

COMPSCI 688: Probabilistic Graphical Models

Lecture 6: Undirected Graphical Models

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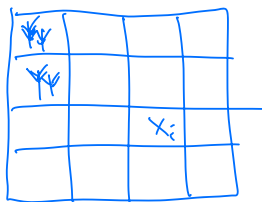
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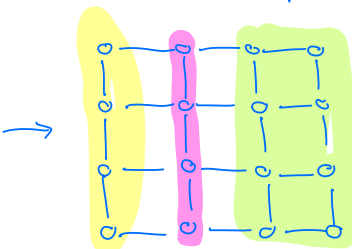
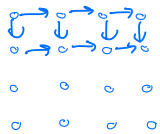
Motivation

Motivating Example

$X_i = 1$ if invasive species in cell i



Bayes net?



$X_A \perp X_B \mid X_S$?

Motivating Example

Markov Properties for Undirected Graphical Model

Undirected graphical models are probability distributions that satisfy a set of conditional independence properties with respect to a *dependence graph* \mathcal{G} . Formally:

- ▶ Let $\mathcal{G} = (V, E)$ be a graph with nodes $V = \{1, \dots, n\}$
- ▶ For $A, B, S \subseteq V$, say that S separates A from B if all paths from A to B in \mathcal{G} go through S , written $\text{sep}_{\mathcal{G}}(A, B | S)$.

The joint distribution of random variables X_1, \dots, X_n satisfies the **global Markov property** with respect to \mathcal{G} if

$$\text{sep}_{\mathcal{G}}(A, B | S) \implies \mathbf{X}_A \perp \mathbf{X}_B \mid \mathbf{X}_S$$

(G)

What form of distribution $p(x_1, \dots, x_n)$ has this property?

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HW due Mon
Quiz due Fri

Bayes nets

- directed
- factorization
- $X_i \perp X_{\text{nd}(i)} \mid X_{\text{pa}(i)}$
- d-separation
- learning (easy)

Undirected graphical models

Markov Random Fields

- undirected
- factorization ("potentials")
- Markov properties based on graph separation
- inference
- learning (harder)

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Warmup: Characterization of Conditional Independence

Recall the definition of conditional independence

$$\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z} \iff p(\mathbf{x}, \mathbf{y} | \mathbf{z}) = p(\mathbf{x} | \mathbf{z}) p(\mathbf{y} | \mathbf{z})$$

Today we'll use two other properties of conditional independence:

1. $\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z} \iff p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \phi_1(\mathbf{x}, \mathbf{z}) \phi_2(\mathbf{y}, \mathbf{z})$ for some ϕ_1, ϕ_2
2. $\mathbf{X} \perp (\mathbf{Y}, \mathbf{W}) \mid \mathbf{Z} \implies \mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}$

Proofs: exercise

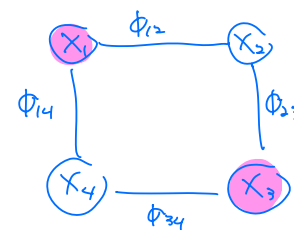
Note: (1) says that conditional independence holds iff the joint distribution factorizes in a certain way, which is very important.

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Markov Random Field Example

Example: $p(x_1, x_2, x_3, x_4) = \phi_{12}(x_1, x_2) \phi_{23}(x_2, x_3) \phi_{34}(x_3, x_4) \phi_{14}(x_1, x_4) \cdot \frac{1}{Z}$

$$= f(x_1, x_2, x_3) \cdot g(x_1, x_3, x_4)$$



$x_2 \perp x_4 \mid x_1$? NO

$\Rightarrow \begin{cases} x_2 \perp x_4 \mid x_1, x_3 \\ x_1 \perp x_3 \mid x_2, x_4 \end{cases}$ (symmetry)

no Bayes net satisfies these CI

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Markov Random Fields $p(x_1, x_2, x_3, x_4) = \frac{1}{Z} \phi_{12}(x_1, x_2) \phi_{123}(x_1, x_2, x_3) \phi_{24}(x_2, x_4)$

$c = \{1, 2, 3\}$ $\mathcal{C} = \{\{1, 2, 3\}, \{1, 2, 3\}, \{2, 3, 4\}\}$

$x_c = (x_1, x_2, x_3)$

A Markov random field is a probability distribution that factorizes over a set of "cliques" \mathcal{C} :

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \phi_c(\mathbf{x}_c), \quad Z = \sum_{\mathbf{x}} \prod_{c \in \mathcal{C}} \phi_c(\mathbf{x}_c)$$

- Each $c \subseteq V = \{1, \dots, n\}$ is a set of indices, or "clique"
- The function ϕ_c is a non-negative *factor* or *potential*. It only depends on x_i for $i \in c$. We say it has *scope* c and define $\text{Scope}(\phi_c) := c$
- Z is the normalizing constant or "partition function"

$f(x_1, x_2, x_3)$
 $\text{Scope}(f) = \{1, 2, 3\}$

Concrete Example

$\mathcal{C} = \{\{1, 2\}, \{2, 3\}\}$ $x_i \in \{0, 1\}$

$p(x_1, x_2, x_3) = \frac{1}{Z} \phi_{12}(x_1, x_2) \phi_{23}(x_2, x_3)$

x_1	x_2	ϕ_{12}
0	0	1
0	1	2
1	0	2
1	1	2

x_2	x_3	ϕ_{23}
0	0	1
0	1	1
1	0	1
1	1	2

x_1	x_2	x_3	$\phi_{12} \cdot \phi_{23}$	$p(x_1, x_2, x_3)$
0	0	0	$1 \cdot 1 = 1$	$1/18$
0	0	1	$1 \cdot 1 = 1$	$1/18$
0	1	0	$2 \cdot 1 = 2$	$2/18$
0	1	1	$2 \cdot 2 = 4$	\vdots
1	0	0	$2 \cdot 1 = 2$	\vdots
1	0	1	$2 \cdot 1 = 2$	\vdots
1	1	0	$2 \cdot 1 = 2$	\vdots
1	1	1	$2 \cdot 2 = 4$	$4/18$
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Dependence Graph

The *dependence graph* $\mathcal{G} = (V, E)$ of the MRF $p(\mathbf{x}) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \phi_c(\mathbf{x}_c)$ is the graph where nodes i and j are connected by an edge if they appear together in some factor:

$$V = \{1, \dots, n\}, \quad E = \{(i, j) : i \in c \text{ and } j \in c \text{ for some } c \in \mathcal{C}\}$$

With this definition, every $c \in \mathcal{C}$ is a clique (fully connected set) in \mathcal{G} .

$p(x_1, x_2, x_3, x_4) = \phi_{12}(x_1, x_2) \underbrace{\phi_{234}(x_2, x_3, x_4)}_{\phi_{234}(x_2, x_3, x_4)} \phi_{34}(x_3, x_4) \frac{1}{Z}$

Factorization and Markov Properties

Factorization

Let \mathcal{G} be a graph. A distribution $p(\mathbf{x})$ factorizes with respect to \mathcal{G} if

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \phi_c(\mathbf{x}_c), \quad \mathcal{C} = \text{cliques}(\mathcal{G}) \quad (\text{F})$$

In other words, it is an MRF with dependence graph \mathcal{G} .

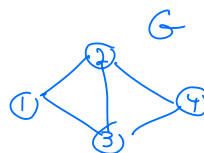
As in Bayes nets, there is a close relationship between factorization and Markov properties obtained from graph separation.

$$p(x_1, x_2, x_3, x_4) = \phi_{123}(x_1, x_2, x_3) \phi_{234}(x_2, x_3, x_4) \cdot \frac{1}{Z}$$

$$\mathcal{C} = \{ \{1, 2, 3\}, \{2, 3, 4\} \}$$

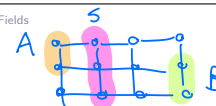


subset of nodes
that is fully
connected



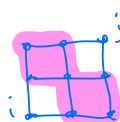
Markov Properties

$$p(x_1, \dots, x_n)$$



The *global Markov property* (G), the *local Markov Property* (L) and *pairwise Markov property* (P) are three different properties of a distribution that hold relative to a graph \mathcal{G} .

every $A \rightarrow B$ path
hits S



$$\text{sep}_{\mathcal{G}}(A, B | S) \implies \mathbf{X}_A \perp \mathbf{X}_B \mid \mathbf{X}_S \quad (\text{G})$$

$$i \in V \implies X_i \perp \mathbf{X}_{V \setminus (\text{nb}(i) \cup \{i\})} \mid \mathbf{X}_{\text{nb}(i)} \quad (\text{L})$$

$$(i, j) \notin E \implies X_i \perp X_j \mid \mathbf{X}_{V \setminus \{i, j\}} \quad (\text{P})$$

Above, $\text{nb}(i)$ is the set of neighbors of node i in \mathcal{G} .

Claim: $(\text{G}) \implies (\text{L}) \implies (\text{P})$

It's easy to see $(\text{G}) \implies (\text{L})$ and $(\text{G}) \implies (\text{P})$ by taking the appropriate choices of A, B, S . We leave $(\text{L}) \implies (\text{P})$ as an exercise.

Markov Property Examples

Markov Property Examples

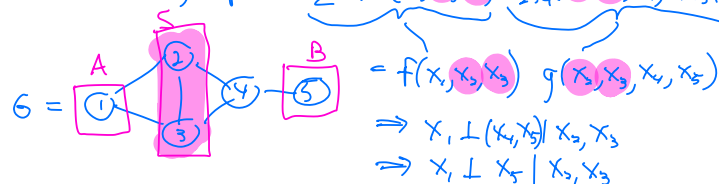
Factorization Implies Markov $\phi(x,z)\phi(y,z) \quad x \perp y | z$

Like in Bayes nets, factorization implies conditional independencies (Markov properties).

Claim: $(F) \Rightarrow (G) \Rightarrow (L) \Rightarrow (P)$

Proof ("by example"): We only need to show $(F) \Rightarrow (G)$.

Assume (F) . $p(x) = \frac{1}{Z} \phi_{123}(x_1, x_2, x_3) \phi_{234}(x_2, x_3, x_4) \phi_{45}(x_4, x_5)$



Want: $\text{sep}_G(A, B | S) \Rightarrow x_A \perp x_B | x_S$

Factorization Implies Markov Proof

Factorization Implies Markov Proof

Suppose $p(x) = \prod_{c \in \mathcal{C}} \phi_c(x_c)$ (assume $1/Z$ is included in one of the factors) and $\text{sep}_G(A, B; S)$. We'll show that $x_A \perp x_B | x_S$.

First, remove S from G . The resulting graph is disconnected and has no paths from A to B

- ▶ Let \tilde{A} be the union of all connected components containing a node from A
- ▶ Let $\tilde{B} = V \setminus \tilde{A}$

Then each $c \in \mathcal{C}$ is a subset of either $\tilde{A} \cup S$ or $\tilde{B} \cup S$

- ▶ Let \mathcal{C}_A be the cliques contained in $\tilde{A} \cup S$
- ▶ Let \mathcal{C}_B be the cliques contained in $\tilde{B} \cup S$

Then

$$\begin{aligned}
 p(\mathbf{x}) &= \prod_{c \in \mathcal{C}_A} \phi_c(\mathbf{x}_c) \prod_{c \in \mathcal{C}_B} \phi_c(\mathbf{x}_c) = h(\mathbf{x}_{\tilde{A}}, \mathbf{x}_S) k(\mathbf{x}_{\tilde{B}}, \mathbf{x}_S) \\
 &\implies \mathbf{X}_{\tilde{A}} \perp \mathbf{X}_{\tilde{B}} \mid \mathbf{X}_S \\
 &\iff (\mathbf{X}_A, \mathbf{X}_{\tilde{A} \setminus A}) \perp (\mathbf{X}_B, \mathbf{X}_{\tilde{B} \setminus B}) \mid \mathbf{X}_S \\
 &\implies \mathbf{X}_A \perp \mathbf{X}_B \mid \mathbf{X}_S
 \end{aligned}$$

Markov Implies Factorization: Hammersley-Clifford Theorem

There is a famous partial converse. For a *positive* distribution, $(P) \Rightarrow (F)$, which implies all the conditions are equivalent:

Theorem (Hammersley-Clifford). If $p(\mathbf{x}) > 0$ for all \mathbf{x} , then

$$(F) \iff (G) \iff (L) \iff (P).$$

The theorem holds for a very general class of distributions, e.g., ones with continuous, discrete, or both types of random variables.