Probabilistic graphical models
CPSC 532c (Topics in AI)
Stat 521a (Topics in multivariate analysis)

Lecture 3

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Monday 20 September, 2004

Administrivia

- Spare stapled copies of the book chapters are outside my door (107). If you take the last unstapled copy, please photocopy and return to the door.
- Please send me comments on the book (errors, unclear parts) in one text file at the end of the semester.
- Mark Crowley is our TA. He will hold a regular discussion section on Fridays 1-2pm, CICSR 304. He will give a Matlab tutorial in the first meeting.

Review: independence properties of DAGs

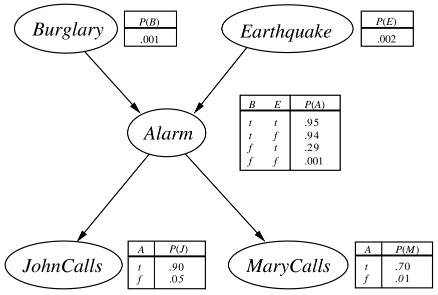
- Defn: let $I_l(G)$ be the set of local independence properties encoded by DAG G, namely:

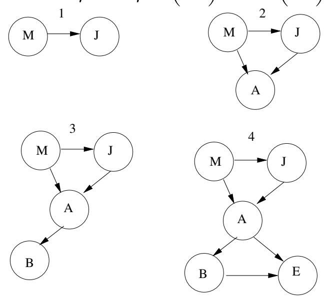
$$\{X_i \perp \text{NonDescendants}(X_i) | \text{Parents}(X_i)\}$$

- Defn: A DAG G is an **I-map** (independence-map) of P if $I_l(G) \subseteq I(P)$.
- A fully connected DAG G is an I-map for any distribution, since $I_l(G) = \emptyset \subseteq I(P)$ for any P.
- Defn: A DAG G is a **minimal I-map** for P if it is an I-map for P, and if the removal of even a single edge from G renders it not an I-map.
- **To construct a minimal I-map**, Pick a node ordering, then let the parents of node X_i be the minimal subset $U \subseteq \{X_1, \ldots, X_{i-1}\}$ s.t. $X_i \perp \{X_1, \ldots, X_i - 1\} \setminus U | U$.

A distribution may have several minimal I-maps

- Suppose the left DAG G perfectly captures all and only the independence properties of some distribution P, i.e., $I(G) = I(P)$.

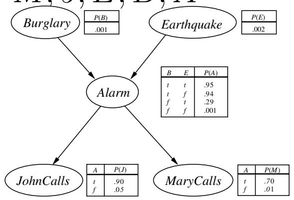


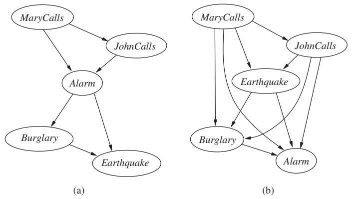


- Now consider a different node ordering: M, J, A, B, E.
- Consider adding parents to node B. Ancestors are M, J, A. We choose A as smallest parent set since $B \perp_G \{M, J\} | A$.

A distribution may have several minimal I-maps

- Order B, E, A, J, M
- Order M, J, A, B, E
- Order M, J, E, B, A

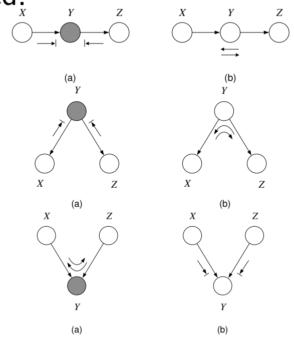




- **All represent exactly the same joint distribution**, but some orderings are better in terms of
  - Representation: easier to understand
  - Inference: faster to compute $P(X_q|x_v)$.
  - Learning: fewer parameters

Global Markov properties of DAGs

- X is **d-separated** (directed-separated) from Y given Z if we can't send a ball from any node in X to any node in Y, where all nodes in Z are shaded.



- Defn: $I(G)$ = all independence properties that correspond to d-separation:

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

Soundness and completeness of d-separation

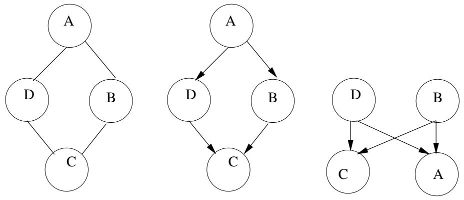
- Defn: P **factorizes over** DAG G if it can be represented as

$$P(X_1, \ldots, X_n) = \prod_i P(X_i|X_{\pi_i})$$

- Thm 3.3.3 (soundness): If P factorizes over G, then $I(H) \subseteq I(P)$.
- Thm 3.3.5 (completeness): If $\neg dsep_G(X; Y|Z)$, then $X \not\perp_P Y|Z$ in some P that factorizes over G.

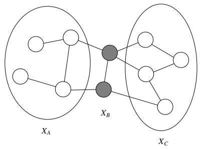
P-maps

- Defn: A DAG G is a **perfect map (P-map)** for a distribution P if $I(P) = I(G)$.
- Thm: not every distribution has a perfect map.
- Pf by counterexample. Suppose we have a model where $A \perp C|\{B, D\}$, and $B \perp D|\{A, C\}$. This cannot be represented by any Bayes net.
- e.g., BN1 wrongly says $B \perp D|A$, BN2 wrongly says $B \perp D$.



Undirected Graphical Models

- Graphs where nodes = random variables, and edges = correlation (direct dependence).
- Defn: Let H be an undirected graph. Then $sep_H(A; C|B)$ iff all paths between A and C go through some nodes in B (simple graph separation).



- Defn: the **global Markov properties** of a UG H are

$$I(H) = \{(X \perp Y|Z) : sep_H(X; Y|Z)\}$$

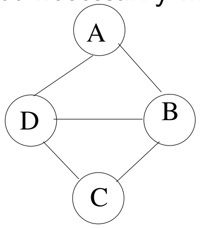
- UGMs also called Markov Random Fields (MRFs) or Markov Networks.

Parameterizing undirected graphical models

- An undirected graph H specifies a **family** of distributions s.t., $I(H) \subseteq I(P)$.
- To specify a *particular* distribution P, we need to add parameters to the graph.
- For Bayes nets, we used **conditional probability distributions (CPDs)**, $P(X_i|X_{\pi_i})$, where $\sum_{X_i} P(X_i|X_{\pi_i}) = 1$.
- For Markov nets, we use **potential functions** or **factors** defined on subsets of completely connected sets of nodes, where $\psi_c(X_c) > 0$.

Cliques

- Defn: a complete subgraph is a fully interconnected set of nodes.
- Defn: a (maximal) clique C is a complete subgraph s.t. any superset $C' \supset C$ is not complete.
- Defn: a sub-clique is a not-necessarily-maximal clique.



- Example: max-cliques = $\{A, B, D\}, \{B, C, D\}$, sub-cliques = edges = $\{A, D\}, \{A, B\}, \ldots$

Undirected graphical models

- Defn: an **undirected graphical model** representing a distribution $P(X_1, \ldots, X_n)$ is an undirected graph H, and a set of positive **potential functions** ψ_c associated with sub-cliques of H, s.t.

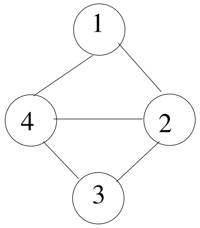
$$P(X_1, \ldots, X_n) = \frac{1}{Z} \prod_{c \in C} \psi_c(x_c)$$

where Z is the **partition function**:

$$Z = \sum_{x_1, \ldots, x_n} \prod_{c \in C} \psi_c(x_c)$$

- Defn: if H is a UGM for P, we say that P **factorizes over** H, or that P **is a Gibbs distribution over** H.

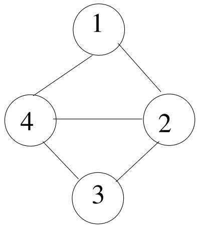
Example of UGM - max cliques



$$P(x_{1:4}) = \frac{1}{Z}\psi_{124}(x_{124}) \times \psi_{234}(x_{234})$$
$$Z = \sum_{x_1,x_2,x_3,x_4} \psi_{124}(x_{124}) \times \psi_{234}(x_{234})$$

- We can represent $P(X_{1:4})$ as two 3D tables instead of one 4D table.

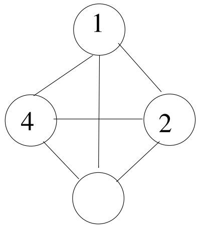
Example of UGM - subcliques



$$\begin{aligned} P(x_{1:4}) &= \frac{1}{Z} \prod_{<ij>} \psi_{ij}(x_{ij}) \\ &= \frac{1}{Z}\psi_{12}(x_{12})\psi_{14}(x_{14})\psi_{23}(x_{23})\psi_{24}(x_{24})\psi_{34}(x_{34}) \\ Z &= \sum_{x_1,x_2,x_3,x_4} \prod_{<ij>} \psi_{ij}(x_{ij}) \end{aligned}$$

- We can represent $P(X_{1:4})$ as five 2D tables instead of one 4D table.

Max cliques vs sub cliques



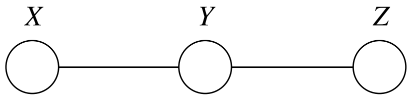
- Max clique version

$$P(X_{1:4}) = \frac{1}{Z}\psi_{1234}(X_{1234})$$

- Sub clique version

$$\begin{aligned} P(X_{1:4}) &= \frac{1}{Z} \prod_{<ij>} \psi_{ij}(x_i, x_j) \\ &= \frac{1}{Z}\psi_{12}(x_{12})\psi_{13}(x_{13})\psi_{14}(x_{14})\psi_{23}(x_{23})\psi_{24}(x_{24})\psi_{34}(x_{34}) \end{aligned}$$

Interpretation of Clique Potentials



- The model implies $\mathbf{x} \perp \mathbf{z} \mid \mathbf{y}$

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

- We can write this as:

$$\begin{aligned} p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x}, \mathbf{y})p(\mathbf{z}|\mathbf{y}) = \psi_{\mathbf{xy}}(\mathbf{x}, \mathbf{y})\psi_{\mathbf{yz}}(\mathbf{y}, \mathbf{z}) \\ p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x}|\mathbf{y})p(\mathbf{z}, \mathbf{y}) = \psi_{\mathbf{xy}}(\mathbf{x}, \mathbf{y})\psi_{\mathbf{yz}}(\mathbf{y}, \mathbf{z}) \end{aligned}$$

cannot have all potentials be marginals
cannot have all potentials be conditionals

- The positive clique potentials can only be thought of as general "compatibility", "goodness" or "happiness" functions over their variables, but not as probability distributions.

Boltzmann Distributions/ log-linear models

- We often represent the clique potentials using their logs:

$$\psi_C(\mathbf{x}_C) = \exp\{-H_C(\mathbf{x}_C)\}$$

for arbitrary real valued "energy" functions $H_C(\mathbf{x}_C)$.
The negative sign is a standard convention.

- This gives the joint a nice additive structure:

$$\mathsf{P}(\mathbf{X}) = \frac{1}{Z}\exp\{-\sum_{\text{cliques } C} H_C(\mathbf{x}_c)\} = \frac{1}{Z}\exp\{-H(\mathbf{X})\}$$

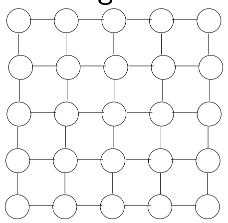
where the sum in the exponent is called the "free energy":

$$H(\mathbf{X}) = \sum_C H_C(\mathbf{x}_c)$$

- In physics, this is called the "Boltzmann distribution".
- In statistics, this is called a log-linear model.

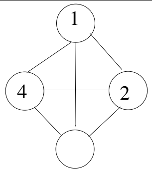
Example: Ising (spin-glass) models

- Nodes are arranged in a regular topology (often a regular packing grid) and connected only to their geometric neighbours.



- Same as sparse Boltzmann machine, where $V_{ij} \neq 0$ iff i, j are neighbors.
- e.g., nodes are pixels, potential function encourages nearby pixels to have similar intensities.
- Potts model = multi-state Ising model.

Example: Boltzmann machines



- A fully connected graph with pairwise (edge) potentials on binary-valued nodes (for $x_i \in \{-1,+1\}$ or $x_i \in \{0,1\}$) is called a **Boltzmann machine**.

$$P(X_{1:4}) = \frac{1}{Z}\prod_{<ij>} \psi_{ij}(x_i, x_j)$$

- where $\psi_{ij}(x_i, x_j) = exp(-H_{ij}(x_i, x_j))$, and

$$H(x_i, x_j) = (x_i - \mu_i)V_{ij}(x_j - \mu_j)$$

- Hence overall energy has form

$$H(x) = \sum_{ij} V_{ij}x_i x_j + \sum_i \alpha_i x_i + C$$

Example: multivariate Gaussian Distribution

- A Gaussian distribution can be represented by a fully connected graph with pairwise (edge) potentials of the form

$$H(\mathbf{x}) = \sum_{ij}(\mathbf{x}_i - \mu_i)V_{ij}(\mathbf{x}_j - \mu_j)$$

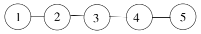
where μ is the mean and V is the inverse covariance (precision) matrix, since

$$P(x_{1:n}) = \frac{1}{Z}e^{-H(x)}$$

- Same as Boltzmann machine except $x_i \in R$.

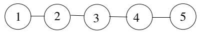
Sparse graph $\equiv$ zeros in precision matrix

- $V_{ij} = 0$ iff no edge between X_i and X_j.
- Chain structured graph $\equiv$ block diagonal precision matrix



$$V = \Sigma^{-1} = \begin{pmatrix} \cdot & \cdot & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & 0 & 0 \\ 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot \end{pmatrix}$$

Sparse precision $\not\Rightarrow$ sparse covariance



$$\Sigma^{-1} = \begin{pmatrix} 1 & 6 & 0 & 0 & 0 \\ 6 & 2 & 7 & 0 & 0 \\ 0 & 7 & 3 & 8 & 0 \\ 0 & 0 & 8 & 4 & 9 \\ 0 & 0 & 0 & 9 & 5 \end{pmatrix} \quad \Sigma = \begin{pmatrix} 0.10 & 0.15 & -0.13 & -0.08 & 0.15 \\ 0.15 & -0.03 & 0.02 & 0.01 & -0.03 \\ -0.13 & 0.02 & 0.10 & 0.07 & -0.12 \\ -0.08 & 0.01 & 0.07 & -0.04 & 0.07 \\ 0.15 & -0.03 & -0.12 & 0.07 & 0.08 \end{pmatrix}$$

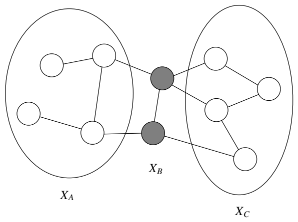
$$\begin{aligned} \Sigma^{-1}_{13} = 0 &\iff X_1 \perp X_3 | X_{nbrs(1)} \\ &\iff X_1 \perp X_3 | X_2 \\ &\not\Rightarrow X_1 \perp X_3 \\ &\iff \Sigma_{13} = 0 \end{aligned}$$

Graphs and distributions

- Let us return to the question of what kinds of distributions can be represented by undirected graphs (ignoring the details of the paticular parameterization).
- Defn: the **global Markov properties** of a UG H are

$$I(H) = \{(X \perp Y | Z) : sep_H(X; Y|Z)\}$$

- Is this definition sound and complete?



Soundness and completeness of global Markov property

- Defn: An UG H is an **I-map** for a distribution P if $I(H) \subseteq I(P)$, i.e., $P \models I(H)$.
- Defn: P is a **Gibbs distribution** over H if it can be represented as

$$P(X_1, \ldots, X_n) = \frac{1}{Z} \prod_{c \in C(H)} \psi_c(x_c)$$

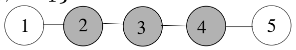
- Thm 5.4.2 (soundness): If P is a Gibbs distribution over H, then H is an I-map of P.
- Thm 5.4.3 (Hammersley-Clifford): Let P be a positive distribution (i.e., $\forall x. P(x) > 0$). If H is an I-map for P, then P can be represented as a Gibbs distribution over H.
- Thm 5.4.5 (completeness): If $\neg sep_H(X; Y|Z)$, then $X \not\perp_P Y|Z$ in some P that factorizes over H.

Local and global Markov properties

- For directed graphs, we defined I-maps in terms of local Markov properties, and derived global independence.
- For undirected graphs, we defined I-maps in terms of global Markov properties, and will now derive local independence.
- Defn: The **pairwise markov independencies** associated with UG $H = (V, E)$ are

$$I_p(H) = \{(X \perp Y) | V \setminus \{X, Y\} : \{X, Y\} \notin E\}$$

- e.g., $X_1 \perp X_5 | \{X_2, X_3, X_4\}$



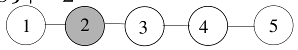
Local Markov properties

- Defn: The **local markov independencies** associated with UG $H = (V, E)$ are

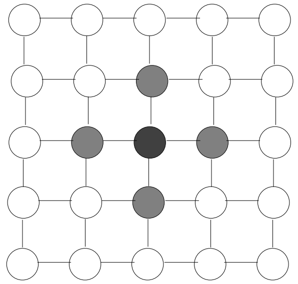
$$I_l(H) = \{(X \perp V \setminus \{X\} \setminus N_H(X) | N_H(X)) : X \in V\}$$

where $N_H(X)$ are the neighbors

- e.g., $X_1 \perp \{X_3, X_4, X_5\} | X_2$

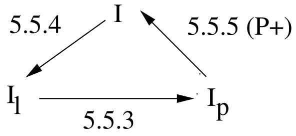


- $N_H(X)$ is also called the **Markov blanket** of X.



Relationship between local and global Markov properties

- Thm 5.5.3. If $P \models I_l(H)$ then $P \models I_p(H)$.
- Thm 5.5.4. If $P \models I(H)$ then $P \models I_l(H)$.
- Thm 5.5.5. If $P > 0$ and $P \models I_p(H)$, then $P \models I(H)$.
- Corollary 5.5.6: If $P > 0$, then $I_l = I_p = I$.
- If $\exists x. P(x) = 0$, then we can construct an example (using deterministic potentials) where $I_p \not\Rightarrow I_l$ or $I_l \not\Rightarrow I$.



I-maps for undirected graphs

- Defn: A Markov network H is a **minimal I-map** for P if it is an I-map, and if the removal of any edge from H renders it not an I-map.
- How can we construct a minimal I-map from a positive distribution P?
- Pairwise method: add edges between all pairs X,Y s.t.

$$P \not\models (X \perp Y | V \setminus \{X, Y\})$$

- Local method: add edges between X and all $Y \in MB_P(X)$, where $MB_P(X)$ is the minimal set of nodes U s.t.

$$P \models (X \perp V \setminus \{X\} \setminus U | U)$$

- Thm 5.5.11/12: both methods induce the unique minimal I-map.
- If $\exists x. P(x) = 0$, then we can construct an example where either method fails to induce an I-map.

Perfect maps

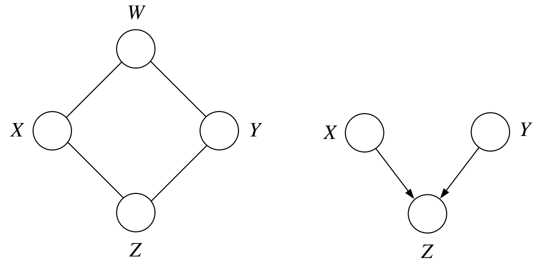
- Defn: A Markov network H is a **perfect map** for P if for any X, Y, Z we have that

$$sep_H(X;Y|Z) \iff P \models (X \perp Y|Z)$$

- Thm: not every distribution has a perfect map.
- Pf by counterexample. No undirected network can capture all and only the independencies encoded in a v-structure $X \rightarrow Z \leftarrow Y$.

Expressive Power

- Can we always convert directed $\leftrightarrow$ undirected?
- No.



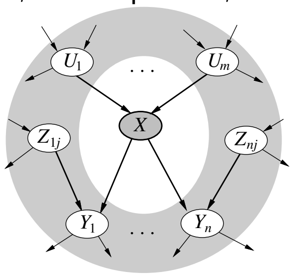
(a) (b)

No directed model can represent these and only these independencies.
$\mathbf{x} \perp \mathbf{y} \mid \{\mathbf{w}, \mathbf{z}\}$
$\mathbf{w} \perp \mathbf{z} \mid \{\mathbf{x}, \mathbf{y}\}$

No undirected model can represent these and only these independencies.
$\mathbf{x} \perp \mathbf{y}$

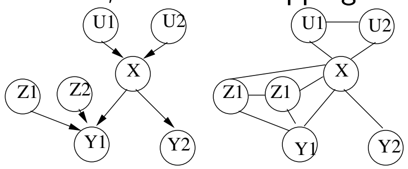
Converting Bayes nets to Markov nets

- Defn: A Markov net H is an I-map for a Bayes net G if $I(H) \subseteq I(G)$.
- We can construct a minimal I-map for a BN by finding the minimal Markov blanket for each node.
- We need to block all active paths coming into node X, from parents, children, and co-parents; so connect them all to X.



Moralization

- Defn: the moral graph $H(G)$ of a DAG is constructed by adding undirected edges between any pair of disconnected ("unmarried") nodes X,Y
  that are parents of a child Z, and then dropping all remaining arrows.

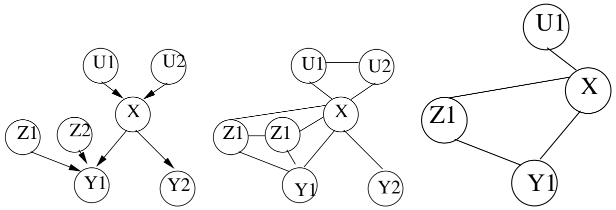


Moralization

- Thm 5.7.5: The moral graph $H(G)$ is the minimal I-map for Bayes net G.
- Pf: moralization loses conditional independence information, and hence is conservative; hence $H(G)$ is an I-map of G. Moralization only introduces where needed to make the semantics of simple separation capture d-separation, hence minimal.

Alternative to d-separation

- Thm 5.7.7. Let X, Y, Z be 3 disjoint sets of nodes in DAG G. Let $U = X \cup Y \cup Z$, let $G^+[U]$ be the induced DAG over Ancestors(U), and let $H' =$ moralize($G^+[U]$) be the moralized ancestral subgraph. Then $dsep_G(X;Y|Z) \iff sep_{H'}(X;Y|Z)$.
- Example: $dsep_G(Z_1;U_1|Y_1)$?



Bayes net to Markov net

- We assign each CPD to one of the clique potentials that contains it, e.g.

$$
\begin{aligned}
P(U,X,Y,Z) &= \frac{1}{Z}\psi(U,X) \times \psi(X,Y,Z) \\
&= \frac{1}{1}P(U)P(X|U) \times P(Y)P(Z|X,Y) \\
&= P(X,U) \times P(Z|X,Y)P(Y)
\end{aligned}
$$