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 → State
  - factor

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.

- Yes.

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.

- Yes.

Is the following statement correct?

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

- No. Sometimes expectations are better.

Is the following statement correct?

- Given two distributions A, B, we have

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

- No.

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.

- No.

What are the applications of inverse graphics?

1. Scene understanding.

2. Data generation.

3. Both.

- 3.

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)

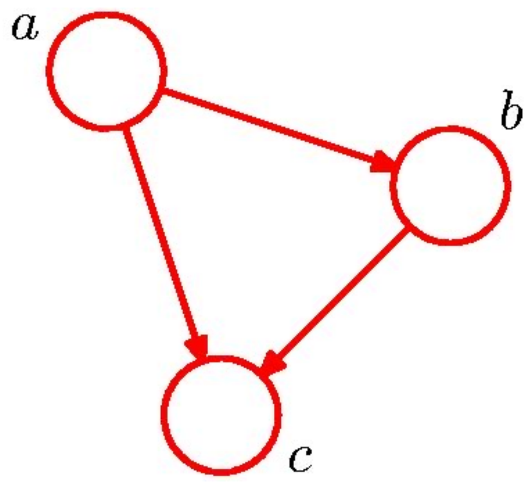
Probabilistic Inference in Table Method

	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

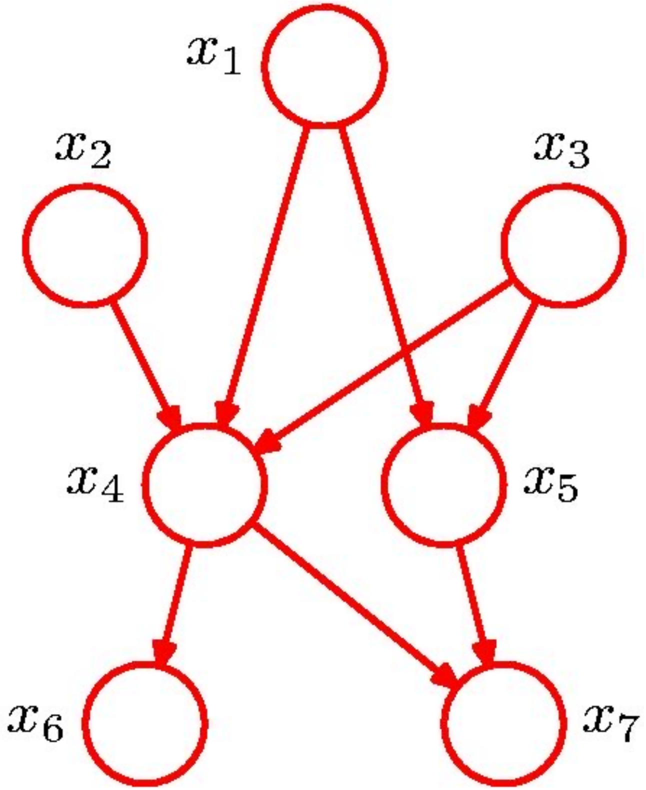
- Directed Acyclic Graph (DAG)



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

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

Bayesian Networks

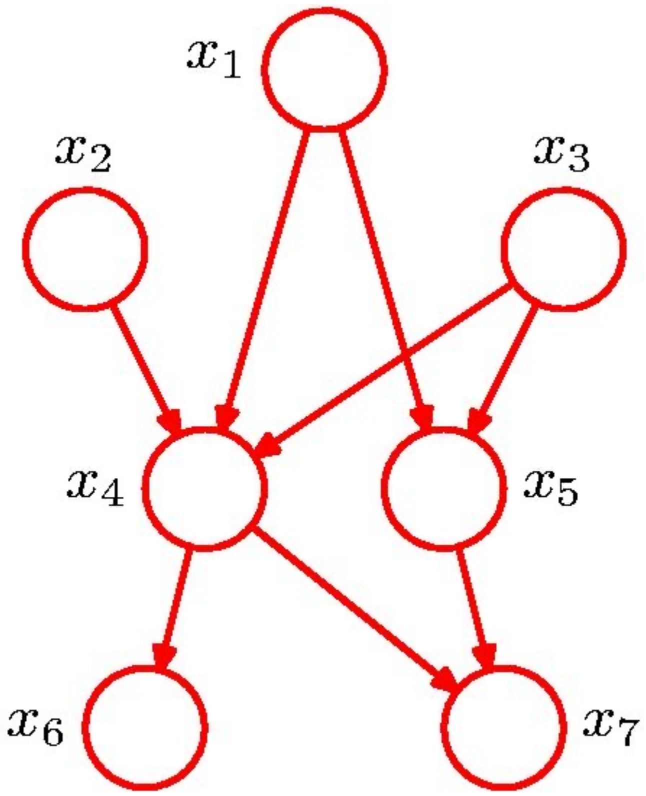


$$
\begin{aligned}
p(x_1, \ldots, x_7) \quad = \quad & p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) \\
& p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)
\end{aligned}
$$

General Factorization

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

Bayesian Networks



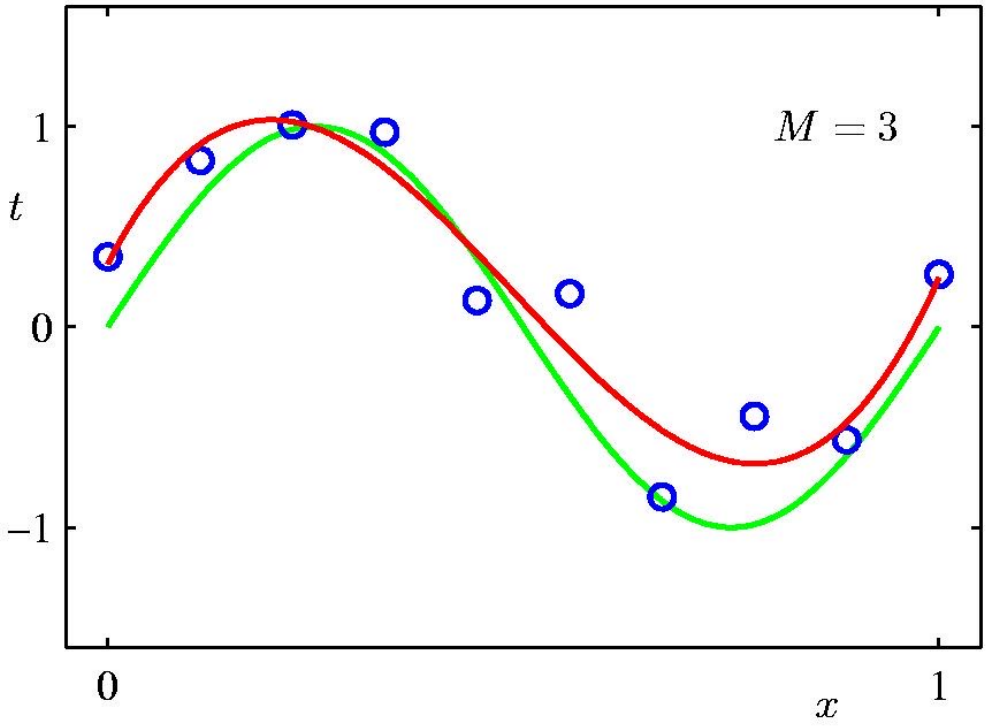
Are x_1 and x_2 independent?

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

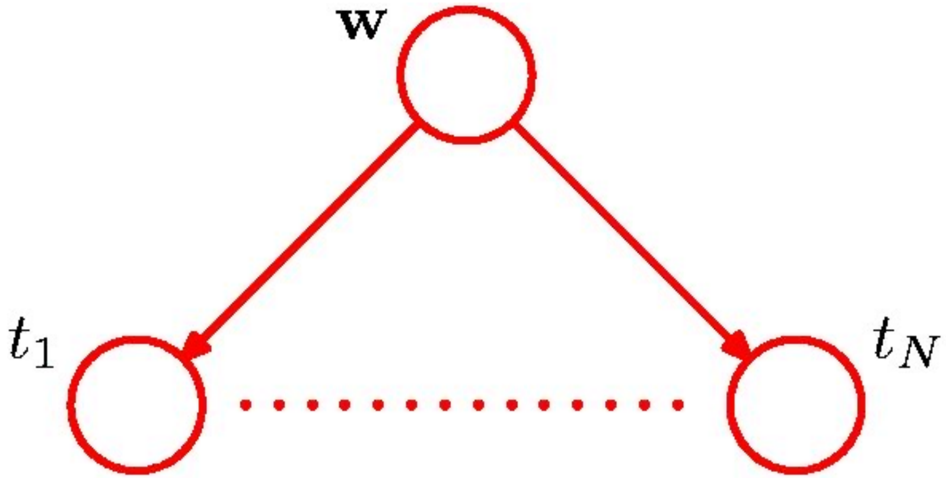
$$y(x, \mathbf{w}) = \sum_{j=0}^{M} w_j x^j$$

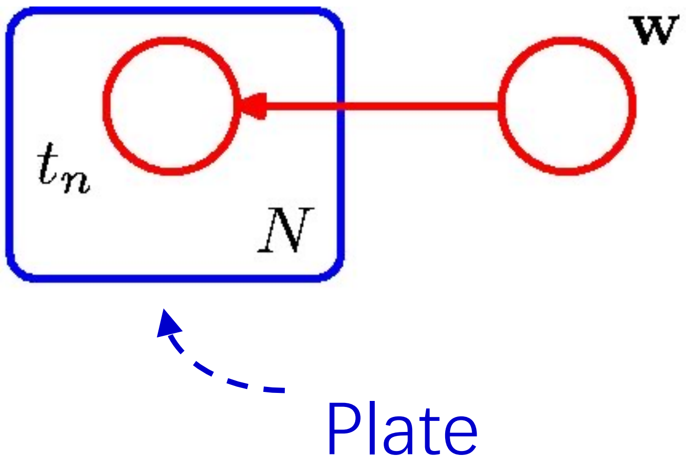
$\mathbf{x}$ is the set of training inputs while $\mathbf{t}$ is their predictions.

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

Example Application: Bayesian Curve Fitting

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





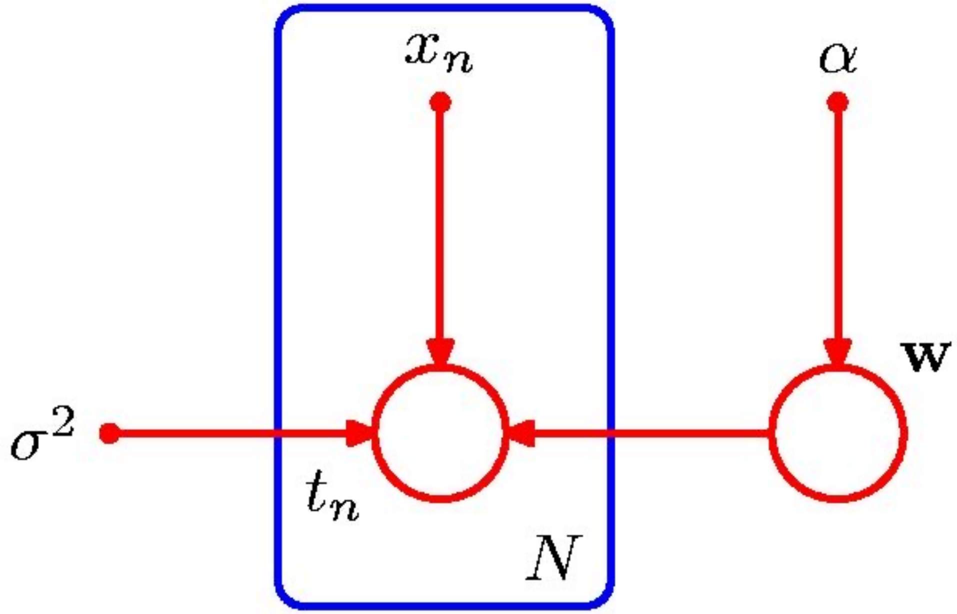
Example Application: Bayesian Curve Fitting

- 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.

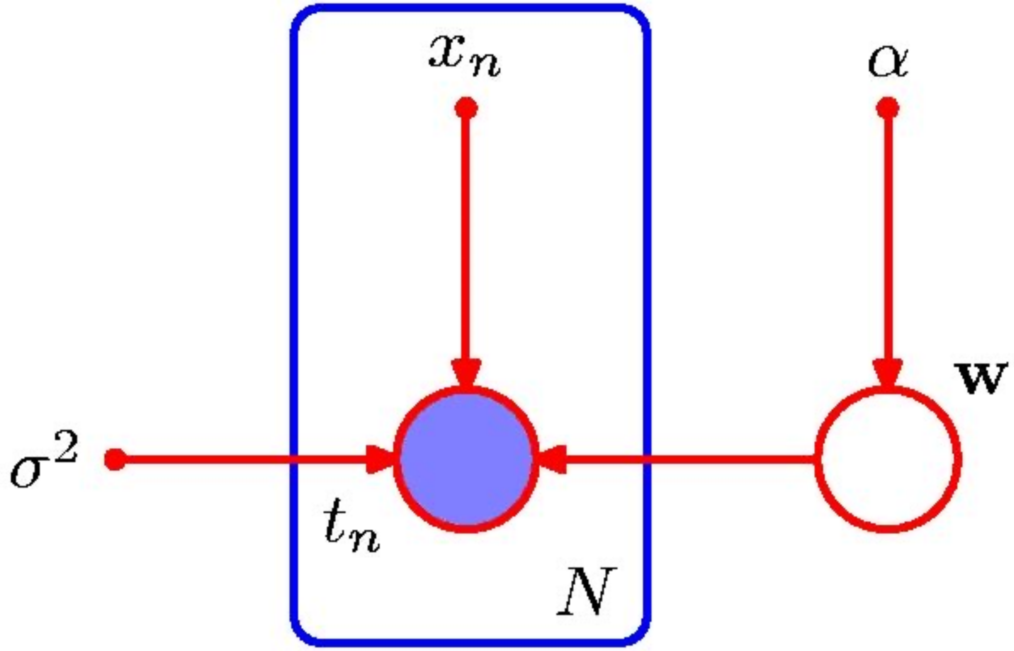
$$p(\mathbf{t}, \mathbf{w} | \mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w}|\alpha) \prod_{n=1}^{N} p(t_n | \mathbf{w}, x_n, \sigma^2).$$



Bayesian Curve Fitting — Learning

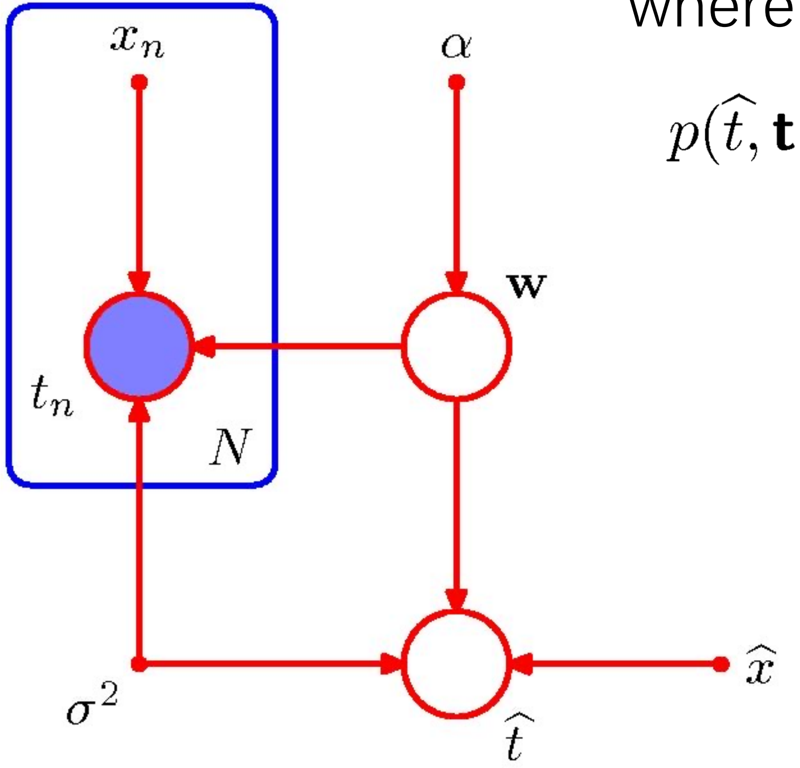
- Condition on data

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



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

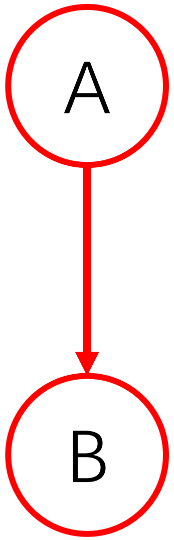
$$p(\widehat{t}, \mathbf{t}, \mathbf{w}|\widehat{x}, \mathbf{x}, \alpha, \sigma^2) =$$
$$\left[\prod_{n=1}^{N} p(t_n|x_n, \mathbf{w}, \sigma^2)\right] p(\mathbf{w}|\alpha) p(\widehat{t}|\widehat{x}, \mathbf{w}, \sigma^2)$$

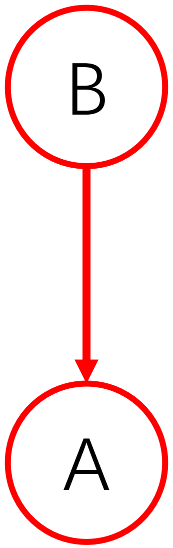
Which model is correct?

A: whether the school bus has a crash

B: whether the teacher is late for the class

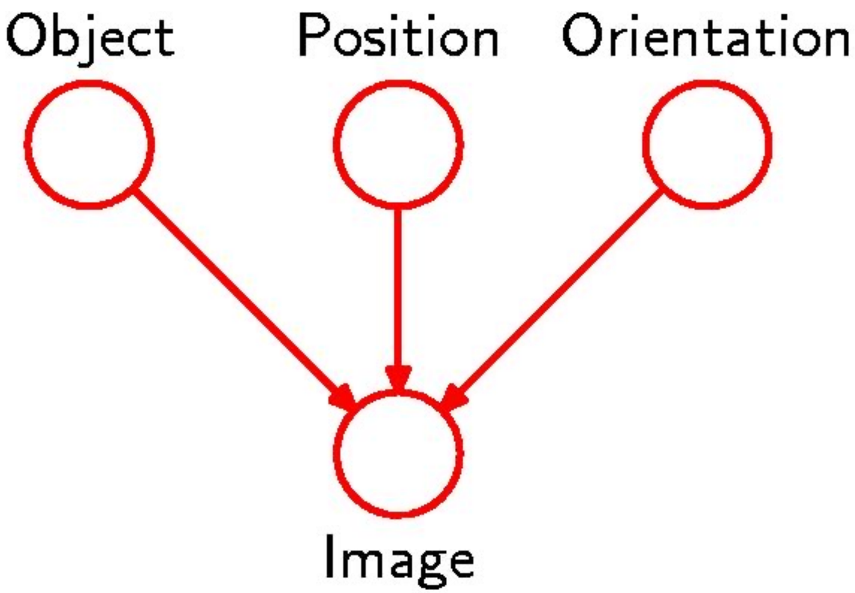
	A= True	A= False
B= True	0.09	0.09
B = False	0.01	0.81





Generative Models

- Causal process for generating images



We will talk about causality in a later lecture!

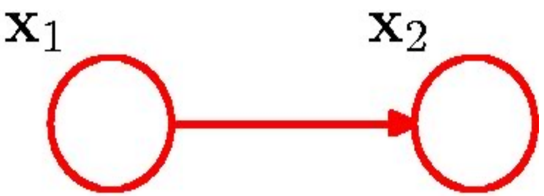
Two Special Cases

- 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

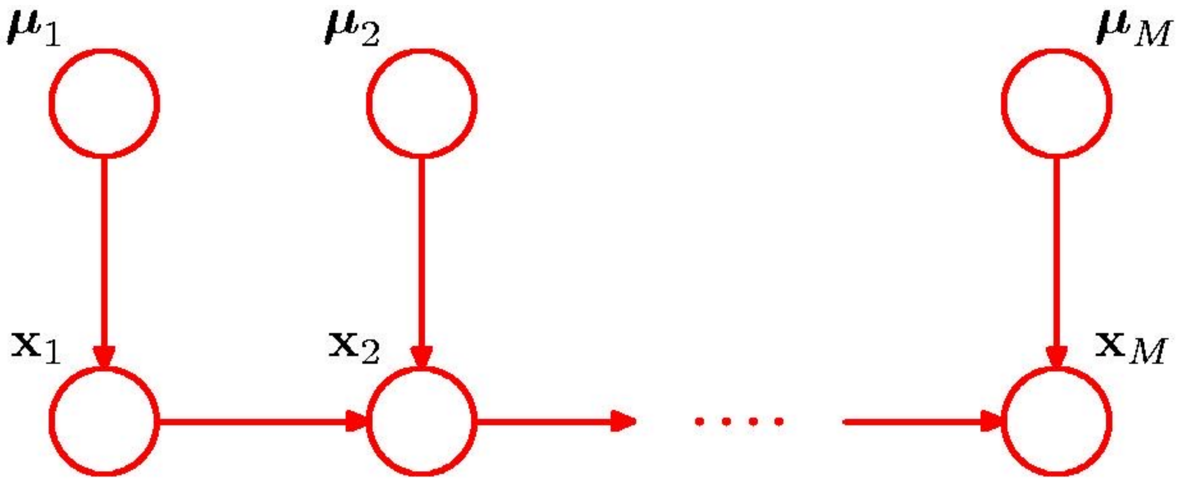
$$\hat{p}(\mathbf{x}_1, \mathbf{x}_2 | \boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_{1k}^{x_{1k}} \prod_{l=1}^{K} \mu_{2l}^{x_{2l}}$$

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



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

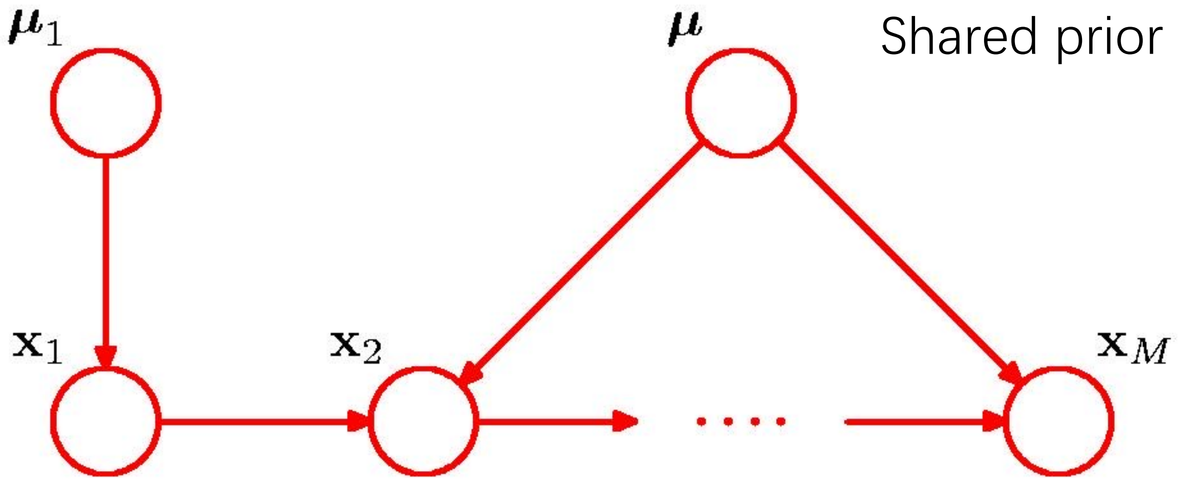
$$p(\boldsymbol{\mu}_m) = \mathrm{Dir}(\boldsymbol{\mu}_m | \boldsymbol{\alpha}_m)$$

Discrete Variables: Bayesian Parameters

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

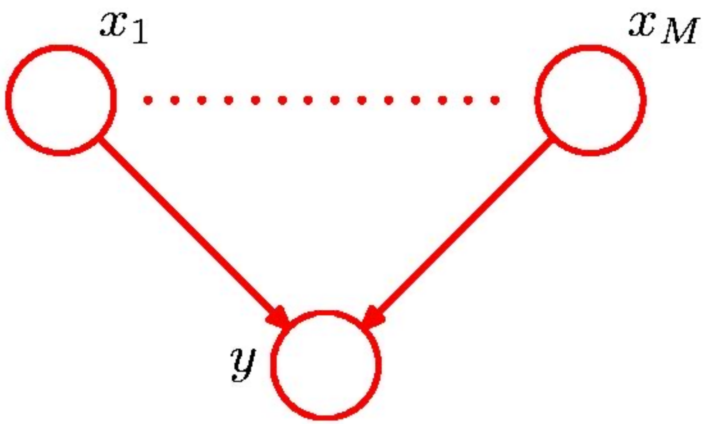
- Further reading: https://towardsdatascience.com/dirichlet-distribution-a82ab942a879

Discrete Variables: Bayesian Parameters



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

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

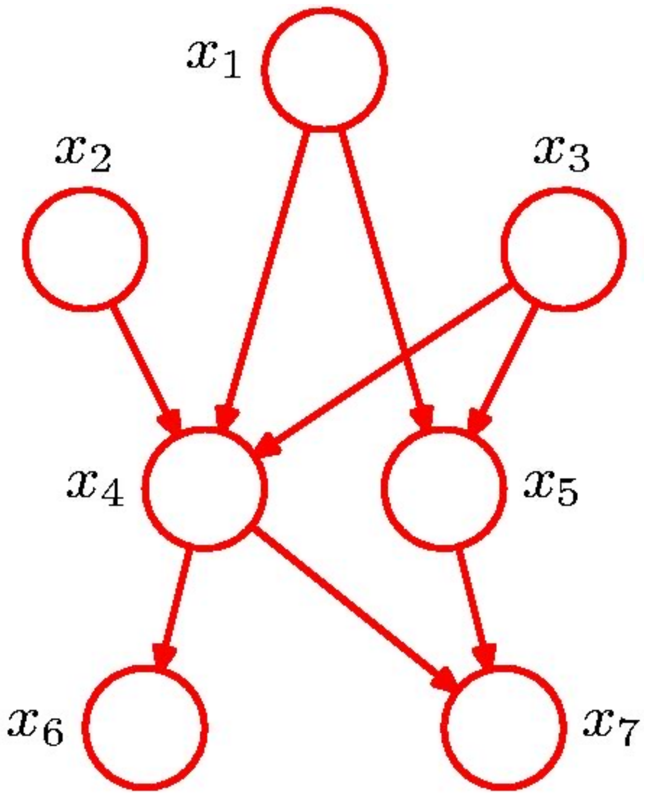
$$p(x_i|\mathrm{pa}_i) = \mathcal{N}\left(x_i \middle| \sum_{j\in\mathrm{pa}_i} w_{ij}x_j + b_i, v_i\right)$$

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

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

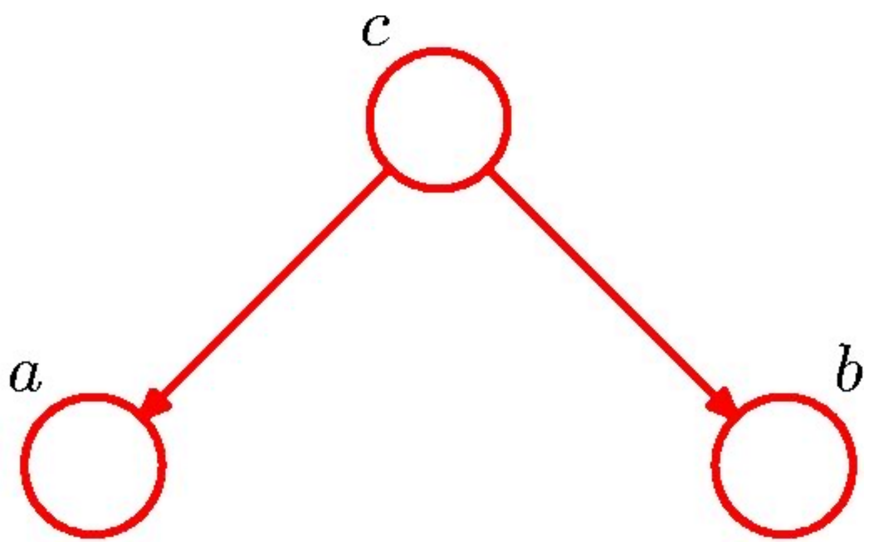
- Equivalently

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

- Notation

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

Conditional Independence: Example 1

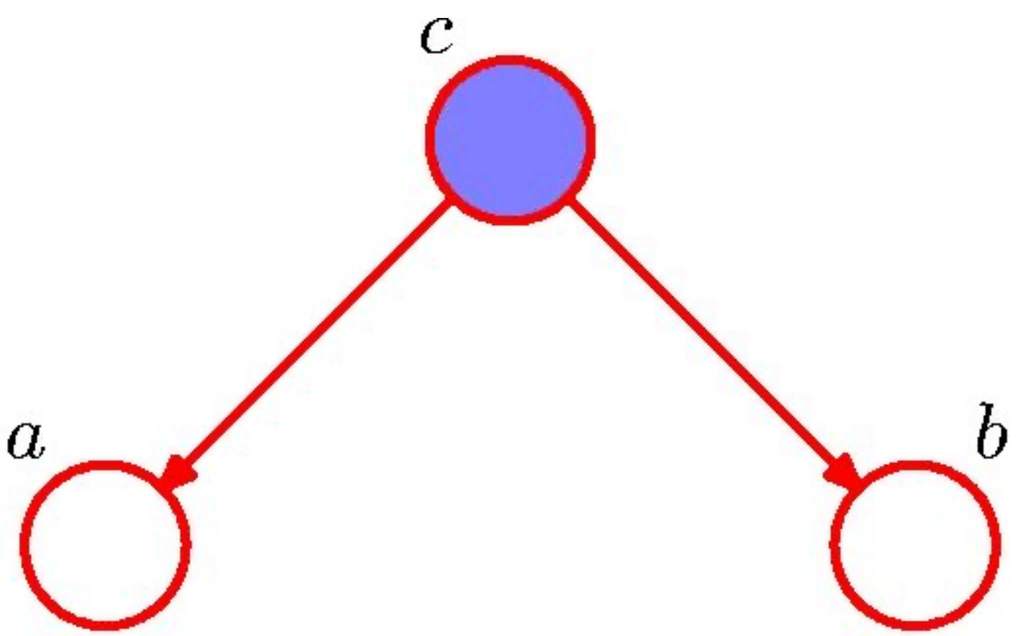


$$p(a,b,c) = p(a|c)p(b|c)p(c)$$

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

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

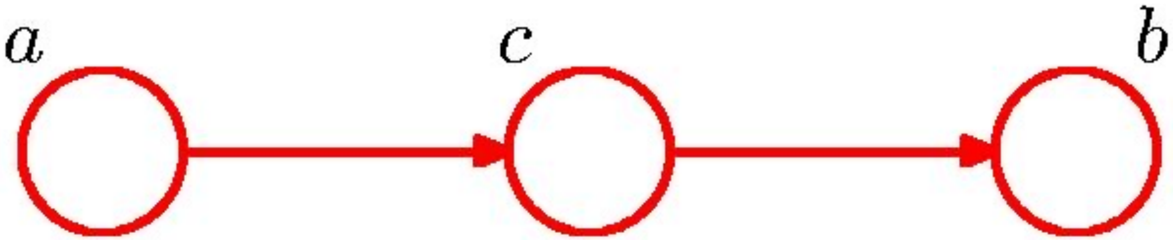
Conditional Independence: Example 1



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

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

Conditional Independence: Example 2

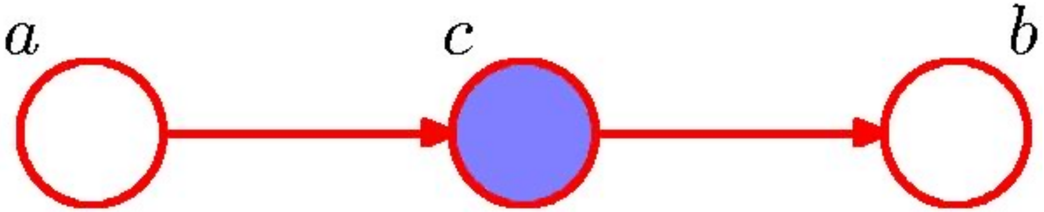


$$p(a, b, c) = p(a)p(c|a)p(b|c)$$

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

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

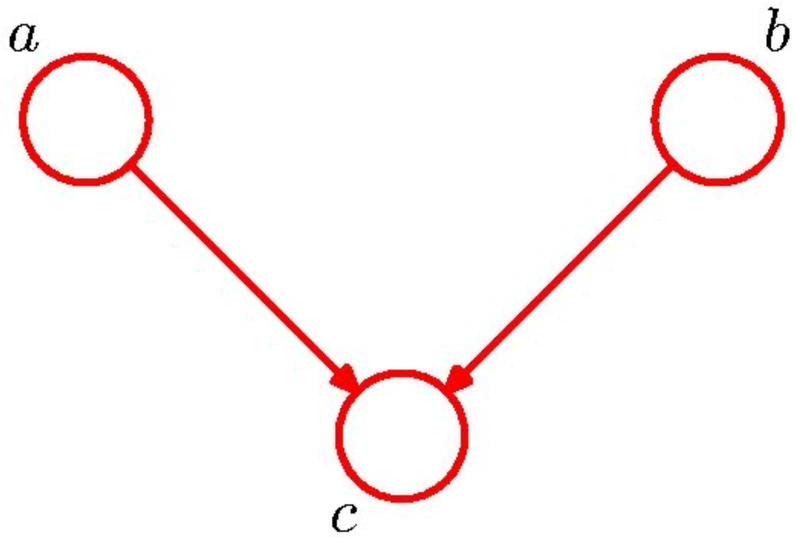
Conditional Independence: Example 2



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

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

Conditional Independence: Example 3



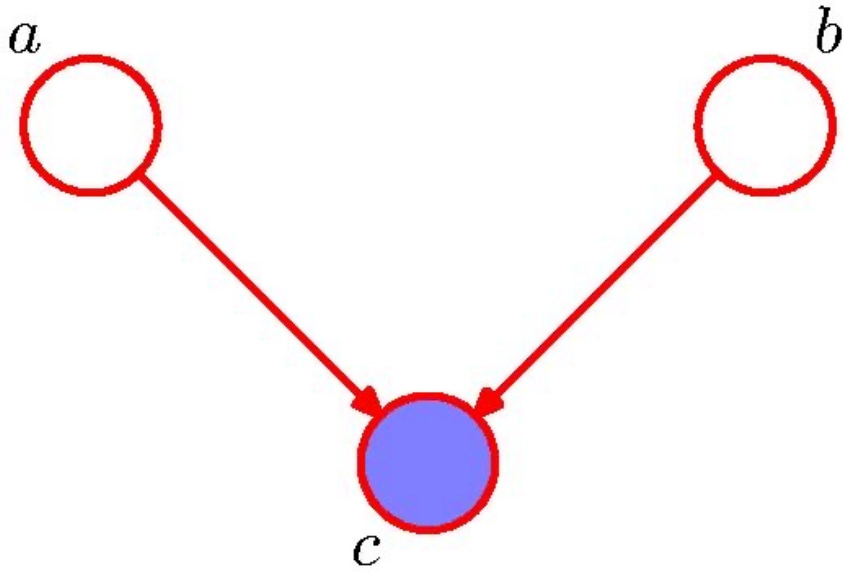
$$p(a, b, c) = p(a)p(b)p(c|a, b)$$

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

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

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

Conditional Independence: Example 3



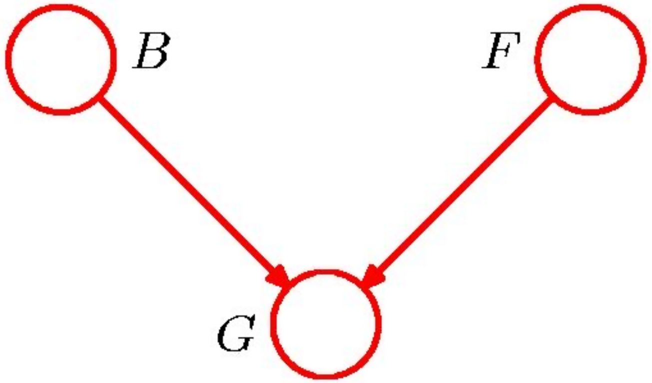
$$
\begin{aligned}
p(a, b|c) &= \frac{p(a, b, c)}{p(c)} \\
&= \frac{p(a)p(b)p(c|a, b)}{p(c)}
\end{aligned}
$$

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

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

“Am I out of fuel?”

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



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

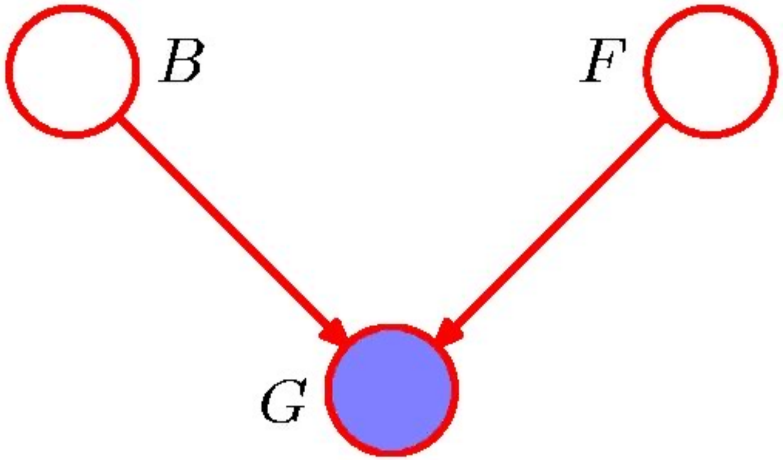
and hence

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

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?”

$$
\begin{aligned}
p(F=0|G=0) &= \frac{p(G=0|F=0)p(F=0)}{p(G=0)} \\
&\simeq 0.257
\end{aligned}
$$

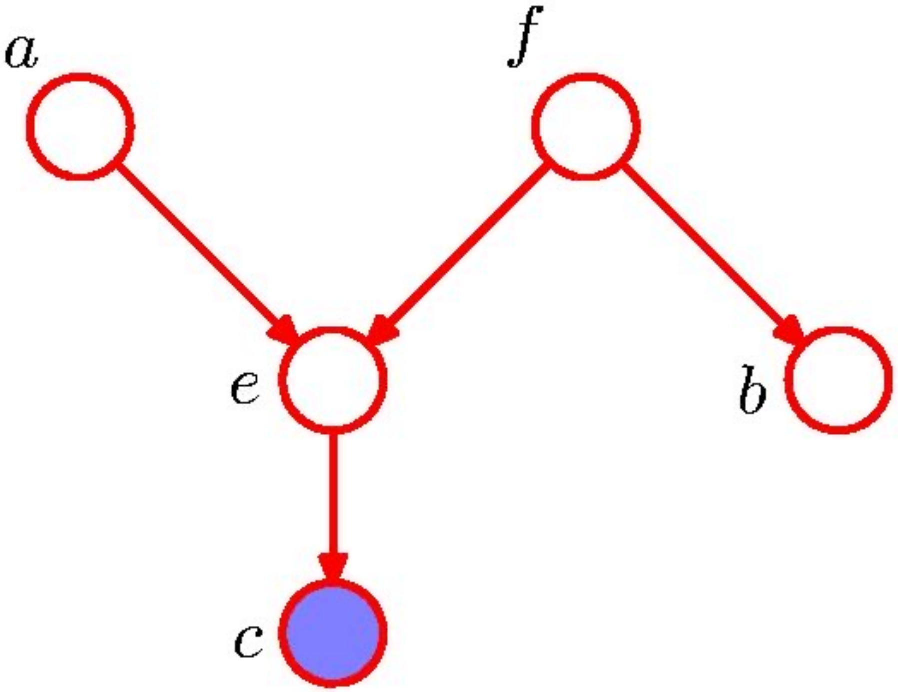


Probability of an empty tank increased by observing G = 0.

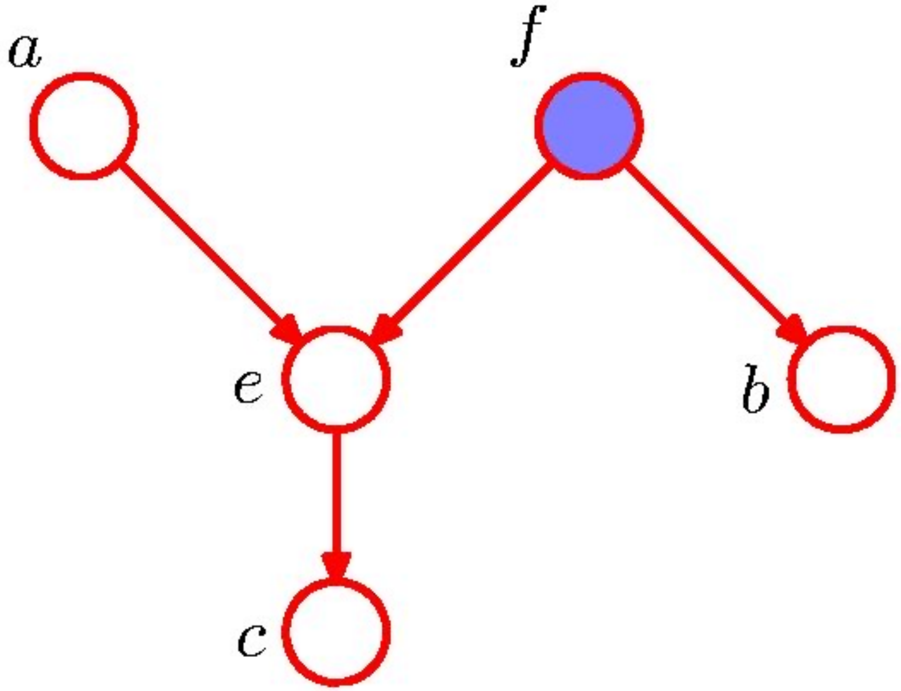
D-separation

- 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

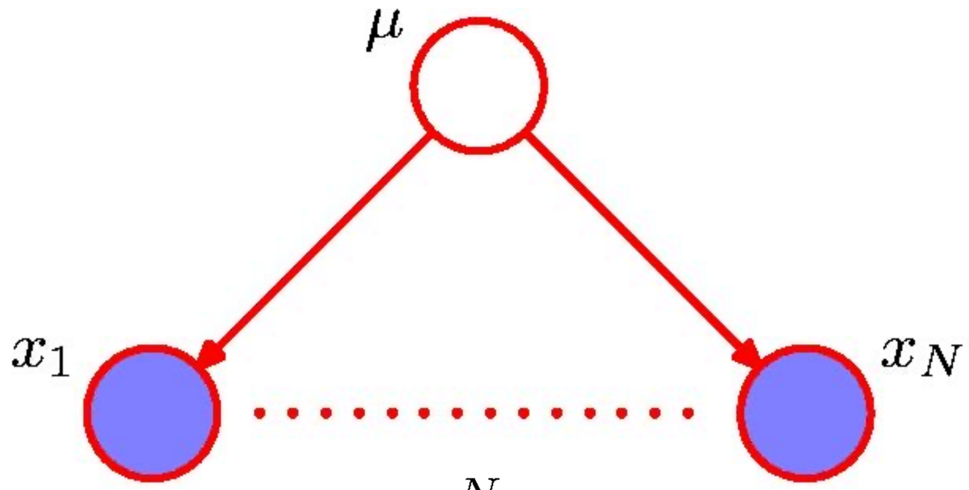


$$a \not\perp\!\!\!\perp b \mid c$$



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

D-separation: I.I.D. Data



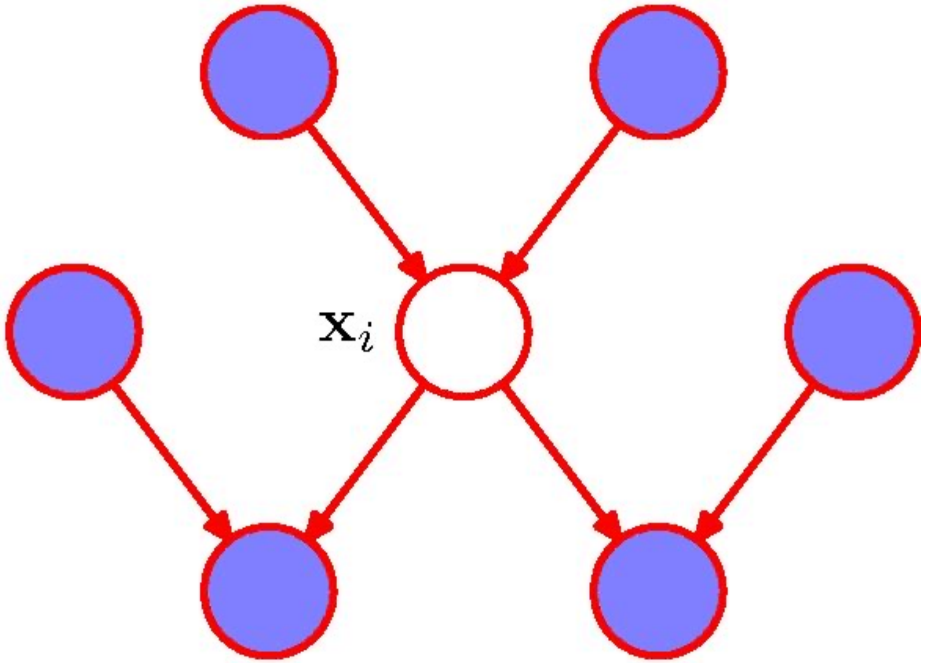
$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu)$$

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

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.

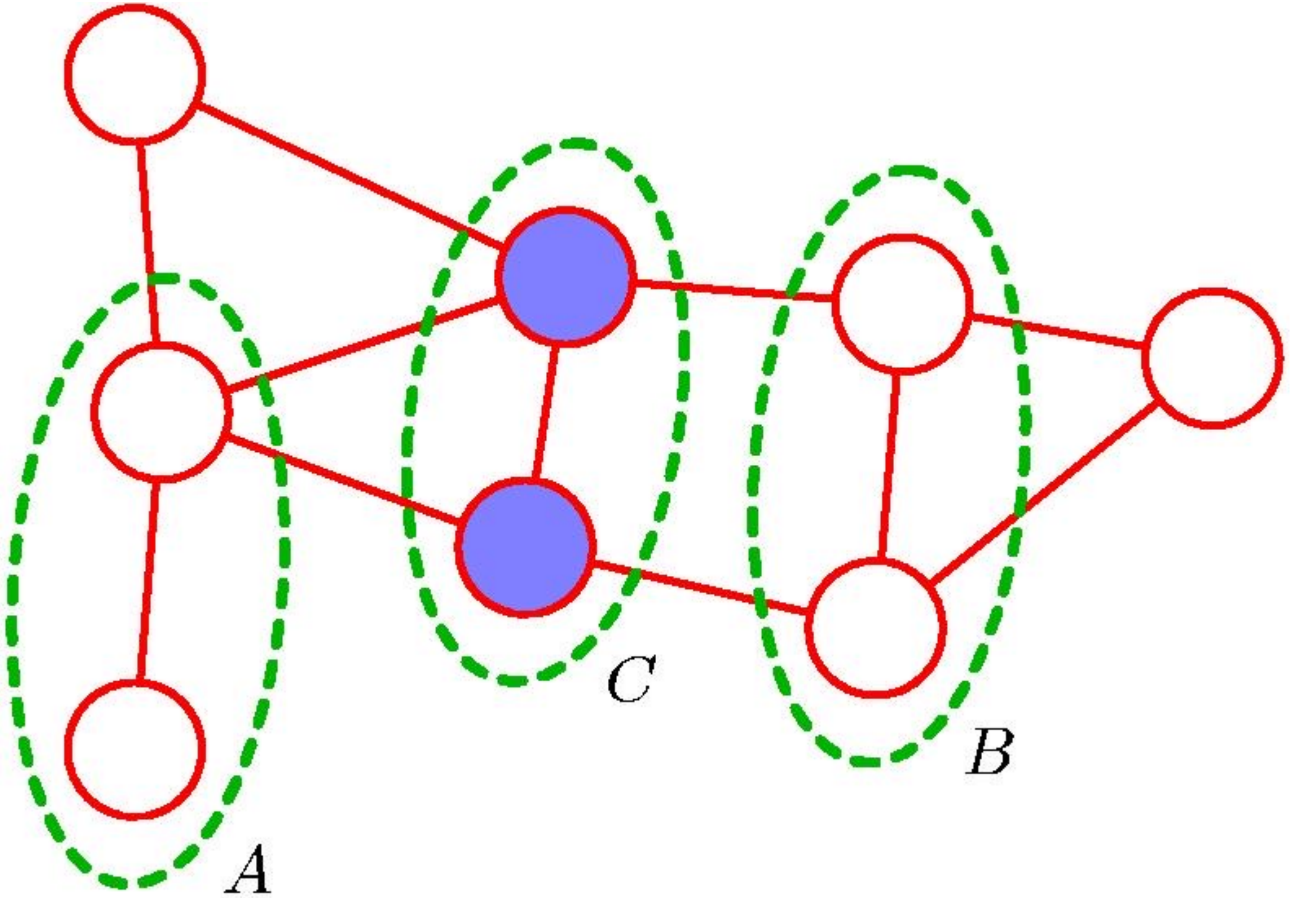
Bayesian Networks: Summary

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

Markov Random Fields

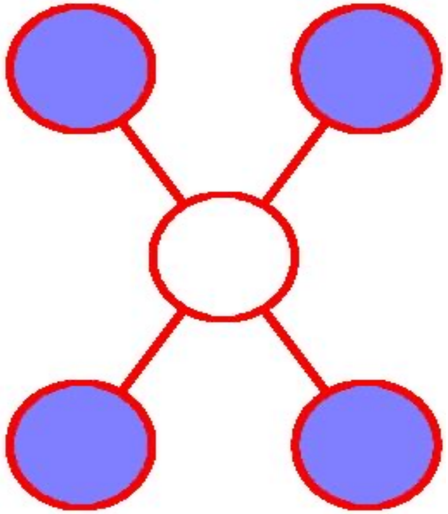
- Undirected
- Markov networks
- One motivation: reasoning about conditional independence is subtle in Bayesian networks. Can we have something simpler?

Markov Random Fields



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

Markov Blanket



Markov Random Fields: Intuitions

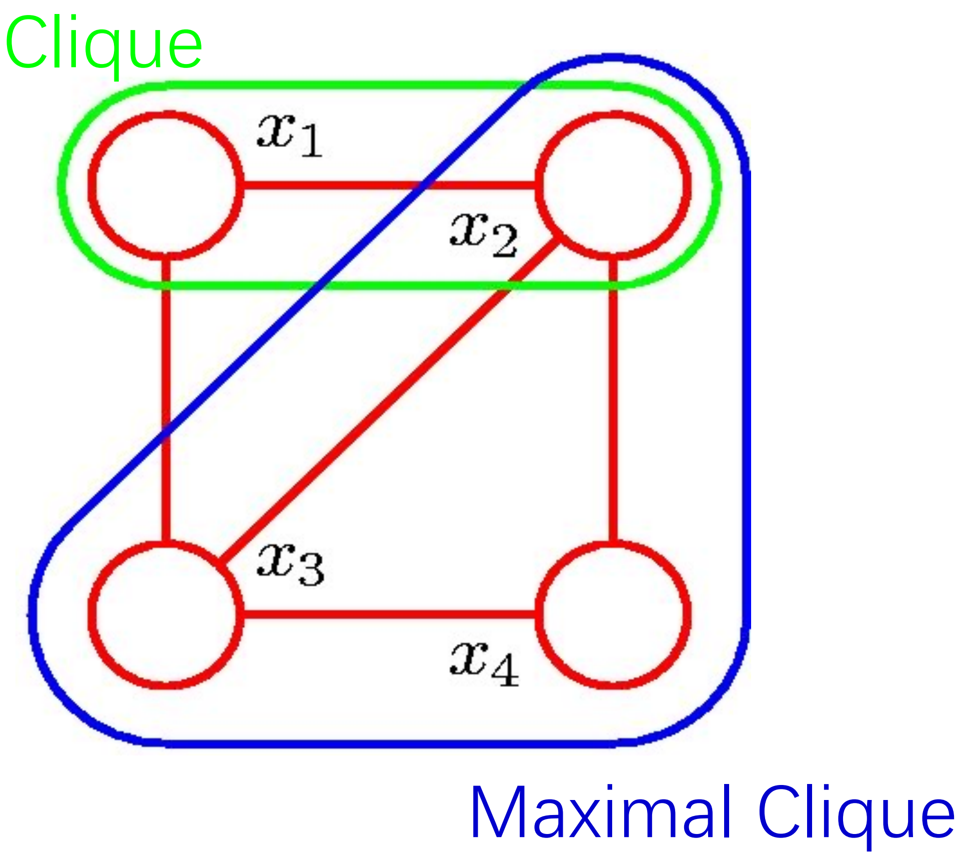
- If x and y are not directly connected, then they should be independent conditioning on the other variables

- $P(x, y \mid V/\{x, y\}) = P(x \mid V/\{x, y\}) * P(y \mid V/\{x, y\})$

- 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

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

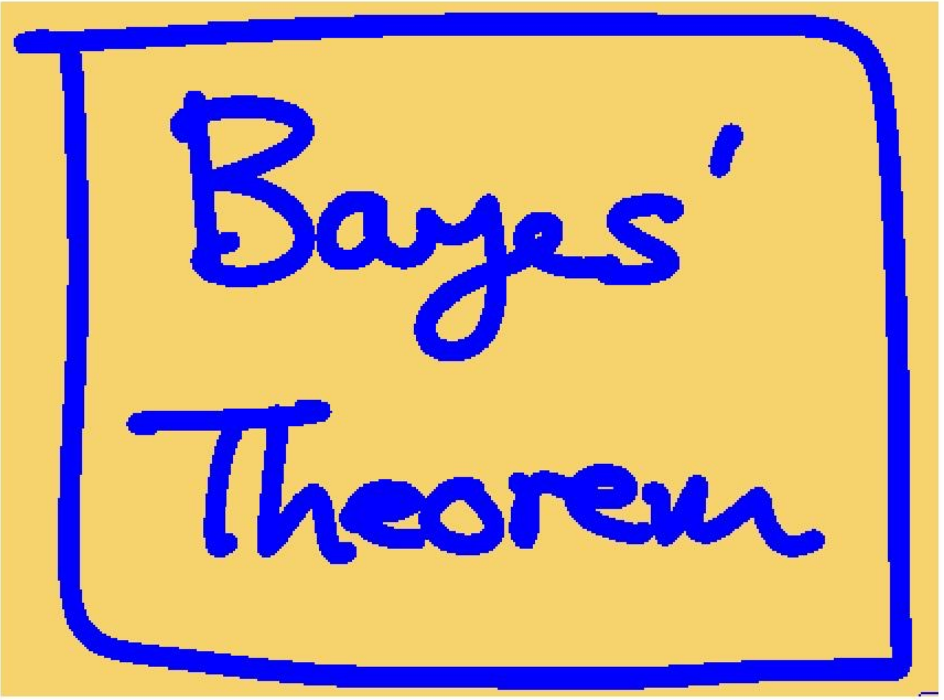
Factorization and Conditional Independence

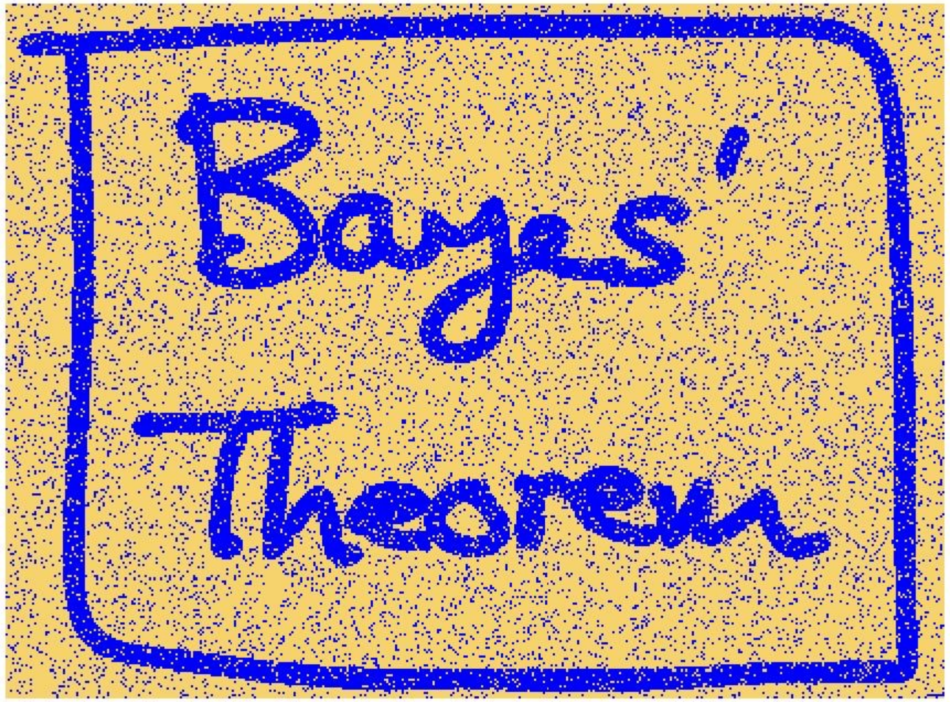
- Given a graph (potential function unknown), let UI be the distributions whose conditional independence fits the graph

- 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





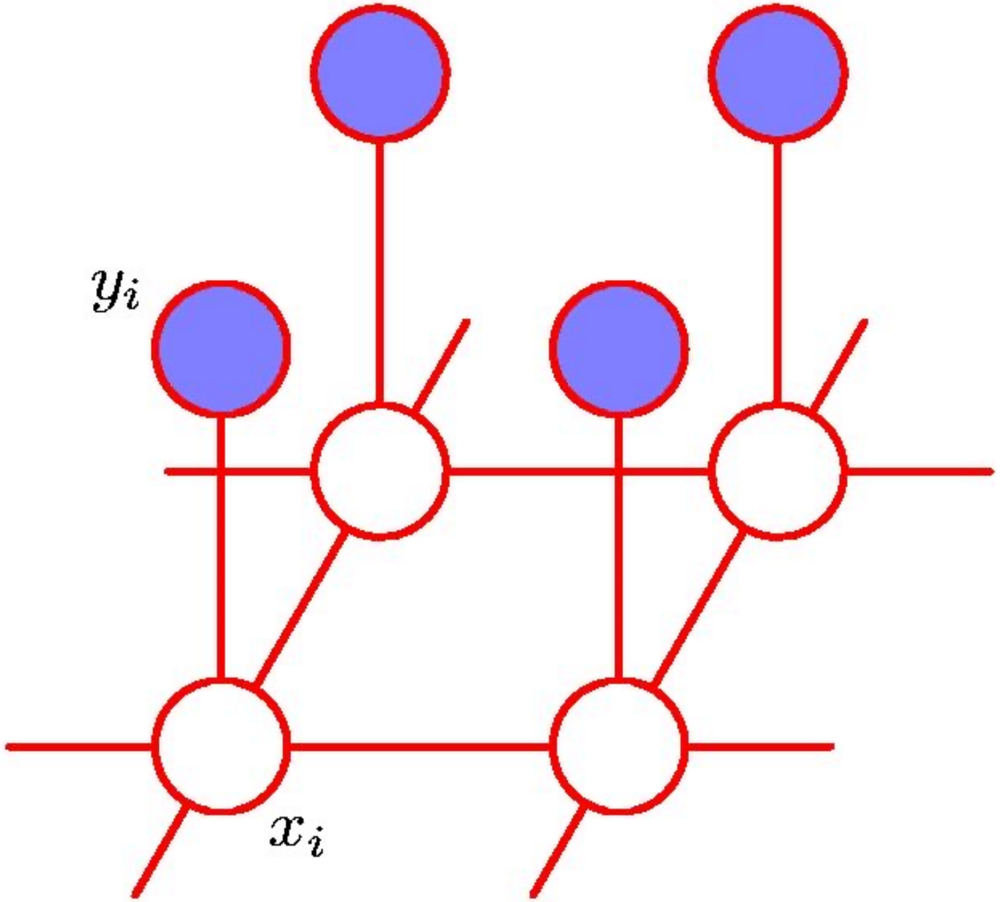
Original Image

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

Noisy Image

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

Illustration: Image De-Noising



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

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

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