Graphical Models

Graphical Models

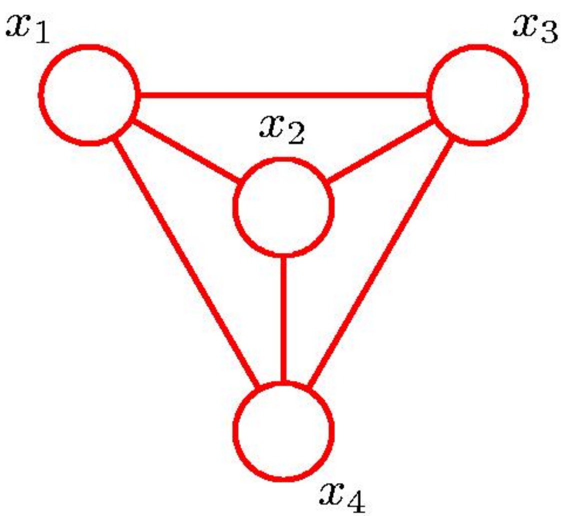
• Probabilistic graphical models provide a powerful framework for representing dependency structure between random variables.

• 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

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

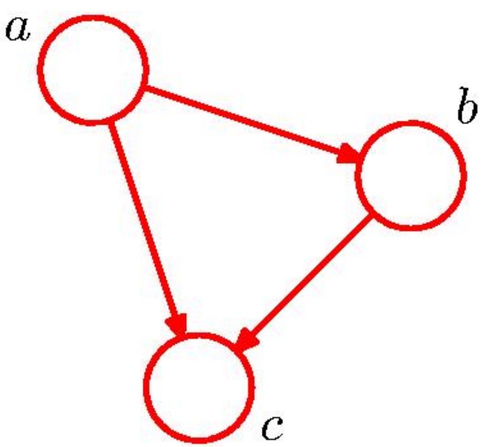
- This decomposition holds for any choice of the joint distribution.

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.

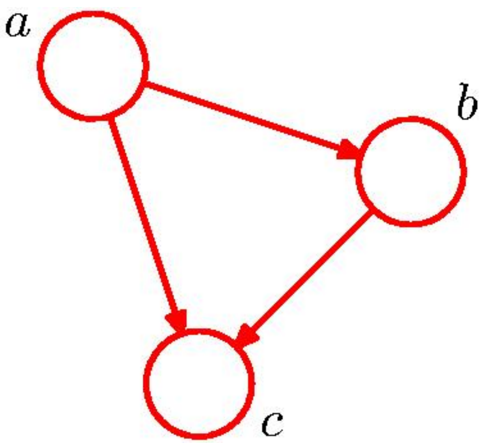
- Hence for the factor $p(c|a, b)$, there will be links from nodes a and b to node c.
- For the factor $p(a)$, there will be no incoming links.

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).

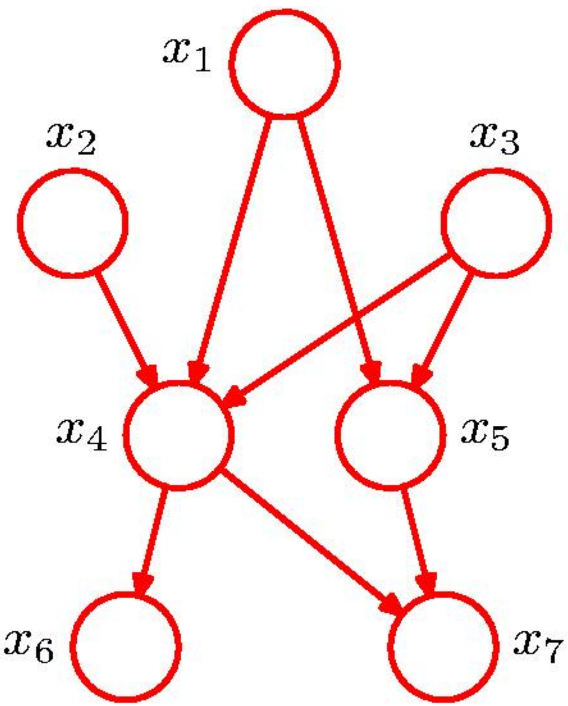
- The joint distribution over K variables factorizes:

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

- 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).

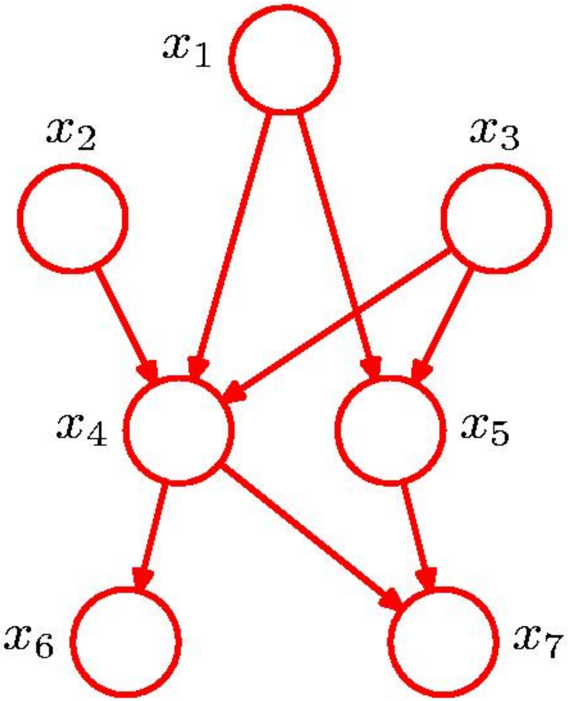
• The joint distribution over $x_1,\ldots,x_7$ can be written as a product of a set of conditional distributions.

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

• 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.

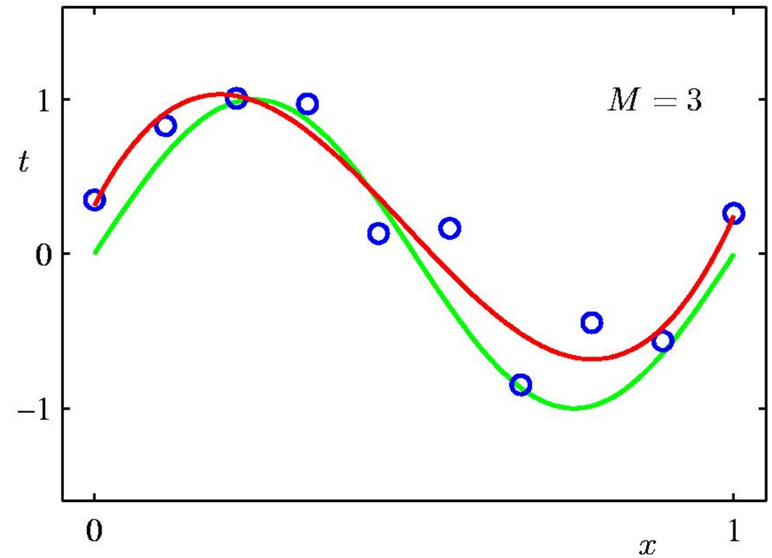
- Important restriction: There must be **no directed cycles!**

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

Bayesian Curve Fitting

- As an example, remember Bayesian polynomial regression model:

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



- We are given inputs $\mathbf{X} = \{x_1, x_2, ..., x_N\}$ and target values $\mathbf{t} = [t_1, t_2, ..., t_N]^T$.

- Given the prior over parameters, the joint distribution is given by:

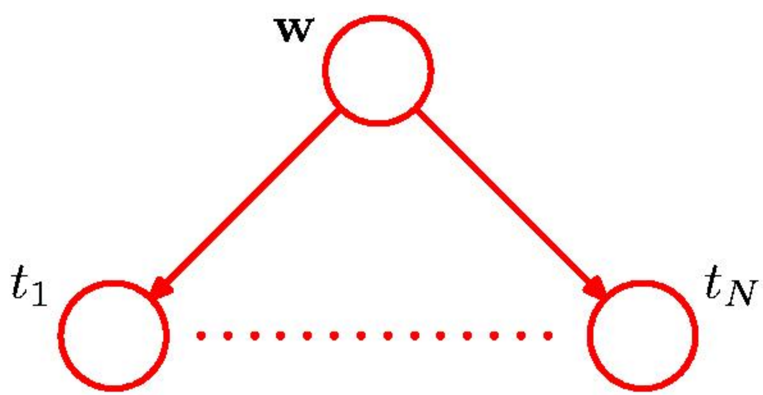
$$p(\mathbf{t}, \mathbf{w}|\mathbf{X}) = \underbrace{p(\mathbf{w})}_{\text{Prior term}} \underbrace{\prod_{i=1}^{N} p(t_n|y(\mathbf{w}, x_n))}_{\text{Likelihood term}}.$$

Prior term Likelihood term

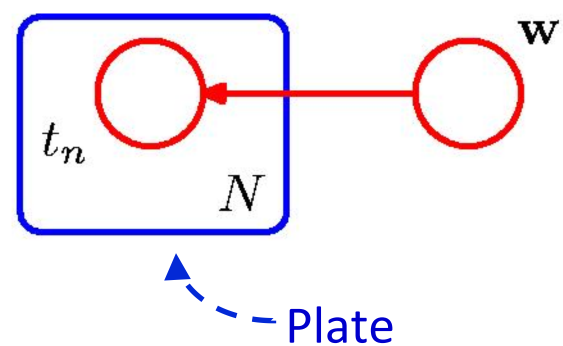
Graphical Representation

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

• This distribution can be represented as a graphical model.



• Same representation using plate notation.



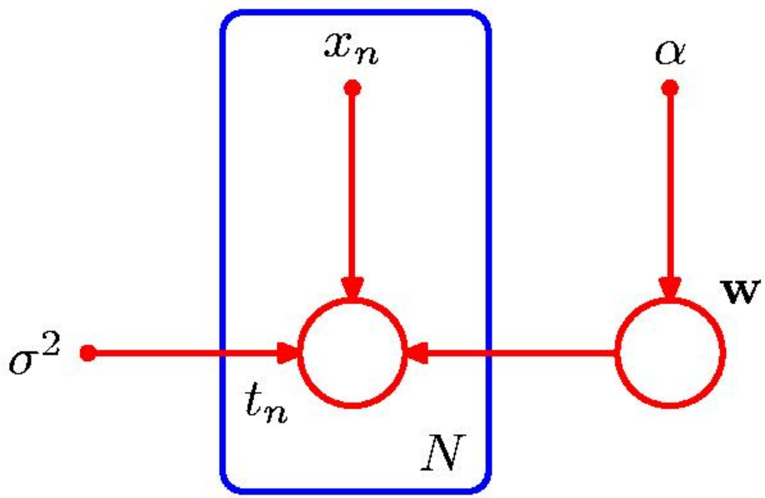
• Compact representation: we introduce a plate that represents N nodes of which only a single example t_n is shown explicitly.

• Note that w and $\mathbf{t} = [t_1, t_2, ..., t_N]^T$ represent random variables.

Graphical Representation

• It will often be useful to make the parameters of the model as well as random variables be explicit.

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



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

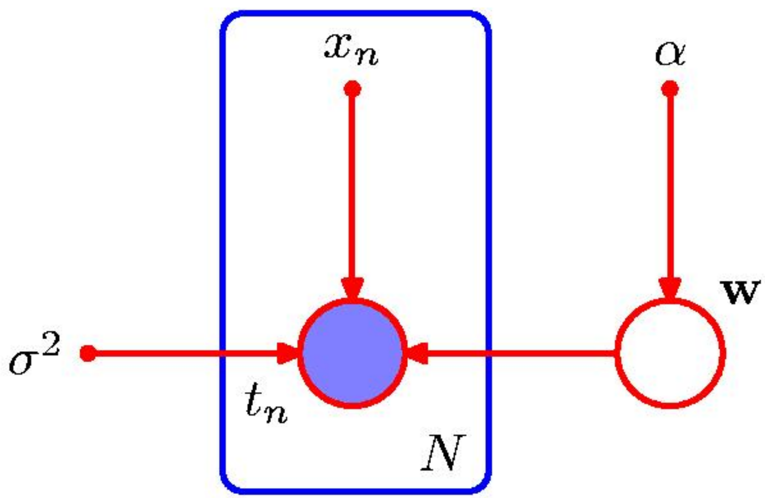
$$p(t_n|\mathbf{w}, x_n, \sigma^2) = \mathcal{N}(t_n|y(\mathbf{w}, x_n), \sigma^2),$$

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

• Random variables will be denoted by open circles and deterministic parameters will be denoted by smaller solid circles.

Graphical Representation

• When we apply a graphical model to a problem in machine learning, we will set some of the variables to specific observed values (e.g. condition on the data).



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

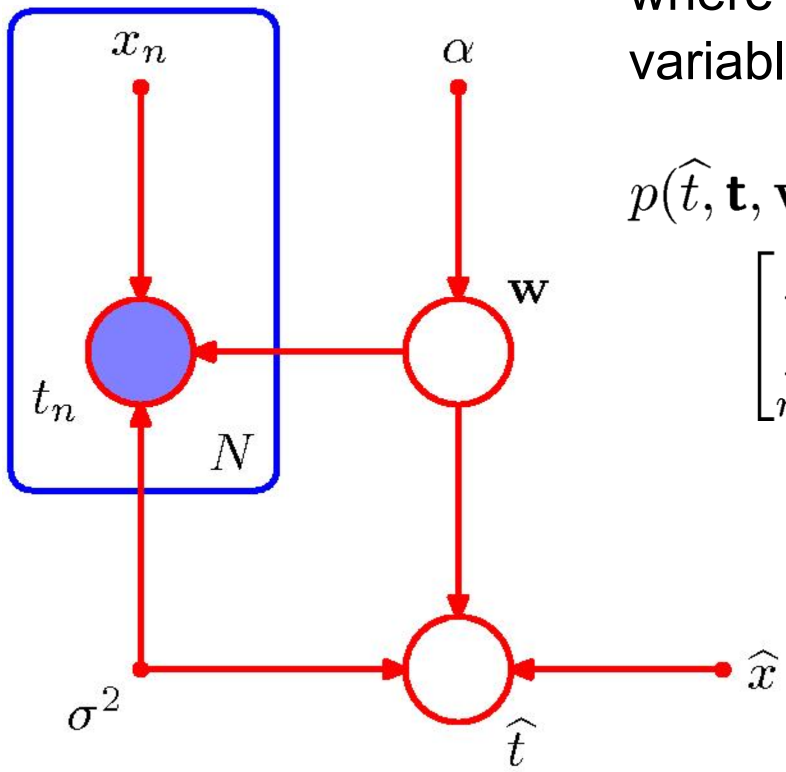
• For example, having observed the values of the targets $\{t_n\}$ on the training data, we wish to infer the posterior distribution over parameters w.

• In this example, we conditioned on observed data $\mathbf{t} = [t_1, t_2, ..., t_N]^T$ by shadowing the corresponding nodes.

Predictive Distribution

- We may also be interested in making predictions for a new input value $\hat{x}$.

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



where the joint distribution of all of the random variables is given by:

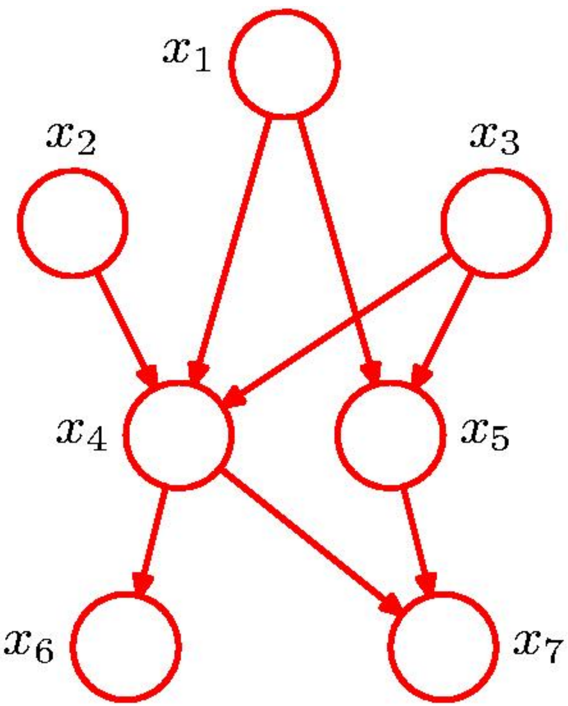
$$p(\widehat{t}, \mathbf{t}, \mathbf{w}|\widehat{x}, \mathbf{x}, \alpha, \sigma^2) = \left[\prod_{n=1}^{N} p(t_n|x_n, \mathbf{w}, \sigma^2)\right] p(\mathbf{w}|\alpha) p(\widehat{t}|\widehat{x}, \mathbf{w}, \sigma^2)$$

- Here we are setting the random variables in t to the specific values observed in the data.

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.

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

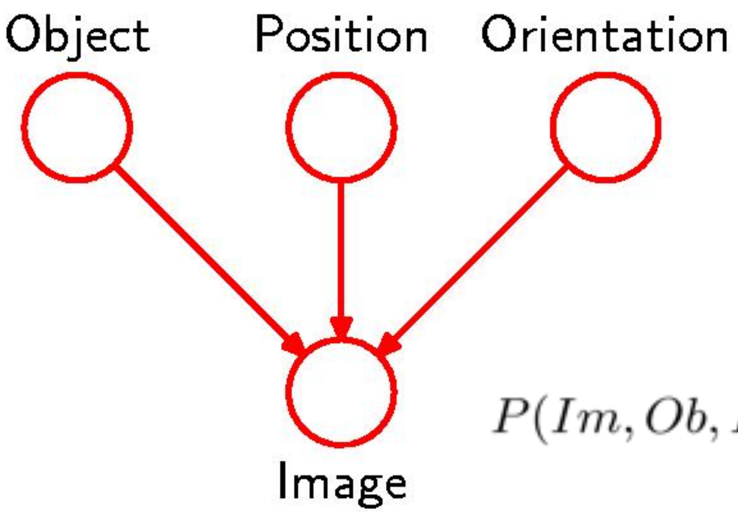
The parent variables are set to their sampled values

- 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.

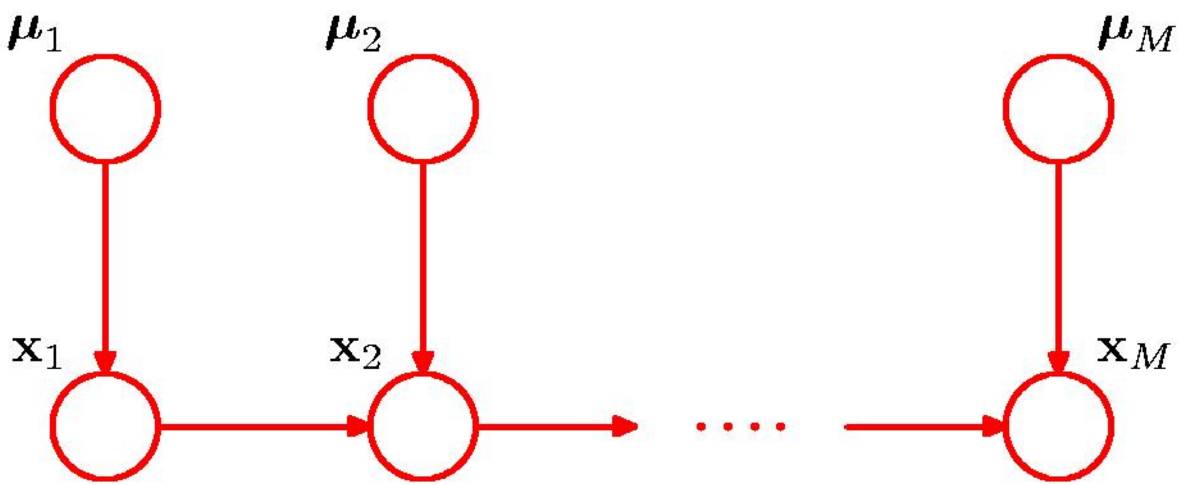
- Total number of parameters: K-1 + (M-1)(K-1)K, which is quadratic in K and linear in the length M of the chain.

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

Adding Priors

• We can turn a graph over discrete random variables into a Bayesian model by introducing Dirichlet priors for the parameters.

• From a graphical model point of view, each node acquires an additional parent representing the Dirichlet distribution over parameters.

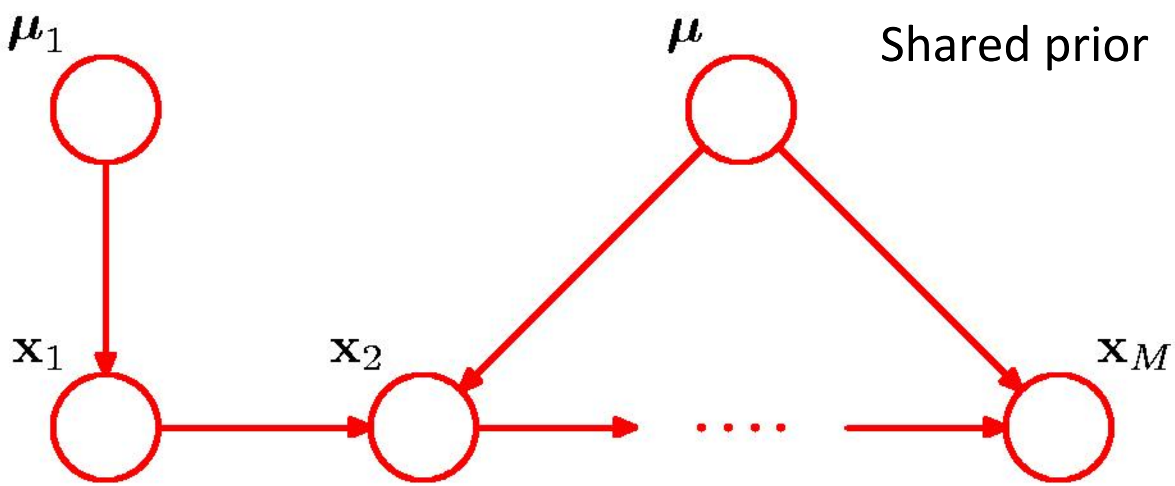


$$p(\{\mathbf{x}_m, \boldsymbol{\mu}_m\}) = p(\mathbf{x}_1|\boldsymbol{\mu}_1)\,p(\boldsymbol{\mu}_1)\prod_{m=2}^{M} p(\mathbf{x}_m|\mathbf{x}_{m-1}, \boldsymbol{\mu}_m)\,p(\boldsymbol{\mu}_m)$$

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

Shared Prior

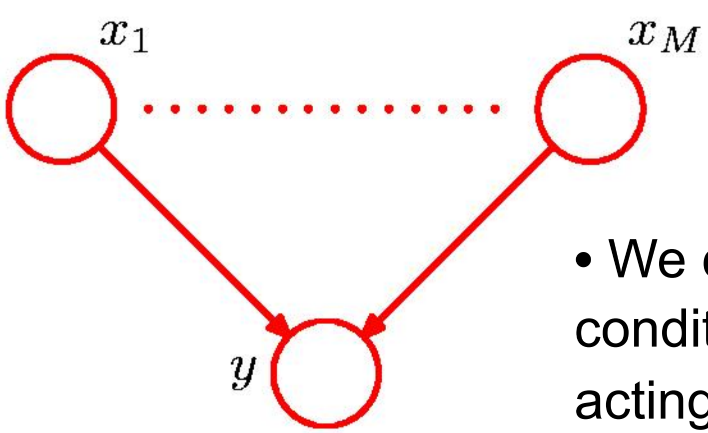
• We can further share the common prior over the parameters governing the conditional distributions.



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

Parameterized 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

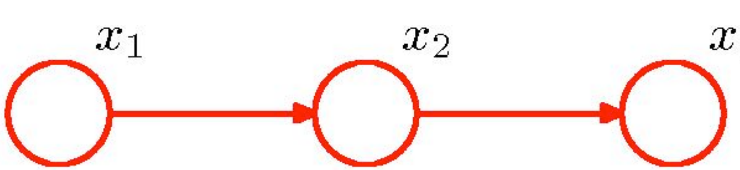
- The log of the joint distribution takes form:

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

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:

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

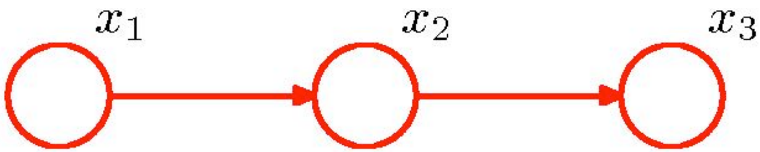
hence

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

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:

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

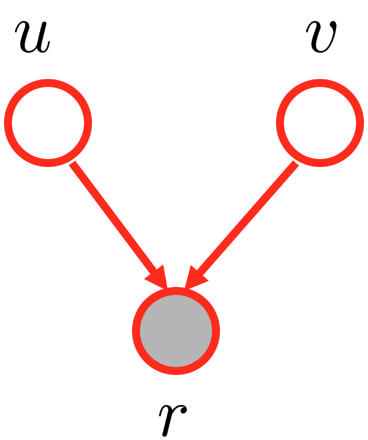
- Consider two cases:

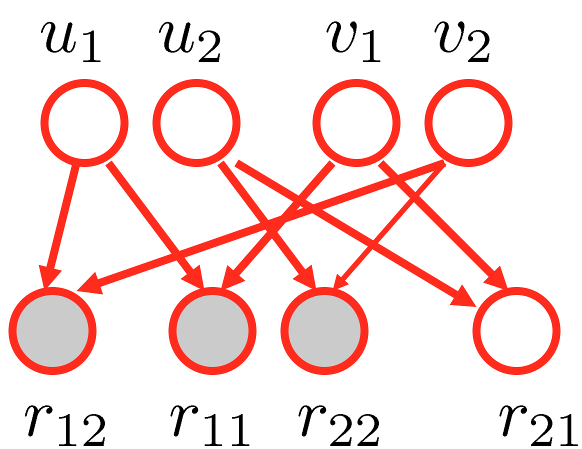
- There are no links in the graph (graph is fully factorized), so that w_{ij}'s are zero. In this case: $\mathbb{E}[\mathbf{x}] = \left[b_1, ..., b_D\right]^T$, and the covariance is diagonal $\operatorname{diag}(v_1, ..., v_D)$. The joint distribution represents D independent univariate Gaussian distributions.

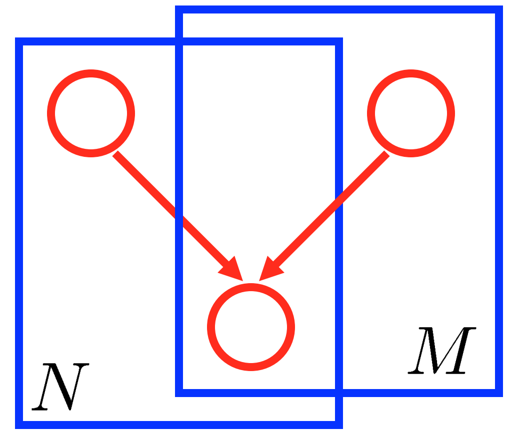
- The graph is fully connected. The total number of parameters is D + D(D-1)/2. The covariance corresponds to a general symmetric covariance matrix.

Bilinear Gaussian Model

- Consider the following model:







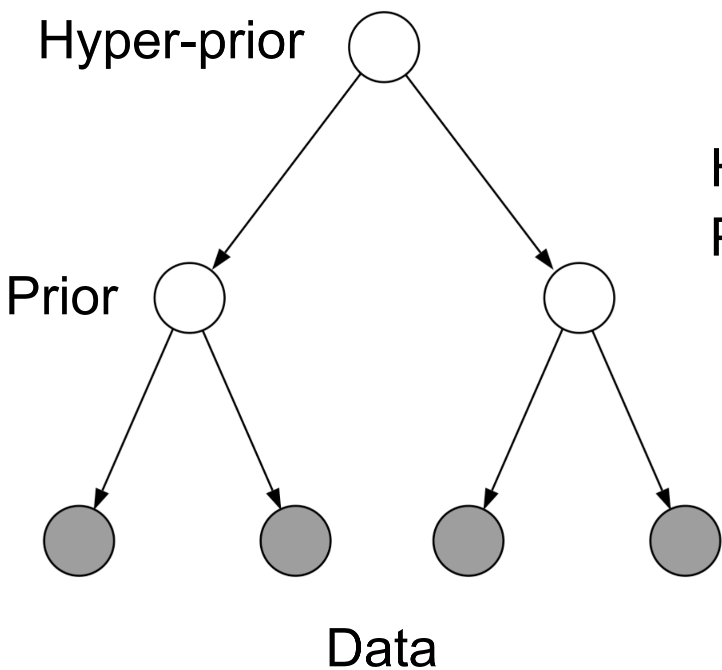
$$u \sim \mathcal{N}(0, 1),$$
$$v \sim \mathcal{N}(0, 1),$$
$$r \sim \mathcal{N}(uv, 1).$$

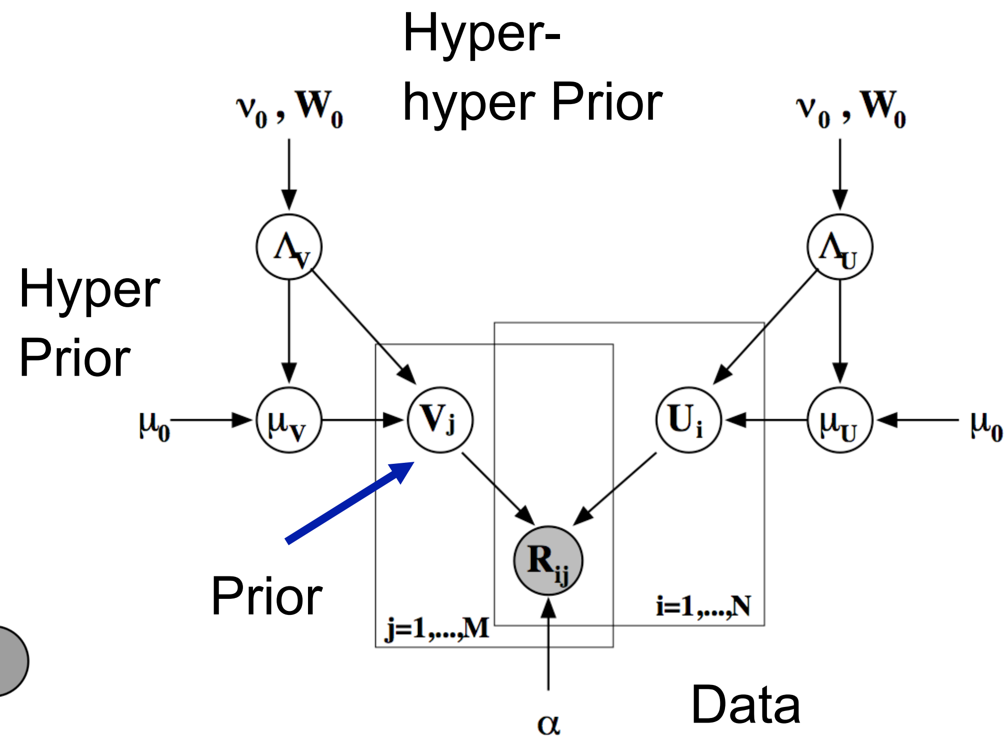
Gaussian terms

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

- 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:

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

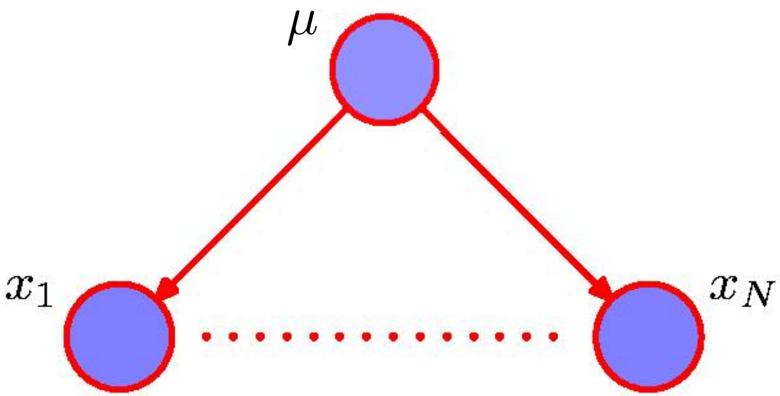
- We will use the notation:

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

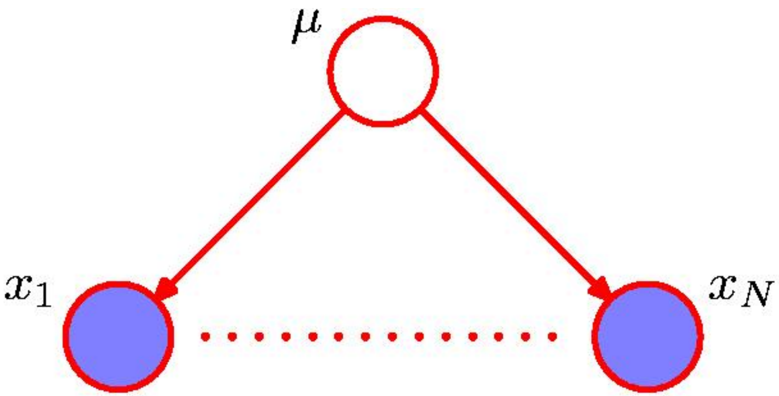
- An important feature of graphical models is that conditional independence properties of the joint distribution can be read directly from the graph without performing any analytical manipulations

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

i.i.d data



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



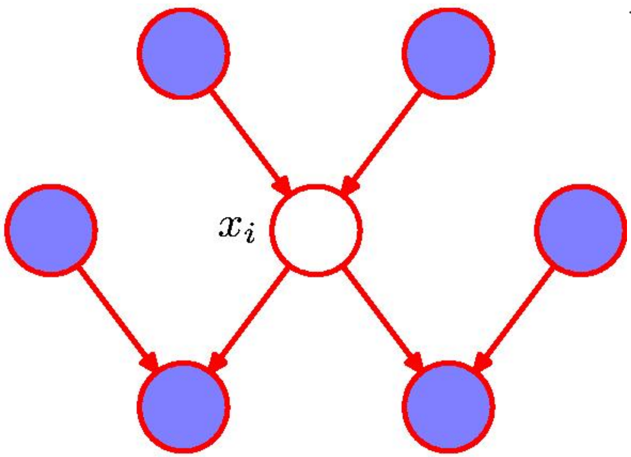
$$p(\mathcal{D}) = \int_{-\infty}^{\infty} p(\mathcal{D}|\mu)p(\mu)\,\mathrm{d}\mu \neq \prod_{n=1}^{N} p(x_n)$$

- Another example of conditional independence is provided by the concept of independent and identically distributed data.
- Consider the problem of finding the posterior distribution over mean μ in Bayesian linear regression model.
- Suppose that we condition on μ and consider the joint over observed variables.
- If we integrate out μ, the observations are no longer independent.

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.



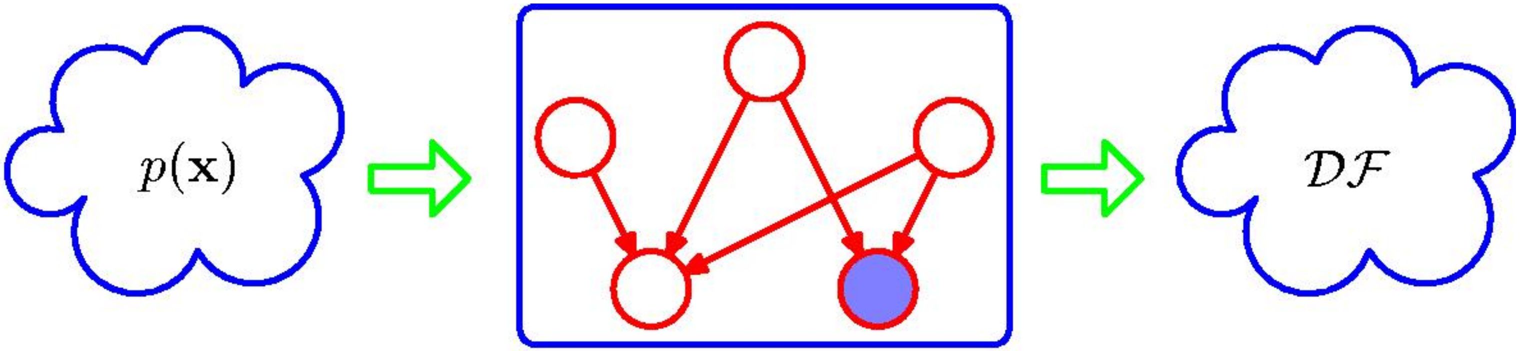
$$p(\mathbf{x}_i|\mathbf{x}_{\{j\neq i\}}) = \frac{p(\mathbf{x}_1,\ldots,\mathbf{x}_M)}{\int p(\mathbf{x}_1,\ldots,\mathbf{x}_M)\,\mathrm{d}\mathbf{x}_i}$$

$$= \frac{\prod_k p(\mathbf{x}_k|\mathrm{pa}_k)}{\int \prod_k p(\mathbf{x}_k|\mathrm{pa}_k)\,\mathrm{d}\mathbf{x}_i}$$

Factors independent of x_i cancel between numerator and denominator.

Directed Graphs as Distribution Filters

- We can view the graphical model as a filter.



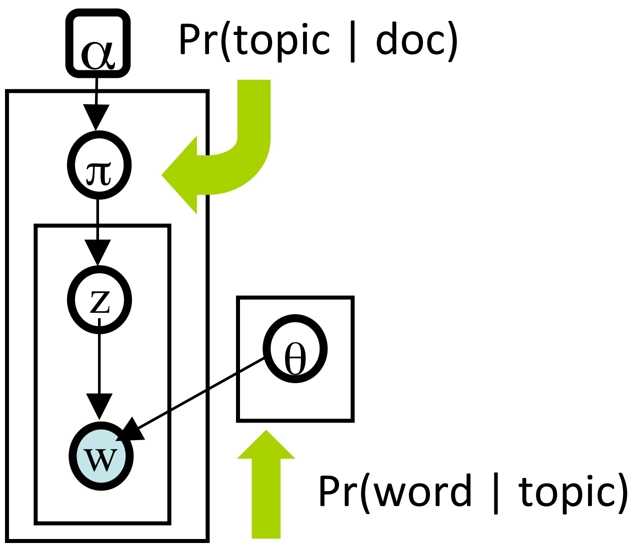
- The joint probability distribution p(x) is allowed through the filter if and only if it satisfies the factorization property.

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

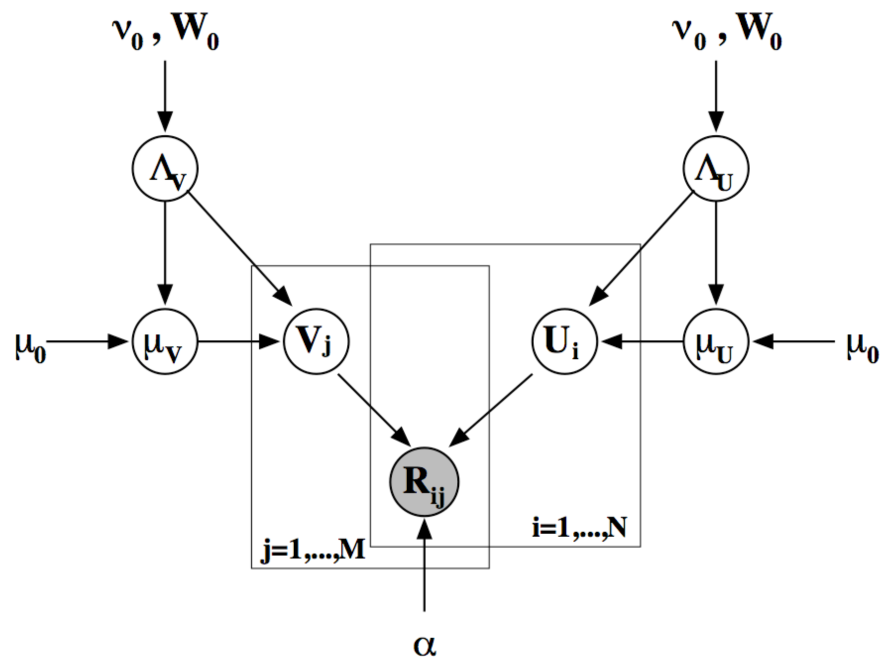
- The fully disconnected graph (no links) corresponds to a joint distribution that factorizes into the product of marginal distributions.

Popular Models

Latent Dirichlet Allocation



Bayesian Probabilistic Matrix Factorization



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

- One of the popular models for collaborative filtering applications.