## CS 3750 Machine Learning Lecture 5

## Markov Random Fields

Milos Hauskrecht
milos@cs.pitt.edu
5329 Sennott Square

## Markov random fields

- Probabilistic models with symmetric dependences.
- Typically models spatially varying quantities

$$
P(x) \propto \prod_{c \in c l(x)} \phi_{c}\left(x_{c}\right)
$$

$\phi_{c}\left(x_{c}\right)$ - A potential function (defined over factors)

- If $\phi_{c}\left(x_{c}\right)$ is strictly positive we can rewrite the definition as:
$P(x)=\frac{1}{Z} \exp \left(-\sum_{c \in c l(x)} E_{c}\left(x_{c}\right)\right) \quad$ - Energy function
- Gibbs (Boltzman) distribution
$Z=\sum_{x \in\{x\}} \exp \left(-\sum_{c \in c l(x)} E_{c}\left(x_{c}\right)\right) \quad$ - A partition function


## Graphical representation of MRFs

An undirected network (also called independence graph)

- $\mathrm{G}=(\mathrm{S}, \mathrm{E})$
- $\mathrm{S}=1,2$, .. N correspond to random variables
- $(i, j) \in E \Leftrightarrow \exists c:\{i, j\} \subset c$ or $\mathrm{x}_{\mathrm{i}}$ and $\mathrm{x}_{\mathrm{j}}$ appear within the same factor c


## Example:

- variables A,B ..H
- Assume the full joint of MRF

$$
\begin{aligned}
& P(A, B, \ldots H) \sim \\
& \phi_{1}(A, B, C) \phi_{2}(B, D, E) \phi_{3}(A, G) \\
& \quad \phi_{4}(C, F) \phi_{5}(G, H) \phi_{6}(F, H)
\end{aligned}
$$



## Markov random fields

- regular lattice (Ising model)

- Arbitrary graph



## Markov random fields

- Pairwise Markov property
- Two nodes in the network that are not directly connected can be made independent given all other nodes
- Local Markov property
- A set of nodes (variables) can be made independent from the rest of nodes variables given its immediate neighbors
- Global Markov property
- A vertex set A is independent of the vertex set B ( A and B are disjoint) given set C if all chains in between elements in A and B intersect C


## Types of Markov random fields

- MRFs with discrete random variables
- Clique potentials can be defined by mapping all cliquevariable instances to $R$
- Example: Assume two binary variables A,B with values $\{\mathrm{a} 1, \mathrm{a} 2, \mathrm{a} 3\}$ and $\{\mathrm{b} 1, \mathrm{~b} 2\}$ are in the same clique c . Then:
$\phi_{c}(A, B) \cong$

| a1 | b1 | 0.5 |
| :---: | :---: | :---: |
| a1 | b2 | 0.2 |
| a2 | b1 | 0.1 |
| a2 | b2 | 0.3 |
| a3 | b1 | 0.2 |
| a3 | b2 | 0.4 |

## Types of Markov random fields

- Gaussian Markov Random Field

$$
\begin{aligned}
& \mathbf{x} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \\
& p(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})=\frac{1}{(2 \pi)^{d / 2}|\boldsymbol{\Sigma}|^{1 / 2}} \exp \left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{T} \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]
\end{aligned}
$$

- Precision matrix $\boldsymbol{\Sigma}^{-1}$
- Variables in $x$ are connected in the network only if they have a nonzero entry in the precision matrix
- All zero entries are not directly connected
- Why?


## Tree decomposition of the graph

- A tree decomposition of a graph G:
- A tree $T$ with a vertex set associated to every node.
- For all edges $\{v, w\} \in \mathrm{G}$ :
 there is a set containing both $v$ and $w$ in $T$.
- For every $v \in \mathrm{G}$ : the nodes in T that contain $v$ form a connected subtree.



## Tree decomposition of the graph

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## Treewidth of the graph

- Width of the tree decomposition: $\max _{i \in I}\left|X_{i}\right|-1$
- Treewidth of a graph

$G: \operatorname{tw}(G)=$ minimum width over all tree decompositions of $G$.



## Trees

Why do we like trees?

- Inference in trees structures can be done in time linear in the number of nodes



## Clique tree

- Clique tree $=$ a tree decomposition of the graph
- Can be constructed:
- from the induced graph

Built by running the variable elimination procedure

- from the chordal graph

Built by running the triangulation algorithm

- We have precompiled the clique tree.
- So how to take advantage of the clique tree to perform inferences?


## VE on the Clique tree

- Variable Elimination on the clique tree
- works on factors
- Makes factor a data structure
- Sends and receives messages
- Cluster graph for set of factors, each node $i$ is associated with a subset (cluster) $\mathrm{C}_{\mathrm{i}}$.
- Family-preserving: each factor's variables are completely embedded in a cluster


## Clique tree properties

- Sepset $S_{i j}=C_{i} \cap C_{j}$
- separation set: Variables $\mathbf{X}$ on one side of sepset are separated from the variables $\mathbf{Y}$ on the other side in the factor graph given variables in $\mathbf{S}$
- Running intersection property
- if $\mathrm{C}_{\mathrm{i}}$ and $\mathrm{C}_{\mathrm{j}}$ both contain X , then all cliques on the unique path between them also contain X



## Message Passing VE

- Query for $\mathrm{P}(\mathrm{J})$
- Eliminate $\mathrm{C}: \quad \tau_{1}(D)=\sum_{C} \pi_{1}^{0}[C, D]$



## Message Passing VE

- Query for P(J)
- Eliminate D: $\tau_{2}(G, I)=\sum_{D} \pi_{2}[G, I, D]$


Message sent from [G,I,D] to [G,S,I]
Message received at [G,S,I] -[G,S,I] updates:

$\pi_{3}[G, S, I]=\tau_{2}(G, I) \times \pi_{3}^{0}[G, S, I]$

## Message Passing VE

- Query for $\mathrm{P}(\mathrm{J})$
- Eliminate I: $\tau_{3}(G, S)=\sum_{I} \pi_{3}[G, S, I]$

$$
\pi_{4}[G, J, S, L]=\tau_{3}(G, S) \times \pi_{4}^{0}[G, J, S, L]
$$

$$
[G, J, S, L] \text { is not ready! }
$$



## Message Passing VE

- Query for $\mathrm{P}(\mathrm{J})$
- Eliminate $\mathrm{H}: \tau_{4}(G, J)=\sum_{H} \pi_{5}[H, G, J]$


Message sent from [H,G,J] to $[G, J, S, L]$


H,G,J
$\pi_{4}[G, J, S, L]=\tau_{3}(G, S) \times \tau_{4}(G, J) \times \pi_{4}^{0}[G, J, S, L]$
And ...

## Message Passing VE

- Query for $\mathrm{P}(\mathrm{J})$
- Eliminate $\mathrm{K}: \quad \tau_{6}(S)=\sum_{K} \pi^{0}[S, K]$


All messages
received at [G,J,S,L] $\uparrow \mathbf{G}, \mathbf{J}$
[G,J,S,L] updates: H,G,J
$\pi_{4}[G, J, S, L]=\tau_{3}(G, S) \times \tau_{4}(G, J) \times \tau_{6}(S) \times \pi_{4}^{0}[G, J, S, L]$
And calculate $\mathbf{P ( J )}$ from it by summing out G,S,L

## Message Passing VE

- [G,J,S,L] clique potential
- ... is used to finish the inference



## Message passing VE

- Often, many marginals are desired
- Inefficient to re-run each inference from scratch
- One distinct message per edge \& direction
- Methods :
- Compute (unnormalized) marginals for any vertex (clique) of the tree
- Results in a calibrated clique tree $\sum_{C_{i}-S_{i j}} \pi_{i}=\sum_{C_{j}-S_{i j}} \pi_{j}$
- Recap: three kinds of factor objects
- Initial potentials, final potentials and messages


## Two-pass message passing VE

- Chose the root clique, e.g. [S,K]
- Propagate messages to the root



## Two-pass message passing VE

- Send messages back from the root


Notation:
number the cliques and denote the messages

$$
\delta_{i \rightarrow j}
$$

## Message Passing: BP

- Graphical model of a distribution
- More edges = larger expressive power
- Clique tree also a model of distribution
- Message passing preserves the model but changes the parameterization
- Different but equivalent algorithm


## Factor division



| $\mathrm{A}=1$ | $\mathrm{~B}=1$ | $0.5 / 0.4=1.25$ |
| :--- | :--- | :--- |
| $\mathrm{~A}=1$ | $\mathrm{~B}=2$ | $0.4 / 0.4=1.0$ |
| $\mathrm{~A}=2$ | $\mathrm{~B}=1$ | $0.8 / 0.4=2.0$ |
| $\mathrm{~A}=2$ | $\mathrm{~B}=2$ | $0.2 / 0.4=2.0$ |
| $\mathrm{~A}=3$ | $\mathrm{~B}=1$ | $0.6 / 0.5=1.2$ |
| $\mathrm{~A}=3$ | $\mathrm{~B}=2$ | $0.5 / 0.5=1.0$ |

Inverse of factor product

## Message Passing: BP

- Each node: multiply all the messages and divide by the one that is coming from node we are sending the message to - Clearly the same as VE

$$
\delta_{i \rightarrow j}=\frac{\sum_{C_{i}-S_{i j}} \pi_{i}}{\delta_{j \rightarrow i}}=\frac{\sum_{C_{i}-S_{i j}} \prod_{k \in N(i)} \delta_{k \rightarrow i}}{\delta_{j \rightarrow i}}=\sum_{C_{i}-S_{i j}} \prod_{k \in N(i) \backslash j} \delta_{k \rightarrow i}
$$

- Initialize the messages on the edges to 1


## Message Passing: BP



Store the last message on the edge and divide
$\delta_{2 \rightarrow 3}=\left(\sum_{B} \pi_{2}^{0}(B, C)\right)$ each passing message by the last stored.

$$
\begin{aligned}
& \pi_{3}(C, D)=\pi_{3}^{0}(C, D) \frac{\delta_{2 \rightarrow 3}}{\mu_{2,3}}=\pi_{3}^{0}(C, D) \sum_{B} \pi_{2}^{0}(B, C) \\
& \mu_{2,3}=\delta_{2 \rightarrow 3}=\left(\sum_{B} \pi_{2}^{0}(B, C)\right) \quad \text { New message }
\end{aligned}
$$

## Message Passing: BP



Store the last message on the edge and divide each passing message by the last stored.

$$
\begin{aligned}
& \pi_{3}(C, D)=\pi_{3}^{0}(C, D) \sum_{B} \pi_{2}^{0}(B, C)=\pi_{3}^{0}(C, D) \mu_{2,3} \\
& \delta_{3->2}=\left(\sum_{D} \pi_{3}(C, D)\right)
\end{aligned}
$$

$$
\pi_{2}(B, C)=\pi_{2}^{0}(B, C) \frac{\delta_{3 \rightarrow 2}}{\mu_{2,3}(C)}=\frac{\pi_{2}^{0}(B, C)}{\mu_{2,3}(C)} \times \sum_{D} \pi_{3}^{0}(C, D) \times \mu_{2,3}(C)=\pi_{2}^{0}(B, C) \times \sum_{D} \pi_{3}^{0}(C, D)
$$

$$
\mu_{2,3}=\delta_{3 \rightarrow 2}=\left(\sum_{D} \pi_{3}(C, D)\right)=\sum_{D} \pi_{3}^{0}(C, D) \sum_{B} \pi_{2}^{0}(B, C) \quad \text { New message }
$$

## Message Passing: BP



$$
\begin{aligned}
& \pi_{2}(B, C)=\pi_{2}^{0}(B, C) \times \sum_{D} \pi_{3}^{0}(C, D) \\
& \pi_{2}(B, C)=\pi_{2}(B, C) \frac{\delta_{3 \rightarrow 2}}{\mu_{2,3}(C)}=\pi_{2}(B, C) \times \frac{\sum_{D}^{D} \pi_{3}^{0}(C, D) \times \sum_{B} \pi_{2}^{0}(B, C)}{\sum_{D} \pi_{3}^{0}(C, D) \times \sum_{B} \pi_{2}^{0}(B, C)}=\pi_{2}(B, C)
\end{aligned}
$$

## Message Propagation: BP

- Lauritzen-Spiegelhalter algorithm
- Two kinds of objects: clique and sepset potentials
- Initial potentials not kept
- Improved "stability" of asynchronous algorithm (repeated messages cancel out)
- New distribution representation
- clique tree potential

$$
\pi_{T}=\frac{\prod_{C_{i} \in T} \pi_{i}\left(C_{i}\right)}{\prod_{\left(C_{i} \leftrightarrow C_{j}\right) \in T} \mu_{i j}\left(S_{i j}\right)}=P_{F}(X)
$$

- Clique tree invariant $=\mathrm{P}_{\mathrm{F}}$


## Loopy belief propagation

- The asynchronous BP algorithm works on clique trees
- What if we run the belief propagation algorithm on a non-tree structure?

- Sometimes converges
- If it converges it leads to an approximate solution
- Advantage: tractable for large graphs


## Loopy belief propagation

- If the BP algorithm converges, it converges to an optimum of the Bethe free energy
See papers:
- Yedidia J.S., Freeman W.T. and Weiss Y. Generalized Belief Propagation, 2000
- Yedidia J.S., Freeman W.T. and Weiss Y. Understanding Belief Propagation and Its Generalizations, 2001

