

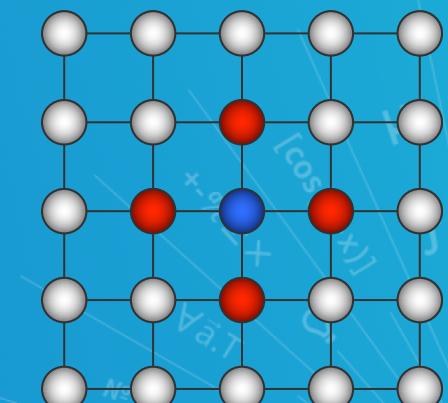
Probabilistic Graphical Models

Representation of undirected GM

Eric Xing

Lecture 3, January 23, 2019

Reading: KF-chap4

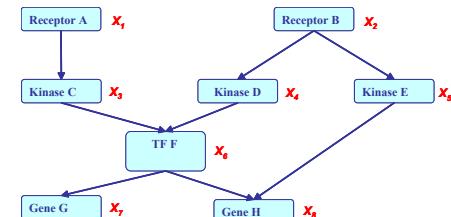




Two types of GMs

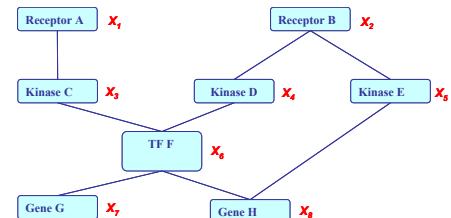
- Directed edges give **causality** relationships (Bayesian Network or Directed Graphical Model):

$$\begin{aligned} & P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8) \\ &= P(X_1) P(X_2) P(X_3|X_1) P(X_4|X_2) P(X_5|X_2) \\ &\quad P(X_6|X_3, X_4) P(X_7|X_6) P(X_8|X_5, X_6) \end{aligned}$$



- Undirected edges simply give **correlations** between variables (Markov Random Field or Undirected Graphical model):

$$\begin{aligned} & P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8) \\ &= \frac{1}{Z} \exp\{E(X_1)+E(X_2)+E(X_3, X_1)+E(X_4, X_2)+E(X_5, X_2) \\ &\quad + E(X_6, X_3, X_4)+E(X_7, X_6)+E(X_8, X_5, X_6)\} \end{aligned}$$





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:

$$\mathcal{I}(\mathcal{G}) = \{X \perp Z|Y : \text{dsep}_{\mathcal{G}}(X; Z|Y)\}$$

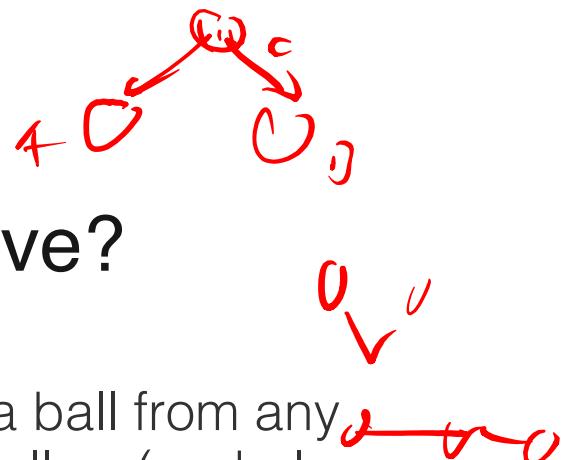
- Defn: A DAG \mathcal{G} is an **I-map** (independence-map) of P if $\mathcal{I}_l(\mathcal{G}) \subseteq \mathcal{I}(P)$
- A fully connected DAG \mathcal{G} is an I-map for any distribution, since $\mathcal{I}_l(\mathcal{G}) = \emptyset \subseteq \mathcal{I}(P)$ for any P .
- Defn: A DAG \mathcal{G} is a **minimal I-map** for P if it is an I-map for P , and if the removal of even a single edge from \mathcal{G} renders it not an I-map.
- A distribution may have several minimal I-maps
 - Each corresponding to a specific node-ordering



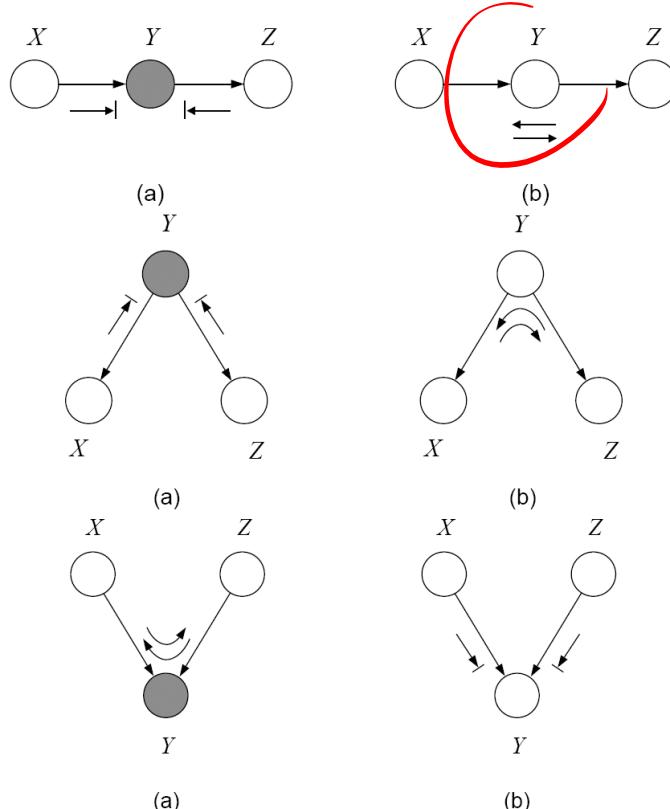


What is in $I(G)$ ---

How to extract D-separation properties? How to prove?



- X is **d-separated** (directed-separated) from Z given Y if we can't send a ball from any node in X to any node in Z using the "*Bayes-ball*" algorithm illustrated below (and plus some boundary conditions):



- **Defn:** $I(G)$ =all independence properties that correspond to d-separation:

$$I(G) = \{X \perp Z | Y : \text{dsep}_G(X; Z | Y)\}$$

- **D-separation is sound and complete (more details later)**

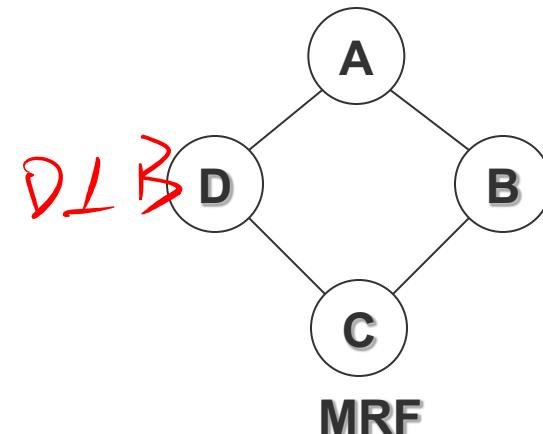
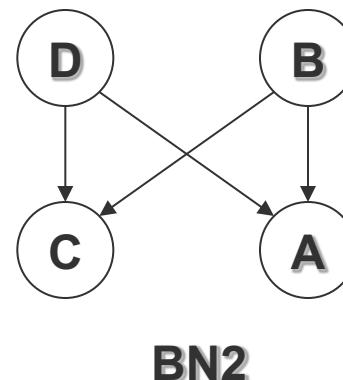
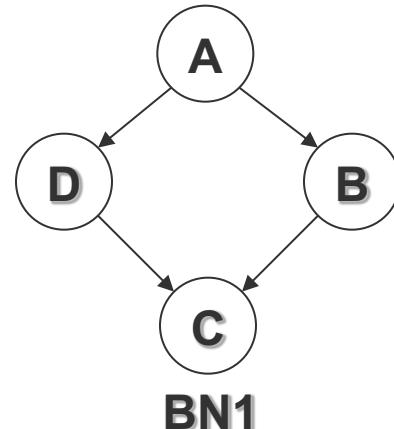




P-maps

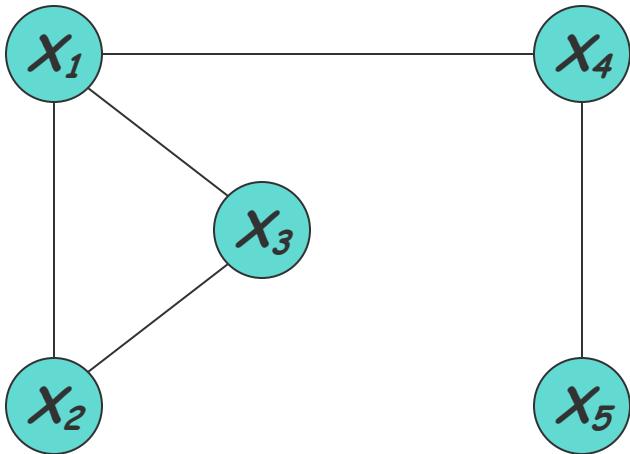
- Defn: A DAG G is a **perfect map** (P-map) for a distribution P if $I(P)=I(G)$.
- Thm: not every distribution has a perfect map as DAG.
 - Pf by counterexample. Suppose we have a model where $A \perp C | \{B, D\}$, and $B \perp D | \{A, C\}$.
This cannot be represented by any Bayes net.
- e.g., BN1 wrongly says $B \perp D | A$, BN2 wrongly says $B \perp D$.

$D \perp B | C$





Undirected graphical models (UGM)

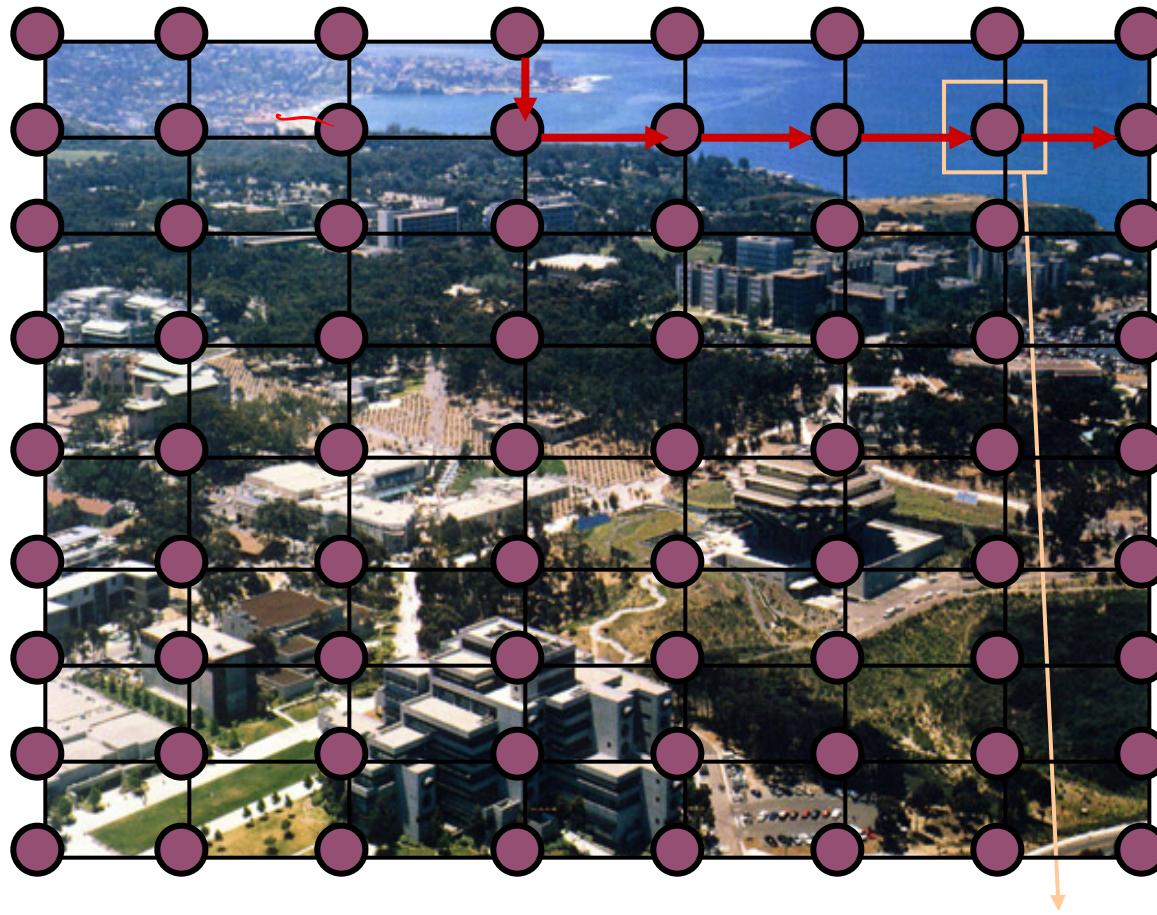


- ❑ Pairwise (non-causal) relationships
- ❑ Can write down model, and score specific configurations of the graph, but no explicit way to generate samples
- ❑ Contingency constraints on node configurations





A Canonical Example: understanding complex scene ...



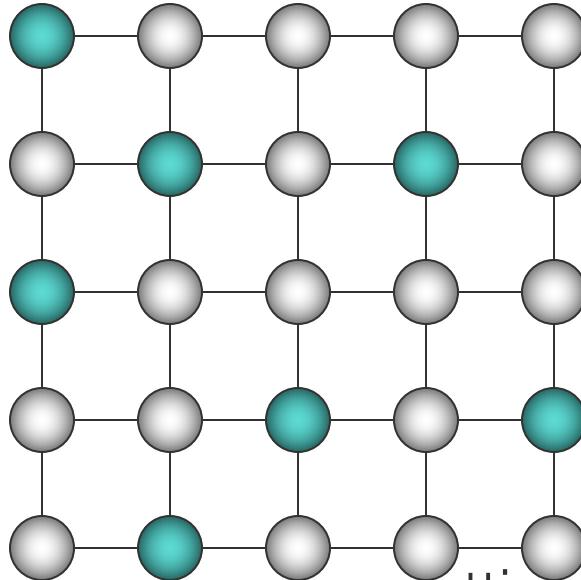
air or water ? ?





A Canonical Example

- The grid model

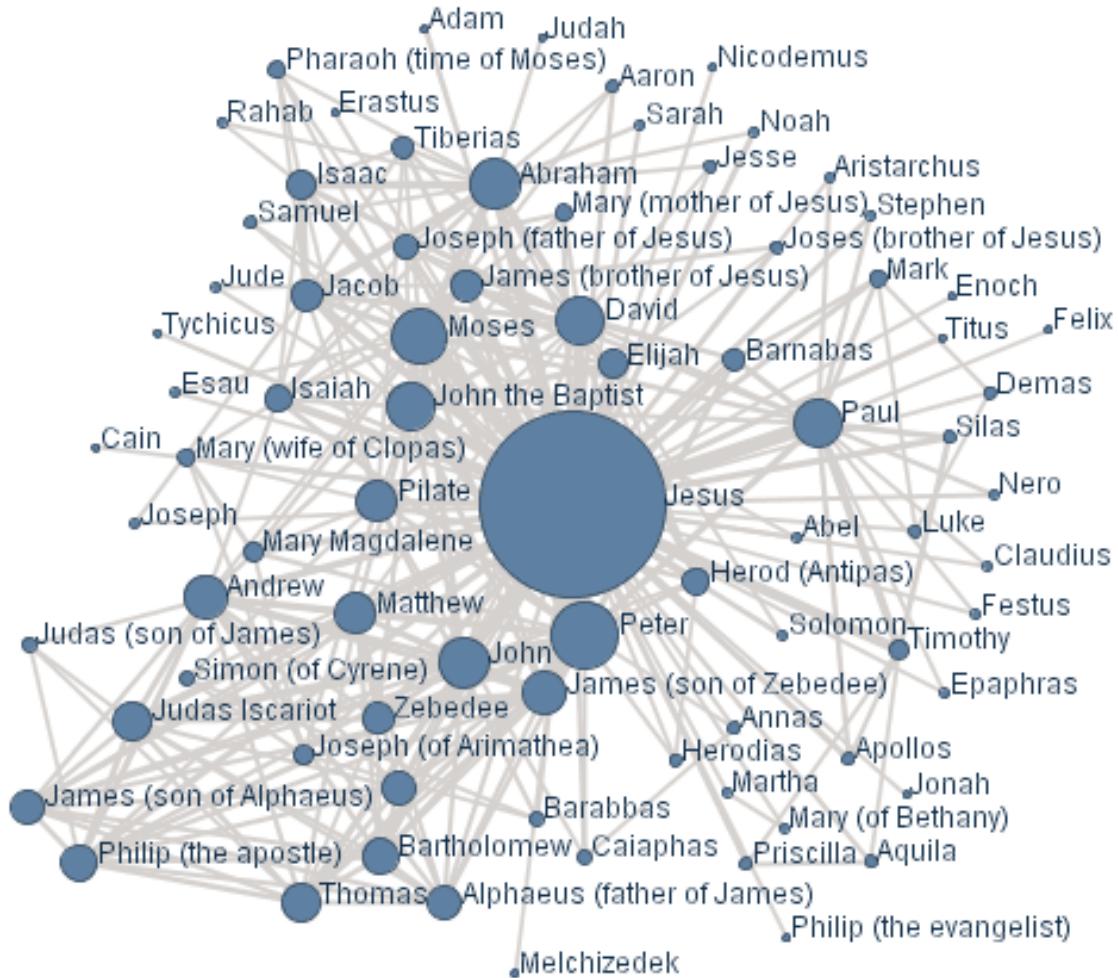


- Naturally arises in image processing, lattice physics, etc.
- Each node may represent a single "pixel", or an atom
 - The states of adjacent or nearby nodes are "coupled" due to pattern continuity or electro-magnetic force, etc.
 - Most likely joint-configurations usually correspond to a "low-energy" state





Social networks



The New Testament Social Networks

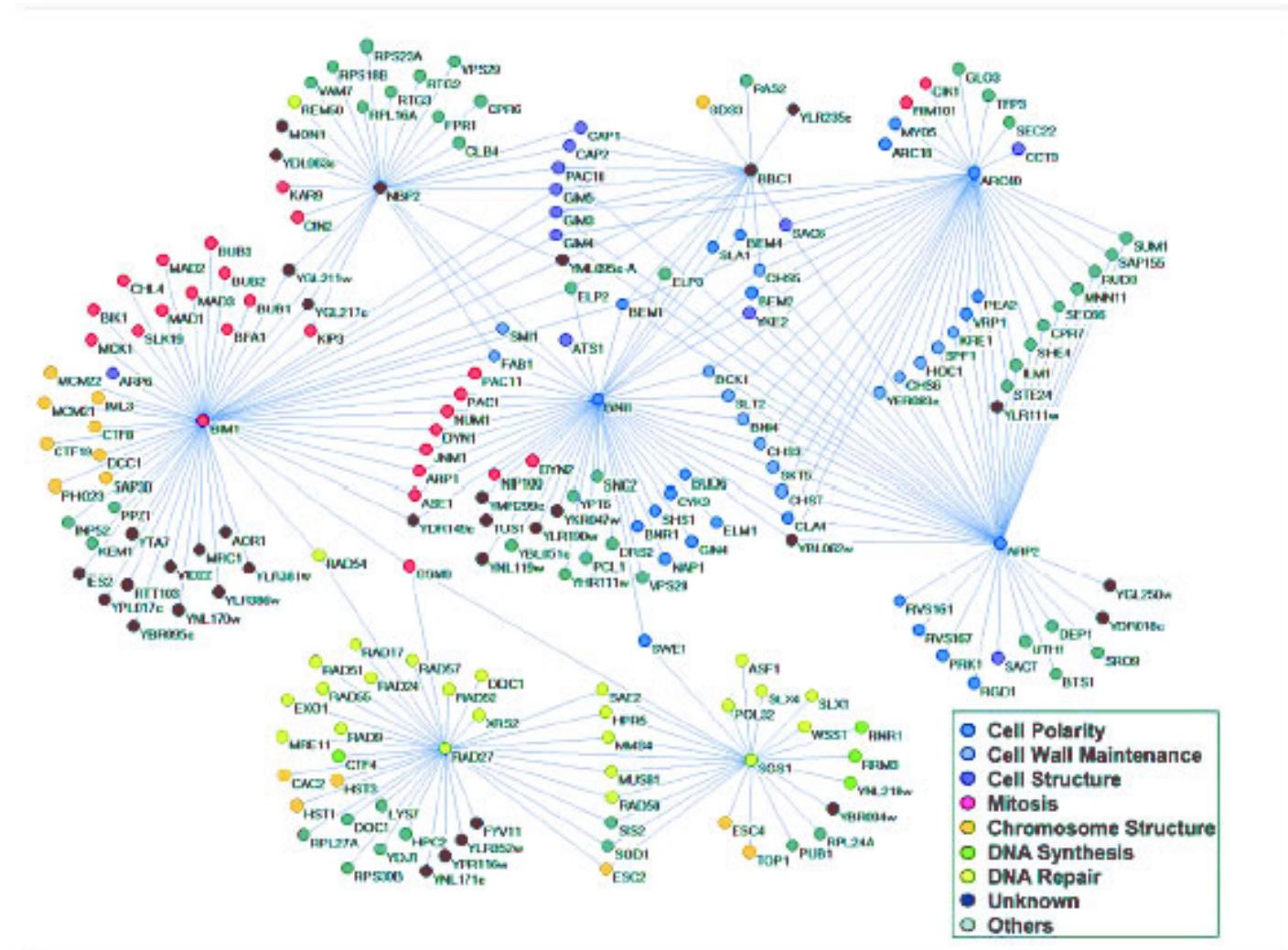
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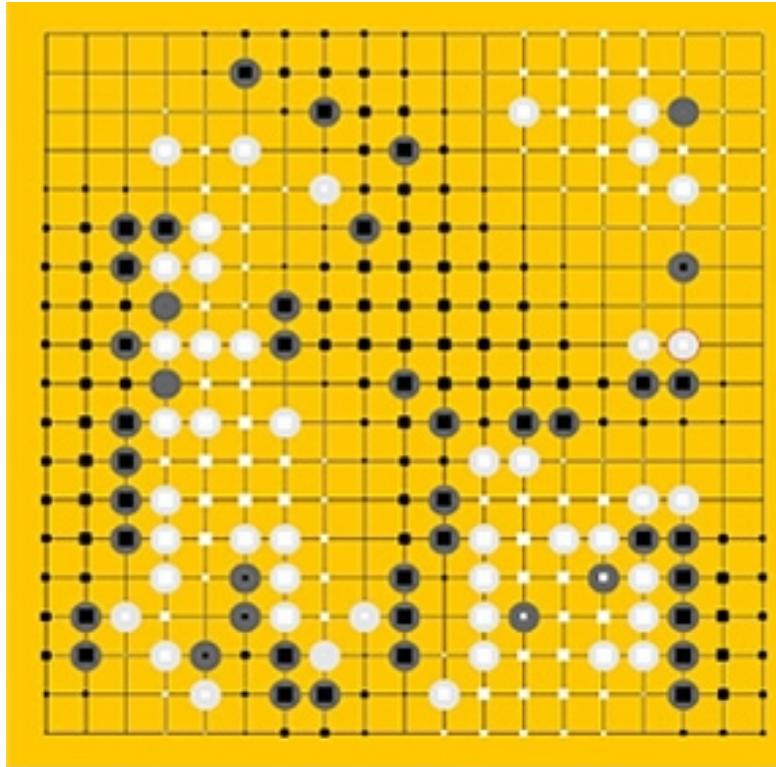


Protein interaction networks





Modeling Go

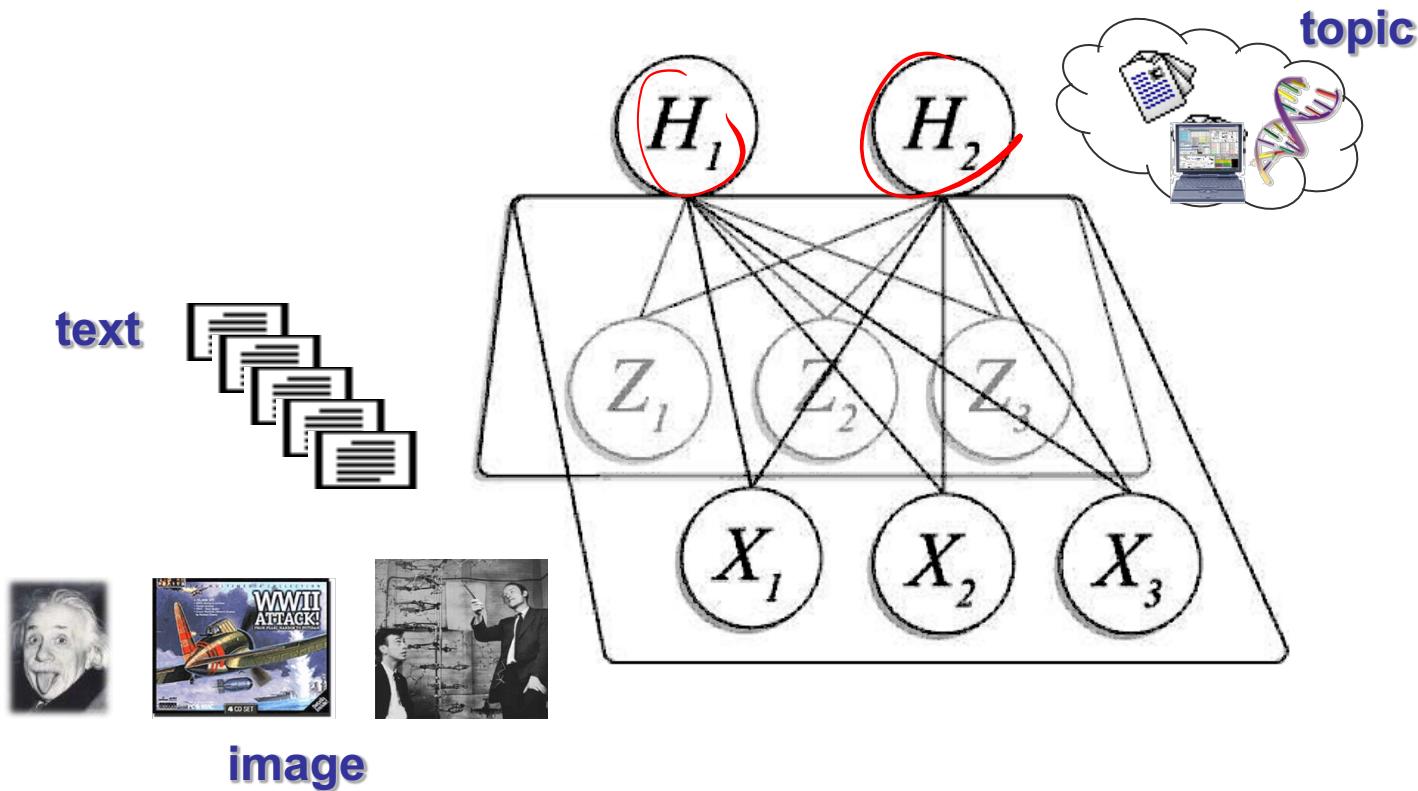


This is the middle position of a Go game.
Overlaid is the estimate for the probability of
becoming black or white for every intersection.
Large squares mean the probability is higher.





Information retrieval





Representation

- Defn: an undirected graphical model represents a distribution $P(X_1, \dots, X_n)$ defined by an undirected graph H , and a set of positive potential functions ψ_c associated with the cliques of H , s.t.

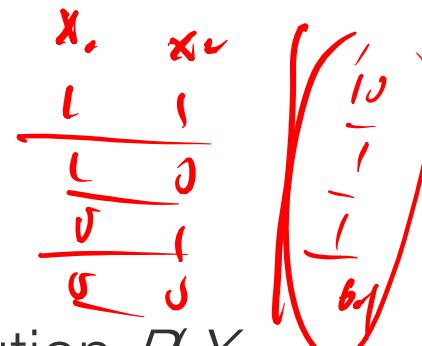
$$P(x_1, \dots, x_n) = \frac{1}{Z} \prod_{c \in C} \psi_c(\mathbf{x}_c)$$

(A Gibbs distribution)

where Z is known as the partition function:

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

- Also known as Markov Random Fields, Markov networks ...
- The potential function can be understood as an contingency function of its arguments assigning "pre-probabilistic" score of their joint configuration.

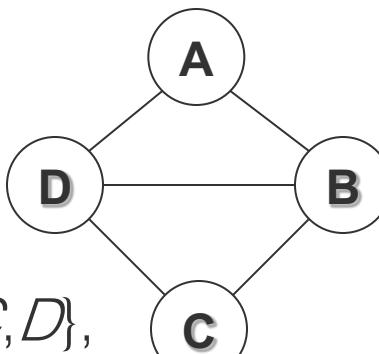




I. Quantitative Specification: Cliques

- For $G = \{V, E\}$, a complete subgraph (clique) is a subgraph $G' = \{V' \subseteq V, E' \subseteq E\}$ such that nodes in V' are fully interconnected
- A (maximal) clique is a complete subgraph s.t. any ~~superset~~ $V'' \supset V'$ is not complete.
- A sub-clique is a not-necessarily-maximal clique.

YC

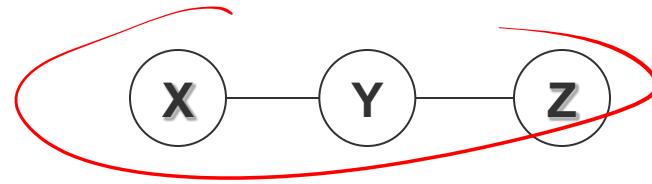


- Example:
 - max-cliques = $\{A, B, D\}, \{B, C, D\}$,
 - sub-cliques = $\{A, B\}, \{C, D\}, \dots \rightarrow$ all edges and singletons





Interpretation of Clique Potentials



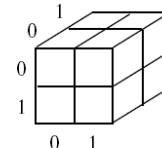
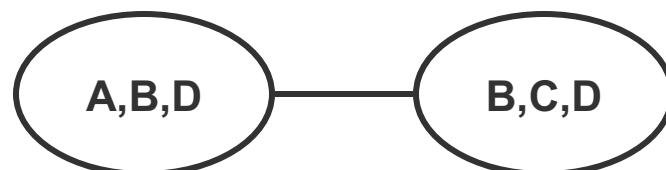
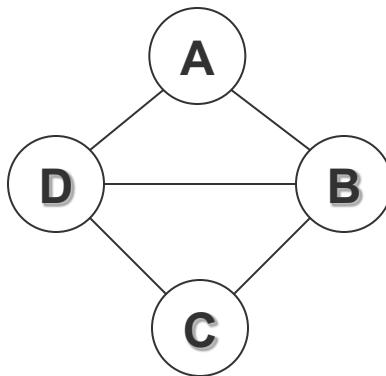
$$\begin{aligned}\phi(x, z) \\ \phi(y, z)\end{aligned}$$

- The model implies $X \perp\!\!\!\perp Y$. This independence statement implies (by definition) that the joint must factorize as:
- We can write this as: $p(x, y, z) = p(y)p(x|y)p(z|y)$, but
 $p(x, y, z) = p(x, y)p(z|y)$
 - **cannot** have all potentials be **marginals**
 - **cannot** have all potentials be **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



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

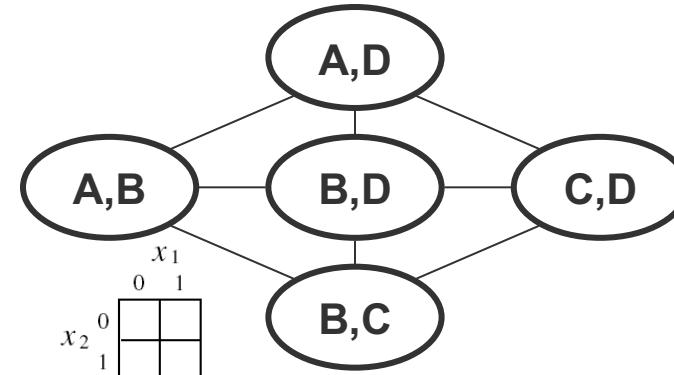
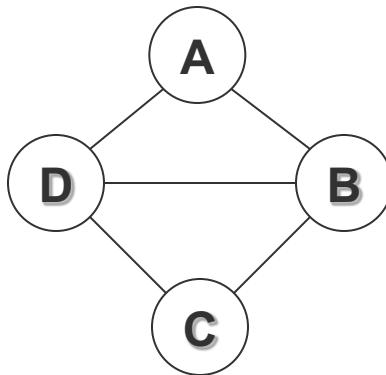
$$Z = \sum_{x_1, x_2, x_3, x_4} \psi_c(x_{124}) \times \psi_c(x_{234})$$

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





Example UGM – using subcliques



$$\begin{aligned} P''(x_1, x_2, x_3, x_4) &= \frac{1}{Z} \prod_{ij} \psi_{ij}(\mathbf{x}_{ij}) \\ &= \frac{1}{Z} \psi_{12}(\mathbf{x}_{12}) \psi_{14}(\mathbf{x}_{14}) \psi_{23}(\mathbf{x}_{23}) \psi_{24}(\mathbf{x}_{24}) \psi_{34}(\mathbf{x}_{34}) \end{aligned}$$

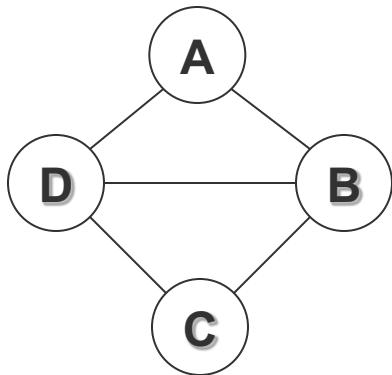
$$Z = \sum_{x_1, x_2, x_3, x_4} \prod_{ij} \psi_{ij}(\mathbf{x}_{ij})$$

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





Example UGM – canonical representation



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

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

- Most general, subsume P' and P'' as special cases
- $I(P)$ vs. $I(P')$ vs. $I(P'')$
- $D(P)$ vs. $D(P')$ vs. $D(P'')$

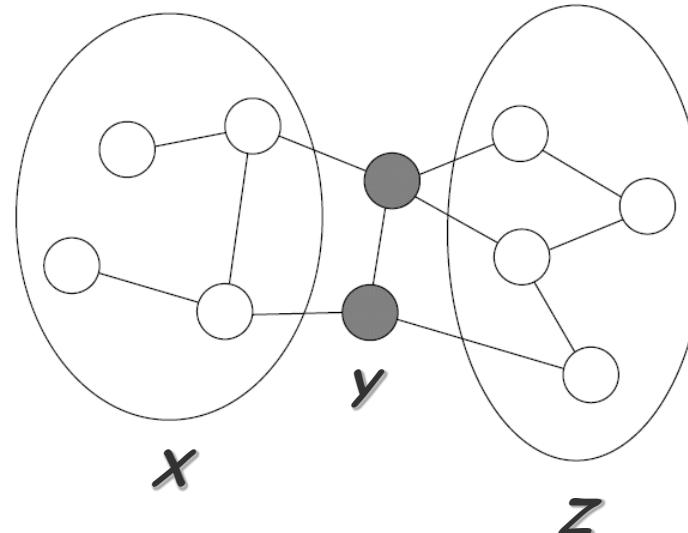




II: Independence properties:

- Now let us ask what kinds of distributions can be represented by undirected graphs (ignoring the details of the particular parameterization).
- Defn: the global ~~Markov~~ properties of a UG H are

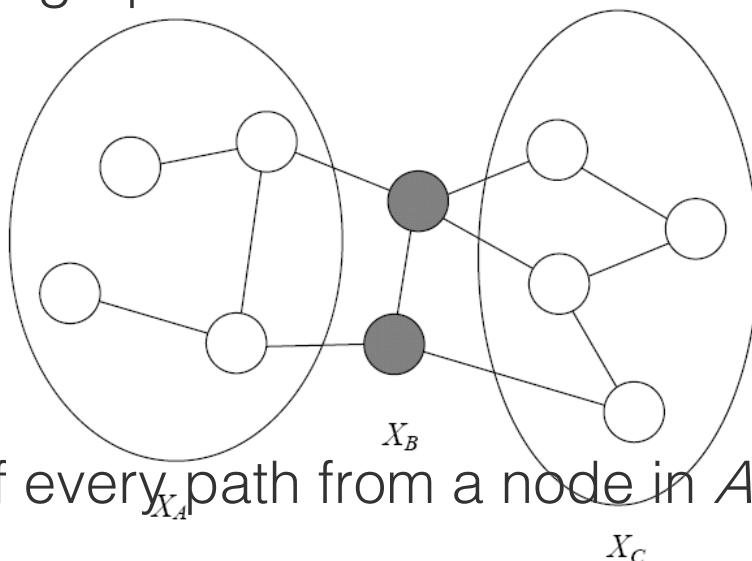
$$\text{I}(H) = \{X \perp Z|Y : \text{sep}_H(X; Z|Y)\}$$





Global Markov Independencies

- Let H be an undirected graph:



- B **separates** A and C if every path from a node in A to a node in C passes through a node in B :
- A probability distribution satisfies the **global Markov property** if for any disjoint A, B, C , such that B separates A and C , A is independent of C given B :

$$I(H) = \{A \perp C | B : \text{sep}_H(A; C | B)\}$$





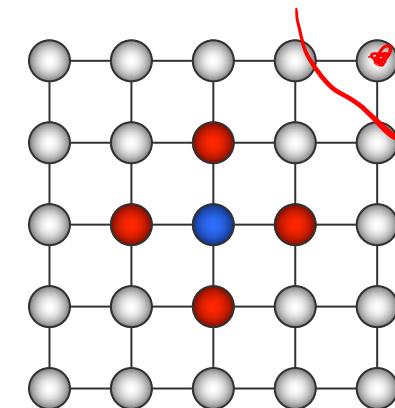
Local Markov independencies

- For each node $X_i \in \mathbf{V}$, there is *unique Markov blanket* of X_i , denoted MB_{X_i} , which is the set of neighbors of X_i in the graph (those that share an edge with X_i)

$$P(X_i | X_{-i}) = P(X_i | MB_i)$$

- Defn:
The *local Markov independencies* associated with H is:

$$I(H): \{X_i \perp \mathbf{V} - \{X_i\} - MB_{X_i} \mid MB_{X_i} : \forall i\},$$



In other words, X_i is independent of the rest of the nodes in the graph given its immediate neighbors





Soundness and completeness of global Markov property

- Defn: An UG H is an I-map for a distribution P if $I(H) \subseteq I(P)$, i.e., P entails $I(H)$.
- Defn: P is a **Gibbs distribution** over H if it can be represented as

$$P(x_1, \dots, x_n) = \frac{1}{Z} \prod_{c \in C} \psi_c(x_c)$$

- Thm (soundness): If \underline{P} is a Gibbs distribution over H , then \underline{H} is an I-map of P .
- Thm (completeness): If $\neg \text{sep}_H(X; Z|Y)$, then $X \perp_P Z|Y$ in **some** P that factorizes over H .





Hammersley-Clifford Theorem

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

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

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

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 .



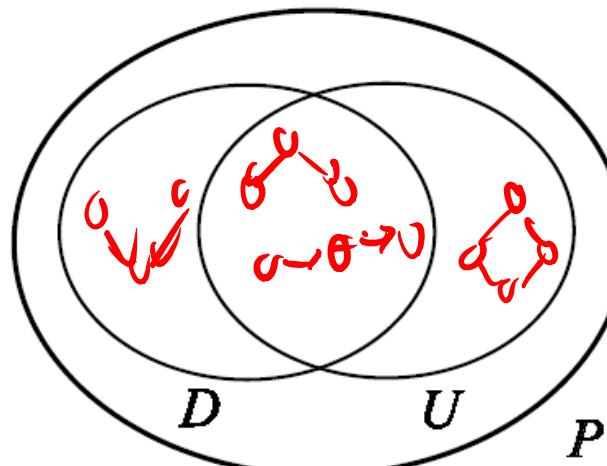


Perfect maps

- Defn: A Markov network H is a perfect map for P if for any $X; Y; Z$ we have that

$$\text{sep}_H(X; Z | Y) \Leftrightarrow P \models (X \perp Z | Y)$$

- Thm: not every distribution has a perfect map as UGM.
 - Pf by counterexample. No undirected network can capture all and only the independencies encoded in a v-structure $X \rightarrow Z \leftarrow Y$.





Exponential Form

$$\begin{matrix} \phi & \psi & H \\ \downarrow & \downarrow & \downarrow \\ \phi & \psi & -H \end{matrix}$$

- Constraining clique potentials to be positive could be inconvenient (e.g., the interactions between a pair of atoms can be either attractive or repulsive). We represent a clique potential $\psi_c(\mathbf{x}_c)$ in an unconstrained form using a real-value "energy" function $\phi_c(\mathbf{x}_c)$:

$$\psi_c(\mathbf{x}_c) = \exp\{-\phi_c(\mathbf{x}_c)\}$$

For convenience, we will call $\phi_c(\mathbf{x}_c)$ a potential when no confusion arises from the context.

- This gives the joint a nice additive structure

$$p(\mathbf{x}) = \frac{1}{Z} \exp\left\{-\sum_{c \in C} \phi_c(\mathbf{x}_c)\right\} = \frac{1}{Z} \exp\{-H(\mathbf{x})\}$$

where the sum in the exponent is called the "free energy":

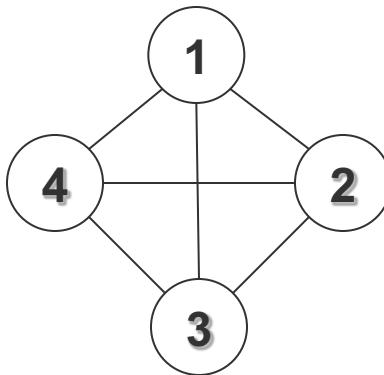
$$H(\mathbf{x}) = \sum_{c \in C} \phi_c(\mathbf{x}_c)$$

- In physics, this is called the "Boltzmann distribution".
- In statistics, this is called a log-linear model.





Example: Boltzmann machines



$x_1 \quad x_2$
 $\vdots \quad \vdots$
 $x_i \quad x_j$
 $\vdots \quad \vdots$

- 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

$$P(x_1, x_2, x_3, x_4) = \frac{1}{Z} \exp \left\{ \sum_{ij} \phi_{ij}(x_i, x_j) \right\} + \sum_i \phi_i$$

$$\Theta = \begin{bmatrix} \theta_{11} & \theta_{12} & \theta_{13} \\ \theta_{21} & \theta_{22} & \dots \\ \vdots & \vdots & \ddots \\ \theta_{n1} & \theta_{n2} & \theta_{nn} \end{bmatrix}$$

- Hence the overall energy function has the form:

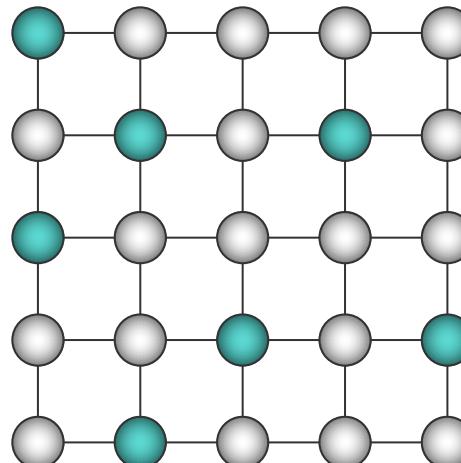
$$H(x) = \sum_{ij} (x_i - \mu) \Theta_{ij} (x_j - \mu) = (x - \mu)^T \Theta (x - \mu)$$





Ising models

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



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

- 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.

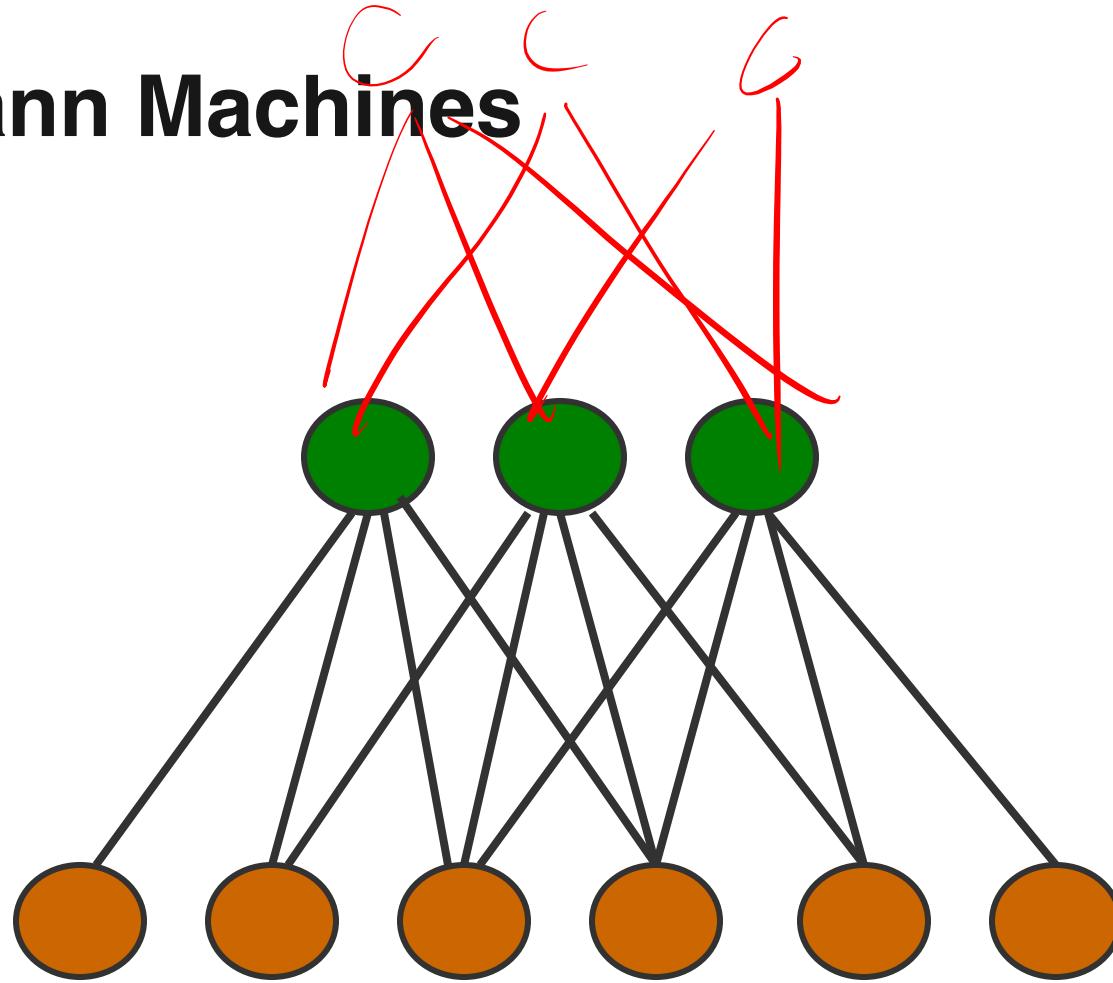




Restricted Boltzmann Machines

hidden units

visible units



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



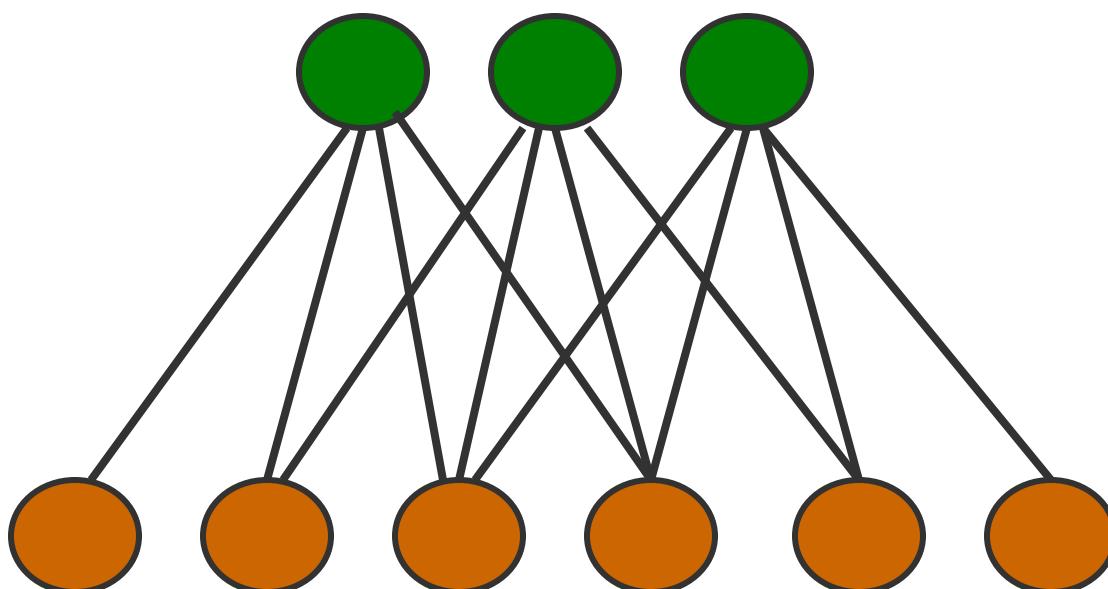


Restricted Boltzmann Machines

The Harmonium (Smolensky –'86)

hidden units

visible units



History:

Smolensky ('86), Proposed the architecture.

Freund & Haussler ('92), The “Combination Machine” (binary), learning with projection pursuit.

Hinton ('02), The “Restricted Boltzman Machine” (binary), learning with contrastive divergence.

Marks & Movellan ('02), Diffusion Networks (Gaussian).

Welling, Hinton, Osindero ('02), “Product of Student-T Distributions” (super-Gaussian)





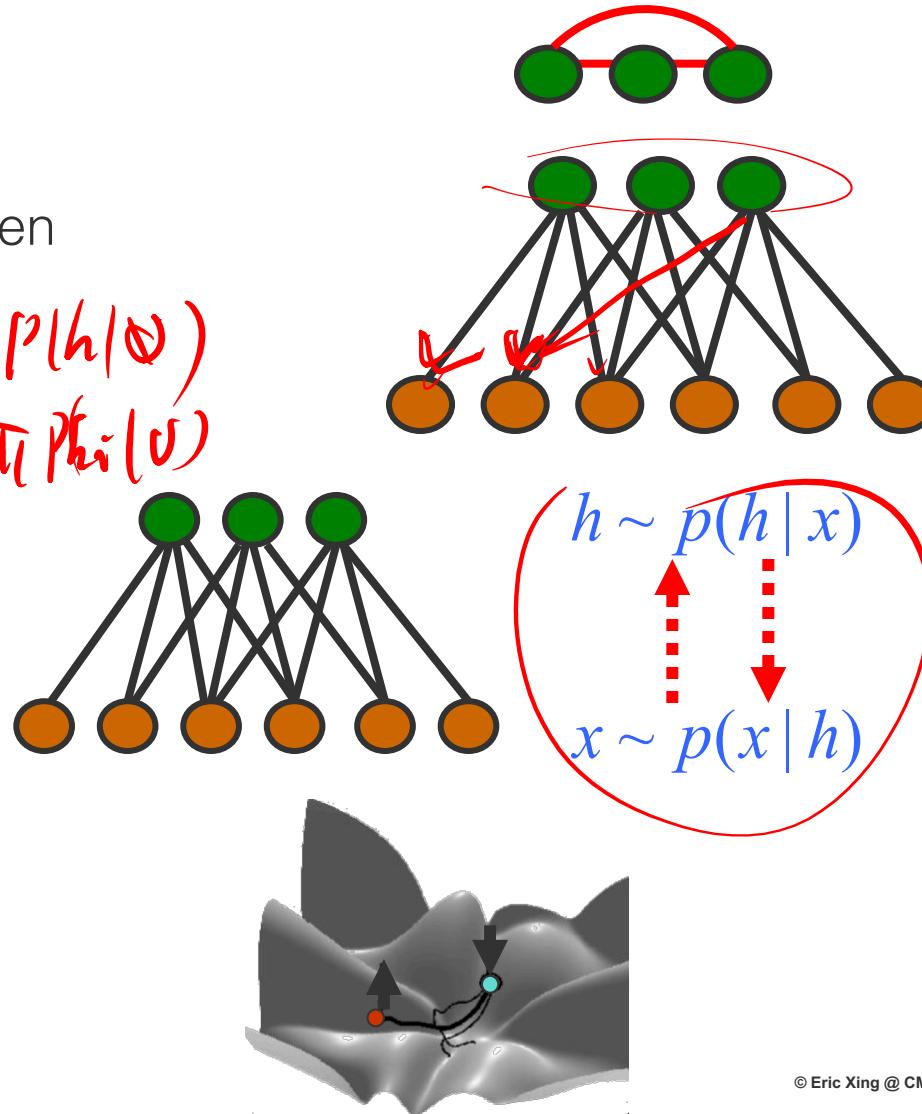
Properties of RBM

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

$$P(\ell | \mathbf{w}) = \prod_i P(\ell_i | \mathbf{w})$$

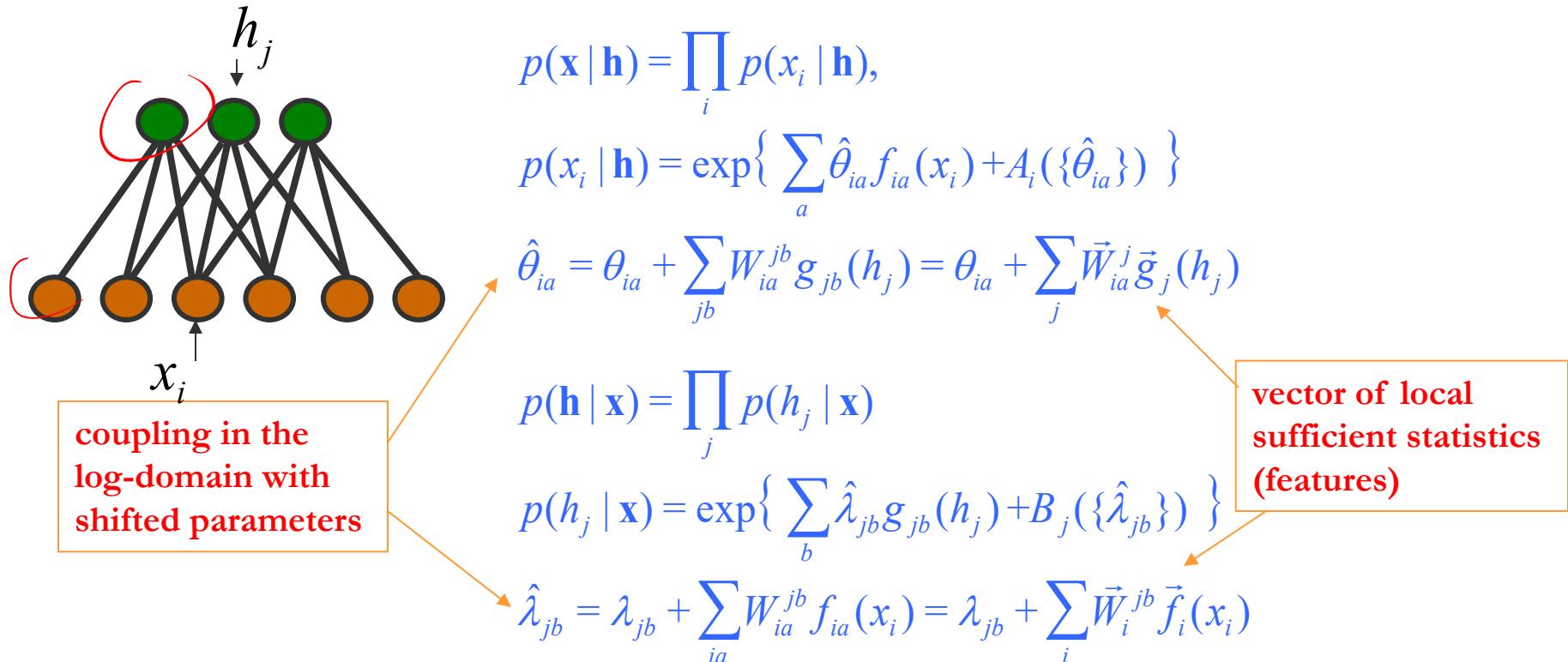
$$\begin{aligned} & P(h | \emptyset) \\ \Rightarrow & \prod_i p_{hi}(v) \end{aligned}$$

- Iterative Gibbs sampling.
- Learning with contrastive divergence





A Constructive Definition



They map to the RBM random field:

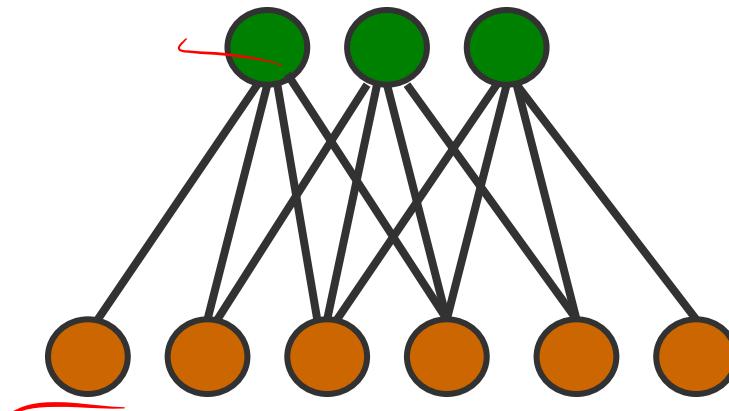
$$p(x, h | \theta) = \exp\left\{ \sum_i \vec{\theta}_i \vec{f}_i(x_i) + \sum_j \vec{\lambda}_j \vec{g}_j(h_j) + \sum_{i,j} \vec{f}_i^T(x_i) \mathbf{W}_{i,j} \vec{g}_j(h_j) \right\}$$





An RBM for Text Modeling

topics



words counts

$h_j = 3$: topic j has strength 3

$$h_j \in \mathbf{R}, \quad \langle h_j \rangle = \sum_i W_{i,j} x_i$$

$x_i = n$: word i has count n

$$x_i \in \mathbf{I}$$

$$\textcircled{p(\mathbf{h} | \mathbf{x})} = \prod_j \text{Normal}_{h_j} \left[\sum_i \vec{W}_{ij} \vec{x}_i, 1 \right]$$

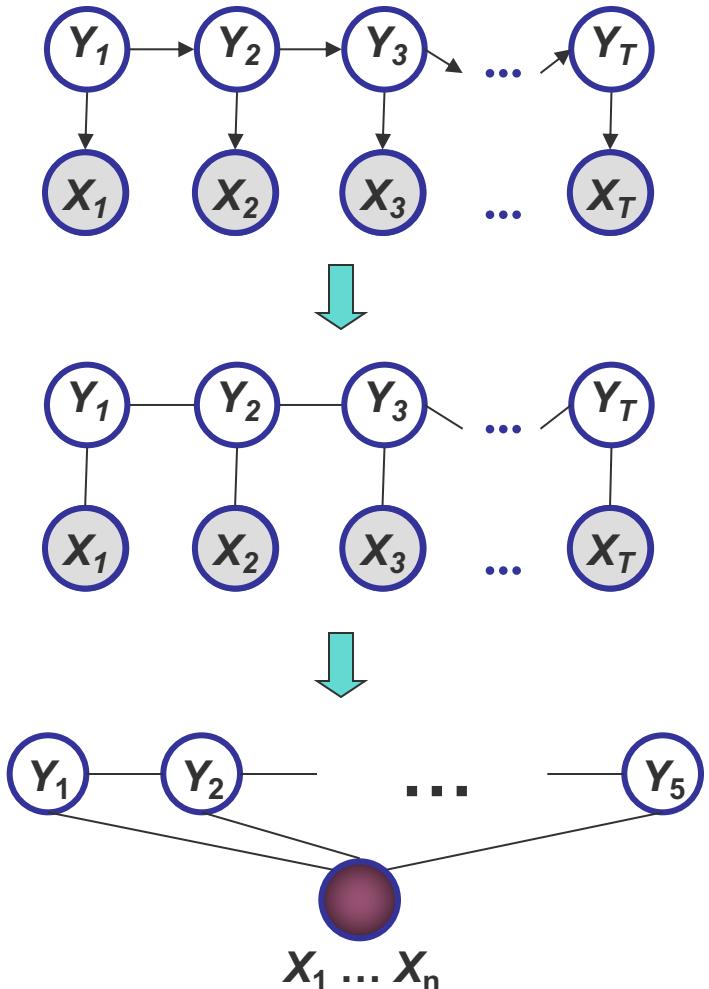
$$\textcircled{p(\mathbf{x} | \mathbf{h})} = \prod_i \text{Bi}_{x_i} \left[N, \frac{\exp(\alpha_j + \sum_j W_{ij} h_j)}{1 + \exp(\alpha_j + \sum_j W_{ij} h_j)} \right]$$

$$\Rightarrow p(\mathbf{x}) \propto \exp \left\{ \sum_i \alpha_i x_i - \log \Gamma(x_i) - \log \Gamma(N - x_i) + \frac{1}{2} \sum_j \left(\sum_i W_{i,j} x_i \right)^2 \right\}$$





Conditional Random Fields



- Discriminative

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

- Doesn't assume that features are independent
- When labeling X_i , future observations are taken into account





Conditional Models

- ❑ Conditional probability $P(\text{label sequence } \mathbf{y} \mid \text{observation sequence } \mathbf{x})$ rather than joint probability $P(\mathbf{y}, \mathbf{x})$
 - ❑ Specify the probability of possible label sequences given an observation sequence
- ❑ Allow arbitrary, non-independent features on the observation sequence \mathbf{X}
- ❑ The probability of a transition between labels may depend on **past** and **future** observations
- ❑ Relax strong independence assumptions in generative models



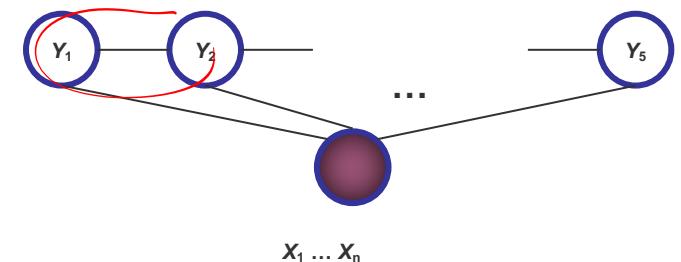


Conditional Distribution

- If the graph $G = (V, E)$ of \mathbf{Y} is a tree, the conditional distribution over the label sequence $\mathbf{Y} = \mathbf{y}$, given $\mathbf{X} = \mathbf{x}$, by the Hammersley Clifford theorem of random fields is:

$$p_{\theta}(\mathbf{y} | \mathbf{x}) \propto \exp \left(\sum_{e \in E, k} \lambda_k f_k(e, \mathbf{y}|_e, \mathbf{x}) + \sum_{v \in V, k} \mu_k g_k(v, \mathbf{y}|_v, \mathbf{x}) \right)$$

- x is a data sequence
- y is a label sequence
- v is a vertex from vertex set V = set of label random variables
- e is an edge from edge set E over V
- f_k and g_k are given and fixed. g_k is a Boolean vertex feature; f_k is a Boolean edge feature
- k is the number of features
- $\theta = (\lambda_1, \lambda_2, \dots, \lambda_n; \mu_1, \mu_2, \dots, \mu_n); \lambda_k$ and μ_k are parameters to be estimated
- $\mathbf{y}|_e$ is the set of components of \mathbf{y} defined by edge e
- $\mathbf{y}|_v$ is the set of components of \mathbf{y} defined by vertex v





Conditional Distribution (cont'd)

- CRFs use the observation-dependent normalization $Z(\mathbf{x})$ for the conditional distributions:

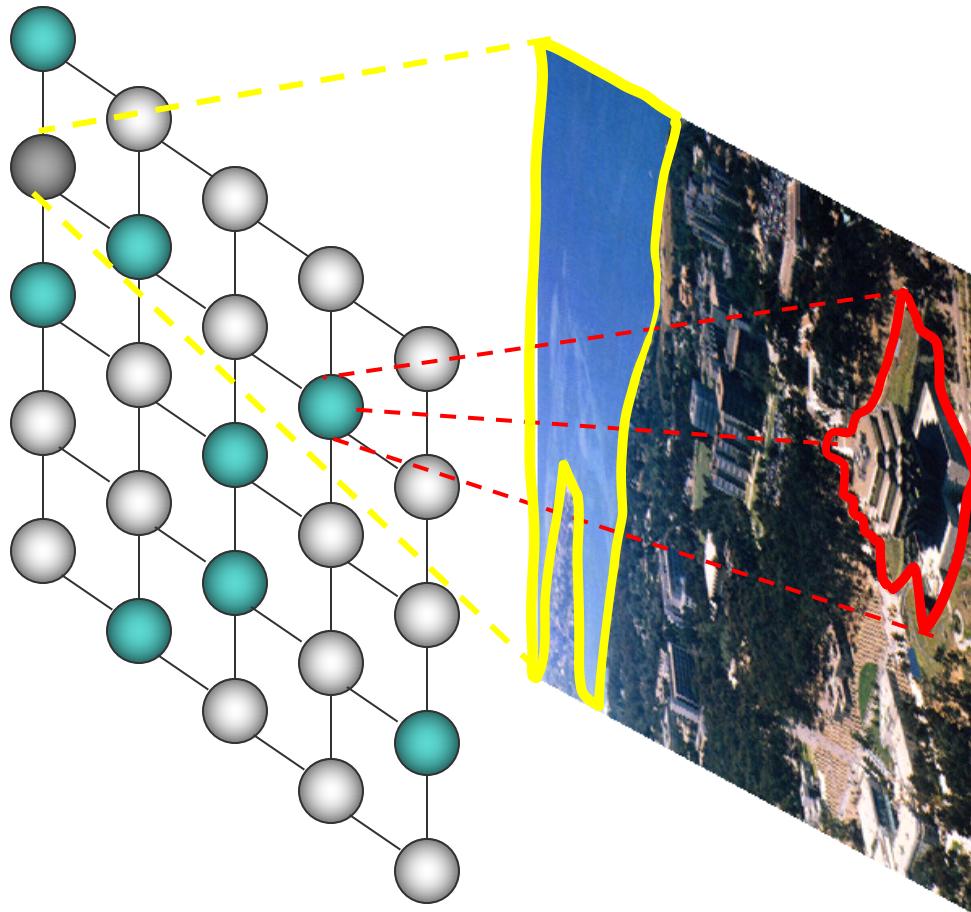
$$p_{\theta}(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z(\mathbf{x})} \exp \left(\sum_{e \in E, k} \lambda_k f_k(e, \mathbf{y}|_e, \mathbf{x}) + \sum_{v \in V, k} \mu_k g_k(v, \mathbf{y}|_v, \mathbf{x}) \right)$$

- $Z(\mathbf{x})$ is a normalization over the data sequence \mathbf{x}





Conditional Random Fields



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

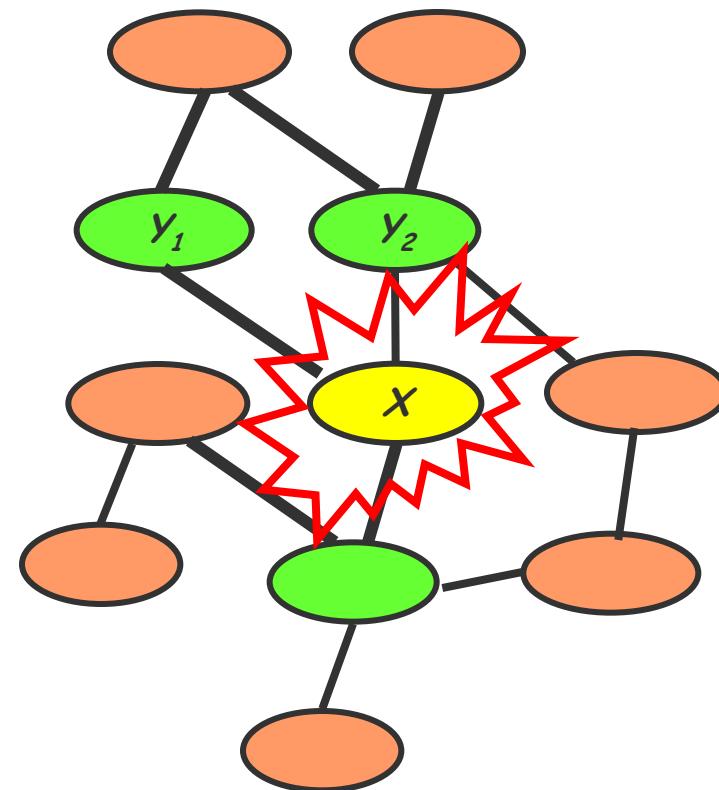
- Allow arbitrary dependencies on input
- Clique dependencies on labels
- Use approximate inference for general graphs





Summary: Conditional Independence Semantics in an MRF

- Structure: an *undirected graph*
- Meaning: a node is **conditionally independent** of every other node in the network given its **Directed neighbors**
- Local contingency functions (**potentials**) and the **cliques in the graph** completely determine the **joint dist.**
- Give correlations between variables, but no explicit way to generate samples





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
- ❑ Learning GM structures:
 - ❑ the Chow-Liu Algorithm





Supplementary:



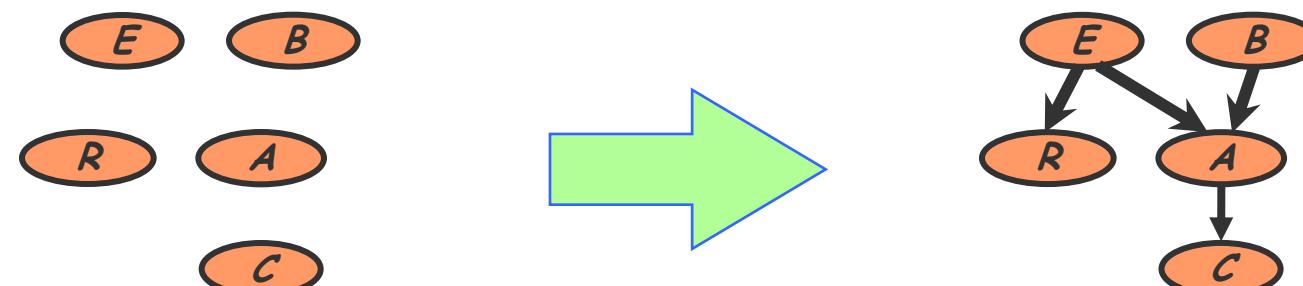


Where is the graph structure come from?

The goal:

- Given set of independent samples (*assignments* of random variables), find the *best* (the most likely?) graphical model topology

ML Structural Learning for completely observed GMs



$$(B, E, A, C, R) = (T, F, F, T, F)$$

$$(B, E, A, C, R) = (T, F, T, T, F)$$

.....

$$(B, E, A, C, R) = (F, T, T, T, F)$$





Information Theoretic Interpretation of ML

$$\begin{aligned}\ell(\theta_G, G; D) &= \log p(D | \theta_G, G) \\ &= \log \prod_n \left(\prod_i p(x_{n,i} | \mathbf{x}_{n, \pi_i(G)}, \theta_{i|\pi_i(G)}) \right) \\ &= \sum_i \left(\sum_n \log p(x_{n,i} | \mathbf{x}_{n, \pi_i(G)}, \theta_{i|\pi_i(G)}) \right) \\ &= M \sum_i \left(\sum_{x_i, \mathbf{x}_{\pi_i(G)}} \frac{\text{count}(x_i, \mathbf{x}_{\pi_i(G)})}{M} \log p(x_i | \mathbf{x}_{\pi_i(G)}, \theta_{i|\pi_i(G)}) \right) \\ &= M \sum_i \left(\sum_{x_i, \mathbf{x}_{\pi_i(G)}} \hat{p}(x_i, \mathbf{x}_{\pi_i(G)}) \log p(x_i | \mathbf{x}_{\pi_i(G)}, \theta_{i|\pi_i(G)}) \right)\end{aligned}$$

From sum over data points to sum over count of variable states





Information Theoretic Interpretation of ML (con'd)

$$\begin{aligned}\ell(\theta_G, G; D) &= \log \hat{p}(D | \theta_G, G) \\ &= M \sum_i \left(\sum_{x_i, \mathbf{x}_{\pi_i(G)}} \hat{p}(x_i, \mathbf{x}_{\pi_i(G)}) \log \hat{p}(x_i | \mathbf{x}_{\pi_i(G)}, \theta_{i|\pi_i(G)}) \right) \\ &= M \sum_i \left(\sum_{x_i, \mathbf{x}_{\pi_i(G)}} \hat{p}(x_i, \mathbf{x}_{\pi_i(G)}) \log \frac{\hat{p}(x_i, \mathbf{x}_{\pi_i(G)}, \theta_{i|\pi_i(G)})}{\hat{p}(\mathbf{x}_{\pi_i(G)})} \frac{\hat{p}(x_i)}{\hat{p}(x_i)} \right) \\ &= M \sum_i \left(\sum_{x_i, \mathbf{x}_{\pi_i(G)}} \hat{p}(x_i, \mathbf{x}_{\pi_i(G)}) \log \frac{\hat{p}(x_i, \mathbf{x}_{\pi_i(G)}, \theta_{i|\pi_i(G)})}{\hat{p}(\mathbf{x}_{\pi_i(G)}) \hat{p}(x_i)} \right) - M \sum_i \left(\sum_{x_i} \hat{p}(x_i) \log \hat{p}(x_i) \right) \\ &= M \sum_i \hat{I}(x_i, \mathbf{x}_{\pi_i(G)}) - M \sum_i \hat{H}(x_i)\end{aligned}$$

Decomposable score and a function of the graph structure





Structural Search

- How many graphs over n nodes? $O(2^{n^2})$
- How many trees over n nodes? $O(n!)$
- But it turns out that we can find exact solution of an optimal tree (under MLE)!
 - Trick: in a tree each node has only one parent!
 - Chow-liu algorithm





Chow-Liu tree learning algorithm

- Objection function:

$$\begin{aligned}\ell(\theta_G, G; D) &= \log \hat{p}(D | \theta_G, G) \\ &= M \sum_i \hat{I}(x_i, \mathbf{x}_{\pi_i(G)}) - M \sum_i \hat{H}(x_i)\end{aligned} \Rightarrow C(G) = M \sum_i \hat{I}(x_i, \mathbf{x}_{\pi_i(G)})$$

- Chow-Liu:

- For each pair of variable x_i and x_j
 - Compute empirical distribution:
 - Compute mutual information:
- Define a graph with node x_1, \dots, x_n
 - Edge (i,j) gets weight

$$\hat{I}(X_i, X_j)$$

$$\begin{aligned}\hat{p}(X_i, X_j) &= \frac{\text{count}(x_i, x_j)}{M} \\ \hat{I}(X_i, X_j) &= \sum_{x_i, x_j} \hat{p}(x_i, x_j) \log \frac{\hat{p}(x_i, x_j)}{\hat{p}(x_i) \hat{p}(x_j)}\end{aligned}$$





Chow-Liu algorithm (con'd)

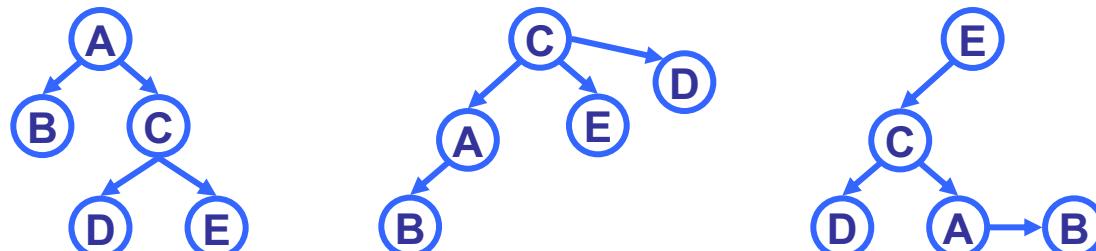
- Objection function:

$$\ell(\theta_G, G; D) = \log \hat{p}(D | \theta_G, G) \\ = M \sum_i \hat{I}(x_i, \mathbf{x}_{\pi_i(G)}) - M \sum_i \hat{H}(x_i) \Rightarrow C(G) = M \sum_i \hat{I}(x_i, \mathbf{x}_{\pi_i(G)})$$

- Chow-Liu:

Optimal tree BN

- Compute maximum weight spanning tree
- Direction in BN: pick any node as root, do breadth-first-search to define directions
- I-equivalence:



$$C(G) = I(A, B) + I(A, C) + I(C, D) + I(C, E)$$





Structure Learning for general graphs

- Theorem:
 - The problem of learning a BN structure with at most d parents is NP-hard for any (fixed) $d \geq 2$
- Most structure learning approaches use heuristics
 - Exploit score decomposition
 - Two heuristics that exploit decomposition in different ways
 - Greedy search through space of node-orders
 - Local search of graph structures

