Probabilistic Graphical Models

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Adapted from the slides of "Pattern Recognition and Machine Learning" Chapter 8

Recap of Last Lecture - WebPPL

WebPPL

- Subset of Javascript
- Probabilistic Constructs
  - Distributions: **Bernoulli, Categorical, Gaussian …**
  - sample → Process
  - condition, observe, factor → State

Recap of Last Lecture - Applications

- Bayesian learning models

$$argmax_{\omega}P(D|\omega) \Rightarrow argmax_{\omega}P(D|\omega) * P(\omega)$$

- Optimal experiment design

$$argmax_{X}\boldsymbol{E}_{p(X,Y)}(D_{KL}(\,m\,|x = X, y = Y\,||m))$$

- Inverse graphics

$$\text{Model}(x) \xrightarrow{\text{Render}(k)} \text{Image}$$

x ~ Distribution

k ~ Distribution
e.g., lightning, angles

condition(Image = Observed)

Is the following statement correct?

- The Bayesian way to do linear regression is strictly more powerful than the conventional way to do linear regression.

Is the following statement correct?

- In a Bayesian learning model, the more training data there is, the less the prediction results will be affected by the prior distribution of the parameters.

Is the following statement correct?

- When using a Bayesian model, one should always use the most likely result in the prediction distribution.

Is the following statement correct?

- Given two distributions A, B, we have

$$D_{KL}(A \,||\, B) = D_{KL}(B \,||\, A) \,.$$

Is the following statement correct?

- The goal of the optimal experiment design is to choose an experiment whose expected result (i.e., output value) is the highest among all experiments.

What are the applications of inverse graphics?

1. Scene understanding.

2. Data generation.

3. Both.

Why do we need graphical models?

- How would you represent a probability distribution, so you can
  - Visualize and design a model.
  - Gain insights about relationships between random variables.
  - Do complex inferences.

Naïve Method

A and B are Bernoulli random variables.

	A= True	A= False
B= True	0.25	0.25
B = False	0.25	0.25

Naïve Method

A and B are Bernoulli random variables.

	A= True	A= False
B= True	0.25	0.25
B = False	0.25	0.25

What questions can we ask?

Probabilistic Inference Problems

- Marginal inference:
  - Let X be the set of random variables, Y be a subset of it, Z = X/Y then marginal inference is to compute

$$P(Y = V_Y) = \Sigma_{V_{Z_i}} P(Y = V_Y, Z = V_{Z_i})$$

- Conditional inference:
  - Let X be the set of random variables, Y and W be subsets of it then conditional inference is to compute

$$P(Y = V_Y \mid W = V_W)$$

Probabilistic Inference in Table Method

	A= True	A= False
B= True	0.25	0.25
B = False	0.25	0.25

$$P(A = True) = P(A = True, B = False) + P(A = True, B = True)$$

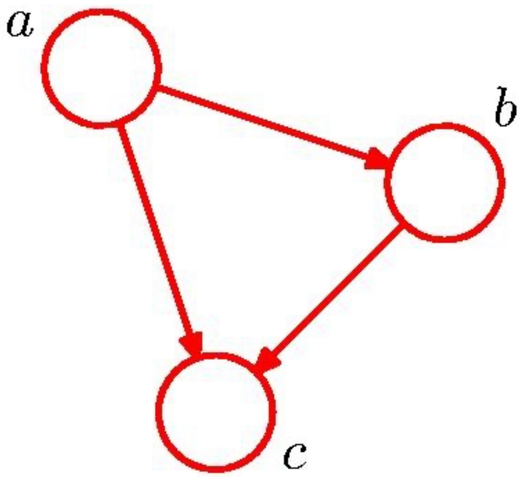
Probabilistic Inference in Table Method

	A= True	A= False
B= True	0.25	0.25
B = False	0.25	0.25

$$P(A = True \mid B = True) = \frac{P(A = True, B = True)}{P(A = True, B = True) + P(A = False, B = True)}$$

Bayesian Networks

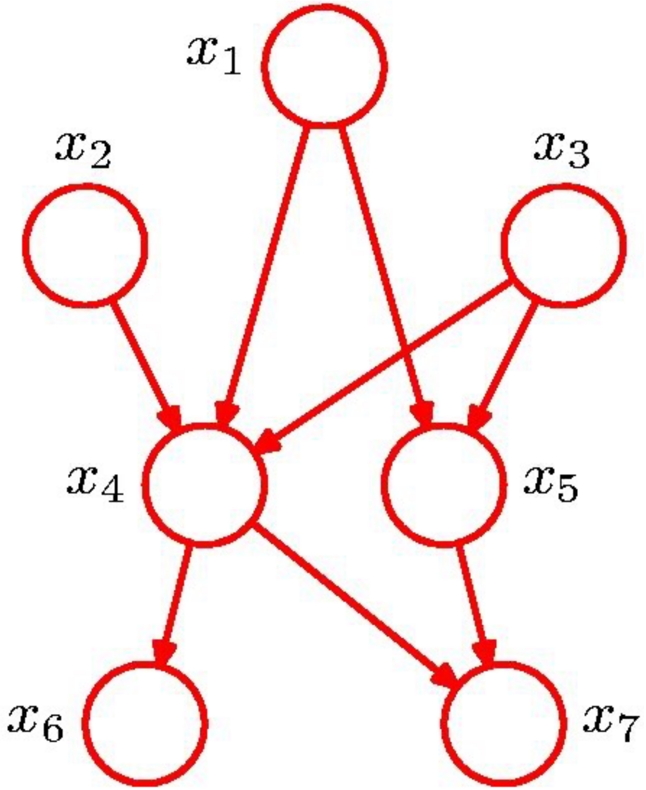
- Directed Acyclic Graph (DAG)



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

$$p(x_1,\ldots,x_K) = p(x_K|x_1,\ldots,x_{K-1})\ldots p(x_2|x_1)p(x_1)$$

Bayesian Networks

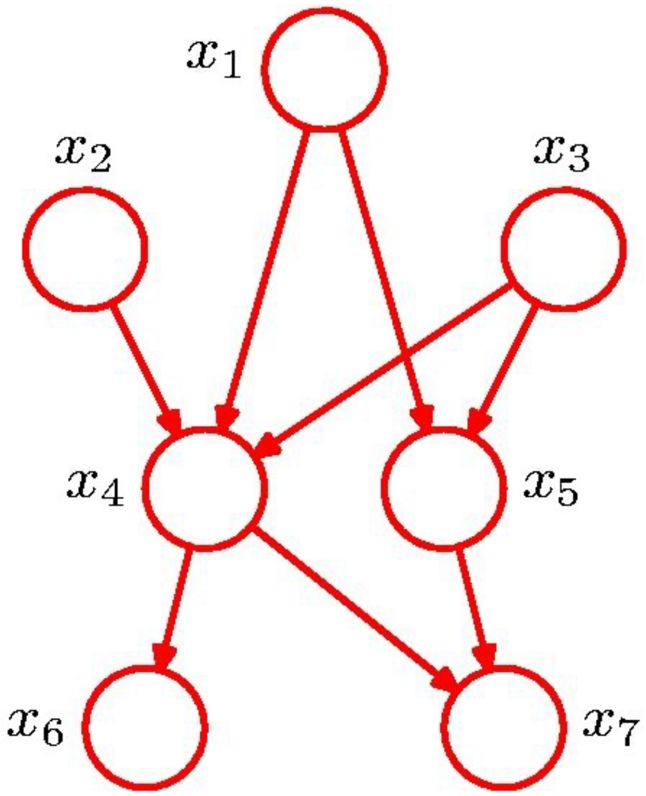


$$p(x_1, \ldots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

General Factorization

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

Bayesian Networks



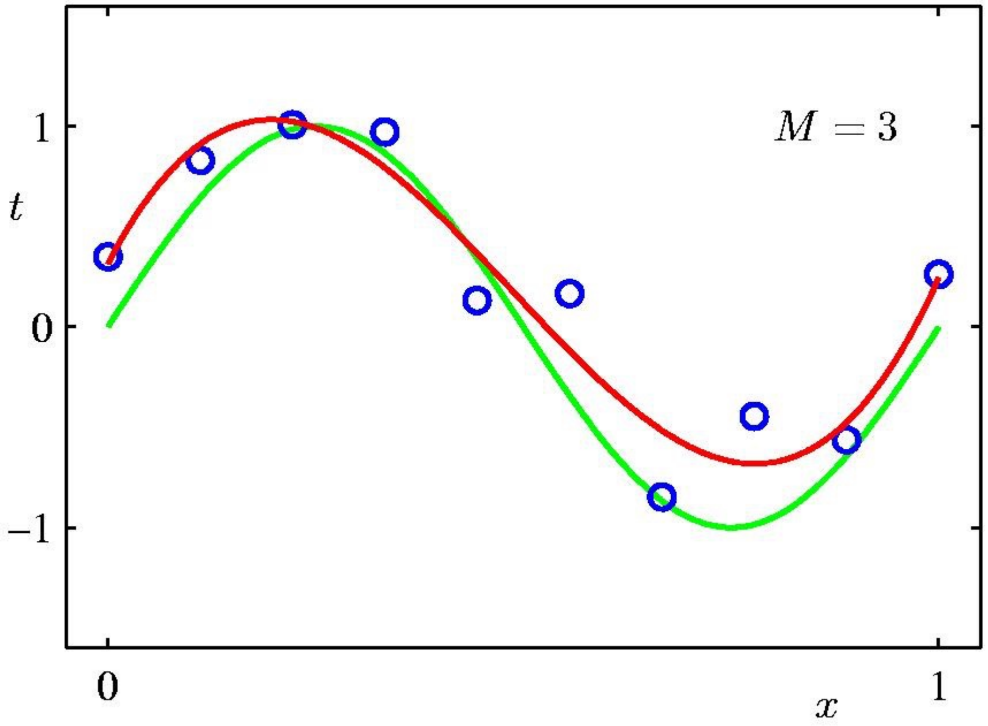
Are x_1 and x_2 independent?

What about x_4 and x_5?

What about x_4 and x_5 when x_1 is fixed?

We will talk about dependence later!

Example Application: Bayesian Curve Fitting



Polynomial

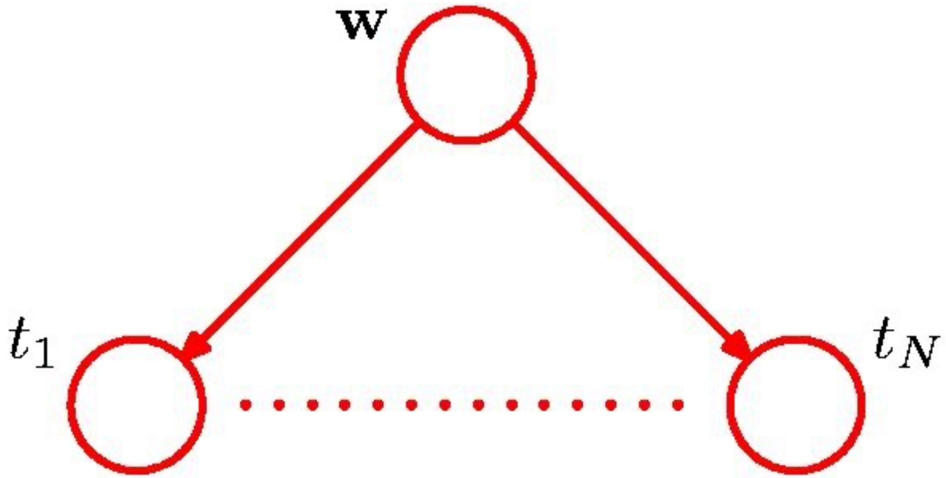
$$y(x, \mathbf{w}) = \sum_{j=0}^{M} w_j x^j$$

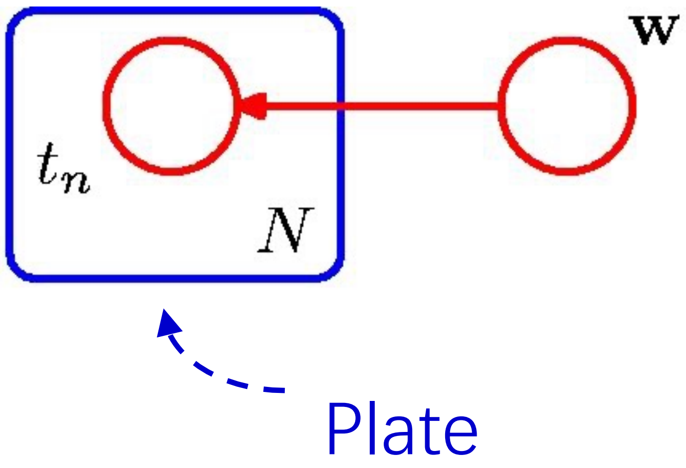
$\mathbf{x}$ is the set of training inputs while $\mathbf{t}$ is their predictions.

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

Example Application: Bayesian Curve Fitting

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





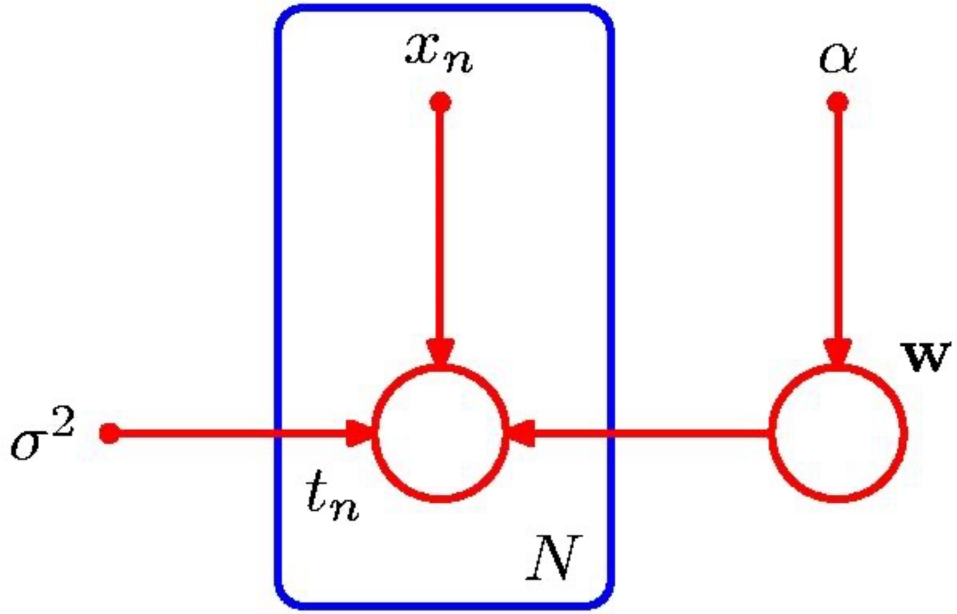
Example Application: Bayesian Curve Fitting

- Input variables and explicit hyperparameters

- α is the parameter of the parameter. For example: $w_i \sim N(\alpha, 1)$

- σ^2 is the variance of the gaussian noise in training.

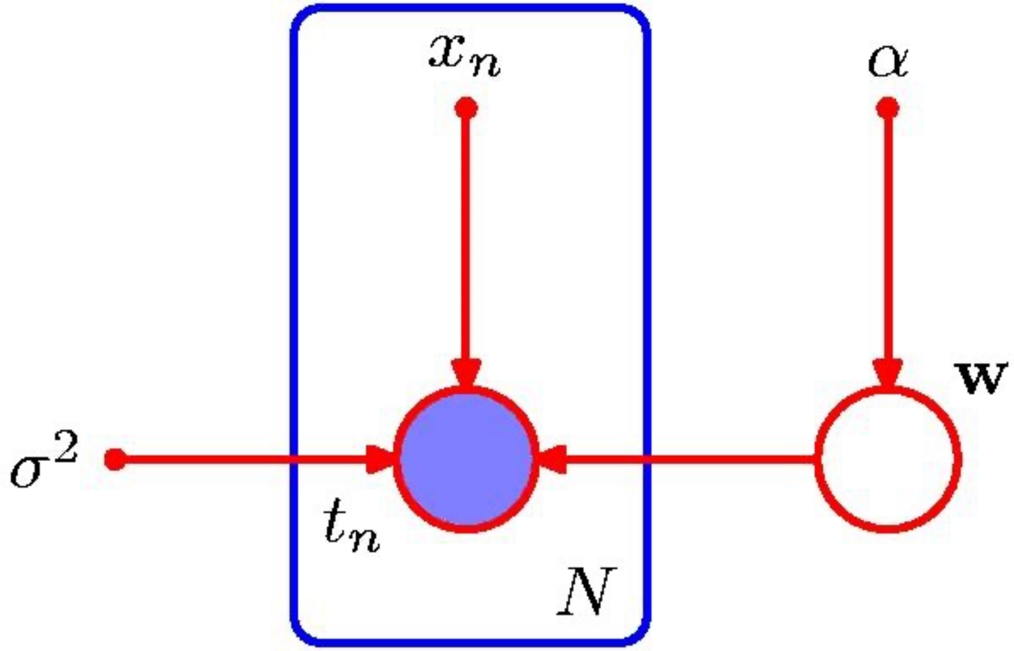
$$p(\mathbf{t}, \mathbf{w} | \mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w}|\alpha) \prod_{n=1}^{N} p(t_n | \mathbf{w}, x_n, \sigma^2).$$



Bayesian Curve Fitting — Learning

- Condition on data

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

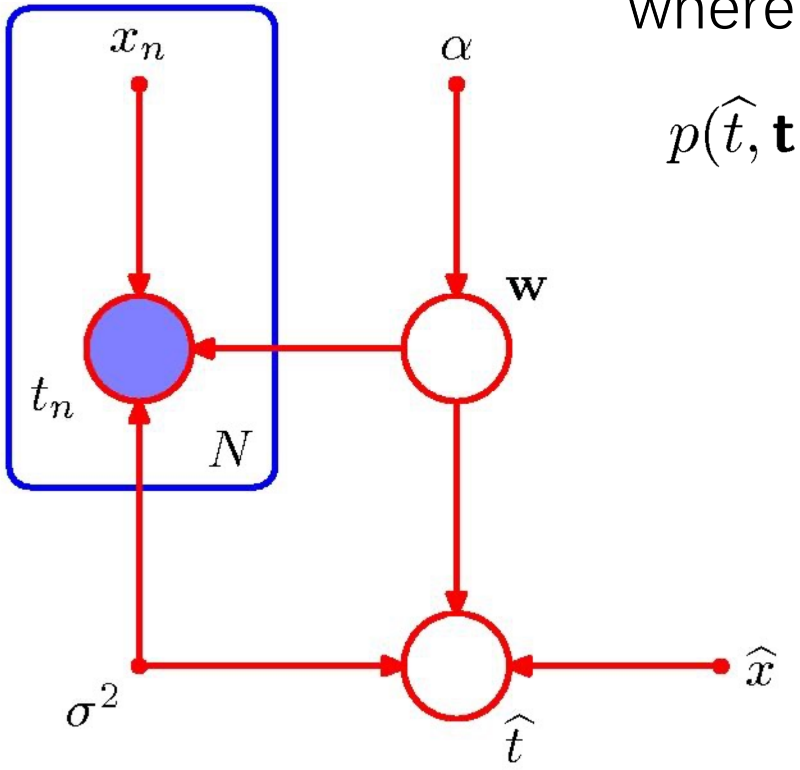


Bayesian Curve Fitting — Prediction

Predictive distribution: $p(\widehat{t}|\widehat{x}, \mathbf{x}, \mathbf{t}, \alpha, \sigma^2) \propto \int p(\widehat{t}, \mathbf{t}, \mathbf{w}|\widehat{x}, \mathbf{x}, \alpha, \sigma^2)\, \mathrm{d}\mathbf{w}$

where

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

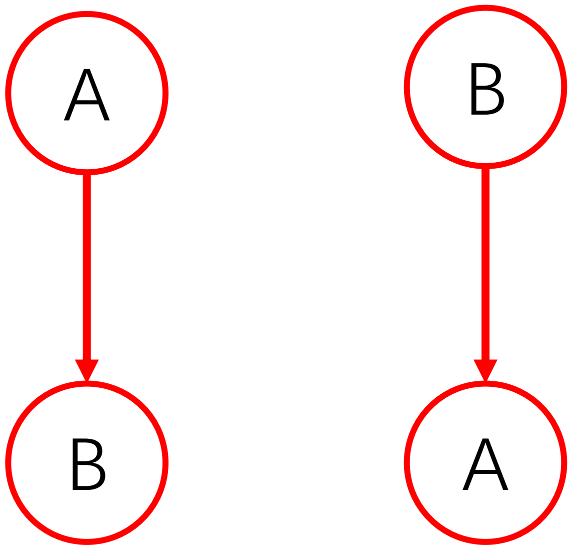


Which model is correct?

A: whether the school bus encounters an accident

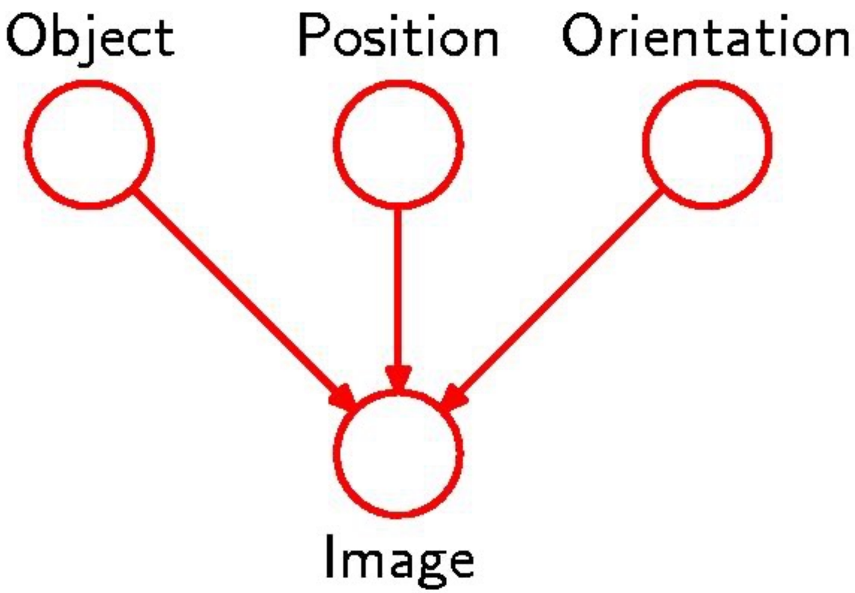
B: whether the teacher is late for the class

	A= True	A= False
B= True	0.09	0.09
B = False	0.01	0.81



Generative Models

- Causal process for generating images



We will talk about causality in a later lecture!

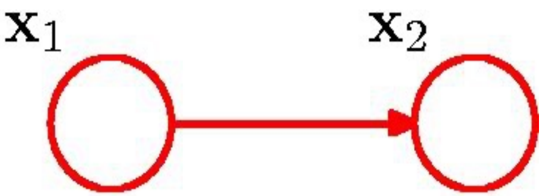
Two Special Cases

- Discrete variables

- Gaussian variables

Discrete Variables

- General joint distribution: $K^2 - 1$parameters



$$p(\mathbf{x}_1, \mathbf{x}_2 | \boldsymbol{\mu}) = \prod_{k=1}^{K} \prod_{l=1}^{K} \mu_{kl}^{x_{1k} x_{2l}}$$

- Independent joint distribution: $2(K - 1)$ parameters

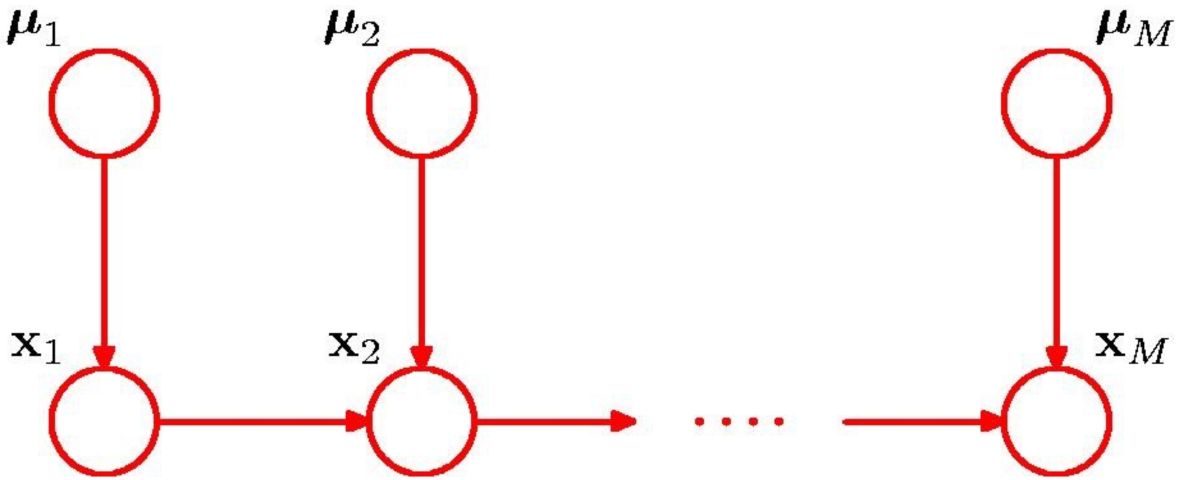
$$\hat{p}(\mathbf{x}_1, \mathbf{x}_2 | \boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_{1k}^{x_{1k}} \prod_{l=1}^{K} \mu_{2l}^{x_{2l}}$$

Discrete Variables

General joint distribution over M variables:
$K^M - 1$ parameters

M -node Markov chain: $K - 1 + (M - 1) K(K - 1)$ parameters

Discrete Variables: Bayesian Parameters



$$p\left(\{\mathbf{x}_m, \boldsymbol{\mu}_m\}\right) = p\left(\mathbf{x}_1 \,|\boldsymbol{\mu}_1\right) p\left(\boldsymbol{\mu}_1\right) \prod_{m=2}^{M} p\left(\mathbf{x}_m | \mathbf{x}_{m-1}, \boldsymbol{\mu}_m\right) p\left(\boldsymbol{\mu}_m\right)$$

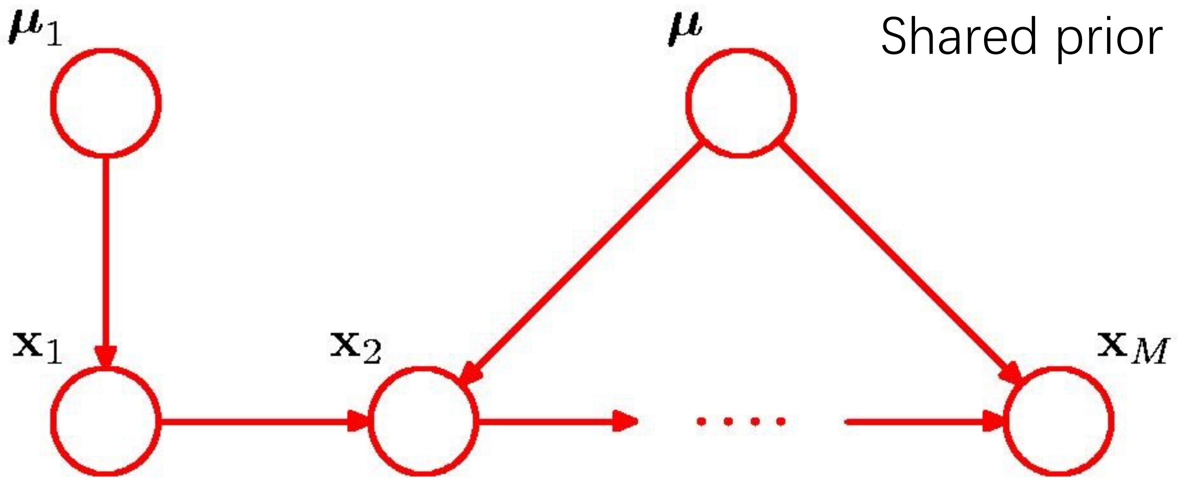
$$p(\boldsymbol{\mu}_m) = \mathrm{Dir}(\boldsymbol{\mu}_m | \boldsymbol{\alpha}_m)$$

Discrete Variables: Bayesian Parameters

- Why are Direchlet distributions used?
  - They are conjugate priors for categorical and binomial distributions.

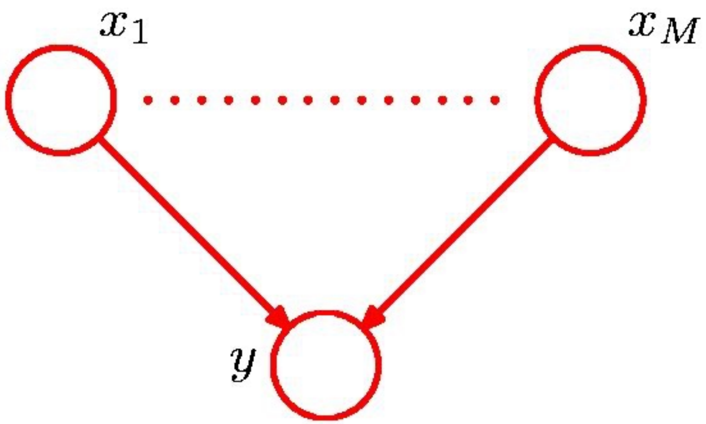
- Further reading: https://towardsdatascience.com/dirichlet-distribution-a82ab942a879

Discrete Variables: Bayesian Parameters



$$p\left(\{\mathbf{x}_m\}, \boldsymbol{\mu}_1, \boldsymbol{\mu}\right) = p\left(\mathbf{x}_1 | \boldsymbol{\mu}_1\right) p\left(\boldsymbol{\mu}_1\right) \prod_{m=2}^{M} p\left(\mathbf{x}_m | \mathbf{x}_{m-1}, \boldsymbol{\mu}\right) p\left(\boldsymbol{\mu}\right)$$

Parameterized Conditional Distributions



If $x_1, \ldots, x_M$ are discrete, K-state variables, $p(y = 1 | x_1, \ldots, x_M)$ in general has $O(K^M)$ parameters.

The parameterized form

$$p(y = 1 | x_1, \ldots, x_M) = \sigma \left(w_0 + \sum_{i=1}^{M} w_i x_i \right) = \sigma(\mathbf{w}^{\mathrm{T}} \mathbf{x})$$

requires only M + 1 parameters

Linear-Gaussian Models

- Directed Graph

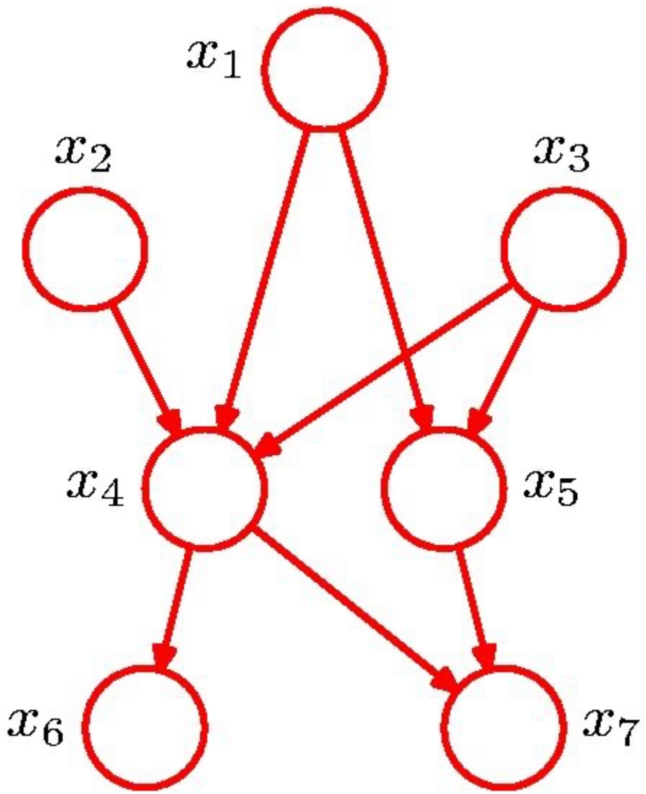
$$p(x_i|\mathrm{pa}_i) = \mathcal{N}\left(x_i \middle| \sum_{j\in\mathrm{pa}_i} w_{ij}x_j + b_i, v_i\right)$$

Each node is Gaussian, the mean is a linear function of the parents.

- Vector-valued Gaussian Nodes

$$p(\mathbf{x}_i|\mathrm{pa}_i) = \mathcal{N}\left(\mathbf{x}_i \middle| \sum_{j\in\mathrm{pa}_i} \mathbf{W}_{ij}\mathbf{x}_j + \mathbf{b}_i, \boldsymbol{\Sigma}_i\right)$$

Recall This Graph



Are x_1 and x_2 independent?

What about x_4 and x_5?

What about x_4 and x_5 when x_1 is fixed?

We will talk about dependence now!

Conditional Independence

- a is independent of b given c

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

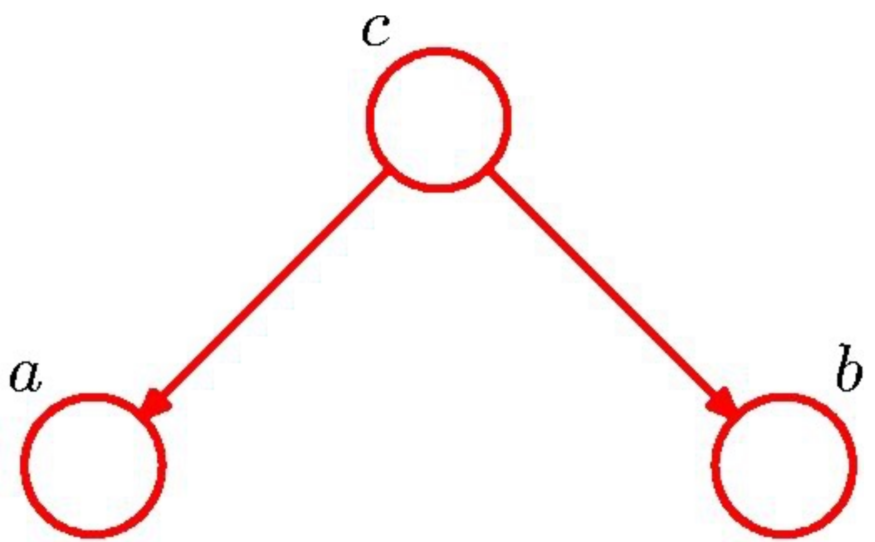
- Equivalently

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

- Notation

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

Conditional Independence: Example 1

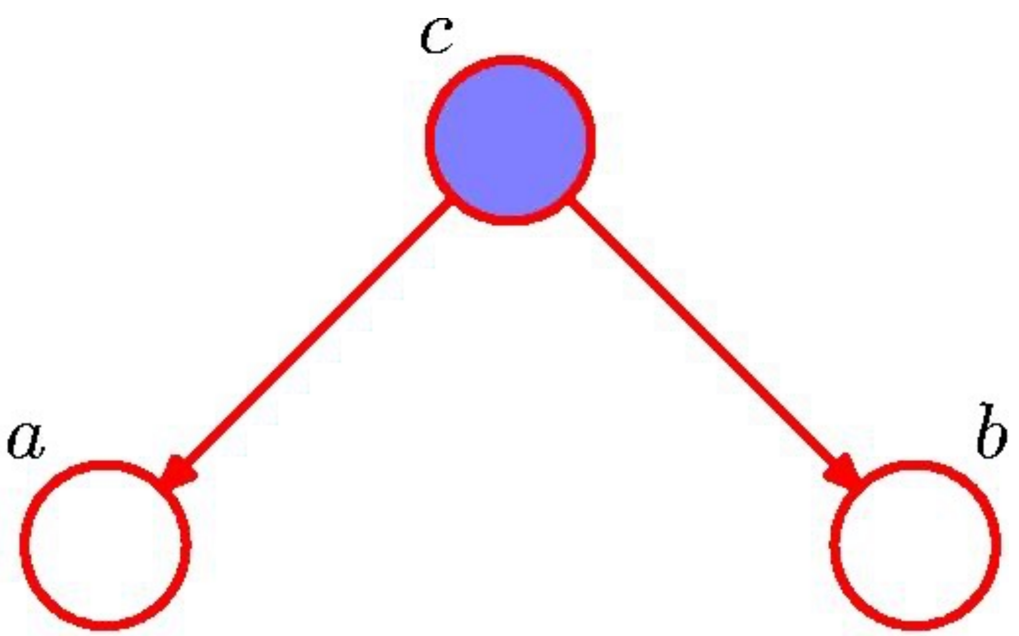


$$p(a, b, c) = p(a|c)p(b|c)p(c)$$

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

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

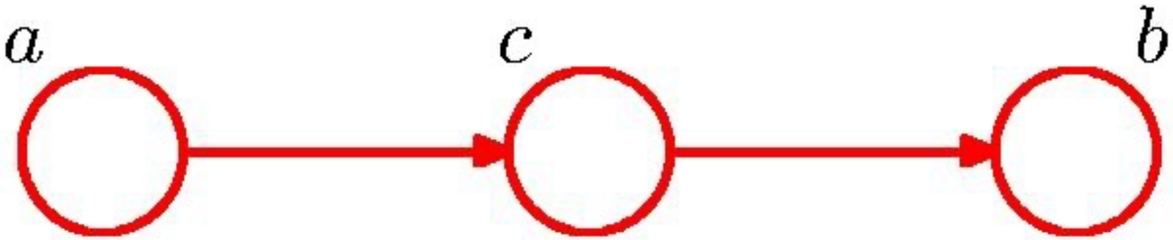
Conditional Independence: Example 1



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

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

Conditional Independence: Example 2

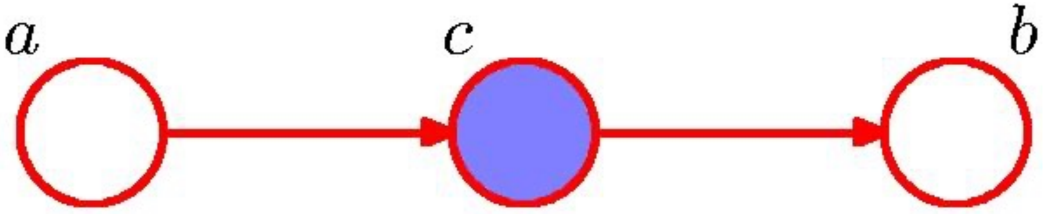


$$p(a,b,c) = p(a)p(c|a)p(b|c)$$

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

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

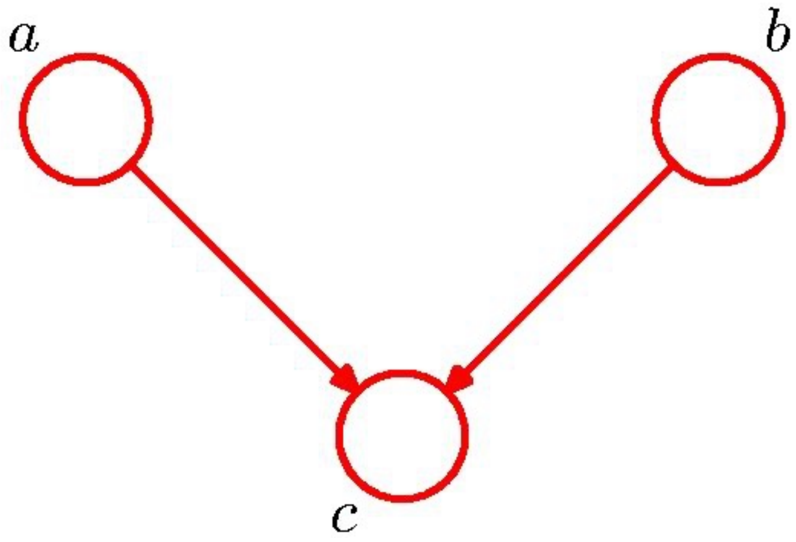
Conditional Independence: Example 2



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

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

Conditional Independence: Example 3



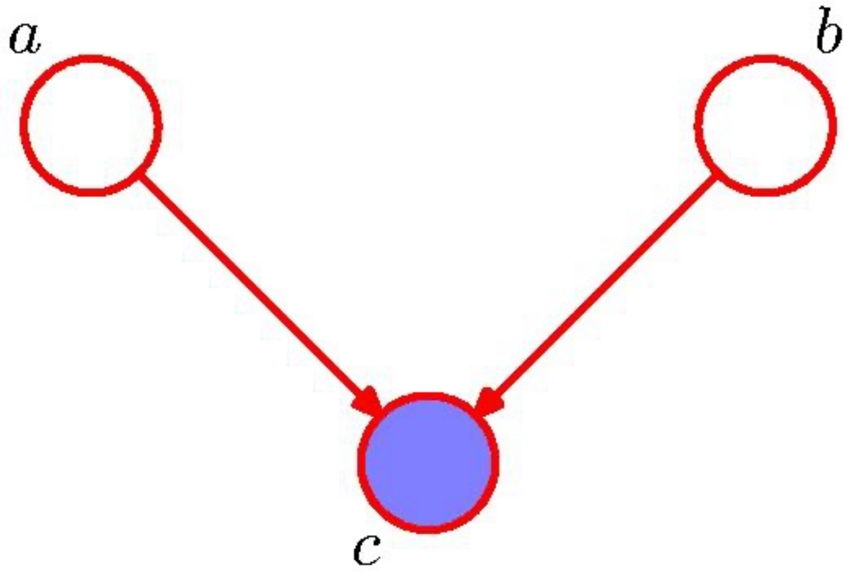
$$p(a,b,c) = p(a)p(b)p(c|a,b)$$

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

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

- Note: this is the opposite of Example 1, with c unobserved.

Conditional Independence: Example 3



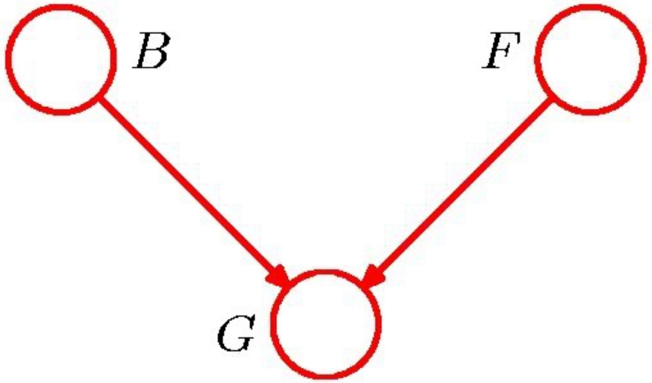
$$p(a,b|c) = \frac{p(a,b,c)}{p(c)} = \frac{p(a)p(b)p(c|a,b)}{p(c)}$$

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

Note: this is the opposite of Example 1, with **c** observed.

"Am I out of fuel?"

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



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

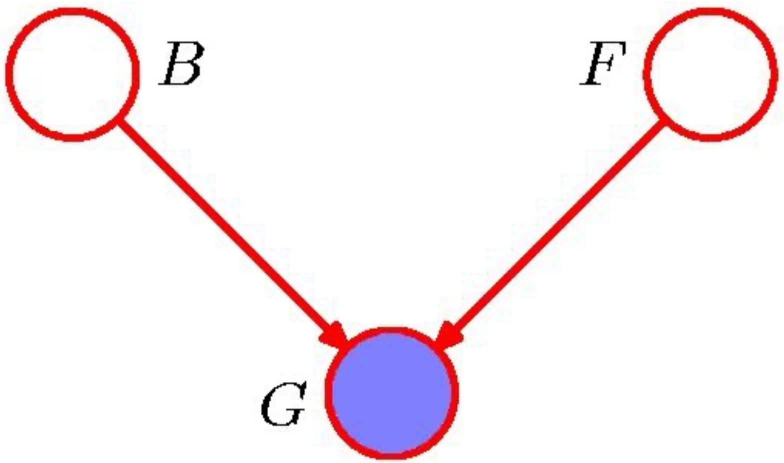
and hence

$$p(F=0) = 0.1$$

B = Battery (0=flat, 1=fully charged)
F = Fuel Tank (0=empty, 1=full)
G = Fuel Gauge Reading
(0=empty, 1=full)

"Am I out of fuel?"

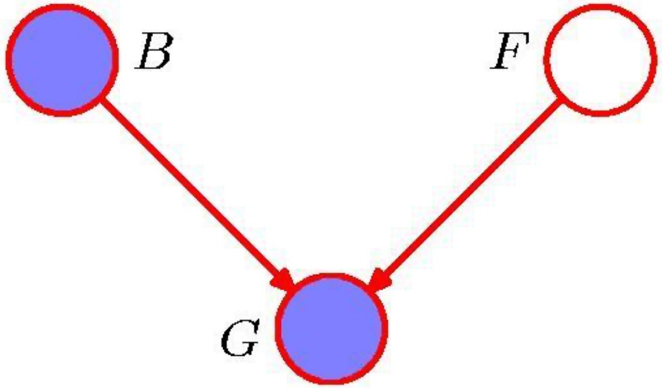
$$p(F=0|G=0) = \frac{p(G=0|F=0)p(F=0)}{p(G=0)} \simeq 0.257$$



Probability of an empty tank increased by observing G = 0.

What if now we also know the battery is flat?

“Am I out of fuel?”



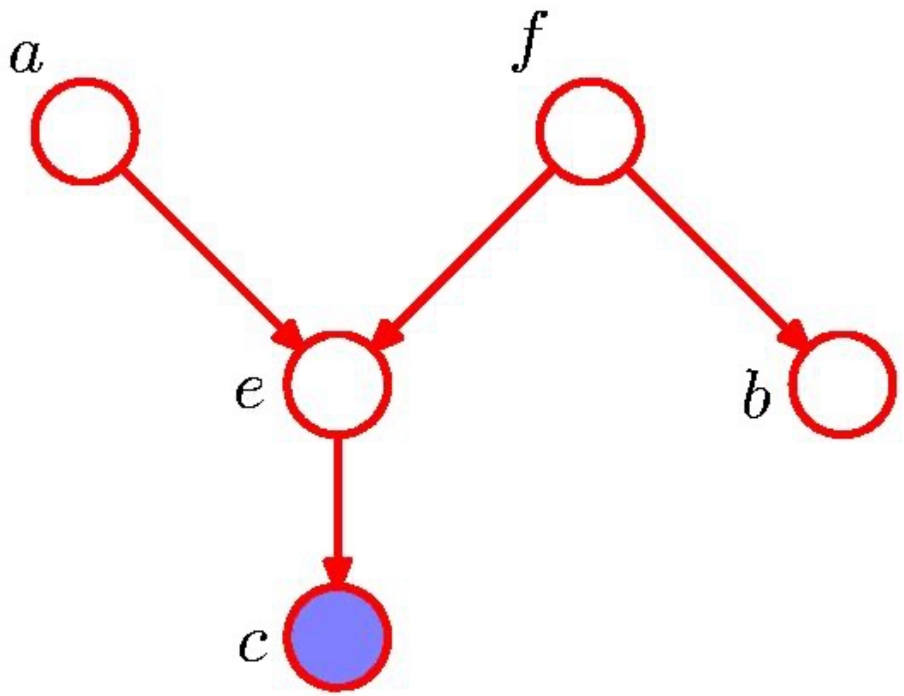
$$
\begin{aligned}
p(F=0|G=0,B=0) &= \frac{p(G=0|B=0,F=0)p(F=0)}{\sum_{F\in\{0,1\}} p(G=0|B=0,F)p(F)} \\
&\simeq 0.111
\end{aligned}
$$

Probability of an empty tank reduced by observing $B = 0$.
This referred to as “explaining away”.

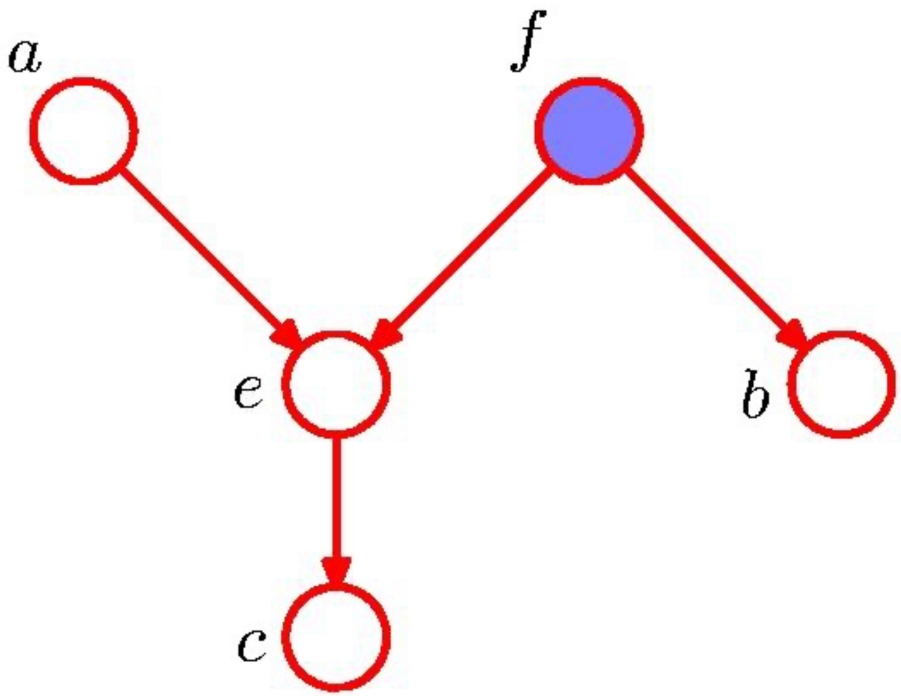
D-separation

- A, B, and C are 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
  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, 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 $A \perp\!\!\!\perp B \mid C$.

D-separation: Example

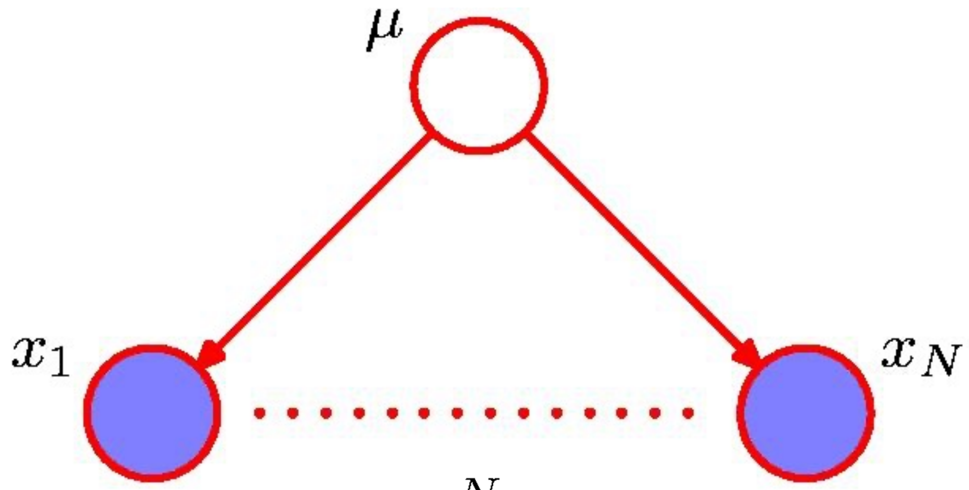


$$a \not\perp\!\!\!\perp b \mid c$$



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

D-separation: I.I.D. Data



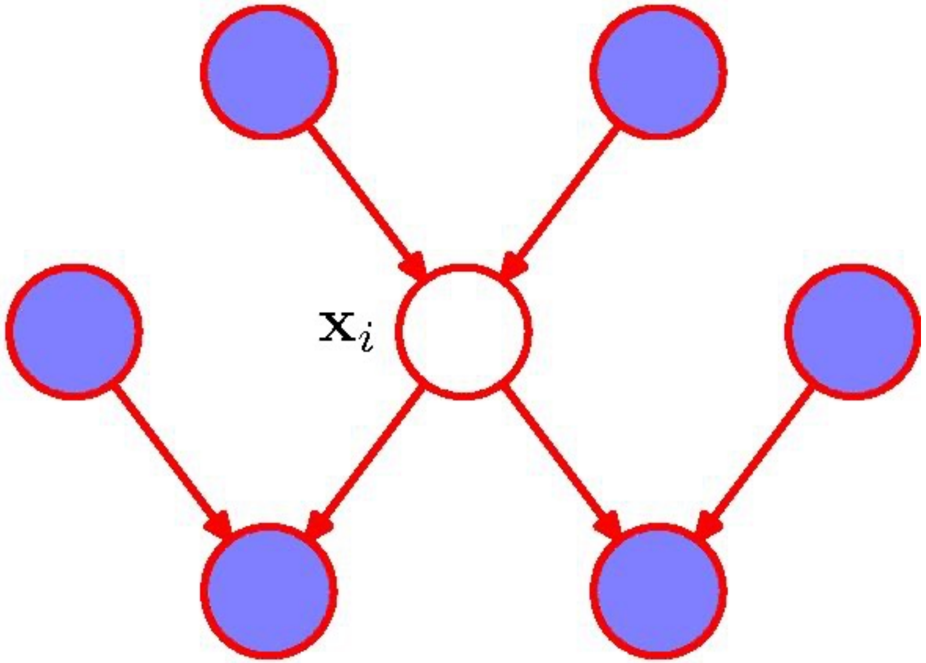
$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu)$$

$$p(\mathcal{D}) = \int_{-\infty}^{\infty} p(\mathcal{D}|\mu)p(\mu)\,\mathrm{d}\mu \neq \prod_{n=1}^{N} p(x_n)$$

Question

- What can D-separation be used for?

The Markov Blanket



$$p(\mathbf{x}_i|\mathbf{x}_{\{j\neq i\}}) = \frac{p(\mathbf{x}_1,\ldots,\mathbf{x}_M)}{\int p(\mathbf{x}_1,\ldots,\mathbf{x}_M)\,\mathrm{d}\mathbf{x}_i} = \frac{\prod_k p(\mathbf{x}_k|\mathrm{pa}_k)}{\int \prod_k p(\mathbf{x}_k|\mathrm{pa}_k)\,\mathrm{d}\mathbf{x}_i}$$

Factors independent of $\mathbf{x}_i$ cancel between numerator and denominator.

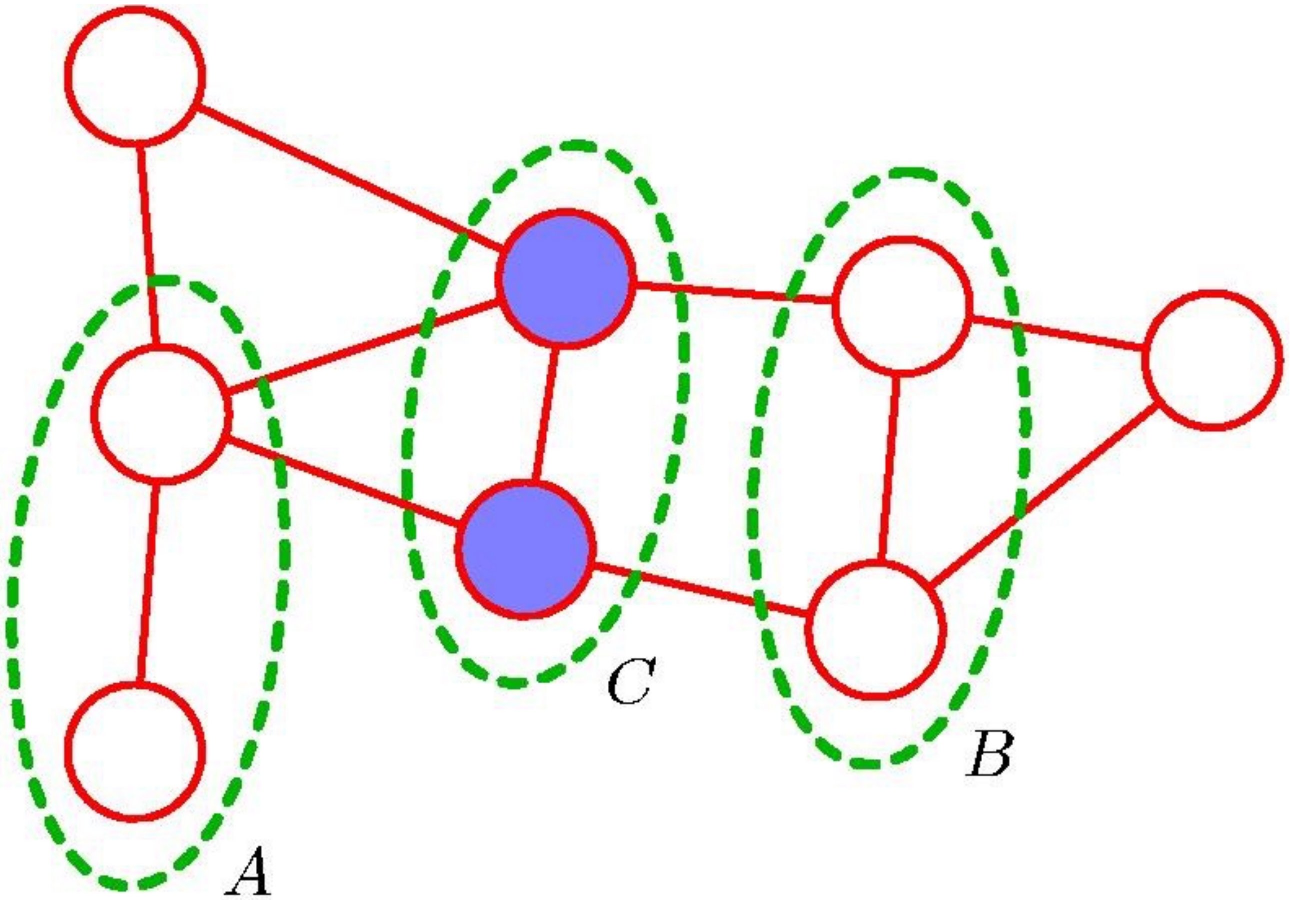
Bayesian Networks: Summary

- Directed
- Factorizations of conditional probabilities
- Reason about the relationships between different variables using conditional independence

Markov Random Fields

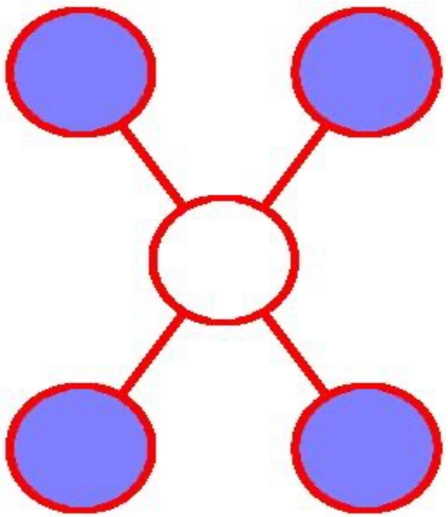
- Undirected
- Markov networks
- One motivation: reasoning about conditional independence is subtle in Bayesian networks. Can we have something simpler?

Markov Random Fields



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

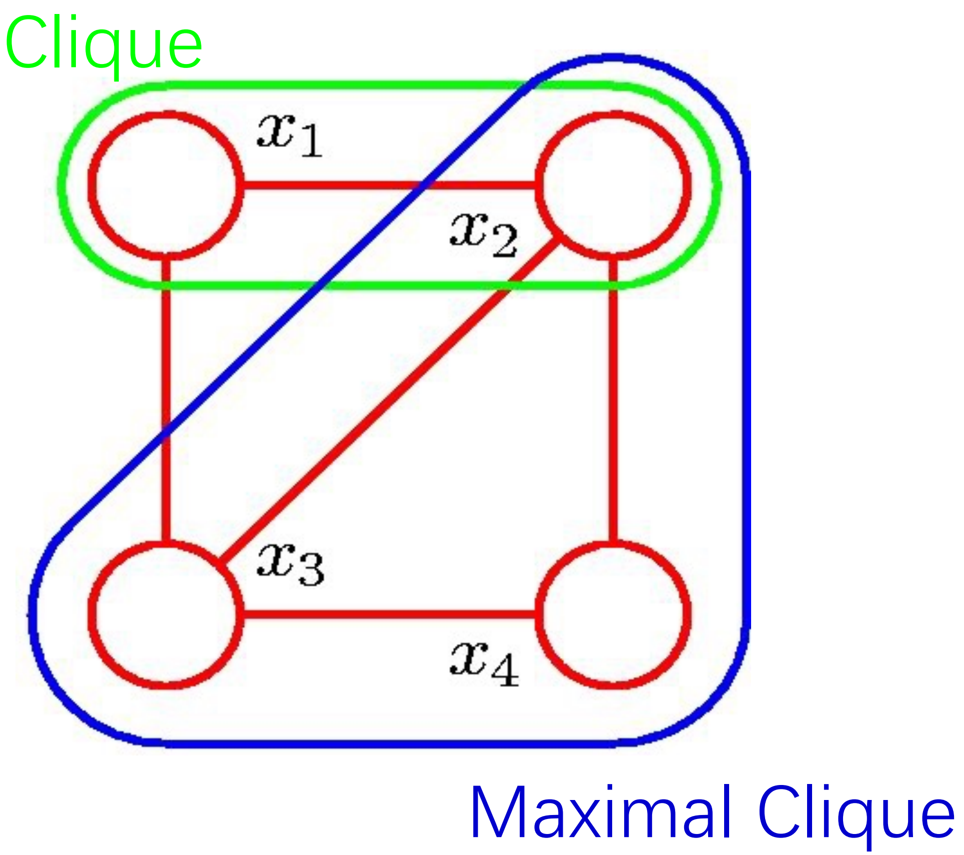
Markov Blanket



Markov Random Fields: Intuitions

- If x and y are not directly connected, then they should be independent conditioning on the other variables
- $P(x, y \,|V/\{x, y\}) = P(x \,|V/\{x, y\}) * P(y \,|V/\{x, y\})$
- x and y should not appear in the same factor
- We should put nodes that are directly connected in the same factor

Cliques and Maximal Cliques



Joint Distribution

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

- where $\psi_C(\mathbf{x}_C)$ is the potential over maximal clique C and

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

- is the normalization coefficient; note: M K-state variables → K^M terms in Z.

- In general, we only require potentials to be positive. One example: Energies and the Boltzmann distribution

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

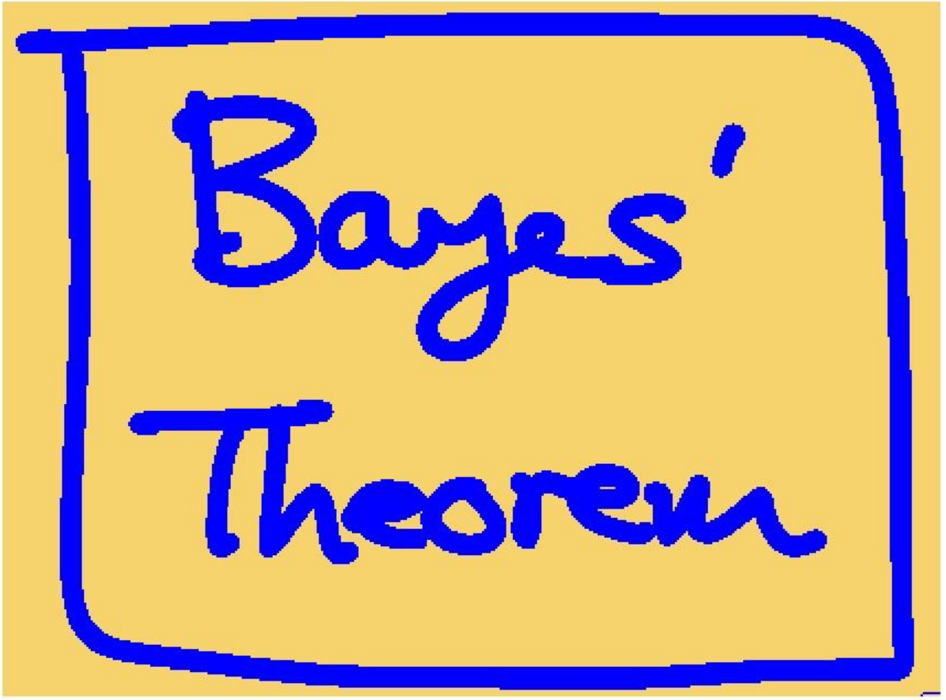
Factorization and Conditional Independence

- Given a graph (potential function unknown), let UI be the distributions whose conditional independence fits the graph

- Let UF be the subset of UI that can be expressed in the factorization form

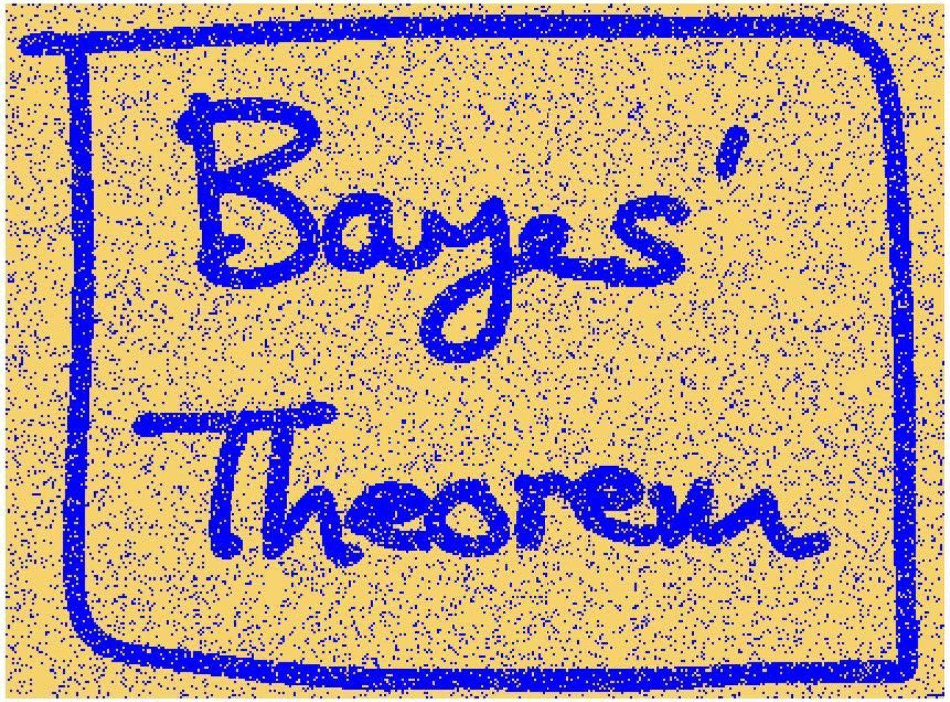
- We have UF = UI: the Hammersley-Clifford theorem (Clifford, 1990)

Illustration: Image De-Noising



Original Image

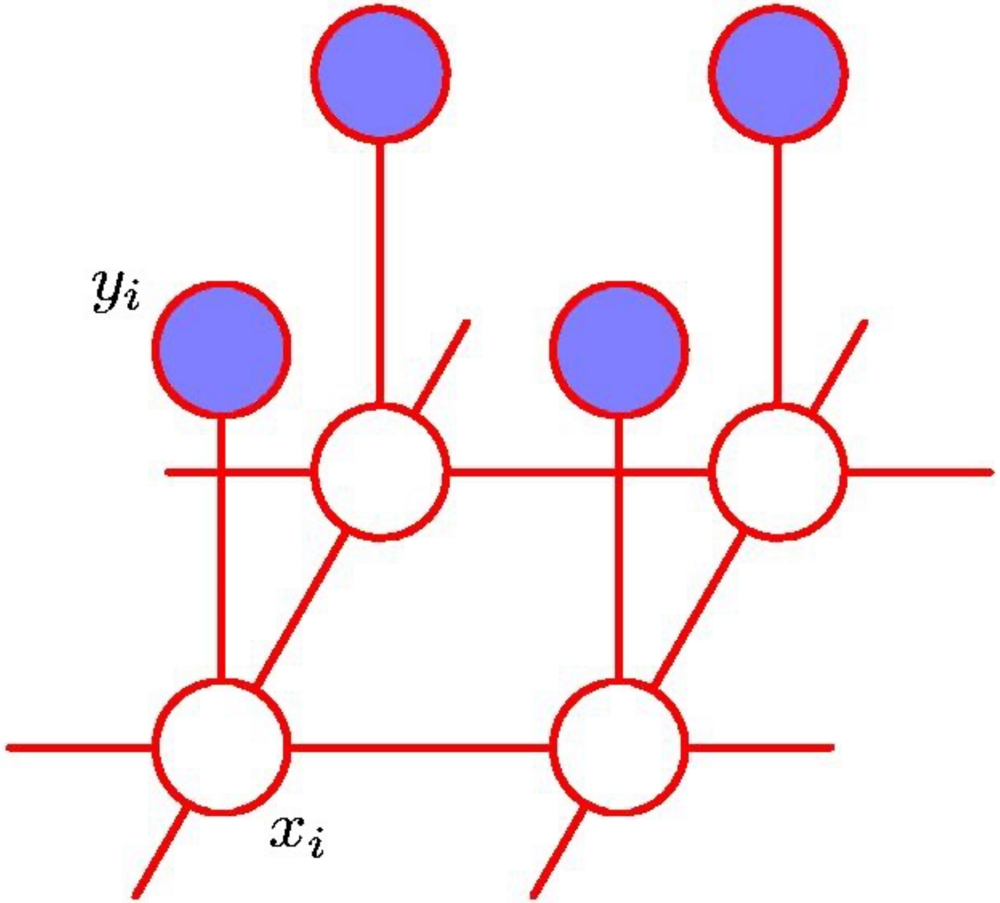
$x_i \in \{-1, 1\}$



Noisy Image

$y_j \in \{-1, 1\}$

Illustration: Image De-Noising



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

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

Special Case: Conditional Random Field

- There two sets of variables X and Y
- The conditional distribution Y|X forms a Markov Random Field
- By observing Y, predict X
- Example: text segmentation: X: text, Y: segments

Summary

- Bayesian networks
  - Directed
  - Factorization of conditional probabilities
  - Conditional independence: D-separation

- Markov random fields
  - Undirected
  - Factorization over maximum cliques

Next Class

- Relationship between directed and undirected models

- Inference