Undirected Graphical Models: Markov Random Fields

Probabilistic Graphical Models

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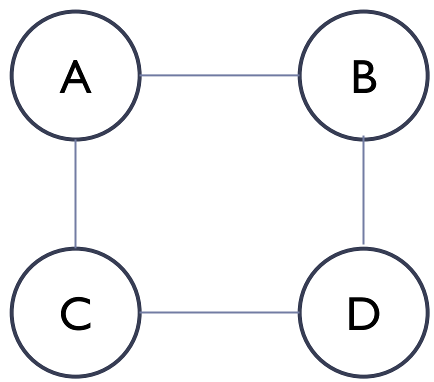
Slides from Dr. Soleymani's PGM course, Sharif University of Technology

Markov Network

- Structure: ***undirected graph***
- Undirected edges show correlations (non-causal relationships) between variables

  - e.g., Spatial image analysis: intensity of neighboring pixels are correlated

Markov Network



MRF: Joint distribution

- Factor $\phi(X_1, \dots, X_k)$
  - $\phi: Val(X_1, \dots, X_k) \rightarrow \mathbb{R}$
  - Scope: $\{X_1, \dots, X_k\}$

- Gibbs Distribution

Joint distribution is parameterized by factors $\boldsymbol{\Phi} = \{\phi_1(\boldsymbol{D}_1), \dots, \phi_K(\boldsymbol{D}_K)\}$:

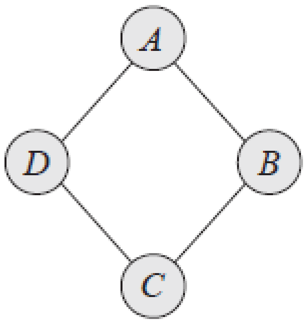
$$P(X_1, \dots, X_N) = \frac{1}{Z} \prod_k \phi_k(\boldsymbol{D}_k)$$

$\boldsymbol{D}_k$: the set of variables in the k-th factor

$$Z = \sum_{\boldsymbol{X}} \prod_k \phi_k(\boldsymbol{D}_k)$$

Z: normalization constant called **partition function**

Misconception example



[Koller & Friedman]

$A = 0$

$\phi_1(A, B)$

a^0	b^0	30
a^0	b^1	5
a^1	b^0	1
a^1	b^1	10

$\phi_2(B, C)$

b^0	c^0	100
b^0	c^1	1
b^1	c^0	1
b^1	c^1	100

$\phi_3(C, D)$

c^0	d^0	1
c^0	d^1	100
c^1	d^0	100
c^1	d^1	1

$\phi_4(D, A)$

d^0	a^0	100
d^0	a^1	1
d^1	a^0	1
d^1	a^1	100

Factors show "compatibilities" between different values of the variables in their scope

A factor is only one contribution to the overall joint distribution.

Relation between factorization and independencies

- Theorem:

  Let $\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{Z}$ be three disjoint sets of variables:

  $P \vDash (\boldsymbol{X} \perp \boldsymbol{Y} | \boldsymbol{Z})$ iff $P(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{Z}) = f(\boldsymbol{X}, \boldsymbol{Z}) g(\boldsymbol{Y}, \boldsymbol{Z})$

  To hold conditional independence property, X_i and X_j that are not directly connected must not appear in the same factor in the distributions belonging to the graph

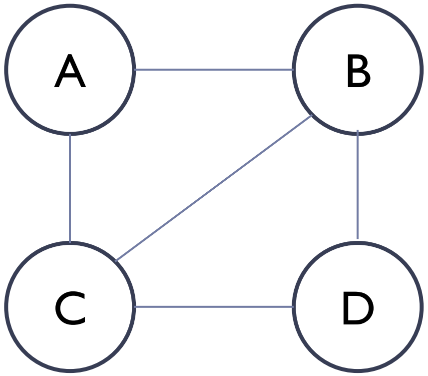
MRF Factorization: clique

Clique: subsets of nodes in the graph that are fully connected (complete subgraph)

Maximal clique: where no superset of the nodes in a clique are also compose a clique, the clique is maximal

Cliques:
{A,B,C}, {B,C,D}, {A,B}, {A,C}, {B,C}, {B,D}, {C,D}, {A}, {B}, {C}, {D}

Max-cliques:
{A,B,C}, {B,C,D}



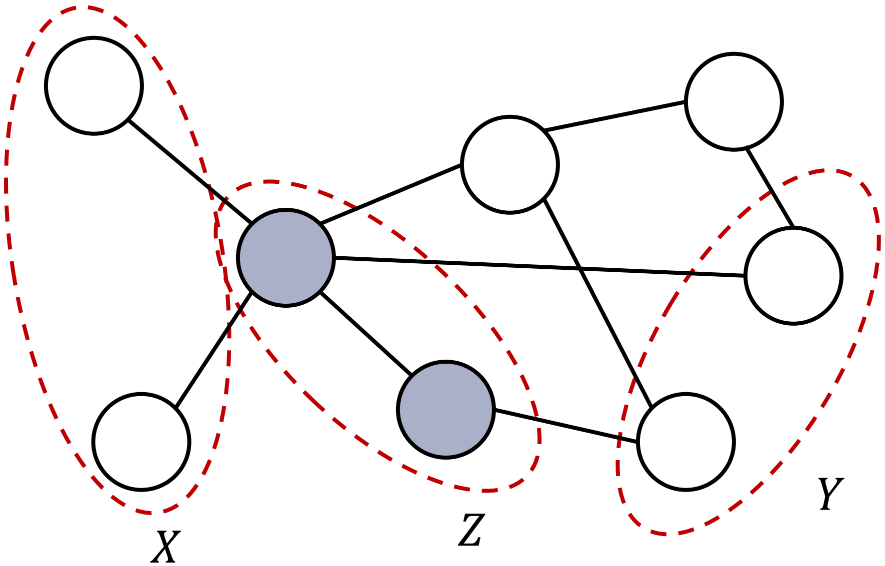
MRF Factorization and pairwise independencies

- A distribution $P_{\boldsymbol{\Phi}}$ with $\boldsymbol{\Phi} = \{\phi_1(\boldsymbol{D}_1), \dots, \phi_K(\boldsymbol{D}_K)\}$ **factorizes** over an MRF H if each $\boldsymbol{D}_k$ is a **complete subgraph** of H

- **Potential functions** and **cliques** in the graph completely determine the **joint** distribution.

MRFs: independencies

Separation in the undirected graph:



A path is active given Z if no node in it is in Z

X and Y are separated given Z if there is no active path between X and Y given Z

$$\text{sep}_H(X, Y|Z)$$

- Global independencies for any disjoint sets A, B, C:
  - $A \perp B|C$

If all paths that connect a node in A to a node in B pass through one or more nodes in set C

MRF: independencies

- Determining conditional independencies in undirected models is much easier than in directed ones

- Conditioning in undirected models can only eliminate dependencies while in directed ones observations can create new dependencies (v-structure)

Factorization & Independence

- Factorization $\Rightarrow$ Independence (<u>soundness of separation criterion</u>)
  - **Theorem:** If P factorizes over H, and $\mathrm{sep}_H(\boldsymbol{X}, \boldsymbol{Y} | \boldsymbol{Z})$ then P satisfies $\boldsymbol{X} \perp \boldsymbol{Y} | \boldsymbol{Z}$ (i.e., H is an I-map of P)
  - $I(H) \subseteq I(P)$

- Independence $\Rightarrow$ Factorization
  - **Theorem** (Hammersley Clifford): For a positive distribution P, if P satisfies $I(H) = \{(\boldsymbol{X} \perp \boldsymbol{Y} | \boldsymbol{Z}) : \mathrm{sep}_H(\boldsymbol{X}, \boldsymbol{Y} | \boldsymbol{Z})\}$ then P factorizes over H

Factorization & Independence

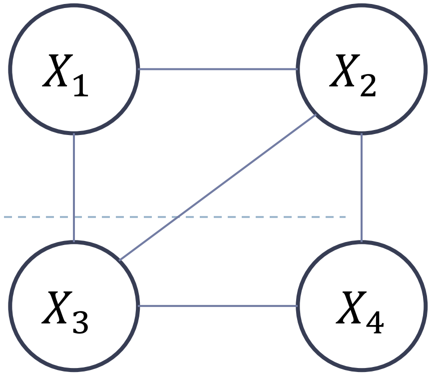
- **Theorem**: Two equivalent views of graph structure for **positive distributions**:
  - If P satisfies all independencies held in H, then it can be factorized on cliques of H
  - If P factorizes over a graph H, we can read from the graph structure, independencies that must hold in P

Interpretation of clique potentials

- Potentials cannot all be marginal or conditional distributions

- A positive clique potential can be considered as general compatibility or goodness measure over values of the variables in its scope

Different factorizations



- Maximal cliques:
  - $P_{\mathbf{\Phi}}(X_1, X_2, X_3, X_4) = \frac{1}{Z}\phi_{123}(X_1, X_2, X_3)\phi_{234}(X_2, X_3, X_4)$
  - $Z = \sum_{X_1, X_2, X_3, X_4} \phi_{123}(X_1, X_2, X_3)\phi_{234}(X_2, X_3, X_4)$
- Sub-cliques:
  - $P_{\mathbf{\Phi}'}(X_1, X_2, X_3, X_4) = \frac{1}{Z}\phi_{12}(X_1, X_2)\phi_{23}(X_2, X_3)\phi_{13}(X_1, X_3)\phi_{24}(X_2, X_4)\phi_{34}(X_3, X_4)$
  - $Z = \sum_{X_1, X_2, X_3, X_4} \phi_{12}(X_1, X_2)\phi_{23}(X_2, X_3)\phi_{13}(X_1, X_3)\phi_{24}(X_2, X_4)\phi_{34}(X_3, X_4)$
- Canonical representation
  - $P_{\mathbf{\Phi}'}(X_1, X_2, X_3, X_4) = \frac{1}{Z}\phi_{123}(X_1, X_2, X_3)\phi_{234}(X_2, X_3, X_4)\phi_{12}(X_1, X_2)\phi_{23}(X_2, X_3)\phi_{13}(X_1, X_3) \times \phi_{24}(X_2, X_4)\phi_{34}(X_3, X_4)\phi_1(X_1)\phi_2(X_2)\phi_3(X_3)\phi_4(X_4)$
  - $Z = \sum_{X_1, X_2, X_3, X_4} \phi_{123}(X_1, X_2, X_3)\phi_{234}(X_2, X_3, X_4)\phi_{12}(X_1, X_2)\phi_{23}(X_2, X_3) \times \phi_{13}(X_1, X_3)\phi_{24}(X_2, X_4)\phi_{34}(X_3, X_4)\phi_1(X_1)\phi_2(X_2)\phi_3(X_3)\phi_4(X_4)$

Pairwise MRF

- All of the factors on single variables or pair of variables (X_i, X_j):

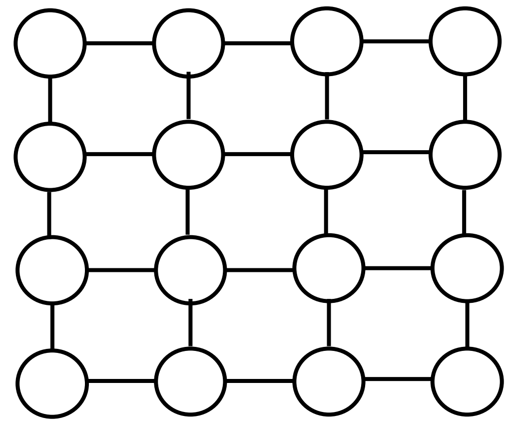
$$P(\boldsymbol{X}) = \frac{1}{Z} \prod_{(X_i, X_j) \in H} \phi_{ij}(X_i, X_j) \prod_i \phi_i(X_i)$$

- Pairwise MRFs are popular (simple special case of general MRFs)

Ising model

- $X_i \in \{-1,1\}$

$$P(\boldsymbol{x}) = \frac{1}{Z}\exp\left\{\sum_i u_i x_i + \sum_{i,j\in E} w_{ij} x_i x_j\right\}$$



- Grid model
  - Image processing, lattice physics, etc.
  - The states of adjacent nodes are related

Binary Image Denoising

- $y_i \in \{-1,1\}$, array of observed noisy pixels
- $x_i \in \{-1,1\}$, noise free image

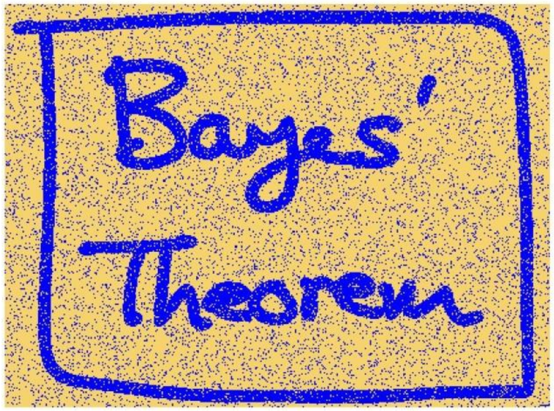
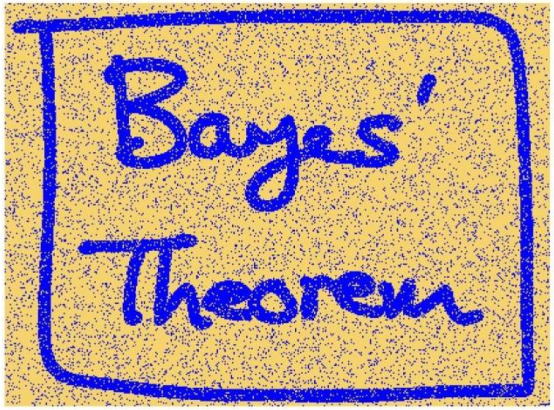
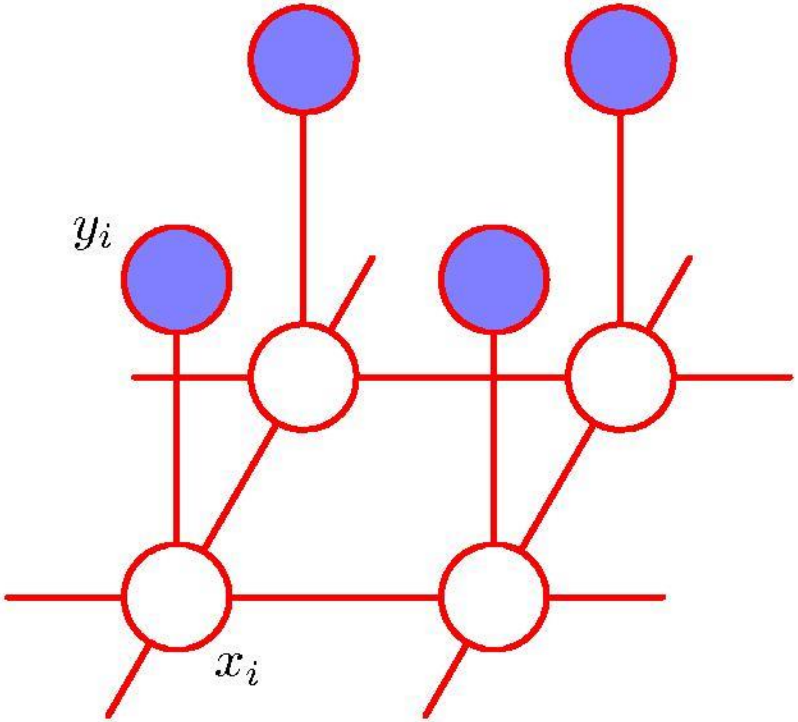


Image denoising





[Bishop]

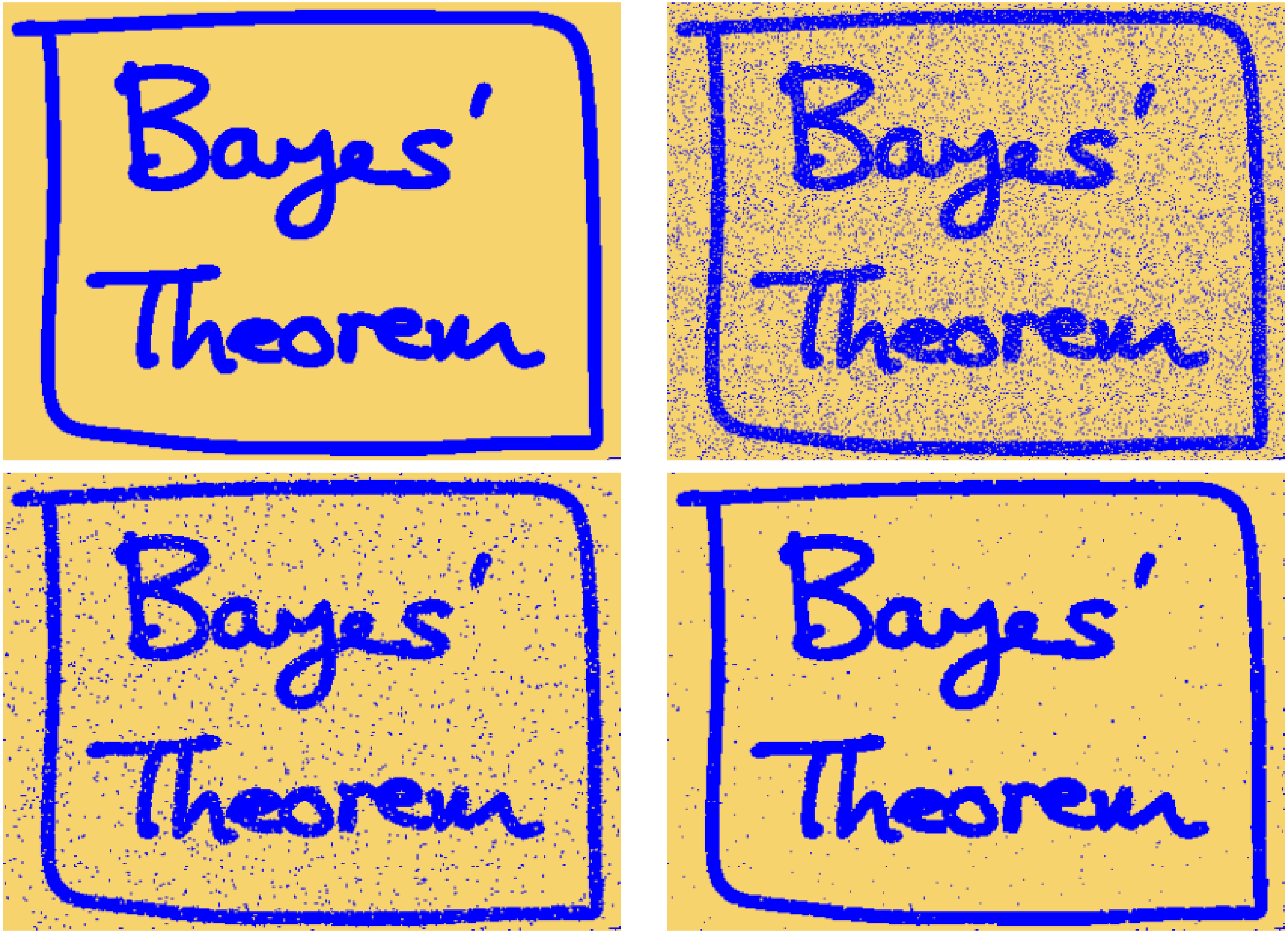
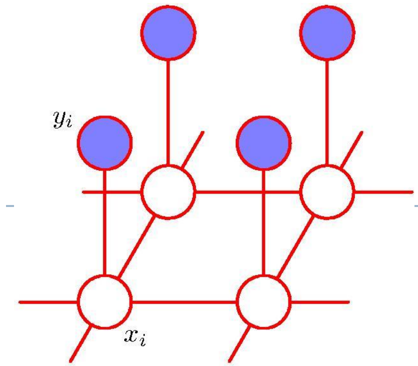


Figure 8.30 Illustration of image de-noising using a Markov random field. The top row shows the original binary image on the left and the corrupted image after randomly changing 10% of the pixels on the right. The bottom row shows the restored images obtained using iterated conditional models (ICM) on the left and using the graph-cut algorithm on the right. ICM produces an image where 96% of the pixels agree with the original image, whereas the corresponding number for graph-cut is 99%.

Image denoising



$$P(\boldsymbol{x}, \boldsymbol{y})$$

$$= \frac{1}{Z} \prod_i \exp\{-\gamma x_i y_i\} \prod_i \exp\{-\beta x_i\} \prod_{i,j \in H} \exp\{-\alpha x_i x_j\}$$

$$= \frac{1}{Z} \exp\left\{-\sum_i \gamma x_i y_i - \sum_i \beta x_i - \sum_{i,j \in H} \alpha x_i x_j\right\}$$

MPA: Most probable assignment of $\boldsymbol{x}$ variables given an evidence $\boldsymbol{y}$

$$\widehat{\boldsymbol{x}} = \operatorname*{argmax}_{\boldsymbol{x}} P(\boldsymbol{x}|\boldsymbol{y})$$

MRF: Markov Blanket

- A variable is conditionally independent of every other variables conditioned only on its neighboring nodes

$$X_i \perp \boldsymbol{X} - \{X_i\} - MB(X_i) \mid MB(X_i)$$

$$MB(X_i) = \{X' \in \boldsymbol{X} | (X_i, X') \in edges\}$$

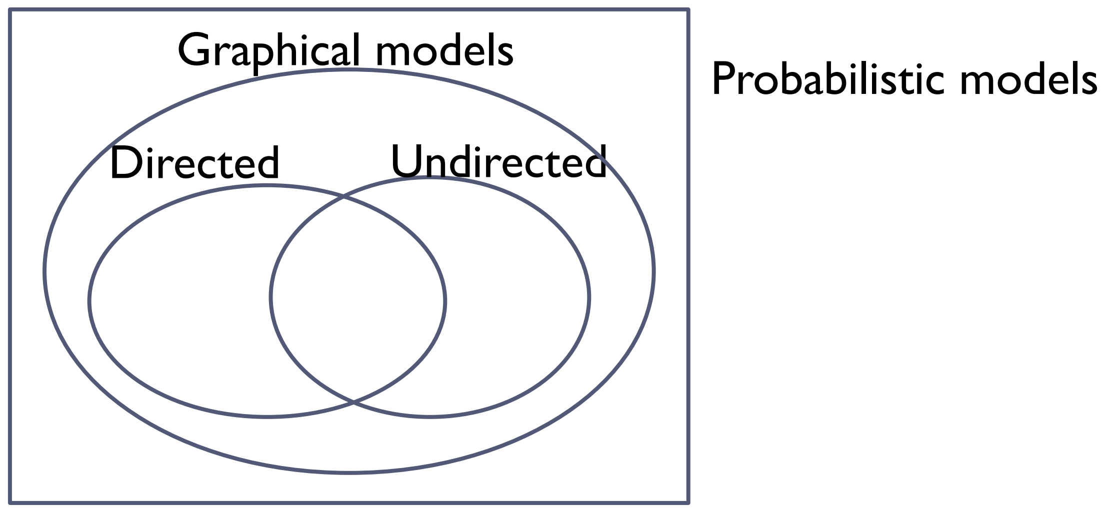
Minimal I-map

- Since we may not find a Markov Network (MN) that is a perfect map of a BN and vice versa, we study the minimal I-map property

- H is a minimal I-map for G if
  - $I(H) \subseteq I(G)$
  - Removal of a single edge in H renders it is not an I-map of G

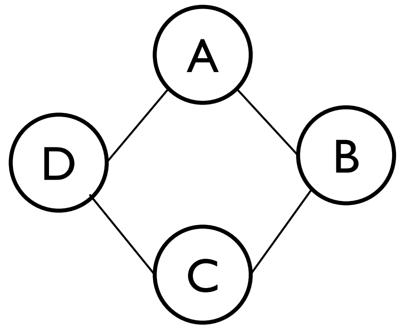
Perfect map of a distribution

- Not every distribution has a MN perfect map
- Not every distribution has a BN perfect map



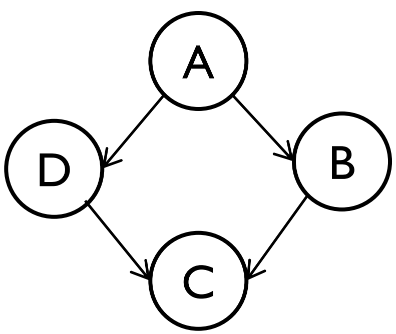
Loop of at least 4 nodes without chord has no equivalent in BNs

- Is there a BN that is a perfect map for this MN?



$A \perp C \mid \{B, D\}$

$B \perp D \mid \{A, C\}$



$A \perp C \mid \{B, D\}$

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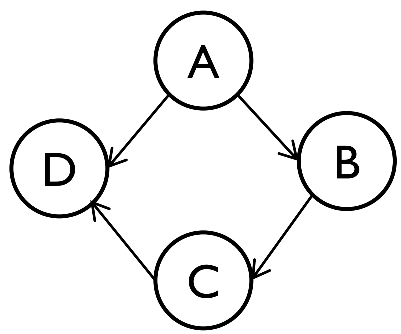
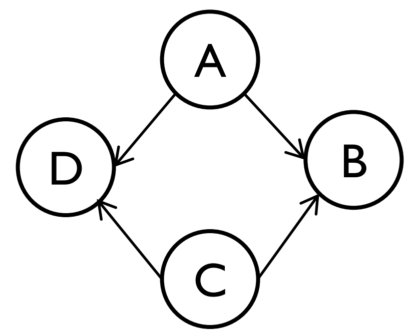


$B \perp D \mid \{A, C\}$

$A \perp C \mid \{B, D\}$

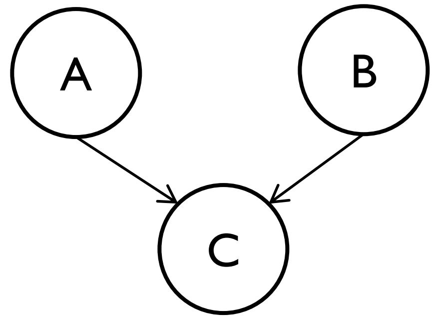


$B \perp D \mid \{A, C\}$

$A \perp C \mid \{B, D\}$

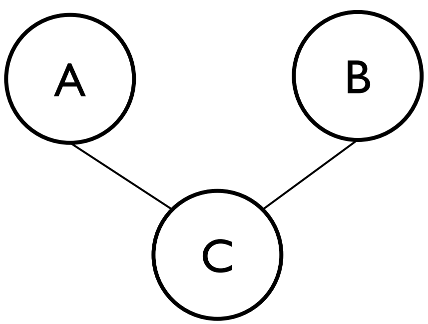
V-structure has no equivalent in MNs

- Is there an MN that is a perfect I-map of this BN?



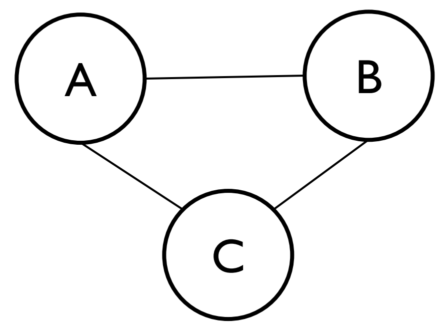
$A \perp B$

$A \perp B | C$



$A \perp B$

$A \perp B | C$



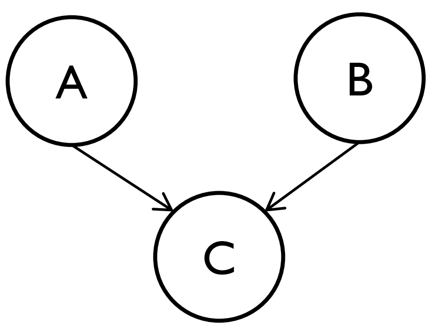
$A \perp B$

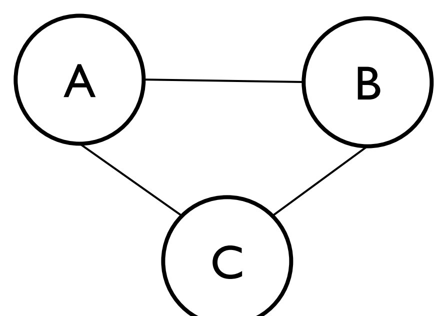
$A \perp B | C$

Minimal I-maps: from DAGs to MNs

- The **moral graph** $M(G)$ of a DAG G is an undirected graph that contains an undirected edge between X and Y if:
  - there is a directed edge between them in either direction
  - X and Y are parents of the same node

- Moralization turns a node and its parent into a fully connected sub-graph





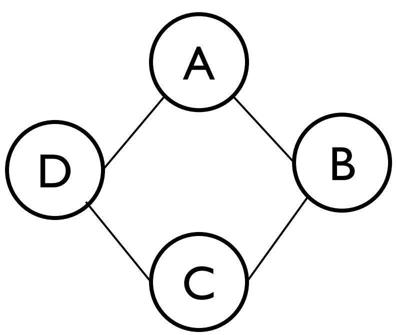
Minimal I-maps: from DAGs to MNs

- **Theorem**: The moral graph $M(G)$ of a DAG G is a minimal I-map for G
  - The moral graph loses some independence information
  - But, we cannot remove any edge from it without appearing new independencies that are not in G
    - all independencies in the moral graph are also satisfied in G
- **Theorem**: If a DAG G is "moral", then its moralized graph $M(G)$ is a perfect I-map of G.

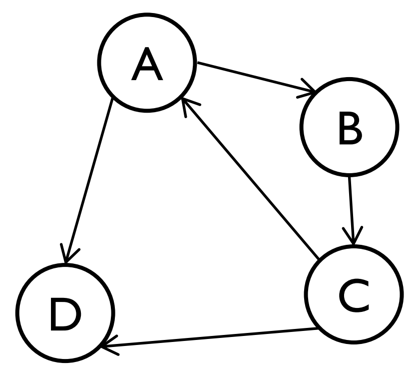
Minimal I-maps: from MNs to DAGs

- **Theorem**: If G is a BN that is minimal I-map for an MN, then G cannot have immoralities.

- **Corollary**: If G is a minimal I-map for an MN then it is **chordal**
  - Any BN that is I-map for an MN must add triangulating edges into the graph



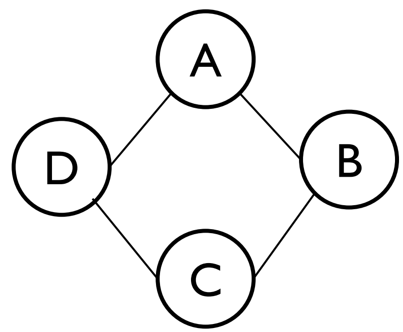
An undirected graph is chordal if any loop with more than three nodes has a chord



G is a minimal I-map of the left MN

Perfect I-map

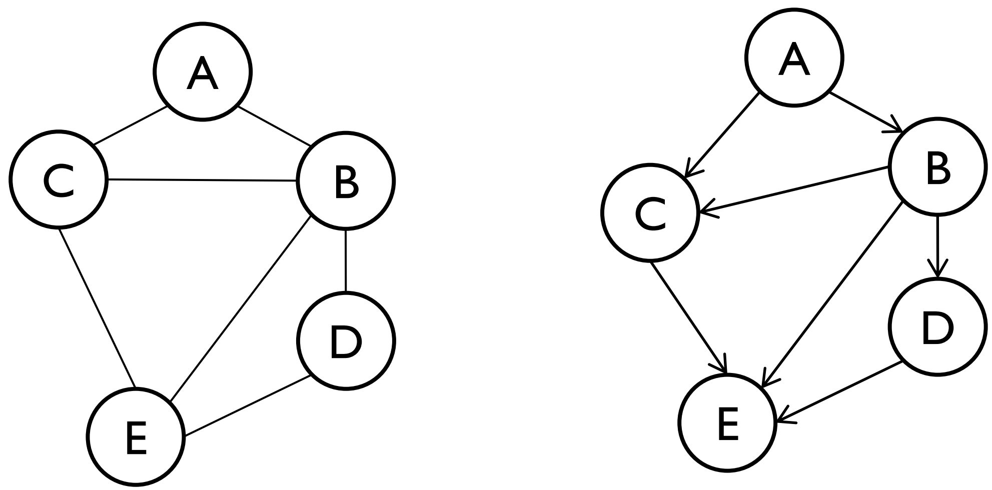
- **Theorem**: Let H be a non-chordal MN. Then there is no BN that is a perfect I-map for H.



$\Rightarrow$ If the independencies in an MN can be exactly represented via a BN then the MN graph is **chordal**

Perfect I-map

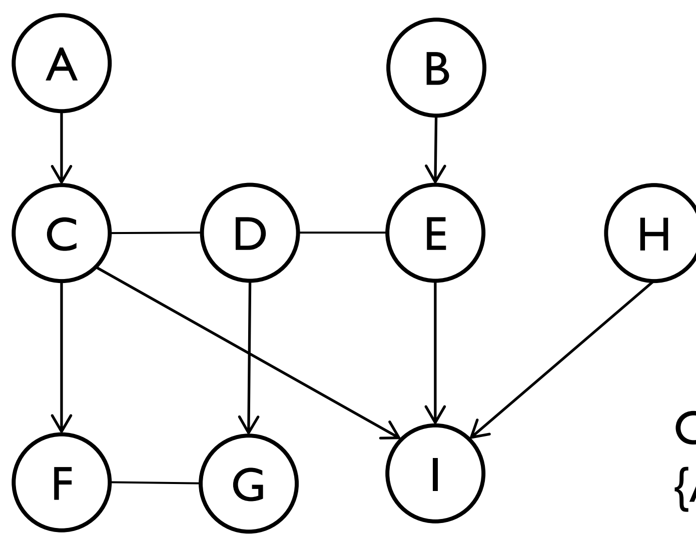
- **Theorem**: Let H be a chordal MN. Then there exists a DAG G that is a perfect I-map for H



⇒ The independencies in a graph can be represented in both type of models **if and only if** the graph is **chordal**

Partially Directed Acyclic Graphs (PDAGs)

- Superset of both directed and undirected graphs
- PDAGs are also called **chain graphs**



Chain components:
{A}, {B}, {C,D,E},{F,G},{H}, {I}

[Koller, PGM book]

Relationship between BNs and MNs: summary

- Directed and undirected models represent different families of independence assumptions
  - Chordal graphs can be represented in both BNs and MNs

- For inference, we can use a single representation for both types of these models
  - simpler design and analysis of the inference algorithm