Stat 521A Lecture 1 Introduction; directed graphical models

1

Outline

- Administrivia
- Overview
- Local markov property, factorization (3.2)
- Global markov property (3.3)
- Deriving graphs from distributions (3.4)

Administrivia

- Class web page www.cs.ubc.ca/~murphyk/Teaching/Stat521A-spring08
- Join groups.google.com/group/stat521a-spring09
- Office hours: Fri 10-11 am
- Final project due Fri Apr 24th
- Weekly homeworks
- Grading
 - Final project: 60%
 - Weekly Assignments: 40%

Auditing

- If you want to 'sit in' on the class, please register for it as 'pass/fail'; you will automatically pass as long as you show up for (most of) the class (no other requirements!)
- If you take it for real credit, you will likely learn more...

Homeworks

Weekly homeworks, out on Tue, due back on Tue

- Collaboration policy:
 - You can collaborate on homeworks if you write the name of your collaborators on what you hand in; however, you must understand everything you write, and be able to do it on your own
- Sickness policy:
 - If you cannot do an assignment, you must come see me in person; a doctor's note (or equivalent) will be required.

Workload

- This class will be quite time consuming.
- Attending lectures: 3h.
- Weekly homeworks: about 3h.
- Weekly reading: about 10h.
- Total: 16h/week.

Pre-requisites

- You should know
 - Basic applied math (calculus, linear algebra)
 - Basic probability/ statistics e.g. what is a covariance matrix, linear/logistic regression, PCA, etc
 - Basic data structures and algorithms (e.g., trees, lists, sorting, dynamic programming, etc)
 - Prior exposure to machine learning (eg CS540) and/or multivariate statistics is strongly recommended

Textbooks

- "Probabilistic graphical models: principles and techniques", Daphne Koller and Nir Friedman (MIT Press 2009, in press).
- We will endeavour to cover the first 900 (of 1100) pages!
- Copies available at Copiesmart copy center in the village (next to McDonalds) from Thursday
- I may hand out some chapters from Michael Jordan's draft book, "Probabilistic graphical models"
- I am writing my own book "Machine learning: a probabilistic approach"; I may hand out some chapters from this during the semester.

Matlab

- Matlab is a mathematical scripting language widely used for machine learning (and engineering and numerical computation in general).
- Everyone should have access to Matlab via their CS or Stats account.
- You can buy a student version for \$170 from the UBC bookstore. Please make sure it has the Stats toolbox.
- Matt Dunham has written an excellent Matlab tutorial which is on the class web site – please study it carefully!

PMTK

- Probabilistic Modeling Toolkit is a Matlab package I am currently developing to go along with my book.
- It uses the latest object oriented features of Matlab 2008a and will not run on older versions.
- It is designed to replace my earlier 'Bayes net toolbox'.
- PMTK will form the basis of some of the homeworks, and may also be useful for projects. (Currently support for GMs is very limited.)
- http://www.cs.ubc.ca/~murphyk/pmtk/

Learning objectives

- By the end of this class, you should be able to
 - Understand basic principles and techniques of probabilistic graphical models
 - Create suitable models for any given problem
 - Derive the algorithm (equations, data structures etc) needed to apply the model to data
 - Implement the algorithm in reasonably efficient Matlab
 - Demonstrate your skills by doing a reasonably challenging project

Ask questions early and often!

I will use Google before asking dumb questions. www.mrburns.nl before asking dumb questions. I will use Google before asking dumb questions I will use Google before asking dumb questions. I will use Google before asking dumb questions. I will use Google before asking dumb question I will use Google before asking dumb questions. I will use Google before asking dumb questions. I will use Google before asking dumb question I will use Google before asking dumb questions. I will use Google before asking dumb questions. I will use Google before asking dumb question I will use Google before asking dumb questions. I will use Google before asking dumb questions. I will use Google before asking dumb question I will use Google before asking dumb questions. I will use Google before asking dumb question I will use Google before asking dumb questions. I will use Google before asking dumb question I will use Google before asking dumb questions. I will use Google before asking dumb question I will use Google before asking dumb questions. I will use Google before asking dumb question I will use Google before asking dumb questions. I will use Google before asking dumb question I will use Google before asking dumb questions. I will use Google before asking dumb question I will use Google before asking dumb question question

Outline

- Administrivia
- →• Overview
 - Local markov property, factorization (3.2)
 - Global markov property (3.3)
 - Deriving graphs from distributions (3.4)

Supervised learning

- Predict output given inputs, ie compute p(h|v)
- Regression: h in R
- Classification: h in {1,...,C}



Structured output learning

- Model joint density of p(h,v) (or maybe p(h|v))
- Then infer p(h|v) state estimation
- MAP estimation (posterior mode) $\mathbf{h}^* = \arg \max_{h_1}, \dots, \arg \max_{h_n} p(\mathbf{h} | \mathbf{v}, \boldsymbol{\theta})$
- Posterior marginals

$$h_1^* = \sum_{h_2} \dots, \sum_{h_n} p(\mathbf{h} | \mathbf{v}, \boldsymbol{\theta})$$

• Also need to estimate parameters and structure

Density estimation

- Model joint density of all variables
- No distinction between inputs and outputs: different subsets of variables can be observed at different times (eg for missing data imputation)
- Can run model in any 'direction'



Water sprinkler joint distribution



p(C, S, R, W)

С	S	r	W	prob
0	0	0	0	0.200
0	0	0	1	0.000
0	0	1	0	0.005
0	0	1	1	0.045
0	1	0	0	0.020
0	1	0	1	0.180
0	1	1	0	0.001
0	1	1	1	0.050
1	0	0	0	0.090
1	0	0	1	0.000
1	0	1	0	0.036
1	0	1	1	0.324
1	1	0	0	0.001
1	1	0	1	0.009
1	1	1	0	0.000
1	1	1	1	0.040

Inference

• Prior that sprinkler is on

$$p(S=1) = \sum_{c=0}^{1} \sum_{r=0}^{1} \sum_{w=0}^{1} p(C=c, S=1, R=r, W=w) = 0.3$$

Posterior that sprinkler is on given that grass is wet

$$p(S = 1|W = 1) = \frac{p(S = 1, W = 1)}{p(W = 1)} = 0.43$$

 Posterior that sprinkler is on given that grass is wet and it is raining

$$p(S=1|W=1,R=1) = \frac{p(S=1,W=1,R=1)}{p(W=1,R=1)} = 0.19$$

Explaining away

Bag of words model

- bag-of-words representation of text documents
- Xi=1 iff word i occurs in document
- Define a joint distribution over bit vectors, p(x1,...,xn)





Inference

- Given word Xi occurs, which other words are likely to co-occur?
- What is the probability of any particular bit vector?
- Sample (generate) documents from joint p(x)

Bayesian classifiers

- Define joint p(y,x) = p(x|y) p(y) on document class label and bit vectors
- Can infer class label using Bayes rule



- If y is hidden, we can use this to cluster documents.
- In both cases, we need to define p(x|y=c)

Naïve Bayes assumption

• The simplest approach is to assume each feature is conditionally independent given the class/cluster Y

$$X_i \perp X_j | Y = c$$

- In this case, we can write $p(\mathbf{x}|y=c) = \prod_{j=1}^d p(x_j|y=c)$
- The number of parameters is reduced from O(C K^d) to O(C K), assuming C classes and K-ary features

Conditional independence

- In general, making CI assumptions is one of the most useful tools in representing joint probability distributions in terms of low-dimensional quantities, which are easier to estimate from data
- Graphical models are a way to represent Cl assumptions using graphs
- The graphs provide an intuitive representation, and enable the derivation of efficient algorithms

Graphical models

- There are many kinds of graphical models
- Directed Acyclic graphs "Bayesian networks"
- Undirected graphs "Markov networks"
- Directed cyclic graphs "dependency networks"
- Partially directed acyclic graphs (PDAGs) "chain graphs"
- Factor graphs
- Mixed ancestral graphs
- Etc
- Today we will focus on DAG models

Outline

- Administrivia
- Overview
- \rightarrow Local markov property, factorization (3.2)
 - Global markov property (3.3)
 - Deriving graphs from distributions (3.4)

CI properties of DAGs

 Defn 3.2.1. A BN structure G is a DAG whose nodes represent rvs X₁,...,X_n. Let Pa(X_i) be the parents of X_i, and Nd(X_i) be the non-descendants of Xi. Then G encodes the following local Markov assumptions:

$$I_{\ell}(G) = \{X_i \perp Nd(X_i) | Pa(X_i)\}$$



Another Example



Red (X8) \perp pink | bue

I-maps

- Def 3.2.2. Let I(P) be the set of independence assertions of the form X \perp Y | Z that hold in P $P \models X \perp Y \mid Z$
- Def 3.2.3. We say G is an I-map for set I if I(G) ⊆ I (hence the graph does not make any false independence assumptions)

I-maps: examples

The second second second second

server a server of the server

• Examples 3.2.4, 3.2.5

X = Y = P(X, Y)	X = Y = P(X, Y)
$x^{0} y^{0} = 0.08$	$x^0 y^0 = 0.4$
$x^0 y^1 = 0.32$	$x^0 y^1 = 0.3$
$x^1 y^0 = 0.12$	$x^1 y^0 = 0.2$
$x^1 y^1 = 0.48$	$x^1 y^1 = 0.1$
Y X Y	· · · · · · · · · · ·
$\begin{pmatrix} 0.08 & 0.32 \\ 0.12 & 0.43 \end{pmatrix} = \begin{pmatrix} 0.4 \\ 0.6 \end{pmatrix} (0.2)$	0.8)
P(X,Y) = P(X) P(Y)	PAXLY
$P \models X \perp I$	
Imaps = X Y, X -> Y, X <- Y	imaps = X -> Y, X <- Y

I-map to factorization

• Def 3.2.5. A distribution P factorizes over a DAG G if it can be written in the form

$$p(X_1,\ldots,X_n) = \prod^n p(X_i | Pa(X_i))$$

- Thm 3.2.7. If G is an lⁱ-map for P, then P factorizes according to G.
- Proof: by the chain rule, we can always write $p(X_1, \dots, X_n) = \prod_{i=1}^n p(X_i | X_{1:i-1})$
- By the local markov assumption, we can drop all the ancestors except the parents. QED.

Student network



 $\begin{array}{l} p(I,D,G,S,L) = & \\ p(I)p(D|I)p(G|I,D)p(S|I,D,G)p(L|I,D,G,S) \\ = & p(I)p(D|)p(G|I,D)p(S|I)p(L|S) \end{array}$

Naïve Bayes classifier

L' J K X d 2

$$p(y, \mathbf{x}) = p(y) \prod_{j=1}^{d} p(x_j | y)$$

Bayes net = DAG + CPD

- A DAG defines a family of distributions, namely all those that factorize in the specified way.
- Def 3.2.6. A Bayes net is a DAG G together with a set of local Conditional Probability Distributions p(X_i|Pa(X_i)).



Water sprinkler BN



p(C, S, R, W) = p(C)p(S|C)p(R|C)p(W|S, R)

34

Joint distribution for sprinkler network

$$p(C, S, R, W) = p(C)p(S|C)p(R|C)p(W|S, R)$$



С	S	r	W	prob
0	0	0	0	0.200
0	0	0	1	0.000
0	0	1	0	0.005
0	0	1	1	0.045
0	1	0	0	0.020
0	1	0	1	0.180
0	1	1	0	0.001
0	1	1	1	0.050
1	0	0	0	0.090
1	0	0	1	0.000
1	0	1	0	0.036
1	0	1	1	0.324
1	1	0	0	0.001
1	1	0	1	0.009
1	1	1	0	0.000
1	1	1	1	0.040

CPDs

- CPDs can be any conditional distribution p(X_i|Pa(X_i))
- If Xi has no parents, this is an unconditional distribution
- For discrete variables, it is common to use tables (conditional multinomials)
- However, CPTs have O(K^{|pa|}) parameters; we will consider more parsimonious representations (such as logistic regression) – see ch 5
- For continuous variables, it is common to use linear regression to define CPDs (see ch 7)

 $p(X_i|Pa(X_i) = \mathbf{u}, \boldsymbol{\theta}_i) = \mathcal{N}(X_i|\mathbf{u}^T\boldsymbol{\theta}_i, \sigma_i^2)$

Representing parameters as nodes

$$Ti$$

$$L$$

$$Y$$

$$X_{1} X_{2} X_{d}$$

$$T T T$$

$$\Phi_{1} \Phi_{2} \Phi_{d}$$

$$p(y, \mathbf{x}, \boldsymbol{\theta}) = p(y|\boldsymbol{\pi})p(\boldsymbol{\pi}) \prod_{j=1}^{d} p(x_j|y, \boldsymbol{\phi}_j)p(\boldsymbol{\phi}_j)$$

We will return to this representation when we discuss parameter estimation DAGs are widely used for Hierarchical Bayesian models

Genetic inheritance

- G(x) = genotype (allele) of person x at given locus, say {A,B,O} x {A,B,O}
- B(x) = phenotype (blood group) in {A,B,O}
- P(B(c)|G(c)) = penetrance model
- P(G(c)|G(p),G(m)) = transmission model
- P(G(c)) = priors for founder nodes



Factorization to I-map

- Thm 3.2.9. If P factorizes over G, then G is an Imap for P.
- Proof (by example)
- We need to show all the local Markov properties hold in P eg. RTP

p(S|I, D, G, L) = p(S|I)



• By factorization and elementary probability,

$$p(S|I, D, G, L) = \frac{p(Q)}{p}$$

$$= \frac{p(S, I, D, G, L)}{p(I, D, G, L)}$$

=
$$\frac{p(I)p(D)p(G|I, D)p(L|G)p(S|I)}{p(I)p(D)p(G|I, D)p(L|G)} = p(S|I)_{39}$$

Outline

- Administrivia
- Overview
- Local markov property, factorization (3.2)
- →• Global markov property (3.3)
 - Deriving graphs from distributions (3.4)

Global Markov properties

• The DAG defines local markov properties

 $I_{\ell}(G) = \{X_i \perp Nd(X_i) | Pa(X_i)\}$

• We would like to be able to determine global markov properties, i.e., statements of the form

 $I(G) = \{ X \perp Y | Z : f(X, Y, Z, G) \}$

for some function f.

- There are several equivalent ways to define f:
- Bayes ball
- d-separation
- Ancestral separation (ch 4)

Chains

• Consider the chain

$$\begin{array}{l} \chi \rightarrow \overleftarrow{} \rightarrow \overleftarrow{} \\ p(x,y,z) = p(x)p(y|x)p(z|y) \end{array}$$

• If we condition and y, x and z are independent

$$p(x, z|y) = \frac{p(x)p(y|x)p(z|y)}{p(y)}$$
$$= \frac{p(x, y)p(z|y)}{p(y)}$$
$$\times \mathcal{M} \neq = p(x|y)p(z|y)$$

Common cause

• Consider the "tent"

$$p(x, y, z) = p(y)p(x|y)p(z|y)$$

Conditioning on Y makes X and Z independent

$$p(x, z|y) = \frac{p(x, y, z)}{p(y)}$$
$$= \frac{p(y)p(x|y)p(z|y)}{p(y)} = p(x|y)p(z|y)$$

V-structure (common effect)

• Consider the v-structure

X

$$p(x, y, z) = p(x)p(z)p(y|x, z)$$

• X and Z are unconditionally independent

$$p(x,z) = \sum_{y} p(x,y,z) = \sum_{y} p(x)p(z)p(y|x,z) = p(x)p(z)$$

but are conditionally dependent

$$p(x, z|y) = \frac{p(x)p(z)p(y|x, z)}{p(y)} \neq f(x)g(z)$$

Explaining away

• Consider the v-structure

- Let X, $Z \in \{0,1\}$ be iid coin tosses.
- Let Y = X + Z.

0

XIF

• If we observe Y, X and Z are coupled.

XXZIT

Explaining away

- Let Y = 1 iff burglar alarm goes off,
- X=1 iff burglar breaks in
- Z=1 iff earthquake occurred



- X and Z compete to explain Y, and hence become dependent
- Intuitively, p(X=1|Y=1) > p(X=1|Y=1,Z=1)

Bayes Ball Algorithm

• $X_A \perp X_B \mid X_C$ if we cannot get a ball from any node in A to any node in B when we shade the variables in C. Balls can get blocked as follows.



Boundary conditions (source X = destn Z)





V-structure First X->Y then Y <- Z





Tent First X <- Y then Y -> Z





 $X_1 \perp X_6 \mid X_2, X_3 ?$





X2 1 X3 / X1, X6 ?

Markov blankets for DAGs

- The Markov blanket of a node is the set that renders it independent of the rest of the graph. $MB(X) = \text{minimal set } Us.t.X \perp X \setminus \{X\} \setminus U|U$
- This is the parents, children and co-parents.

$$p(X_{i}|X_{-i}) = \frac{p(X_{i}, X_{-i})}{\sum_{x} p(X_{i}, X_{-i})}$$

$$= \frac{p(X_{i}, U_{1:n}, Y_{1:m}, Z_{1:m}, R)}{\sum_{x} p(x, U_{1:n}, Y_{1:m}, Z_{1:m}, R)}$$

$$= \frac{p(X_{i}|U_{1:n})[\prod_{j} p(Y_{j}|X_{i}, Z_{j})]P(U_{1:n}, Z_{1:m}, R)}{\sum_{x} p(X_{i} = x|U_{1:n})[\prod_{j} p(Y_{j}|X_{i} = x, Z_{j})]P(U_{1:n}, Z_{1:m}, R)}$$

$$= \frac{p(X_{i}|U_{1:n})[\prod_{j} p(Y_{j}|X_{i} = x, Z_{j})]P(U_{1:n}, Z_{1:m}, R)}{\sum_{x} p(X_{i} = x|U_{1:n})[\prod_{j} p(Y_{j}|X_{i} = x, Z_{j})]}$$

 $p(X_i|X_{-i}) \propto p(X_i|Pa(X_i)) \prod_{Y_j \in ch(X_i)} p(Y_j|Pa(Y_j))$

Useful for Gibbs sampling

Another example



Red node (X8) indep of rest (black) given MB (blue parents, green children, pink co-parents)

Active trails

- Whenever influence can flow from to Y via Z, we say that the trail X <-> Y <-> Z is active.
- Causal trail: X -> Z -> Y. Active iff Z not obs.
- Evidential trail: X <- Z <- Y. Active iff Z not obs
- Common cause: X <- Z -> Y. Active iff Z not obs
- Common effect; X -> Z <- Y. Active iff either Z or one of its descendants is observed.
- Def 3.3.1. Let G be a BN structure, and X1 <-> ... <-> Xn be a trail in G. Let E be a subset of nodes. The trail is active given E if
- Whenever we have a v-structure X_{i-1} -> X_i <- X_{i+1}, then X_i or one of its desc is in E
- No other node along the trail is in E

Example

- D-> G <- I -> S not active for E={}
- D-> G <- I ->S is active for E={L}
- D-> G <- I ->S not active for E={L,I}
- Non-monotonic



d-separation

Def 3.3.2, We say X and Y are d-separated given Z, denoted d-sep_G(X;Y|Z), if there is no active trail between any node in X to any node in Y, given Z. The set of such independencies is denoted

 $I(G) = \{ X \perp Y | Z : \mathsf{dsep}_G(X; Y | Z) \}$

- Thm 3.3.3. (Soundness of dsep). If P factorizes according to G, then $I(G) \subseteq I(P)$.
- False thm (completeness of dsep). For any P that factorizes according to G, if $X \perp Y \mid Z$ in I(P), then desp_G(X;Y|Z) (i.e., P is faithful to G)

Faithfulness

- Def 3.3.4. A distribution P is faithful to G if, whenever X ⊥ Y
 | Z in I(P), we have dsep_G(X;Y|Z) i.e., there are no "non-graphical" independencies buried in the parameters
- A simple unfaithful distribution, with Imap A->B:

Such distributions are "rare"

 Thm 3.3.7. For almost all distributions P that factorize over G (ie except for a set of measure zero in the space of CPD parameterizations), we have that I(P)=I(G)

Markov equivalence

- A DAG defines a set of distributions. Different DAGs may encode the same set and hence are indistinguishable given observational data.
- Def 3.3.10. DAGs G1 and G2 are I-equivalent if I(G1)=I(G2). The set of all DAGs can be partitioned into I-equivalence classes.

Identifying I-equivalence

- Def 3.3.11. The skeleton of a DAG is an undirected graph obtained by dropping the arrows.
- Thm 3.3.12. If G1 and G2 have the same skeleton and the same v-structures, they are I-equivalent.
- However, there are structures that are I-equiv but do not have same v-structures (eg fully connected DAG).
- Def 3.3.13. A v-structure X->Z<-Y is an immorality if there is no edge between X and Y (unmarried parents who have a child)
- Thm 3.3.14. G1 and G2 have the same skeleton and set of immoralities iff they are I-equiv.







I Rit Tritit

l't *P*^ℓ



59

Markov properties of DAGs

- DF: F factorizes over G
- DG: $I(G) \subseteq I(P)$
- DL: $I_I(G) \subseteq I(P)$



Outline

- Administrivia
- Overview
- Local markov property, factorization (3.2)
- Global markov property (3.3)
- \rightarrow Deriving graphs from distributions (3.4)

Deriving graphs from distributions

- So far, we have discussed how to derive distributions from graphs.
- But how do we get the DAG?
- Assume we have access to the true distribution P, and can answer questions of the form

 $P \models X \perp Y | Z$

- For finite data samples, we can approximate this oracle with a CI test – the frequentist approach to graph structure learning (see ch 18)
- What DAG can be used to represent P?

Minimal I-map

- The complete DAG is an I-map for any distribution (since it encodes no CI relations)
- Def 3.4.1. A graph K is a minimal I-map for a set of independencies I if it is an I-map for I, and if the removal of even a single edge from K renders it not an I-map.
- To derive a minimal I-map, we pick an arbitrary node ordering, and then find some minimal subset U to be X_i's parents, where

 $X_i \perp \{X_1, \ldots, X_{i-1}\} \setminus U | U$

• (K2 algorithm replace this CI test with a Bayesian scoring metric: sec 18.4.2).

Effect of node ordering

- "Bad" node orderings can result in dense, unintuitive graphs.
- Eg L,S,G,I,D. Add L. Add S: must add L as parent, since $P \not\models L \perp S$ Add G: must add L,S as parents.



Figure 3.8 Three minimal 1-maps for $P_{electrat}$, induced by different orderings: [4] D, I, S, G, L [6] L, S, G, I, D [C] L, D, S, I, G

Perfect maps

- Minimal I-maps can have superfluous edges.
- Def 3.4.2. Graph K is a perfect map for a set of independencies I if I(K)=I. K is a perfect map for P if I(K)=I(P).
- Not all distributions can be perfectly represented by a DAG.
- Eg let Z = xor(X,Y) and use some independent prior on X, Y. Minimal I-map is X -> Z <- Y. However, X ⊥ Z in I(P), but not in I(G).
- Eg. A \perp C | {B,D} and B \perp D | {A,C}



Finding perfect maps

- If P has a perfect map, we can find it in polynomial time, using an oracle for the CI tests.
- We can only identify the graph up to I-equivalence, so we return the PDAG that represents the corresponding equivalence class.
- The method* has 3 steps (see sec 3.4.3)
 - Identify undirected skeleton
 - Identify immoralities
 - Compute eclass (compelled edges)
- This algorithm has been used to claim one can infer causal models from observational data, but this claim is controversial

Algorithm due to Verma & Pearl 1991, Spirtes, Glymour, Scheines 1993, Meek 1995