10707
Deep Learning

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Graphical Models

Graphical Models

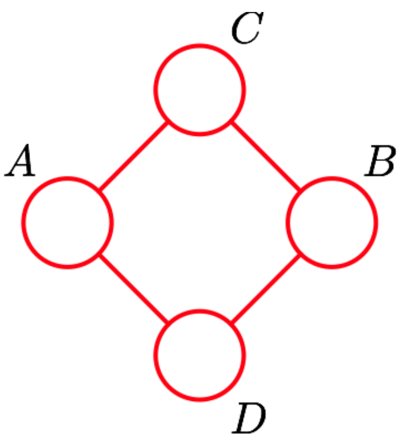
• Probabilistic graphical models provide a powerful framework for representing dependency structure between random variables.

• 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.

Undirected Graphical Models

Directed graphs are useful for expressing causal relationships between random variables, whereas undirected graphs are useful for expressing soft constraints between random variables



- The joint distribution defined by the graph is given by the product of non-negative potential functions over the maximal cliques (connected subset of nodes).

$$p(\mathbf{x}) = \frac{1}{\mathcal{Z}} \prod_C \phi_C(x_C) \qquad \mathcal{Z} = \sum_{\mathbf{x}} \prod_C \phi_C(x_C)$$

where the normalizing constant $\mathcal{Z}$ is called a partition function.

- For example, the joint distribution factorizes:

$$p(A, B, C, D) = \frac{1}{\mathcal{Z}} \phi(A, C)\phi(C, B)\phi(B, D)\phi(A, D)$$

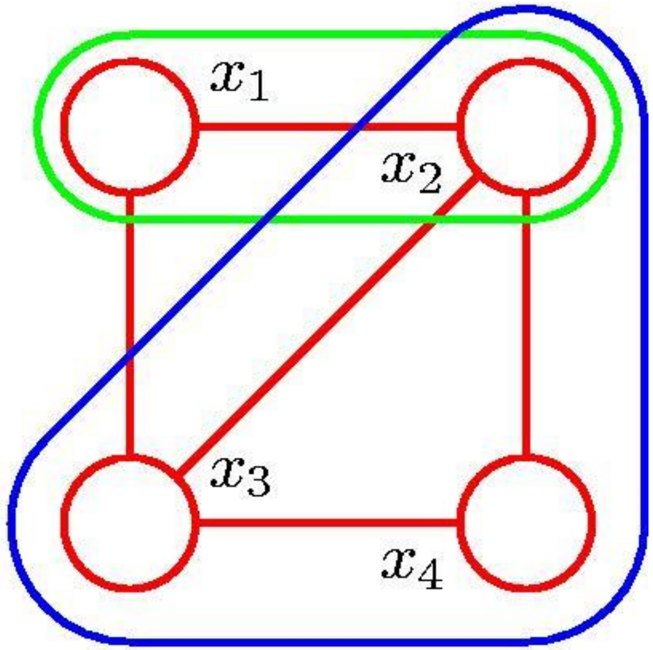
- Let us look at the definition of cliques.

Cliques

- The subsets that are used to define the potential functions are represented by maximal cliques in the undirected graph.

- Clique: a subset of nodes such that there exists a link between all pairs of nodes in a subset.

- Maximal Clique: a clique such that it is not possible to include any other nodes in the set without it ceasing to be a clique.



- This graph has 5 cliques:

$$\{x_1, x_2\}, \{x_2, x_3\}, \{x_3, x_4\},$$
$$\{x_4, x_2\}, \{x_1, x_3\}.$$

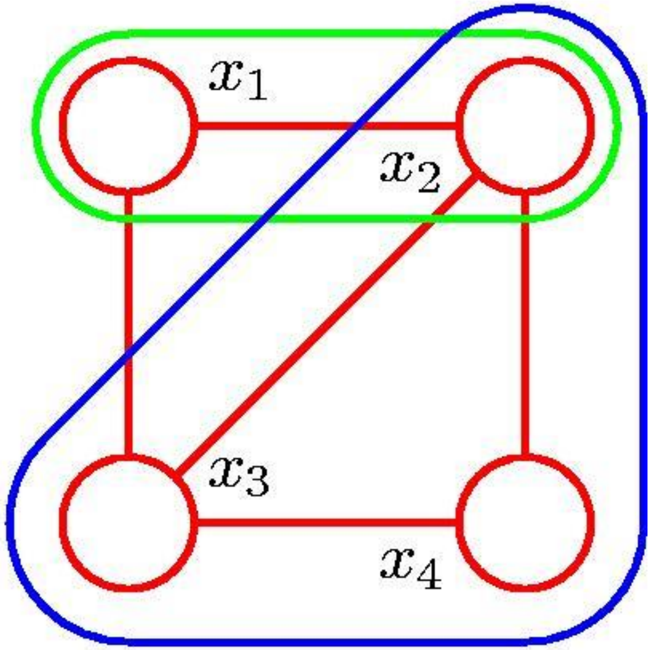
- Two maximal cliques:

$$\{x_1, x_2, x_3\}, \{x_2, x_3, x_4\}.$$

Using Cliques to Represent Subsets

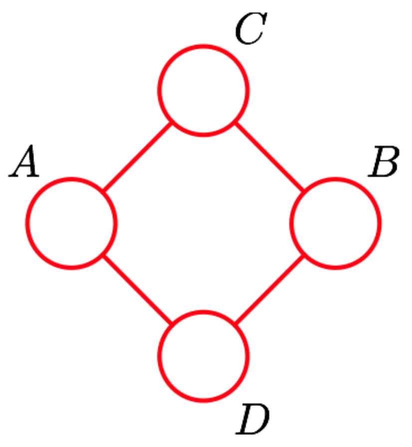
- If the potential functions only involve two nodes, an undirected graph has a nice representation.

- If the potential functions involve more than two nodes, using a different factor graph representation is much more useful.



- For now, let us consider only potential functions that are defined over two nodes.

Markov Random Fields (MRFs)



$$p(\mathbf{x}) = \frac{1}{Z}\prod_C \phi_C(x_C)$$

- Each potential function is a mapping from the joint configurations of random variables in a clique to non-negative real numbers.
- The choice of potential functions is not restricted to having specific probabilistic interpretations.

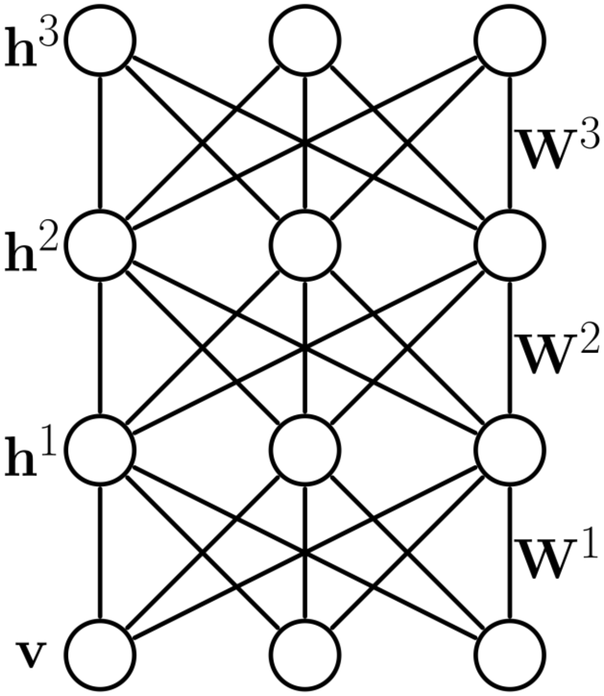
Potential functions are often represented as exponentials:

$$p(\mathbf{x}) = \frac{1}{Z}\prod_C \phi_C(x_C) = \frac{1}{Z}\exp(-\sum_C E(x_c)) = \underbrace{\frac{1}{Z}\exp(-E(\mathbf{x}))}_{\text{Boltzmann distribution}}$$

where E(x) is called an energy function.

MRFs with Hidden Variables

For many interesting real-world problems, we need to introduce hidden or latent variables.



- Our random variables will contain both visible and hidden variables x=(v,h).

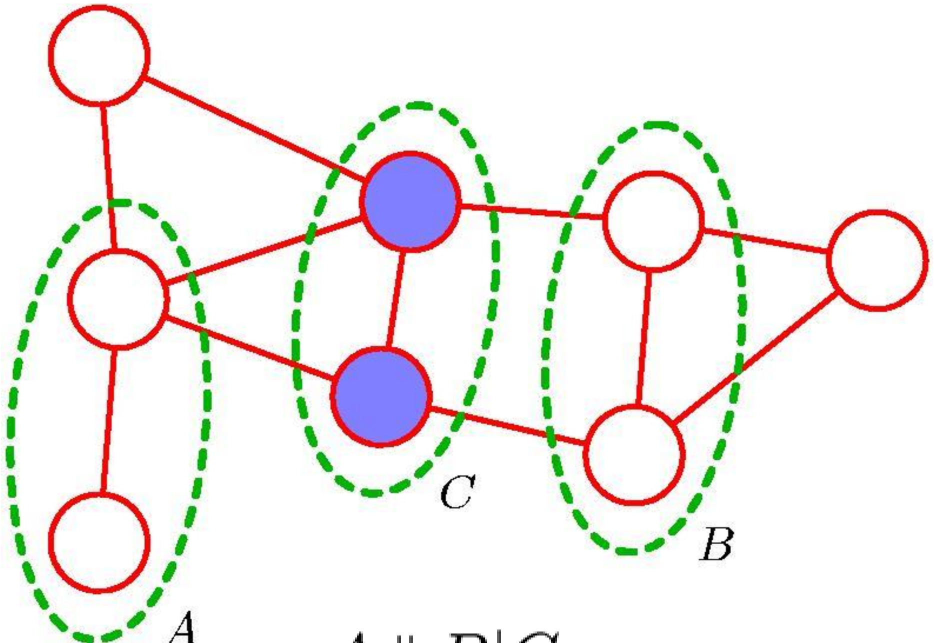
$$p(\mathbf{v}) = \frac{1}{\mathcal{Z}} \sum_{\mathbf{h}} \exp(-E(\mathbf{v}, \mathbf{h}))$$

- In general, computing both partition function and summation over hidden variables will be intractable, except for special cases.

- Parameter learning becomes a very challenging task.

Conditional Independence

- Conditional Independence is easier compared to directed models:



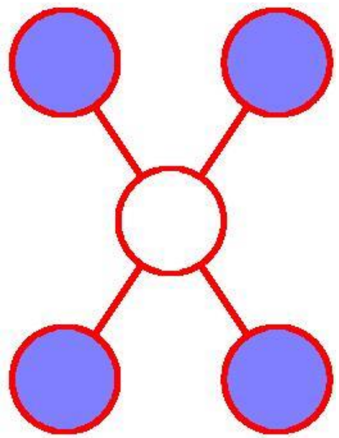
$$A \perp\!\!\!\perp B \mid C$$

- Observation blocks a node.
- Two sets of nodes are conditionally independent if the observations block all paths between them.

Markov Blanket

- The Markov blanket of a node is simply all of the directly connected nodes.

Markov Blanket

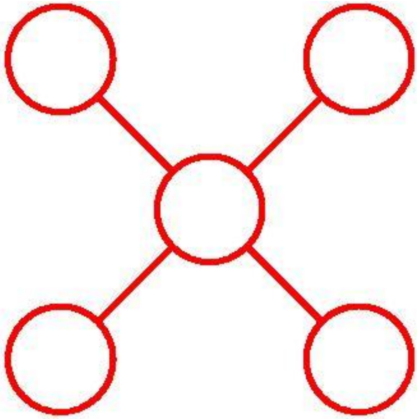


- This is simpler than in directed models, since there is no explaining away.

- The conditional distribution of x_i conditioned on all the variables in the graph is dependent only on the variables in the Markov blanket.

Conditional Independence and Factorization

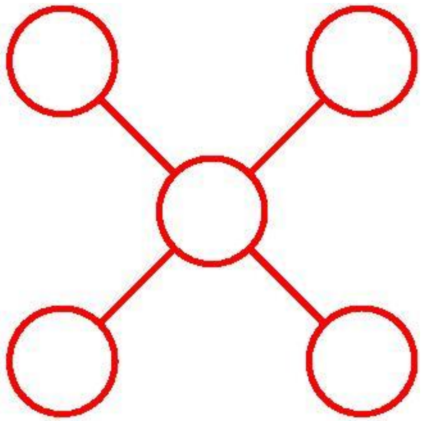
- Consider two sets of distributions:
  - The set of distributions consistent with the conditional independence relationships defined by the undirected graph.
  - The set of distributions consistent with the factorization defined by potential functions on maximal cliques of the graph.
- The Hammersley-Clifford theorem states that these two sets of distributions are the same.



$$p(\mathbf{x}) = \frac{1}{Z} \prod_C \phi_C(x_C)$$

Interpreting Potentials

• In contrast to directed graphs, the potential functions **do not have a specific probabilistic interpretation**.



$$p(\mathbf{x}) = \frac{1}{\mathcal{Z}} \prod_C \phi_C(x_C) = \frac{1}{\mathcal{Z}} \exp(-\sum_C E(x_c))$$

• This gives us greater flexibility in choosing the potential functions.

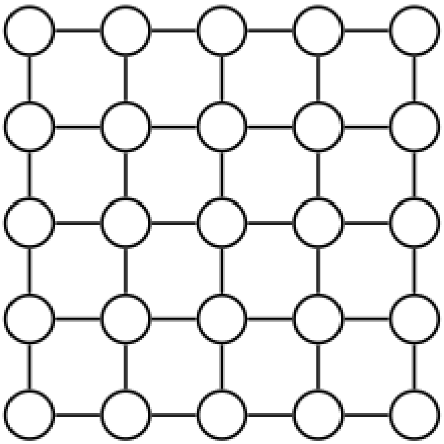
• We can view the potential function as expressing which configuration of the local variables are preferred to others.

• Global configurations with relatively high probabilities are those that find a good balance in satisfying the (possibly conflicting) influences of the clique potentials.

• So far we did not specify the nature of random variables, discrete or continuous.

Discrete MRFs

- MRFs with all discrete variables are widely used in many applications.
- MRFs with binary variables are sometimes called Ising models in statistical mechanics, and Boltzmann machines in machine learning literature.



- Denoting the binary valued variable at node j by $x_j \in \{0, 1\}$, the Ising model for the joint probabilities is given by:

$$P_\theta(\mathbf{x}) = \frac{1}{\mathcal{Z}(\theta)} \exp\Big(\sum_{ij \in E} x_i x_j \theta_{ij} + \sum_{i \in V} x_i \theta_i \Big)$$

- The conditional distribution is given by logistic:

$$P_\theta(x_i = 1 | \mathbf{x}_{-i}) = \frac{1}{1 + \exp(-\theta_i - \sum_{ij \in E} x_j \theta_{ij})},$$

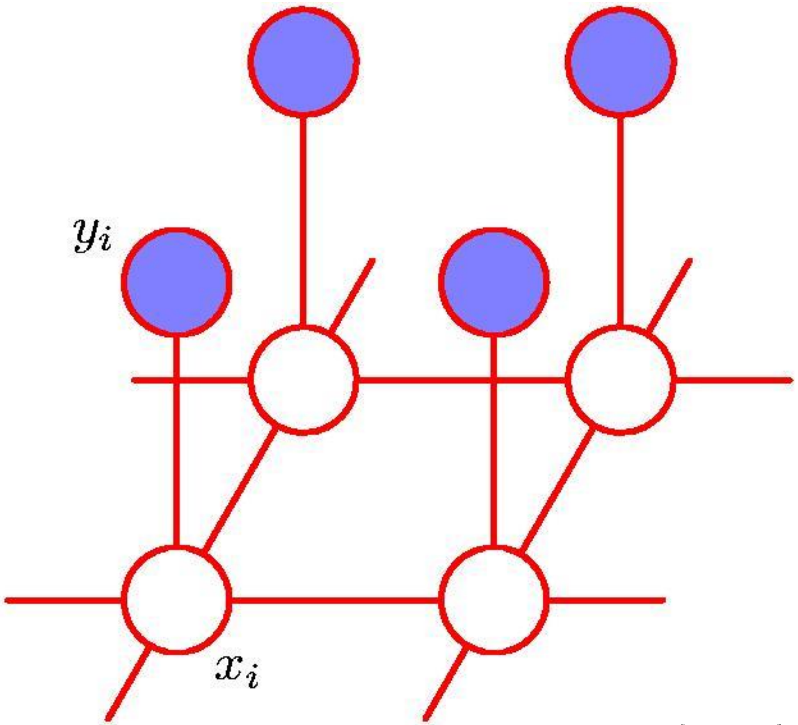
where x_{-i} denotes all nodes except for i.

Hence the parameter θ_{ij} measures the dependence of x_i on x_j, conditional on the other nodes.

Example: Image Denoising

- Let us look at the example of noise removal from a binary image.

- Let the observed noisy image be described by an array of binary pixel values: $y_j \in \{-1, +1\}$, i=1,…,D.



- We take a noise-free image $x_j \in \{-1, +1\}$, and randomly flip the sign of pixels with some small probability.

Bias term

Neighboring pixels are likely to have the same sign

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

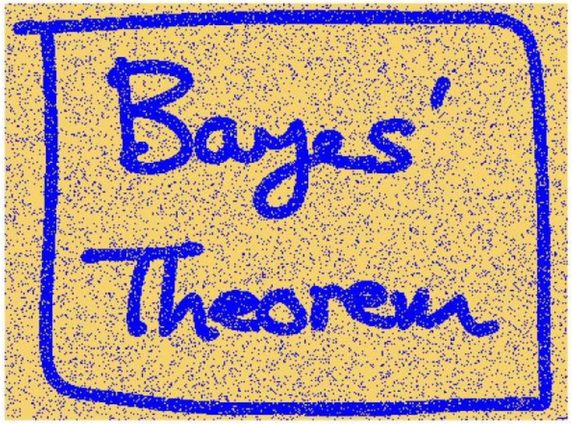
Noisy and clean pixels are likely to have the same sign

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

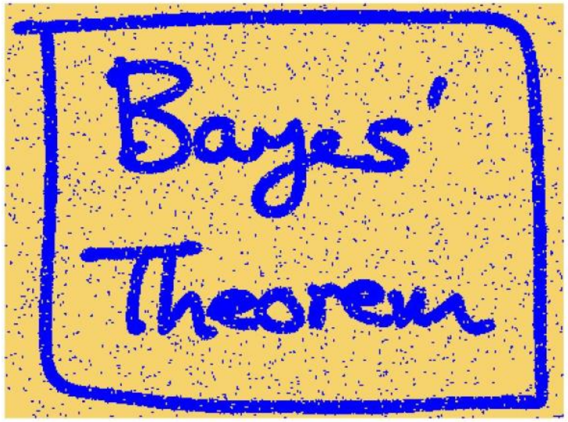
Iterated Conditional Modes

- Iterated conditional modes: coordinate-wise gradient descent.
- Visit the unobserved nodes sequentially and set each x to whichever of its two values has the lowest energy.
  - This only requires us to look at the Markov blanket, i.e. the connected nodes.
  - Markov blanket of a node is simply all of the directly connected nodes.

Original Image



Noisy Image



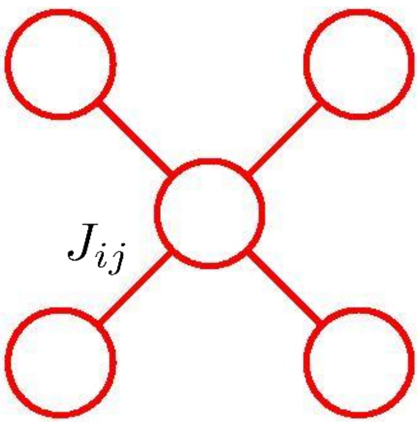
ICM

Gaussian MRFs

• We assume that the observations have a multivariate Gaussian distribution with mean ¹ and covariance matrix § .

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

• Since the Gaussian distribution represents at most second-order relationships, it automatically encodes a pairwise MRF. We rewrite:



$$P(\mathbf{x}) = \frac{1}{\mathcal{Z}} \exp(-\frac{1}{2}\mathbf{x}^T J \mathbf{x} + \mathbf{g}^T \mathbf{x}),$$

where

$$J = \Sigma^{-1}, \qquad \mu = J^{-1}\mathbf{g}.$$

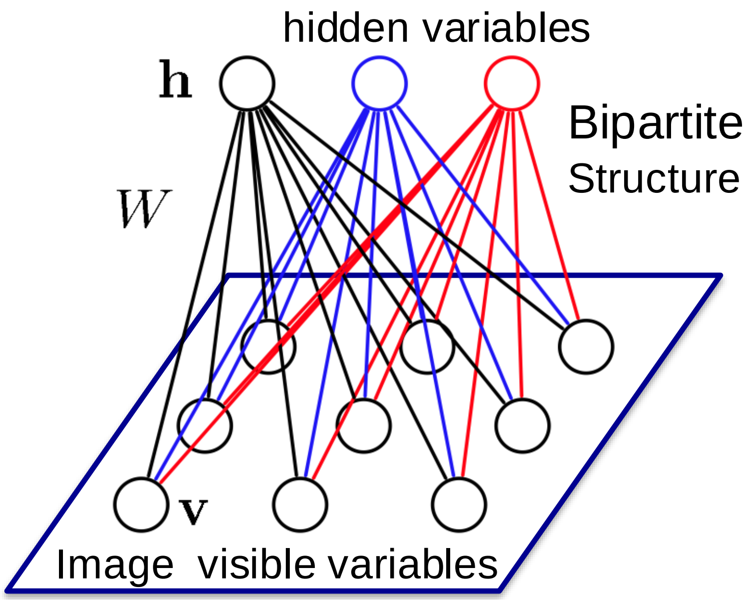
• The positive definite matrix J is known as the information matrix and is sparse with respect to the given graph: $\mathbf{x}^T J \mathbf{x} = \sum_i J_{ii} x_i^2 + 2 \sum_{ij \in E} J_{ij} x_i x_j,$

$$\text{if } (i,j) \neq E, \text{ then } J_{ij} = 0.$$

• The information matrix is sparse, but the covariance matrix is not sparse.

Restricted Boltzmann Machines

- For many real-world problems, we need to introduce hidden variables.
- Our random variables will contain visible and hidden variables x=(v,h).



Stochastic binary visible variables $\mathbf{v} \in \{0,1\}^D$ are connected to stochastic binary hidden variables $\mathbf{h} \in \{0,1\}^F$.

The energy of the joint configuration:

$$E(\mathbf{v},\mathbf{h};\theta) = -\sum_{ij} W_{ij} v_i h_j - \sum_i b_i v_i - \sum_j a_j h_j$$

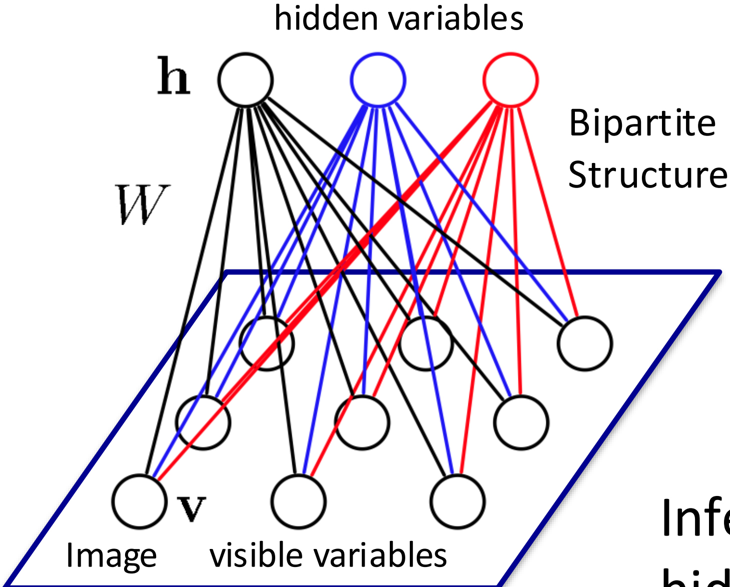
$\theta = \{W, a, b\}$ model parameters.

Probability of the joint configuration is given by the Boltzmann distribution:

$$P_\theta(\mathbf{v},\mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\big(-E(\mathbf{v},\mathbf{h};\theta)\big) = \underbrace{\frac{1}{\mathcal{Z}(\theta)}}_{\text{partition function}} \prod_{ij} \underbrace{e^{W_{ij} v_i h_j}}_{\text{potential functions}} \prod_i e^{b_i v_i} \prod_j e^{a_j h_j}$$

$$\mathcal{Z}(\theta) = \sum_{\mathbf{h},\mathbf{v}} \exp\big(-E(\mathbf{v},\mathbf{h};\theta)\big)$$

Restricted Boltzmann Machines



Restricted: No interaction between hidden variables

Inferring the distribution over the hidden variables is easy:

$$P(\mathbf{h}|\mathbf{v}) = \underbrace{\prod_j P(h_j|\mathbf{v})}_{\text{Factorizes: Easy to compute}} \quad P(h_j = 1|\mathbf{v}) = \frac{1}{1 + \exp(-\sum_i W_{ij} v_i - a_j)}$$

Similarly:

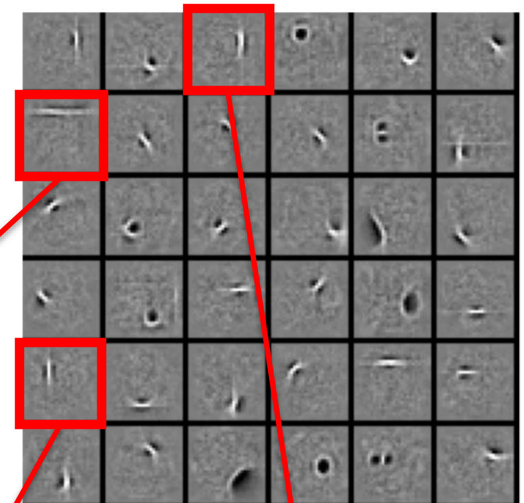
$$P(\mathbf{v}|\mathbf{h}) = \prod_i P(v_i|\mathbf{h}) \quad P(v_i = 1|\mathbf{h}) = \frac{1}{1 + \exp(-\sum_j W_{ij} h_j - b_i)}$$

Markov random fields, Boltzmann machines, log-linear models.

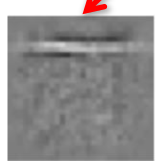
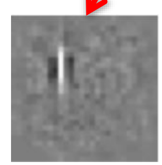
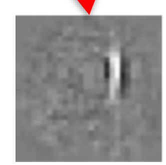
Restricted Boltzmann Machines

Observed Data
Subset of 25,000 characters

Learned W: “edges”
Subset of 1000 features



Most hidden variables are off

New Image:  $= \sigma\Big(0.99 \times$  $+ \; 0.97 \times$  $+ \; 0.82 \times$  $\ldots\Big)$

$p(h_7 = 1|v)$ $\quad$ $p(h_{29} = 1|v)$

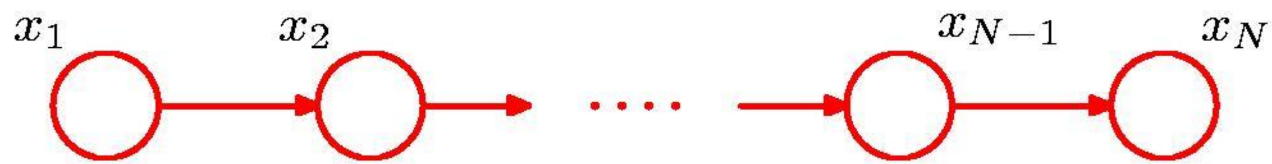
$\sigma(x) = \frac{1}{1+\exp(-x)}$

Logistic Function: Suitable for modeling binary images

Represent:  as $P(\mathbf{h}|\mathbf{v}) = [0,\, 0,\, 0.82,\, 0,\, 0,\, 0.99,\, 0,\, 0 \,\ldots\,]$

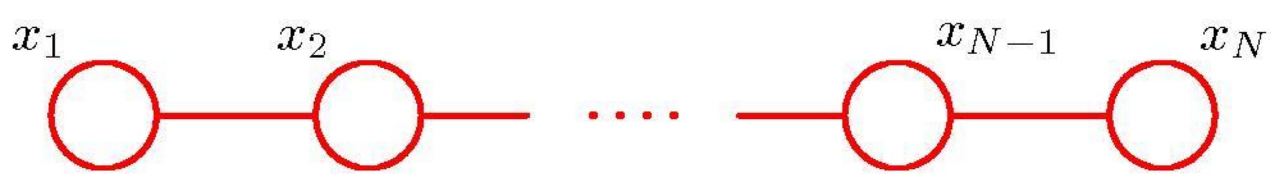
Relation to Directed Graphs

- Let us try to convert directed graph into an undirected graph:



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

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



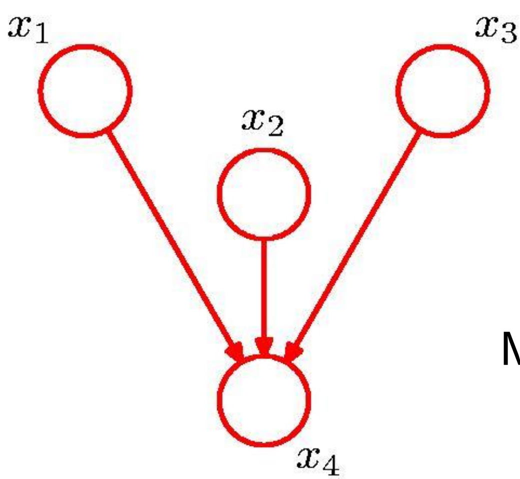
Directed vs. Undirected

- Directed Graphs can be more precise about independencies than undirected graphs.

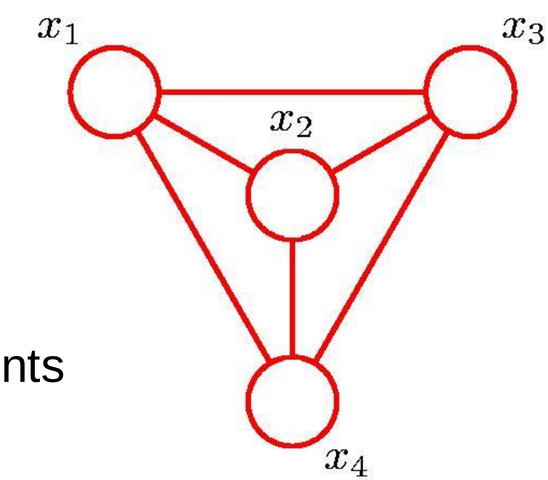
$$p(\mathbf{x}) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$$

$$p(\mathbf{x}) = \frac{1}{\mathcal{Z}}\psi(x_1, x_2, x_3, x_4)$$

need 4th order clique



Moralize: Marry the parents



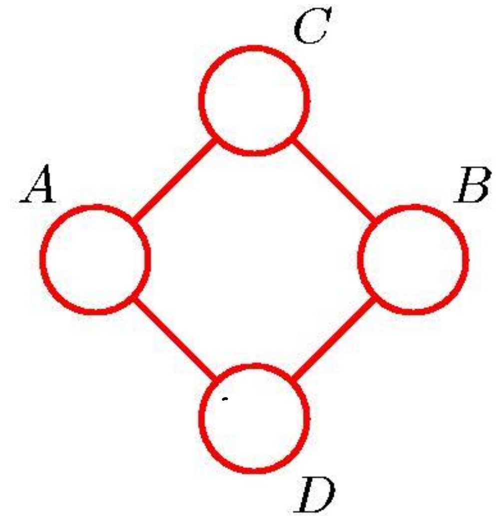
- All the parents of x_4 can interact to determine the distribution over x_4.
- The directed graph represents independencies that the undirected graph cannot model.

- To represent the high-order interaction in the directed graph, the undirected graph needs a fourth-order clique.
- This fully connected graph exhibits no conditional independence properties

Undirected vs. Directed

- Undirected Graphs can be more precise about independencies than directed graphs

  - There is no directed graph over four variables that represents the same set of conditional independence properties.



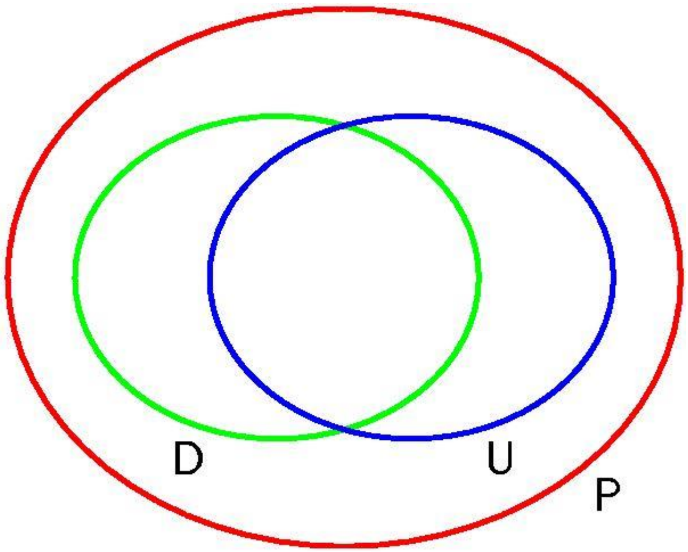
$$A \not\perp\!\!\!\perp B \mid \emptyset$$

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

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

Directed vs. Undirected

• If every conditional independence property of the distribution is reflected in the graph and vice versa, then the graph is a perfect map for that distribution.



• Venn diagram:

- The set of all distributions P over a given set of random variables.
- The set of distributions D that can be represented as a perfect map using directed graph.
- The set of distributions U that can be represented as a perfect map using undirected graph.

• We can extend the framework to graphs that include both directed and undirected graphs.