2018 CS420, Machine Learning, Lecture 8

Probabilistic Graphical Models

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http://wnzhang.net/teaching/cs420/index.html

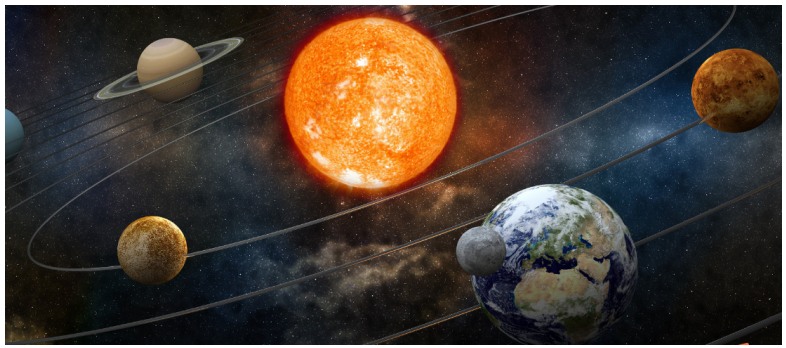
Content of This Lecture

- Introduction
- Bayes Networks (Directed Graphs)
- Markov Networks (Undirected Graphs)
- Inferences in Graphical Models

Reference: Chapter 8 of Pattern Recognition and Machine Learning by Chris Bishop

Review: Data Science

- Physics
  - Goal: discover the underlying principle of the world



  - Solution: build the model of the world from observations

$$F = G\frac{m_1 m_2}{r^2}$$

- Data Science
  - Goal: discover the underlying principle of the data

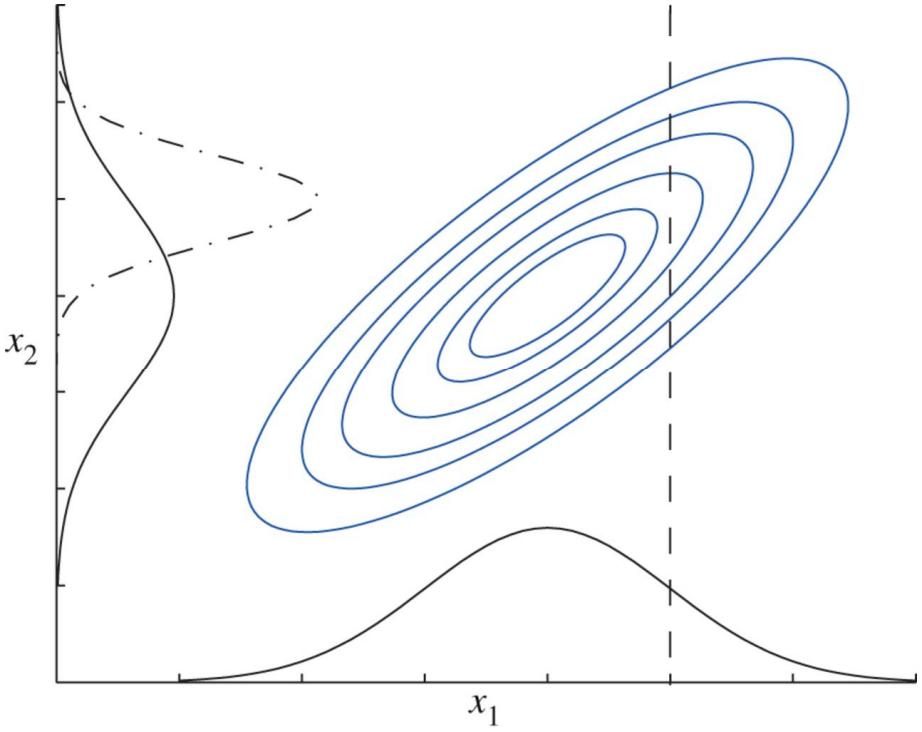
  - Solution: build the model of the data from observations

$$p(x) = \frac{e^{f(x)}}{\sum_{x'} e^{f(x')}}$$

Data Science

- Mathematically
  - Find joint data distribution $p(x)$
  - Then the conditional distribution $p(x_2|x_1)$
- E.g., Gaussian distribution
  - Multivariate

$$p(x) = \frac{e^{-(x-\mu)^\top \Sigma^{-1}(x-\mu)}}{\sqrt{|2\pi\Sigma|}}$$



- Univariate

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

A Simple Example in User Behavior Modelling

Interest	Gender	Age	BBC Sports	PubMed	Bloomberg Business	Spotify
Finance	Male	29	Yes	No	Yes	No
Sports	Male	21	Yes	No	No	Yes
Medicine	Female	32	No	Yes	No	No
Music	Female	25	No	No	No	Yes
Medicine	Male	40	Yes	Yes	Yes	No

- Joint data distribution

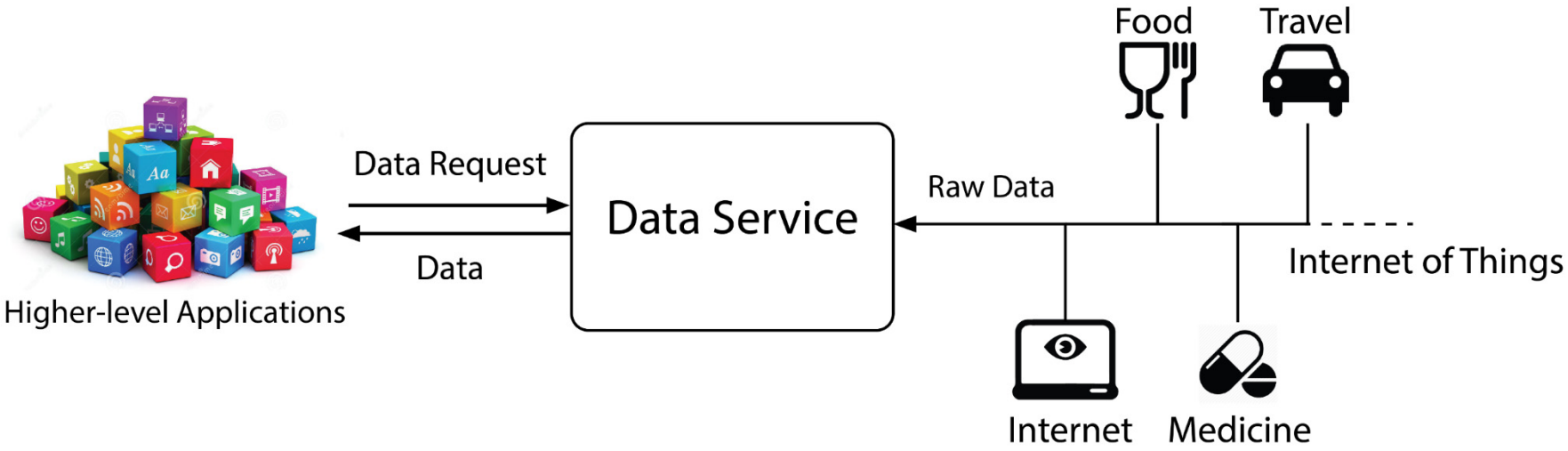
p(Interest=Finance, Gender=Male, Age=29, Browsing=BBC Sports,Bloomberg Business)

- Conditional data distribution

p(Interest=Finance | Browsing=BBC Sports, Bloomberg Business)

p(Gender=Male | Browsing=BBC Sports, Bloomberg Business)

Data Technology



Key Problem of Data Science

- How to build the data model?

- Specifically, how to model the joint data distribution $p(x)$?

  - For example, the data of temperature and people's cloth

Temperature	Cloth	Probability
Hot	Shirt	48%
Hot	Coat	12%
Cold	Shirt	8%
Cold	Coat	32%

Data Probabilistic Modeling

Temperature	Cloth	Probability
Hot	Shirt	48%
Hot	Coat	12%
Cold	Shirt	8%
Cold	Coat	32%

- From the table, we can directly build a joint distribution model

P(temperature=hot, cloth=shirt) = 48%
P(temperature=hot, cloth=coat) = 12%
P(temperature=cold, cloth=shirt) = 8%
P(temperature=cold, cloth=coat) = 32%

  - to estimate and maintain 2×2 = 4 probabilities

Data Probabilistic Modeling

- What if we have a high dimensional data

Temperature	Cloth	Gender	Weekday	Probability
Hot	Shirt	Male	Monday	2.4%
Hot	Coat	Female	Friday	1.2%
Cold	Shirt	Female	Sunday	3.8%
Cold	Coat	Male	Thursday	3.1%
…				

  - Directly build a joint distribution model to estimate and maintain $2\times2\times2\times7 = 56$ probabilities
    - Exponential complexity

  - We should find a better way to model the data distribution

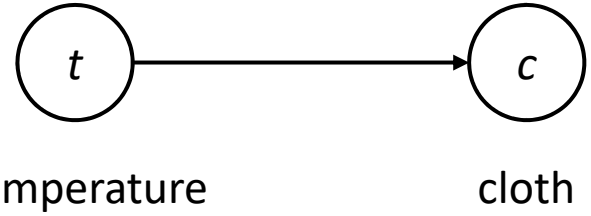
Domain Knowledge

Temperature	Cloth	Probability
Hot	Shirt	48%
Hot	Coat	12%
Cold	Shirt	8%
Cold	Coat	32%

- Build data dependency with domain knowledge
  - People choose clothes according to the temperature
  - Thus the cloth variable depends on the temperature variable

$$p(t, c) = p(t)p(c|t)$$

P(temperature=hot) = 60%
P(temperature=cold) = 40%

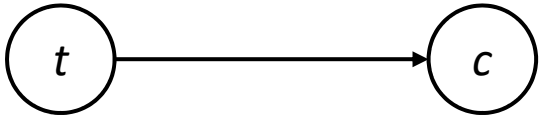


P(cloth=shirt|temperature=hot) = 80%
P(cloth=coat|temperature=hot) = 20%
P(cloth=shirt|temperature=cold) = 20%
P(cloth=coat|temperature=cold) = 80%

Graphical Model

- Graphical model is a methodology to formulate such data dependency from any domain knowledge
  - Bayesian network (directed graphs)

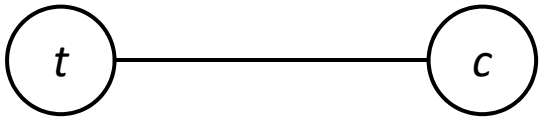
$$p(t, c) = p(t)p(c|t)$$



temperature cloth

  - Markov network (undirected graphs)

$$p(t, c) = \frac{e^{\phi(t,c)}}{\sum_{t',c'} e^{\phi(t',c')}}$$



temperature cloth

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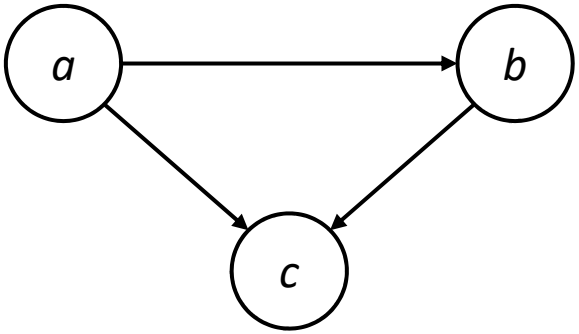
A Simple Bayesian Network

- Consider an arbitrary joint distribution $p(a, b, c)$
- One may apply the product rule of probability

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

Symmetrical w.r.t. *a*, *b* and *c*

Asymmetrical w.r.t. *a*, *b* and *c*

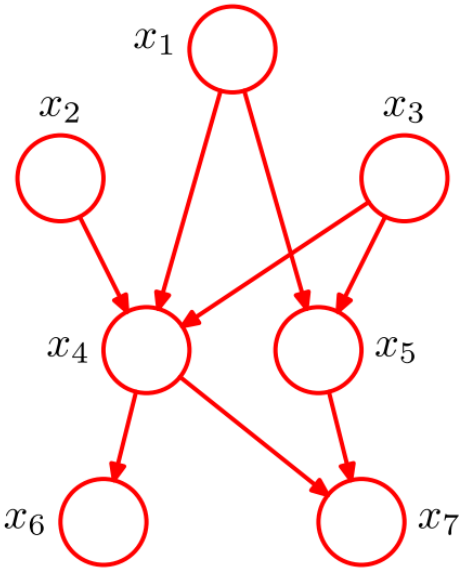


- One of the powerful aspects of graphical models is that a specific graph can make probabilistic statements for a broad class of distributions
- We say this graph is **fully connected** because there is a link between every pair of nodes

A More Complex Bayesian Network

- A 7-dimensional data distribution

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



- For a graph with *K* nodes, the joint distribution is

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

Parent nodes of x_k

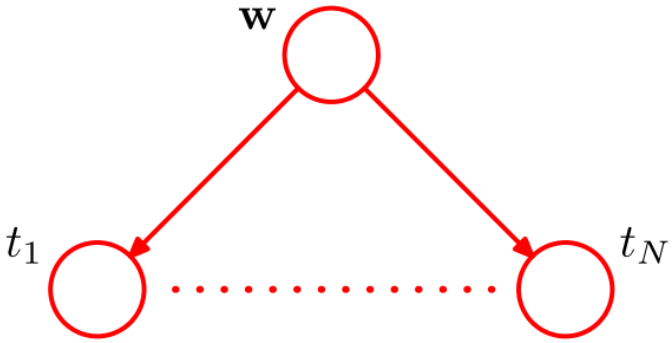
- An important restriction: directed acyclic graphs (DAGs)

An ML Example

- For the training data $D = \{(x_i, t_i)\}$
- We build a linear prediction model with observation Gaussian noise

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

Prior distribution

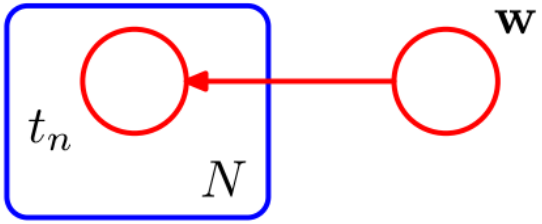


- More explicitly

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

$$p(t_i|x_i, \mathbf{w}, \sigma^2) = \mathcal{N}(t_i|\mathbf{w}^\top x_i, \sigma^2)$$

$$p(\mathbf{t}, \mathbf{w}|\mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w}|\alpha) \prod_{i=1}^{N} p(t_i|x_i, \mathbf{w}, \sigma^2)$$



An alternative, more compact, representation of the graph

An ML Example

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- We build a linear prediction model with observation Gaussian noise

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

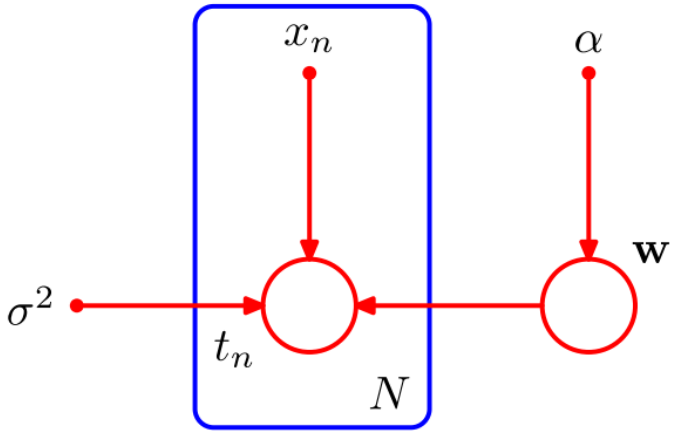
Prior distribution

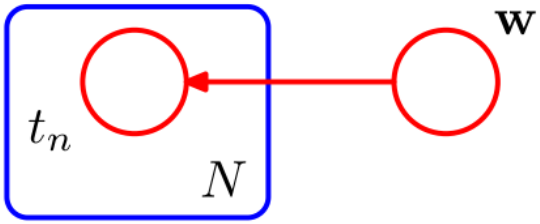
- More explicitly

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

$$p(t_i|x_i, \mathbf{w}, \sigma^2) = \mathcal{N}(t_i|\mathbf{w}^\top x_i, \sigma^2)$$

$$p(\mathbf{t}, \mathbf{w}|\mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w}|\alpha) \prod_{i=1}^{N} p(t_i|x_i, \mathbf{w}, \sigma^2)$$





An alternative, more compact, representation of the graph

Posterior Distribution

- With $\{t_n\}$ observed, we can evaluate the posterior distribution of coefficients ***w***

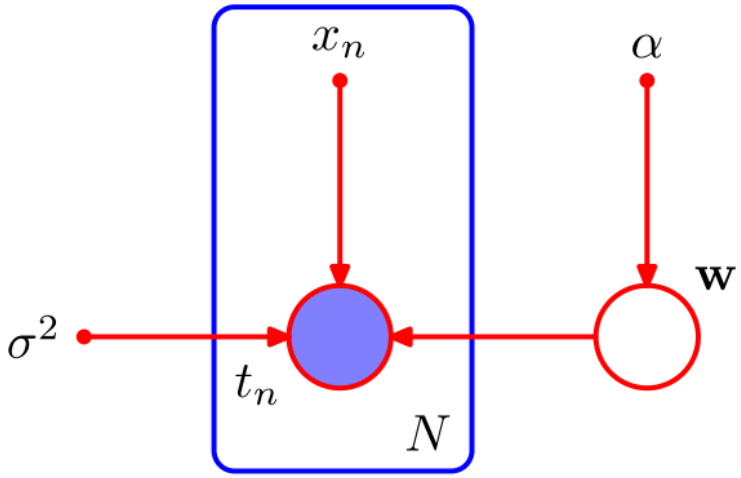
$$p(\mathbf{w}|\mathbf{t}) = \frac{p(\mathbf{w})p(\mathbf{t}|\mathbf{w})}{p(\mathbf{t})}$$

$$\propto p(\mathbf{w}) \prod_{i=1}^{N} p(t_i|\mathbf{w})$$

Posterior distribution

Prior distribution

Data likelihood



Maximum A Posteriori Estimation

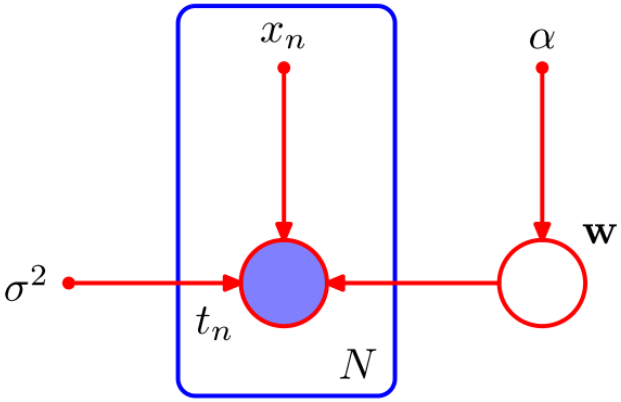
- Maximum A Posteriori (MAP) estimation of the model coefficients $\mathbf{w}$

$$\max_{\mathbf{w}} p(\mathbf{w}|\mathbf{t}) = \max_{\mathbf{w}} p(\mathbf{w},\mathbf{t}) = \max_{\mathbf{w}} p(\mathbf{w})p(\mathbf{t}|\mathbf{w})$$

$$p(\mathbf{w})p(\mathbf{t}|\mathbf{w}) = p(\mathbf{w}|\alpha)\prod_{i=1}^{N} p(t_i|x_i,\mathbf{w},\sigma^2)$$

$$= \mathcal{N}(\mathbf{w}|\mathbf{0},\alpha)\prod_{i=1}^{N}\mathcal{N}(t_i|\mathbf{w}^\top\mathbf{x},\sigma^2)$$

$$= \frac{1}{\sqrt{(2\pi\alpha)^d}}\exp\Big(-\frac{\mathbf{w}^\top\mathbf{w}}{2\alpha^d}\Big)\prod_{i=1}^{N}\frac{1}{\sqrt{2\pi\sigma^2}}\exp\Big(-\frac{(t_i-\mathbf{w}^\top\mathbf{x})^2}{2\sigma^2}\Big)$$



$$\log p(\mathbf{w})p(\mathbf{t}|\mathbf{w}) = -\frac{\mathbf{w}^\top\mathbf{w}}{2\alpha^d} - \sum_{i=1}^{N}\frac{(t_i-\mathbf{w}^\top\mathbf{x})^2}{2\sigma^2} + \text{const}$$

Equivalent to $\min_{\mathbf{w}} \frac{\sigma^2}{\alpha^d}\|\mathbf{w}\|^2 + \sum_{i=1}^{N}(t_i-\mathbf{w}^\top\mathbf{x})^2$ i.e., ridge regression with square loss

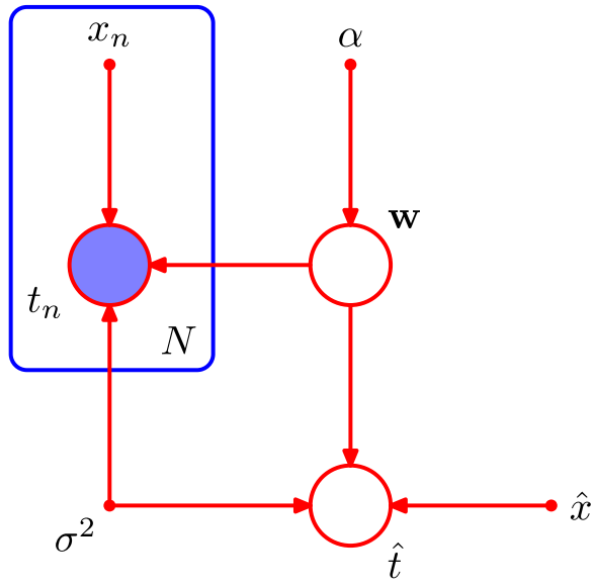
Prediction on New Instance

- Given a new input value $\hat{x}$, predict the corresponding probability distribution for its label $\hat{t}$
  - Joint distribution of random variables

$$p(\hat{t}, \mathbf{t}, \mathbf{w}|\hat{x}, \mathbf{x}, \alpha, \sigma^2) = \left[\prod_{i=1}^{N} p(t_i|x_i, \mathbf{w}, \sigma^2)\right] p(\mathbf{w}|\alpha) p(\hat{t}|\hat{x}, \mathbf{w}, \sigma^2)$$

  - Marginalize out the coefficients ***w***

$$\begin{aligned} p(\hat{t}|\hat{x}, \mathbf{x}, \mathbf{t}, \alpha, \sigma^2) &= \frac{p(\hat{t}, \mathbf{t}|\hat{x}, \mathbf{x}, \alpha, \sigma^2)}{p(\mathbf{t})} \\ &\propto p(\hat{t}, \mathbf{t}|\hat{x}, \mathbf{x}, \alpha, \sigma^2) \\ &= \int p(\hat{t}, \mathbf{t}, \mathbf{w}|\hat{x}, \mathbf{x}, \alpha, \sigma^2) d\mathbf{w} \end{aligned}$$



Conditional Independence

- Consider three variables *a*, *b*, and *c*
- Suppose that the conditional distribution of *a*, given *b* and *c*, is such that it does not depend on the value of *b*

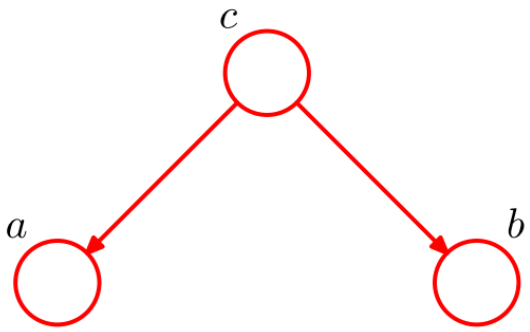
$$p(a|b,c) = p(a|c)$$

- We say that *a* is conditionally independent of *b* given *c*
- A slightly different presentation

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

- A notation for conditional independence

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

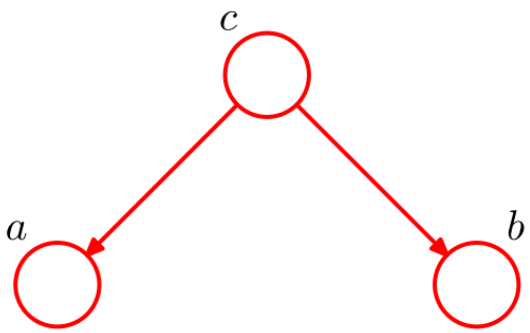


Conditional Independence in Graph

- Conditional independence properties of the joint distribution can be read directly from the graph
- Example 1: tail-to-tail
  - With *c* unobserved

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

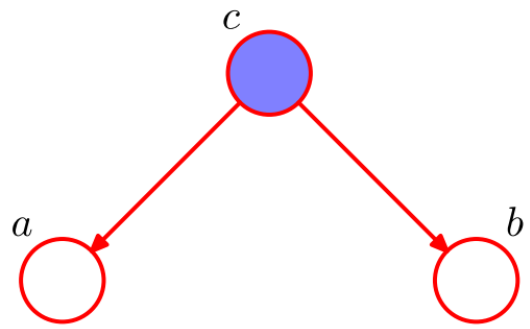
Not conditional independence $a \not\perp\!\!\!\perp b \mid \emptyset$



  - With *c* observed

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

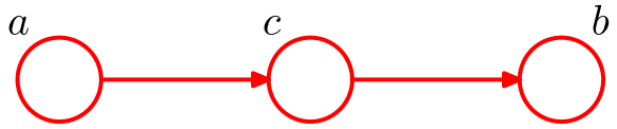
Conditional independence $a \perp\!\!\!\perp b \mid c$



Conditional Independence in Graph

- Example 2: head-to-tail
  - With *c* unobserved

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



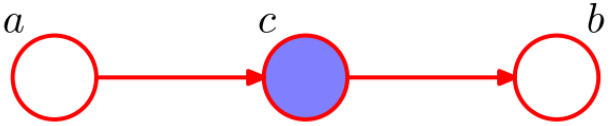
Not conditional independence $a \not\perp\!\!\!\perp b \mid \emptyset$

  - With *c* observed

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

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

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



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

Conditional Independence in Graph

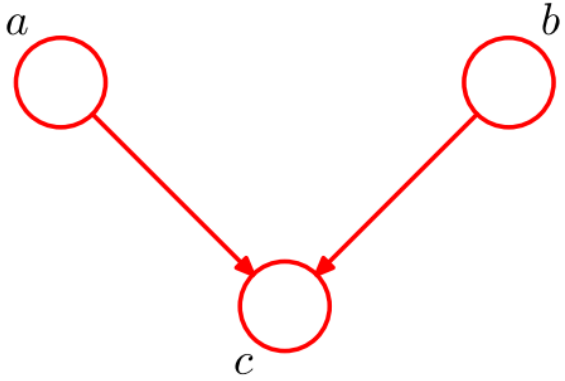
- Example 3: head-to-head
  - With *c* unobserved

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

Marginalize both sides over *c*

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

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

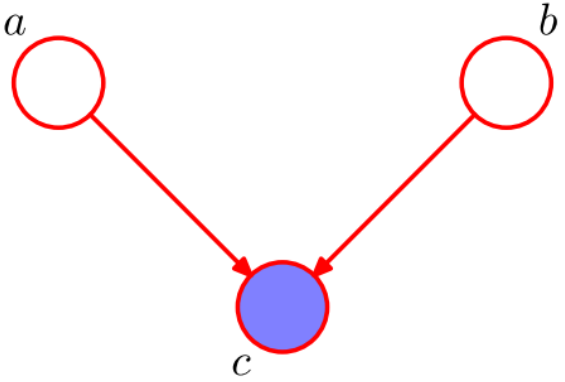


  - With *c* observed

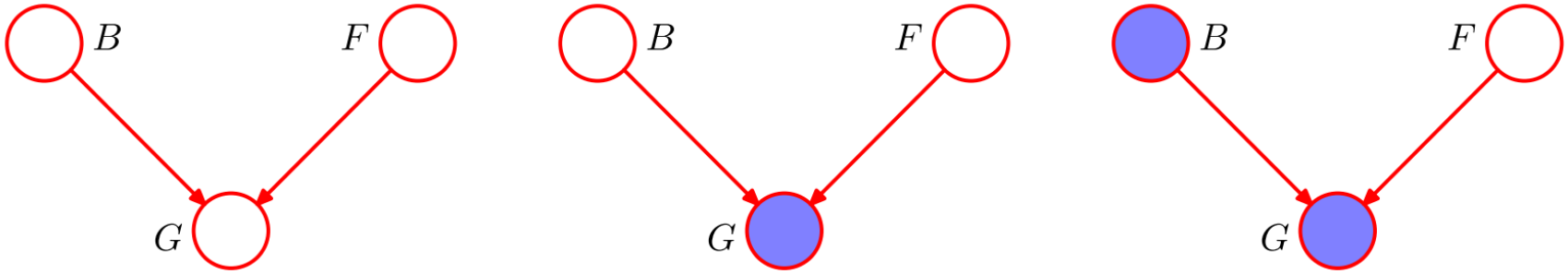
$$p(a,b|c) = \frac{p(a,b,c)}{p(c)}$$

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

Not conditional independence $a \not\perp\!\!\!\perp b \mid c$



Understanding head-to-head Case



- Variables
  - *B*: battery state, either charged (*B*=1) or flat (*B*=0)
  - *F*: fuel tank state, either full of fuel (*F*=1) or empty (*F*=0)
  - *G*: electric fuel gauge, either full (*G*=1) or empty (*G*=0)

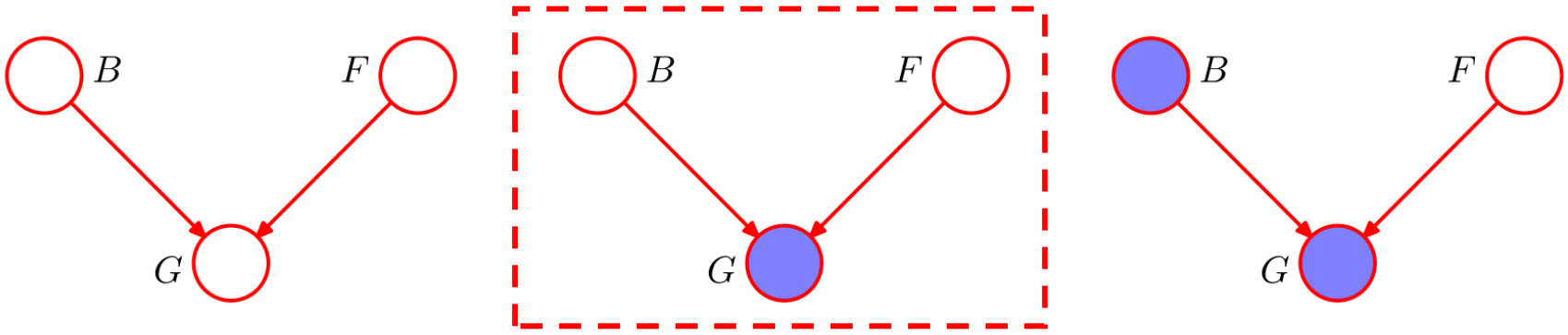
- (Conditional) probabilities

$$p(B=1) = 0.9$$
$$p(F=1) = 0.9$$

$$p(G=1|B=1,F=1) = 0.8$$
$$p(G=1|B=1,F=0) = 0.2$$
$$p(G=1|B=0,F=1) = 0.2$$
$$p(G=1|B=0,F=0) = 0.1$$

All remaining probabilities are determined by the requirement that probabilities sum to one

Understanding head-to-head Case



- If we observe the fuel gauge reads empty, i.e., *G*=0

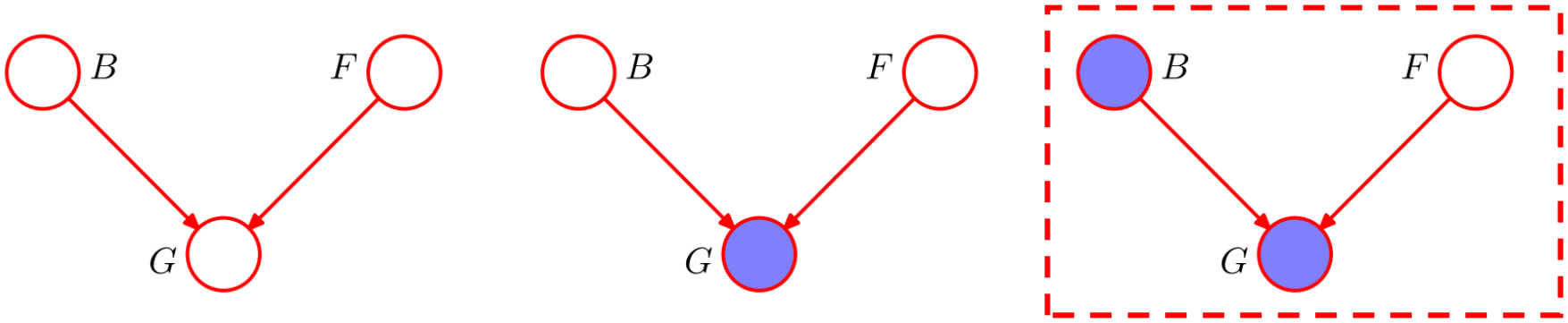
$$p(G=0) = \sum_{B\in\{0,1\}} \sum_{F\in\{0,1\}} p(G=0|B,F)p(B)p(F) = 0.315$$

$$p(G=0|F=0) = \sum_{B\in\{0,1\}} p(G=0|B,F=0)p(B) = 0.81$$

$$p(F=0|G=0) = \frac{p(G=0|F=0)p(F=0)}{p(G=0)} \simeq 0.257 > p(F=0) = 0.1$$

Thus observing that the gauge reads empty makes it more likely that the tank is indeed empty

Understanding head-to-head Case



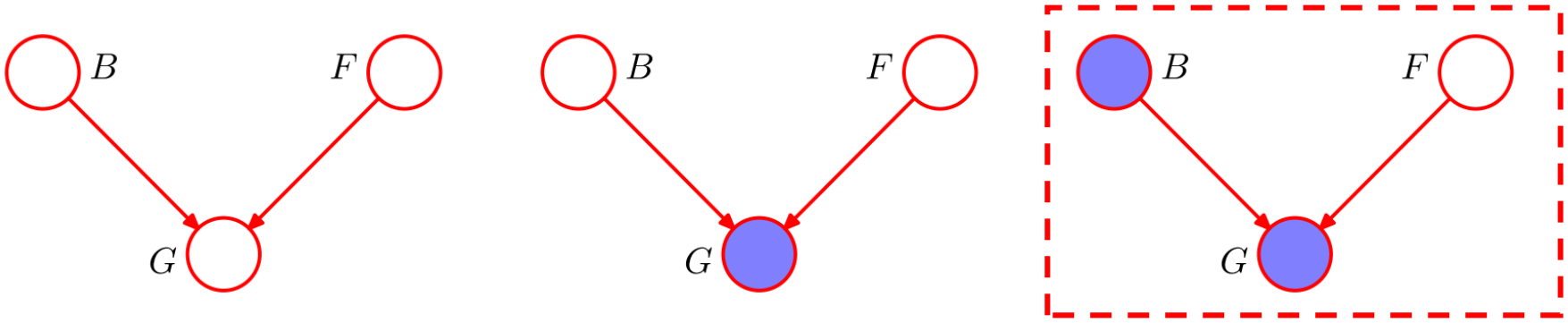
- If we observe the fuel gauge reads empty, i.e., *G*=0

$$p(F=0|G=0) = \frac{p(G=0|F=0)p(F=0)}{p(G=0)} \simeq 0.257 > p(F=0) = 0.1$$

$$p(F=0|G=0,B=0) = \frac{p(G=0|B=0,F=0)p(F=0)}{\sum_{F\in\{0,1\}} p(G=0|B=0,F)p(F)} \simeq 0.111 > p(F=0) = 0.1$$

- The probability that the tank is empty has decreased (from 0.257 to 0.111) as a result of the observation of the state of the battery
- **Explaining away**: the battery is flat explains away the observation that the fuel gauge reads empty

Understanding head-to-head Case



- If we observe the fuel gauge reads empty, i.e., *G*=0

$$p(F=0|G=0) = \frac{p(G=0|F=0)p(F=0)}{p(G=0)} \simeq 0.257 > p(F=0) = 0.1$$

$$p(F=0|G=0,B=0) = \frac{p(G=0|B=0,F=0)p(F=0)}{\sum_{F\in\{0,1\}} p(G=0|B=0,F)p(F)} \simeq 0.111 > p(F=0) = 0.1$$

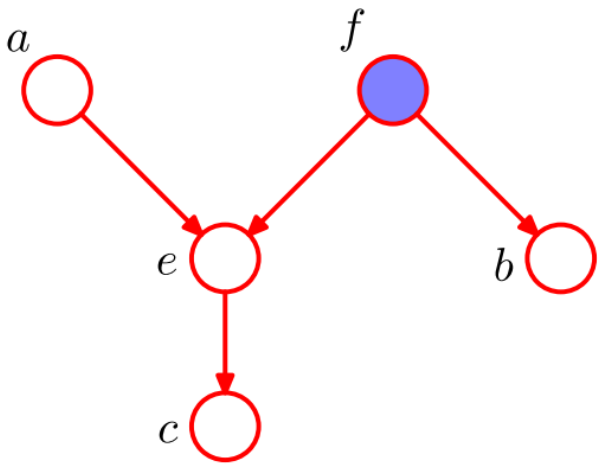
- Note that the probability $p(F=0|G=0,B=0)$ ~ 0.111 is greater than the prior probability $p(F=0)=0.1$ because the observation that the fuel gauge reads zero still provides some evidence in favor of an empty fuel tank.

D-separation

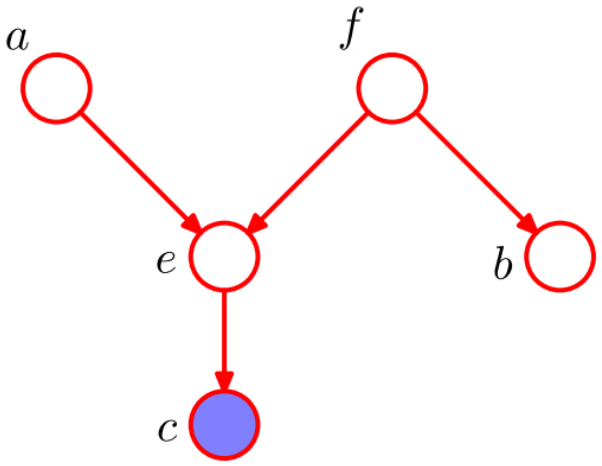
- Consider a general directed graph in which *A*, *B*, and *C* are arbitrary nonintersecting sets of nodes.
- Any such path is said to be blocked if it includes a node such that either
  a) the arrows on the path meet either head-to-tail or tail-to-tail at the node, and the node is in the set *C*, or
  b) the arrows meet head-to-head at the node, and neither the node, nor any of its descendants, is in the set *C*.
- If all paths are blocked, then *A* is said to be d-separated from *B* by *C*, and the joint distribution over all of the variables in the graph will satisfy

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

D-separation Illustration



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

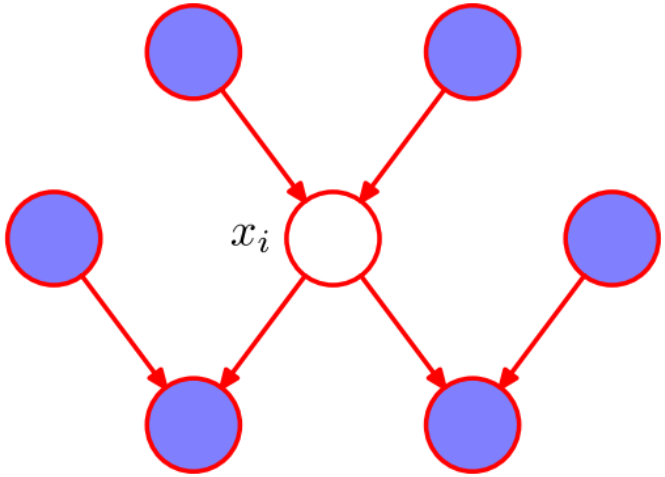


$a \not\perp\!\!\!\perp b \mid c$

- *A*, *B*, *C* satisfy $A \perp\!\!\!\perp B \mid C$ if
  a) 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
  b) the arrows meet head-to-head at the node, and neither the node, nor any of its descendants, is in the set *C*.

Markov Blanket in Bayesian Network

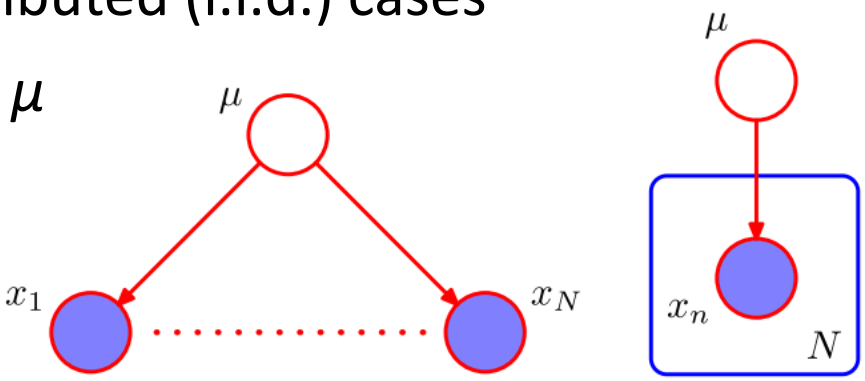
- The Markov blanket of a node x_i comprises the set of parents, children and co-parents of the children.
- It has the property that the conditional distribution of x_i, conditioned on all the remaining variables in the graph, is dependent only on the variables in the Markov blanket.



i.i.d. Cases

- Independent identically distributed (i.i.d.) cases
- Goal: given **x** observed, infer μ

$$p(\mu|D) \propto p(\mu)p(D|\mu)$$
$$= p(\mu)\prod_{i=1}^{N} p(x_i|\mu)$$



- If we integrate over μ, the observations are in general independent

$$p(D) = \int p(D|\mu)p(\mu)d\mu \neq \prod_{i=1}^{N} p(x_i)$$

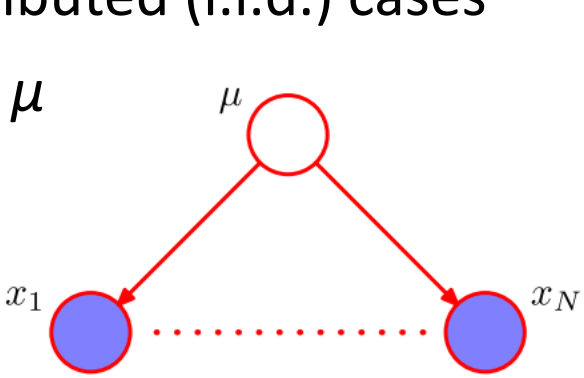
- We may say these data instances are jointly distributed.

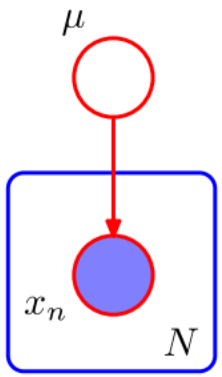
i.i.d. Cases

- Independent identically distributed (i.i.d.) cases
- Goal: given **x** observed, infer μ

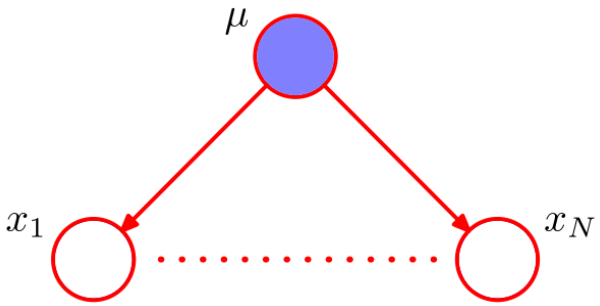
$$p(\mu|D) \propto p(\mu)p(D|\mu)$$

$$= p(\mu)\prod_{i=1}^{N} p(x_i|\mu)$$





- If we condition on μ and consider the joint distribution of the observations
  - A unique path from x_i to x_j
  - The path is tail-to-tail w.r.t. μ
  - Thus the path is blocked given μ observed



- Data instances are independent conditioned on the model

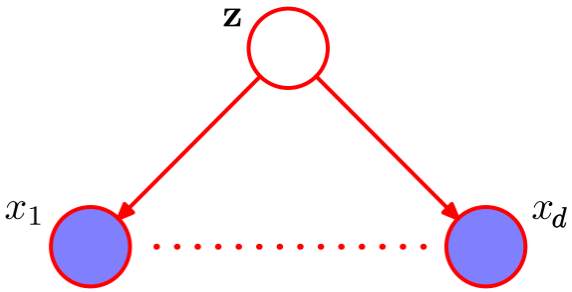
Naive Bayes Classification Model

- *K*-class classification
- The classes **z** are represented in 1-of-*K* encoding vector
  - Multinomial prior $p(\mathbf{z}|\boldsymbol{\mu})$
  - μ_k is the prior probability of class C_k
- Each data instance (e.g. a piece of text) is represented by a *d*-dimensional vector **x** (each dimension as a word)
  - The generation of **x** conditioned on **z** is $p(\mathbf{x}|\mathbf{z})$
  - The principle of naive Bayes is the conditional independence of x_j's

$$p(\mathbf{x}|\mathbf{z}) = \prod_{j=1}^{d} p(x_j|\mathbf{z})$$

- Class label inference

$$p(\mathbf{z}|\mathbf{x}) \propto p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|\boldsymbol{\mu})$$



Multinomial Naive Bayes

- Each class *y* is modeled as a histogram of words
  - *y*=*y*(**z**) is the index of 1 in **z**

$$\theta_y = (\theta_{y1}, \theta_{y2}, \ldots, \theta_{yn})$$

- The parameter ϑ_y is estimated as

$$\hat{\theta}_{yi} = \frac{N_{yi} + \alpha}{N_y + \alpha d}$$

  - N_{yi} is the count of word *i* appears in any instance of class *y* in the training set
  - N_y is the total count of all words for class *y*

$$p(\mathbf{z}|\mathbf{x}) \propto p(\mathbf{z}|\boldsymbol{\mu}) p(\mathbf{x}|\mathbf{z}) = p(\mathbf{z}|\boldsymbol{\mu}) \prod_{i=1}^{d} \theta_{y(\mathbf{z})i}$$

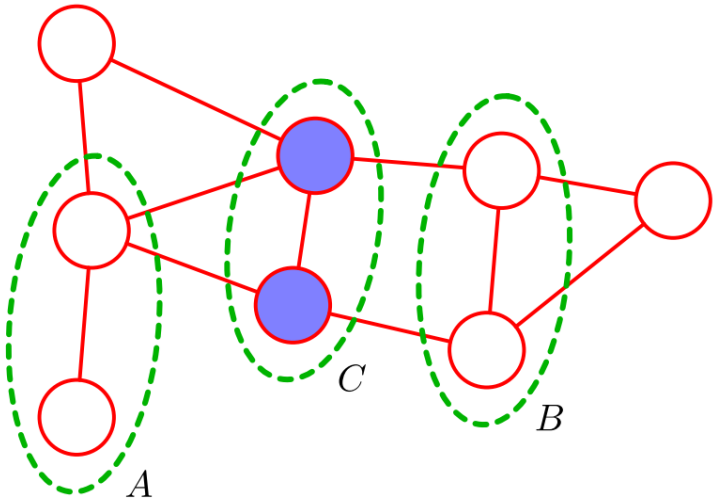
Content of This Lecture

- Introduction
- Bayes Networks (Directed Graphs)
- Markov Networks (Undirected Graphs)
- Inferences in Graphical Models

Markov Random Fields

- Undirected network, also called Markov network
- Compared to Bayes Network, it is more straightforward to ascertain the conditional independence in Markov network:
  - If all paths linking any nodes in A and B is blocked by the nodes in C, then

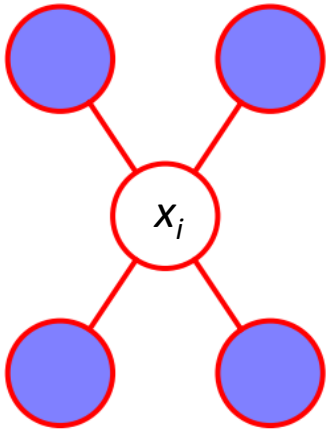
$$A \perp\!\!\!\perp B \mid C$$



Markov Blanket in Markov Network

- For an undirected graph, the Markov blanket of a node x_i consists of the set of neighboring nodes.

- It has the property that the conditional distribution of x_i , conditioned on all the remaining variables in the graph, is dependent only on the variables in the Markov blanket.



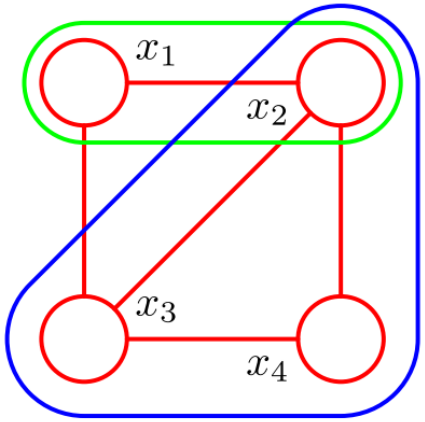
Conditional Independence in Markov Network

- Consider two nodes x_i and x_j that are not connected by a link, then these variables must be conditionally independent given all other nodes in the graph

$$p(x_i, x_j|\mathbf{x}_{\setminus\{i,j\}}) = p(x_i|\mathbf{x}_{\setminus\{i,j\}})p(x_j|\mathbf{x}_{\setminus\{i,j\}})$$

- The factorization of the joint distribution must therefore be such that x_i and x_j do not appear in the same factor

An Example of Cliques in Markov Networks



- **Clique**: a subset of the nodes in a graph in which the nodes are fully connected
- A Markov network of four nodes $\{x_1, x_2, x_3, x_4\}$
  - 5 two-node cliques $\{x_1, x_2\}$, $\{x_2, x_3\}$, $\{x_3, x_4\}$, $\{x_2, x_4\}$, $\{x_1, x_3\}$
  - 2 maximal cliques $\{x_1, x_2, x_3\}$, $\{x_2, x_3, x_4\}$

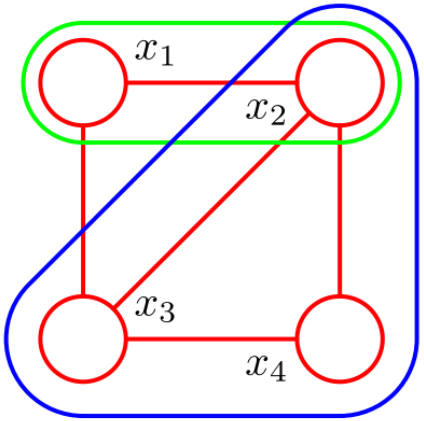
  - Note that $\{x_1, x_2, x_3, x_4\}$ is not a clique

Joint Distribution Decomposition

- Define the factors in the decomposition of the joint distribution to be functions of the variables in the cliques
- Let *C* denote a clique and the set of variables in it as $\mathbf{x}_C$

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

Potential function



$$p(\mathbf{x}) = \frac{1}{Z} \psi_{\{2,3,4\}}(x_2, x_3, x_4) \psi_{\{1,2,3\}}(x_1, x_2, x_3)$$

- The quantity *Z*, also called the partition function, is a normalization factor

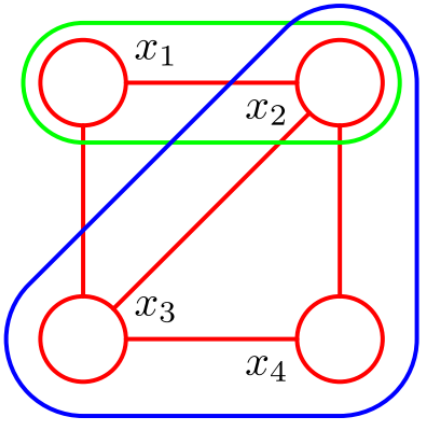
$$Z = \sum_{\mathbf{x}} \prod_C \psi_C(\mathbf{x}_C)$$

Joint Distribution Decomposition

- Define the factors in the decomposition of the joint distribution to be functions of the variables in the cliques
- Let *C* denote a clique and the set of variables in it as $\mathbf{x}_C$

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

Potential function



- Potential function satisfies $\psi_C(\mathbf{x}_C) \geq 0$ to ensure the probability is non-negative
- Potential functions can be defined with domain knowledge

Energy Function for Potential

- If we define the potential function to be strictly positive, i.e.,

$$\psi_C(\mathbf{x}_C) > 0$$

- It is convenient to express the potential functions as exponentials

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

- $E(\mathbf{x}_C)$ is called an energy function
- With such an exponential representation, the distribution $p(\mathbf{x})$ is called Boltzmann distribution

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

Boltzmann Distribution

- Boltzmann distribution is a probability distribution, probability measure, or frequency distribution of particles in a system over various possible states

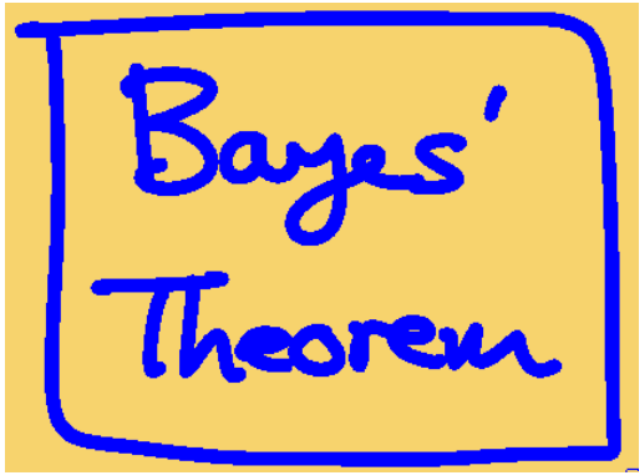
$$p(s) = \frac{e^{-E(s)/kT}}{\sum_{s'} e^{-E(s')/kT}}$$

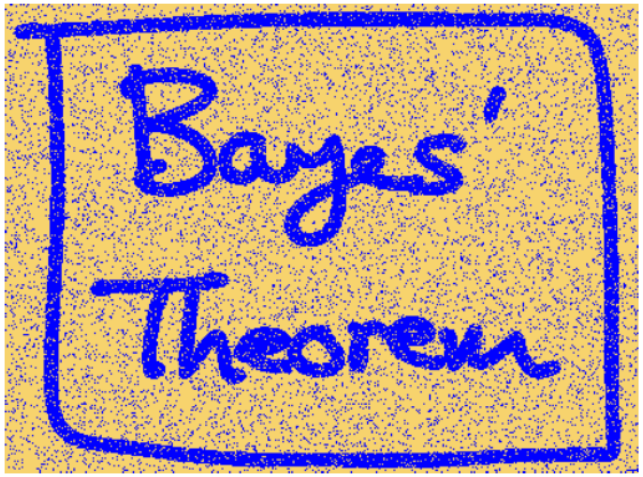
  - *s* denotes a particular state
  - *E*(*s*) is the state energy
  - $k = 1.381 \times 10^{-23}$ J/K is Boltzmann constant
  - *T* is thermodynamic temperature

- Low-energy state is more stable, i.e., with higher probability

MRF Application Example: Image Denoising

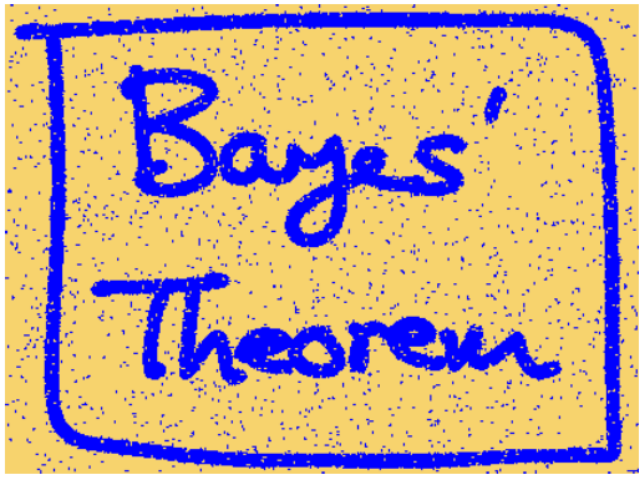
Original Image

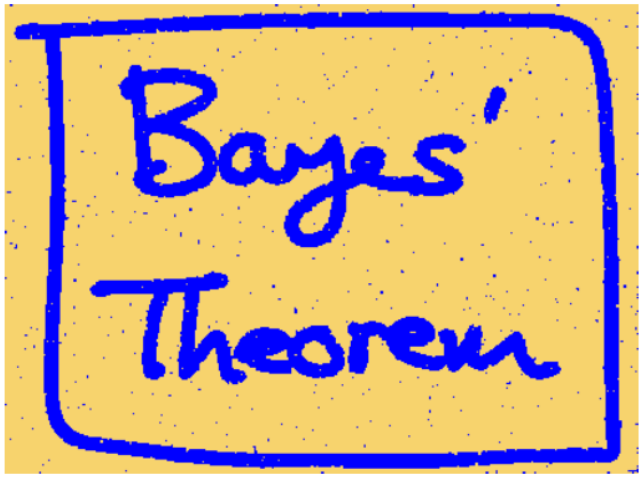




Corrupted Image

Denoised By ICM





Denoised By Graph-Cut

MRF Application Example: Image Denoising

- Observed noisy image is described by an array of binary pixel values

$$y_i \in \{-1, +1\},\ i = 1, \ldots, d$$ runs over all pixels

- Suppose the ground-truth noise-free image

$$x_i \in \{-1, +1\},\ i = 1, \ldots, d$$

- Noise generation: randomly flipping the sign of pixels with some small probability, e.g., 10%

- Model assumptions
  - There is a strong correlation between x_i and y_i
  - There is a strong correlation between neighboring pixels x_i and x_j

MRF for Image Denoising

- Model assumptions
  - There is a strong correlation between x_i and y_i
  - There is a strong correlation between neighboring pixels x_i and x_j
- Model
  - For the cliques $\{x_i, y_i\}$

$$E(\{x_i, y_i\}) = -\eta x_i y_i$$

  - For the cliques $\{x_i, x_j\}$

$$E(\{x_i, x_j\}) = -\beta x_i x_j$$

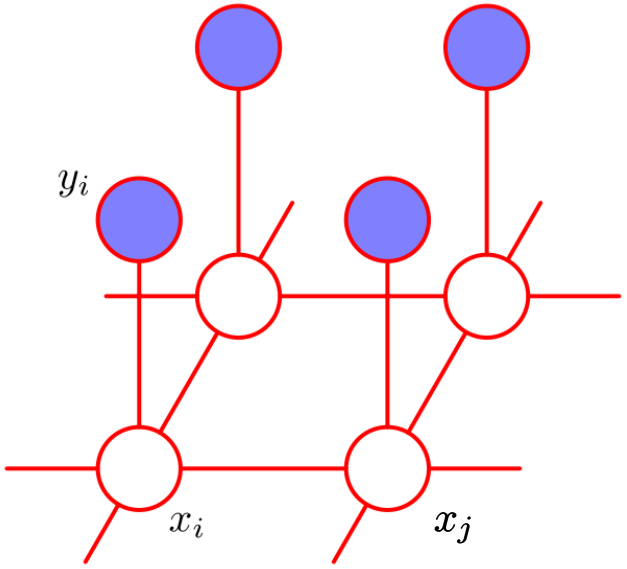
  - Moreover, for each $\{x_i\}$

$$E(\{x_i\}) = h x_i$$

  - Complete energy function

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

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

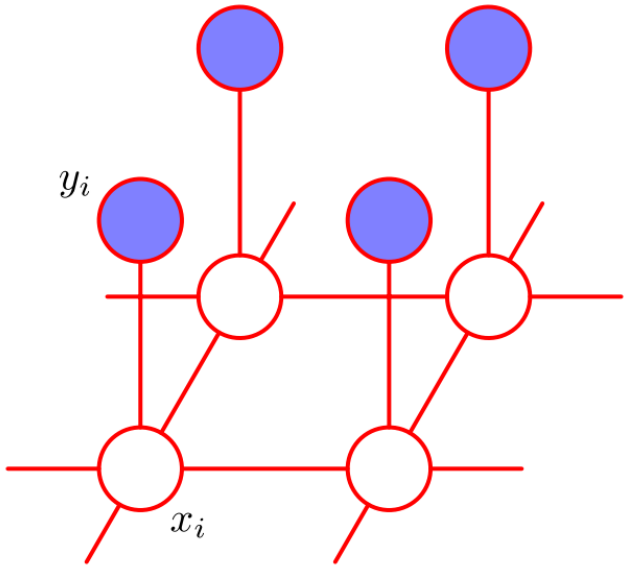


Solution: Iterated Conditional Modes (ICM)

- Objective

$$\max_{\mathbf{x}} p(\mathbf{x}|\mathbf{y}) = \max_{\mathbf{x}} p(\mathbf{x}, \mathbf{y})$$ Given **y** observed

- Idea: coordinate-wise gradient ascent
  - For each node x_j, check which one of x_j=+1 or -1 leads to lower $E(\mathbf{x},\mathbf{y})$
  - Implementation β=1.0, η=2.1 and h=0



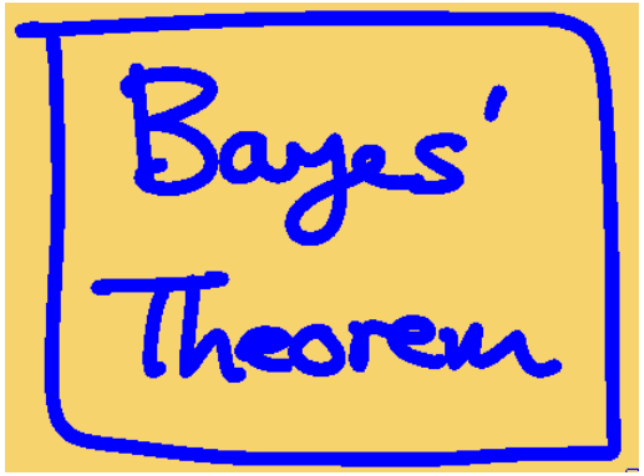
- Energy function

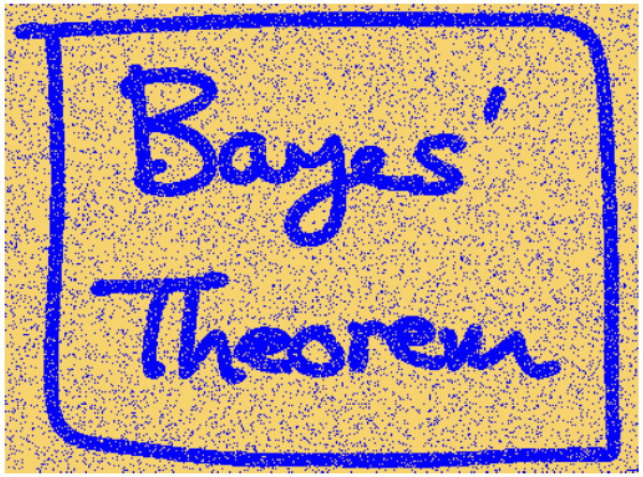
$$E(\mathbf{x}, \mathbf{y}) = h \sum_i x_i - \beta \sum_{i,j} x_i x_j - \eta \sum_i x_i y_i$$

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

MRF Application Example: Image Denoising

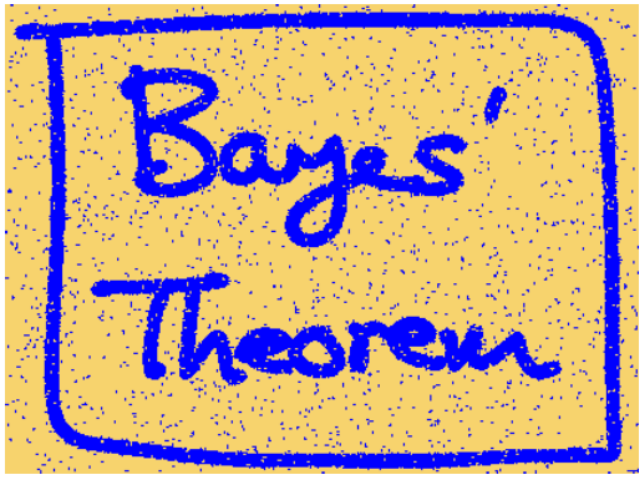
Original Image

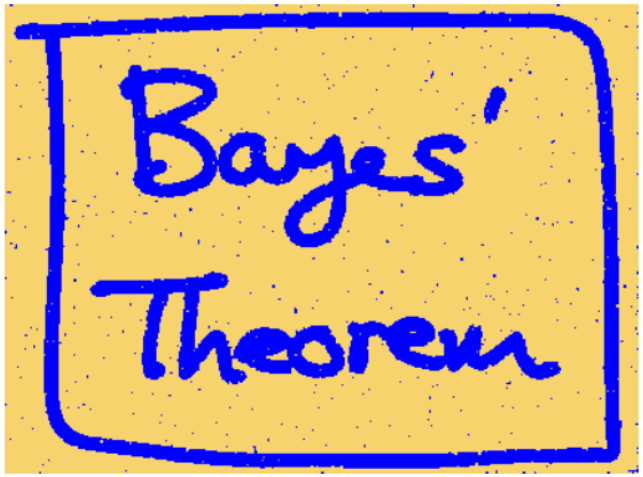




Corrupted Image

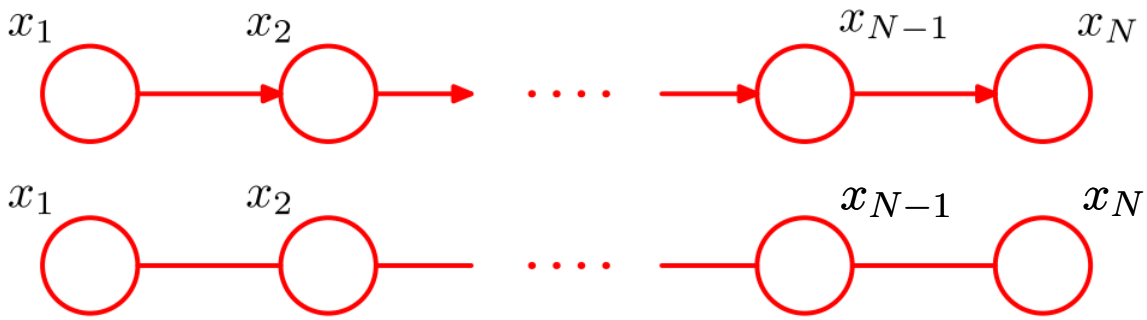
Denoised By ICM





Denoised By Graph-Cut

Directed Graphs vs. Undirected Graphs



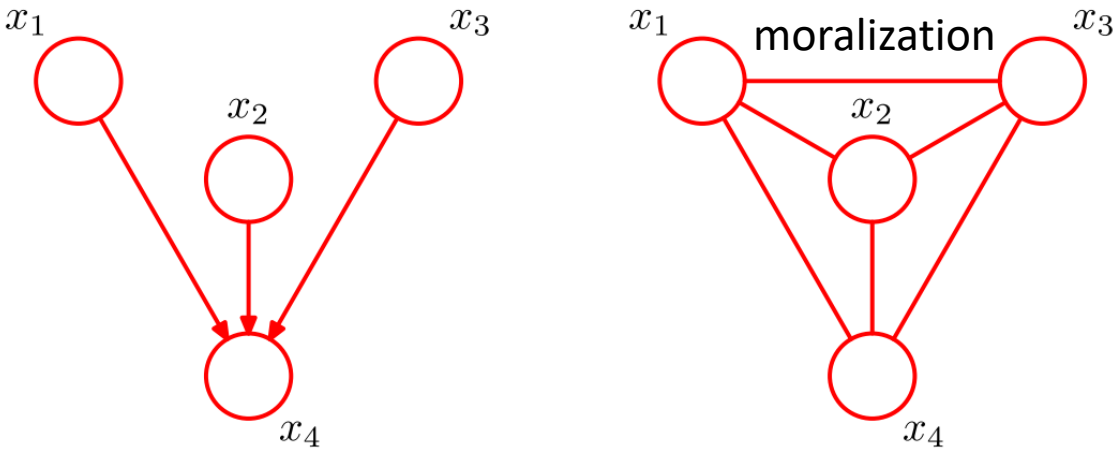
- Convert a directed graph to an undirected graph
  - Directed graphical model

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

  - Undirected graphical model

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

Directed Graphs vs. Undirected Graphs



- Convert a directed graph to an undirected graph
  - Directed graphical model

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

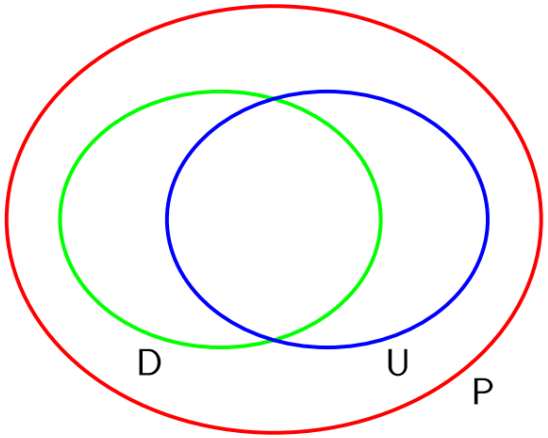
  - Undirected graphical model

$$p(\mathbf{x}) = \frac{1}{Z}\psi_{1,2,3,4}(x_1, x_2, x_3, x_4)$$

Moralization: marrying the parents

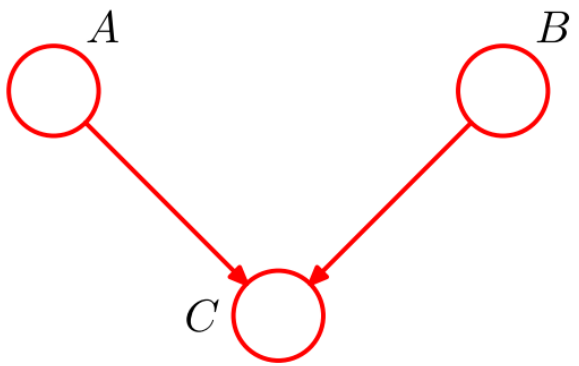
Directed Graphs vs. Undirected Graphs

- Although each directed graph can be converted into an undirected graph
  - One brute-force solution is to use a fully connected undirected graph
- Directed and undirected graphs can express different conditional independence properties



- P: all possible distributions
- D/U: distributions that can be represented by directed/undirected graphs

Directed Graphs vs. Undirected Graphs

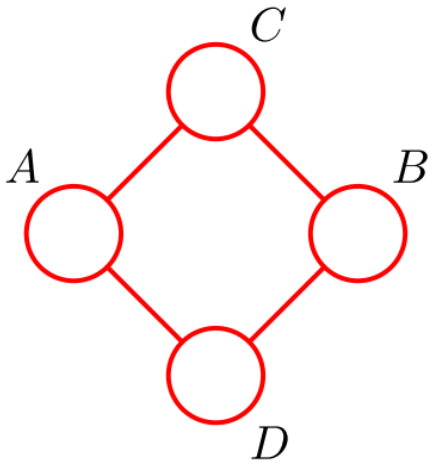


A directed graph whose conditional independence properties cannot be expressed using an undirected graph over the same three variables

- Directed graph

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

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



An undirected graph whose conditional independence properties cannot be expressed in terms of a directed graph over the same variables

- Undirected graph

$$A \not\perp\!\!\!\perp B \mid \emptyset,\ C \perp\!\!\!\perp D \mid A \cup B$$

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

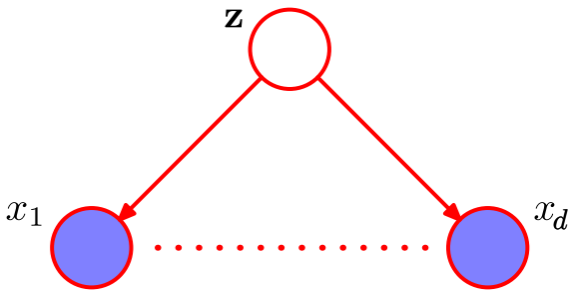
Content of This Lecture

- Introduction
- Bayes Networks (Directed Graphs)
- Markov Networks (Undirected Graphs)
- Inferences in Graphical Models

Variable Inference and Parameter Estimation

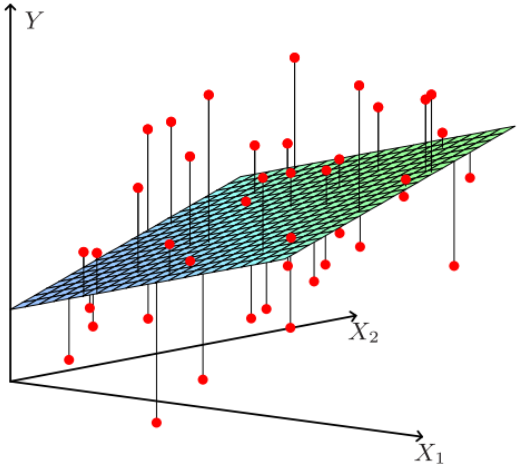
- Random variable inference
  - Infer the posterior distribution of random variables given their prior and the observed data

$$p(\mathbf{z}|\mathbf{x}) \propto p(\mathbf{z}|\boldsymbol{\mu})p(\mathbf{x}|\mathbf{z})$$



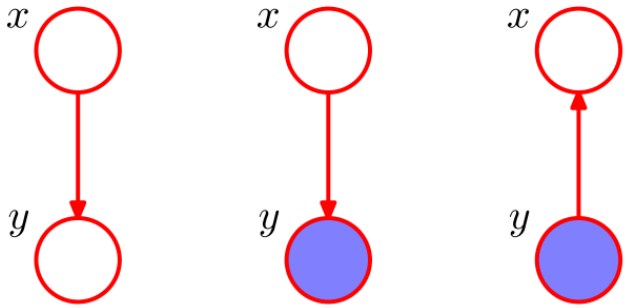
- Parameter estimation
  - Find the optimal parameter value for an objective, e.g., minimum loss or maximum likelihood

$$\hat{\theta} = \arg\min_{\theta} \mathcal{L}(D;\theta)$$



Tzikas, Dimitris G., Aristidis C. Likas, and Nikolaos P. Galatsanos. "The variational approximation for Bayesian inference." *IEEE Signal Processing Magazine* 25.6 (2008): 131-146.

A Basic Case for Inference



- Joint distribution of two random variables *x* and *y*

$$p(x, y) = p(x)p(y|x)$$

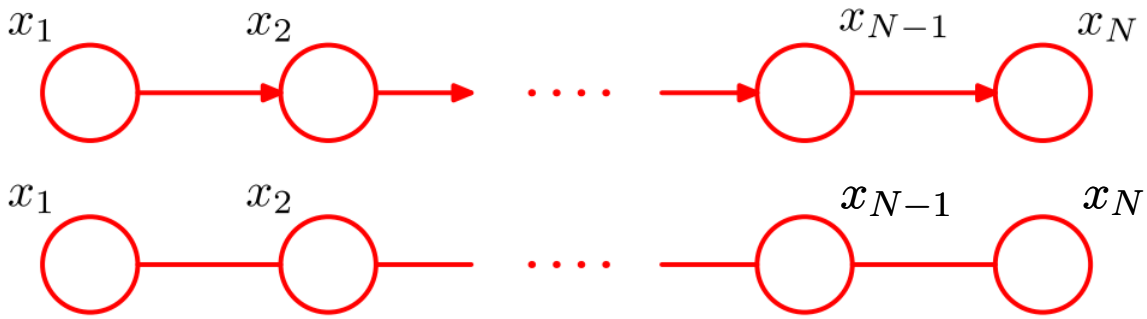
- The marginal distribution of *y*

$$p(y) = \sum_{x'} p(x')p(y|x')$$

- The inverse conditional distribution

$$p(x|y) = \frac{p(x)p(y|x)}{p(y)}$$

Inference on a Chain



- Joint distribution

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

- Discrete variable setting
  - *N* nodes represent discrete variables each having *K* states
  - Each potential function $\psi_{n-1,n}(x_{n-1}, x_n)$ comprises a $K \times K$ table
  - Thus the joint distribution has $(N\text{-}1)K^2$ parameters

Calculate the Marginal Distribution

- Inference problem of finding the marginal distribution $p(x_n)$

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

- A brute-force solution
  - Sum up K^{N-1} values, introducing exponential complexity $O(K^{N-1})$
- An efficient dynamic programming solution
  - Exploit the conditional independence properties

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

general sum-product algorithm $ab + ac = a(b + c)$

DP for Calculating Marginal Distribution

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

- Conditional independence
  - The potential $\psi_{N-1,N}(x_{N-1}, x_N)$ is the only one that depends on x_N

$$\begin{aligned}
p(x_n) &= \sum_{x_1}\cdots\sum_{x_{n-1}}\sum_{x_{n+1}}\cdots\sum_{x_N} p(\mathbf{x}) \\
&= \frac{1}{Z}\sum_{x_1}\cdots\sum_{x_{n-1}}\sum_{x_{n+1}}\cdots\sum_{x_N}\psi_{1,2}(x_1, x_2)\cdots\psi_{N-1,N}(x_{N-1}, x_N) \\
&= \frac{1}{Z}\sum_{x_1}\cdots\sum_{x_{n-1}}\sum_{x_{n+1}}\cdots\sum_{x_{N-1}}\psi_{1,2}(x_1, x_2)\cdots\psi_{N-2,N-1}(x_{N-2}, x_{N-1})\sum_{x_N}\psi_{N-1,N}(x_{N-1}, x_N)
\end{aligned}$$

general sum-product algorithm $ab + ac = a(b + c)$

DP for Calculating Marginal Distribution

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

- Conditional independence
  - The potential $\psi_{1,2}(x_1, x_2)$ is the only one the depends on x_1

$$\begin{aligned} p(x_n) &= \sum_{x_1}\cdots\sum_{x_{n-1}}\sum_{x_{n+1}}\cdots\sum_{x_N} p(\mathbf{x}) \\ &= \frac{1}{Z}\sum_{x_n}\cdots\sum_{x_{n+1}}\sum_{x_{n-1}}\cdots\sum_{x_1}\psi_{N-1,N}(x_{N-1}, x_N)\cdots\psi_{1,2}(x_1, x_2) \\ &= \frac{1}{Z}\sum_{x_n}\cdots\sum_{x_{n+1}}\sum_{x_{n-1}}\cdots\sum_{x_2}\psi_{N-1,N}(x_{N-1}, x_N)\cdots\psi_{1,2}(x_1, x_2)\sum_{x_1}\psi_{1,2}(x_1, x_2) \end{aligned}$$

DP for Calculating Marginal Distribution

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

- Conditional independence
  - The potential $\psi_{1,2}(x_1, x_2)$ is the only one that depends on x_1

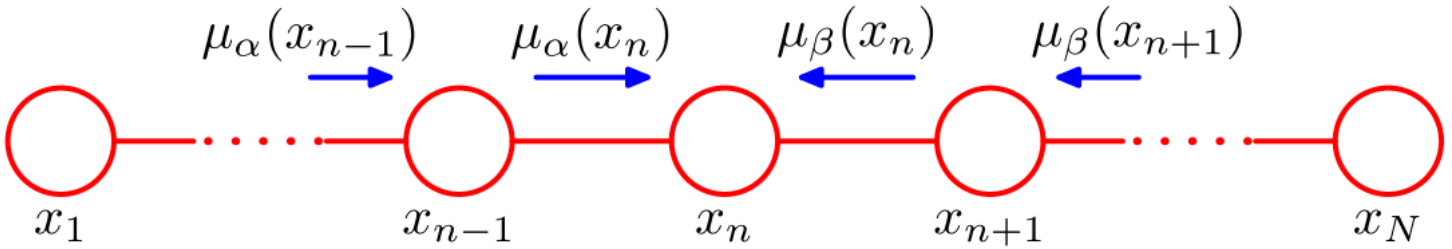
$$p(x_n) = \frac{1}{Z}\underbrace{\left[\sum_{x_{n-1}}\psi_{n-1,n}(x_{n-1}, x_n)\cdots\left[\sum_{x_2}\psi_{2,3}(x_2, x_3)\left[\sum_{x_1}\psi_{1,2}(x_1, x_2)\right]\right]\cdots\right]}_{\mu_\alpha(x_n)}$$

$$\underbrace{\left[\sum_{x_{n+1}}\psi_{n,n+1}(x_n, x_{n+1})\cdots\left[\sum_{x_N}\psi_{N-1,N}(x_{N-1}, x_N)\right]\cdots\right]}_{\mu_\beta(x_n)}$$

Complexity $O(NK^2)$

Interpretation: Message Passing

- Passing of local messages around on the graph



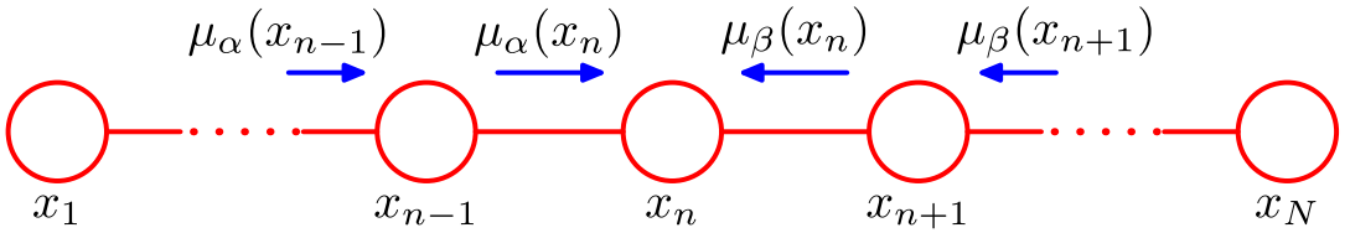
$$p(x_n) = \frac{1}{Z}\underbrace{\left[\sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \cdots \left[\sum_{x_2} \psi_{2,3}(x_2, x_3)\left[\sum_{x_1} \psi_{1,2}(x_1, x_2)\right]\right] \cdots\right]}_{\mu_\alpha(x_n)}$$

$$\underbrace{\left[\sum_{x_{n+1}} \psi_{n,n+1}(x_n, x_{n+1}) \cdots \left[\sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N)\right] \cdots\right]}_{\mu_\beta(x_n)}$$

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

Interpretation: Message Passing

- Passing of local messages around on the graph



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

- Message passes recursively

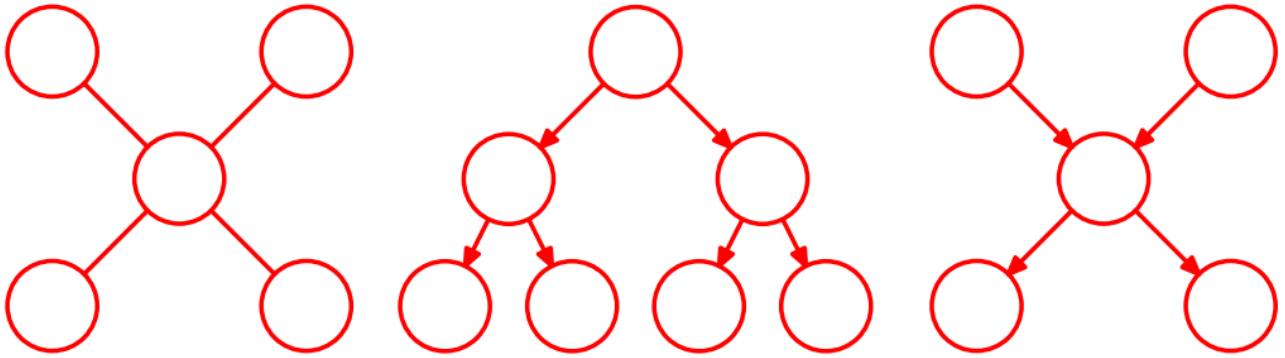
$$\mu_\alpha(x_n) = \sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n)\Big[\sum_{x_{n-2}} \psi_{n-2,n-1}(x_{n-2}, x_{n-1}) \sum_{x_{n-3}} \cdots\Big]$$

$$= \sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n)\mu_\alpha(x_{n-1})$$

- With the start

$$\mu_\alpha(x_2) = \sum_{x_1} \psi_{1,2}(x_1, x_2)$$

Tree Graphical Models



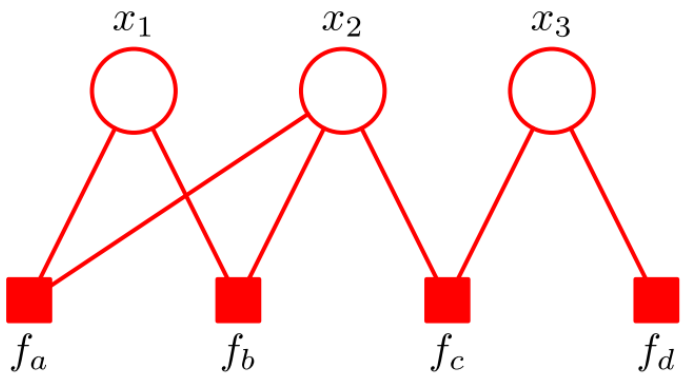
Undirected tree Directed tree Directed polytree

- **Undirected graph tree**: graph in which there is one, and only one, path between any pair of nodes
- **Directed graph tree**: there is a single node, called the root, which has no parents, and all other nodes have one parent
  - Thus the moralization step will not add any links
- **Polytree**: nodes in a directed graph that have more than one parent, but there is still only one path (ignoring the direction of the arrows) between any two nodes
- Before introducing inference algorithm, let's discuss a general form: factor graph

Factor Graphs

- Observations: Both directed and undirected graphs allow a global function of several variables to be expressed as a product of factors over subsets of those variables
- Factor graphs make this decomposition explicit by introducing additional nodes for the factors

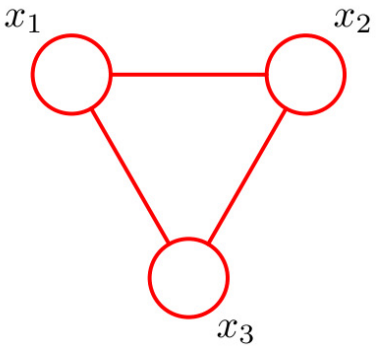
$$p(\mathbf{x}) = \prod_s f_s(\mathbf{x}_s)$$



Factor graphs are said to be bipartite

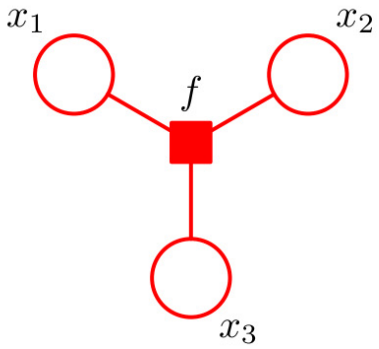
Factor Graphs

- Undirected graphs to factor graphs



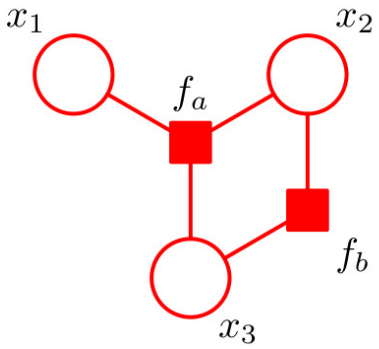
An undirected graph with a single clique potential

$$\psi(x_1, x_2, x_3)$$



A factor graph representing the same distribution with factor

$$f(x_1, x_2, x_3) = \psi(x_1, x_2, x_3)$$

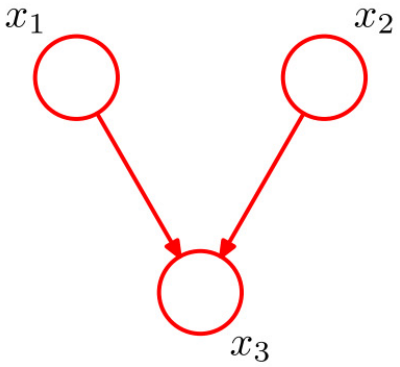


Another factor graph representing the same distribution

$$f_a(x_1, x_2, x_3) f_b(x_1, x_2) = \psi(x_1, x_2, x_3)$$

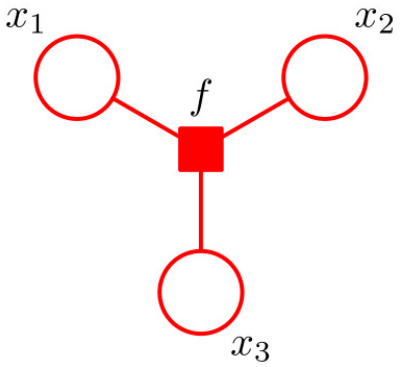
Factor Graphs

- Directed graphs to factor graphs



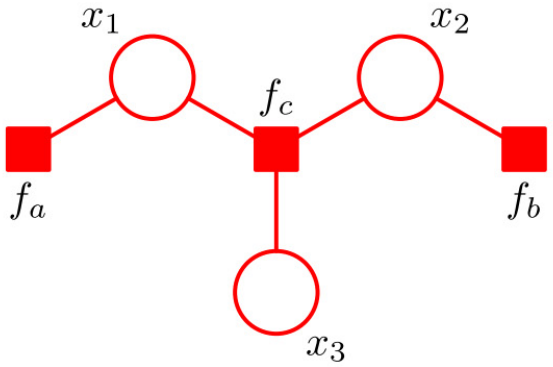
A directed graph with factorization

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



A factor graph representing the same distribution with factor

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



Another factor graph representing the same distribution

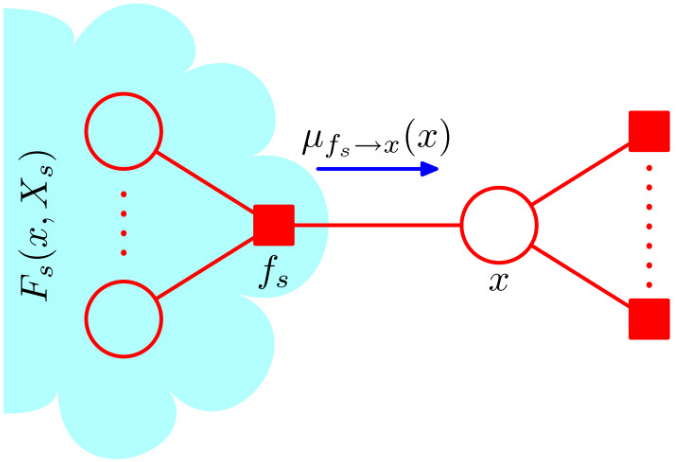
$$f_a(x_1) = p(x_1)$$
$$f_b(x_2) = p(x_2)$$
$$f_c(x_1,x_2,x_3) = p(x_3|x_1,x_2)$$

Inference on a Tree: Sum-Product

- Consider the marginal of a particular variable *x* on the factor graph tree

$$p(x) = \sum_{\mathbf{x}\setminus x} p(\mathbf{x}) \qquad\qquad p(x) = \prod_{s\in \mathrm{ne}(x)} F_s(x, X_s)$$

  - ne(*x*): set of neighbor factors of *x*
  - X_s: set of all variables in the subtree connected to the variable node *x* via the factor node
  - $F_s(x, X_s)$: the product of all the factors in the group associated with factor f_s



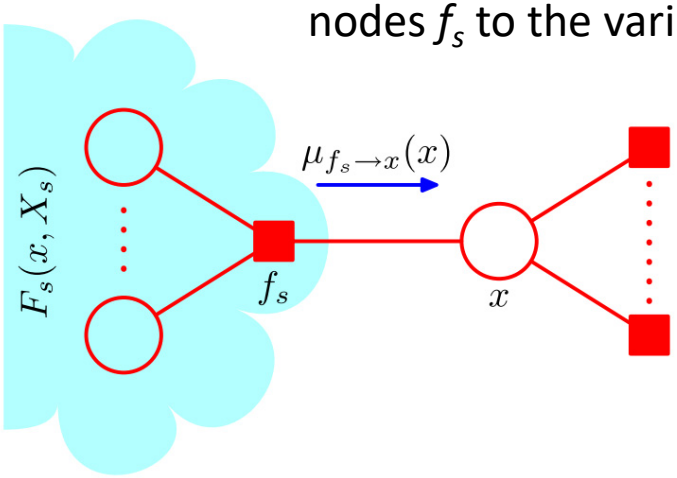
Message Passing

- Consider the marginal of a particular variable *x* on the factor graph tree

$$p(x) = \prod_{s \in \mathrm{ne}(x)} \left[\sum_{X_s} F_s(x, X_s) \right]$$

$$\equiv \prod_{s \in \mathrm{ne}(x)} \mu_{f_s \to x}(x)$$

messages from the factor nodes f_s to the variable node *x*



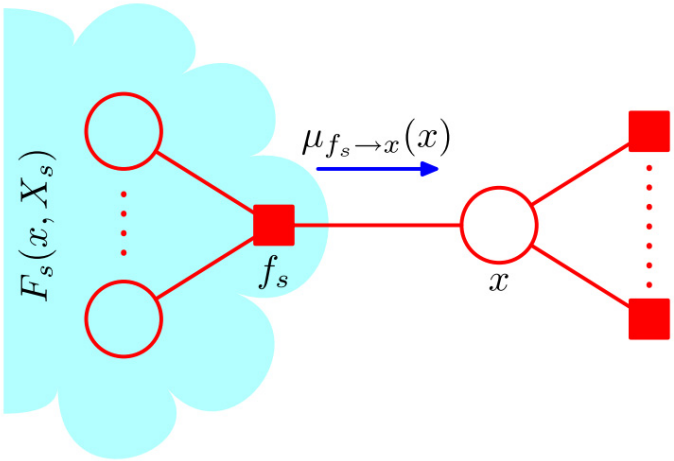
Message Passing Iteration

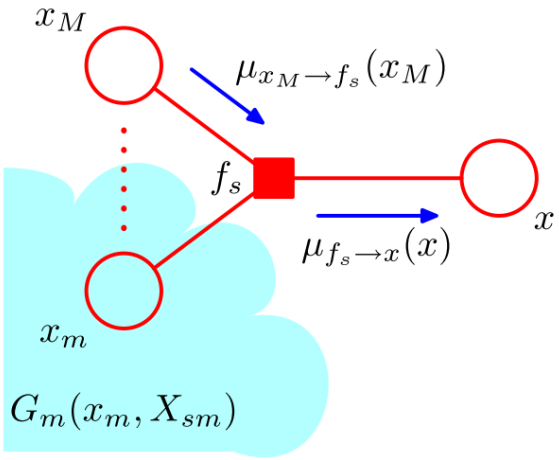
- Denote $\{x, x_1, \ldots, x_M\}$ as the set of variables on which the factor f_s depends, then

$$F_s(x, X_s) = f_s(x, x_1, \ldots, x_M) G_1(x_1, X_{s1}) \cdots G_M(x_M, X_{sM})$$

$$\mu_{f_s \to x}(x) = \sum_{x_1} \cdots \sum_{x_M} f_s(x, x_1, \ldots, x_M) \prod_{m \in \mathrm{ne}(f_s) \setminus x} \left[\sum_{X_{sm}} G_m(x_m, X_{sm}) \right]$$

$$= \sum_{x_1} \cdots \sum_{x_M} f_s(x, x_1, \ldots, x_M) \prod_{m \in \mathrm{ne}(f_s) \setminus x} \mu_{x_m \to f_s}(x_m)$$



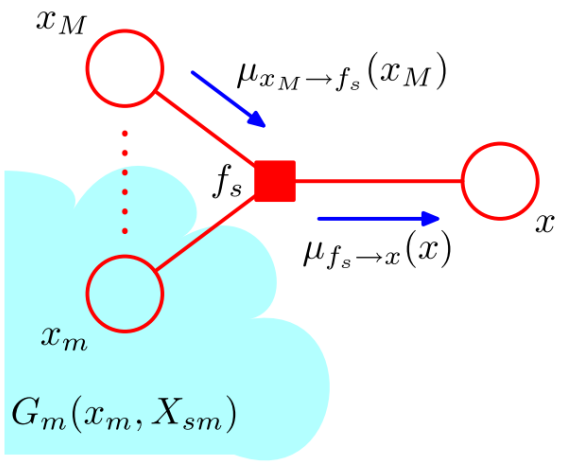


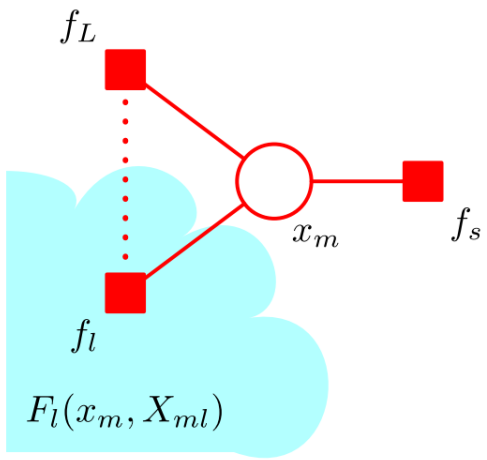
Message Passing Iteration

- Denote $\{x, x_1, \ldots, x_M\}$ as the set of variables on which the factor f_s depends, then

$$F_s(x, X_s) = f_s(x, x_1, \ldots, x_M) G_1(x_1, X_{s1}) \cdots G_M(x_M, X_{sM})$$

$$G_m(x_m, X_{sm}) = \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} F_l(x_m, X_{ml})$$





Two Types of Messages

- Messages from factor nodes to variable nodes

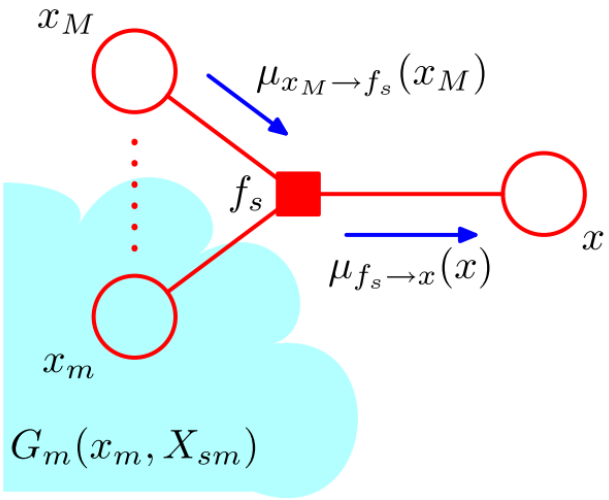
$$\mu_{f_s \to x}(x) = \sum_{X_s} F_s(x, X_s)$$

$$F_s(x, X_s) = f_s(x, x_1, \ldots, x_M) G_1(x_1, X_{s1}) \cdots G_M(x_M, X_{sM})$$

- Messages from variable nodes to factor nodes

$$\mu_{x_m \to f_s}(x_m) = \sum_{X_{sm}} G_m(x_m, X_{sm})$$

$$G_m(x_m, X_{sm}) = \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} F_l(x_m, X_{ml})$$



Two Types of Messages

- Relationships of two types of messages

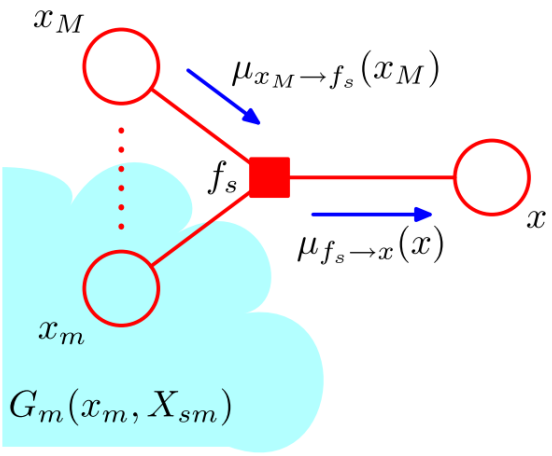
$$\mu_{x_m \to f_s}(x_m) = \sum_{X_{sm}} G_m(x_m, X_{sm})$$

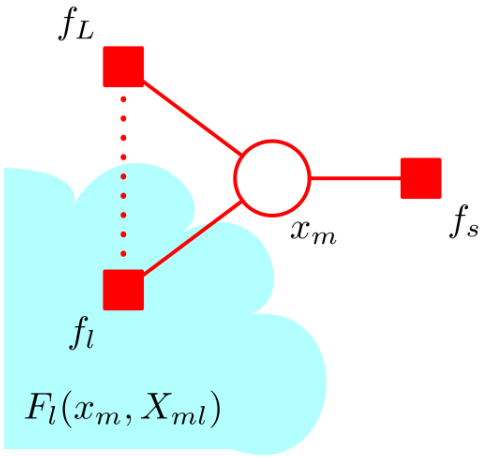
$$= \sum_{X_{sm}} \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} F_l(x_m, X_{ml})$$

(Tree structure)

$$= \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} \left[\sum_{X_{ml}} F_l(x_m, X_{ml}) \right]$$

$$= \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} \mu_{f_l \to x_m}(x_m)$$





Start of Recursion

$$\mu_{x \to f}(x) = 1 \qquad \mu_{f \to x}(x) = f(x)$$

- Messages from variable nodes to factor nodes

$$\mu_{x_m \to f_s}(x_m) = \sum_{X_{sm}} G_m(x_m, X_{sm})$$

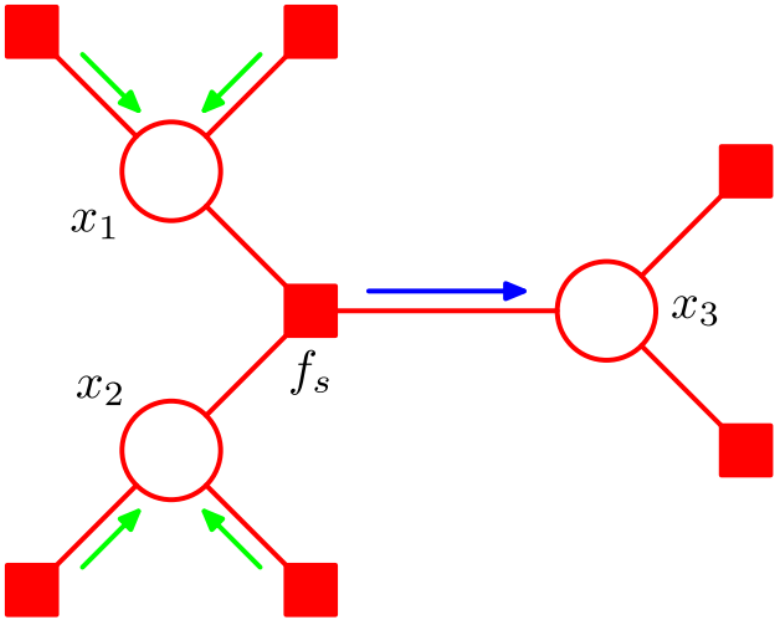
$$G_m(x_m, X_{sm}) = \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} F_l(x_m, X_{ml})$$

- Messages from factor nodes to variable nodes

$$\mu_{f_s \to x}(x) = \sum_{X_s} F_s(x, X_s)$$

$$F_s(x, X_s) = f_s(x, x_1, \ldots, x_M) G_1(x_1, X_{s1}) \cdots G_M(x_M, X_{sM})$$

Marginal of Variables of a Factor

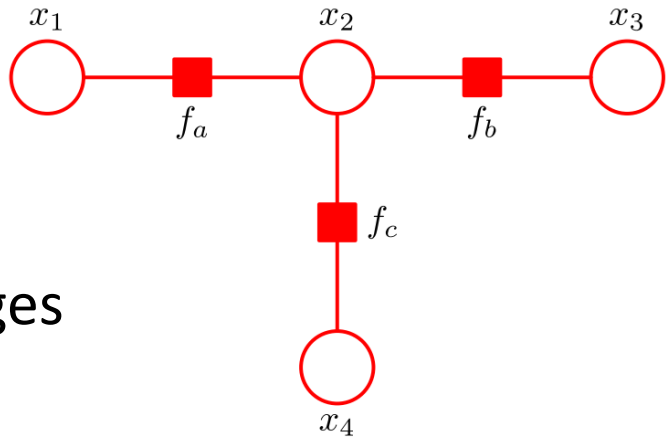


$$p(\mathbf{x}_s) = f_s(\mathbf{x}_s) \prod_{i \in \mathrm{ne}(f_s)} \mu_{x_i \to f_s}(x_i)$$

An Example for Practice

- Unnormalized joint distribution

$$\tilde{p}(\mathbf{x}) = f_a(x_1, x_2) f_b(x_2, x_3) f_c(x_2, x_4)$$



- Designate node x_3 as the root, messages

$$\mu_{x_1 \to f_a}(x_1) = 1$$

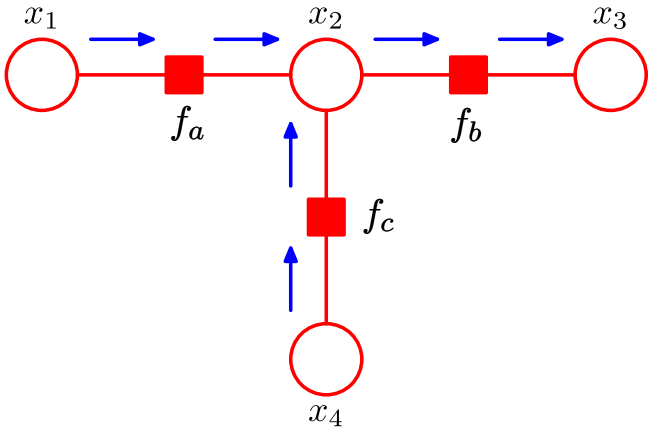
$$\mu_{f_a \to x_2}(x_2) = \sum_{x_1} f_a(x_1, x_2)$$

$$\mu_{x_4 \to f_c}(x_4) = 1$$

$$\mu_{f_c \to x_2}(x_2) = \sum_{x_4} f_c(x_2, x_4)$$

$$\mu_{x_2 \to f_b}(x_2) = \mu_{f_a \to x_2}(x_2) \mu_{f_c \to x_2}(x_2)$$

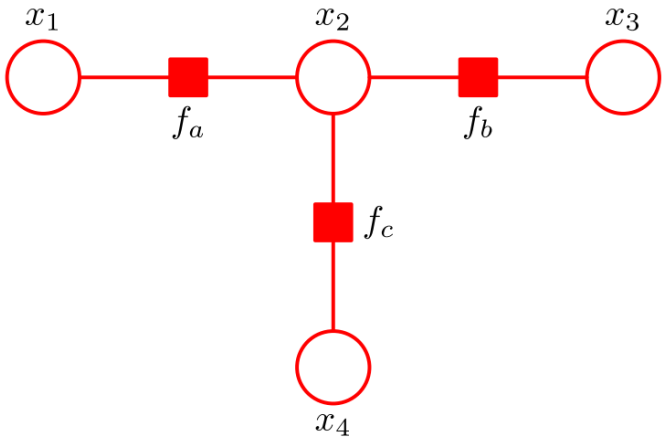
$$\mu_{f_b \to x_3}(x_3) = \sum_{x_2} f_b(x_2, x_3) \mu_{x_2 \to f_b}$$



An Example for Practice

- Unnormalized joint distribution

$$\tilde{p}(\mathbf{x}) = f_a(x_1, x_2) f_b(x_2, x_3) f_c(x_2, x_4)$$



- Messages from the root node out to the leaf nodes

$$\mu_{x_3 \to f_b}(x_3) = 1$$

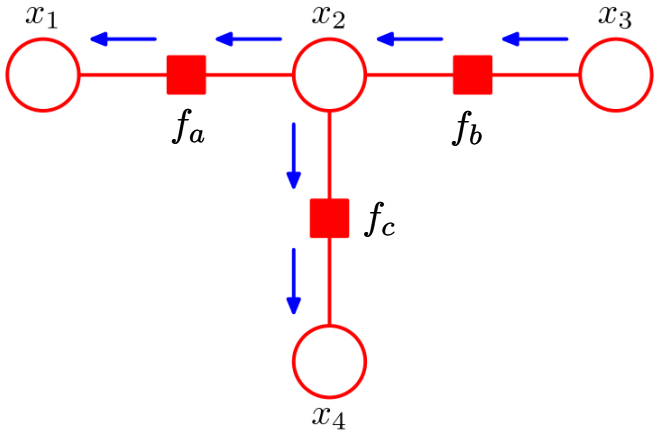
$$\mu_{f_b \to x_2}(x_2) = \sum_{x_3} f_b(x_2, x_3)$$

$$\mu_{x_2 \to f_a}(x_2) = \mu_{f_b \to x_2}(x_2) \mu_{f_c \to x_2}(x_2)$$

$$\mu_{f_a \to x_1}(x_2) = \sum_{x_2} f_a(x_1, x_2) \mu_{x_2 \to f_a}(x_2)$$

$$\mu_{x_2 \to f_c}(x_2) = \mu_{f_a \to x_2}(x_2) \mu_{f_b \to x_2}(x_2)$$

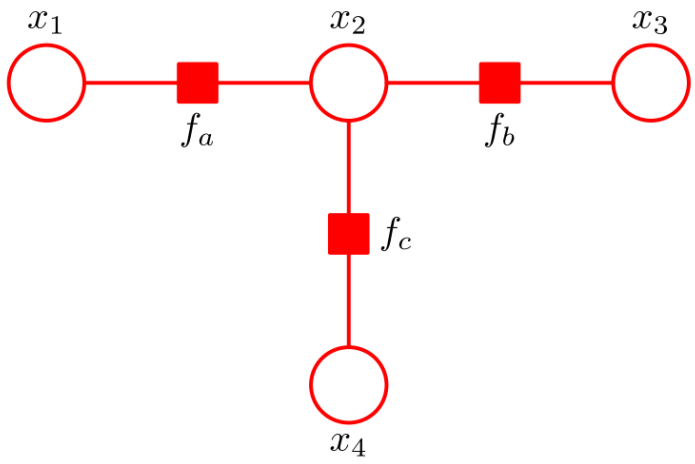
$$\mu_{f_c \to x_4}(x_4) = \sum_{x_2} f_c(x_2, x_4) \mu_{x_2 \to f_c}(x_2)$$



An Example for Practice

- Verify the marginal $p(x_2)$

$$\begin{aligned}\tilde{p}(x_2) &= \mu_{f_a \to x_2}(x_2)\mu_{f_b \to x_2}(x_2)\mu_{f_c \to x_2}(x_2) \\ &= \left[\sum_{x_1} f_a(x_1, x_2)\right]\left[\sum_{x_3} f_b(x_2, x_3)\right]\left[\sum_{x_4} f_c(x_2, x_4)\right] \\ &= \sum_{x_1}\sum_{x_3}\sum_{x_4} f_a(x_1, x_2) f_b(x_2, x_3) f_c(x_2, x_4) \\ &= \sum_{x_1}\sum_{x_3}\sum_{x_4} \tilde{p}(\mathbf{x})\end{aligned}$$



Consistent with

$$p(x) = \sum_{\mathbf{x} \setminus x} p(\mathbf{x})$$

Conditioned on Observed Variables

- Suppose we partition **x** into
  - hidden variables **h**
  - observed variables $\mathbf{v} = \hat{\mathbf{v}}$
- For the calculation $p(h|\mathbf{v} = \hat{\mathbf{v}}) = \sum_{\mathbf{x} \setminus h} p(\mathbf{x})$
  - We just need to update $p(\mathbf{x})$ as

$$p(\mathbf{x}) \leftarrow p(\mathbf{x}) \prod_i I(v_i = \hat{v}_i)$$

- The sum-product algorithm is efficient