Inference and Representation

DS-GA-1005, CSCI-GA.2569

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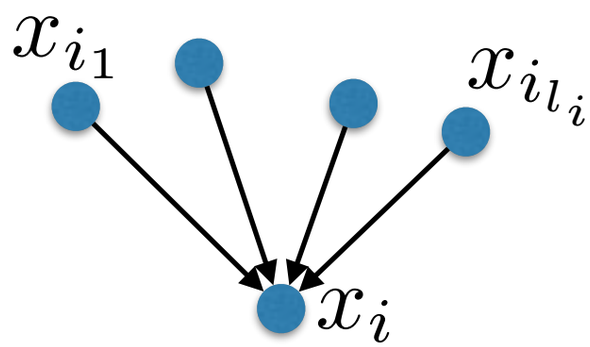
Lecture 1: Bayesian Networks

- We've seen that reducing the scope of conditional probability is critical in order to beat the curse of dimensionality.

$$p_G(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i \mid x_{i_1}, \ldots x_{i_{l_i}}) \ .$$

- Q: How to describe those dependencies?
- Given a directed acyclic graph $G = (V, E)$ we encode a model as
  - One node $i \in V$ for each random variable.
  - One conditional probability distribution per node, where conditional factors become the parents in the graph:



$$\{x_{i_1}, \ldots, x_{i_{l_i}}\} := x_{Pa(i}$$

- Properties of the joint distribution are now expressed in terms of the graph.
  - algorithms for inference
  - complexity questions.

Lect.1: Conditional Independence

- In a specific graphical model, conditional probabilities have missing terms:

$$p(X_i \mid X_{i_1}, \ldots, X_{i_{l_i}}) \text{ instead of } p(X_i \mid X_1, \ldots, X_{i-1})$$

- Thus

$$X_i \perp X_j \mid X_{Pa(i)} \text{ for } j < i,\ j \notin Pa(i).$$

- In fact,

missing variables in the local conditional probabilities

$\Updownarrow$

missing edges in the corresponding graph

Independence Maps

- Given a directed acyclic graph G, we denote by $I(G)$ the set of conditional independencies implied by it.
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- G is a *minimal independence map* if pruning G (thus enlarging $I(G)$) makes it not an i-map.
  - Each node ordering may correspond to a different minimal i-map.
- G is a *perfect independence map* for p if $I(G) = I(p)$
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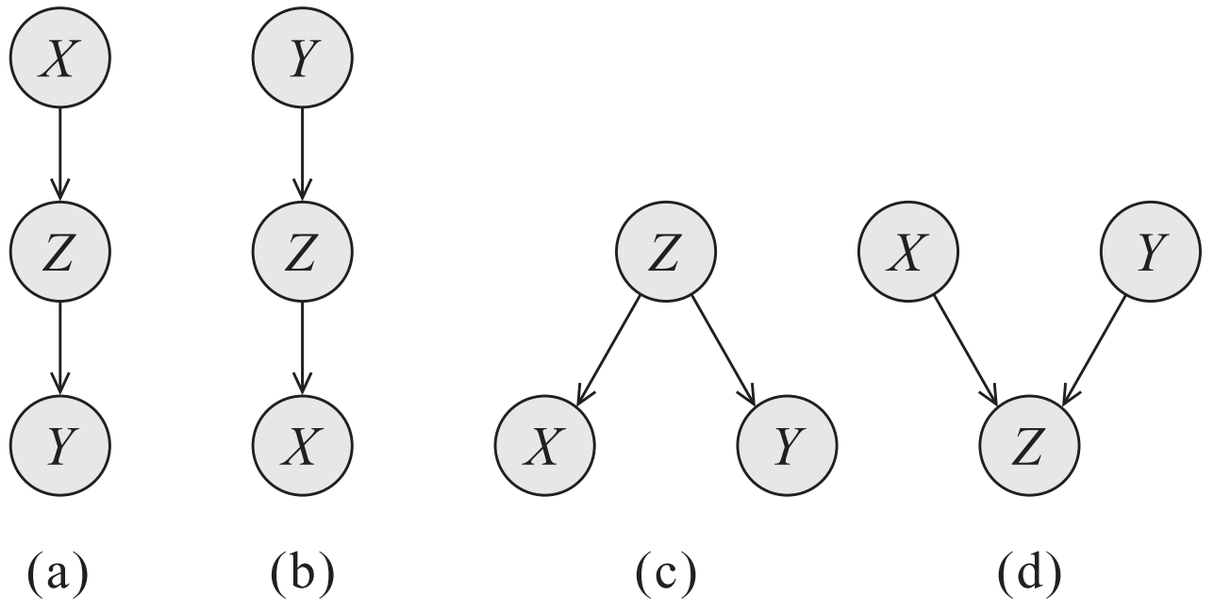
  - Q: Does every distribution have a perfect map?
  - $X, Y \sim \mathrm{Ber}(0.5)$, $Z = X \text{ XOR } Y$.

Equivalent Graph Structures

- Two different BNs can be equivalent: they encode the same conditional independence assumptions.
- Which of these are equivalent?



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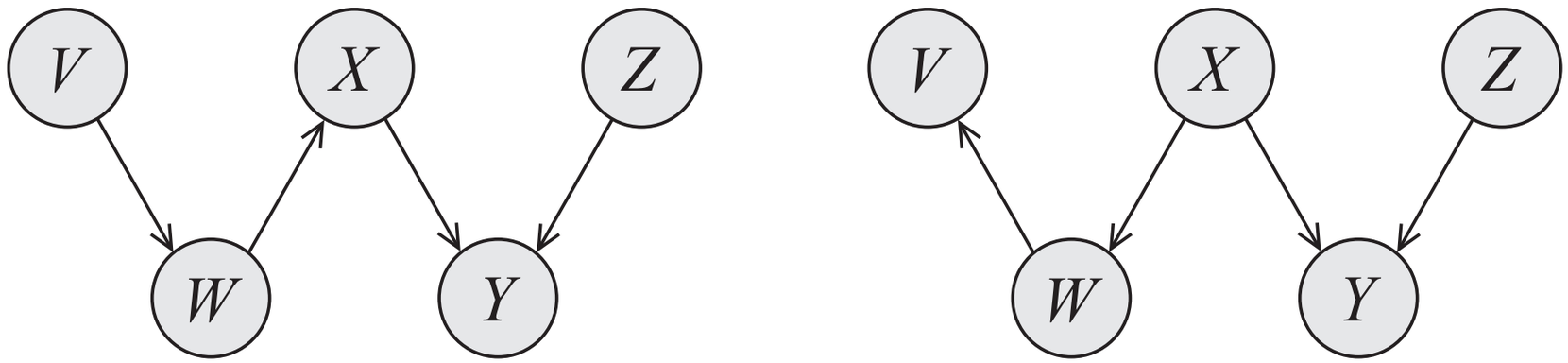

Summary: Bayesian Networks

- A Bayesian Network corresponds to a particular factorization of the joint distribution:

$$p(X_1, \ldots, X_n) = \prod_{i \in V} p(X_i \mid X_{Pa(i)})$$

- How well a BN corresponds to a given probabilistic model?
  - Given a directed acyclic graph G, we denote by $I(G)$ the set of conditional independencies implied by it.
  - Given a joint distribution p, we denote by $I(p)$ the set of conditional independencies satisfied by it.
  - G is a *perfect independence map* for p if $I(G) = I(p)$.
- No unicity: Different BNs can result in the same conditional independencies (different topological order)
- No existence: There exist p without perfect independence map.

Lecture 2

- Undirected Graphical Models (Markov Random Fields)
  - Definitions
  - Conditional Independence
  - Examples: The Ising Model

- Factor Graphs

- From Bayesian to Markov networks

- Parameter Estimation

Pros/Cons of Directed Models

$$p(X_1, \ldots, X_n) = \prod_{i \in V} p(X_i \mid X_{Pa(i)})$$

- Pros:
  - They allow efficient sampling (generative model): follow topological order.
  - Local factors directly interpreted as conditional probabilities.

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- Q: How to palliate some of its problems?

Undirected Graphical Models

- Consider a graph $G = (V, E)$, with
  - V in 1-to-1 correspondence with our set of rvs $X_1, \ldots, X_n$.
  - E: set of undirected edges within V.

- In the directed case, we started with the parametrization

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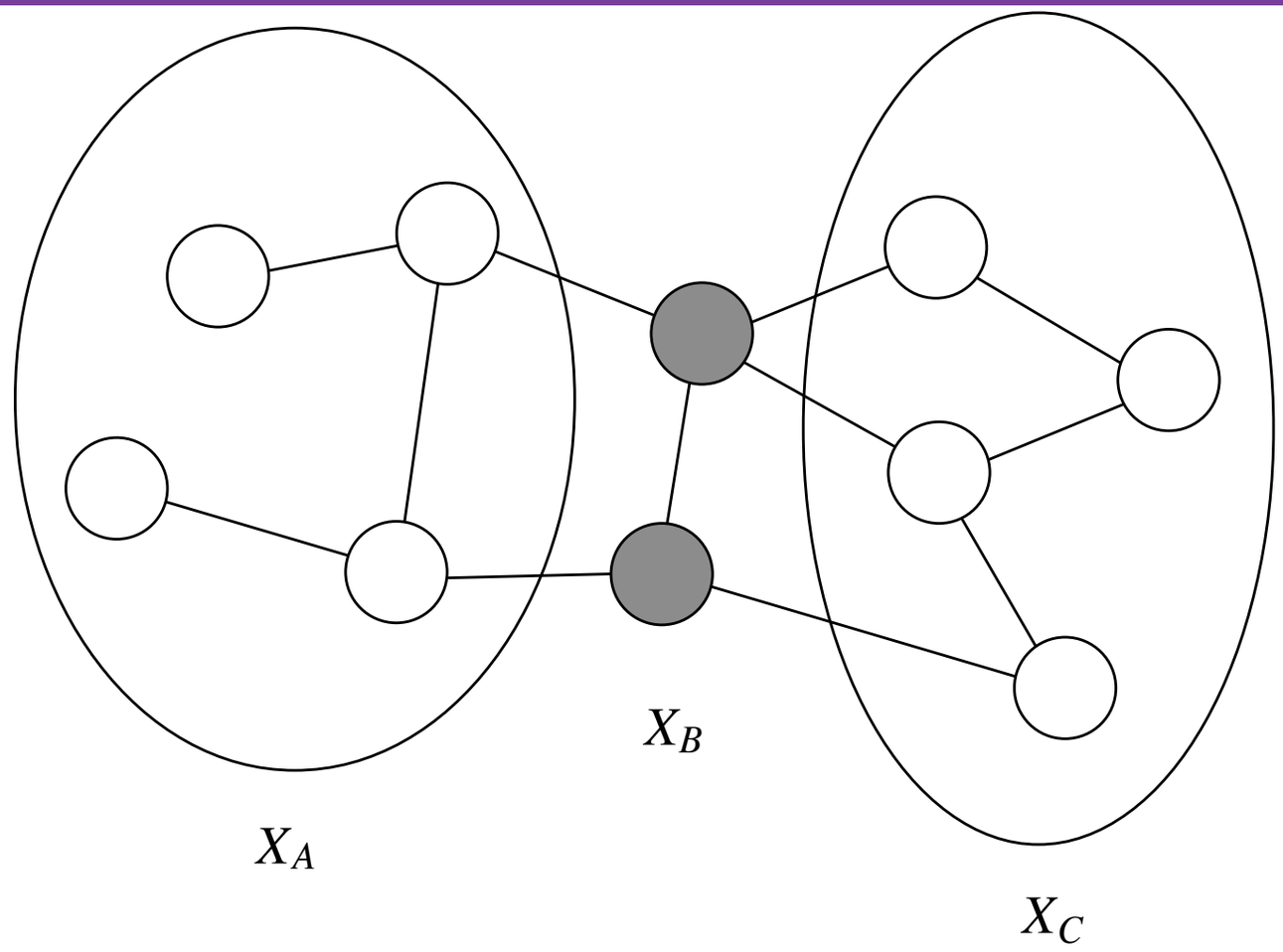
- In the undirected case, we do the opposite:

Given subsets of nodes A, B and C,

$X_A \perp X_B \mid X_C$ when nodes X_B separate nodes X_A from X_C.

Undirected Graphical Models



- Remark:
  - When we say $X_A \perp X_B \mid X_C$ holds for a given graph G, we mean that it is true *for every probability distribution associated with* G.
  - When we say that $X_A \perp X_B \mid X_C$ does not hold for a given G means that *some distributions that factor according to* G *do not satisfy it*.

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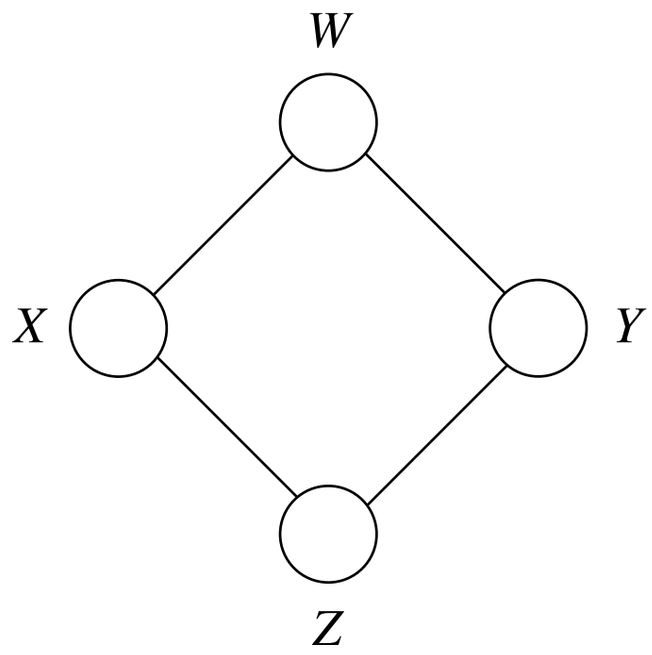

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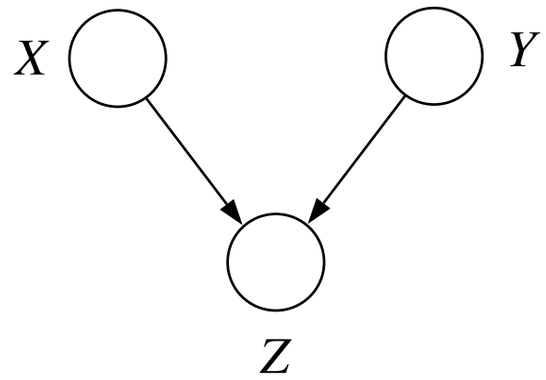

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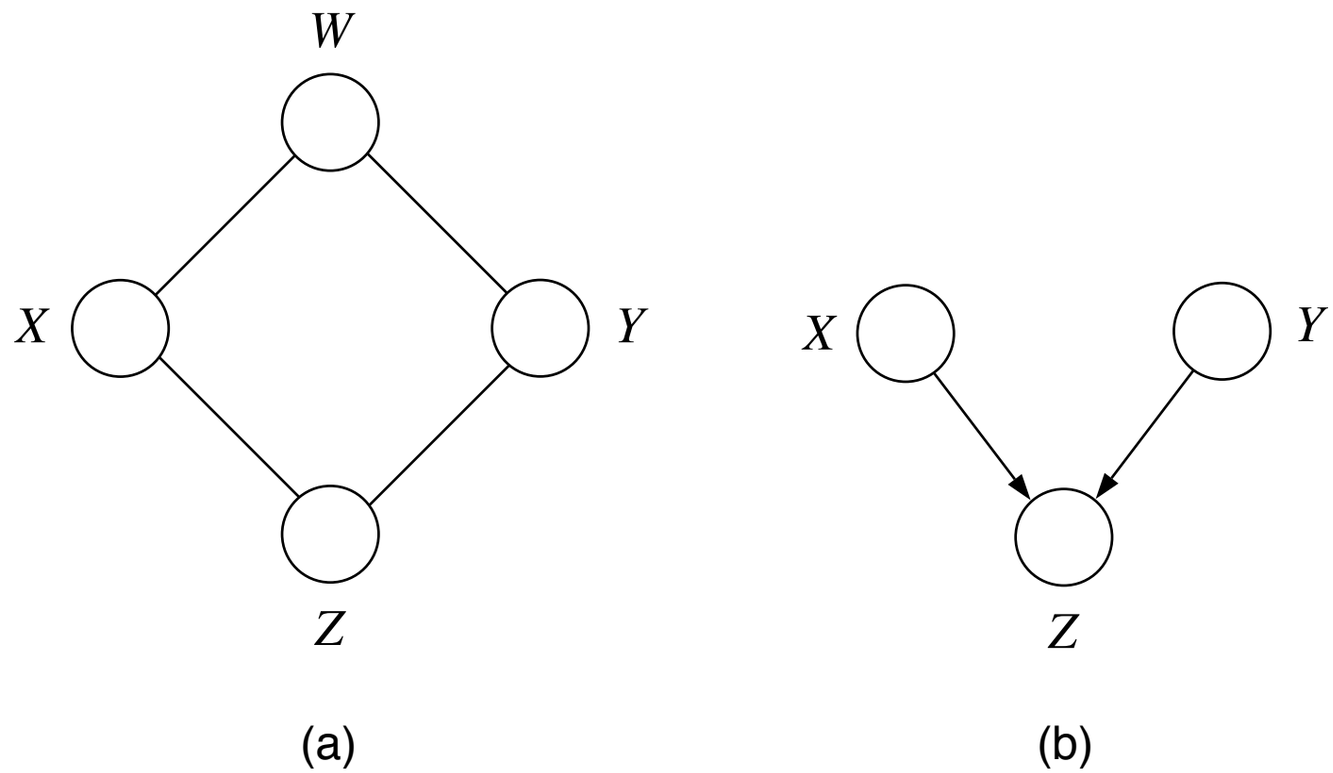

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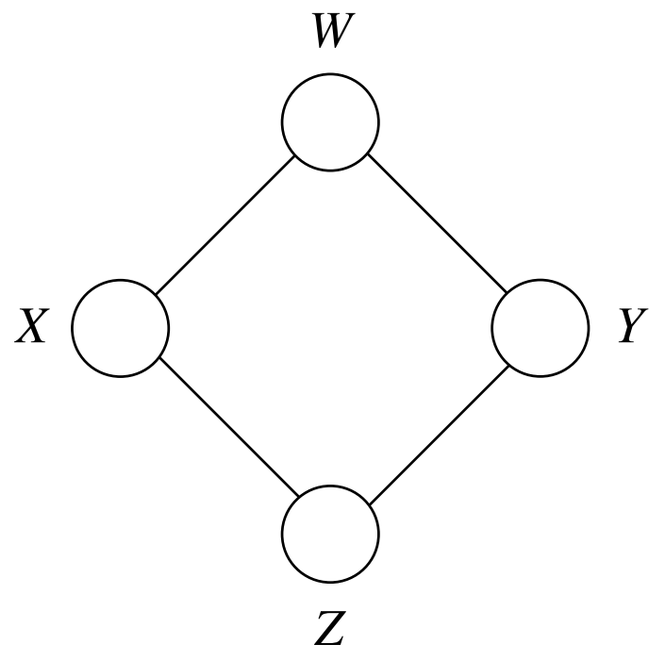

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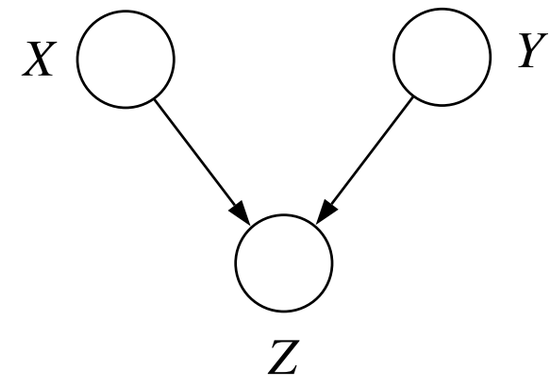

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– In (b), no undirected 3-node graph can represent $X \perp Y$ $(\text{without implying also } X \perp Z \text{ or } Y \perp Z)$

Undirected Graphical Models

- Q: How to parametrize those models? (from graph to distribution)
- In the directed setting, we used conditional probabilities as "building blocks" for the joint distribution:

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- We cannot do this now: how to select "parents" from children locally so that it is globally consistent?

- We still want to obtain a factorization of p as a product of "local factors".

Undirected Graphical Models

- We want to obtain a factorization $p(x_1, \ldots, x_n) = \prod_{C \in \mathcal{C}} \psi_C(x_C)$
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  - Suppose one of the factors C contains both x_i and x_j
  - In general, this will violate

$$p(x_i, x_j \mid \{x_k\}) = p(x_i \mid \{x_k\}_k) \cdot p(x_j \mid \{x_k\}_k)$$

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  - If X_C form a maximal clique, arbitrary functions $\psi(x_C)$ capture all possible dependencies within the clique.
- So, by considering

$$\mathcal{C} = \text{ set of maximal cliques of } G$$

$$\psi_C(x_C) : \text{non-negative potential function (not necessarily normalized)}$$

- We have $p(x) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(x_C)$, $Z = \int dx \prod_{C \in \mathcal{C}} \psi_C(x_C)$.

partition function

Interpretation of Potential Functions

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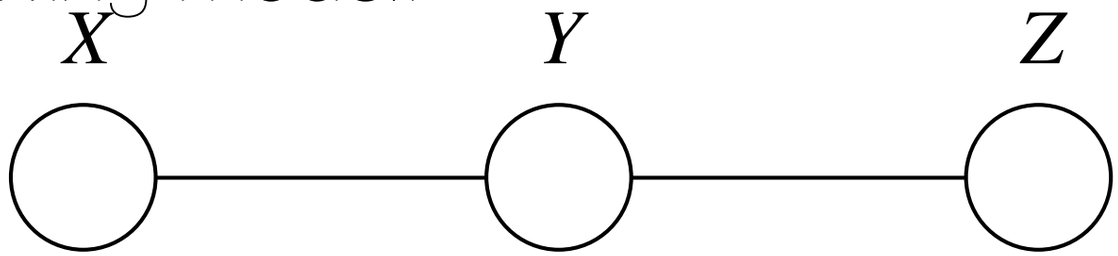

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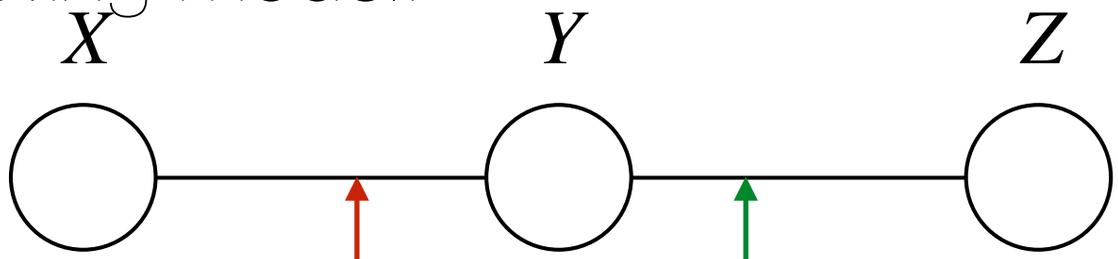

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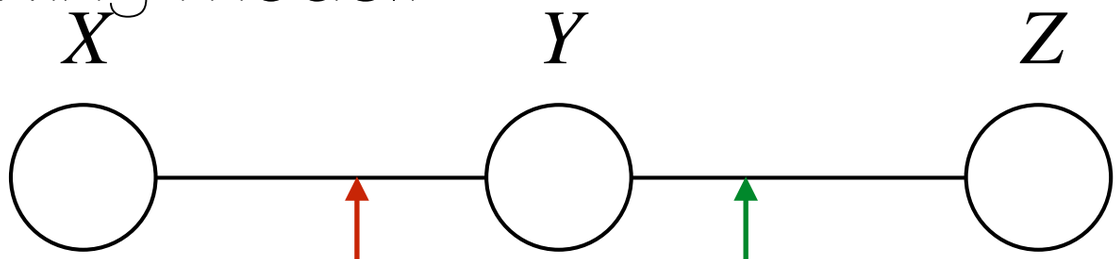

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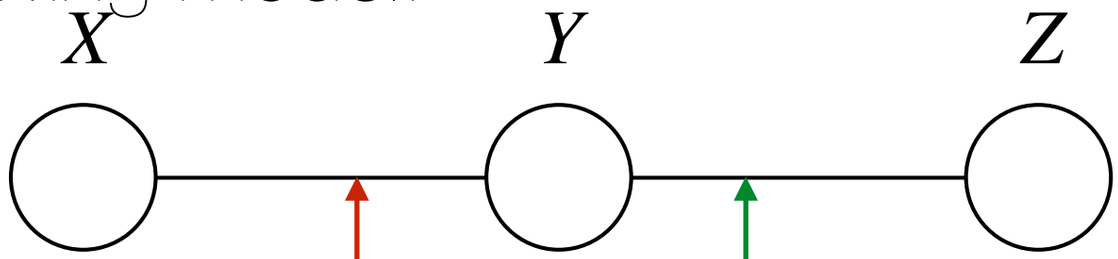

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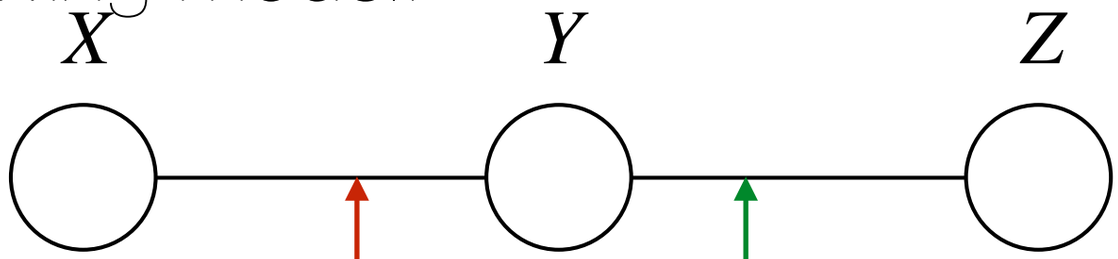

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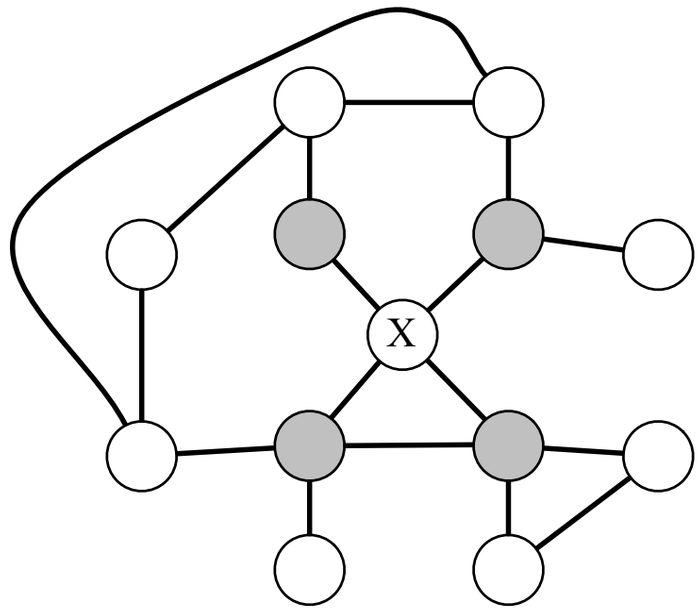
- In general, $p(x, y, z) \neq p(x, y)p(y, z)$.

$$p(x, y, z) = p(x, y)p(y, z) \Rightarrow p(y) = 0 \text{ , or } p(y) = 1 \text{ .}$$

Markov Blanket

- **A set $A \subseteq \mathcal{X}$ is a Markov Blanket of X if $X \notin A$ and if A is a minimal set of nodes such that $X \perp (\mathcal{X} \setminus (A \cup X)) \mid A$.**
- In undirected graphical models, the Markov Blanket of a variable is precisely its neighbors in the graph:



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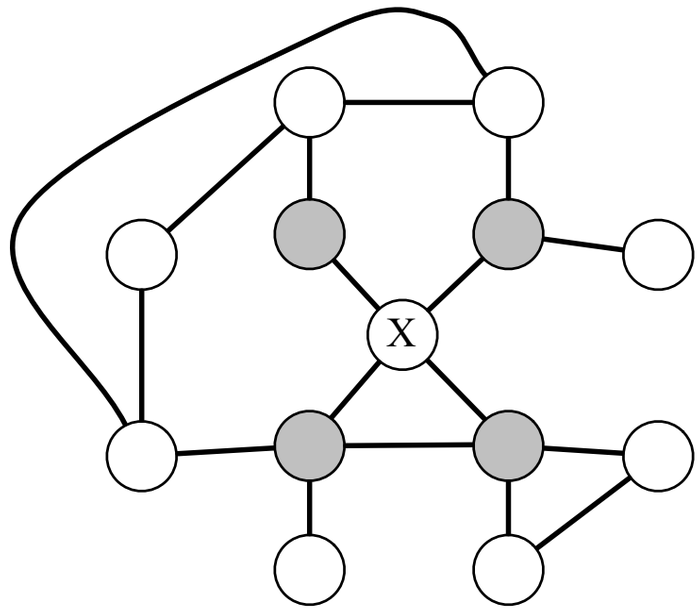
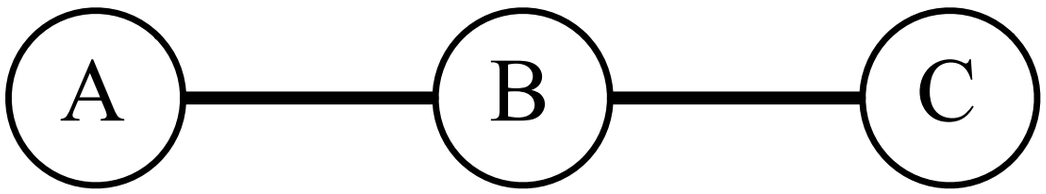


- *X* is independent of the rest of nodes conditioned on its neighbors.

Independence Through Separation

- We illustrate notion of Markov Blanket with the following example:



$$p(a,b,c) = \frac{1}{Z}\psi_{AB}(a,b)\psi_{BC}(b,c) \ .$$

- Let us verify $A \perp C \mid B$

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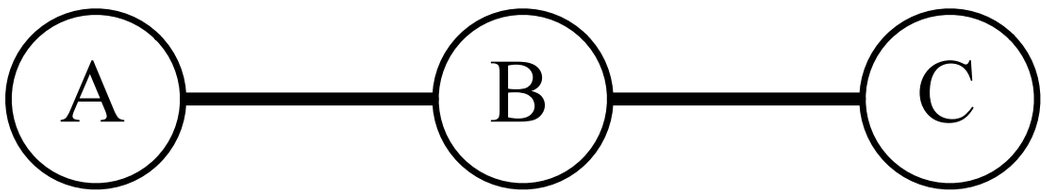

$$p(a,b,c) = \frac{1}{Z}\psi_{AB}(a,b)\psi_{BC}(b,c) \ .$$

- Let us verify $A \perp C \mid B$

$$p(a \mid b) = \frac{p(a,b)}{p(b)} = \frac{\sum_{c'} \psi_{AB}(a,b)\psi_{BC}(b,c')}{\sum_{a',c'} \psi_{AB}(a',b)\psi_{BC}(b,c')}$$

$$= \frac{\left(\sum_{c'} \psi_{BC}(b,c')\right) \psi_{AB}(a,b)}{\left(\sum_{c'} \psi_{BC}(b,c')\right) \left(\sum_{a'} \psi_{AB}(a',b)\right)}$$

$$= \frac{\psi_{AB}(a,b)}{\sum_{a'} \psi_{AB}(a',b)}$$

- In general, separability holds when a variable is conditioned on its Markov Blanket.

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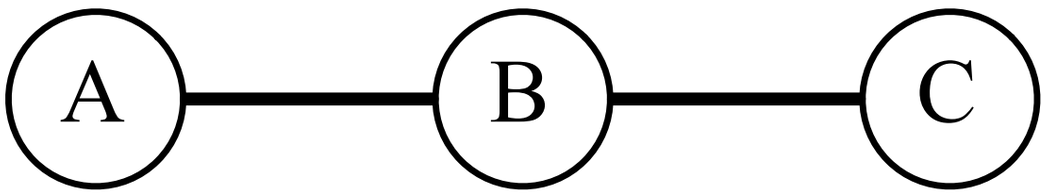

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- It follows that

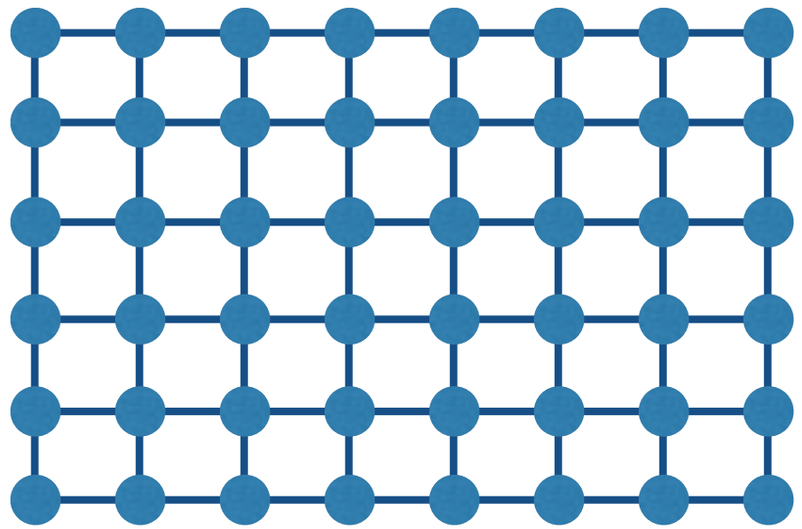
$$\begin{aligned} p(a,c\,|b) &= \frac{p(a,b,c)}{p(b)} = \frac{\psi_{AB}(a,b)\psi_{BC}(b,c)}{\sum_{a',c'}\psi_{AB}(a',b)\psi_{BC}(b,c')} \\ &= \frac{\psi_{AB}(a,b)}{\sum_{a'}\psi_{AB}(a',b)} \cdot \frac{\psi_{BC}(b,c)}{\sum_{c'}\psi_{BC}(b,c')} \\ &= p(a \mid b)p(c \mid b) \ . \end{aligned}$$

- Also, conditional probabilities do not "care" about partition function.

Example: Ising Model

- Consider a collection of *spins* or magnets, taking discrete ± 1 values, arranged in a lattice configuration.
- Spins interact with their neighbors in the lattice, either by attracting each other to have same state (ferromagnetism) or by repulsing each other (anti-ferromagnetism).

1d lattice (Ising, 1924)



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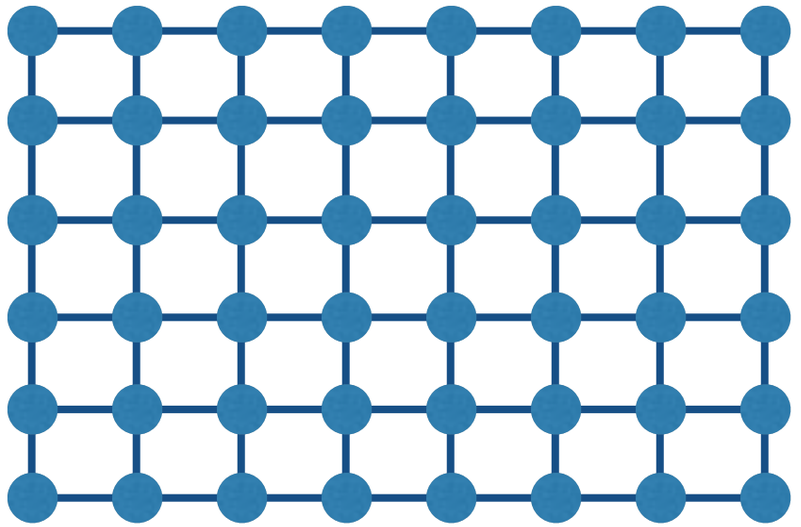

2d lattice (Onsager, 1944)

- $i \in \mathcal{L}$: 1d/2d Lattice $X_i = \pm 1$: state of each spin

$$p(X_1, \ldots, X_n) = \frac{1}{Z} \exp\left(- \sum_{i<j} w_{i,j} X_i X_j - \sum_i u_i X_i \right) .$$

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  - $w_{i,j} > 0$: ferromagnetic interactions (why?)
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- From statistical mechanics, we can interpret the exponent

$$H(X) = -\sum_{i<j} w_{i,j} X_i X_j - \sum_i u_i X_i$$

as an energy quantity (in fact, it is the Hamiltonian of the system).

Boltzmann/Gibbs distributions

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- β: **inverse temperature parameter.**
  - controls the "order" of the system.
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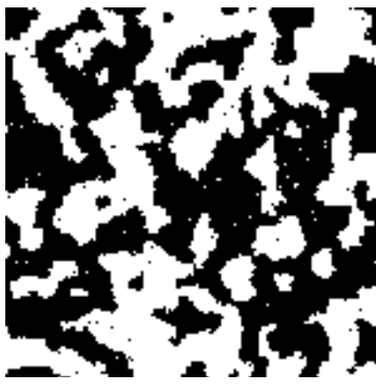
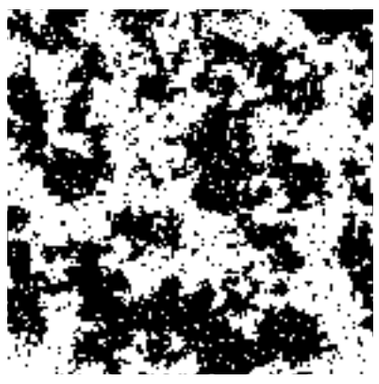
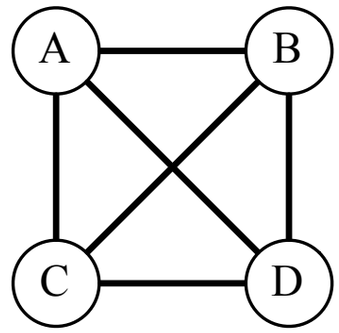




2d Ising decreasing β.

Factor Graphs

- Recall clique vs maximal clique ambiguity:



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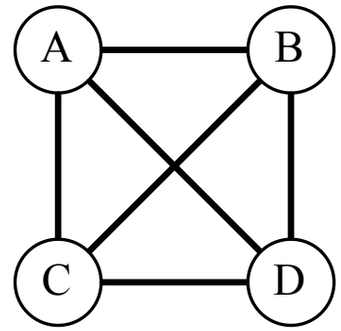

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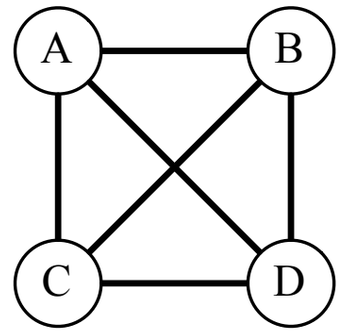

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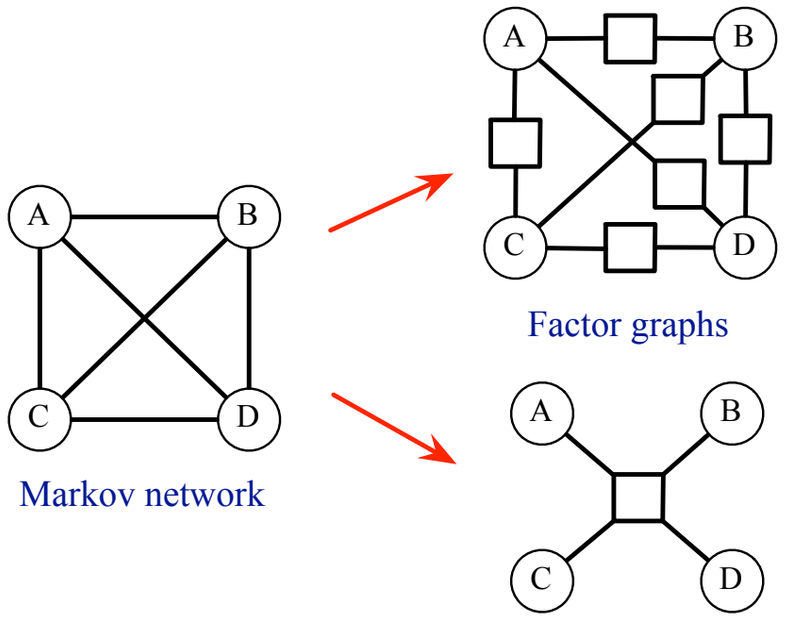
- Q: How to resolve the ambiguity of the graphical representation?

Factor Graphs

- A *factor graph* is a bipartite graph where
  - nodes correspond to **both** random variables $\{X_i\}_{i \leq n}$ and potential factors $\{\psi_C\}_{C \in \mathcal{C}}$.
  - edges can only be drawn between variable and factor nodes (if variable X_i appears in factor ψ_C).



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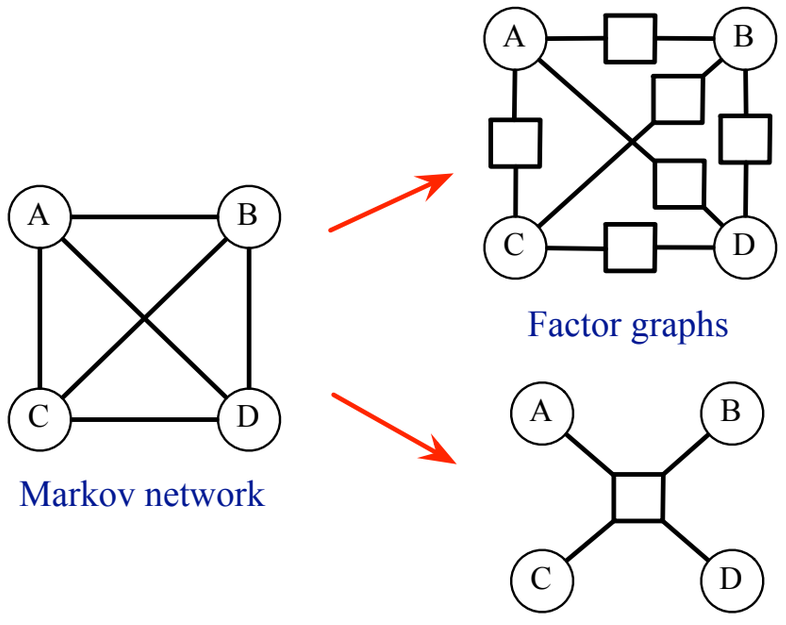

- Factor graphs do not have the clique vs maximal clique ambiguity (why?).
- Same probabilistic model, different graphical representation.

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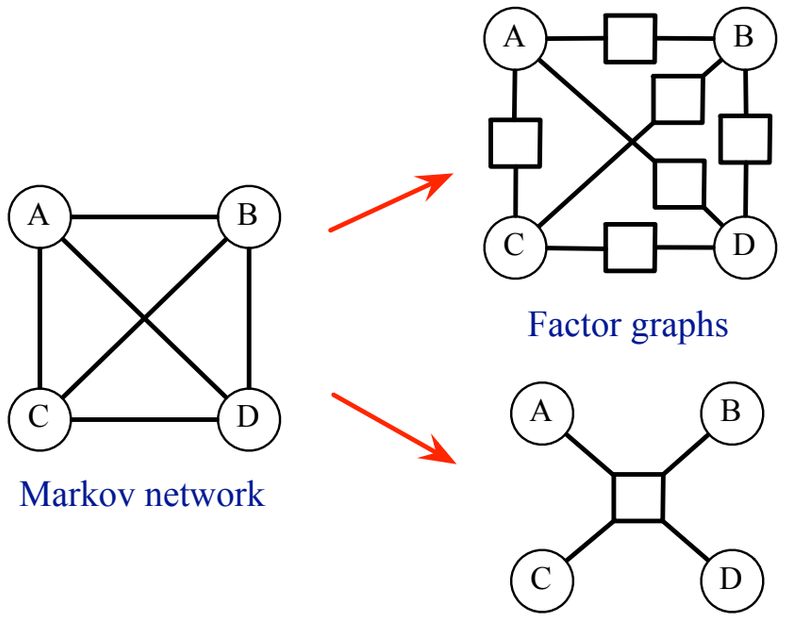
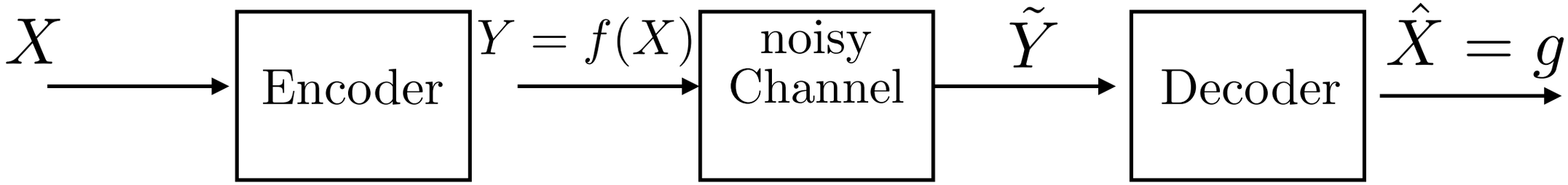


- Also, any Bayesian Network or any Markov Random Field can be represented as factor graphs (why?)

Example: LDPC Codes

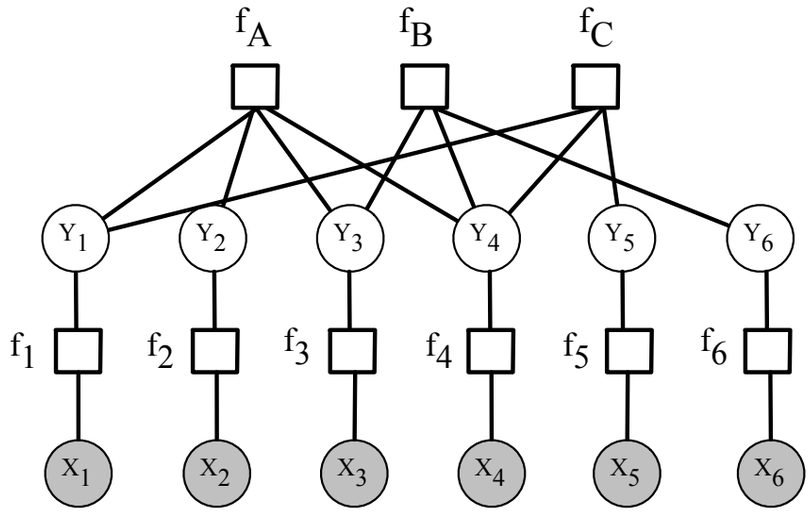
- Error-correcting codes are ubiquitous in digital communications.
- Basic Principle: given a sequence $X = (X_1, \ldots, X_n)$ of discrete (e.g binary) symbols to be transmitted, *encode* it to $Y = f(X)$ bits prior to transmit, in order to increase error robustness. $m \geq n$



- Long history in Information Theory
  - Parity codes
  - Also Group Theory and Algebraic Geometry.

LDPC Codes

- Low-density parity-check codes (Gallager, 60s):



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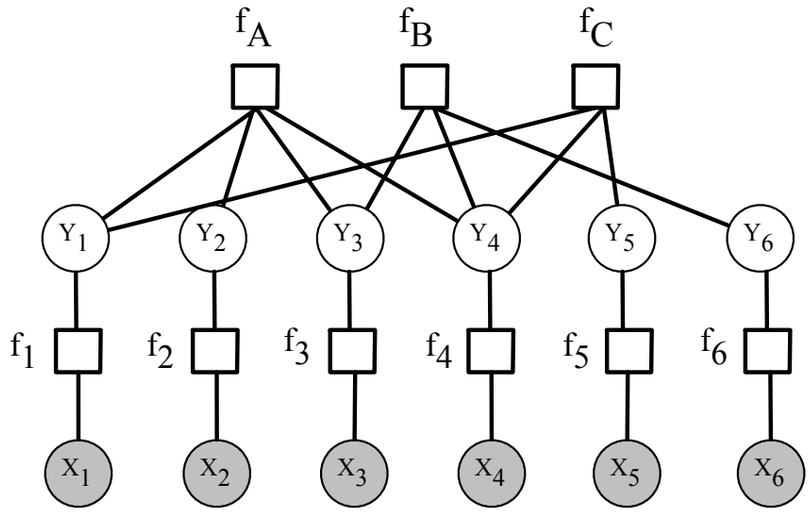

- Each of the top row factors provides a parity constraint:

$$f_A(Y_1, Y_2, Y_3, Y_4) = \begin{cases} 1 & \text{if } Y_1 \oplus Y_2 \oplus Y_3 \oplus Y_4 = 0 \ , \\ 0 & \text{otherwise.} \end{cases}$$

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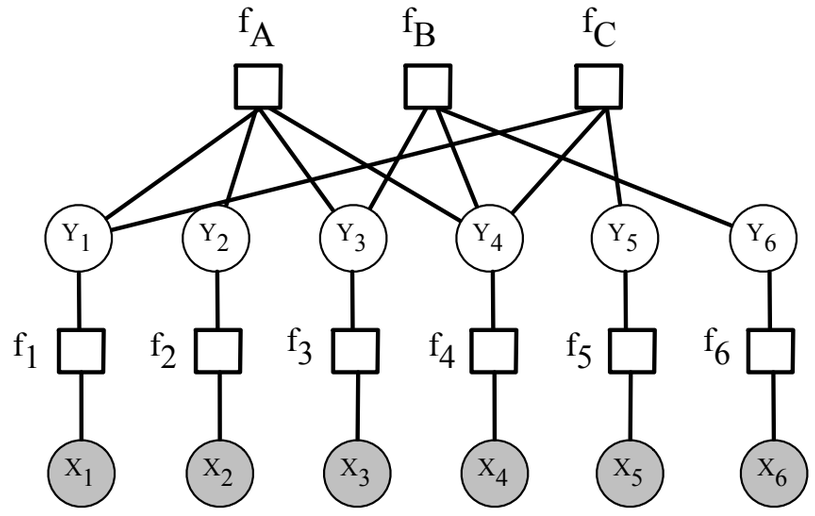

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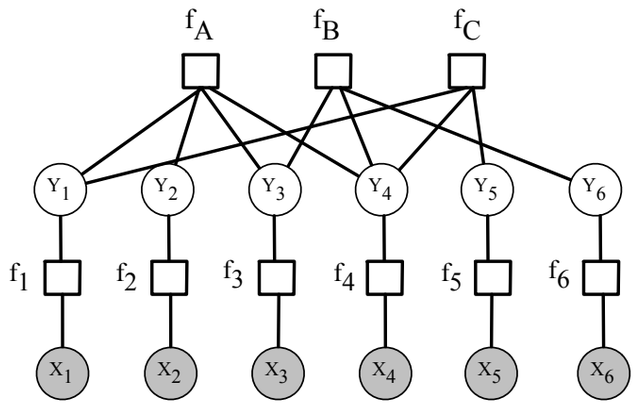
- The three top factors together imply that the only assignments Y with non-zero probability are:

000000, 011001, 110010, 101011, 111100, 100101, 001110, 010111

- Noise model: $f_i(X_i, Y_i) = p(X_i \mid Y_i) \ .$

LDPC Codes



- Q: How to decode from observed data?

$$\hat{Y} = \arg\max_{\mathbf{Y}} p(\mathbf{Y} \mid X = x) \quad \text{(Maximum a Posteriori inference)}$$

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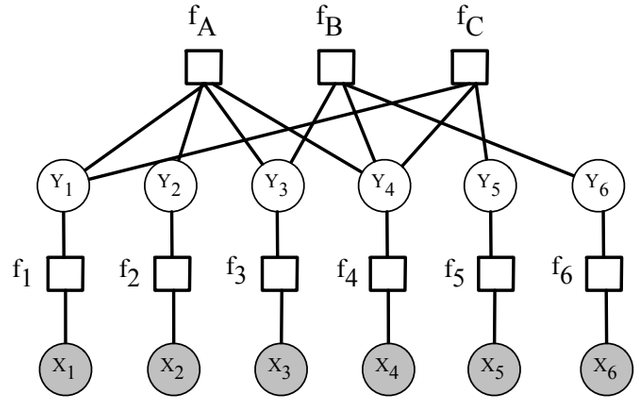

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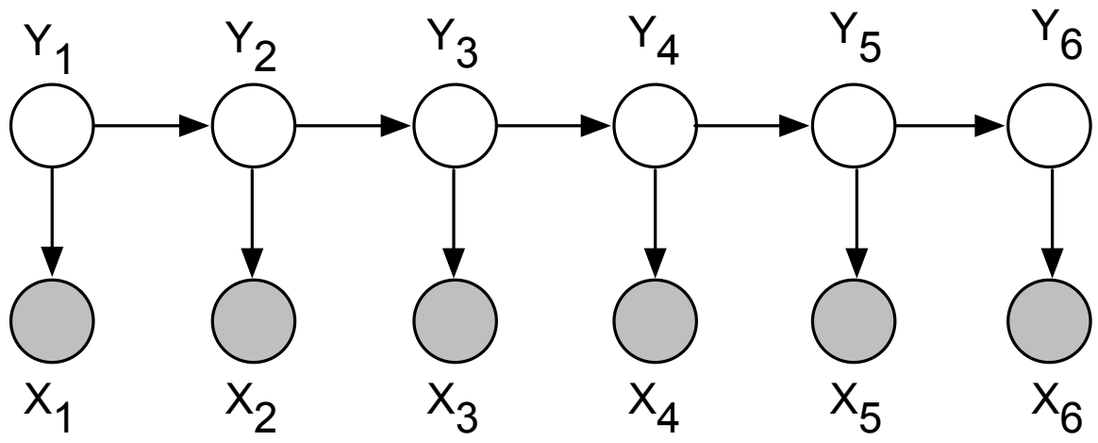
- For general $p(\mathbf{Y}, X) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(Y_C, X_C)$, we have

$$\hat{Y} = \arg\max_{\mathbf{Y}} \sum_{C \in \mathcal{C}} \log \psi_C(Y_C, X_C)$$

- We will see several approaches to solve this later on
  - Belief Propagation on trees.

BNs and MRFs

- So far, we have seen two formalisms to model joint distributions with graphs:
  - Directed Acyclic from Bayes Chain Rule: Bayesian Networks.
  - Undirected graphs: Markov Random Fields.
- Q: To what extent we can "translate" between formalisms?
- Ex: What is the equivalent undirected network for the HMM?



Moralization

- Algorithm to map a Bayesian Network to a Markov Network.
- Given $G = (V, E)$ DAG, we define $M(G)$ an undirected graph over V, with edge between X_i and X_j whenever
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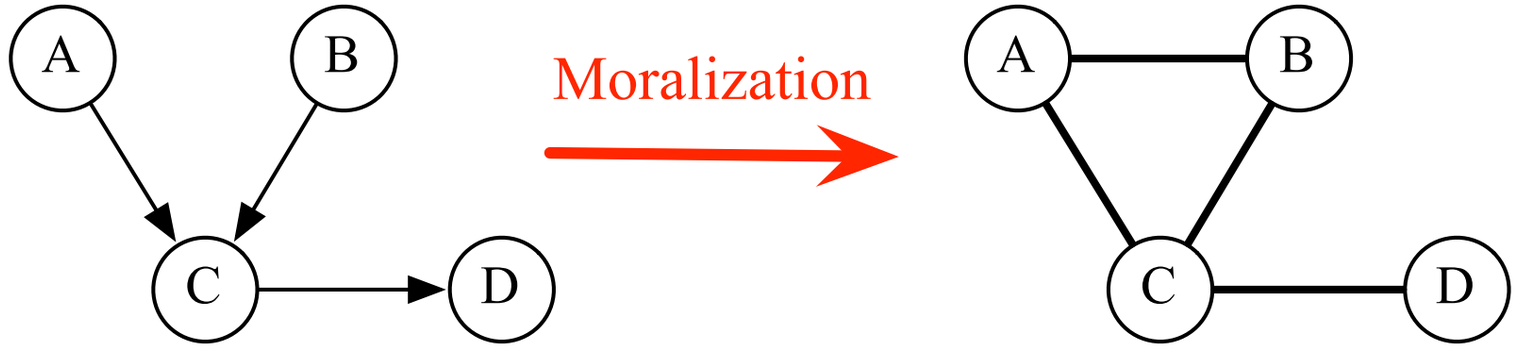

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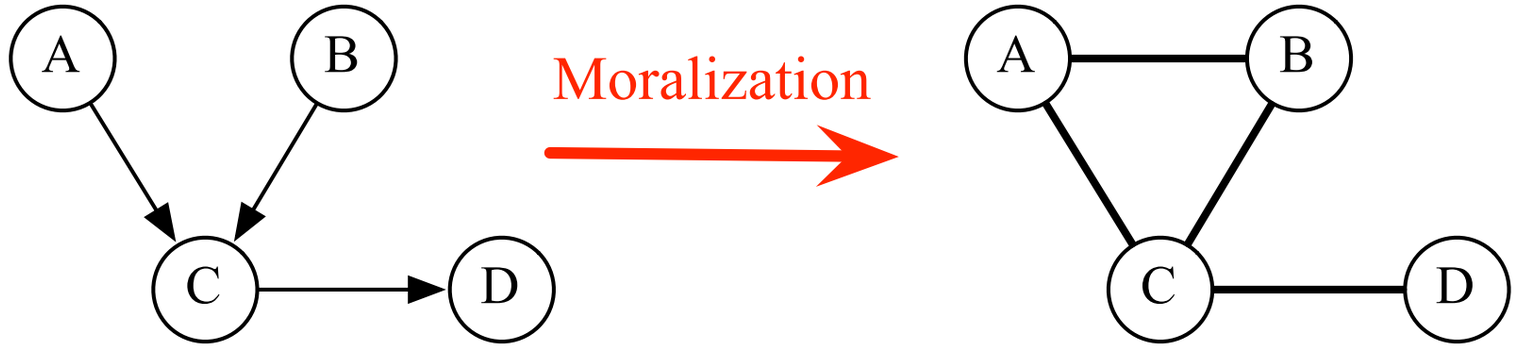

- In $M(G)$, we can no longer tell that $A \perp B$.
  - V-structures disappear, but we can still model "explaining away" with e.g. sparsity priors.

Moralization

- Equivalently, this rule is obtained by mapping factorization of joint distribution.

$$\underbrace{p(x_1,\ldots,x_n) = \prod_i p(x_i \mid x_{Pa(i)})}_{\text{Bayesian Net}} \quad \Longleftrightarrow \quad \underbrace{p(x_1,\ldots,x_n) = \frac{1}{Z}\prod_{C\in\mathcal{C}} \psi_C(x_C)}_{\text{MRF}}$$

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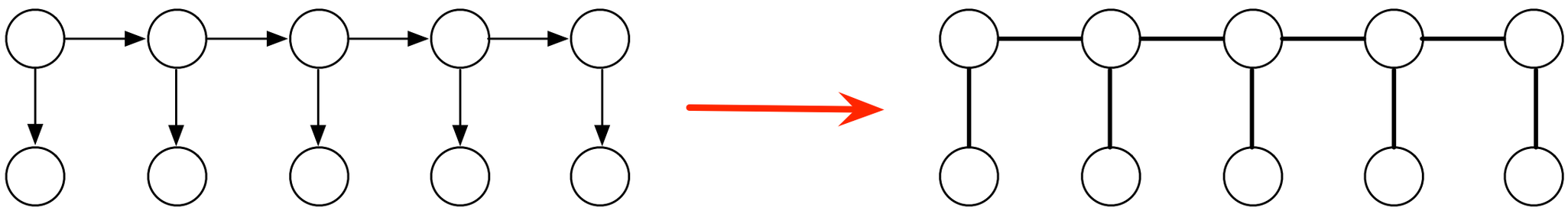
- Each node generates a factor in the resulting factor graph:

$$\psi_{C_i}(x_{C_i}) := p(x_i \mid x_{Pa(i)}) \ , \ C_i = \{i\} \cup Pa(i) \ .$$

- Ex: Hidden Markov Model:



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- Converse true?
  - Not in general.

Hammersley-Clifford Theorem

- However, if we assume that p is positive, i.e. $p(x) > 0$ for all x,
- Then we have

Theorem [H-C]: An undirected graph G is an I-map for a positive distribution $p(x)$ iff p is a Gibbs distribution that factorizes over G.

- It provides a parametrization for any distribution that complies with a series of conditional independence assumptions (Markov Property).

- Positivity condition is needed!

Global Markov but not Factorizing

- Consider 4 binary random variables A, B, C, D, and the following distribution:

$$p(A=1,B=1,C=1,D=1)=\frac{1}{8}\ ,\ p(A=1,B=1,C=0,D=1)=\frac{1}{8}$$
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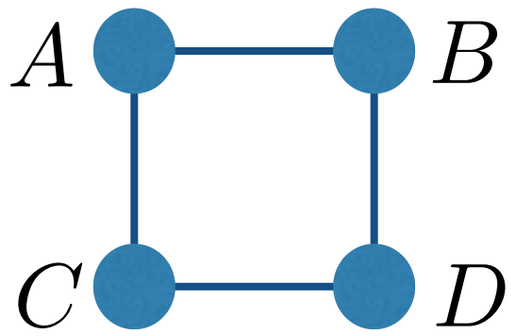

- Do we have $I(G) \subseteq I(p)$?

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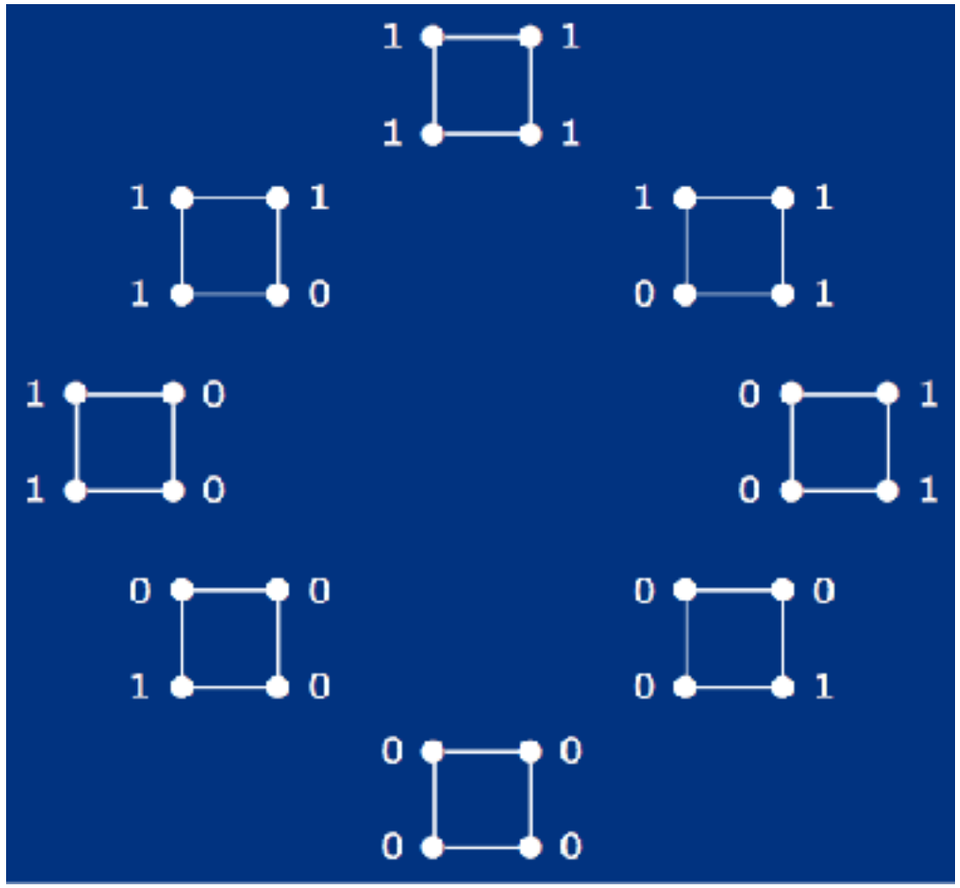

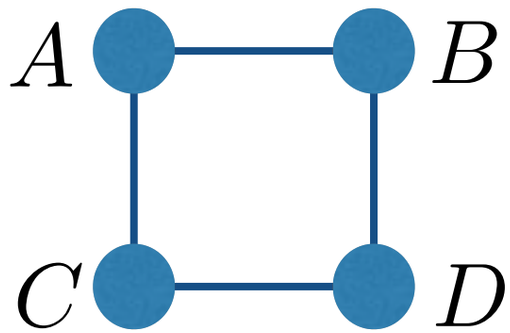

- Do we have $I(G) \subseteq I(p)$?

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

  - Observe that conditioning on opposite corners always yields one corner deterministic, and $X \perp Y$ **whenever** X **or** Y **are deterministic.**

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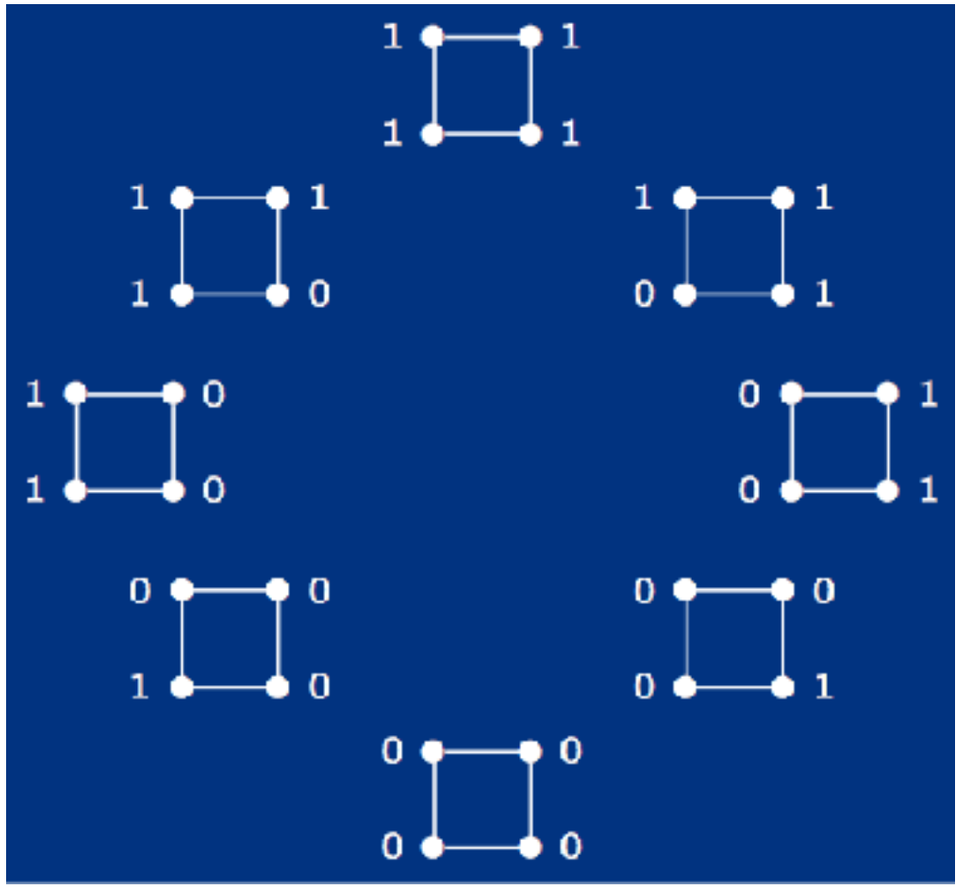

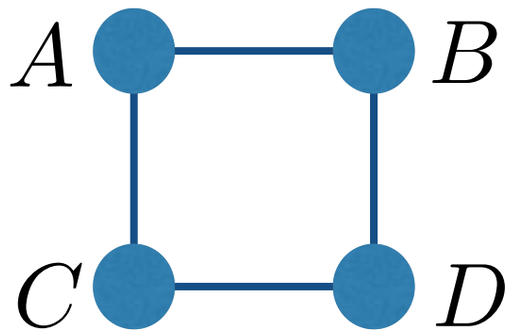

- Is p a Gibbs distribution?

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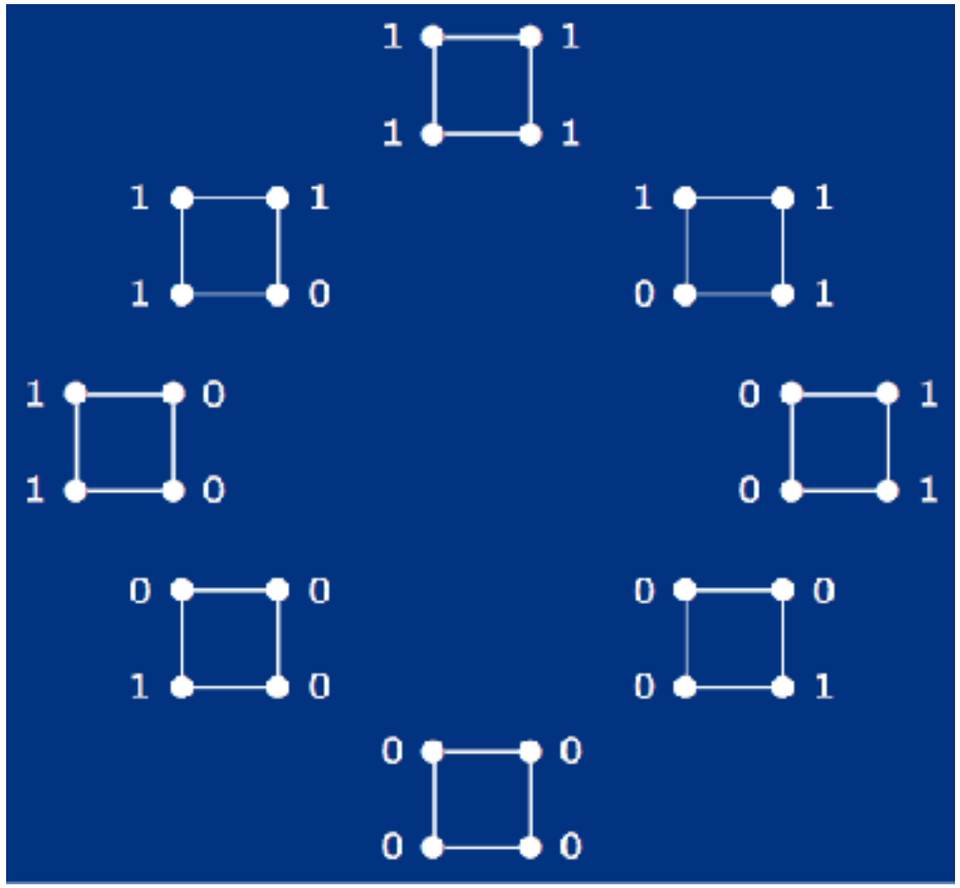

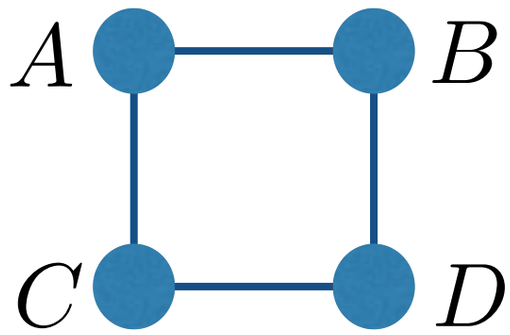

- Is p a Gibbs distribution?
  - Assume $p(x) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(x_C)$

    so all these factors are strictly positive

    $0 < Z \cdot p(0,0,0,0) = \psi_{AB}(0,0)\psi_{BD}(0,0)\psi_{DC}(0,0)\psi_{CA}(0,0)$
  - Trying all 8 positive events implies all factors are strictly positive!

Parameter Estimation

- So far, we have described two families of graphical models, with pros and cons.
- In practice, given some dataset, how to choose which one? Which parameters?
- We assume data is sampled from an underlying (unknown) distribution p^*, associated to some network model $\mathcal{M}^* = (G^*, \theta^*)$

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- Samples $\{\mathbf{X}^1, \ldots, \mathbf{X}^L\} \sim p^*$ iid.
- In order to "search" for $\mathcal{M}^*$, we parametrize the search within a family of graphical models
  - We can learn both model parameters for a fixed graph structure,
  - or both structure and parameters.

Task-driven inference

- Depending on the task, we might want to perform different kinds of estimation.
    1. Density Estimation: we are interested in the joint distribution, which can be subsequently used to perform any inference query.
    2. Prediction: we are only interested in a specific set of conditional distribution, e.g classification, or output prediction.
    3. Structural discovery: We are interested in the graph itself (not so much the parameters), e.g. determining dependencies between genes.

- (1) is typically harder than (2). (3) is typically harder than (2) and (1).

Parameter Estimation

- Let us focus on (1) first. $\{\mathbf{X}^1, \ldots, \mathbf{X}^L\} \sim p^* \text{ iid.}$
- Suppose $p^* = p_{\theta^*} \text{ for some } \theta^*.$
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- Two main approaches for parameter estimation:
  - Maximum Likelihood Estimation:

$$E(\theta) = \log p(\{\mathbf{X}^1, \ldots, \mathbf{X}^L\} \mid \theta) = \sum_{l<L} \log p(\mathbf{X}^l \mid \theta)$$

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  - Under appropriate assumptions, $\hat{\theta}_{MLE}$ is
    - consistent (as sample size grows, $\hat{\theta}_{MLE} \to \theta^* \text{ (in probability)}$
    - asymptotically efficient (no other consistent estimator has lower asymptotic mean-squared error).
  - However, in general this estimation is computationally intractable.

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- Two main approaches for parameter estimation:
  - Method of Moments:

$$\text{Consider measurable functions } g_1, \ldots, g_S.$$

$$(\text{e.g. } g_i(\mathbf{x}) = x_{i_1} x_{i_2})$$

For each θ, we have $\mu_s(\theta) = \mathbb{E}_{X \sim p_\theta}(g_s(\mathbf{X})) \quad s = 1 \ldots S$

For appropriate choice of moments/functions, system is invertible:

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We estimate μ by replacing expectations with empirical averages:

$$\hat{\mu}_s = \frac{1}{L} \sum_{l \leq L} g_s(X^l) \quad s = 1 \ldots S$$

And we plug-in the estimator for θ: $\hat{\theta}_{MM} = F(\hat{\mu})$

MLE in Bayesian Networks

- Let us illustrate ML estimation on BN, assuming we know the Bayesian structure G .

$$p(x_1, \ldots, x_n; \theta) = \prod_{i=1}^{n} p(x_i \mid x_{Pa(i)}; \theta)$$

- Given iid samples $\{X^1, \ldots, X^L\}$, its log-likelihood is

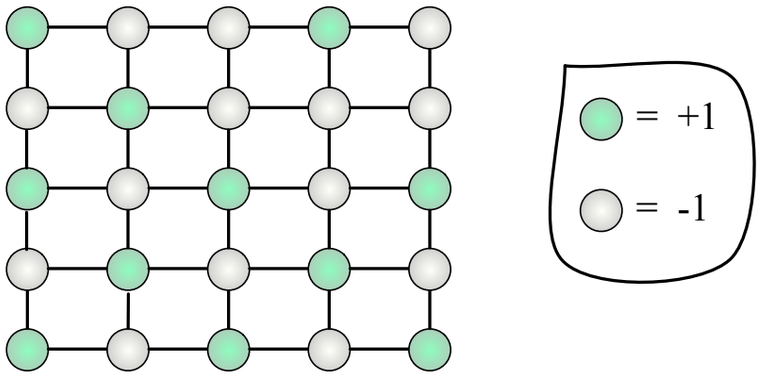
$$E(\theta) = \sum_{l \leq L} \sum_{i \leq n} \log p(X_i^l \mid X_{Pa(i)}^l; \theta)$$

$$= \sum_{i \leq n} \sum_{l \leq L} \log p(X_i^l \mid X_{Pa(i)}^l; \theta_i) \ .$$

  - so the estimation is separable across different factors, breaking the curse of dimensionality.

- Q: How about Markov Random Fields?

Parameter Estimation in MRFs



$$p(x_1, \cdots, x_n) = \frac{1}{Z} \exp\left(\sum_{i<j} w_{i,j} x_i x_j - \sum_i u_i x_i\right)$$

- In a MRF, we also have a factorization into local potentials…

$$p(x_1, \ldots, x_n; \theta) = \frac{1}{Z(\theta)} \prod_{C \in \mathcal{C}} \psi_C(x_C; \theta) \ .$$

- … but the partition function entangles the estimation!

$$\sum_{l \leq L} \log p(X^l; \theta) = \sum_{l \leq L} \left(\sum_{C \in \mathcal{C}} \log \psi(X^l_C; \theta) - \log Z(\theta) \right) \ .$$

Lecture 2 Summary

- Bayesian Networks are compelling models, which offer lightweight generative process and parameter estimation.
- However, many phenomena (physics, and other areas to come) require different probabilistic models
- Markov Random Fields offer a more general alternative
  - Easier to encode exchangeable properties of the data distributions.
  - Conditional Independences are more easily extracted from the graph.
  - Generation, inference and parameter estimation require special machinery (lectures 4-7).
  - BN can be embedded as MRFs through *Moralization*.
- Factor Graphs are flexible representations that include both BN and MRFs.