Representation of undirected GM

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Review

Review: Directed Graphical Model

- Represent distribution of the form

$$p(X_1, \cdots, X_n) = \prod_{i=1}^{n} p(X_i | \pi(X_i))$$

Parents of X_i

- Factorizes in terms of local conditional probabilities
- Each node has to maintain $p(X_i | \pi(X_i))$
- Each variable is Conditional Independent of its non-descendants given its parents

the nodes before X_i that are not its parents X_i

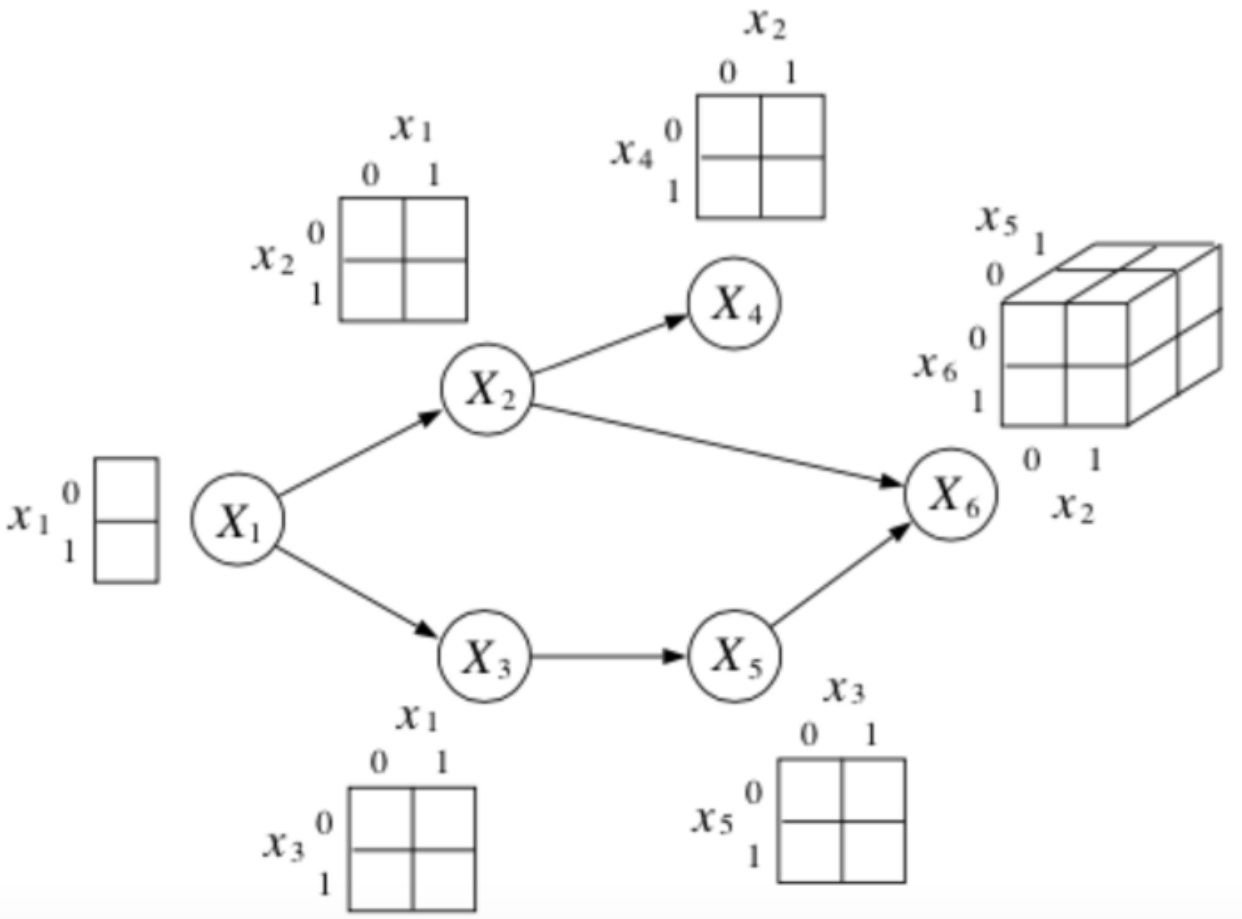
Parents of X_i

$$X_i \perp\!\!\!\perp \tilde{\pi}(X_i) | \pi(X_i)$$

- Such an ordering is a "topological" ordering (i.e., parents have lower numbers than their children)

Review: Directed Graphical Model

For discrete variables, each node stores a conditional probability table (CPT)

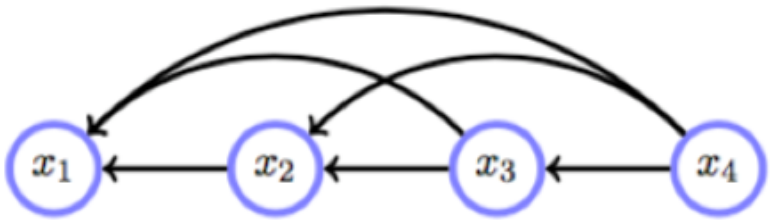


Review: independence properties of DAGs

- **Defn**: let $\mathcal{I}_l(\mathcal{G})$ be the set of local independence properties encoded by DAG $\mathcal{G}$, namely:

$$\mathcal{I}_\ell(\mathcal{G}) = \{X \perp\!\!\!\perp Z | dsep_{\mathcal{G}}(X; Z|Y)\}$$

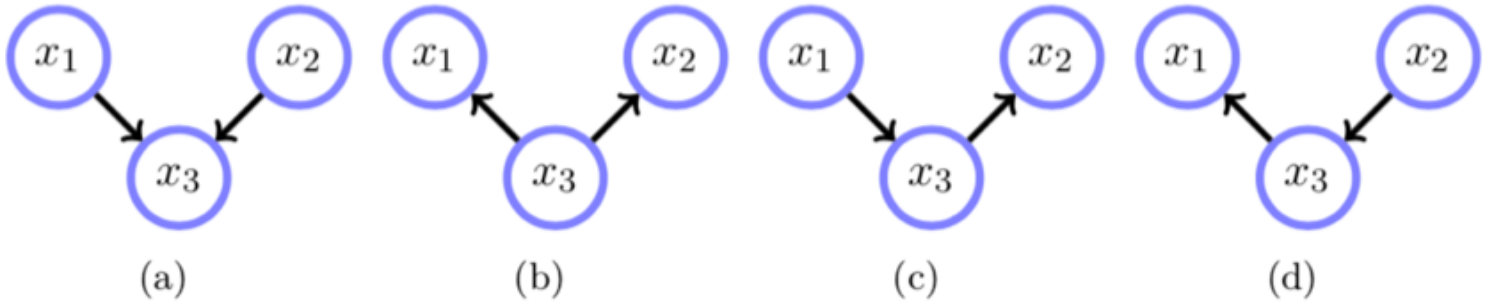
- **Defn**: A DAG $\mathcal{G}$ is an **I-map** (independence-map) of P if $\mathcal{I}_l(\mathcal{G}) \subseteq \mathcal{I}(P)$
- A fully connected DAG $\mathcal{G}$ is an I-map for any distribution, since $\mathcal{I}_l(\mathcal{G}) = \varnothing \subseteq \mathcal{I}(P)$ for any P.



$$\begin{aligned} p(x_1, \ldots, x_n) &= p(x_1|x_2, \ldots, x_n)p(x_2, \ldots, x_n) \\ &= p(x_1|x_2, \ldots, x_n)p(x_2|x_3, \ldots, x_n)p(x_3, \ldots, x_n) \\ &= p(x_n)\prod_{i=1}^{n-1} p(x_i|x_{i+1}, \ldots, x_n) \end{aligned}$$

Review: I-equivalence

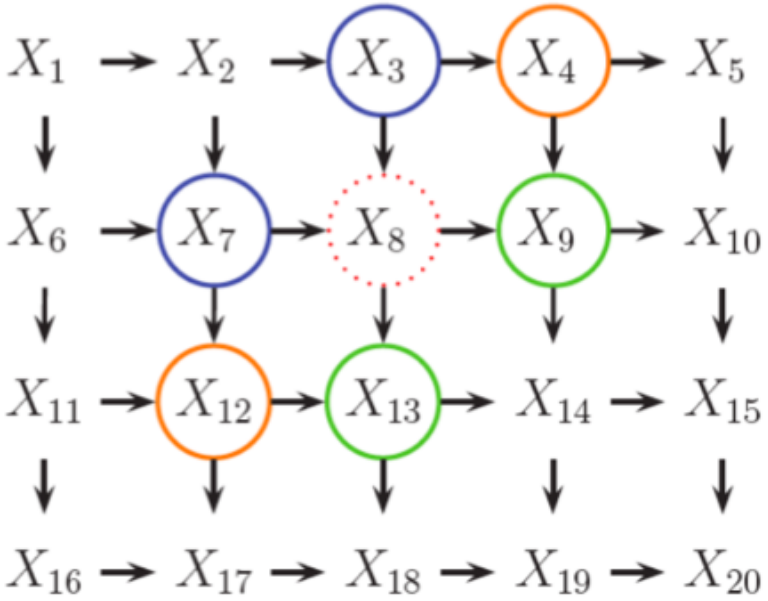
- Which graphs satisfy $\mathcal{I}(\mathcal{G}) = \{x_1 \perp\!\!\!\perp x_2 | x_3\}$?

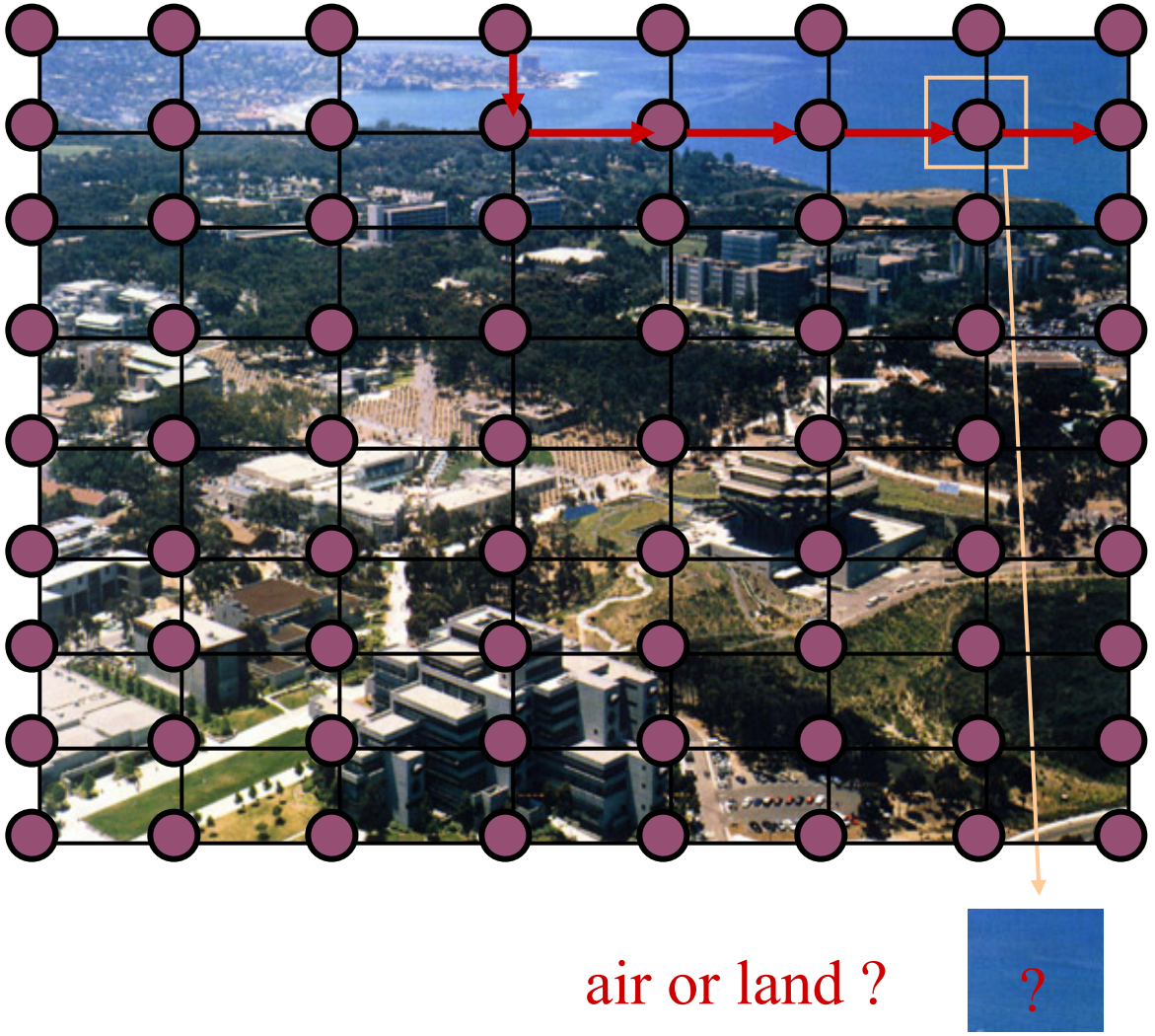


- **Defn :** The *skeleton* of a Bayesian network graph G over $\boldsymbol{V}$ is an undirected graph over $\boldsymbol{V}$ that contains an edge $\{X, Y\}$ for every edge (X, Y) in G.

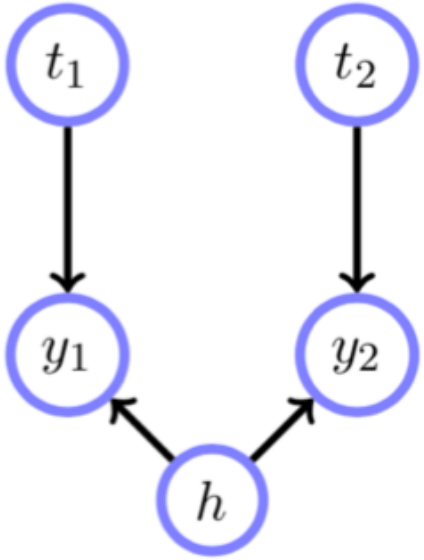
Why Undirected GM?

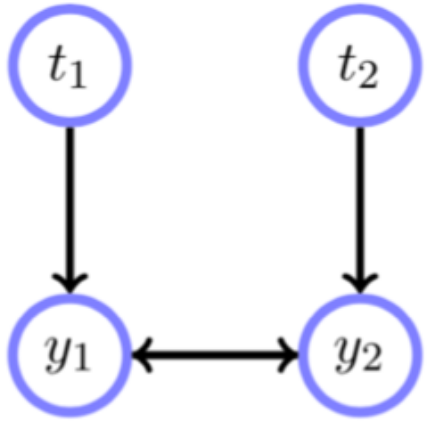
DGM is not always a good choice…





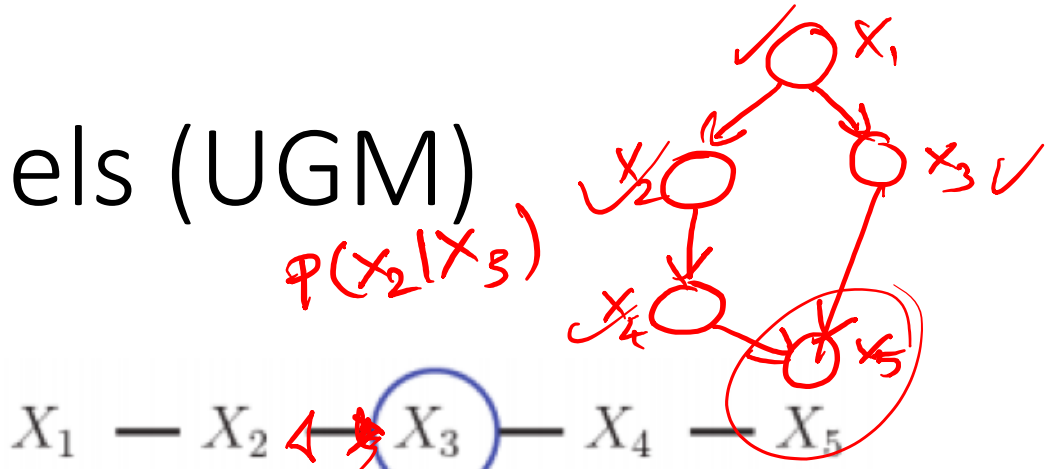
DGM is not always a good choice…



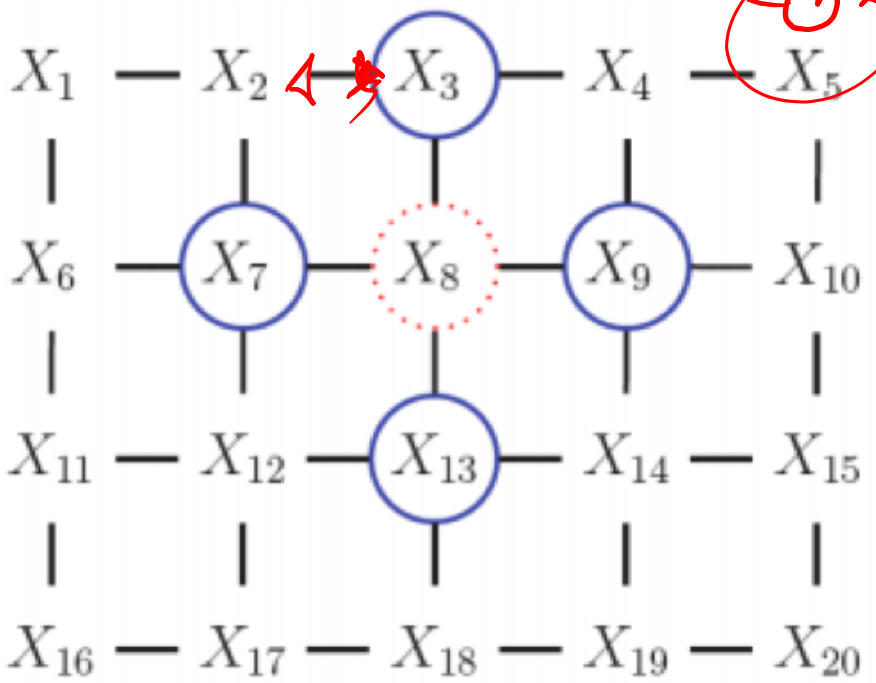


What if we cannot observe h ?

Undirected Graphical Models (UGM)

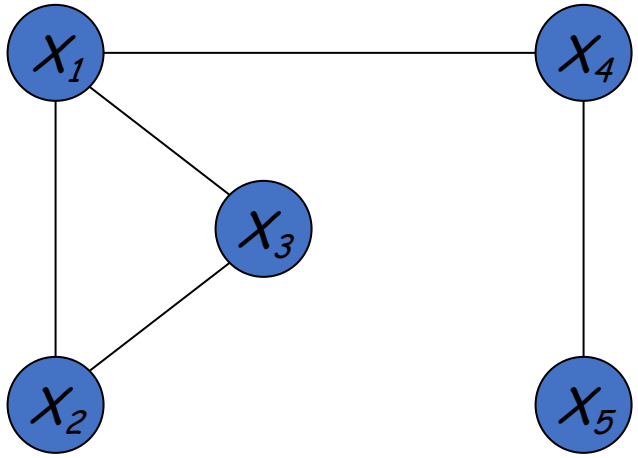


- As in DGM, the nodes in the graph represent the variables
- Edges represent probabilistic interaction between neighboring variables
- Parametrization?
  - In DGM we used CPD (conditional probabilities) to represent distribution of a node given others
  - For undirected graphs, we use a more symmetric parameterization that captures the affinities between related variables.
  - Differences:
    - Pairwise (non-causal) relationships
    - No explicit way to generate samples



What is UGM
and
What are they good for?

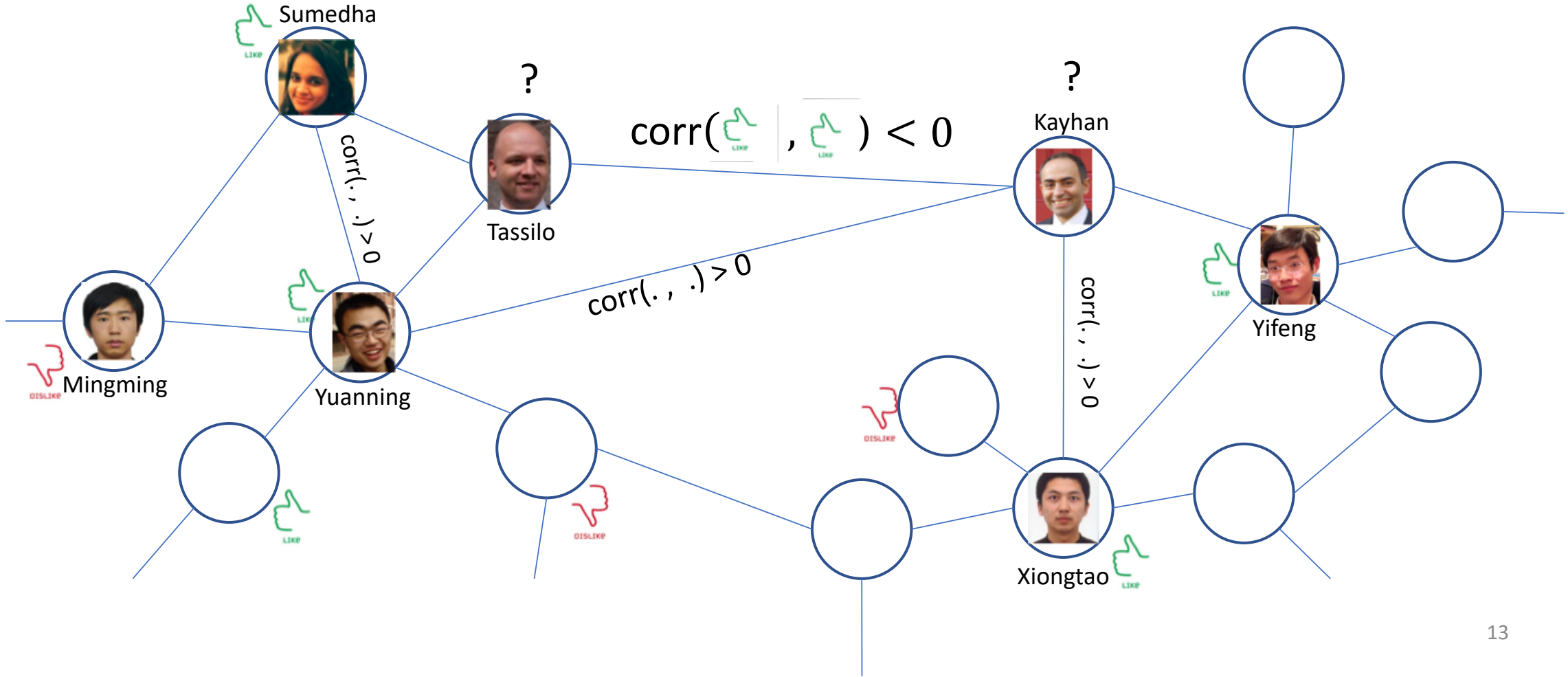
Undirected graphical models (UGM)



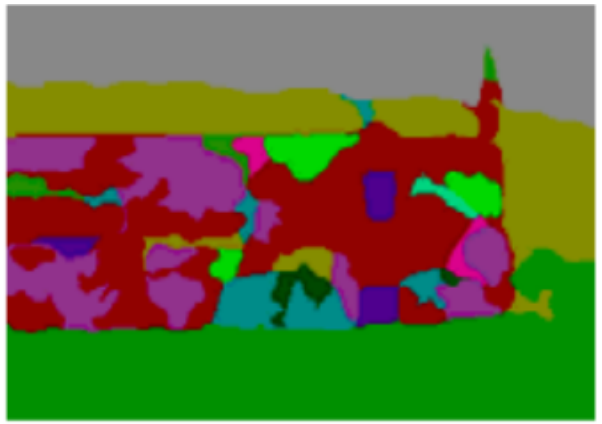
- Pairwise (non-causal) relationships
- Can write down model, and score specific configurations of the graph, but no explicit way to generate samples
- Contingency constrains on node configurations

Social networks

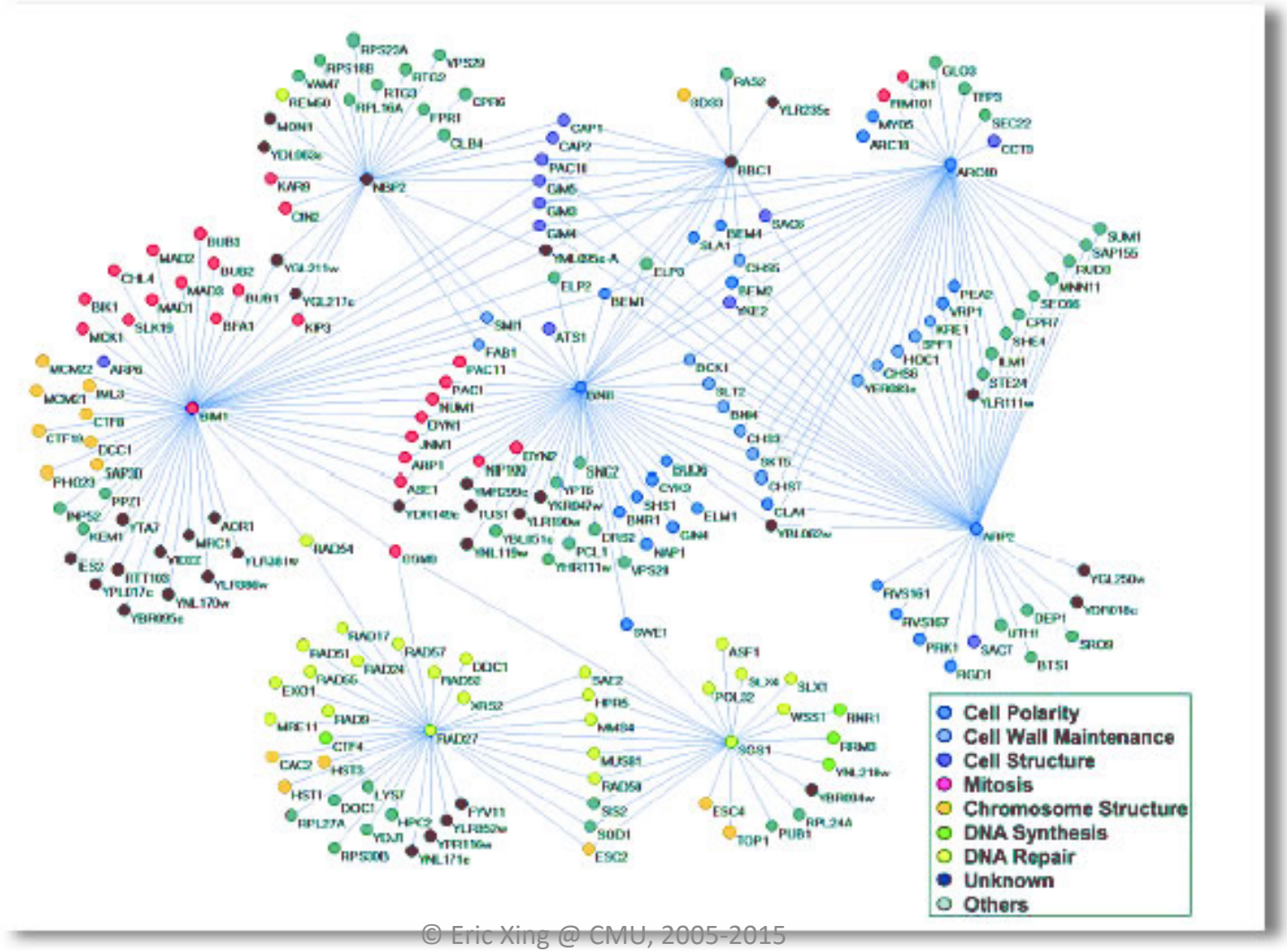
Opinions of the students about HW0.
Query: Did Tassilo like the HW0 given a few observation?
Links represent correlation between classmates.



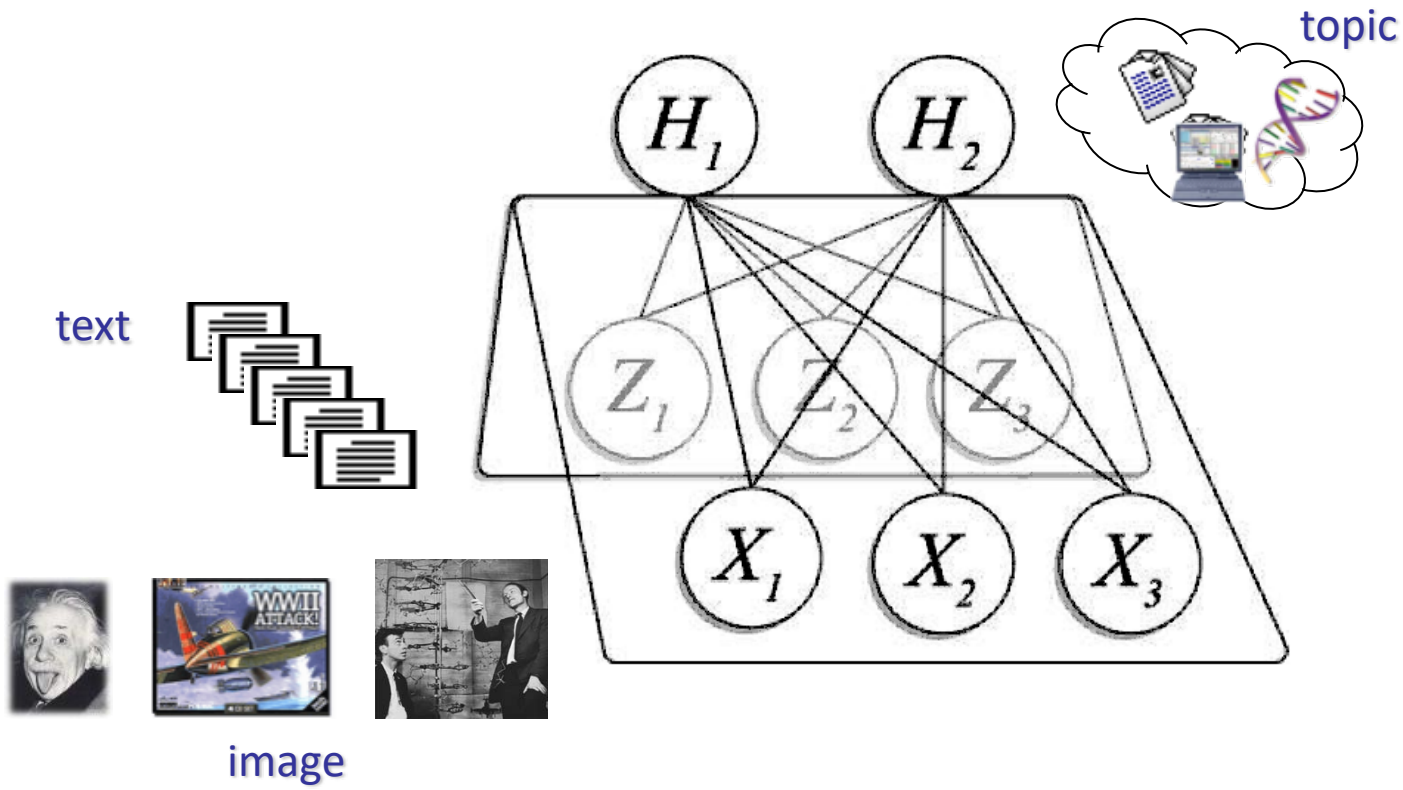
A Canonical Example: understanding complex scene …



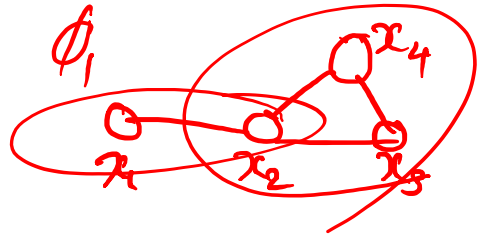
Protein interaction networks



Information retrieval

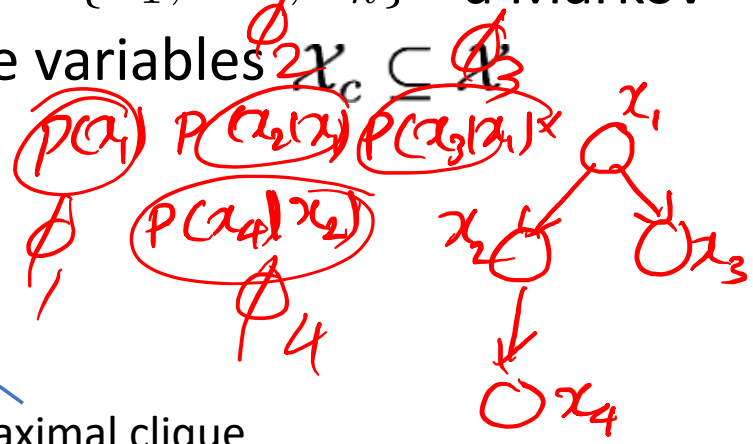


Undirected graphical models (UGM)



Defn (also called Markov Network): For a set of variables $\mathcal{X} = \{x_1, \ldots, x_n\}$ a Markov network is defined as a product of potentials on subsets of the variables $\mathcal{X}_c \subseteq \mathcal{X}$

$$p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{c=1}^{C} \phi_c(\mathcal{X}_c)$$

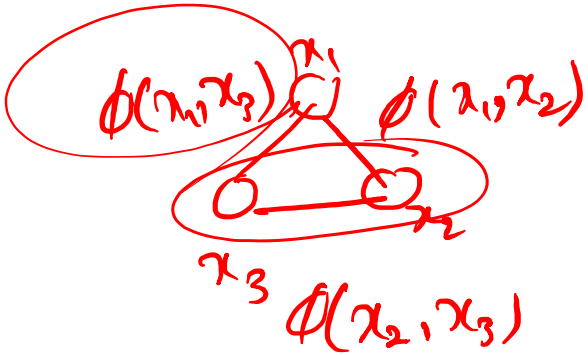


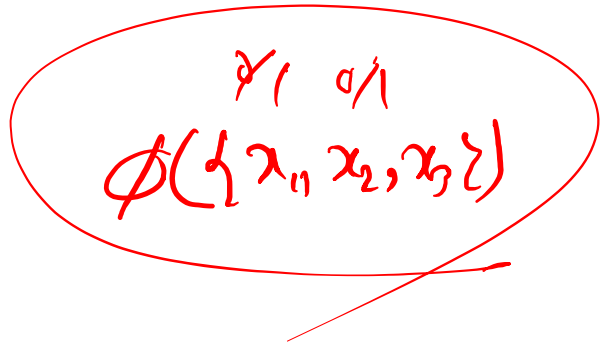
Normalizer to ensure it is a p is a probability

This is called potential ≥ 0 (this does not have to be probability)

Maximal clique

Def: A maximal clique is a clique that cannot be extended by including one more adjacent vertex, meaning it is not a subset of a larger clique.



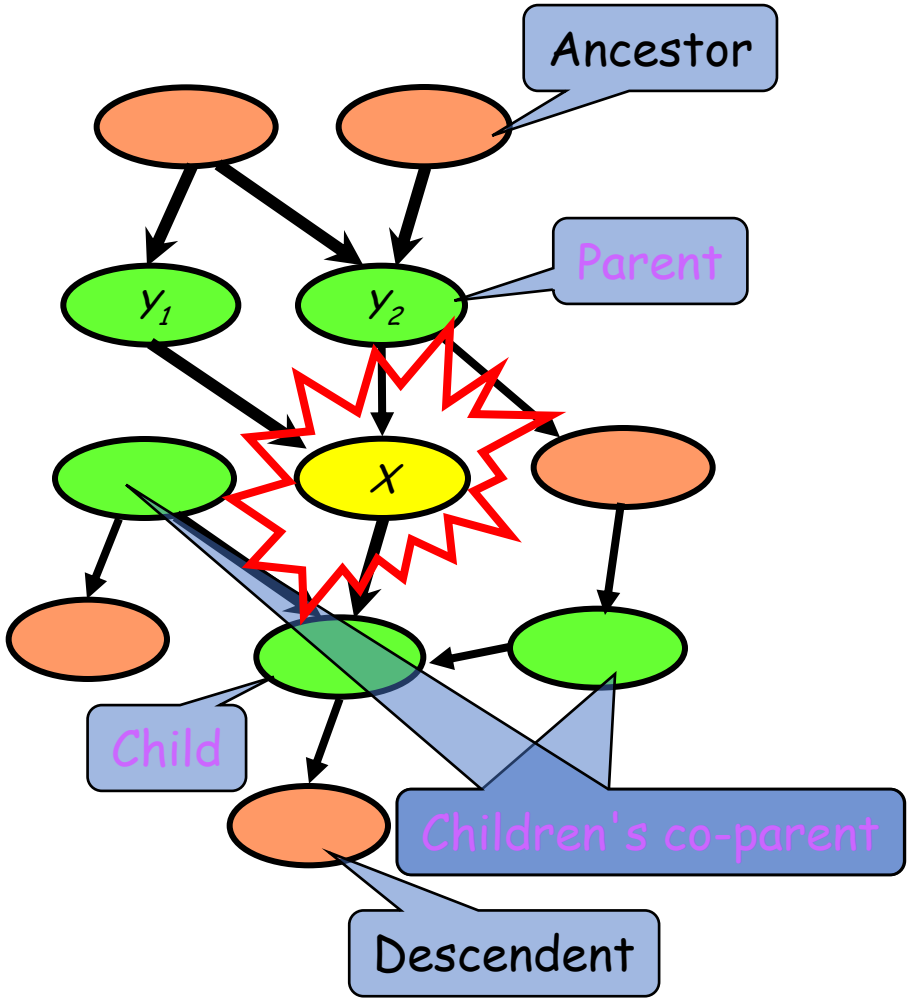


Independence

Remember the Markov Blanket for BN

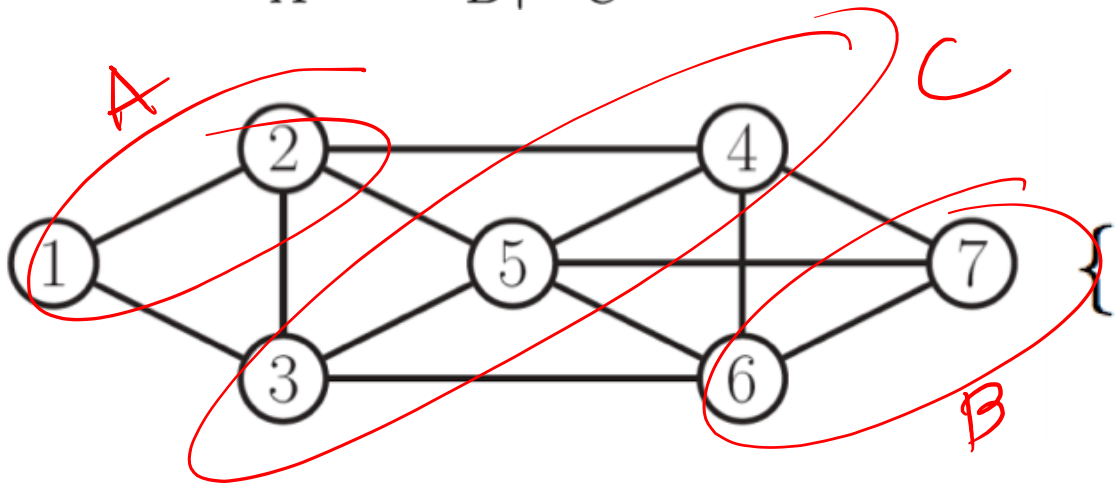
Structure: *DAG*

- Meaning: a node is conditionally independent of every other node in the network outside its Markov blanket



About Conditional Independence

Global Markov Property: $X_A \perp\!\!\!\perp X_B | X_C$ if and only if C separates A from B (there is no path connecting them)



$$\{1,2\} \perp \{6,7\} | \{3,4,5\}$$

Markov Blanket (local property) is the set of nodes that renders a node t conditionally independent of all the other nodes in the graph

$$t \perp\!\!\!\perp \mathcal{V} - mb(t) - \{t\} | mb(t)$$

All nodes in the graph

Markov Blanket

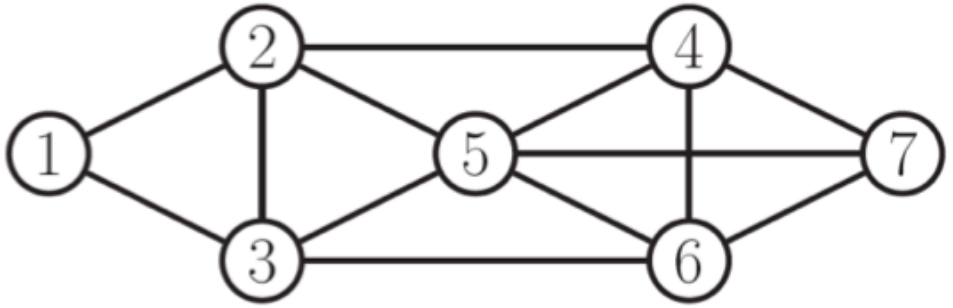
$$mb(5) = \{2,3,4,6,7\}$$

Example of Dependencies

Pairwise: $1 \perp 7 | \text{rest}$

Local: $1 \perp \text{rest} | 2, 3$

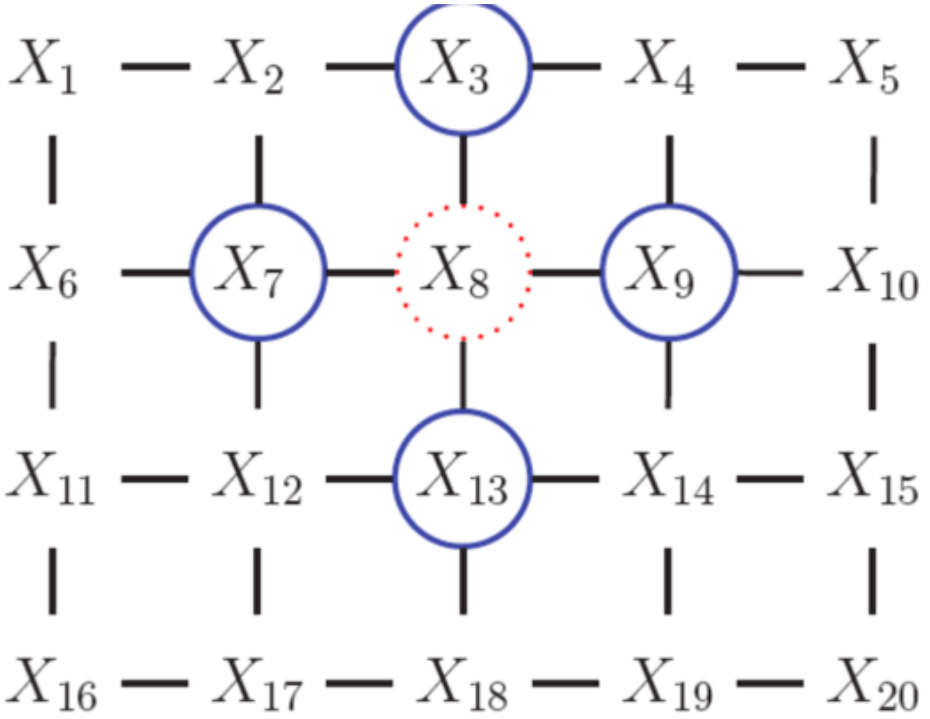
Global: $1, 2 \perp 6, 7 | 3, 4, 5$



$1 \perp 7 | \text{rest}?,\ 1 \perp 20 | \text{rest}?, 1 \perp 2 | \text{rest}?$

$1 \perp \text{rest} | ?,\ 8 \perp \text{rest} | ?$

$1, 2 \perp 15, 20 | ?$



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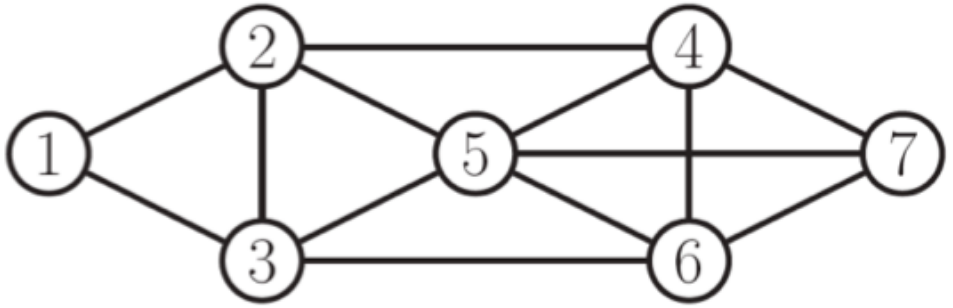
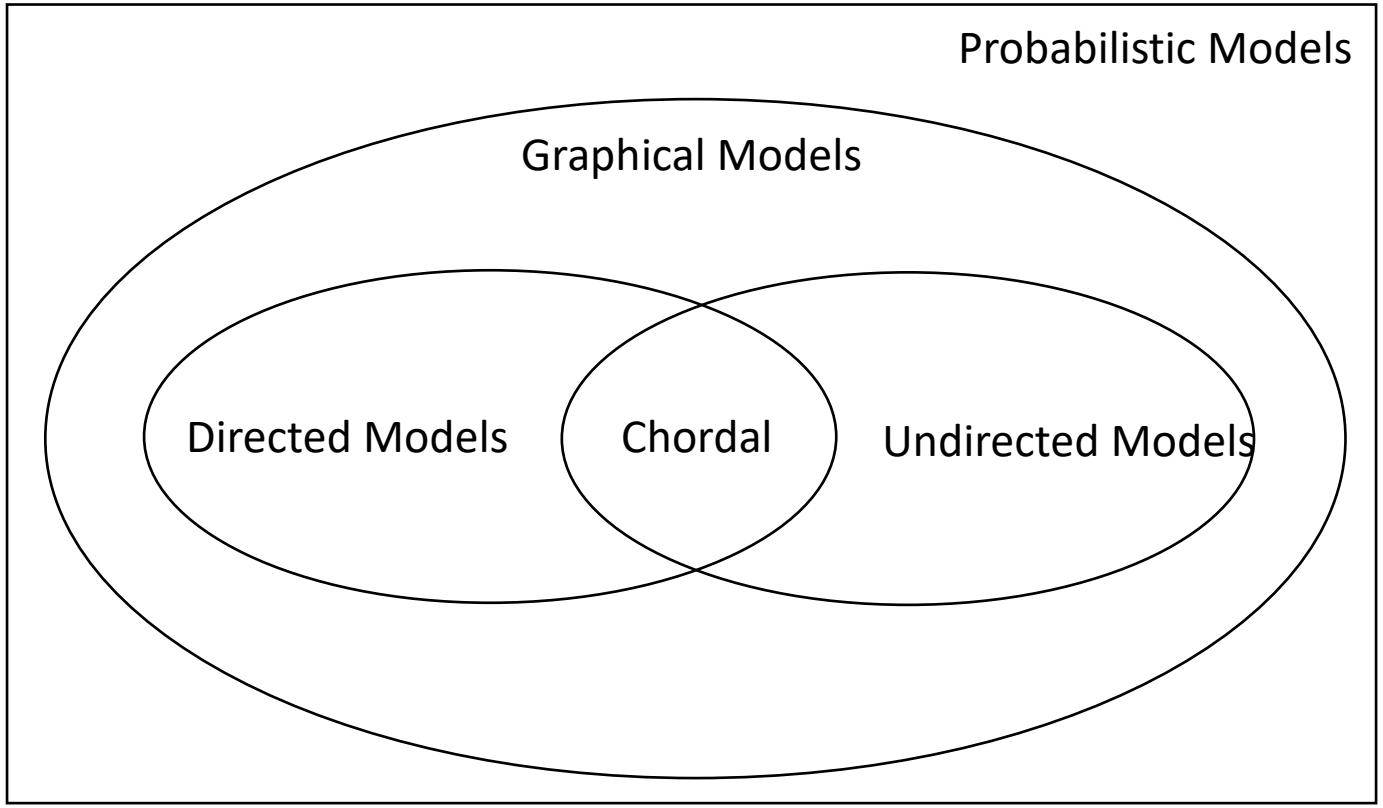


Global $\Longrightarrow$ Local $\Longrightarrow$ Pairwise

$p(x) > 0$

For proof: See page 119 of the book by Koller and Friedman

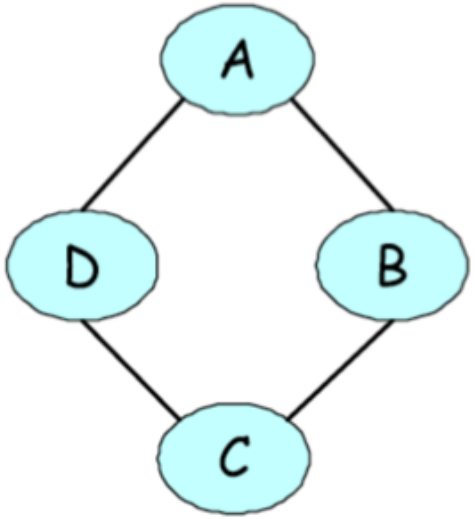
UGM and DGM



Triangulation: UGM $\Longrightarrow$ DGM

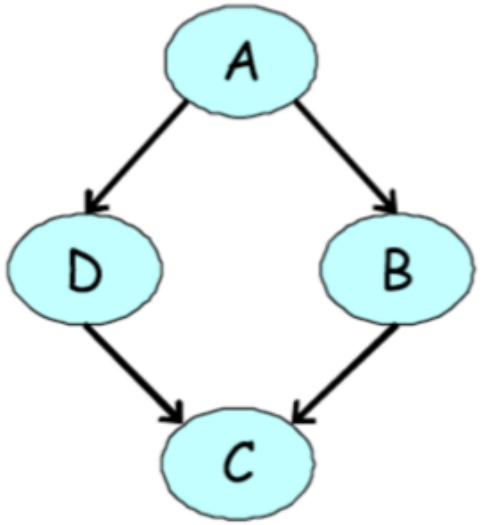
Moralization: DGM $\Longrightarrow$ UGM

Not all UGM can be represented as DGM



$A \perp C|D, B$

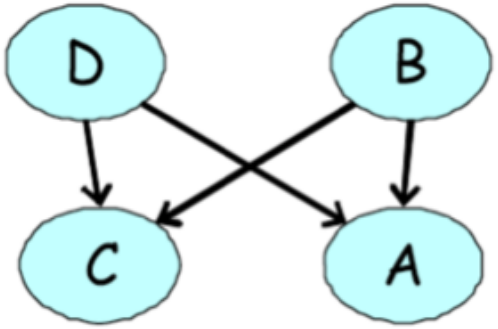
$B \perp D|A, C$



$A \perp C|D, B$

$B \perp D|A, C$ X

$D \perp\!\!\!\perp B \mid \emptyset$

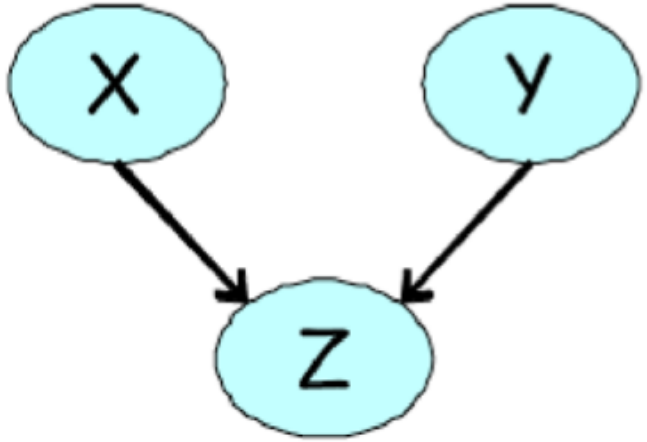


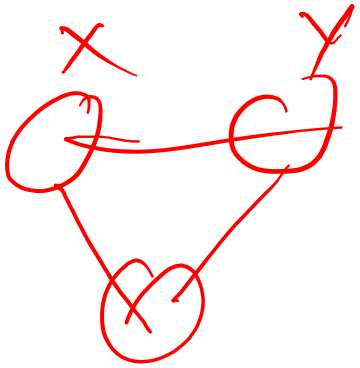
$A \perp C|D, B$

$B \perp D|A, C$ X

In this graph, B and D are marginally independent

Not all DGM can be represented as UGM





Undirected model fails to capture the marginal independence $(X \perp Y)$ that holds in the directed model at the same time as $\neg(X \perp Y|Z)$

What is this “Clique”?

Undirected graphical models (UGM)

Defn (also called Markov Network): For a set of variables $\mathcal{X} = \{x_1, \cdots, x_n\}$ a Markov network is defined as a product of potentials on subsets of the variables $\mathcal{X}_c \subseteq \mathcal{X}$

$$p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{c=1}^{C} \phi_c(\mathcal{X}_c)$$

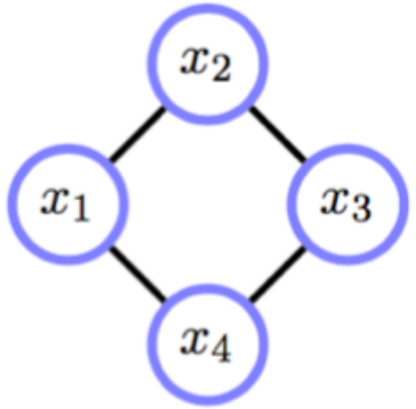
Normalizer to ensure it is a p is a probability

This is called potential ≥ 0 (this does not have to be probability)

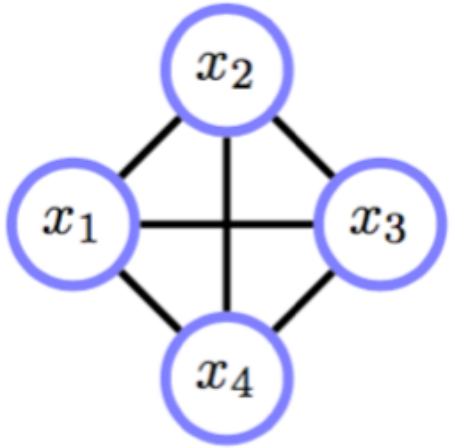
Maximal clique

Def: A maximal clique is a clique that cannot be extended by including one more adjacent vertex, meaning it is not a subset of a larger clique.

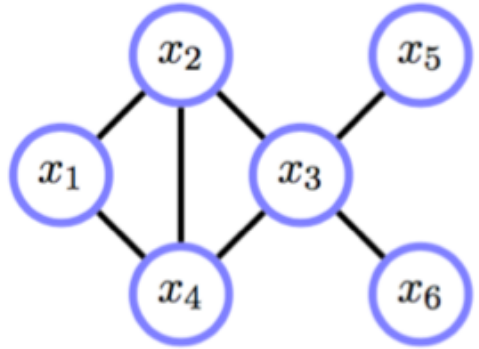
Examples



$$\phi(x_1, x_2)\phi(x_2, x_3)\phi(x_3, x_4)\phi(x_4, x_1)/Z_a$$

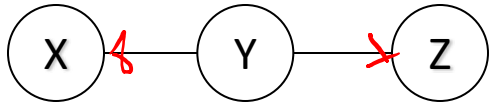


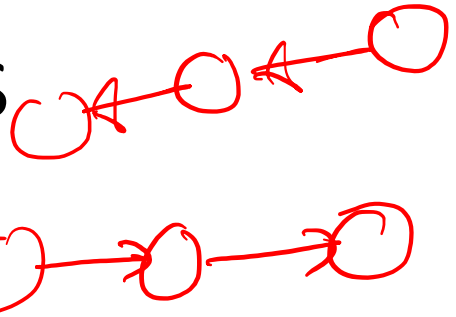
$$\phi(x_1, x_2, x_3, x_4)/Z_b$$



$$\phi(x_1, x_2, x_4)\phi(x_2, x_3, x_4)\phi(x_3, x_5)\phi(x_3, x_6)/Z_c$$

Interpretation of Clique Potentials





- The model implies $X \perp\!\!\!\perp Z|Y$. This independence statement implies (by definition) that the joint must factorize as:

$$p(x,y,x) = p(y)p(x|y)p(z|y)$$

…but also we can write it

$$p(x,y)p(z|y)$$

…but also …

$$p(x|y)p(z,y)$$

$$\phi_1(x,y)$$

$$\phi_2(y,x)$$

…but also …

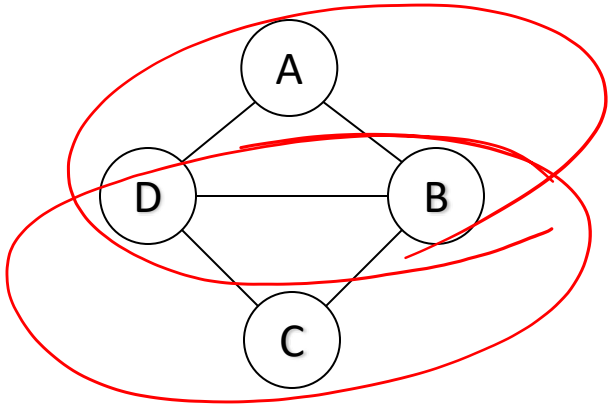
$$\frac{f_1(x,y)}{Z_1}\frac{f_2(y,z)}{Z_2}$$

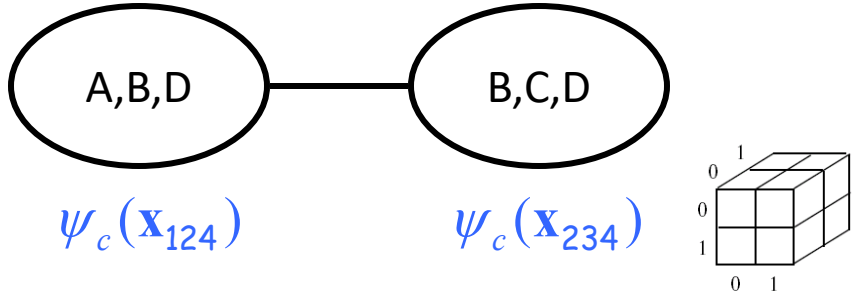
Interpretation of Clique Potentials

Take-home message about potentials:

- Those are not necessarily marginals or conditionals.
- The positive clique potentials can only be thought of as general "compatibility", "goodness" or "happiness" functions over their variables, but not as probability distributions.

Example UGM – using max cliques



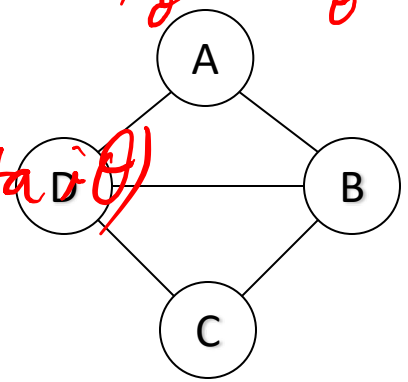


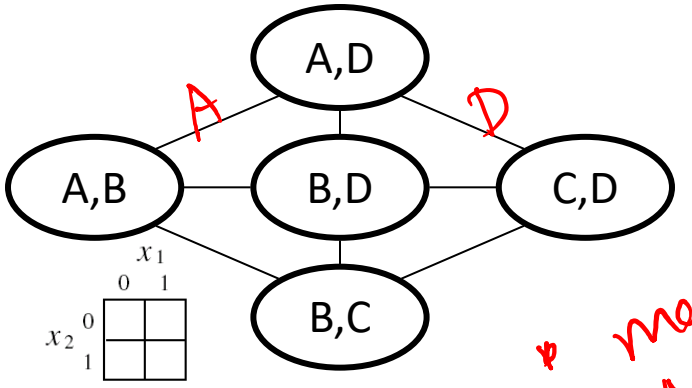
$$P'(x_1, x_2, x_3, x_4) = \frac{1}{Z}\psi_c(\mathbf{x}_{124}) \times \psi_c(\mathbf{x}_{234})$$

$$Z = \sum_{x_1, x_2, x_3, x_4} \psi_c(\mathbf{x}_{124}) \times \psi_c(\mathbf{x}_{234})$$

- For discrete nodes, we can represent $P(X_{1:4})$ as two 3D tables instead of one 4D table

Example UGM – using subcliques



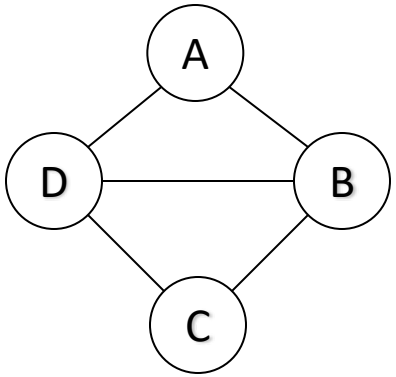


$$P''(x_1, x_2, x_3, x_4) = \frac{1}{Z}\prod_{ij}\psi_{ij}(\mathbf{x}_{ij})$$

$$Z = \sum_{x_1,x_2,x_3,x_4}\prod_{ij}\psi_{ij}(\mathbf{x}_{ij}) \qquad = \frac{1}{Z}\psi_{12}(\mathbf{x}_{12})\psi_{14}(\mathbf{x}_{14})\psi_{23}(\mathbf{x}_{23})\psi_{24}(\mathbf{x}_{24})\psi_{34}(\mathbf{x}_{34})$$

- We can represent $P(X_{1:4})$ as 5 2D tables instead of one 4D table
- Pair MRFs, a popular and simple special case
- Are two graphs equivalent ($\mathcal{I}(P')$ and $\mathcal{I}(P'')$)?

Example UGM – canonical representation



$$P(x_1, x_2, x_3, x_4)$$

$$= \frac{1}{Z}\psi_c(\mathbf{x}_{124}) \times \psi_c(\mathbf{x}_{234})$$
$$\times \psi_{12}(\mathbf{x}_{12})\psi_{14}(\mathbf{x}_{14})\psi_{23}(\mathbf{x}_{23})\psi_{24}(\mathbf{x}_{24})\psi_{34}(\mathbf{x}_{34})$$
$$\times \psi_1(x_1)\psi_2(x_2)\psi_3(x_3)\psi_4(x_4)$$

$$Z = \sum_{x_1, x_2, x_3, x_4} \begin{array}{l} \psi_c(\mathbf{x}_{124}) \times \psi_c(\mathbf{x}_{234}) \\ \times \psi_{12}(\mathbf{x}_{12})\psi_{14}(\mathbf{x}_{14})\psi_{23}(\mathbf{x}_{23})\psi_{24}(\mathbf{x}_{24})\psi_{34}(\mathbf{x}_{34}) \\ \times \psi_1(x_1)\psi_2(x_2)\psi_3(x_3)\psi_4(x_4) \end{array}$$

- Most general, subsume P' and P'' as special cases

Hammersley-Clifford Theorem

- If arbitrary potentials are utilized in the following product formula for probabilities,

$$P(x_1,\ldots,x_n)=\frac{1}{Z}\prod_{c\in C}\psi_c(\mathbf{x}_c)$$

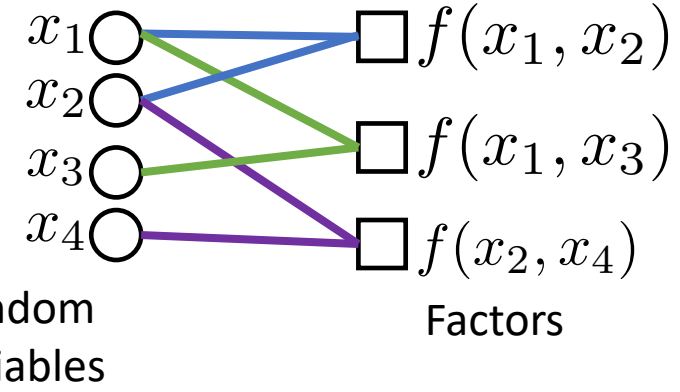
$$Z=\sum_{x_1,\ldots,x_n}\prod_{c\in C}\psi_c(\mathbf{x}_c)$$

  then the family of probability distributions obtained is exactly that set which **respects** the *qualitative specification* (the conditional independence relations) described earlier

- **Thm :** Let P be a positive distribution over $\mathbf{V}$, and *H* a Markov network graph over $\mathbf{V}$. If *H* is an I-map for P, then P is a Gibbs distribution over *H*.

Factor Graphs

Factor Graph

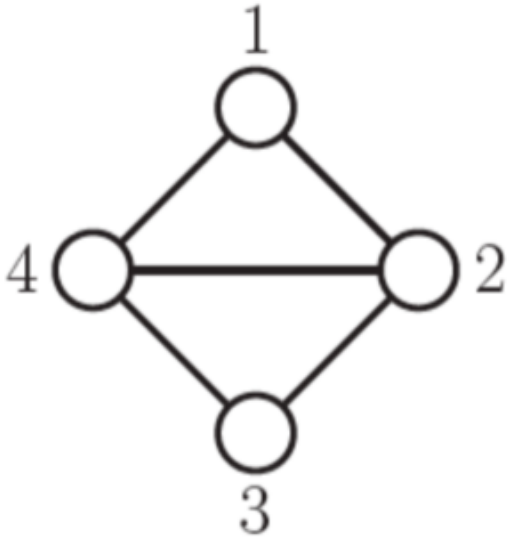


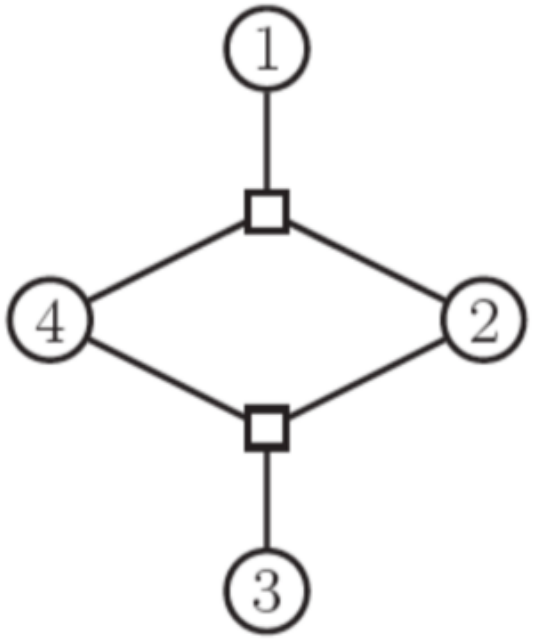
- A factor graph is a graphical model representation that unifies directed and undirected models
- It is an undirected bipartite graph with two kinds of nodes.
  - Round nodes represent variables,
  - Square nodes represent factors

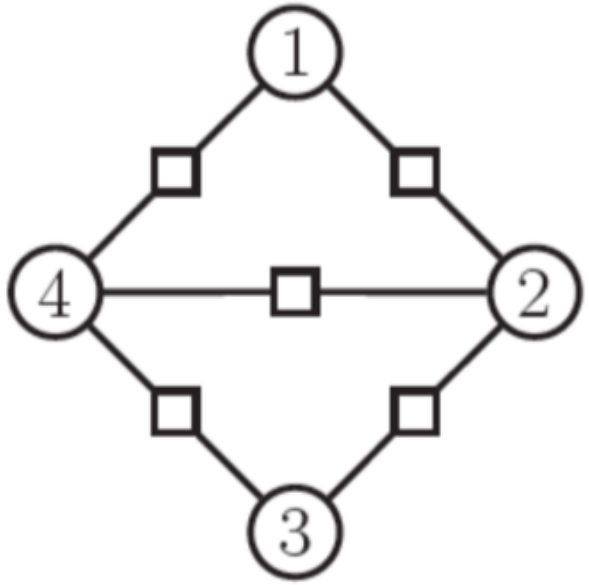
and there is an edge from each variable to every factor that mentions it.

- Represents the distribution more uniquely than a graphical model

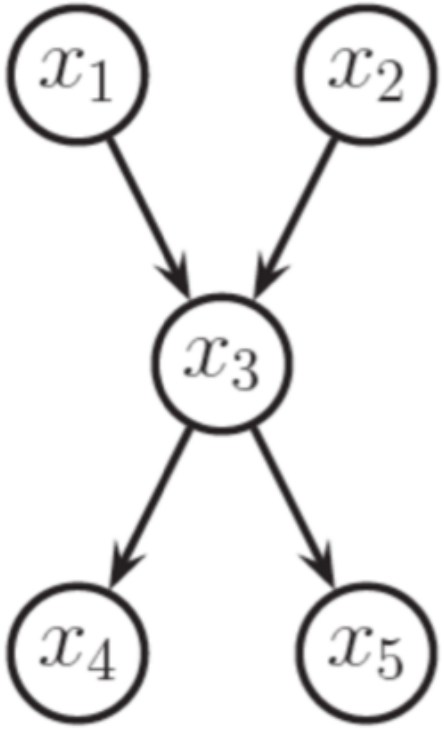
Factor Graph for UGM

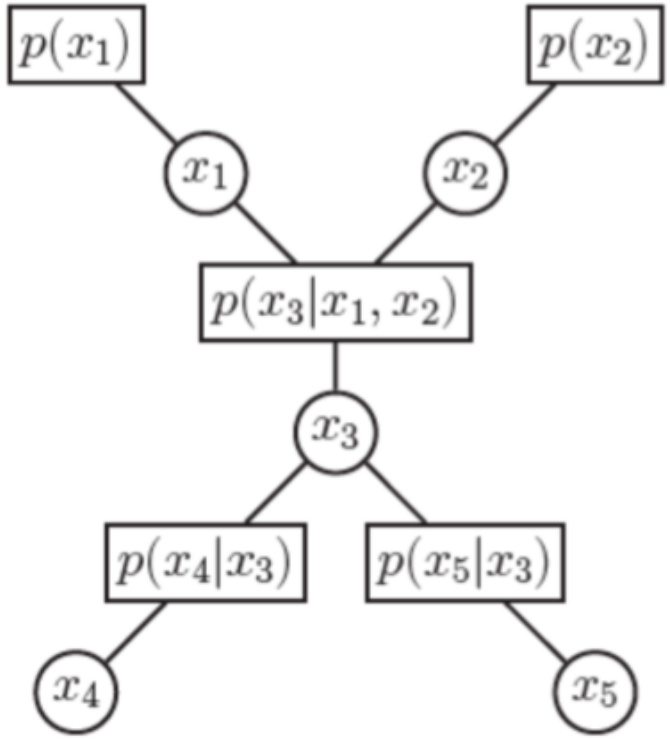






Factor Graph for DGM





One factor per CPD (conditional distribution) and connect the factor to all the variables that use the CPD

Practical Examples

Exponential Form

Remember the Gibbs distribution:

$$p(x_1, \cdots, x_n) = \frac{1}{Z} \prod_{c=1}^{C} \psi_c(\mathcal{X}_c)$$

So-called Potentials > 0

$$p(x_1, \cdots, x_n) = \frac{1}{Z} \prod_{c=1}^{C} \exp\left(-\phi_c(\mathcal{X}_c)\right)$$

Energy of the clique, can be positive/negative

Free Energy of the system (log of prob):

$$H(x_1, \cdots, x_n) = \sum_c \phi_c(\mathcal{X}_c)$$

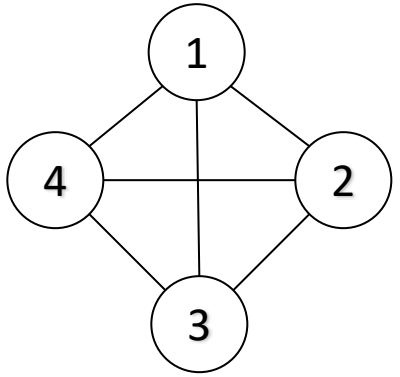
A powerful parametrization (log-linear model):

$$H(x_1, \cdots, x_n; \theta) = \sum_c f_c(\mathcal{X}_c)^T \theta_c$$

Param

Feature function

Example: Boltzmann machines



A fully connected graph with pairwise (edge) potentials on binary-valued nodes (for $x_i \in \{-1, +1\}$ or $x_i \in \{0,1\}$) is called a Boltzmann machine

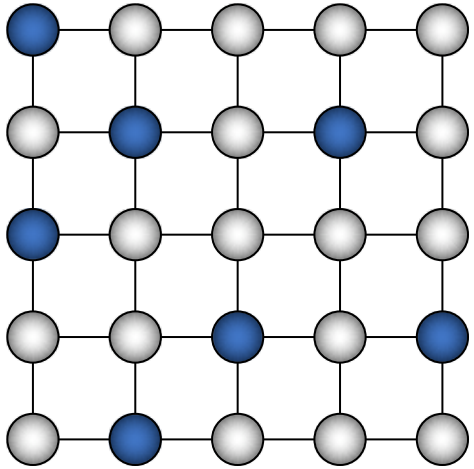
$$p(x_1, x_2, x_3, x_4; \theta; \alpha) = \frac{1}{Z(\theta, \alpha)} \exp\left[\sum_{ij} \theta_{ij} x_i x_j + \sum_i \alpha_i x_i\right]$$

Hence the overall energy function has a quadratic form.

$$H(\mathbf{x}; \Theta, \mu) = (\mathbf{x} - \mu)^T \Theta (\mathbf{x} - \mu)$$

Ising models

- Nodes are arranged in a regular topology (often a regular packing grid) and connected only to their geometric neighbors.

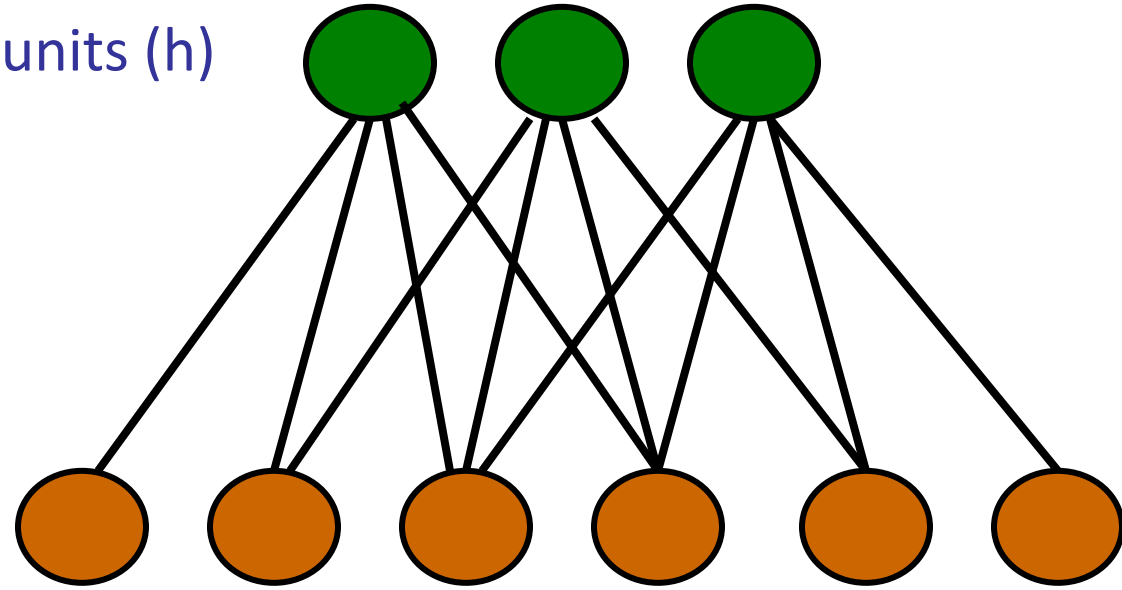


$$p(X) = \frac{1}{Z}\exp\left\{\sum_{i,j\in N_i}\theta_{ij}X_iX_j + \sum_i \theta_{i0}X_i\right\}$$

- Same as sparse Boltzmann machine, where $\theta_{ij}\neq 0$ iff i, j are neighbors.
  - e.g., nodes are pixels, potential function encourages nearby pixels to have similar intensities.
- Potts model: multi-state Ising model.

Restricted Boltzmann Machines (RBM)

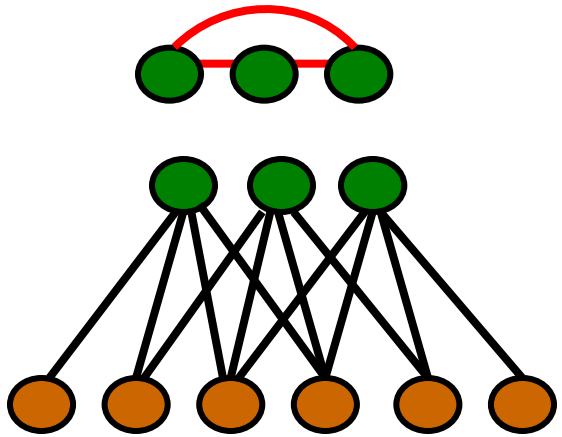
- Observed can pixels, signal in speech, word in a document
- Unobserved has “a notion” of summary of data
- One can use it as building block for more complicated models



$$p(x, h; \theta) = \exp\left(\sum_i \theta_i \phi_i(x) + \sum_j \theta_j \phi_j(h_j) + \sum_{i,j} \theta_{i,j}(x_i, h_j) - A(\theta)\right)$$

Properties of RBM

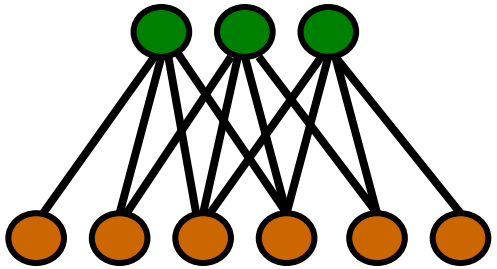
- Factors are marginally *dependent*.



- Factors are conditionally *independent* given observations on the visible nodes.

$$p(h_1, \cdots, h_M|\mathbf{x}) = \prod_m p(h_m|\mathbf{x})$$

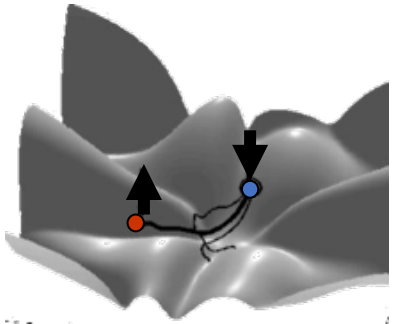
- Iterative Gibbs sampling to generate pairs of (x,h).



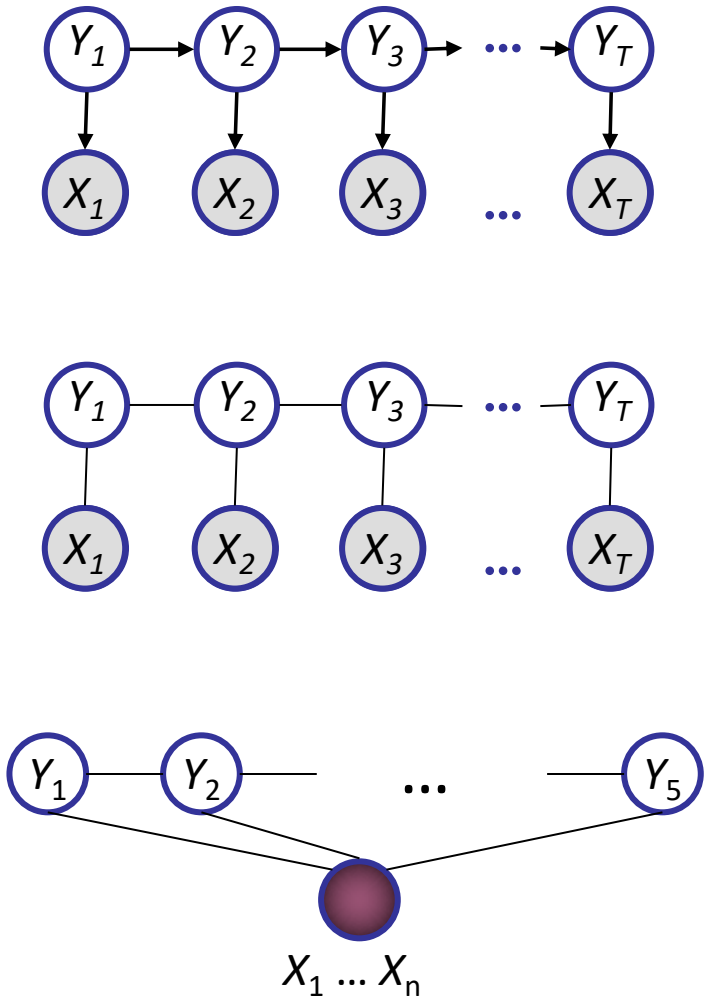
$$h \sim p(h \mid x)$$

$$x \sim p(x \mid h)$$

- Learning with contrastive divergence



Conditional Random Fields



- For example: part of speech labeling
- We are interested in Discriminative (not joint):

$$p_\theta(y \mid x) = \frac{1}{Z(\theta, x)} \exp\left\{\sum_c \theta_c f_c(x, y_c)\right\}$$

Summary

- Undirected graphical models capture “relatedness”, “coupling”, “co-occurrence”, “synergism”, etc. between entities
  - Local and global independence properties identifiable via graph separation criteria
  - Defined on clique potentials
- Can be used to define either joint or conditional distributions
- Generally intractable to compute likelihood due to presence of “partition function”
  - Therefore not only inference, but also likelihood-based learning is difficult in general
- Important special cases:
  - Ising models
  - RBM
  - CRF