

Probabilistic Graphical Models

Representation of undirected GM

Eric Xing Lecture 3, February 22, 2014



Reading: KF-chap4

Two types of GMs

• Directed edges give causality relationships (Bayesian Network or Directed Graphical Model):

 $P(X_{1}, X_{2}, X_{3}, X_{4}, X_{5}, X_{6}, X_{7}, X_{8})$

 $= P(X_1) P(X_2) P(X_3/X_1) P(X_4/X_2) P(X_5/X_2)$ $P(X_6/X_3, X_4) P(X_7/X_6) P(X_8/X_5, X_6)$



 Undirected edges simply give correlations between variables (Markov Random Field or Undirected Graphical model):

 $P(X_{1}, X_{2}, X_{3}, X_{4}, X_{5}, X_{6}, X_{7}, X_{8})$

$$= \frac{1/Z}{E(X_1) + E(X_2) + E(X_3, X_1) + E(X_4, X_2) + E(X_5, X_2)} + \frac{E(X_6, X_3, X_4) + E(X_7, X_6) + E(X_8, X_5, X_6)}{E(X_8, X_5, X_6)}$$



Review: independence properties of DAGs



 Defn: let *I*_l(*G*) be the set of local independence properties encoded by DAG *G*, namely:

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

- Defn: A DAG G is an I-map (independence-map) of P if I_l(G)⊆ I(P)
- A fully connected DAG *G* is an I-map for any distribution, since *I*_l(*G*)=∅⊆ *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.
- A distribution may have several minimal I-maps
 - Each corresponding to a specific node-ordering

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 as DAG.
 - Pf by counterexample. Suppose we have a model where $A \perp C \mid \{B, D\}$, and $B \perp D \mid \{A, C\}$.

This cannot be represented by any Bayes net.

• e.g., BN1 wrongly says $B \perp D \mid A$, BN2 wrongly says $B \perp D$.



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This cannot be represented by any Bayes net.

- e.g., BN1 wrongly says $B \perp D \mid A$, BN2 wrongly says $B \perp D$.
- The fact that G is a minimal I-map for P is far from a guarantee that G captures the independence structure in P
- The P-map of a distribution *is* unique up to I-equivalence between networks. That is, a distribution P can have many P-maps, but all of them are I-equivalent.

Undirected graphical models (UGM)





- Pairwise (non-causal) relationships
- Can write down model, and score specific configurations of the graph, but no explicit way to generate samples
- Contingency constrains on node configurations

A Canonical Examples: understanding complex scene ...







air or water ?

Canonical example

• The grid model



- Naturally arises in image processing, lattice physics, etc.
- Each node may represent a single "pixel", or an atom
 - The states of adjacent or nearby nodes are "coupled" due to pattern continuity or electro-magnetic force, etc.
 - Most likely joint-configurations usually correspond to a "low-energy" state

Social networks





The New Testament Social Networks



Protein interaction networks



Modeling Go



This is the middle position of a Go game. Overlaid is the estimate for the probability of becoming black or white for every intersection. Large squares mean the probability is higher.

Information retrieval



image

Representation



Defn: an undirected graphical model represents a distribution P(X₁,...,X_n) defined by an undirected graph H, and a set of positive *potential functions* y_c associated with the cliques of H, s.t.

$$P(x_1,\ldots,x_n) = \frac{1}{Z} \prod_{c \in C} \psi_c(\mathbf{x}_c)$$

where Z is known as the partition function:

$$Z = \sum_{x_1, \dots, x_n} \prod_{c \in C} \psi_c(\mathbf{x}_c)$$

- Also known as Markov Random Fields, Markov networks ...
- The *potential function* can be understood as an contingency function of its arguments assigning "pre-probabilistic" score of their joint configuration.

Global Markov Independencies

• Let *H* be an undirected graph:



- *B* separates *A* and *C* if every path from a node in *A* to a node in *C* passes through a node in *B*: $sep_H(A;C|B)$
- A probability distribution satisfies the *global Markov property* if for any disjoint *A*, *B*, *C*, such that *B* separates *A* and *C*, *A* is independent of *C* given *B*: $I(H) = \{A \perp C | B : sep_H(A; C | B)\}$

Local Markov independencies

• For each node $X_i \in \mathbf{V}$, there is *unique Markov blanket* of X_i , denoted MB_{Xi} , which is the set of neighbors of X_i in the graph (those that share an edge with X_i)

• Defn:

The local Markov independencies associated with H is:

$$I_{\ell}(H): \{X_i \perp \mathbf{V} - \{X_i\} - MB_{Xi} \mid MB_{Xi}: \forall i\},\$$

In other words, X_i is independent of the rest of the nodes in the graph given its immediate neighbors

Summary: Conditional Independence Semantics in an MRF



Structure: an *undirected* graph

- Meaning: a node is conditionally independent of every other node in the network given its Directed neighbors
- Local contingency functions (potentials) and the cliques in the graph completely determine the joint dist.
- Give correlations between variables, but no explicit way to generate samples



I. Quantitative Specification: Cliques



- For G={V,E}, a complete subgraph (clique) is a subgraph
 G'={V'⊆V,E'⊆E} such that nodes in V' are fully interconnected
- A (maximal) clique is a complete subgraph s.t. any superset
 V"⊃V' is not complete.
- A sub-clique is a not-necessarily-maximal clique.



- Example:
 - max-cliques = {*A*,*B*,*D*}, {*B*,*C*,*D*},
 - sub-cliques = $\{A, B\}, \{C, D\}, \dots \rightarrow$ all edges and singletons

Gibbs Distribution and Clique Potential



• Defn: an undirected graphical model represents a distribution $P(X_1, ..., X_n)$ defined by an undirected graph H, and **a set** of positive **potential functions** ψ_c associated with cliques of H, s.t.

$$P(x_1,\ldots,x_n) = \frac{1}{Z} \prod_{c \in C} \psi_c(\mathbf{x}_c)$$

(A Gibbs distribution)

where Z is known as the partition function:

$$Z = \sum_{x_1, \dots, x_n} \prod_{c \in C} \psi_c(\mathbf{x}_c)$$

- Also known as Markov Random Fields, Markov networks ...
- The *potential function* can be understood as an contingency function of its arguments assigning "pre-probabilistic" score of their joint configuration.



Interpretation of Clique Potentials



• The model implies X⊥Z|Y. This independence statement implies (by definition) that the joint must factorize as:

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

• We can write this as:

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

- **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.

Example UGM – using max cliques





$$(x_{1}, x_{2}, x_{3}, x_{4}) = \frac{-\psi_{c}(\mathbf{x}_{124}) \times \psi_{c}(\mathbf{x}_{234})}{Z}$$
$$Z = \sum_{x_{1}, x_{2}, x_{3}, x_{4}} \psi_{c}(\mathbf{x}_{124}) \times \psi_{c}(\mathbf{x}_{234})$$

• For discrete nodes, we can represent $P(X_{1:4})$ as two 3D tables instead of one 4D table



Example UGM – using subcliques



- We can represent $P(X_{1:4})$ as 5 2D tables instead of one 4D table
- Pair MRFs, a popular and simple special case
- I(P') vs. I(P") ? D(P') vs. D(P")

Example UGM – canonical representation





 $P(x_{1}, x_{2}, x_{3}, x_{4})$ $= \frac{1}{Z} \psi_{c}(\mathbf{x}_{124}) \times \psi_{c}(\mathbf{x}_{234})$ $\times \psi_{12}(\mathbf{x}_{12}) \psi_{14}(\mathbf{x}_{14}) \psi_{23}(\mathbf{x}_{23}) \psi_{24}(\mathbf{x}_{24}) \psi_{34}(\mathbf{x}_{34})$ $\times \psi_{1}(x_{1}) \psi_{2}(x_{2}) \psi_{3}(x_{3}) \psi_{4}(x_{4})$

 $\begin{aligned}
& \psi_c(\mathbf{x}_{124}) \times \psi_c(\mathbf{x}_{234}) \\
Z &= \sum_{x_1, x_2, x_3, x_4} & \times \psi_{12}(\mathbf{x}_{12}) \psi_{14}(\mathbf{x}_{14}) \psi_{23}(\mathbf{x}_{23}) \psi_{24}(\mathbf{x}_{24}) \psi_{34}(\mathbf{x}_{34}) \\
& \times \psi_1(x_1) \psi_2(x_2) \psi_3(x_3) \psi_4(x_4)
\end{aligned}$

- Most general, subsume P' and P" as special cases
- I(P) vs. I(P') vs. I(P")
 D(P) vs. D(P') vs. D(P")



Hammersley-Clifford Theorem

• If arbitrary potentials are utilized in the following product formula for probabilities,

$$P(x_1, \dots, x_n) = \frac{1}{Z} \prod_{c \in C} \psi_c(\mathbf{x}_c)$$
$$Z = \sum_{x_1, \dots, x_n} \prod_{c \in C} \psi_c(\mathbf{x}_c)$$

then the family of probability distributions obtained is exactly that set which **respects** the *qualitative specification* (the conditional independence relations) described earlier

• **Thm**: Let P be a positive distribution over V, and H a Markov network graph over V. If <u>H is an I-map for P</u>, then P is a Gibbs distribution over H.

II: Independence properties: global independencies



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

 $I(H) = \left\{ X \perp Z | Y \right\} : \operatorname{sep}_{H}(X; Z | Y) \right\}$



• 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* entails I(H).
- Defn: P is a Gibbs distribution over H if it can be represented as

$$P(\mathbf{x}_1,\ldots,\mathbf{x}_n) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \psi_c(\mathbf{x}_c)$$

- Thm (soundness): If *P* is a Gibbs distribution over *H*, then *H* is an I-map of *P*.
- Thm (completeness): If ¬sep_H(X; Z | Y), then X ∠_P Z | Y in some P that factorizes over H.

Local and global Markov properties revisit



- 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

 $\mathbf{I}_{p}(H) = \left\{ X \perp Y \middle| V \setminus \{X, Y\} : \{X, Y\} \notin E \right\}$

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



Local Markov properties

 A distribution has the *local Markov property* w.r.t. a graph *H*=(V,E) if the conditional distribution of variable given its neighbors is independent of the remaining nodes

 $\mathbf{I}_{l}(H) = \left\{ X \perp \mathbf{V} \setminus \left(X \cup N_{H}(X) \right) \middle| N_{H}(X) \right) : X \in \mathbf{V} \right\}$

- **Theorem** (Hammersley-Clifford): If the distribution is strictly positive and satisfies the local Markov property, then it factorizes with respect to the graph.
- $N_{H}(X)$ is also called the Markov blanket of X.



Relationship between local and global Markov properties

- Thm 5.5.5. If $P \models I_{l}(H)$ then $P \models I_{p}(H)$.
- Thm 5.5.6. If P = I(H) then $P = I_{I}(H)$.
- Thm 5.5.7. If P > 0 and $P \models I_p(H)$, then $P \models I(H)$.
- **Corollary (5.5.8):** The following three statements are equivalent for a *positive distribution* P:
 - $P \models I_{l}(H)$ $P \models I_{p}(H)$ $P \models I(H)$
 - This equivalence relies on the positivity assumption.
 - We can design a distribution locally

Perfect maps

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

$$\operatorname{sep}_{H}(X; Z | Y) \Leftrightarrow P \models (X \perp Z | Y)$$

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



Exponential Form



• Constraining clique potentials to be positive could be inconvenient (e.g., the interactions between a pair of atoms can be either attractive or repulsive). We represent a clique potential $\psi_c(\mathbf{x}_c)$ in an unconstrained form using a real-value "energy" function $\phi_c(\mathbf{x}_c)$:

$$\psi_c(\mathbf{x}_c) = \exp\{-\phi_c(\mathbf{x}_c)\}$$

For convenience, we will call $\phi_c(\mathbf{x}_c)$ a potential when no confusion arises from the context.

• This gives the joint a nice additive strcuture

$$p(\mathbf{x}) = \frac{1}{Z} \exp\left\{-\sum_{c \in C} \phi_c(\mathbf{x}_c)\right\} = \frac{1}{Z} \exp\left\{-H(\mathbf{x})\right\}$$

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

$$H(\mathbf{x}) = \sum_{c \in C} \phi_c(\mathbf{x}_c)$$

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

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Example: Boltzmann machines



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

$$P(x_1, x_2, x_3, x_4) = \frac{1}{Z} \exp\left\{\sum_{ij} \phi_{ij}(x_{ij}, x_j)\right\}$$
$$= \frac{1}{Z} \exp\left\{\sum_{ij} \theta_{ij} x_i x_j + \sum_i \alpha_i x_i + C\right\}$$

• Hence the overall energy function has the form:

$$H(x) = \sum_{ij} (x_i - \mu) \Theta_{ij} (x_j - \mu) = (x - \mu)^T \Theta(x - \mu)$$

Restricted Boltzmann Machines



 $p(x,h \mid \theta) = \exp \left\{ \sum_{i} \theta_{i} \phi_{i}(x_{i}) + \sum_{j} \theta_{j} \phi_{j}(h_{j}) + \sum_{i,j} \theta_{i,j} \phi_{i,j}(x_{i},h_{j}) - A(\theta) \right\}$

Restricted Boltzmann Machines



The Harmonium (Smolensky –'86)

hidden units





visible units

History:

Smolensky ('86), Proposed the architechture.

Freund & Haussler ('92), The "Combination Machine" (binary), learning with projection pursuit. Hinton ('02), The "Restricted Boltzman Machine" (binary), learning with contrastive divergence. Marks & Movellan ('02), Diffusion Networks (Gaussian).

Welling, Hinton, Osindero ('02), "Product of Student-T Distributions" (super-Gaussian)

Properties of RBM

- Factors are marginally dependent.
- Factors are conditionally *independent* given observations on the visible nodes.

 $P(\ell \mid \mathbf{w}) = \prod_{i} P(\ell_i \mid \mathbf{w})$

• Iterative Gibbs sampling.

• Learning with contrastive divergence



A Constructive Definition



A Constructive Definition



They map to the RBM random field:

$$p(x,h \mid \theta) = \exp\left\{ \sum_{i} \vec{\theta}_{i} \vec{f}_{i}(x_{i}) + \sum_{j} \vec{\lambda}_{j} \vec{g}_{j}(h_{j}) + \sum_{i,j} \vec{f}_{i}^{T}(x_{i}) \mathbf{W}_{i,j} \vec{g}_{j}(h_{j}) \right\}$$



An RBM for Text Modeling





 $h_j = 3$: topic j has strength 3 $h_j \in \mathbf{R}, \qquad \langle h_j \rangle = \Sigma_i W_{i,j} x_i$

 $x_i = n$: word i has count n

words counts

$$p(\mathbf{h} \mid \mathbf{x}) = \prod_{j} \operatorname{Normal}_{h_{j}} \left[\sum_{i} \vec{W}_{ij} \vec{x}_{i}, 1 \right]$$

$$p(\mathbf{x} \mid \mathbf{h}) = \prod_{i} \operatorname{Bi}_{x_{i}} \left[N, \frac{\exp(\alpha_{j} + \sum_{j} W_{ij} h_{j})}{1 + \exp(\alpha_{j} + \sum_{j} W_{ij} h_{j})} \right]$$

$$\Rightarrow p(\mathbf{x}) \propto \exp\left\{ \left(\sum_{i} \alpha_{i} x_{i} - \log \Gamma(x_{i}) - \log \Gamma(N - x_{i}) \right) + \frac{1}{2} \sum_{j} \left(\sum_{i} W_{i,j} x_{i} \right)^{2} \right\}$$

 $x_i \in \mathbf{I}$



Conditional Random Fields



• Discriminative

$$p_{\theta}(y \mid x) = \frac{1}{Z(\theta, x)} \exp\left\{\sum_{c} \theta_{c} f_{c}(x, y_{c})\right\}$$

• Doesn't assume that features are independent

• When labeling *X_i* future observations are taken into account

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Conditional Models



- Conditional probability *P*(label sequence y | observation sequence x) rather than joint probability *P*(y, x)
 - Specify the probability of possible label sequences given an observation sequence
- Allow arbitrary, non-independent features on the observation sequence X
- The probability of a transition between labels may depend on past and future observations
- Relax strong independence assumptions in generative models

Conditional Distribution



$$p_{\theta}(\mathbf{y} \mid \mathbf{x}) \propto \exp\left(\sum_{e \in E, k} \lambda_k f_k(e, \mathbf{y} \mid_e, \mathbf{x}) + \sum_{v \in V, k} \mu_k g_k(v, \mathbf{y} \mid_v, \mathbf{x})\right)$$

- x is a data sequence
- y is a label sequence
- *v* is a vertex from vertex set V = set of label random variables
- e is an edge from edge set E over V
- f_k and g_k are given and fixed. g_k is a Boolean vertex feature; f_k is a Boolean edge feature
- *k* is the number of features
- $\theta = (\lambda_1, \lambda_2, \dots, \lambda_n; \mu_1, \mu_2, \dots, \mu_n); \lambda_k \text{ and } \mu_k$ are parameters to be estimated
- y|_e is the set of components of y defined by edge e
- y|_v is the set of components of y defined by vertex v



Conditional Distribution (cont'd)



$$p_{\theta}(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z(\mathbf{x})} \exp\left(\sum_{e \in E,k} \lambda_k f_k(e, \mathbf{y} \mid_e, \mathbf{x}) + \sum_{v \in V,k} \mu_k g_k(v, \mathbf{y} \mid_v, \mathbf{x})\right)$$

• $Z(\mathbf{x})$ is a normalization over the data sequence \mathbf{x}

Conditional Random Fields



 $\boldsymbol{p}_{\theta}(\boldsymbol{y} \mid \boldsymbol{x}) = \frac{1}{Z(\theta, \boldsymbol{x})} \exp\left\{\sum_{c} \theta_{c} \boldsymbol{f}_{c}(\boldsymbol{x}, \boldsymbol{y}_{c})\right\}$

- Allow arbitrary dependencies on input
- Clique dependencies on labels
- Use approximate inference for general graphs

Summary

- Undirected graphical models capture "relatedness", "coupling", "co-occurrence", "synergism", etc. between entities
- Local and global independence properties identifiable via graph separation criteria
- Defined on clique potentials
- Generally intractable to compute likelihood due to presence of "partition function"
 - Therefore not only inference, but also likelihood-based learning is difficult in general
- Can be used to define either joint or conditional distributions
- Important special cases:
 - Ising models
 - RBM
 - CRF