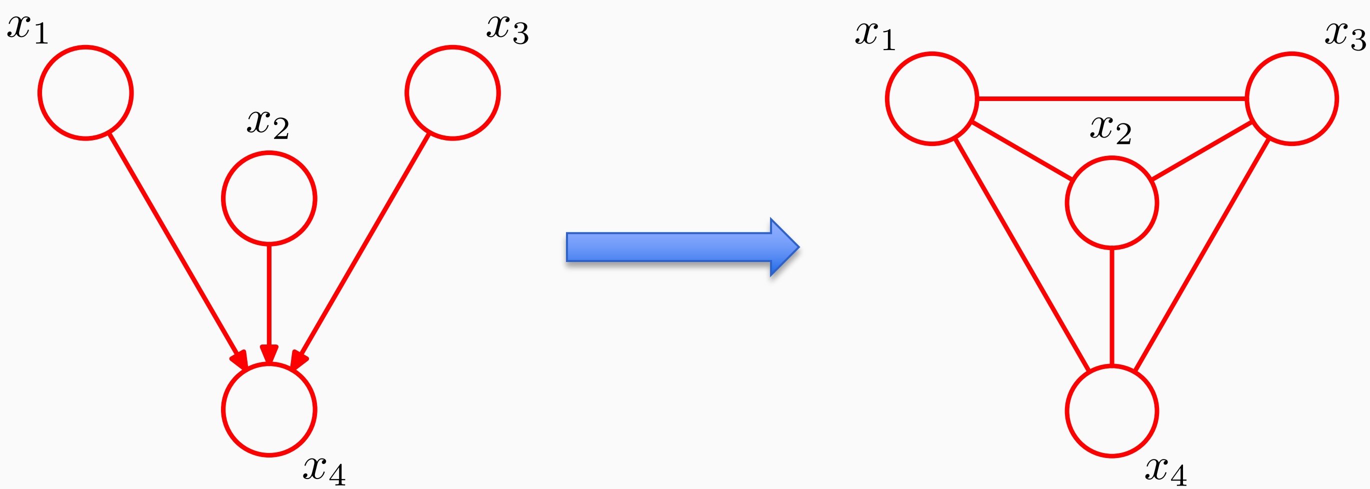
$$p(\mathbf{x}) = \underbrace{p(x_1)p(x_2|x_1)}\, p(x_3|x_2) \cdots p(x_N|x_{N-1})$$

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



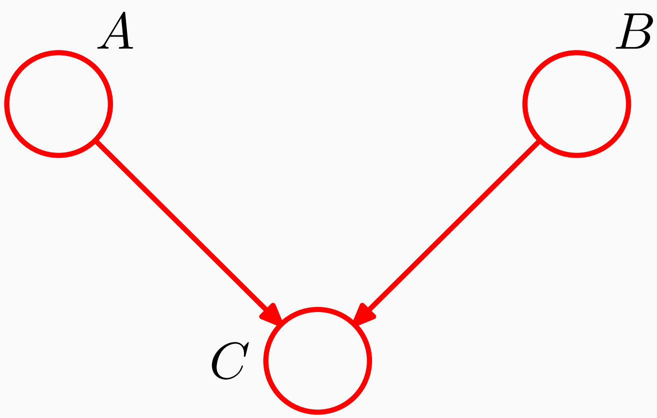
How to convert directed to undirected graphs

Add additional links: “marrying parents”, i.e., moralization



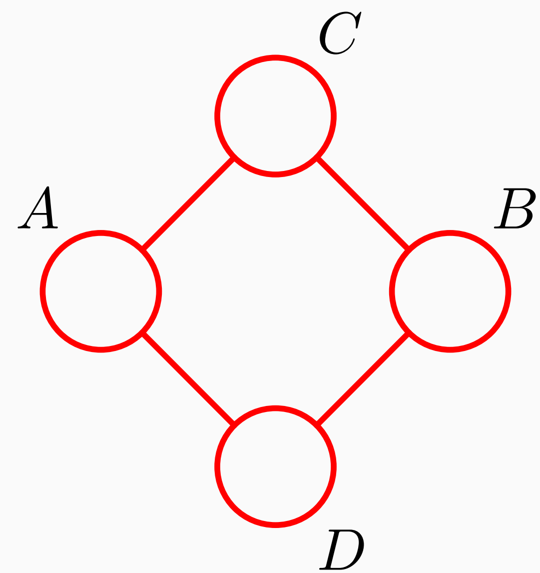
$$p(\mathbf{x}) \quad = \quad p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) = \psi(x_1, x_2, x_3, x_4)$$

Directed vs. undirected graphs



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

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



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

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

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

What you need to know

- How to construct Bayes networks and Markov random field
- How to convert a BN to MRF (moralization)
- BN is an acyclic directed graph, why? (Bayes’ Rule)
- Conditional independence
- Head-to-tail, tail-to-tail and head-to-head
- Explain away effect
- D-separation (Bayes ball algorithm)
- BNs are NOT equivalent to MRFs!