

Probabilistic Graphical Models

Undirected Models

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Fall 2019

Learning objectives

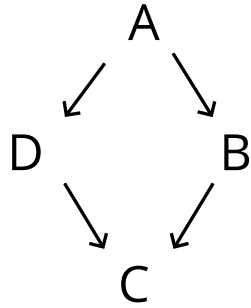
Markov networks:

- how it represents a prob. dist.
 - independence assumptions
 - factorization
 - representations:
 - factor-graph
 - log-linear models
- Hammersley-Clifford theorem

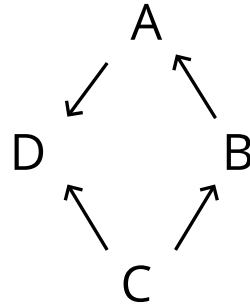
Challenge

Given the following set of CIs draw their DAG

$$\mathcal{I}(P) = \{(A \perp C \mid B, D), (D \perp B \mid A, C)\}$$



OR

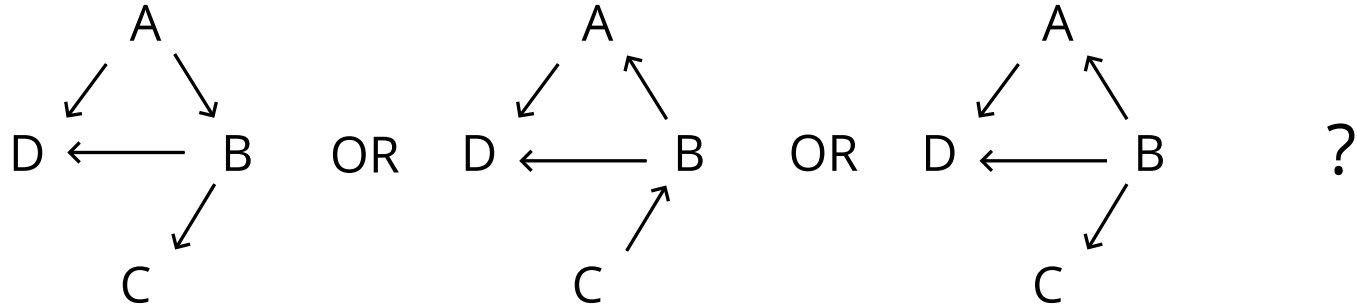


?

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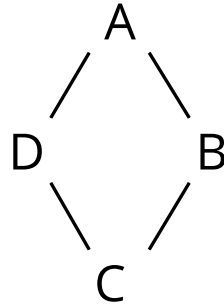
a DAG cannot be a P-map for P
an undirected model can!

Challenge

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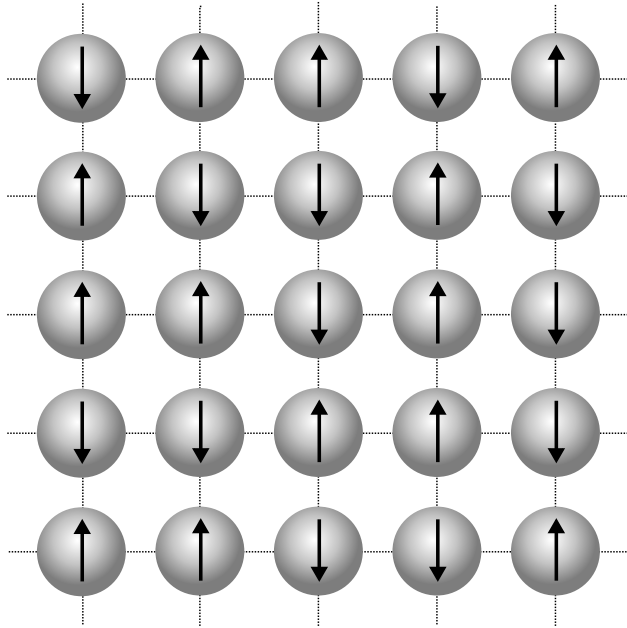
$$\mathcal{I}(P) = \{(A \perp C \mid B, D), (D \perp B \mid A, C)\}$$

a DAG cannot be a P-map for P
an undirected model can!



Motivation

Statistical physics: **Ising model** of ferromagnetism

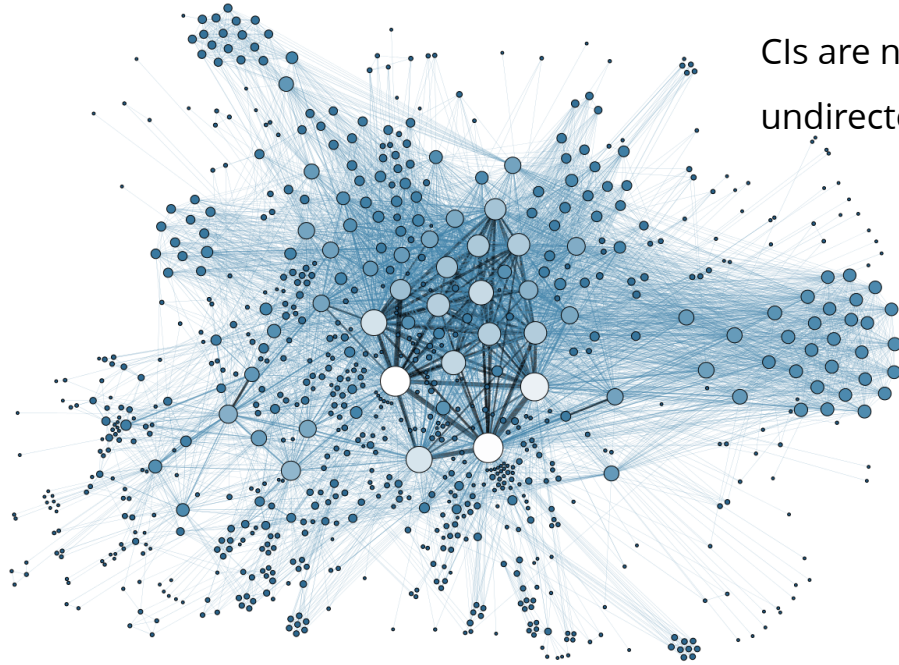


CIIs are naturally expressed using an undirected model

Image: <https://web.stanford.edu/~peastman/statmech/phasetransitions.html>

Motivation

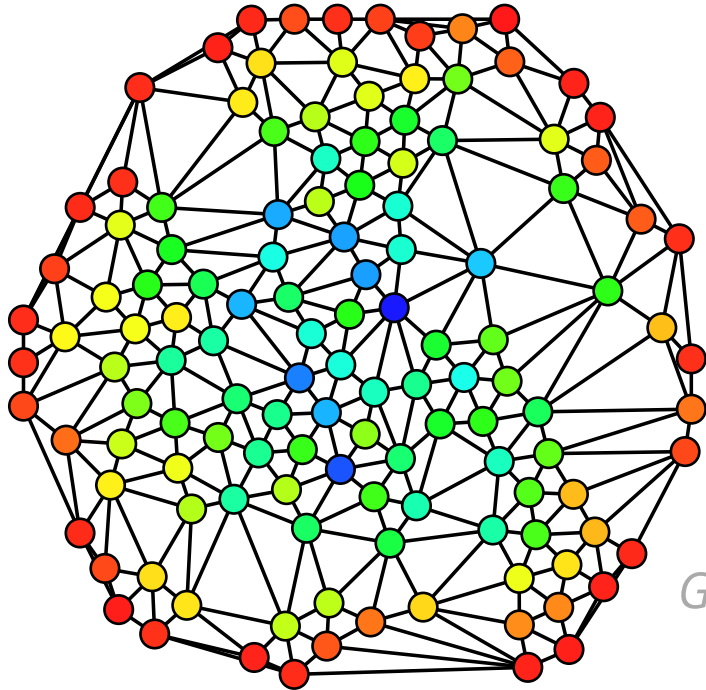
Social sciences



CIs are naturally expressed using an undirected model

Motivation

Combinatorial problems



CIs are naturally expressed using an undirected model

Graph coloring

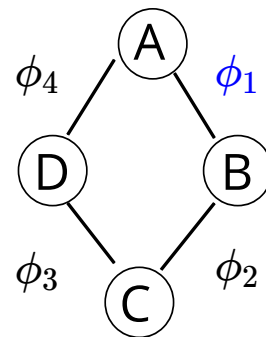
Factorization in Markov networks

$$P(A, B, C, D) = \frac{1}{Z} \phi_1(A, B) \phi_2(B, C) \phi_3(C, D) \phi_4(A, D)$$

$$Z = \sum_{a,b,c,d} \phi_1(a, b) \phi_2(b, c) \phi_3(c, d) \phi_4(a, d)$$

is a **normalization constant** (*partition function*)

$\phi_1 : Val(A, B) \rightarrow [0, +\infty)$ is called a **factor** (*potential*)



MRF: Conditional Independencies

$$P(A, B, C, D) = \underbrace{\left(\frac{1}{Z} \phi_1(A, B) \phi_2(B, C)\right)}_{f(B, A, C)} \underbrace{\phi_3(C, D) \phi_4(A, D)}_{g(D, A, C)}$$

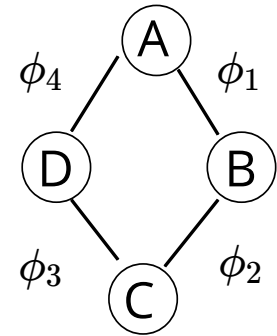
↓ assignment (?)

$$P \models (B \perp D \mid A, C)$$

$$P(A, B, C, D) = \left(\frac{1}{Z} \phi_1(A, B) \phi_2(A, D)\right) \phi_3(C, D) \phi_4(B, C)$$

↓

$$P \models (A \perp C \mid B, D)$$



Product of factors

$$P(A, B, C, D) = \frac{1}{Z} \phi_1(A, B) \phi_2(B, C) \phi_3(C, D) \phi_4(A, D)$$

$$\psi(A, B, C) : Val(A, B, C) \rightarrow \mathfrak{R}^+$$

$$\phi_1 : Val(A, B) \rightarrow \mathfrak{R}^+$$

a^1	b^1	0.5
a^1	b^2	0.8
a^2	b^1	0.1
a^2	b^2	0
a^3	b^1	0.3
a^3	b^2	0.9

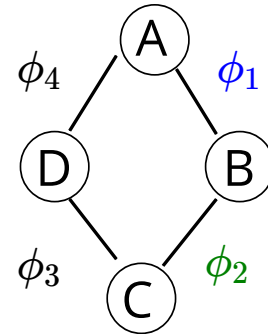
$$\phi_2 : Val(B, C) \rightarrow \mathfrak{R}^+$$

b^1	c^1	0.5
b^1	c^2	0.7
b^2	c^1	0.1
b^2	c^2	0.2



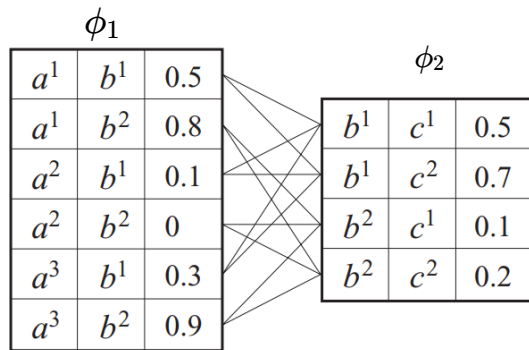
a^1	b^1	c^1	$0.5 \cdot 0.5 = 0.25$
a^1	b^1	c^2	$0.5 \cdot 0.7 = 0.35$
a^1	b^2	c^1	$0.8 \cdot 0.1 = 0.08$
a^1	b^2	c^2	$0.8 \cdot 0.2 = 0.16$
a^2	b^1	c^1	$0.1 \cdot 0.5 = 0.05$
a^2	b^1	c^2	$0.1 \cdot 0.7 = 0.07$
a^2	b^2	c^1	$0 \cdot 0.1 = 0$
a^2	b^2	c^2	$0 \cdot 0.2 = 0$
a^3	b^1	c^1	$0.3 \cdot 0.5 = 0.15$
a^3	b^1	c^2	$0.3 \cdot 0.7 = 0.21$
a^3	b^2	c^1	$0.9 \cdot 0.1 = 0.09$
a^3	b^2	c^2	$0.9 \cdot 0.2 = 0.18$

$Val(A) \times Val(B) \times Val(C)$ similar to a 3D tensor



Q: Do factors represent marginals?

Simplified example: $P(A, B, C) = \frac{1}{Z} \phi_1(A, B) \phi_2(B, C)$



$P(A, B, C) \times Z$

a^1	b^1	c^1	$0.5 \cdot 0.5 = 0.25$
a^1	b^1	c^2	$0.5 \cdot 0.7 = 0.35$
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$$Z = .25 + .35 + \dots = 1.55$$

Marginal probabilities:

$$P(a^1, b^1) = (.25 + .35) / Z \approx .38$$

$$P(a^1, b^2) = (.08 + .16) / Z \approx .15$$

Compare to ϕ_1

$$\phi_1(a^1, b^1) = .5$$

$$\phi_1(a^1, b^2) = .8$$

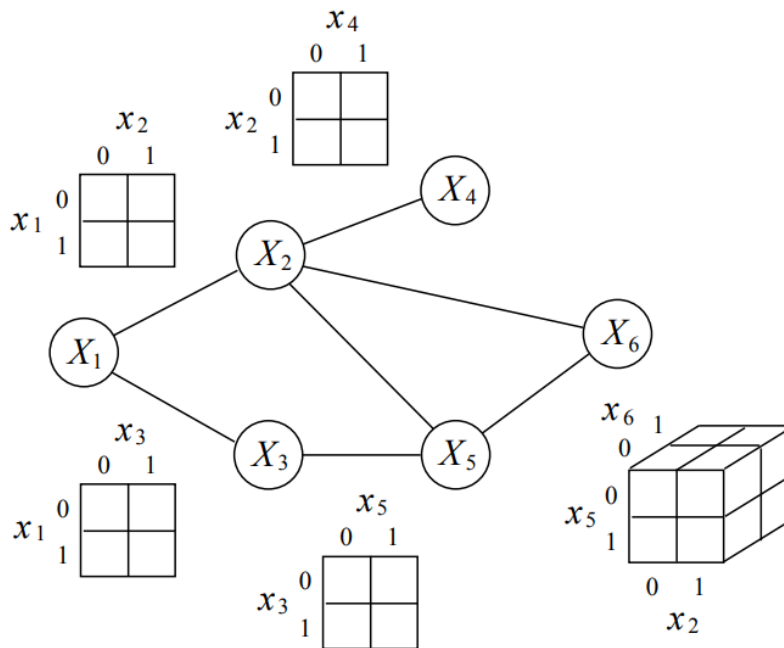
Factorization: general form

\mathbf{P} factorizes over the *cliques*

$$P(\mathbf{X}) = \frac{1}{Z} \prod_k \phi_k(\mathbf{D}_k)$$

Gibbs distribution

Can always convert to factorization over *maximal cliques*



Factorization: general form

\mathbf{P} factorizes over cliques

$$P(\mathbf{X}) = \frac{1}{Z} \prod_k \phi_k(\mathbf{D}_k)$$

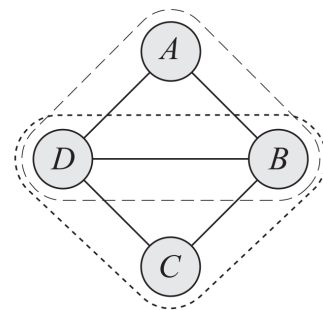
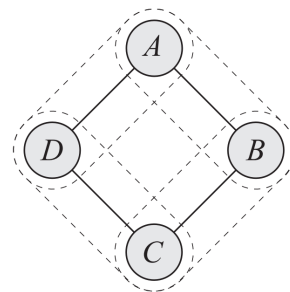
Rewrite as factorization over **maximal cliques**

- original form of \mathbf{P}

$$P(A, B, C, D) = \phi_1(A, B)\phi_2(A, D)\phi_3(B, D)\phi_4(C, D)\phi_5(B, C)$$

- factorized over cliques

$$P(A, B, C, D) = \psi_1(A, B, C)\psi_2(B, C, D)$$



Factorized form: **directed vs undirected**

Markov Networks:

$$P(\mathbf{X}) = \frac{1}{Z} \prod_k \phi_k(\mathbf{D}_k)$$

Bayesian Networks:

$$P(\mathbf{X}) = \prod_k P(X_i | Pa_{X_i})$$

- No *partition function*
- Each factor is a *cond. distribution*
- One factor per variable

Conditioning on the **evidence**

given $P(\mathbf{X}) \propto \prod_k \phi_k(\mathbf{D}_k)$, how to obtain $P(\mathbf{X} | U = u)$?

fix the evidence in the relevant factors $P(\mathbf{X} | U = u) \propto \prod_k \phi_k[U = u]$

$\phi_k(A, B, C)$

a^1	b^1	c^1	$0.5 \cdot 0.5 = 0.25$
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conditioned on $C = c^1$



$\phi_k[C = c]$

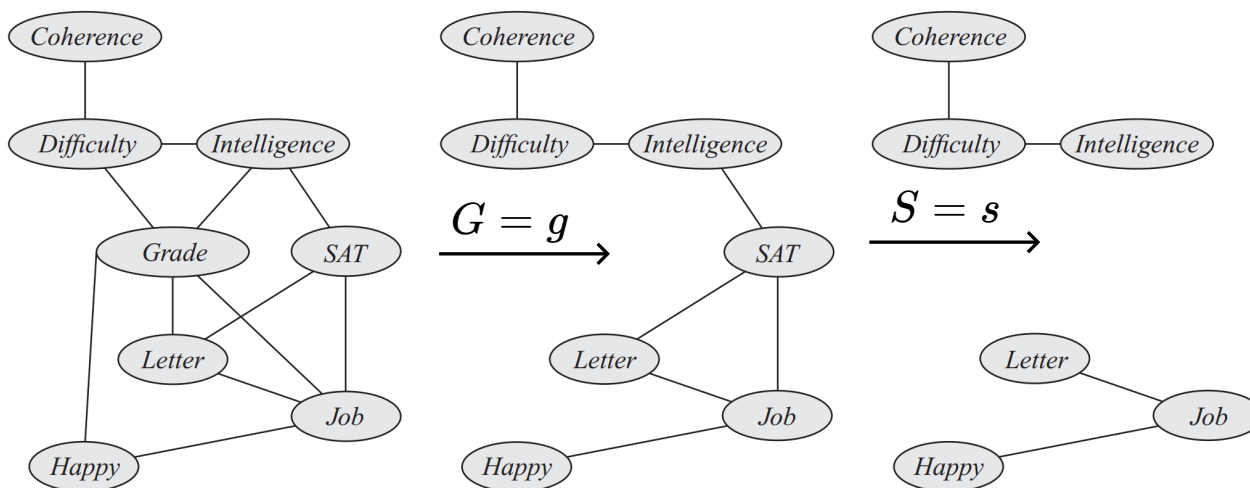
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reduced factor

Conditioning on the **evidence**

effect on the graphical model

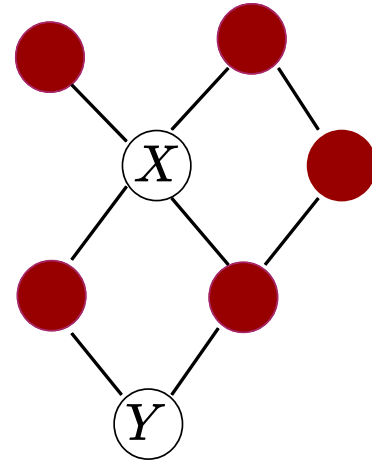
- cannot create new dependencies
- compare this to colliders in **Bayes-nets**



Pairwise conditional independencies

Non-adjacent nodes are independent given everything else

$$X \perp Y \mid \mathcal{X} - \{X, Y\}$$

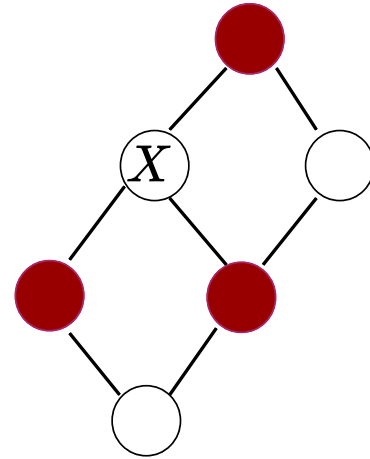


Local conditional Independencies

$MB^{\mathcal{H}}(X)$: **Markov blanket** of node X in graph H

$$X \perp \mathcal{X} - X - MB^{\mathcal{H}}(X) \mid MB^{\mathcal{H}}(X)$$

Given its Markov blanket X is independent of every other variable



Local conditional Independencies

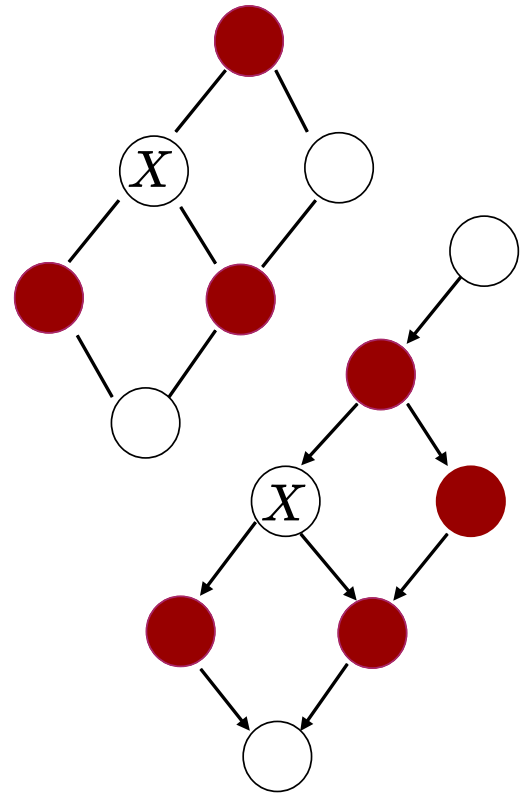
$MB^{\mathcal{H}}(X)$: **Markov blanket** of X in graph H

$$X \perp \mathcal{X} - X - MB^{\mathcal{H}}(X) \mid MB^{\mathcal{H}}$$

$MB^{\mathcal{G}}(X)$: **Markov blanket** of X in DAG G

- Parents
- *Children*
- *Parents of children*

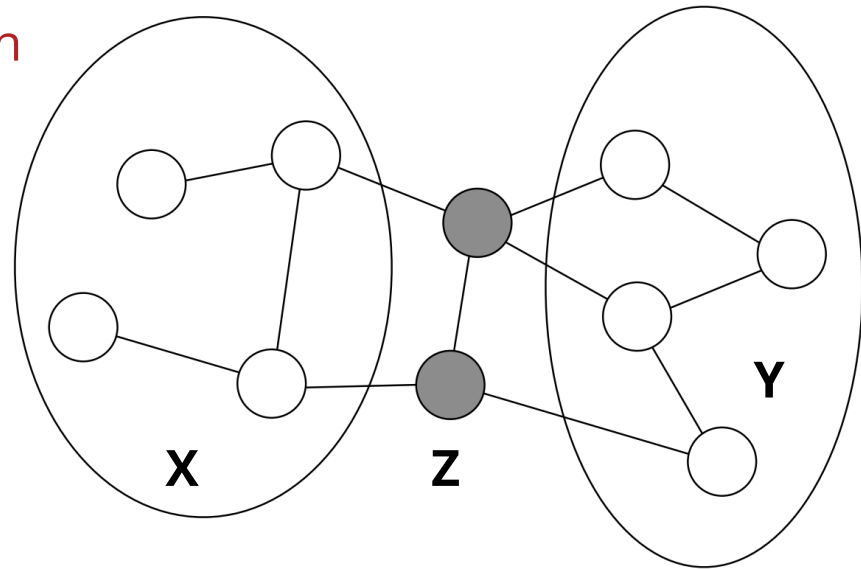
$$X \perp \mathcal{X} - X - MB^{\mathcal{G}}(X) \mid MB^{\mathcal{G}}$$



Global conditional Independencies

$X \perp Y \mid Z$ iff every path between **X** and **Y** is blocked by **Z**

much simpler than **D-separation**



Relationship between the three

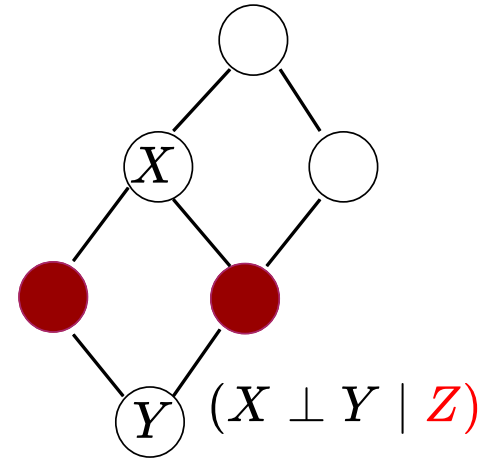
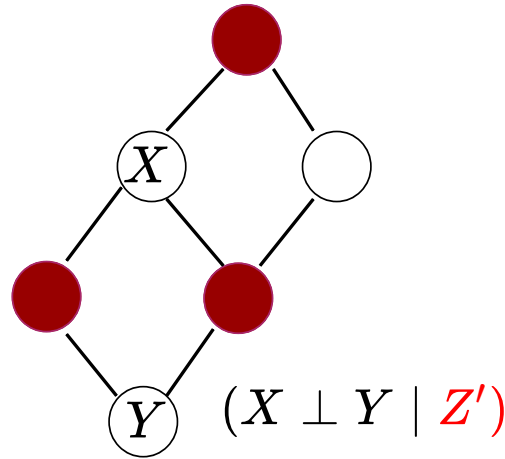
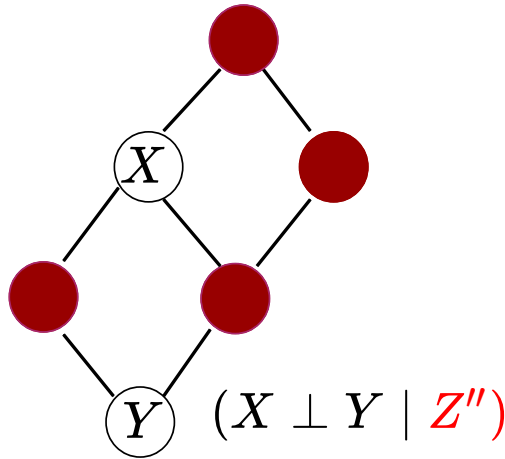
pairwise \mathcal{I}_p



local \mathcal{I}_ℓ



global \mathcal{I}



Relationship between the three

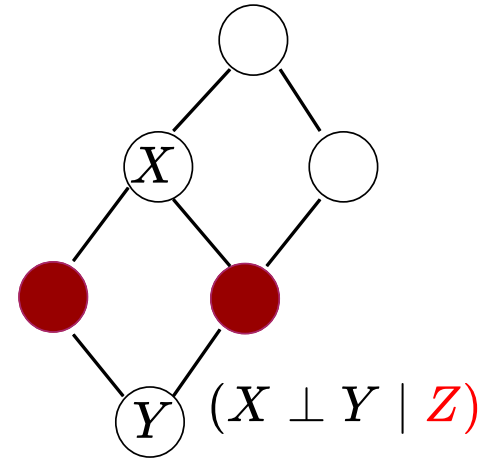
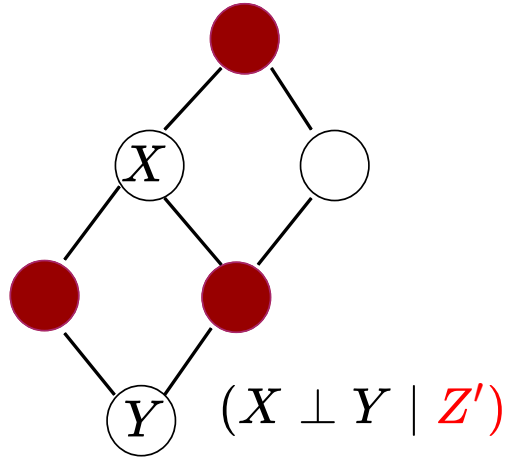
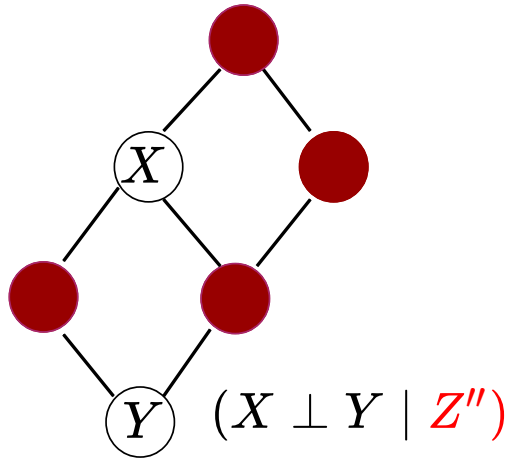
pairwise \mathcal{I}_p



local \mathcal{I}_ℓ



global \mathcal{I}



$P > 0$: pairwise $\mathcal{I}_p \Rightarrow$

local \mathcal{I}_ℓ



global \mathcal{I}

Factorization & independence

Recall this relationship in **Bayesian Networks**:

- **Factorization** according to a DAG
- **Local & global** CIs

Equivalent

Is it similar for **Markov Networks**?

- **Factorization** according to an *undirected graph*
- **Pairwise, local & global** CIs

Equivalent?

(same family of distributions)

Factorization & Independence

Is it similar for **Markov Networks**?

- **Factorization** according to an *undirected graph*
- **Pairwise, local & global** CIs

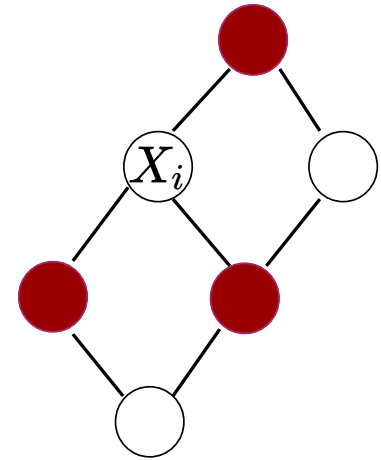


Short answer:

- for positive distributions they are equivalent

Factorization \Rightarrow CI

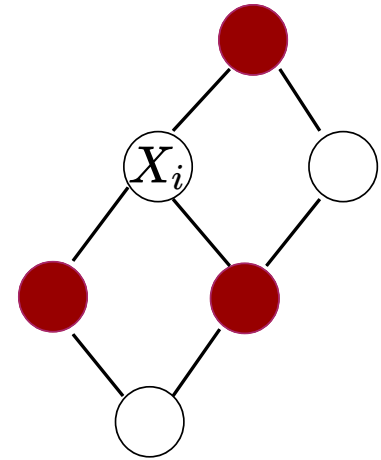
given $P(\mathbf{X}) \propto \prod_k \phi_k(\mathbf{C}_k)$ does **local** CI hold?



Factorization \Rightarrow CI

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proof



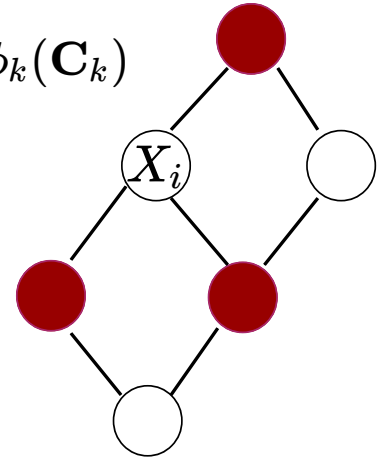
Factorization \Rightarrow CI

given $P(\mathbf{X}) \propto \prod_k \phi_k(\mathbf{C}_k)$ does **local** CI hold?

proof

$$\begin{aligned} P(\mathbf{X}) &\propto \prod_k \phi_k(\mathbf{C}_k) = \prod_{\mathbf{C}_k \in MB(X_i)} \phi_k(\mathbf{C}_k) \prod_{\mathbf{C}_k \notin MB(X_i)} \phi_k(\mathbf{C}_k) \\ &= f(X_i, MB(X_i)) g(\mathcal{X} - X_i) \quad \Rightarrow \end{aligned}$$

$$X_i \perp \mathcal{X} - MB^{\mathcal{H}}(X_i) - X_i \mid MB^{\mathcal{H}}(X_i)$$



CI \Rightarrow factorization

Hammersely-Clifford theorem:

If P is *strictly positive* satisfying CI $\mathcal{I}(\mathcal{H})$
then P factorizes over \mathcal{H}

proof

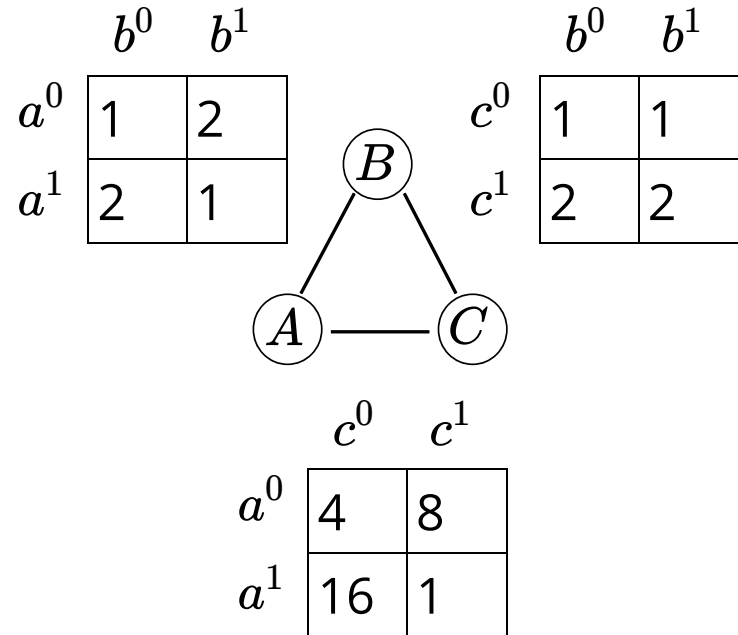
needs canonical parametrization



Parametrization: **redundancy**

is this representation of P unique?

$$P(A, B, C) \propto \phi_1(A, B)\phi_2(B, C)\phi_3(C, A)$$

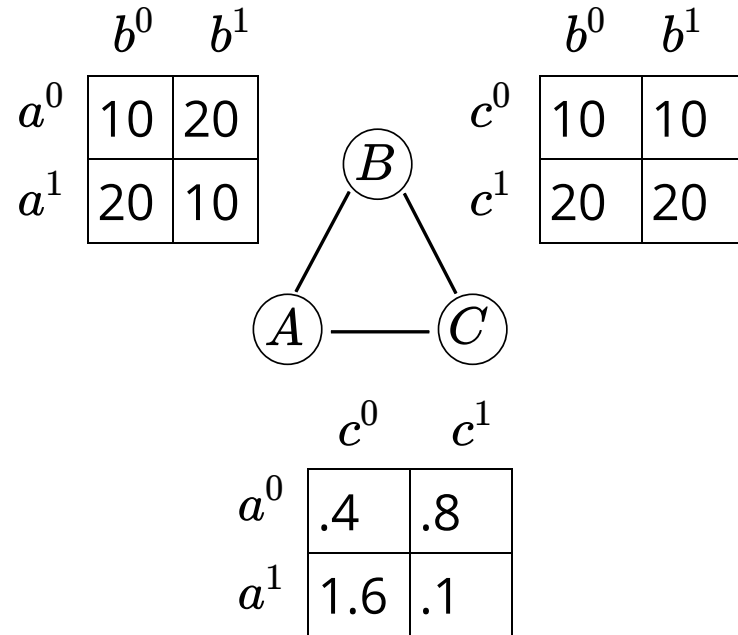


Parametrization: **redundancy**

is this representation of P unique?

$$P(A, B, C) = \frac{1}{Z} \phi_1(A, B) \phi_2(B, C) \phi_3(C, A)$$

multiplying all factors by a constant
only affects **Z**



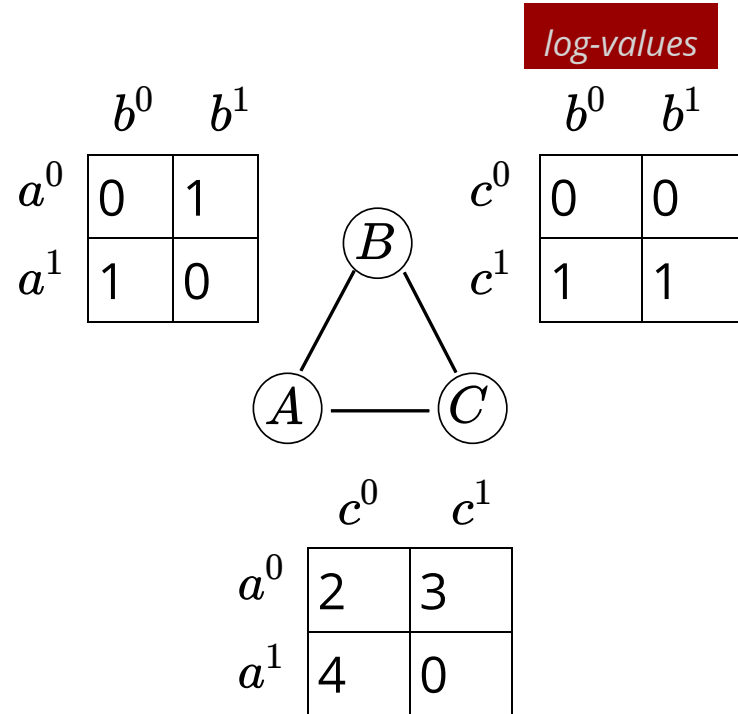
Parametrization: **redundancy**

is this representation of P unique?

$$P(A, B, C) = \frac{1}{Z} \phi_1(A, B) \phi_2(B, C) \phi_3(C, A)$$

use the logarithmic form

$$P(A, B, C) = \frac{1}{Z} 2^{(\psi_1(A,B) + \psi_2(B,C) + \psi_3(C,A))}$$



Parametrization: **redundancy**

Is this representation of P unique?

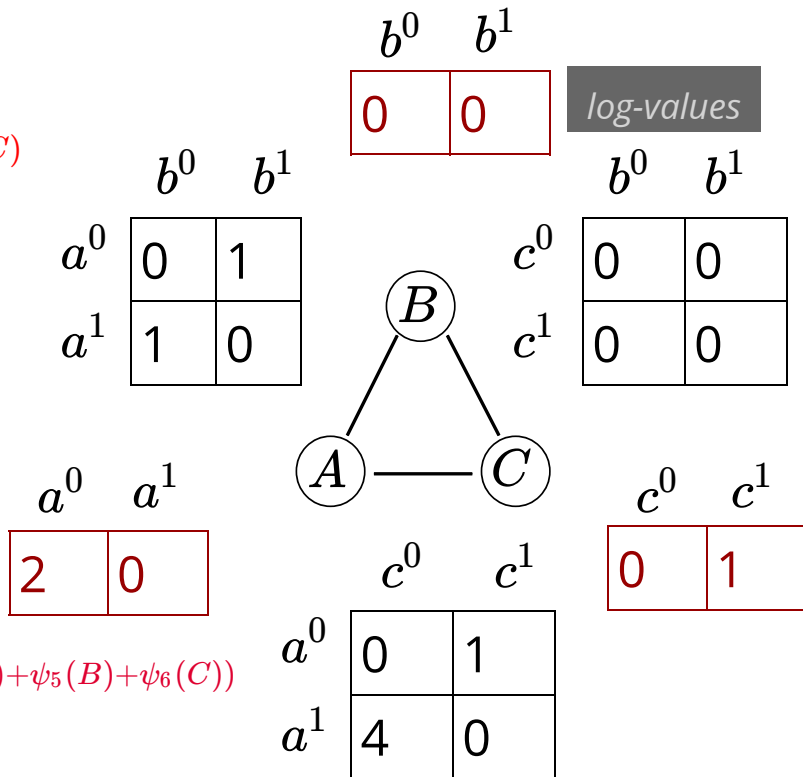
$$P(A, B, C) = \frac{1}{Z} \phi_1(A, B) \phi_2(B, C) \phi_3(C, A) \phi_4(B) \phi_5(A) \phi_6(C)$$

use the logarithmic form

$$P(A, B, C) = \frac{1}{Z} 2^{(\psi_1(A, B) + \psi_2(B, C) + \psi_3(C, A))}$$

simplify using local potentials

$$P(A, B, C) = \frac{1}{Z} 2^{(\psi_1(A, B) + \psi_2(B, C) + \psi_3(C, A) + \psi_4(A) + \psi_5(B) + \psi_6(C))}$$



Parametrization: **redundancy**

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$$P(A, B, C) = \frac{1}{Z} \phi_1(A, B) \phi_2(B, C) \phi_3(C, A) \phi_5(A) \phi_6(C)$$

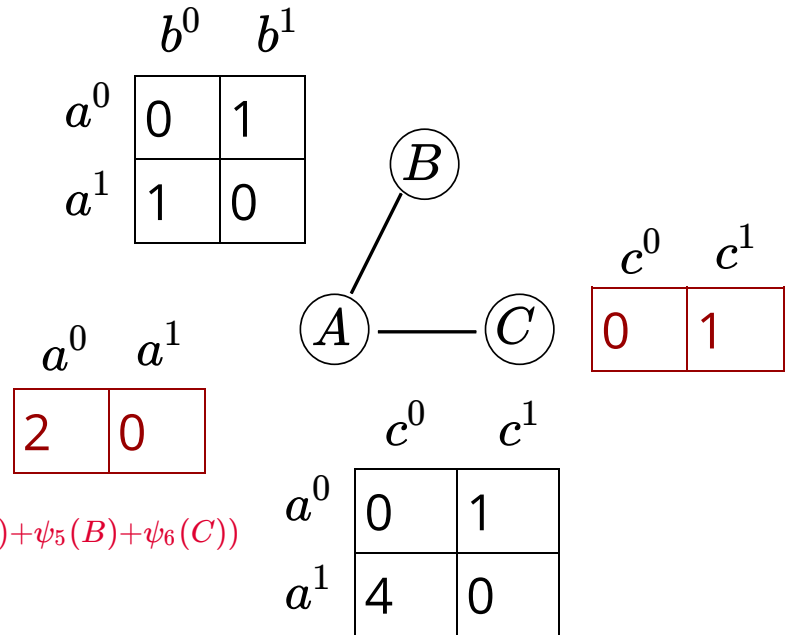
log-values

use the logarithmic form

$$P(A, B, C) = \frac{1}{Z} 2^{(\psi_1(A,B) + \psi_2(B,C) + \psi_3(C,A))}$$

simplify using local potentials

$$P(A, B, C) = \frac{1}{Z} 2^{(\psi_1(A,B) + \psi_2(B,C) + \psi_3(C,A) + \psi_4(A) + \psi_5(B) + \psi_6(C))}$$



Parametrization: example (Ising model)

Ising model: $Val(X_i) = \{-1, +1\}$ $p(\mathbf{x}) = \frac{1}{Z(t)} \exp\left(-\frac{1}{t}\left(\sum_i h_i x_i + \frac{1}{2} \sum_{i,j \in \mathcal{E}} x_i J_{ij} x_j\right)\right)$

can represent all positive, pairwise Markov networks over the binary domain

		interactions		local field	
		-1	+1	-1	+1
-1	J	-J			
+1	-J	J		-h	h

log-values

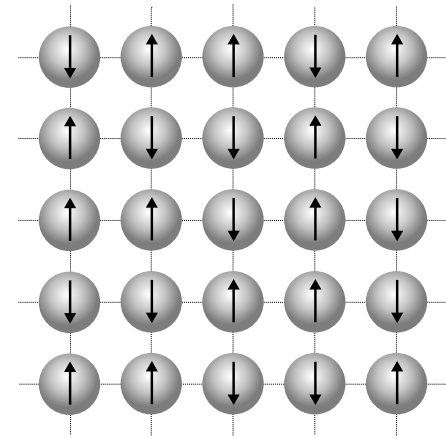


Image: <https://web.stanford.edu/~peastman/statmech/phasetransitions.html>

Parametrization: example (Boltzmann machine)

Boltzmann machine: $Val(X_i) = \{0, 1\}$

$$p(\mathbf{x}) = \frac{1}{Z} \exp \left(- \sum_i b_i x_i - \frac{1}{2} \sum_{i,j \in \mathcal{E}} x_i W_{ij} x_j \right)$$

interaction weights		local bias	
	-1	+1	
-1	0	0	
+1	0	J	
		-1	+1
		0	h

log-values

Parametrization: **log-linear model**

for a positive distribution:

$$P(\mathbf{X}) \propto \prod_k \phi_k(\mathbf{D}_k) = \exp\left(-\sum_k \underbrace{\psi_k(\mathbf{D}_k)}_{\text{energy}} - \log(\phi_k(\mathbf{D}_k))\right)$$

Parametrization: **log-linear model**

for a positive distribution:

$$P(\mathbf{X}) \propto \prod_k \phi_k(\mathbf{D}_k) = \exp\left(- \sum_k \underbrace{\psi_k(\mathbf{D}_k)}_{\text{energy}} - \log(\phi_k(\mathbf{D}_k))\right)$$

linearly parameterize it:

$$P_w(\mathbf{X}) \propto \exp\left(- \sum_k w_k \underbrace{f_k(\mathbf{D}_k)}_{\text{feature/sufficient statistics}}\right)$$

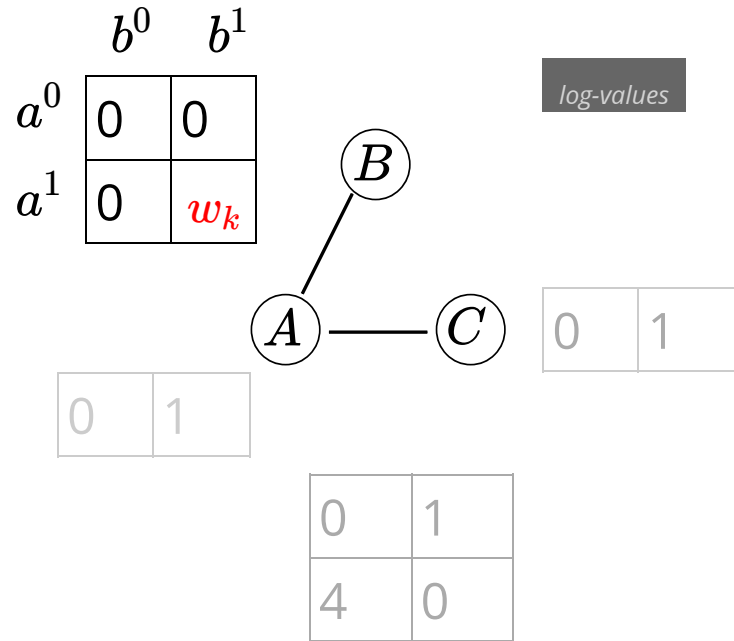
Parametrization: **log-linear model**

features in **discrete** distributions:

$$P_w(\mathbf{X}) \propto \exp\left(-\sum_k w_k f_k(\mathbf{D}_k)\right)$$



$$f_{1,1}(A, B) = \mathbb{I}(A = a^1, B = b^1)$$



Parametrization: log-linear model

$$P_w(\mathbf{X}) \propto \exp\left(-\sum_k w_k f_k(\mathbf{D}_k)\right)$$

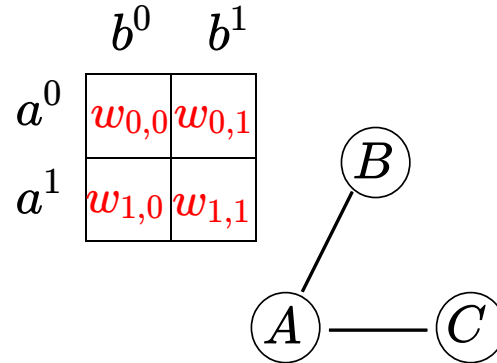


$$f_{1,1}(A, B) = \mathbb{I}(A = a^1, B = b^1)$$

$$f_{0,1}(A, B) = \mathbb{I}(A = a^0, B = b^1)$$

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log-values

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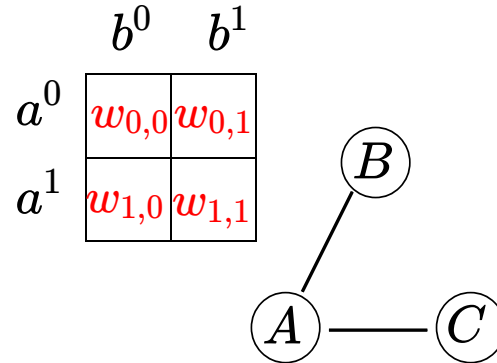


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Overparameterized model: $\{w_k\} \rightarrow P_w$ is not one-to-one

Parametrization: **log-linear model**

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Redundant \equiv linearly dependent features



$$\sum_k \alpha_k f_k(\mathbf{D}) = \alpha \quad \forall \mathbf{D}$$

$$P_w(\mathbf{X}) \propto \exp\left(-\sum_k w_k f_k(\mathbf{D}_k)\right) \propto \exp\left(-\sum_k (w_k + \alpha_k) f_k(\mathbf{D}_k)\right) \propto P_{w+\alpha}(\mathbf{X})$$

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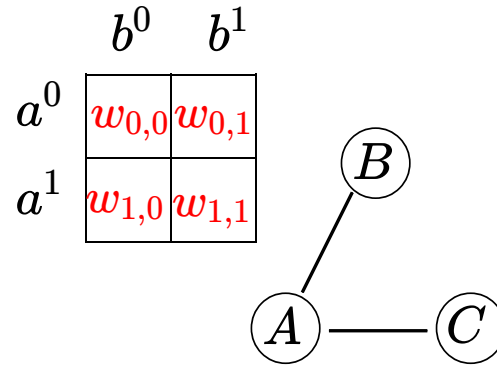


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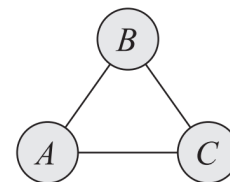
Linear dependency of features:

$$f_{0,0}(A, B) + f_{1,0}(A, B) + f_{0,1}(A, B) + f_{1,1}(A, B) = 1$$

Parametrization: **factor-graph**

Markov network representation:

- ✓ • identifies CI
- defines the factorized form
- ☹️ ■ is not fine-grained enough



$$P(A, B, C) = \phi_1(A, B)\phi_2(B, C)\phi_3(C, A) \quad ?$$

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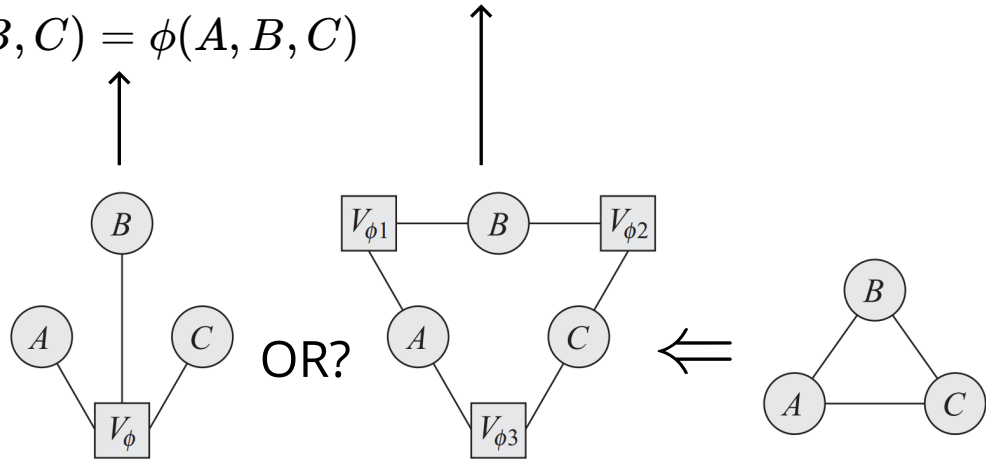
Parametrization: **factor-graph**

use a bipartite structure:

- factors (square)
- variables (circle)

$$P(A, B, C) = \phi_1(A, B)\phi_2(B, C)\phi_3(C, A)$$

$$P(A, B, C) = \phi(A, B, C)$$



Summary

- similar to directed models:
 - **factorization** of the probability over cliques
 - set of **conditional independencies**
 - (pariwise, local, global)

$P > 0 \Rightarrow$
same family of dists.

Summary

- similar to directed models:
 - **factorization** of the probability over cliques
 - set of **conditional independencies**
 - (pariwise, local, global)
- **parametrization**
 - **redundancy** (same dist. different params/factors)
 - **log-linear model**
 - **factor-graph** (finer-grained specification of the factors)

$P > 0 \Rightarrow$
same family of dists.

Bonus Slides

Parametrization: **canonical form**

reparameterize a given Gibbs dist.

$$P(\mathbf{X}) \propto \exp\left(-\sum_k \psi_k(\mathbf{D}_k)\right)$$

such that low order interactions are automatically moved to smaller cliques

need to fixed an assignment $\xi^* = (x_1^*, \dots, x_n^*)$ e.g., $\xi^* = (0, \dots, 0)$

Mobius inversion lemma

For two functions $f, g : 2^{\mathcal{X}} \rightarrow \mathfrak{R}$ defined over all subsets $\mathcal{Z} \subseteq \mathcal{X}$ the following are equivalent:

$$\forall \mathcal{Z} \subseteq \mathcal{X} \quad f(\mathcal{Z}) = \sum_{\mathcal{S} \subseteq \mathcal{Z}} g(\mathcal{S})$$

$$\forall \mathcal{Z} \subseteq \mathcal{X} \quad g(\mathcal{Z}) = \sum_{\mathcal{S} \subseteq \mathcal{Z}} (-1)^{|\mathcal{Z}-\mathcal{S}|} f(\mathcal{S})$$

Mobius inversion

Parametrization: **canonical form**

Given a *fixed an assignment* $\xi^* = (x_1^*, \dots, x_n^*)$ e.g., $\xi^* = (0, \dots, 0)$

$f(x_Z) \triangleq \log P(x_Z, \xi_{-Z}^*)$ is defined for all $Z \subseteq \{1, \dots, N\}$

$$f(x) = \log P(x)$$

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Its *Mobius inversion*: $g(x_Z) = - \sum_{S \subseteq Z} (-1)^{|Z-S|} \log P(x_S, \xi_{-S}^*)$

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Problem: one factor per subset of nodes

Proof of Hammersly-Clifford theorem:

When Z is not a clique $\psi_Z(x_Z)$ becomes zero.

Proof of the **Hammersley-Clifford**

Recap:

- fix an assignment
- define factors over each subset of nodes as:

$$\psi(x_Z) = \sum_{S \subseteq Z} (-1)^{|Z-S|} \log P(x_S, \xi_{-S}^*)$$

- if Z is not a clique in \mathcal{H} then $\exists_{i,j \in Z} X_i \perp X_j \mid \mathbf{X} - \{X_i, X_j\}$
 - we can show that $\psi_Z(x_Z) = 0 \quad \forall x_Z$