

CSC535: Probabilistic Graphical Models

Probabilistic Graphical Models

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Graphical Models

A variety of graphical models can represent the same probability distribution



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A variety of graphical models can represent the same probability distribution



[Source: Erik Sudderth, PhD Thesis]

Outline

Directed graphical models

- Bayes Nets
- Conditional dependence

Undirected graphical models

- Markov random fields (MRFs)
- Factor graphs

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From Probabilities to Pictures

A probabilistic graphical model allows us to pictorially represent a probability distribution

Probability Model: $p(x_1, x_2, x_3) =$ $p(x_1)p(x_2)p(x_3 | x_1, x_2)$ Graphical Model: x_l x_2 x_3

Conditional distribution on each RV is dependent on its parent nodes in the graph

Directed Graphical Models

Directed models are generative models...



$$p(C, X_1, X_2) = p(C)p(X_1 \mid C)p(X_2 \mid C)$$

The graph and the formula say exactly the same thing. (The graph has very specific semantics.)

...tells how data are generated (called ancestral sampling)

Step 1 Sample root node (prior): $c \sim p(C)$

Step 2 Sample children, given sample of parent (likelihood): $x_1 \sim p(X_1 \mid C = c)$ $x_2 \sim p(X_2 \mid C = c)$

Inference



Denote observed data with shaded nodes,

$$X_1 = x_1 \qquad \qquad X_2 = x_2$$

Infer *latent* variable C via Bayes' rule:

$$p(c \mid x_1, x_2) = \frac{p(c)p(x_1 \mid c)p(x_2 \mid c)}{p(x_1, x_2)}$$

- This is (obviously) a simple example
- Models and inference task can get really complicated
- But the fundamental concepts and approach are the same

Chain Rule of Probability

Recall the **probability chain rule** says that we can decompose any joint distribution as a product of conditionals....

 $p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2)p(x_4 \mid x_1, x_2, x_3)$

Valid for any ordering of the random variables...

 $p(x_1, x_2, x_3, x_4) = p(x_3)p(x_1 \mid x_3)p(x_4 \mid x_1, x_3)p(x_2 \mid x_1, x_3, x_4)$

For a collection of N RVs and any permutation ρ :

$$p(x_1, \dots, x_N) = p(x_{\rho(1)}) \prod_{i=2}^N p(x_{\rho(i)} \mid x_{\rho(i-1)}, \dots, x_{\rho(1)})$$

Conditional Independence

Recall two RVs X and Y are conditionally independent given Z (or $X \perp Y \mid Z$) iff:

 $p(X \mid Y, Z) = p(X \mid Z)$

Idea Apply chain rule with ordering that exploits conditional independencies to simplify the terms



 x_3

Ex. Suppose $x_4 \perp x_1 \mid x_3$ and $x_2 \perp x_4 \mid x_1$ then: $p(x) = p(x_3)p(x_1 \mid x_3)p(x_4 \mid x_1, x_3)p(x_2 \mid x_1, x_3, x_4)$ $= p(x_3)p(x_1 \mid x_3)p(x_4 \mid x_3)p(x_2 \mid x_1, x_3)$

Can visualize conditional dependencies using **directed acyclic graph** (DAG)

General Directed Graphs

Def. A <u>directed graph</u> is a graph with edges $(s, t) \in \mathcal{E}$ (arcs) connecting parent vertex $s \in \mathcal{V}$ to a child vertex $t \in \mathcal{V}$

 x_3

 x_2

 x_1

 x_4

Def. Parents of vertex $t \in \mathcal{V}$ are given by the set of nodes with arcs pointing to t,

$$\operatorname{Pa}(t) = \{s : (s,t) \in \mathcal{E}\}$$

<u>Children</u> of $t \in \mathcal{V}$ are given by the set,

$$Ch(t) = \{t : (t,k) \in \mathcal{E}\}\$$

<u>Ancestors</u> are parents-of-parents. <u>Descendants</u> are children-of-children. Model factors are normalized conditional distributions:

$$p(x) = \prod_{s \in \mathcal{V}} p(x_s \mid x_{\operatorname{Pa}(s)})$$
Parents of node s

Directed acyclic graph (DAG) specifies factorized form of joint probability:

 $p(x) = p(x_3)p(x_1 \mid x_3)p(x_4 \mid x_3)p(x_2 \mid x_1, x_3)$

Locally normalized factors yield globally normalized joint probability



Shading & Plate Notation

Convention: Shaded nodes are observed, open nodes are latent/hidden/unobserved



Inference



Example: Gaussian Mixture Model

Bayes nets are easily simulated via <u>ancestral sampling</u>...



Sample all nodes with no parents, then children, etc., to terminals. Can sample nodes at same level in parallel.

What is the joint factorization?



p(a,b,c) = p(a)p(b)p(c)

Are a and b independent ($a \perp b$)?



p(a,b,c) = p(a)p(b)p(c)

p(a,b,c) = p(a)p(b|a)p(c|a,b)



Note there are **no conditional independencies**

Three interesting cases



Head-to-tail

Three interesting cases



For each case, consider two questions:

- 1) Is $a \perp b$?
- 2) Is $a \perp b \mid c$? (i.e. c is observed)

Case one (tail-to-tail)



Is $a \perp b$?

Case one (tail-to-tail)



Intuition *c* generates, both, *a* and *b*. Knowing *a* tells you something about *c* (via Bayes rule p(c|a)) which in turn generates b...information is exchanged

Can prove by counterexample (HW problem)



Is $a \perp b \mid c$?



$$\begin{split} p(a,b,c) &= p(c)p(a|c)p(b|c) \quad \text{(what the graph represents in general)} \\ p(a,b|c) &= p(a|c)p(b|c) \quad \text{(with c observed)} \\ \end{split}$$
This is the definition of $a \perp b|c$

Case one (tail-to-tail) summary



Tail-to-tail case

With no conditioning = no independence With conditioning = independence





If you know *a*, that informs you about *c*, which informs you about *b*.



The graph represents p(a,b,c) = p(a)p(c|a)p(b|c)



The graph represents p(a,b,c) = p(a)p(c|a)p(b|c)

Algebraically, $p(a,b) = \sum_{c} p(a,b,c) = p(a) \sum_{c} p(c|a) p(b|c)$

If $a \perp b$ then the above would also have to be equal to p(a)p(b)

$$p(a,b) = \sum_{c} p(a,b,c) = p(a) \sum_{c} p(c|a) p(b|c)$$

If $a \perp b$ then the above **also** equals p(a)p(b)

To prove the claim that a λ b we can construct a counter example where the above is false.

Homework Question





$$p(a,b \mid c) = \frac{p(a,b,c)}{p(c)}$$
$$= \frac{p(a)p(c|a)p(b|c)}{p(c)}$$

(definition)

(why?)





$$p(a,b | c) = \frac{p(a,b,c)}{p(c)}$$
$$= \frac{p(a)p(c|a)p(b|c)}{p(c)}$$
$$= \frac{p(a)p(a|c)p(c)p(b|c)}{p(a)p(c)}$$
$$= p(a|c)p(b|c)$$

(definition)

(from graph)

(Bayes on p(c|a))

(why?)



$$p(a,b \mid c) = \frac{p(a,b,c)}{p(c)}$$
$$= \frac{p(a)p(c|a)p(b|c)}{p(c)}$$
$$= \frac{p(a)p(a|c)p(c)p(b|c)}{p(a)p(c)}$$
$$= p(a|c)p(b|c)$$

(definition)

(from graph)

(Bayes on p(c|a))

(canceling factors)
Case two (head-to-tail) summary



Head-to-tail case

With no conditioning = no independence With conditioning = independence

(Same as tail-to-tail case!)

Case three (head-to-head)

Are a and b independent ($a \perp b$)?



$$p(a,b) = \sum_{c} p(a)p(b)p(c \mid a, b) = p(a)p(b)$$

Are a and b conditionally independent ($a \perp b \mid c$)?



p(a,b,c) = p(a)p(b)p(c|a,b)

Are a and b conditionally independent ($a \perp b \mid c$)?

$$p(a,b|c) = \frac{p(a,b,c)}{p(c)}$$

$$p(a,b|c) = \frac{p(a,b,c)}{p(c)}$$

$$p(a,b|c) = \frac{p(a,b,c)}{p(c)}$$

$$p(a,b) = \frac{p(a,b,c)}{p(c)}$$

$$p(a|c) = \frac{p(a)p(b)p(c|a,b)}{p(c)}$$

$$p(a|c)p(b|c) \quad \text{(in general)}$$

$$unless the algebra reduces to something obviously false, we typically look for a counter example}$$

Both latent variables must explain same observed data so become dependent



Phenomenon in Bayes networks known as **explaining away**



Markov Properties

How can we be sure a PGM is **correct** for a distribution p(x)?



It must satisfy **all** of the conditional independencies of p(x), then we say p(x) **is Markov with respect to** the graph.

Bayes Ball Algorithm

To test if $X \perp Z \mid Y$ imagine rolling a "ball" from X towards Z



Bayes Ball Algorithm

To test if $X \perp Z \mid Y$ imagine rolling a "ball" from X towards Z



Directed Separation (d-Separation)

To test if $X_A \perp X_B \mid X_C$ roll ball from every node in X_A ...



Tests for property of *directed separation* (d-separation): if X_C separates / blocks X_A from X_B then $X_A \perp X_B \mid X_C$

Administrative Items

- HW2 Due Tonight
- HW3 Out Tonight
 - Due Wednesday, 2/16
 - Bayesian inference and Bayes Nets
 - 4 Questions
 - 6 Points

Bayes Ball Algorithm

Y

Blocks

 $X \perp Z \mid Y$

Y

Doesn't

Block

Ζ

Ζ

 $X \not\perp Z$



Question Is X conditionally independent of all other nodes in graph given its **parents** and **children?**



Question Is X conditionally independent of all other nodes in graph given its **parents** and **children?**

Answer No. It still depends on coparents.

WHY?



Question Is X conditionally independent of all other nodes in graph given its **parents** and **children?**

Answer No. It still depends on coparents.

WHY?

Head-to-head conditional dependence from *explaining away property*



We refer to this conditioning set as the *Markov Blanket* of X...

X conditionally independent of all other nodes, given its Markov blanket

Definition A RV X with distribution p(x) that is Markov w.r.t. Bayes Net with graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ has a **Markov blanket** given by:

 $Mb(X) = Pa(X) \cup Ch(X) \cup CoPa(X)$

For any $Y \notin Mb(X)$:

 $X \perp Y \mid \mathrm{Mb}(X)$



Markov blanket used to simplify inference and distribute computation (e.g. Gibbs sampler, variational inference, etc.)

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Directed graphical models

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- Conditional dependence

Undirected graphical models

- Markov random fields (MRFs)
- Factor graphs

Model factors are normalized conditional distributions:

 x_3

 x_2

 \mathcal{X}_1

 x_4

$$p(x) = \prod_{s \in \mathcal{V}} p(x_s \mid x_{\operatorname{Pa}(s)})$$
Parents of node s

Locally normalized factors yield globally normalized joint probability

Often difficult to specify joint in terms of product of normalized probabilities...

Markov Random Field

Specify joint as product of unnormalized functions...



- More general class of models than Bayes Nets
- Any Bayes Net easily convertes to MRF by dropping local normalizers
- MRF→Bayes Net not straighfortward

Factorized Probability Distributions

A probability distribution over RVs $x = (x_1, \ldots, x_d)$ can be written as a product of factors,

$$p(x) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \psi_c(x_c)$$

Where:

- C a collection of subsets of indices $\{1, \ldots, d\}$
- $\psi(\cdot)$ are nonnegative *factors* (or *potential functions*)
- *Z* the normalizing constant (or *partition function*)

$$Z = \int \prod_{c \in \mathcal{C}} \psi_c(x_c) \, dx_c$$

Undirected Graphical Models

A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a set of vertices \mathcal{V} and edges \mathcal{E} . An edge $(s, t) \in \mathcal{E}$ connects two vertices $s, t \in \mathcal{V}$.



In **undirected models** edges are specified irrespective of node ordering so that,

 $(s,t)\in \mathcal{E} \Leftrightarrow (t,s)\in \mathcal{E}$

Distributions are typically specified with unknown normalization (easier to specify),

$$p(x) \propto \prod_{c \in \mathcal{C}} \psi_c(x_c)$$

Markov Random Fields (MRFs)

A factor $\psi_c(x_c)$ corresponds to a clique $c \in C$ (fully connected subgraph) in the MRF

An MRF does not imply a unique factorization, for example all the following are "*valid*":

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

Complete Graph



Markov Random Fields (MRFs)

A factor $\psi_c(x_c)$ corresponds to a clique $c \in C$ (fully connected subgraph) in the MRF

An MRF does not imply a unique factorization, for example all the following are "*valid*":

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

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



Markov Random Fields (MRFs)

A factor $\psi_c(x_c)$ corresponds to a clique $c \in C$ (fully connected subgraph) in the MRF

Pairwise MRF



An MRF does not imply a unique factorization, for example all the following are "*valid*":

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

A minimal factorization is one where all factors are maximal cliques (not a strict subset of any other clique) in the MRF

Example



Example: Image Denoising

Noisy Image



Bayes' Theorem

Latent Image

Problem Given observed image corrupted by i.i.d. noise, infer "clean" denoised image.

Example: Image Denoising

Model Assume binary image with latent pixels $x_i \in \{0, 1\}$ and observed $y_i \in \{0, 1\}$.

Observed pixels randomly flipped i.i.d.,

 $\log \phi_i(x_i) = \eta x_i y_i$ Eta parameter controls noise

Neighboring pixels should appear similar,

 $\log \phi_{ij}(x_i, x_j) = \beta x_i x_j$ Beta parameter controls smoothness

Full MRF (in "energy" form):

$$E(x,y) = -\sum_{i} \log \phi_i(x_i) - \sum_{(i,j)} \log \phi_{ij}(x_i, x_j)$$

Often specify MRF in "energy" or negative log-probability form (minimize energy → maximize probability)

[Source: Bishop, C. PRML]



Normalizing MRFs

Joint probability of *image denoising* model,

$$p(x,y) = \frac{1}{Z} \exp\left\{-E(x,y)\right\}$$

Normalization (a.k.a. partition function) for N pixel image:

$$Z = \sum_{x_1} \sum_{x_2} \dots \sum_{x_N} \exp\left\{-E(x, y)\right\}$$

O(2^N) terms

Normalization not always possible in closed-form : i.e. need to sum over *all possible N-pixel images*

Often ignore Z and specify MRFs up to proportionality...

Simulation



Bayes Nets Straightforward simulation via <u>ancestral sampling</u> successively samples from conditionals:

$$p(\mathbf{x}) = \prod_{i \in \mathcal{V}} p(x_i \mid x_{\operatorname{Pa}(i)})$$

 $x_i \sim p(x_i \mid x_{\operatorname{Pa}(i)})$

Undirected Graphs Sampling not as straightforward...

- Lack locally normalized conditionals to sample from
- Lack partial ordering of nodes

We will return to this when we discuss Markov chain Monte Carlo

Conditional Independence (Undirected)

We say x_A and x_C are *independent* or $x_A \perp x_C$ if:

 $p(x_A, x_C) = p(x_A)p(x_C)$

We say they are *conditionally independent* or $x_A \perp x_C \mid x_B$ if:

$$p(x_A, x_C \mid x_B) = p(x_A \mid x_B)p(x_C \mid x_B)$$

Def. We say p(x) is globally Markov w.r.t. \mathcal{G} if $x_A \perp x_C \mid x_B$ in any separating set of \mathcal{G} .



Conditional independence in undirected graphical models is defined by separating sets

Global & Local Markov Properties

Global Markov Property

- Set B separates A from C if all paths from A to C pass through B
- By definition, distribution is Markov if and only if for any B separating A and C:

$$p(x_A, x_C \mid x_B) = p(x_A \mid x_B)p(x_C \mid x_B)$$

$$p(x_A \mid x_B, x_C) = p(x_A \mid x_B) \quad p(x_C \mid x_B, x_A) = p(x_C \mid x_B)$$

Local Markov Property

• Given its *neighbors*, each node is independent of all other variables

$$p(x_s \mid x_{\mathcal{V} \setminus s}) = p(x_s \mid x_{\Gamma(s)})$$

$$\Gamma(s) = \{t \in \mathcal{V} \mid (s, t) \in \mathcal{E}\}$$
Markov blanket only includes immediate neighbors (we needed co-parents in Bayes nets)

 This local Markov property is a special case of the global Markov property
 Source: Erik Sudde **Thorem (Hammersley-Clifford).** Let C denote the set of cliques of an undirected graph G. A probability distribution defined as a normalized product of non-negative potential functions on those cliques is then always Markov with respect to G:

$$p(x) \propto \prod_{c \in \mathcal{C}} \psi_c(x_c)$$

Conversely, any strictly positive density which is Markov with respect to \mathcal{G} can be represented in this factored form.



Pairwise Markov Random Field

Often easier to specify and do inference on pairwise model



$$p(x,y) \propto \prod_{s \in \mathcal{V}} \psi_s(x_s,y) \prod_{(s,t) \in \mathcal{E}} \psi_{st}(x_s,x_t)$$

Likelihood Prior

Restricted class of MRFs

- 2-node factor exists for every edge
- Explicit factorization of joint distribution
- High-order factors not always easily decomposed into pairwise terms

Example: Image Segmentation



Pairwise MRF energy: $-\log p(x, y) = \log Z + \sum \psi_i(x_i, y_i) + \sum \psi_{i,j}(x_i, x_j)$

Don't need to specify normalized conditionals as in Bayes Nets

Low energy configurations = $\stackrel{i}{\text{High probability}}$ (*i*,*j*)

L2 Likelihood: $\psi_i(x_i, y_i) = ||x_i - y_i||^2$ Potts model: $\psi_{i,j}(x_i, x_j) = \mathbb{I}(x_i = x_j)$

MAP (minimum energy) configuration = Piecewise constant regions

Transformations of Undirected Models



Conditioning on C makes A and B independent:

[Source: Erik Sudderth]

Factor Graphs

A hypergraph $\mathcal{H} = (\mathcal{V}, \mathcal{F})$ where a hyperedge $f \in \mathcal{F}$ is a subset of vertices $f \subset \mathcal{V}$.

Factor node for each product term in the joint factorization:

 $\begin{array}{l} \text{Graphical model makes} \\ \text{factorization explicit} \end{array} p(x) \propto \prod_{f \in \mathcal{F}} \psi_f(x_f) \end{array}$

 X_2

 X_{5}

 X_3

where $x_f = \{x_i : i \in f\}$ the set of variables in factor *f*. For example:

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

Example: Low Density Parity Check Codes

Factor Graph Representation



Problem Setup

- A code *t* is transmitted over a noisy
- Received code *r* is corrupted by noise
- Estimate the most probable code that was sent *t** (*maximum a posteriori*)

Transmitted Code
 Received Code

$$t \sim p(t)$$
 $r \mid t \sim p(r \mid t)$

 Noisy
 Decoder

 Channel
 Decoder
Example: Low Density Parity Check Codes



- Valid codes have zero parity: $p(t) \propto \mathbb{I}(Ht = 0 \mod 2)$
- Chanel noise model arbitrary, e.g. flip bits w/ ϵ probability:

$$p(r \mid t) = \prod_{n} p(r_n \mid t_n) = \prod_{n} (1 - \epsilon)^{\mathbb{I}(r_n = t_n)} \epsilon^{\mathbb{I}(r_n \neq t_n)}$$
n-th bit

Recap: Directed Models

• Distribution factorized as product of conditionals via chain rule

 $p(x_1, x_2, x_3, x_4) = p(x_3)p(x_1 \mid x_3)p(x_4 \mid x_1, x_3)p(x_2 \mid x_1, x_3, x_4)$

Choose ordering where terms simplify due to conditional independence

Eg. Suppose $x_4 \perp x_1 \mid x_3$ and $x_2 \perp x_4 \mid x_1$ then:

 $p(x) = p(x_3)p(x_1 \mid x_3)p(x_4 \mid x_3)p(x_2 \mid x_1, x_3)$

 Directed graph encodes factorized distribution via conditional independence properties



 Straightforward simulation via ancestral sampling

 x_1

Tail-to-tail

Head-to-head

Head-to-tail

Recap: Undirected Model

- Joint factorization as nonnegative factors (potentials) over subsets: $p(x) \propto \prod_{f \in \mathcal{F}} \psi_f(x_f)$
- Easier to specify models compared to Bayes nets since:
 - Factors do not need to be normalized conditional probabilities
 - May specify up to unknown normalization constant
- Easier to verify Markov independence via separating sets
- Factorization ambiguous in MRFs, but explicit in factor graphs (factor graphs generally preferred)
- Simulation is not easy in general. Can't do ancestral sampling.

