Probabilistic Graphical Models

Undirected Graphical Models

Probabilistic Graphical Models

Directed graphical models

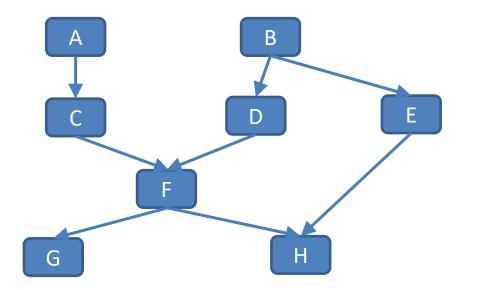
- Bayes Nets
- Conditional dependence

Undirected graphical models

- Markov random fields (MRFs)
- Factor graphs

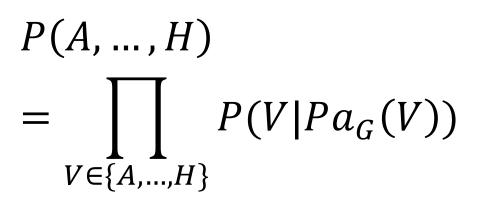
From Markov Condition to Factorization

A Directed Acyclic Graph



A joint Probability Distribution

P(A, B, C, D, E, F, G, H)



Markov Condition:

Every variable is independent of its nondescendants given its parents (in the graph)

Summary

BN: DAG + Distribution

The distribution factorizes according to the graph based on the Markov condition: Every variable is independent from its non-descendants (in the graph) based on its parents (in the graph)

D-separation allows us to read the independencies from the graph. sound (dsep->ind) and complete (dcon->dep in some distribution that factorizes according to G)

If $I(G) \subseteq I(P)$ then G is an I-Map for P

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Summary

BN: DAG + Distribution

```
If I(G) \subseteq I(P) then G is an I-Map for P
```

If *G* is an I-Map for *P* and every chat stems from removing an edge from *G* is not an I-Map for *P*, *G* is minimal I-Map for *P*

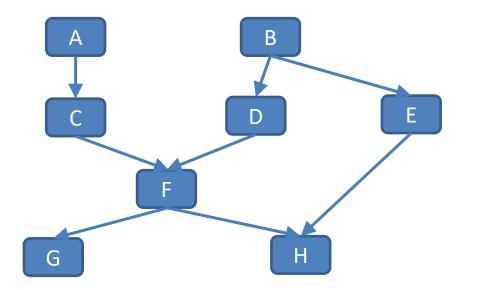
If I(G) = I(P) then G is a perfect map for P

If I(G) = I(G'), G and G' are Markov Equivalent (I-Equivalent)

The Markov Boundary of *Y* is the set of Parents, Children and Spouses of *G*

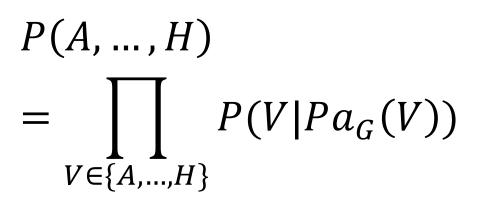
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Example: Misconception

Four students who get together in pairs to work on homeworks.

Only the following pairs meet:

Alice and Bob; Bob and Charles; Charles and Debbie; Debbie and Alice.

(Alice and Charles just can't stand each other, and Bob and Debbie had a relationship that ended badly.) Probability of having misunderstood something in the class

Example: Misconception

Four students who get together in pairs to work on homeworks.

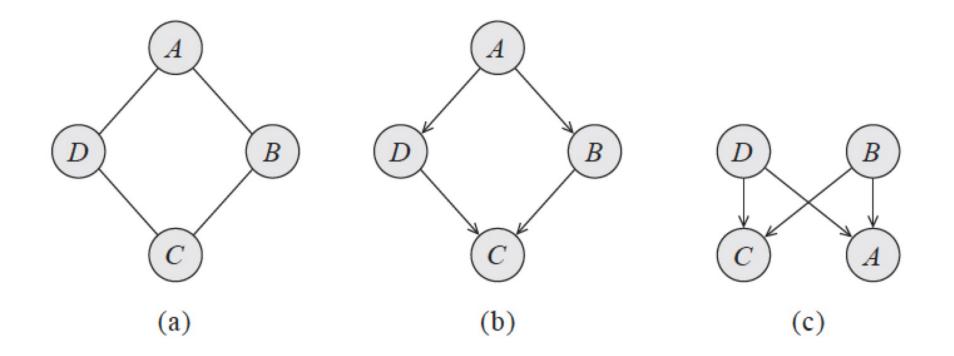
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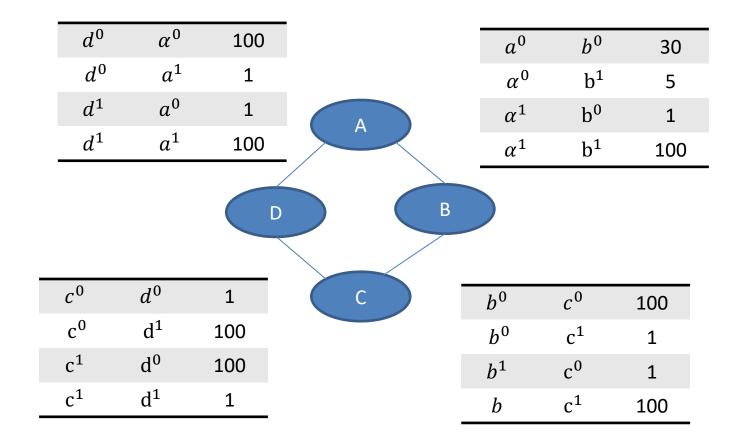
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Ind(A, C|B,D) Ind(B, D|A, C)

Example: Misconception



Pairwise Markov Networks



Factors

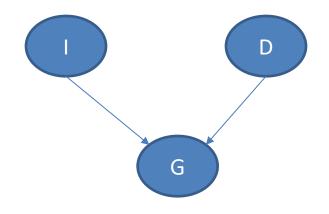
A factor $\phi(X_{1, \dots, X_{k}})$ $\phi: \operatorname{Val}(X_{1}, \dots, X_{k}) \to \mathbb{R}$ Scope = $\{X_{1, \dots, X_{k}}\}$

Fundamental building block for defining distributions in high-dimensional spaces

Set of basic operations for manipulating these probability distributions

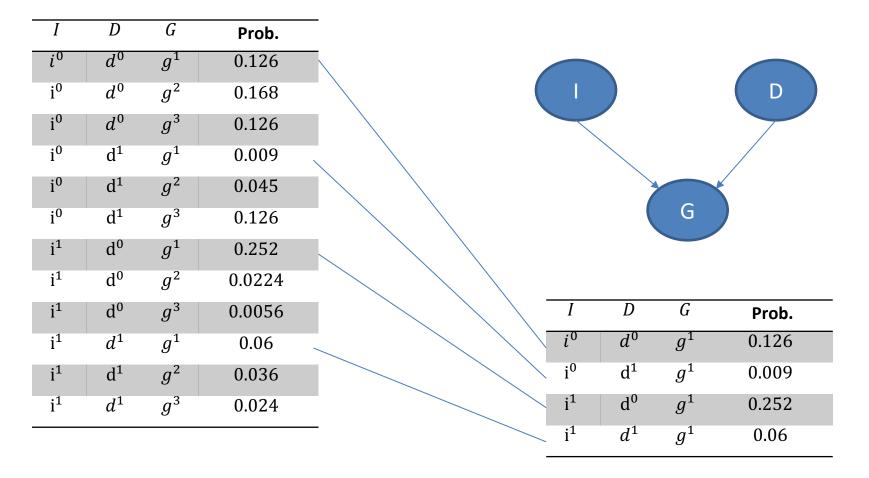
Example: JPD

| Ι | D | G | Prob. |
|----------------|----------------|---------|--------|
| i ⁰ | d^0 | g^{1} | 0.126 |
| i ⁰ | d^0 | g^2 | 0.168 |
| i ⁰ | d^0 | g^3 | 0.126 |
| i ⁰ | d ¹ | g^1 | 0.009 |
| i ⁰ | d1 | g^2 | 0.045 |
| i ⁰ | d ¹ | g^3 | 0.126 |
| i ¹ | d ⁰ | g^1 | 0.252 |
| i ¹ | d ⁰ | g^2 | 0.0224 |
| i ¹ | d ⁰ | g^3 | 0.0056 |
| i ¹ | d^1 | g^1 | 0.06 |
| i ¹ | d ¹ | g^2 | 0.036 |
| i ¹ | d^1 | g^3 | 0.024 |



Scope = $\{I, D, G\}$

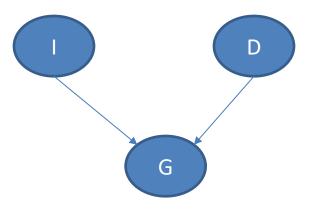
Unnormalized measure



Scope = $\{I, D\}$

Conditional Distribution

| Ι | D | G | Prob. |
|----------------|----------------|-------|--------|
| i ⁰ | d^0 | g^1 | 0.126 |
| i ⁰ | d^0 | g^2 | 0.168 |
| i ⁰ | d^0 | g^3 | 0.126 |
| i ⁰ | d^1 | g^1 | 0.009 |
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| i ¹ | d ⁰ | g^1 | 0.252 |
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| i ¹ | d^1 | g^1 | 0.06 |
| i ¹ | d ¹ | g^2 | 0.036 |
| i ¹ | d^1 | g^3 | 0.024 |



| | g^1 | g^2 | g^3 |
|---------------------------------|-------|-------|-------|
| i ⁰ , d ⁰ | 0.3 | 0.4 | 0.3 |
| i ⁰ , d ¹ | 0.05 | 0.25 | 0.7 |
| i ¹ , d ⁰ | 0.9 | 0.08 | 0.02 |
| i ¹ , d ¹ | 0.5 | 0.3 | 0.2 |

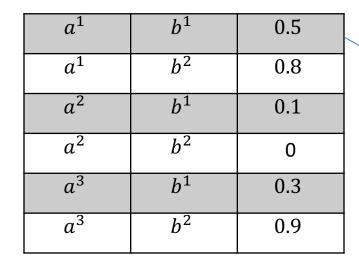
Scope = $\{I, D, G\}$

General Factors

| D | А | $\phi(D, A)$ |
|-------|------------|--------------|
| d^0 | α^0 | 100 |
| d^0 | a^1 | 1 |
| d^1 | a^0 | 1 |
| d^1 | a^1 | 100 |

Scope = $\{D, A\}$

Factor Product



| / | b^1 | <i>c</i> ¹ | 0.5 |
|---|-----------------------|-----------------------|-----|
| | b^1 | <i>c</i> ² | 0.7 |
| | <i>b</i> ² | <i>c</i> ¹ | 0.1 |
| | <i>b</i> ² | <i>c</i> ² | 0.2 |

Let *X*, *Y*, and *Z* be three disjoint sets of variables, and let $\phi_1(X, Y)$ and $\phi_2(Y, Z)$ be two factors. We define the factor product $\phi_1 \times \phi_2$ to be a factor ψ : Val $(X, Y, Z) \mapsto \mathbb{R}$ as follows:

 $\psi(X, Y, Z) = \phi_1(X, Y) \cdot \phi_2(Y, Z)$

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

Factor Marginalization

| a ¹ | b^1 | <i>C</i> ¹ | $0.5 \cdot 0.5 = 0.25$ |
|-----------------------|-----------------------|-----------------------|------------------------|
| a ¹ | b^1 | <i>c</i> ² | $0.5 \cdot 0.7 = 0.35$ |
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$$\phi(a^1,c^1) = \sum_b \phi(a^1,c^1,b)$$

| a ¹ | c ¹ | 033 |
|-----------------------|-----------------------|------|
| <i>a</i> ¹ | <i>c</i> ² | 0.51 |
| a^2 | <i>c</i> ¹ | 0.05 |
| a ² | <i>c</i> ² | 0.07 |
| a ³ | <i>c</i> ¹ | 0.24 |
| a ³ | <i>c</i> ² | 0.39 |

Let *X* be a set of variables, and $Y \notin X$ a variable. Let $\phi(X, Y)$ be a factor. We define the factor marginalization of *Y* in ϕ , denoted $\sum_{Y} \phi$, to be a factor ψ over *X* such that:

$$\psi(\mathbf{X}) = \sum_{\mathbf{Y}} \phi(\mathbf{X}, \mathbf{Y})$$

This operation is also called summing out of *Y* in ψ .

Factor Reduction

| <i>a</i> ¹ | b^1 | C ¹ | $0.5 \cdot 0.5 = 0.25$ |
|-----------------------|-----------------------|-----------------------|------------------------|
| <i>a</i> ¹ | b^1 | <i>c</i> ² | $0.5 \cdot 0.7 = 0.35$ |
| <i>a</i> ¹ | <i>b</i> ² | <i>C</i> ¹ | $0.8 \cdot 0.1 = 0.08$ |
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| <i>a</i> ² | <i>b</i> ¹ | <i>C</i> ¹ | $0.1 \cdot 0.5 = 0.05$ |
| <i>a</i> ² | b^1 | <i>c</i> ² | $0.1 \cdot 0.7 = 0.07$ |
| <i>a</i> ² | <i>b</i> ² | C ¹ | $0 \cdot 0.1 = 0$ |
| <i>a</i> ² | <i>b</i> ² | <i>c</i> ² | $0 \cdot 0.2 = 0$ |
| <i>a</i> ³ | b^1 | C ¹ | $0.3 \cdot 0.5 = 0.15$ |
| <i>a</i> ³ | b^1 | <i>c</i> ² | $0.3 \cdot 0.7 = 0.21$ |
| <i>a</i> ³ | <i>b</i> ² | <i>C</i> ¹ | $0.9 \cdot 0.1 = 0.09$ |
| <i>a</i> ³ | <i>b</i> ² | <i>c</i> ² | $0.9 \cdot 0.2 = 0.18$ |

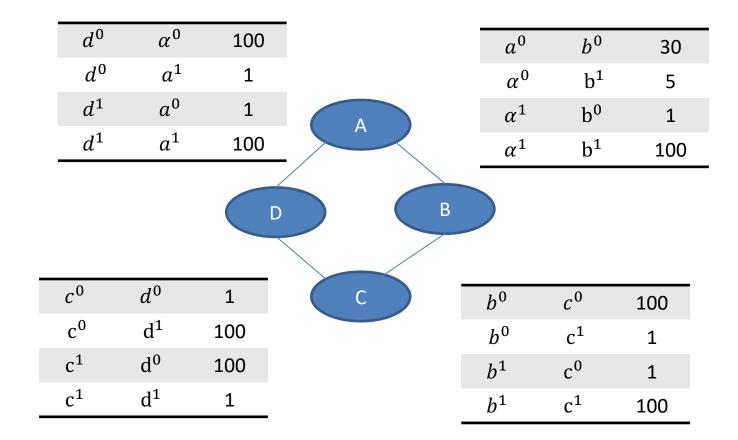
| <i>a</i> ¹ | b^1 | C ¹ | 0.25 |
|-----------------------|-----------------------|-----------------------|------|
| <i>a</i> ¹ | <i>b</i> ² | <i>c</i> ¹ | 0.08 |
| a ² | b^1 | <i>C</i> ¹ | 0.05 |
| <i>a</i> ² | <i>b</i> ² | <i>c</i> ¹ | 0 |
| <i>a</i> ³ | b^1 | C ¹ | 0.15 |
| a^3 | <i>b</i> ² | c^1 | 0.09 |

Let $\phi(Y)$ be a factor, and U = u an assignment for $U \subseteq Y$. We define the reduction of the factor ϕ to the context U = u, denoted $\phi[U = u]$ (and abbreviated $\phi[u]$), to be a factor over scope Y' = Y - U, such that

 $\phi[\boldsymbol{u}](\boldsymbol{y}') = \phi(\boldsymbol{y}', \boldsymbol{u})$

For $U \not\subset Y$, we define $\phi[u]$ to be $\phi[U' = u']$, where $U' = U \cap Y$, and $u' = u \langle U' \rangle$, where $u \langle U' \rangle$ denotes the assignment in u to the variables in U'.

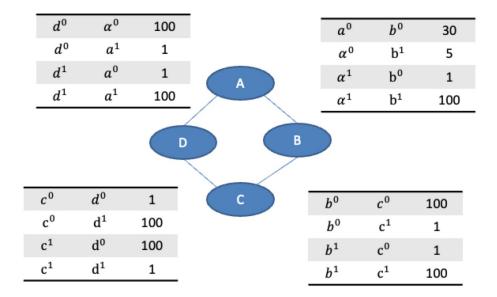
Pairwise Markov Networks



Pairwise Markov Networks

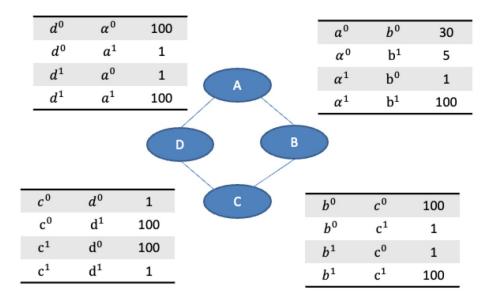
| | Assigr | Unnomalized | | |
|-----------------------|-----------------------|-----------------------|-----------------------|---------|
| <i>a</i> ⁰ | <i>b</i> ⁰ | <i>c</i> ⁰ | d^0 | 300000 |
| <i>a</i> ⁰ | <i>b</i> ⁰ | <i>c</i> ⁰ | d^1 | 300000 |
| <i>a</i> ⁰ | <i>b</i> ⁰ | <i>c</i> ¹ | d^0 | 300000 |
| <i>a</i> ⁰ | <i>b</i> ⁰ | <i>c</i> ¹ | d^1 | 30 |
| <i>a</i> ⁰ | <i>b</i> ¹ | <i>c</i> ⁰ | d^0 | 500 |
| <i>a</i> ⁰ | <i>b</i> ¹ | <i>c</i> ⁰ | d^1 | 500 |
| <i>a</i> ⁰ | <i>b</i> ¹ | <i>c</i> ¹ | d^0 | 5000000 |
| a ⁰ | <i>b</i> ¹ | <i>c</i> ¹ | d^1 | 500 |
| <i>a</i> ¹ | <i>b</i> ⁰ | <i>c</i> ⁰ | d^0 | 100 |
| <i>a</i> ¹ | <i>b</i> ⁰ | <i>c</i> ⁰ | d^1 | 1000000 |
| <i>a</i> ¹ | <i>b</i> ⁰ | <i>c</i> ¹ | d^0 | 100 |
| <i>a</i> ¹ | <i>b</i> ⁰ | <i>c</i> ¹ | d^1 | 100 |
| <i>a</i> ¹ | <i>b</i> ¹ | <i>c</i> ⁰ | d^0 | 10 |
| <i>a</i> ¹ | <i>b</i> ¹ | <i>c</i> ⁰ | d^1 | 100000 |
| <i>a</i> ¹ | <i>b</i> ¹ | <i>c</i> ¹ | d^0 | 100000 |
| <i>a</i> ¹ | <i>b</i> ¹ | <i>c</i> ¹ | <i>d</i> ¹ | 100000 |

 $\tilde{P}(A, B, C, D) = \phi(A, B)\phi(B, C)\phi(C, D)\phi(D, A)$ $P(A, B, C, D) = \frac{1}{Z}\phi(A, B)\phi(B, C)\phi(C, D)\phi(D, A)$



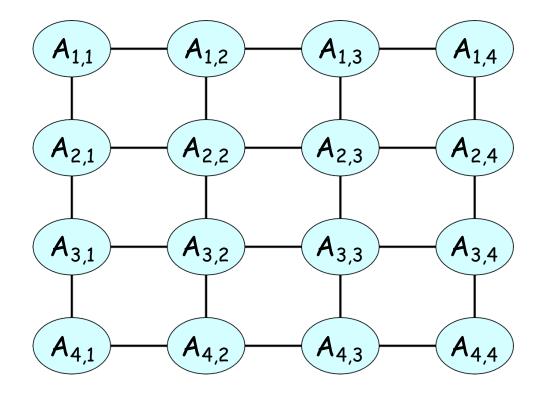
Eyeballing probabilities is hard

| <i>a</i> ⁰ | b^0 | 0.13 |
|-----------------------|----------------|------|
| α^0 | b^1 | 0.69 |
| α^1 | b ⁰ | 0.14 |
| α^1 | b ¹ | 0.04 |

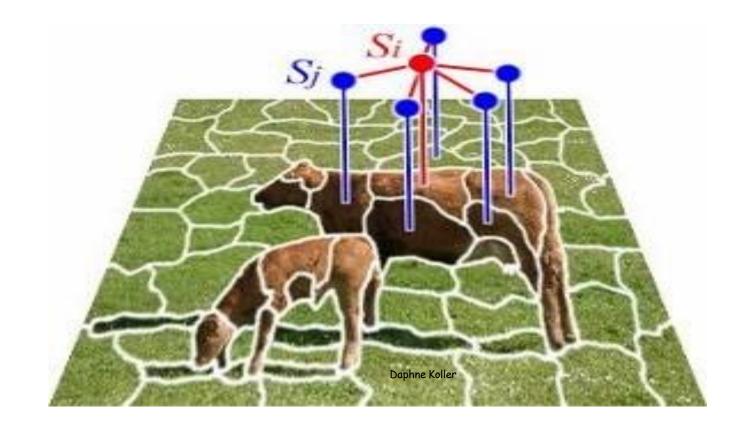


Pairwise Markov Networks

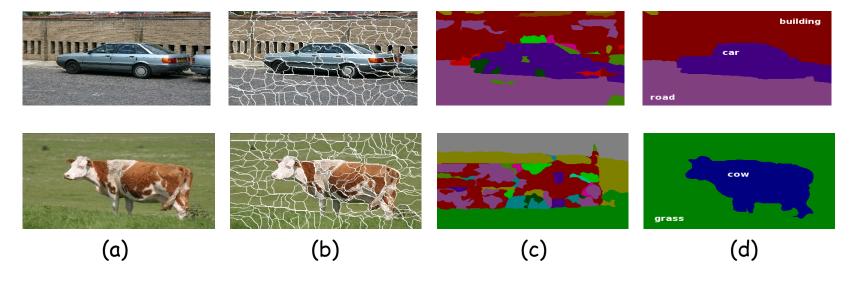
A pairwise Markov network is an undirected graph whose nodes are $X_1, ..., X_n$ and each edge $X_i - X_j$ is associated with a factor (potential) $\phi_{ij} (X_i - X_j)$



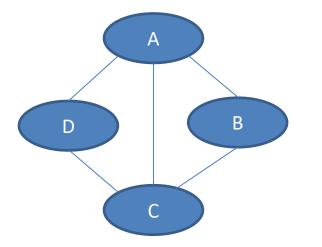
Example: Image Segmentation



Example: Image Segmentation



Daphne Koller

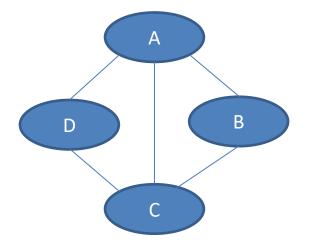


Consider a fully connected pairwise Markov network over $X_1, ..., X_n$ where each X_i has d values. How many parameters does the network have?

a. $O(d^n)$

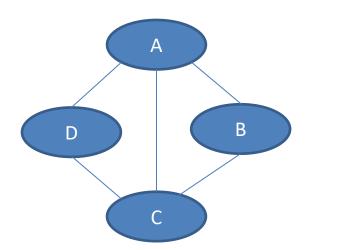
- b. $O(n^d)$
- *c.* $O(n^2d^2)$

d. 0(*nd*)



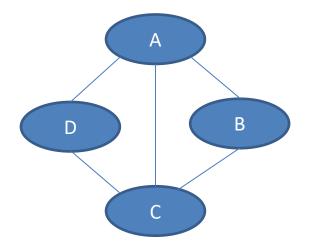
$$a^1$$
 b^1 c^1 0.25 a^1 b^1 c^2 0.35 a^1 b^2 c^1 0.08 a^1 b^2 c^2 0.16 a^2 b^1 c^1 0.05 a^2 b^1 c^2 0.07 a^2 b^2 c^1 0 a^3 b^1 c^2 0.15 a^3 b^1 c^2 0.21 a^3 b^2 c^2 0.18

$$\Phi = \{\phi_1(\boldsymbol{D}_1), \dots, \phi_k(\boldsymbol{D}_k)\}$$
$$\tilde{P}_{\Phi}(X_1, \dots, X_n) = \prod_i \phi_i(\boldsymbol{D}_i)$$



$$\Phi = \{\phi_1(\boldsymbol{D}_1), \dots, \phi_k(\boldsymbol{D}_k)\}$$
$$\tilde{P}_{\Phi}(X_1, \dots, X_n) = \prod_i \phi_i(\boldsymbol{D}_i)$$
$$Z_{\Phi} = \sum_{X_1, \dots, X_n} \tilde{P}_{\Phi}(X_1, \dots, X_n)$$

| <i>a</i> ¹ | <i>b</i> ¹ | <i>c</i> ¹ | 0.25 |
|-----------------------|-----------------------|-----------------------|------|
| a ¹ | <i>b</i> ¹ | <i>c</i> ² | 0.35 |
| <i>a</i> ¹ | <i>b</i> ² | c^1 | 0.08 |
| <i>a</i> ¹ | <i>b</i> ² | <i>c</i> ² | 0.16 |
| a ² | <i>b</i> ¹ | <i>c</i> ¹ | 0.05 |
| a ² | <i>b</i> ¹ | c^2 | 0.07 |
| a ² | <i>b</i> ² | <i>c</i> ¹ | 0 |
| a ² | <i>b</i> ² | <i>c</i> ² | 0 |
| <i>a</i> ³ | <i>b</i> ¹ | c^1 | 0.15 |
| a ³ | <i>b</i> ¹ | <i>c</i> ² | 0.21 |
| a ³ | <i>b</i> ² | <i>C</i> ¹ | 0.09 |
| <i>a</i> ³ | <i>b</i> ² | <i>c</i> ² | 0.18 |

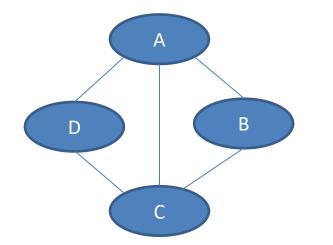


$$\Phi = \{\phi_1(\boldsymbol{D}_1), \dots, \phi_k(\boldsymbol{D}_k)\}$$
$$\tilde{P}_{\Phi}(X_1, \dots, X_n) = \prod_i \phi_i(\boldsymbol{D}_i)$$
$$Z_{\Phi} = \sum_{X_1, \dots, X_n} \tilde{P}_{\Phi}(X_1, \dots, X_n)$$

$$P_{\phi}(X_1, \dots, X_n) = \frac{1}{Z_{\phi}} \prod_i \phi_i(\boldsymbol{D}_i)$$

| <i>a</i> ¹ | <i>b</i> ¹ | c ¹ | 0.25 |
|-----------------------|-----------------------|-----------------------|------|
| <i>a</i> ¹ | <i>b</i> ¹ | <i>c</i> ² | 0.35 |
| <i>a</i> ¹ | <i>b</i> ² | C ¹ | 0.08 |
| <i>a</i> ¹ | <i>b</i> ² | <i>c</i> ² | 0.16 |
| a ² | <i>b</i> ¹ | <i>c</i> ¹ | 0.05 |
| <i>a</i> ² | b^1 | c^2 | 0.07 |
| a ² | <i>b</i> ² | c^1 | 0 |
| a ² | <i>b</i> ² | c^2 | 0 |
| a ³ | <i>b</i> ¹ | <i>c</i> ¹ | 0.15 |
| a ³ | <i>b</i> ¹ | c^2 | 0.21 |
| <i>a</i> ³ | <i>b</i> ² | <i>c</i> ¹ | 0.09 |
| <i>a</i> ³ | <i>b</i> ² | c^2 | 0.18 |

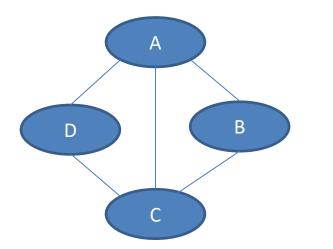
Induced Markov Network



A-B if A and B appear together in some factor.

 $\Phi = \left\{ \phi_{A,B,C}(A,B,C), \phi_{A,C,D}(A,C,D) \right\}$

Factorization

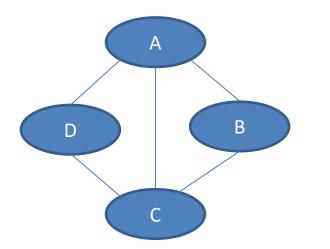


A-B if A and B appear together in some function.

We say G factorizes according to (over) P if there exists a set of factors $\Phi = \{\phi_1(D_1), \dots, \phi_k(D_k)\}$ such that G is the induced graph for Φ

A graph does not imply a unique factorization

Factorization

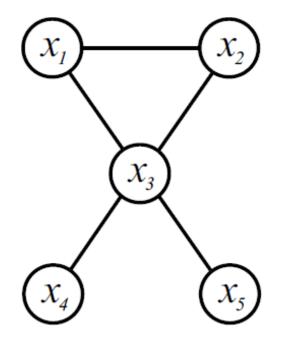


A-B if A and B appear together in some function.

We say G factorizes according to (over) P if there exists a set of factors $\Phi = \{\phi_1(D_1), \dots, \phi_k(D_k)\}$ such that G is the induced graph for Φ A *minimal factorization* is one where all factors are *maximal cliques* (not a strict subset of any other clique) in the MRF

A graph does not imply a unique factorization

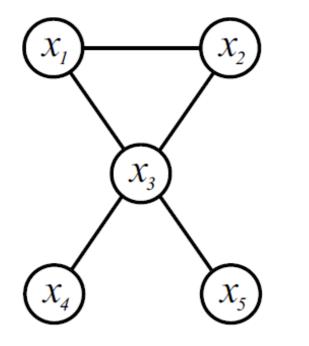
Example



Find the minimal factorization

Find a valid factorization that is not minimal

Example

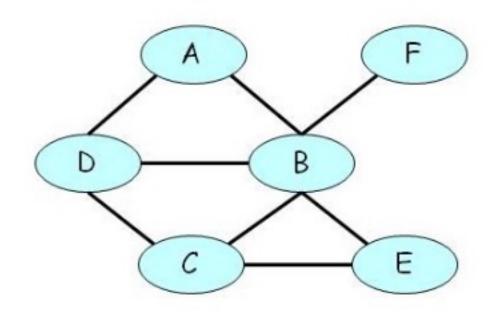


Find the minimal factorization

Find a valid factorization that is not minimal

 $\psi(x_1, x_2, x_3)\psi(x_3, x_4)\psi(x_3, x_5)$ $\psi(x_1, x_2)\psi(x_2, x_3)\psi(x_1, x_3)\psi(x_3, x_4)\psi(x_3, x_5)$

Separation in Markov Networks



Definition:

X and Y are *separated* in H given Z if there is no active trail in H between X and Y given Z

Active trail: Undirected path Conditioning on a node on the path blocks the path

Factorization and Independence

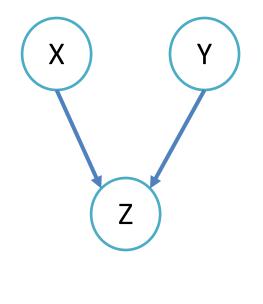
Factorization \Rightarrow Independence

Theorem: If P factorizes over (according to) H, and sep_H(**X**, **Y** | **Z**) then Ind(**X**, **Y** | **Z**) in P

If P factorizes over H, then H is an I-map of P

Independence⇒ Factorization **Theorem (**Hammersley Clifford): If H is an I-Map for P, and P is a positive distribution, then P factorizes over H

Markov Networks and DAGs



G

If G is a perfect map for P Find an MN that is a perfect map for P

Markov Networks and DAGs



If G is a perfect map for P Find an MN that is a perfect map for P Going from BN to MN you lose some independencies

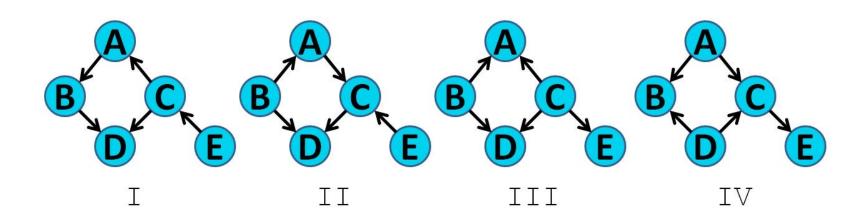
I-equivalence

E

B

G

Which networks are Markov Equivalent to G?



Practice

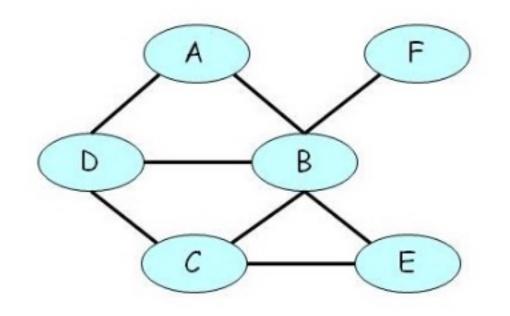
E

B

G

Find a MN that is an I-Map of the probability induced by G

Practice: Separations



Log-linear Representation

$$\tilde{P} = \prod_{i} \phi_{i}(\boldsymbol{D}_{i}) \qquad \tilde{P} = \exp\left(-\sum_{j} w_{j} f_{j}(\boldsymbol{D}_{j})\right)$$

Original parameterization

Log-linear parameterization

Features are functions (like factors) without the non-negativity assumption. Each feature has a single weight. Different features can have the same scope.

Log-linear Representation

$$\phi(X_1, X_2) = \begin{pmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{pmatrix}$$
 $f_{12}^{ij} = I(X_1 = i \text{ and } X_2 = j)$

One feature for each i, j value

$$\phi(X_2, X_3) = \exp\left(-\sum_{kl} w_{kl} f_{ij}^{kl}(X_1, X_2)\right)$$

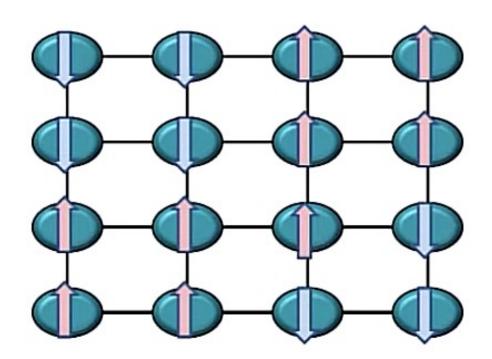
$$w_{kl} = -\log(a_{kl})$$

Example: Ising Models

$$E(x_1, \dots, x_n) = -\sum_{i < j} w_{i,j} x_i x_j - \sum_i u_i x_i$$
$$x_i \in \{-1, 1\}$$
$$f_{i,j}(X_i, X_j) = X_i \cdot X_j$$
$$P(\mathbf{X}) \propto e^{-\frac{1}{T}E(\mathbf{X})}$$

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As T grows, w_{ij} 's become smaller

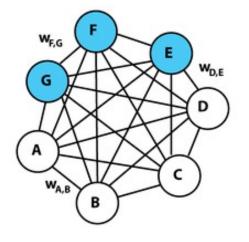
20

60 80 100

80 100 120

Example: Boltzman machine

$$E = -\sum_{i < j} w_{ij} s_i s_j + -\sum_i \theta_i s_i$$
$$s_i \in \{0, 1\}$$



- w_{ij} is the connection strength between unit *j* and unit *i*.
- s_i is the state, $s_i \in \{0,1\}$, of unit *i*.
- θ_i is the bias of unit *i* in the global energy function. ($-\theta_i$ is the activation threshold for the unit.)

Model for neural activation