10417/10617
Intermediate Deep Learning:
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https://deeplearning-cmu-10417.github.io/

Graphical Models I

Graphical Models

- Probabilistic graphical models provide a powerful framework for representing dependency structure between random variables.

- Graphical models offer several useful properties:

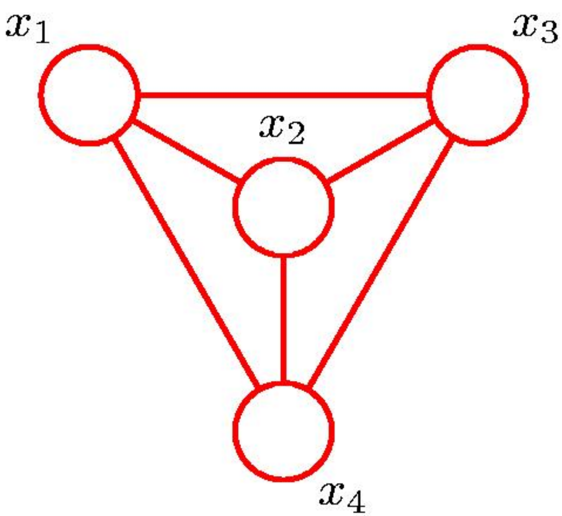
  - They provide a simple way to visualize the structure of a probabilistic model and can be used to motivate new models.

  - They provide various insights into the properties of the model, including conditional independence.

  - Complex computations (e.g. inference and learning in sophisticated models) can be expressed in terms of graphical manipulations.

Graphical Models

• A graph contains a set of nodes (vertices) connected by links (edges or arcs)



• In a probabilistic graphical model, each node represents a random variable, and links represent probabilistic dependencies between random variables.

• The graph specifies the way in which the joint distribution over all random variables decomposes into a product of factors, where each factor depends on a subset of the variables.

• Two types of graphical models:

- Bayesian networks, also known as Directed Graphical Models (the links have a particular directionality indicated by the arrows)
- Markov Random Fields, also known as Undirected Graphical Models (the links do not carry arrows and have no directional significance).

• Hybrid graphical models that combine directed and undirected graphical models, such as Deep Belief Networks.

Bayesian Networks

- Directed Graphs are useful for expressing causal relationships between random variables.

- Let us consider an arbitrary joint distribution $p(a,b,c)$ over three random variables a,b, and c.

- Note that at this point, we do not need to specify anything else about these variables (e.g. whether they are discrete or continuous).

- By application of the product rule of probability (twice), we get

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

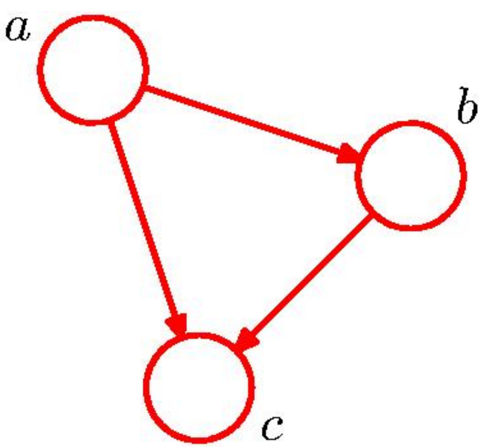
- This decomposition holds for any choice of the joint distribution.

Bayesian Networks

- By application of the product rule of probability (twice), we get

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

- Represent the joint distribution in terms of a simple graphical model:



- Introduce a node for each of the random variables.
- Associate each node with the corresponding conditional distribution in above equation.
- For each conditional distribution we add directed links to the graph from the nodes corresponding to the variables on which the distribution is conditioned.

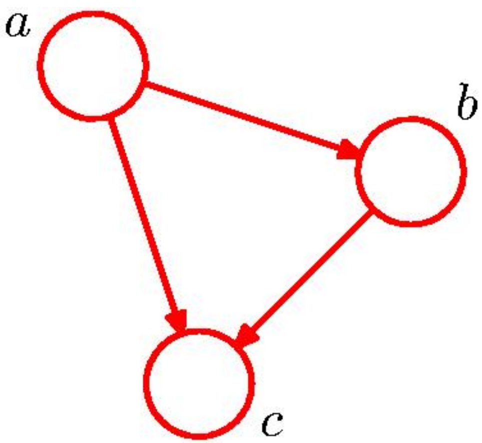
- Hence for the factor $p(c|a,b)$, there will be links from nodes a and b to node c.
- For the factor $p(a)$, there will be no incoming links.

Bayesian Networks

- By application of the product rule of probability (twice), we get

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

- If there is a link going from node a to node b, then we say that:



  - node a is a parent of node b.
  - node b is a child of node a.

- For the decomposition, we choose a specific ordering of the random variables: a,b,c.

- If we chose a different ordering, we would get a different graphical representation (we will come back to that point later).

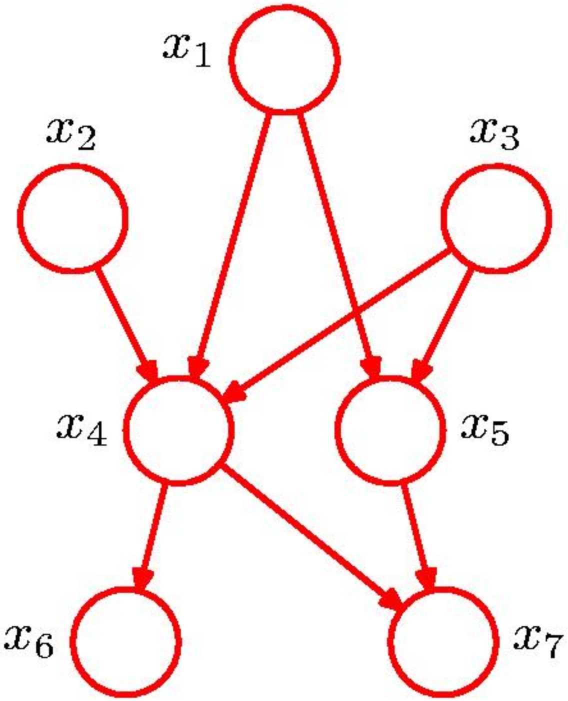
- The joint distribution over K variables factorizes:

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

- If each node has incoming links from all lower numbered nodes, then the graph is fully connected; there is a link between all pairs of nodes.

Bayesian Networks

- Absence of links conveys certain information about the properties of the class of distributions that the graph conveys.



- Note that this graph is not fully connected (e.g. there is no link from x_1 to x_2).

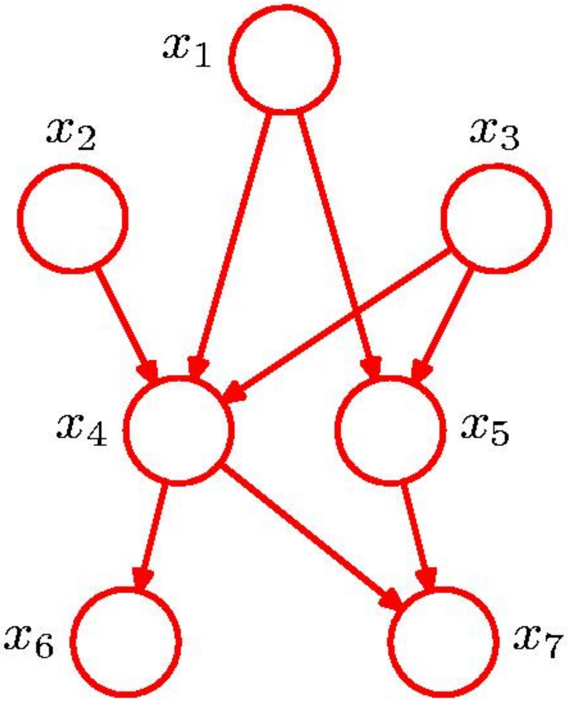
- The joint distribution over $x_1,\ldots,x_7$ can be written as a product of a set of conditional distributions.

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

- Note that according to the graph, x_5 will be conditioned only on x_1 and x_3.

Factorization Property

• The joint distribution defined by the graph is given by the product of a conditional distribution for each node conditioned on its parents:



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

where pa_k denotes a set of parents for the node x_k.

• This equation expresses a key factorization property of the joint distribution for a directed graphical model.

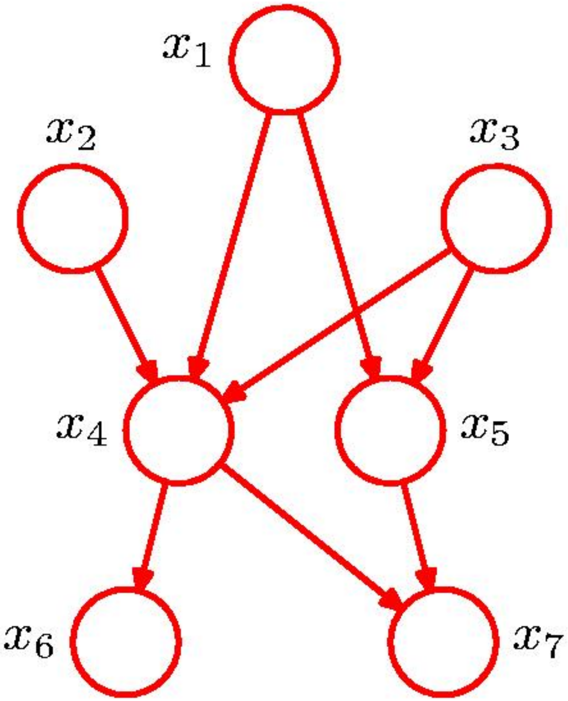
• Important restriction: There must be **no directed cycles!**

• Such graphs are also called directed acyclic graphs (DAGs).

Ancestral Sampling

- Consider a joint distribution over K random variables $p(x_1, x_2, ..., x_K)$ that factorizes as:

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



- Our goal is draw a sample from this distribution.
- Start at the top and sample in order.

$$\hat{x}_1 \sim p(x_1)$$
$$\hat{x}_2 \sim p(x_2)$$
$$\hat{x}_3 \sim p(x_3)$$
$$\hat{x}_4 \sim p(x_4|\hat{x}_1, \hat{x}_2, \hat{x}_3)$$
$$\hat{x}_5 \sim p(x_5|\hat{x}_1, \hat{x}_3)$$

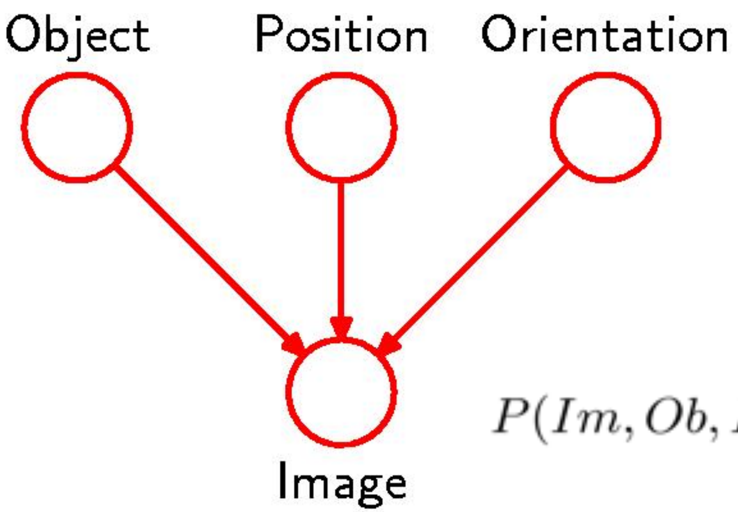
The parent variables are set to their sampled values

- To obtain a sample from the marginal distribution, e.g. $p(x_2, x_5)$, we sample from the full joint distribution, retain $\hat{x}_2, \hat{x}_5$, and discard the remaining values.

Generative Models

- Higher-level nodes will typically represent latent (hidden) random variables.
- The primary role of the latent variables is to allow a complicated distribution over observed variables to be constructed from simpler (typically exponential family) conditional distributions.

Generative Model of an Image



- Object identity, position, and orientation have independent prior probabilities.
- The image has a probability distribution that depends on the object identity, position, and orientation (likelihood function).

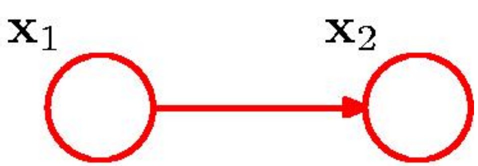
$$P(Im, Ob, Po, Or) = \underbrace{P(Im|Ob, Po, Or)}_{\text{Likelihood}}\underbrace{P(Ob)P(Po)P(Or)}_{\text{Prior}}$$

- The graphical model captures the causal process, by which the observed data was generated (hence the name generative models).

Discrete Variables

• We now examine the discrete random variables.

• Assume that we have two discrete random variables x_1 and x_2, each of which has K states.



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

• Using 1-of-K encoding, we denote the probability of observing both $x_{1k}=1$, $x_{2l}=1$ by the parameter μ_{kl}, where x_{1k} denotes the k^{th} component of x_1 (similarly for x_2).

• This distribution is governed by $K^2 - 1$ parameters.

• The total number of parameters that must be specified for an arbitrary joint distribution over M random variables is K^M-1 (corresponds to a fully connected graph).

• Grows exponentially in the number of variables M!

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.

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

- We dropped the link between the nodes, so each variables is described by a separate multinomial distribution.

Discrete Variables

- In general:
  - Fully connected graphs have completely general distributions and have exponential K^M-1 number of parameters (too complex).
  - If there are no links, the joint distribution fully factorizes into the product of the marginals, and has M(K-1) parameters (too simple).
  - Graphs that have an intermediate level of connectivity allow for more general distributions compared to the fully factorized one, while requiring fewer parameters than the general joint distribution.

- Let us look at the example of the chain graph.

Chain Graph

• Consider an M-node Markov chain:

• The marginal distribution $p(\mathbf{x}_1)$ requires K-1 parameters.

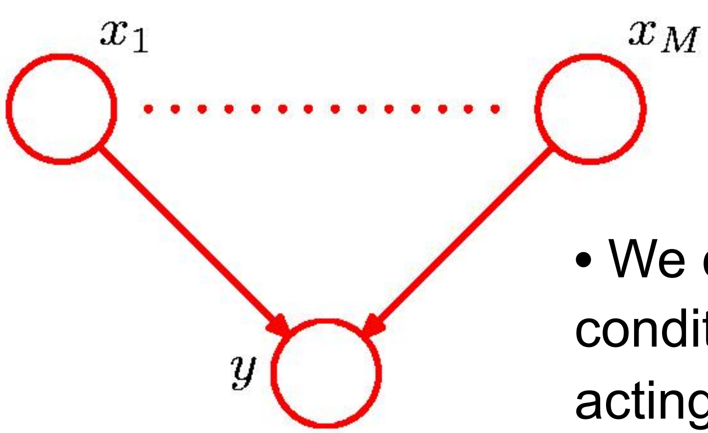
• The remaining conditional distributions $p(\mathbf{x}_i|\mathbf{x}_{i-1}), i = 2, ..., M$ require K(K-1) parameters.

• Total number of parameters: K-1 + (M-1)(K-1)K, which is quadratic in K and linear in the length M of the chain.

• This graphical model forms the basis of a simple Hidden Markov Model.

Parameterized Models

- We can use parameterized models to control exponential growth in the number of parameters.



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.

- We can obtain a more parsimonious form of the conditional distribution by using a logistic function acting on a linear combination of the parent variables:

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

- This is a more restricted form of conditional distribution, but it requires only M+1 parameters (linear growth in the number of parameters).

Linear Gaussian Models

- So far we worked with joint probability distributions over a set of discrete random variables (expressed as nodes in directed acyclic graphs).

- We now show how a multivariate Gaussian distribution can be expressed as a directed graph corresponding to a linear Gaussian model.

- Consider an arbitrary acyclic graph over D random variables, in which each node represent a single continuous Gaussian distribution with its mean given by the linear function of the parents:

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

where w_{ij} and b_i are parameters governing the mean, and v_i is the variance.

Linear Gaussian Models

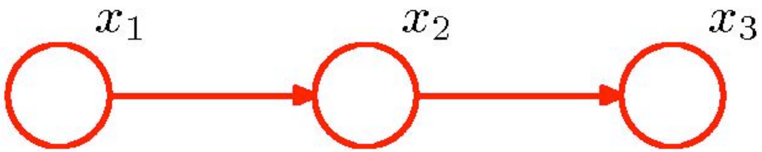
- The log of the joint distribution takes form:

$$\ln p(\mathbf{x}) = \sum_{i=1}^{D} \ln p(x_i|\mathrm{pa}_i) = -\sum_{i=1}^{D} \frac{1}{2v_i} \left(x_i - \sum_{j\in \mathrm{pa}_i} w_{ij}x_j - b_i \right)^2 + \mathrm{const},$$

where 'const' denotes terms independent of x.

- This is a quadratic function of x, and hence the joint distribution p(x) is a multivariate Gaussian.

- For example, consider a directed graph over three Gaussian variables with one missing link:



Computing the Mean

- We can determine the mean and covariance of the joint distribution. Remember:

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

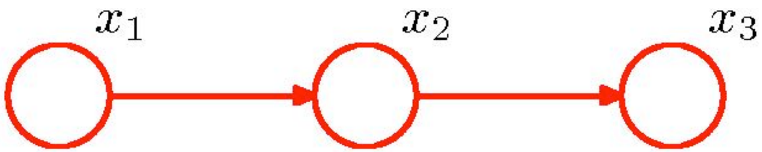
hence

$$x_i = \sum_{j \in \mathrm{pa}_i} w_{ij} x_j + b_i + \sqrt{v_i}\epsilon_i, \qquad \epsilon_i \sim \mathcal{N}(0,1),$$

so its expected value:

$$\mathbb{E}[x_i] = \sum_{j \in \mathrm{pa}_i} w_{ij} \mathbb{E}[x_j] + b_i.$$

- Hence we can find components: $\mathbb{E}[\mathbf{x}] = \left[\mathbb{E}[x_1], ..., \mathbb{E}[x_D]\right]$ by doing ancestral pass: start at the top and proceed in order (see example):



Computing the Covariance

- We can obtain the i,j element of the covariance matrix in the form of a recursion relation:

$$\begin{aligned}\mathrm{cov}[x_i, x_j] &= \mathbb{E}\left[(x_i - \mathbb{E}[x_i])(x_j - \mathbb{E}[x_j])\right] \\ &= \mathbb{E}\left[(x_i - \mathbb{E}[x_i])\left(\sum_{k \in \mathrm{pa}_j} w_{jk}(x_k - \mathbb{E}[x_k]) + \sqrt{v_i}\epsilon_j\right)\right] \\ &= \sum_{k \in \mathrm{pa}_j} w_{jk}\mathrm{cov}[x_i, x_k] + I_{ij}v_j.\end{aligned}$$

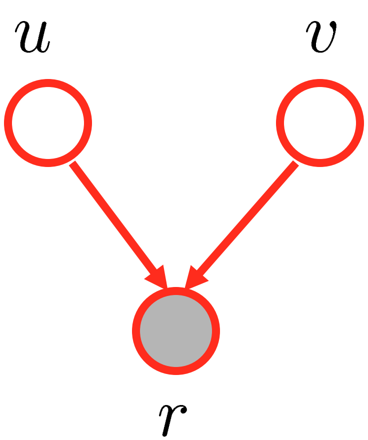
- Consider two cases:

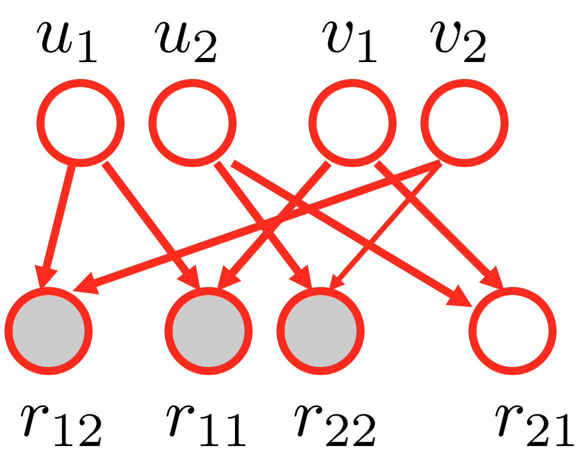
- There are no links in the graph (graph is fully factorized), so that w_{ij}'s are zero. In this case: $\mathbb{E}[\mathbf{x}] = \left[b_1, ..., b_D\right]^T$, and the covariance is diagonal $\mathrm{diag}(v_1, ..., v_D)$. The joint distribution represents D independent univariate Gaussian distributions.

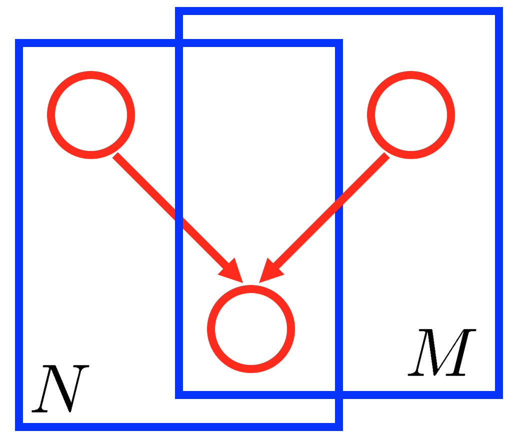
- The graph is fully connected. The total number of parameters is D + D(D-1)/2. The covariance corresponds to a general symmetric covariance matrix.

Bilinear Gaussian Model

- Consider the following model:







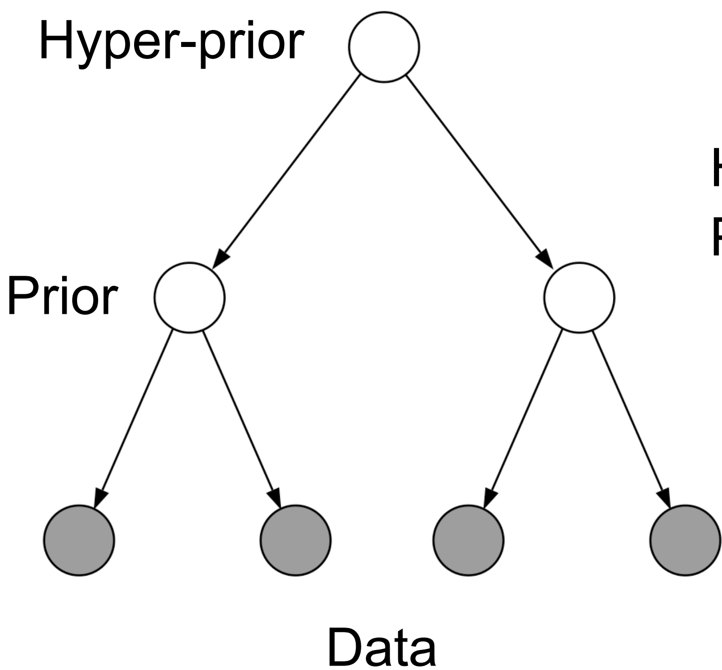
$$u \sim \mathcal{N}(0,1),$$
$$v \sim \mathcal{N}(0,1),$$
$$r \sim \mathcal{N}(uv,1).$$

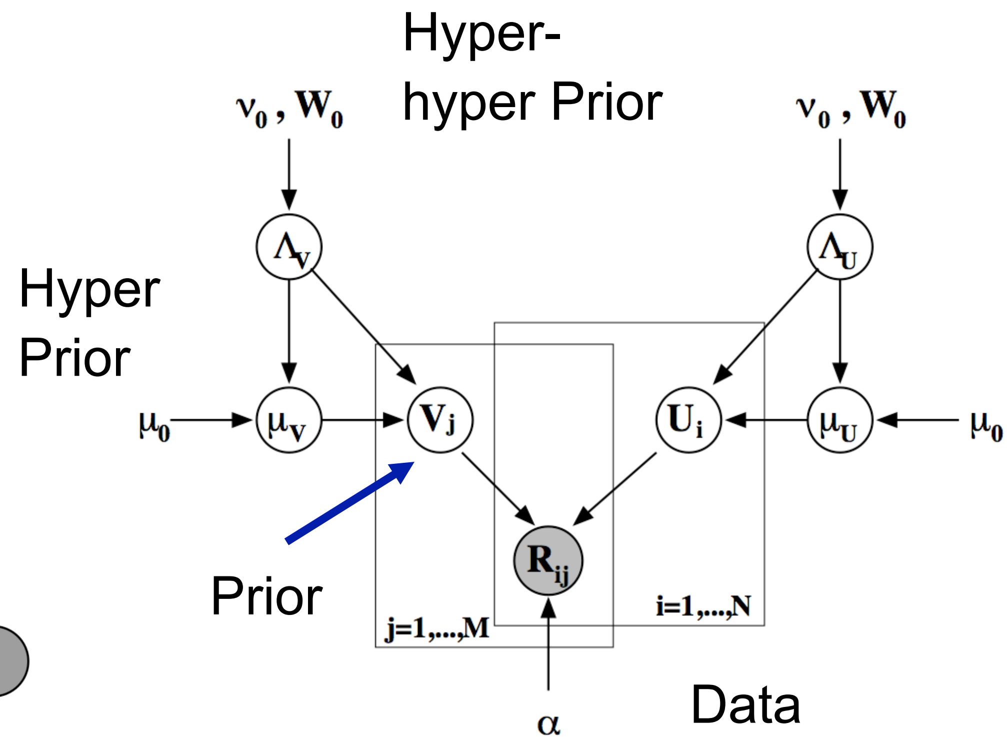
Gaussian terms

$$u_i \sim \mathcal{N}(0,1), \; i = 1, ..., N$$
$$v_j \sim \mathcal{N}(0,1), \; j = 1, ..., M$$
$$r_{ij} \sim \mathcal{N}(u_i v_j, 1).$$

- The mean is given by the product of two Gaussians.

Hierarchical Models





Conditional Independence

- We now look at the concept of conditional independence.
- a is independent of b given c:

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

- Equivalently:

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

- We will use the notation:

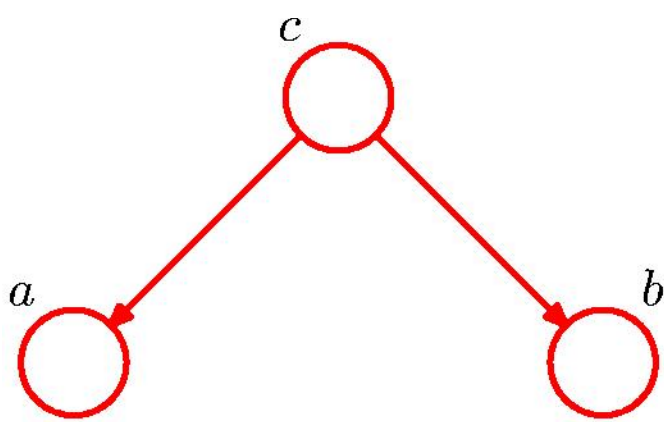
$$a \perp\!\!\!\perp b \mid c$$

- An important feature of graphical models is that conditional independence properties of the joint distribution can be read directly from the graph without performing any analytical manipulations

- The general framework for achieving this is called d-separation, where d stands for ‘directed’ (Pearl 1988).

Example 1: Tail-to-Tail Node

- The joint distribution over three variables can be written:



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

- If none of the variables are observed, we can examine whether a and b are independent:

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

- In general, this does not factorize into the product $p(a,b) = p(a)p(b)$.

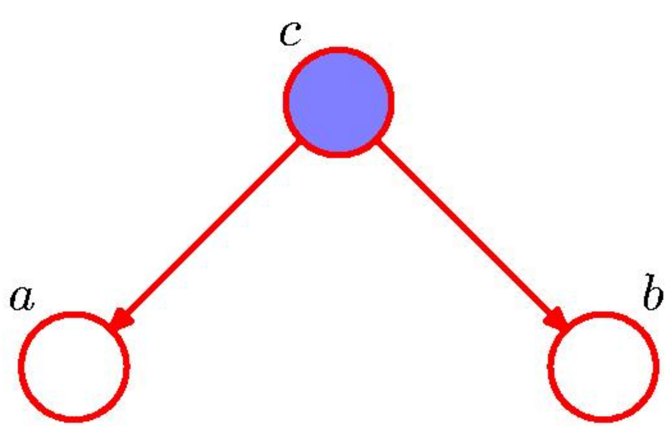
$$a \not\perp\!\!\!\perp b \mid \emptyset$$

- a and b have a common cause.

- The node c is said to be tail-to-tail node with respect to this path (the node is connected to the tails of the two arrows).

Example 1: Tail-to-Tail Node

- Suppose we condition on the variable c:



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

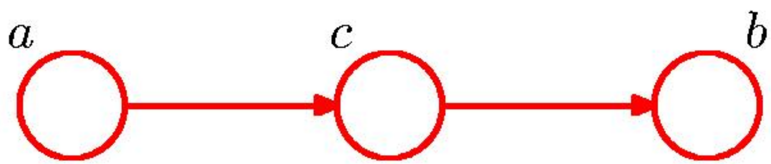
- We obtain conditional independence property:

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

- Once c has been observed, a and b can no longer have any effect on each other. They become independent.

Example 2: Head-to-Tail Node

- The joint distribution over three variables can be written:



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

- If none of the variables are observed, we can examine whether a and b are independent:

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

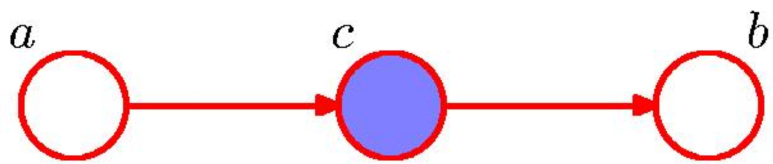
$$a \not\perp\!\!\!\perp b \mid \emptyset$$

- If c is not observed, a can influence c, and c can influence b.

- The node c is said to be head-to-tail node with respect to the path from node a to node b.

Example 2: Head-to-Tail Node

- Suppose we condition on the variable c:



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

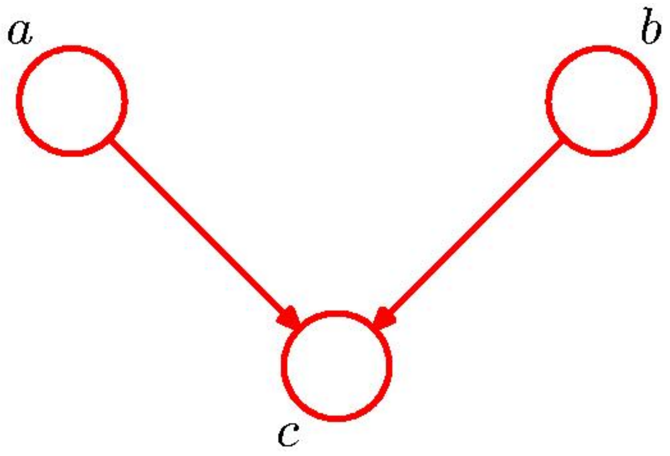
- We obtain conditional independence property:

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

- If c is observed, the value of a can no longer influence b.

Example 3: Head-to-Head Node

- The joint distribution over three variables can be written:



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

- If none of the variables are observed, we can examine whether a and b are independent:

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

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

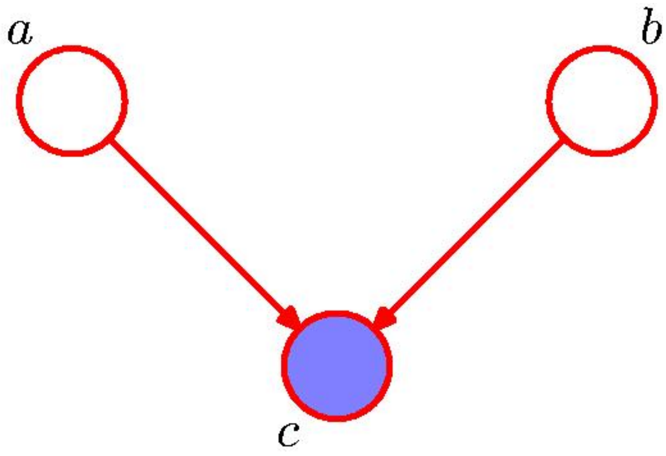
- Opposite to Example 1.

- An unobserved descendant has no effect.

- The node c is said to be head-to-head node with respect to the path from a to b (because it connects to the heads of two arrows).

Example 3: Head-to-Head Node

- Suppose we condition on the variable c:



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

- In general, this does not factorize into the product.

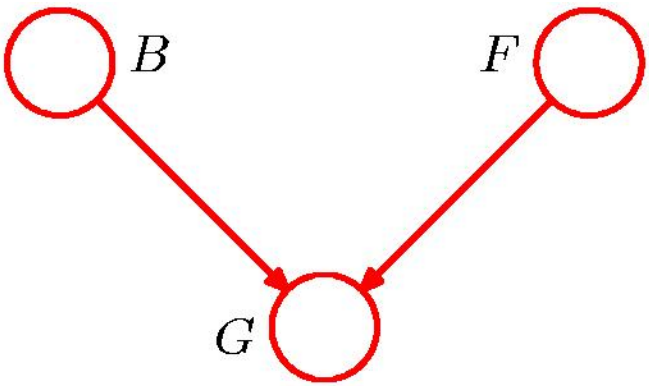
$$a \not\perp\!\!\!\perp b \mid c$$

- Opposite to Example 1.

- If the descendant (or any of its descendants) is observed, its value has implications for both a and b,

Fuel Example

- Consider the following example over three binary random variables:



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

and hence

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

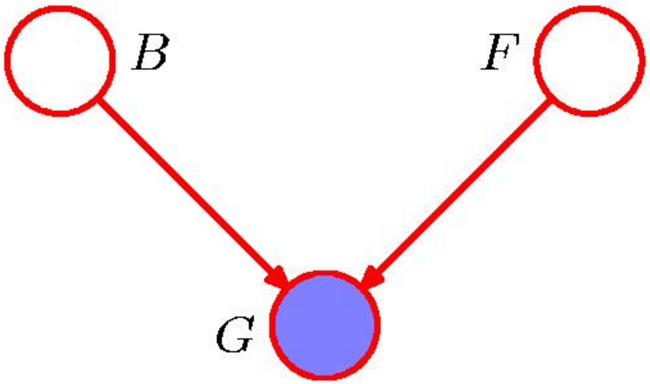
B = Battery (0=dead, 1=fully charged)
F = Fuel Tank (0=empty, 1=full)
G = Fuel Gauge Reading (0=empty, 1=full)

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

Fuel Example

- Suppose that we observe that the Fuel Gauge Reading is empty G = 0.

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



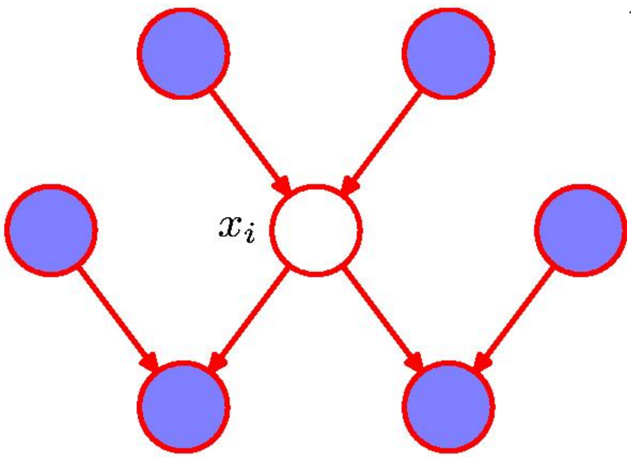
- Probability of an empty tank increased by observing G = 0.

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

Markov Blanket in Directed Models

- The Markov blanket of a node is the minimal set of nodes that must be observed to make this node independent of all other nodes

- In a directed model, the Markov blanket includes parents, children and co-parents (i.e. all the parents of the node's children) due to explaining away.

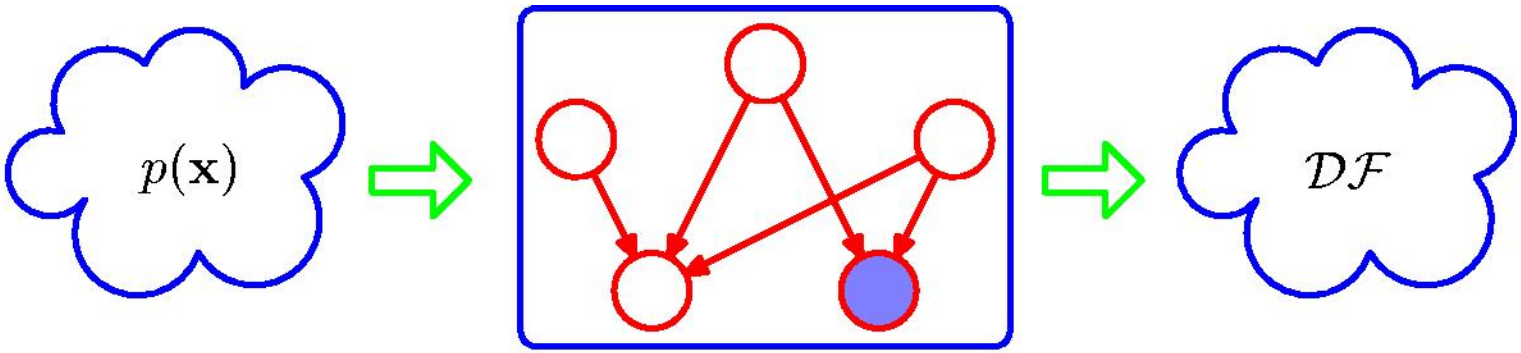


$$p(\mathbf{x}_i|\mathbf{x}_{\{j\neq i\}}) = \frac{p(\mathbf{x}_1,\ldots,\mathbf{x}_M)}{\int p(\mathbf{x}_1,\ldots,\mathbf{x}_M)\,\mathrm{d}\mathbf{x}_i} = \frac{\prod_k p(\mathbf{x}_k|\mathrm{pa}_k)}{\int \prod_k p(\mathbf{x}_k|\mathrm{pa}_k)\,\mathrm{d}\mathbf{x}_i}$$

Factors independent of x_i cancel between numerator and denominator.

Directed Graphs as Distribution Filters

- We can view the graphical model as a filter.



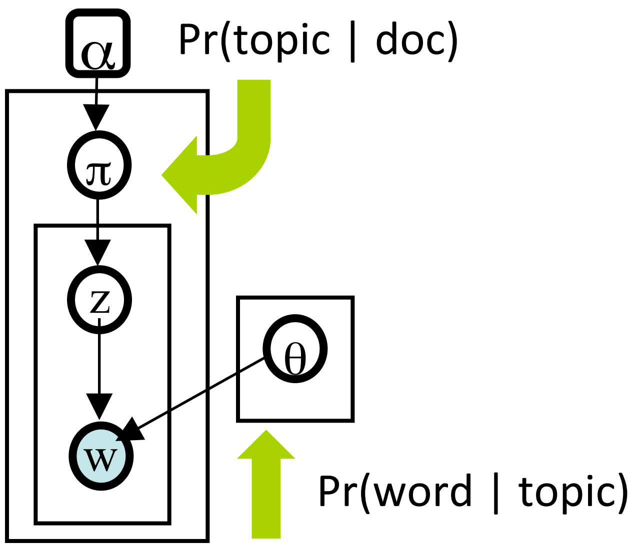
- The joint probability distribution p(x) is allowed through the filter if and only if it satisfies the factorization property.

- Note: The fully connected graph exhibits no conditional independence properties at all.

- The fully disconnected graph (no links) corresponds to a joint distribution that factorizes into the product of marginal distributions.

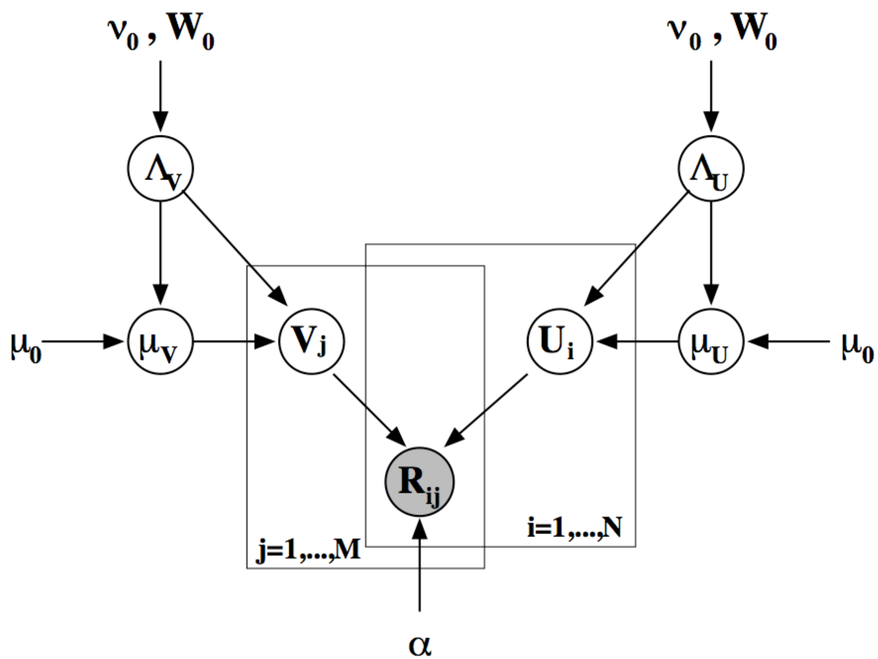
Popular Models

Latent Dirichlet Allocation



• One of the popular models for modeling word count vectors. We will see this model later.

Bayesian Probabilistic Matrix Factorization



• One of the popular models for collaborative filtering applications.