Graphical models

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Probabilistic modeling

- Given: several variables: $x_1, \ldots x_n$, n is large.
- Task: build a joint distribution function $\Pr(x_1, \ldots x_n)$
- Goal: Answer several kind of projection queries on the distribution

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- Task: build a joint distribution function $\Pr(x_1, \ldots x_n)$
- Goal: Answer several kind of projection queries on the distribution
- Basic premise
  - Explicit joint distribution is dauntingly large
  - Queries are simple marginals (sum or max) over the joint distribution.

Example

- Variables are attributes are people.

Age	Income	Experience	Degree	Location
10 ranges	7 scales	7 scales	3 scales	30 places

- An explicit joint distribution over all columns not tractable: number of combinations: $10 \times 7 \times 7 \times 3 \times 30 = 44100$.
- Queries: Estimate fraction of people with
  - Income $>$ 200K and Degree="Bachelors",
  - Income $<$ 200K, Degree="PhD" and experience $>$ 10 years.
  - Many, many more.

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  - Ad hoc methods of combining these into a single estimate
- Go beyond pairwise correlations: conditional independencies
  - income $\not\perp\!\!\!\perp$ age, but income $\perp\!\!\!\perp$ age $\mid$ experience
  - experience $\perp\!\!\!\perp$ degree, but experience $\not\perp\!\!\!\perp$ degree $\mid$ income

Graphical models make explicit an efficient joint distribution from these independencies

Graphical models

Model joint distribution over **several** variables as a product of smaller factors that is

1. *Intuitive* to represent and visualize
   - Graph: represent structure of dependencies
   - Potentials over subsets: quantify the dependencies
2. *Efficient* to query
   - given values of any variable subset, reason about probability distribution of others.
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Graphical models = graph theory + probability theory.

Graphical models in use

- Roots in statistical physics for modeling interacting atoms in gas and solids [1900]
- Early usage in genetics for modeling properties of species [1920]
- AI: expert systems (1970s-80s)
- Now many new applications:
  - Error Correcting Codes: Turbo codes, impressive success story (1990s)
  - Robotics and Vision: image denoising, robot navigation.
  - Text mining: information extraction, duplicate elimination, hypertext classification, help systems
  - Bio-informatics: Secondary structure prediction, Gene discovery
  - Data mining: probabilistic classification and clustering.

Part I: Outline

1. Representation
   - Directed graphical models: Bayesian networks
   - Undirected graphical models
2. Inference Queries
   - Exact inference on chains
   - Variable elimination on general graphs
   - Junction trees
3. Approximate inference
   - Generalized belief propagation
   - Sampling: Gibbs, Particle filters
4. Constructing a graphical model
   - Graph Structure
   - Parameters in Potentials
5. General framework for Parameter learning in graphical models
6. References

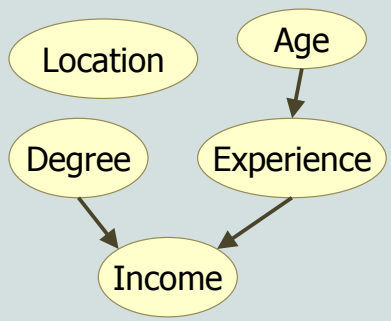
Representation

Structure of a graphical model: Graph + Potential

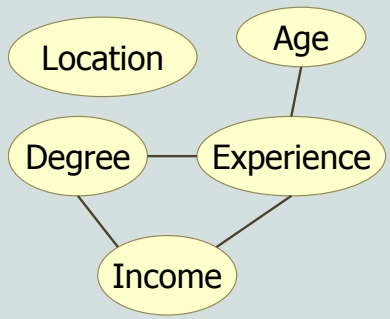
Graph

- Nodes: variables $\mathbf{x} = x_1, \ldots x_n$
  - Continuous: Sensor temperatures, income
  - Discrete: Degree (one of Bachelors, Masters, PhD), Levels of age, Labels of words
- Edges: direct interaction
  - Directed edges: Bayesian networks
  - Undirected edges: Markov Random fields

Directed



Undirected



Representation

Potentials: $\psi_c(\mathbf{x}_c)$

- Scores for assignment of values to subsets c of directly interacting variables.
- Which subsets? What do the potentials mean?
  - Different for directed and undirected graphs

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Probability

Factorizes as product of potentials

$$\Pr(\mathbf{x} = x_1, \ldots x_n) \propto \prod \psi_S(\mathbf{x}_S)$$

Directed graphical models: Bayesian networks

- Graph G: directed acyclic
  - Parents of a node: $\mathrm{Pa}(x_i) =$ set of nodes in G pointing to x_i

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$$\psi_i(x_i, \mathrm{Pa}(x_i)) = \Pr(x_i | \mathrm{Pa}(x_i)$$

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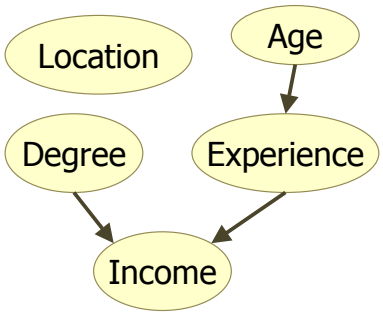
- Probability distribution

$$\Pr(x_1 \ldots x_n) = \prod_{i=1}^{n} \Pr(x_i|pa(x_i))$$

Example of a directed graph



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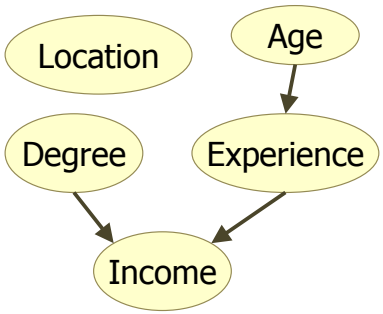

$\psi_1(L) = \Pr(L)$

NY	CA	London	Other
0.2	0.3	0.1	0.4

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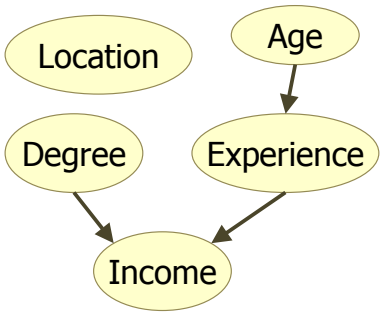

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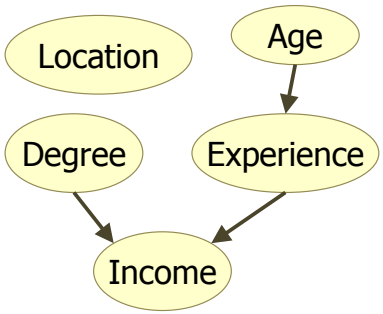

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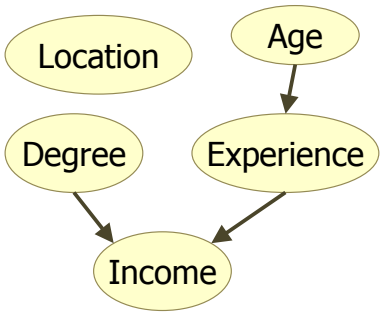

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$\psi_2(E, A) = \Pr(E|A)$

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30–45	0.4	0.5	0.1
$>$ **45**	0.1	0.1	0.8

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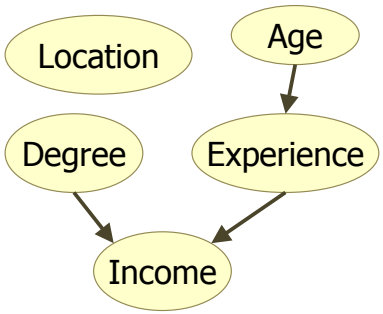

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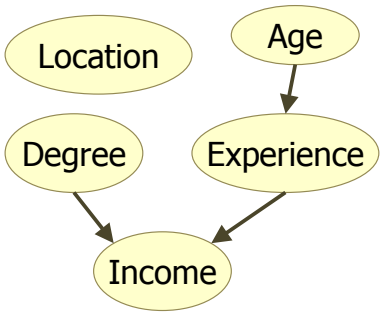
$\psi_2(I, E, D) = \Pr(I|D, A)$

3 dimensional table, or a histogram approximation.

Example of a directed graph



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Probability distribution

$$\Pr(\mathbf{x} = L, D, I, A, E) = \Pr(L)\Pr(D)\Pr(A)\Pr(E|A)\Pr(I|D, E)$$

Conditional Independencies

- Given three sets of variables X, Y, Z, set X is conditionally independent of Y given Z ($X \perp\!\!\!\perp Y|Z$) iff

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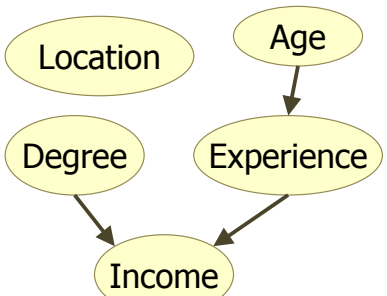
$$x_i \perp\!\!\!\perp ND(x_i)|Pa(x_i)$$

- $L \perp\!\!\!\perp E, D, A, I$
- $A \perp\!\!\!\perp L, D$
- $E \perp\!\!\!\perp L, D|A$
- $I \perp\!\!\!\perp A|E, D$



CIs and Factorization

Theorem

Local CI $\Longrightarrow$ *Factorization*

Proof.

- $x_1, x_2, \ldots, x_n$ topographically ordered (parents before children).
- Local CI: $\Pr(x_i|x_1, \ldots, x_{i-1}) = \Pr(x_i|Pa(x_i))$
- Chain rule:
  $\Pr(x_1, \ldots, x_n) = \prod_i \Pr(x_i|x_1, \ldots, x_{i-1}) = \prod_i \Pr(x_i|Pa(x_i))$

Global Cls in a BN

Three sets of variables X, Y, Z. If Z d-separates X from Y in BN then, $X \perp\!\!\!\perp Y | Z$.
In a directed graph H, Z d-separates X from Y if all paths P from any X to Y is blocked by Z.
A path P is blocked by Z when

1. $x_1 \rightarrow x_2 \rightarrow \ldots x_k$ and $x_i \in Z$
2. $x_1 \leftarrow x_2 \leftarrow \ldots x_k$ and $x_i \in Z$
3. $x_1 \ldots \leftarrow x_i \rightarrow \ldots x_k$ and $x_i \in Z$
4. $x_1 \ldots \rightarrow x_i \leftarrow \ldots x_k$ and $x_i \notin Z$ and $Desc(x_i) \notin Z$

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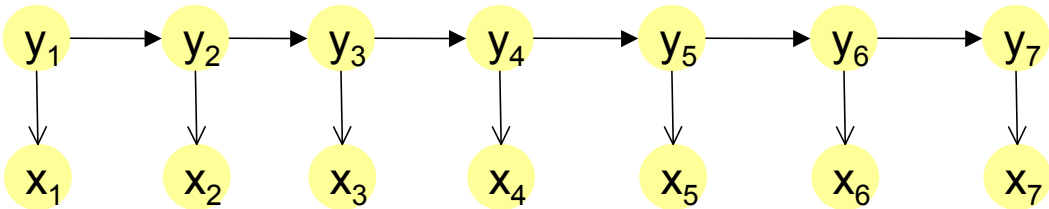
Theorem

The d-separation test identifies the complete *set of conditional independencies that hold in* all *distributions that conform to a given Bayesian network.*

Popular Bayesian networks

- Hidden Markov Models: speech recognition, information extraction



  - State variables: discrete phoneme, entity tag
  - Observation variables: continuous (speech waveform), discrete (Word)
- Kalman Filters: State variables: continuous
  - Discussed later
- Topic models for text data
  1. Principled mechanism to categorize multi-labeled text documents while incorporating priors in a flexible generative framework
  2. Application: news tracking
- QMR (Quick Medical Reference) system
- PRMs: Probabilistic relational networks:

Undirected graphical models

- Graph G: arbitrary undirected graph
- Useful when variables interact symmetrically, no natural parent-child relationship
- Example: labeling pixels of an image.
- Potentials $\psi_C(\mathbf{y}_C)$ defined on arbitrary cliques C of G.
- $\psi_C(\mathbf{y}_C)$: Any arbitrary non-negative value, cannot be interpreted as probability.

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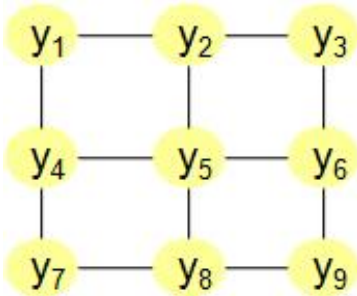

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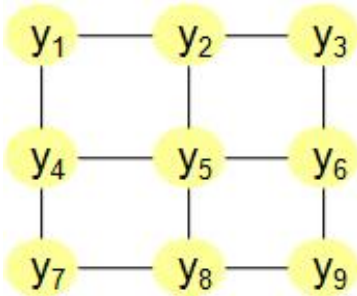
- Probability distribution

$$\Pr(y_1 \dots y_n) = \frac{1}{Z} \prod_{C \in G} \psi_C(\mathbf{y}_C)$$

where $Z = \sum_{\mathbf{y}'} \prod_{C \in G} \psi_C(\mathbf{y}'_C)$ (partition function)

Undirected graphical models



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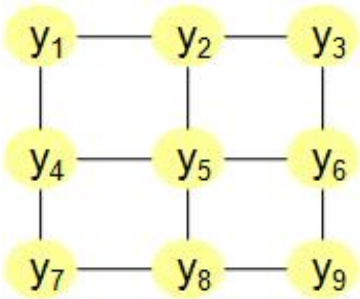

$y_i = 1$ (part of foreground), 0 otherwise.

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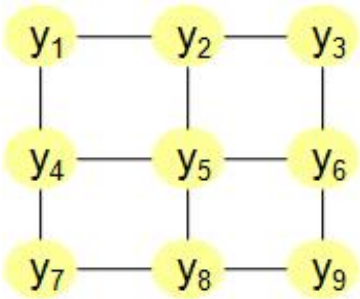

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- Node potentials
  - $\psi_1(0) = 4$, $\psi_1(1) = 1$
  - $\psi_2(0) = 2$, $\psi_2(1) = 3$
  - ....
  - $\psi_9(0) = 1$, $\psi_9(1) = 1$

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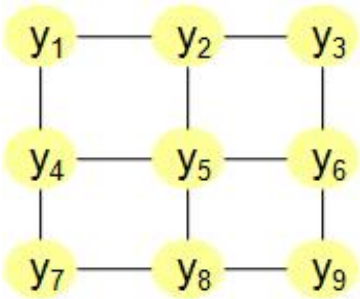

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- Edge potentials: Same for all edges
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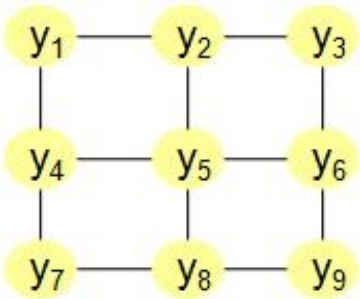

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  - $\psi(0,0) = 5$, $\psi(1,1) = 5$, $\psi(1,0) = 1, \psi(0,1) = 1$
- Probability: $\Pr(y_1 \dots y_9) \propto \prod_{k=1}^{9} \psi_k(y_k) \prod_{(i,j) \in E(G)} \psi(y_i, y_j)$

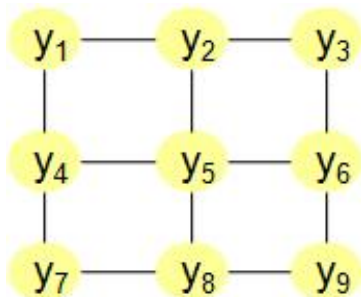
Conditional independencies (CIs) in an undirected graphical model

Let $V = \{y_1, \ldots, y_n\}$.

1. Local CI: $y_i \perp\!\!\!\perp V - ne(y_i) - \{y_i\} | ne(y_i)$
2. Pairwise CI: $y_i \perp\!\!\!\perp y_j | V - \{y_i, y_j\}$ if edge (y_i, y_j) does not exist.
3. Global CI: $X \perp\!\!\!\perp Y | Z$ if Z separates X and Y in the graph.

Equivalent when the distribution is positive.

1. $y_1 \perp\!\!\!\perp y_3, y_5 y_6, y_7, y_8, y_9 | y_2, y_4$
2. $y_1 \perp\!\!\!\perp y_3 | y_2, y_4, y_5, y_6, y_7, y_8, y_9$
3. $y_1, y_2, y_3 \perp\!\!\!\perp y_7, y_8, y_9 | y_4, y_5, y_6$



Relationship between Local-CI and Global-CI

Let G be a undirected graph over $V = x_1, \ldots, x_n$ nodes and $P(x_1, \ldots, x_n)$ be a distribution. If P satisfies Global-CIs of G, then P will also satisfy the local-CIs of G but the reverse is not always true.
We will show this with an example.
Consider a distribution over 5 binary variables: $P(x_1, \ldots, x_5)$ where $x_1 = x_2$, $x_4 = x_5$ and $x_3 = x_2 \mathrm{A}ND x_4$.
Let G be

$$x_1 \text{ ——— } x_2 \text{ ——— } x_3 \text{ ——— } x_4 \text{ ——— } x_5$$

All 5 local CIs in the graph: e.g. $x_1 \perp\!\!\!\perp \{x_3, x_4, x_5\} | x_2$ etc hold in the graph.
However, the global CI: $x_2 \perp\!\!\!\perp x_4 | x_3$ does not hold.

Relationship between Local-CI and Pairwise-CI

Let G be a undirected graph over $V = x_1, \ldots, x_n$ nodes and $P(x_1, \ldots, x_n)$ be a distribution. If P satisfies Local-CIs of G, then P will also satisfy the pairwise-CIs of G but the reverse is not always true. We will show this with an example.

Consider a distribution over 3 binary variables: $P(x_1, x_2, x_3)$ where $x_1 = x_2 = x_3$. That is, $P(x_1, x_2, x_3) = 1/2$ when all three are equal and 0 otherwise.

Let G be

$$x_1 \text{ ——— } x_2 \qquad\qquad x_3$$

All 2 pairwise CIs in the graph: e.g. $x_1 \perp\!\!\!\perp \{x_3\} | x_2$ and $x_2 \perp\!\!\!\perp \{x_3\} | x_1$ hold in the graph.

However, the local CI: $x_1 \perp\!\!\!\perp x_3$ does not hold.

Factorization implies Global-CI

Theorem

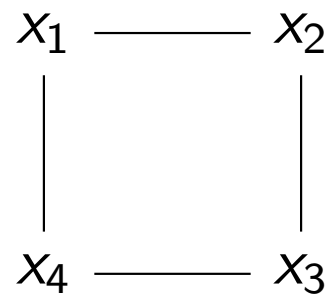
Let G be a undirected graph over $V = x_1, \ldots, x_n$ nodes and $P(x_1, \ldots, x_n)$ be a distribution. If P can be factorized as per the cliques of G, then P will also satisfy the global-CIs of G

Proof.

Discussed in class. □

Global-CI does not imply factorization.

But global-CI does not imply factorization. Consider a distribution over 4 binary variables: $P(x_1, x_2, x_3, x_4)$
Let G be



Let $P(x_1, x_2, x_3, x_4) = 1/8$ when x_1, x_2, x_3, x_4 takes values from this set $=\{0000,1000,1100,1110,1111,0111,0011,0001\}$. In all other cases it is zero. One can painfully check that all four globals CIs in the graph: e.g. $x_1 \perp\!\!\!\perp \{x_3\}|x_2, x_4$ etc hold in the graph.
Now let us look at factorization. The factors correspond to the edges in $\psi(x_1, x_2)$. Each of the four possible assignment of each factor will get a positive value. But that cannot represent the zero probability for cases like $x_1, x_2, x_3, x_4 = 0101$.

Fractorization and CIs

Theorem

(Hammerseley Clifford Theorem) If a positive distribution $P(x_1, \ldots, x_n)$ *confirms to the pairwise CIs of a UDGM* G*, then it can be factorized as per the cliques* C *of* G *as*

$$P(x_1, \ldots, x_n) \propto \prod_{C \in G} \psi_C(\mathbf{y}_C)$$

Proof.

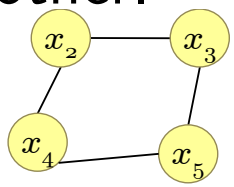
Skipped. □

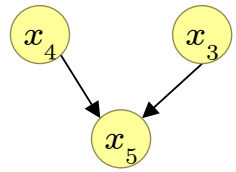
Popular undirected graphical models

- Interacting atoms in gas and solids [1900]
- Markov Random Fields in vision for image segmentation
- Conditional Random Fields for information extraction
- Social networks
- Bio-informatics: annotating active sites in a protein molecules.

Comparing directed and undirected graphs

- Some distributions can only be expressed in one and not the other.





- Potentials
  - Directed: conditional probabilities, more intuitive
  - Undirected: arbitrary scores, easy to set.
- Dependence structure
  - Directed: Complicated d-separation test
  - Undirected: Graph separation: $A \perp\!\!\!\perp B \mid C$ iff C separates A and B in G.
- Often application makes the choice clear.
  - Directed: Causality
  - Undirected: Symmetric interactions.

Part I: Outline

1. Representation
   - Directed graphical models: Bayesian networks
   - Undirected graphical models
2. Inference Queries
   - Exact inference on chains
   - Variable elimination on general graphs
   - Junction trees
3. Approximate inference
   - Generalized belief propagation
   - Sampling: Gibbs, Particle filters
4. Constructing a graphical model
   - Graph Structure
   - Parameters in Potentials
5. General framework for Parameter learning in graphical models
6. References

Inference queries

1. *Marginal probability queries over a small subset of variables:*
   - Find Pr(Income='High & Degree='PhD')
   - Find Pr(pixel $y_9 = 1$)

$$\Pr(x_1) = \sum_{x_2 \ldots x_n} \Pr(x_1 \ldots x_n)$$

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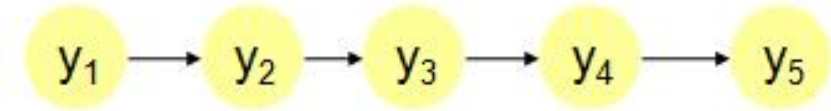
2. *Most likely labels of remaining variables:* (MAP queries)
   - Find most likely entity labels of all words in a sentence
   - Find likely temperature at sensors in a room

$$\mathbf{x}^* = \text{argmax}_{x_1 \ldots x_n} \Pr(x_1 \ldots x_n)$$

Exact inference on chains

- Given,
  - Graph 

  - Potentials: $\psi_i(y_i, y_{i+1})$
  - $Pr(y_1, \ldots y_n) = \prod_i \psi_i(y_i, y_{i+1})$
- Find, $\Pr(y_i)$ for any i, say $\Pr(y_5 = 1)$
  - Exact method: $\Pr(y_5 = 1) = \sum_{y_1, \ldots y_4} Pr(y_1, \ldots y_4, 1)$ requires exponential number of summations.
  - A more efficient alternative...

Exact inference on chains

$$\Pr(y_5 = 1) = \sum_{y_1,\ldots y_4} Pr(y_1, \ldots y_4, 1)$$

$$= \sum_{y_1} \sum_{y_2} \sum_{y_3} \sum_{y_4} \psi_1(y_1, y_2)\psi_2(y_2, y_3)\psi_3(y_3, y_4)\psi_4(y_4, 1)$$

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$$= \sum_{y_1}\sum_{y_2} \psi_1(y_1, y_2) \sum_{y_3} \psi_2(y_2, y_3) \sum_{y_4} \psi_3(y_3, y_4)\psi_4(y_4, 1)$$

Exact inference on chains

$$
\begin{aligned}
\Pr(y_5 = 1) &= \sum_{y_1,\ldots y_4} Pr(y_1, \ldots y_4, 1) \\
&= \sum_{y_1}\sum_{y_2}\sum_{y_3}\sum_{y_4} \psi_1(y_1, y_2)\psi_2(y_2, y_3)\psi_3(y_3, y_4)\psi_4(y_4, 1) \\
&= \sum_{y_1}\sum_{y_2} \psi_1(y_1, y_2) \sum_{y_3} \psi_2(y_2, y_3) \sum_{y_4} \psi_3(y_3, y_4)\psi_4(y_4, 1) \\
&= \sum_{y_1}\sum_{y_2} \psi_1(y_1, y_2) \sum_{y_3} \psi_2(y_2, y_3) B_3(y_3)
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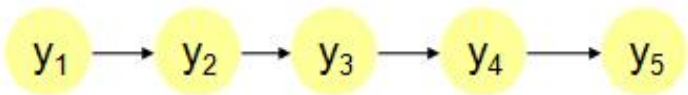
\end{aligned}
$$

An alternative view: flow of beliefs $B_i(.)$ from node $i+1$ to node i



Adding evidence

Given fixed values of a subset of variables $\mathbf{x}_e$ (evidence), find the

1. *Marginal probability queries over a small subset of variables:*
   - Find Pr(Income='High | Degree='PhD')

$$\Pr(x_1) = \sum_{x_2 \ldots x_m} \Pr(x_1 \ldots x_n | \mathbf{x}_e)$$

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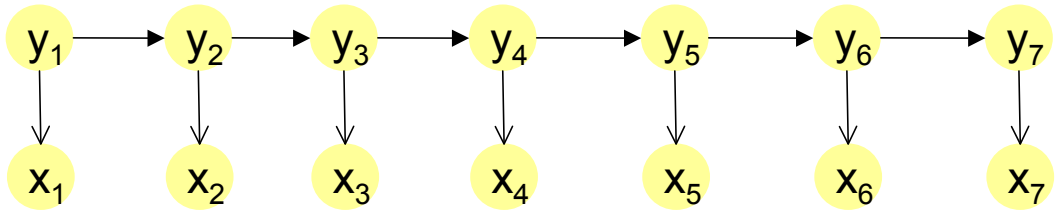
2. *Most likely labels of remaining variables:* (MAP queries)
   - Find likely temperature at sensors in a room given readings from a subset of them

$$\mathbf{x}^* = \text{argmax}_{x_1 \ldots x_m} \Pr(x_1 \ldots x_n | \mathbf{x}_e)$$

Easy to add evidence, just change the potential.

Inference in HMMs

- Given,
  - Graph 

  - Potentials: $\Pr(y_i|y_{i-1}), \Pr(x_i|y_i)$
  - Evidence variables: $\mathbf{x} = x_1 \ldots x_n = o_1 \ldots o_n$.
- Find most likely values of the hidden state variables.

  $\mathbf{y} = y_1 \ldots y_n$

$$\text{argmax}_{\mathbf{y}} \Pr(\mathbf{y}|\mathbf{x} = \mathbf{o})$$

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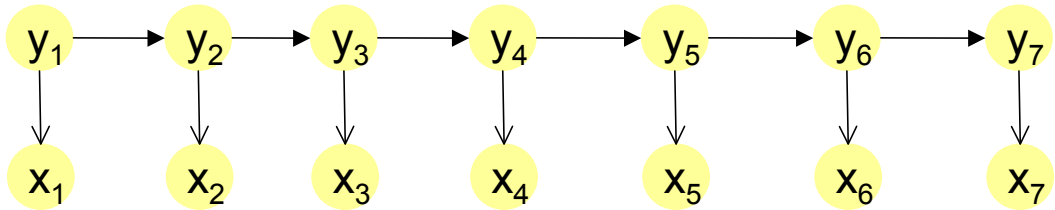
  - Graph 

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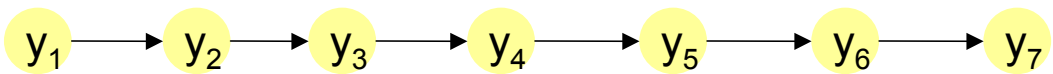
- Define $\psi_i(y_{i-1}, y_i) = \Pr(y_i|y_{i-1}) \Pr(x_i = o_i|y_i)$
- Reduced graph only a single chain of y nodes.



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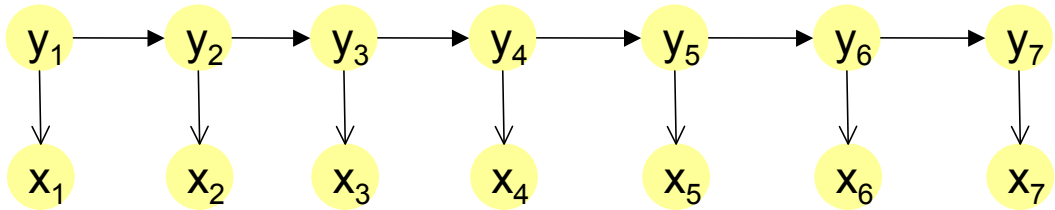
  - Graph 

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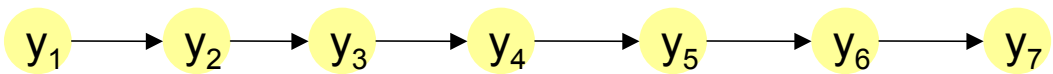

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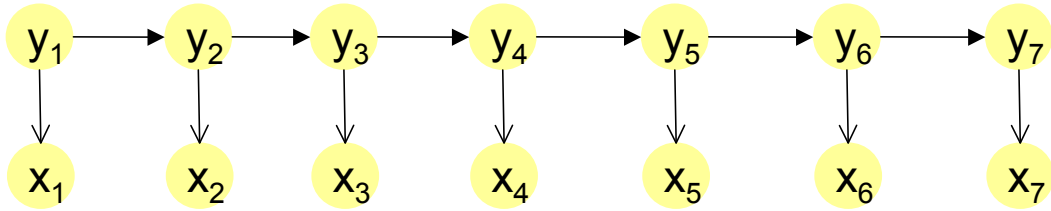
  - Graph 

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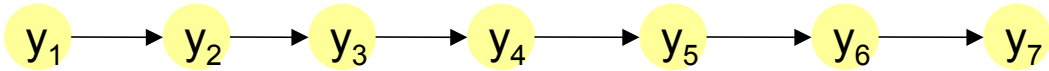

- Algorithm same as earlier, just replace "Sum" with "Max"

This is the well-known Viterbi algorithm

Variable elimination on general graphs

- Given, arbitrary sets of potentials $\psi_C(x_C)$, $C =$ cliques in a graph G.
- Find, $Z = \sum_{x_1,\ldots,x_n} \prod_C \psi_C(x_C)$

$x_1, \ldots x_n =$ good ordering of variables
$\mathcal{F} = \psi_C(x_C)$, $C =$ cliques in a graph G.
for $i = 1 \ldots n$ **do**
  $\mathcal{F}_i =$ factors in $\mathcal{F}$ that contain x_i
  $M_i =$ product of factors in $\mathcal{F}_i$
  $m_i = \sum_{x_i} M_i$
  $\mathcal{F} = \mathcal{F} - \mathcal{F}_i \cup \{m_i\}$
end for

Example: Variable elimination

- Given, $\psi_{12}(x_1, x_2)$, $\psi_{24}(x_2, x_4)$, $\psi_{23}(x_2, x_3)$, $\psi_{45}(x_4, x_5)$, , $\psi_{35}(x_3, x_5)$.
- Find, $Z = \sum_{x_1,\ldots,x_5} \psi_{12}(x_1, x_2)\psi_{24}(x_2, x_4)\psi_{23}(x_2, x_3)\psi_{45}(x_4, x_5)\psi_{35}(x_3, x_5)$.

1. x_1: $\prod\{\psi_{12}(x_1, x_2)\} \rightarrow M_1(x_1, x_2) \xrightarrow{\sum_{x_1}} m_1(x_2)$

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2. x_2: $\prod\{\psi_{24}(x_2, x_4), \psi_{23}(x_2, x_3), m_1(x_2)\} \rightarrow M_2(x_2, x_3, x_4) \xrightarrow{\sum_{x_2}} m_2(x_3, x_4)$

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3. x_3:$\prod\{\psi_{35}(x_3, x_5), m_2(x_3, x_4)\} \rightarrow M_3(x_3, x_4, x_5) \xrightarrow{\sum_{x_3}} m_3(x_4, x_5)$

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4. x_4:$\prod\{\psi_{45}(x_4, x_5), m_3(x_4, x_5)\} \rightarrow M_4(x_4, x_5) \xrightarrow{\sum_{x_4}} m_4(x_5)$

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5. x_5:$\prod\{m_5(x_5)\} \rightarrow M_5(x_5) \xrightarrow{\sum_{x_5}} Z$

Choosing a variable elimination order

- Complexity of VE $O(nm^w)$ where w is the maximum number of variables in any factor.
- Wrong elimination order can give rise to very large intermediate factors.
- Example: eliminating x_2 first will give a factor of size 4.
- Given an example where the penalty can be really severe (?)
- Choosing the optimal elimination order is NP hard for general graphs.
- Polynomial time algorithm exists for chordal graphs.
  - A graph is chordal or triangulated if all cycles of length greater than three have a shortcut.
- Optimal triangulation of graphs is NP hard. (Many heuristics)

Junction tree algorithm

- An optimal general-purpose algorithm for exact marginal/MAP queries
- Simultaneous computation of many queries
- Efficient data structures
- Complexity: $O(m^w N)$ w= size of the largest clique in (triangulated) graph, m = number of values of each discrete variable in the clique. $\rightarrow$ linear for trees.
- Basis for many approximate algorithms.
- Many popular inference algorithms special cases of junction trees
  - Viterbi algorithm of HMMs
  - Forward-backward algorithm of Kalman filters

Junction tree

Junction tree JT of a triangulated graph G with nodes $x_1, \ldots, x_n$ is a tree where

- Nodes = cliques of G
- Edges ensure that if any two nodes contain a variable x_i then x_i is present in every node in the unique path between them (Running intersection property).

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Constructing a junction tree

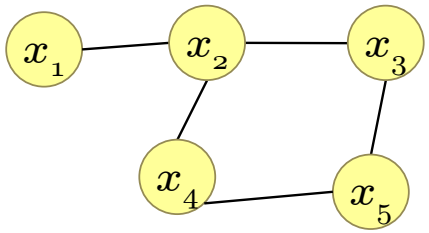
Efficient polynomial time algorithms exist for creating a JT from a triangulated graph.

1. Enumerate a covering set of cliques
2. Connect cliques to get a tree that satisfies the running intersection property.

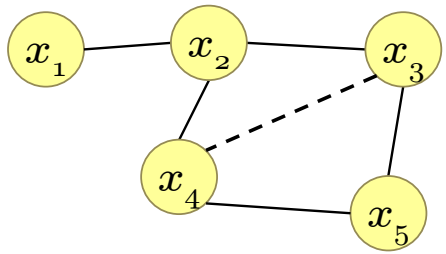
If graph is non-triangulated, triangulate first using heuristics, optimal triangulation is NP-hard.

Creating a junction tree from a graphical model

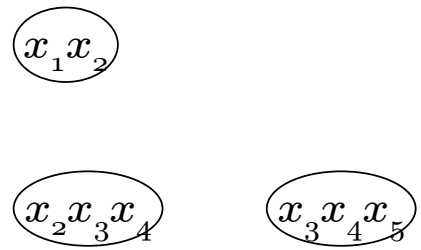
1. Starting graph



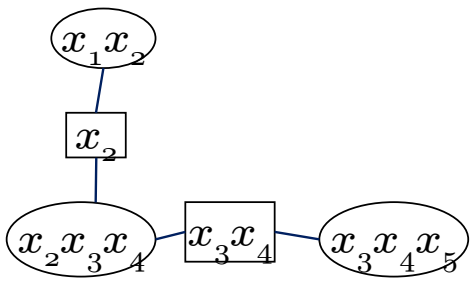
2. Triangulate graph



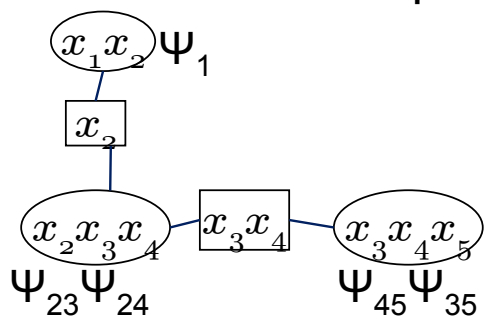
3. Create clique nodes



4. Create tree edges such that variables connected.



5) Assign potentials to exactly one subsumed clique node.



Finding cliques of a triangulated graph

Theorem

Every triangulated graph has a simplicial vertex, that is, a vertex whose neighbors form a complete set.

Input: Graph G. n = number of vertices of G
for $i = 1, \ldots, n$ **do**
  π_i = pick any simplicial vertex in G
  $C_i = \{\pi_i\} \cup Ne(\pi_i)$
  remove π_i from G
end for
Return maximal cliques from $C_1, \ldots C_n$

Connecting cliques to form junction tree

Separator variables = intersection of variables in the two cliques joined by an edge.

Theorem

A clique tree that satisfies the running intersection property maximizes the number of separator variables.

Input: Cliques: $C_1, \ldots C_k$
Form a complete weighted graph H with cliques as nodes and edge weights = size of the intersection of the two cliques it connects.
T = maximum weight spanning tree of H
Return T as the junction tree.

Belief propagation on junction trees

- Each node c
  - sends *belief* $B_{c \to c'}(.)$ to each of its neighbors c'
    - ⋆ once it has beliefs from every other neighbor $N(c) - \{c'\}$.
  - $B_{c \to c'}(.)$ = belief that clique c has about the distribution of labels to common variables $s = c \cap c'$

$$B_{c \to c'}(\mathbf{x}_s) = \sum_{\mathbf{x}_{c-s}} \psi_c(\mathbf{x}_c) \prod_{d \in N(c) - \{c'\}} B_{d \to c}(\mathbf{x}_{d \cap c})$$

Replace "sum" with "max" for MAP queries.

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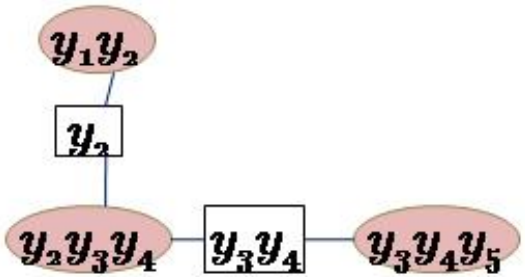
Replace "sum" with "max" for MAP queries.

Compute marginal probability of any variable x_i as

1. c = clique in JT containing x_i
2. $\Pr(x_i) \propto \sum_{\mathbf{x}_{c-x_i}} \psi_c(\mathbf{x}_c) \prod_{d \in N(c)} B_{d \to c}(\mathbf{x}_{d \cap c})$

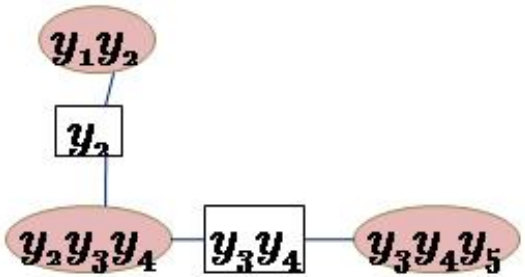
Example



$$\psi_{234}(\mathbf{y}_{234}) = \psi_{23}(\mathbf{y}_{23})\psi_{34}(\mathbf{y}_{34})$$
$$\psi_{345}(\mathbf{y}_{345}) = \psi_{35}(\mathbf{y}_{35})\psi_{45}(\mathbf{y}_{45})$$
$$\psi_{234}(\mathbf{y}_{12}) = \psi_{12}(\mathbf{y}_{12})$$

1. Clique "12" sends belief $B_{12\to234}(y_2) = \sum_{y_1} \psi_{12}(\mathbf{y}_{12})$ to its only neighbor.

Example



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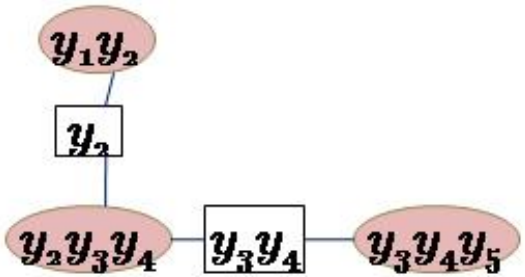
Example



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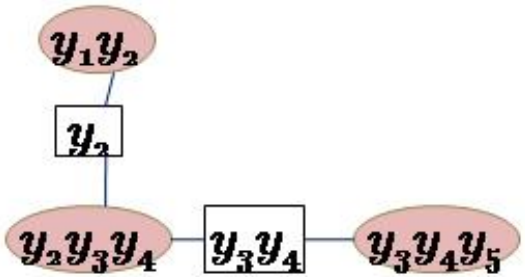
3. Clique "234" sends belief $B_{234\to345}(\mathbf{y}_{34}) = \sum_{y_2} \psi_{234}(\mathbf{y}_{234}) B_{12\to234}(y_2)$ to "345"

Example



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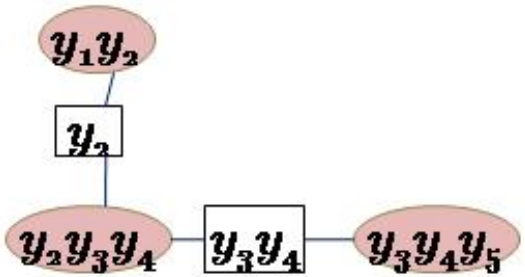
4. Clique "234" sends belief $B_{234\to12}(y_2) = \sum_{y_4} \psi_{234}(\mathbf{y}_{234}) B_{345\to234}(\mathbf{y}_{34})$ to "12"

Example



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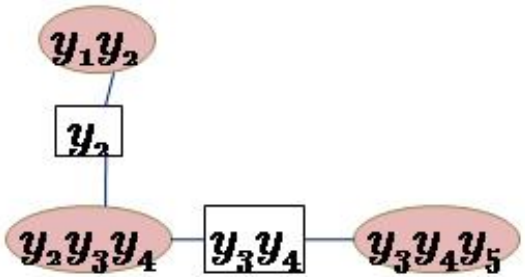

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$\Pr(y_1) \propto \sum_{y_2} \psi_{12}(\mathbf{y}_{12}) B_{234\to12}(y_2)$

Part I: Outline

1. Representation
   - Directed graphical models: Bayesian networks
   - Undirected graphical models
2. Inference Queries
   - Exact inference on chains
   - Variable elimination on general graphs
   - Junction trees
3. Approximate inference
   - Generalized belief propagation
   - Sampling: Gibbs, Particle filters
4. Constructing a graphical model
   - Graph Structure
   - Parameters in Potentials
5. General framework for Parameter learning in graphical models
6. References

Why approximate inference

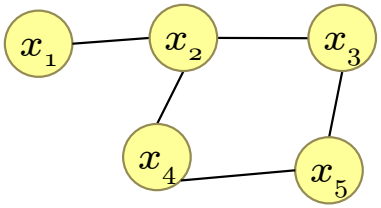
- Exact inference is NP hard. Complexity: $O(w^m)$
  - w= tree width = size of the largest clique in (triangulated) graph-1,
  - m = number of values of each discrete variable in the clique.
- Many real-life graphs produce large cliques on triangulation
  - A $n \times n$ grid has a tree width of n
  - A Kalman filter on K parallel state variables influencing a common observation variable, has a tree width of size $K + 1$

Generalized belief propagation

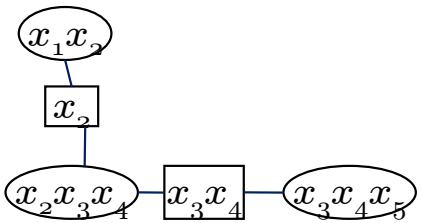
- Approximate junction tree with a cluster graph where
  1. Nodes = arbitrary clusters, not cliques in triangulated graph. Only ensure all potentials subsumed.
  2. Separator nodes on edges = *subset* of intersecting variables.
- Special case: factor graphs.

Example cluster graph

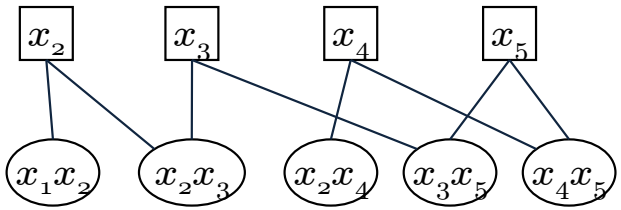
Starting graph



Junction tree.



Cluster graph



Belief propagation in cluster graphs

- Graph can have loops, tree-based two-phase method not applicable.
- Many variants on scheduling order of propagating beliefs.
  - Simple loopy belief propagation [**?**]
  - Tree-reweighted message passing [**?**, **?**]
  - Residual belief probagation [**?**]
- Many have no guarantees of convergence. Specific tree-based orders do [**?**]
- Works well in practice, default method of choice.

MCMC (Gibbs) sampling

- Useful when all else failes, guaranteed to converge to the optimal over infinite number of samples.
- Basic premise: easy to compute conditional probability $\Pr(x_i|\text{fixed values of remaining variables})$

Algorithm

- Start with some initial assignment, say $\mathbf{x}^1 = [x_1, \ldots, x_n] = [0, \ldots, 0]$
- For several iterations
  - For each variable x_i
    Get a new sample $\mathbf{x}^{t+1}$ by replacing value of x_i with a new value sampled according to probability $\Pr(x_i|x_1^t, \ldots x_{i-1}^t, x_{i+1}^t, \ldots, x_n^t)$

Others

- Combinatorial algorithms for MAP [**?**].
- Greedy algorithms: relaxation labeling.
- Variational methods like mean-field and structured mean-field.
- LP and QP based approaches.

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Graph Structure

1. Manual: Designed by domain expert
   - Used in applications where dependency structure is well-understood
   - Example: QMR systems, Kalman filters, Vision (Grids), HMM for speech recognition and IE.
2. Learned from examples
   - NP hard to find the optimal structure.
   - Widely researched, mostly posed as a branch and bound search problem.
   - Useful in dynamic situations

Parameters in Potentials

1. Manual: Provided by domain expert
   - Used in infrequently constructured graphs, example QMR systems
   - Also where potentials are an easy function of the attributes of connected graphs, example: vision networks.
2. Learned: from examples
   - More popular since difficult for humans to assign numeric values
   - Many variants of parameterizing potentials.
     1. Table potentials: each entry a parameter, example, HMMs
     2. Potentials: combination of shared parameters and data attributes: example, CRFs.

Learning potentials

Given sample $D = \{\mathbf{x}^1, \ldots, \mathbf{x}^N\}$ of data generated from a distribution $P(\mathbf{x})$ represented by a graphical model with known structure G, learn potentials $\psi_C(\mathbf{x}_C)$.
Two dimensions:

1. All variables observed or not.
    1. Fully observed: each training sample $\mathbf{x}^i$ has all n variables observed.
    2. Partially observed: a subset of the variables are observed.
2. Potentials coupled with a log-partition function or not.
    1. No: Closed form solutions
    2. Yes: Potentials attached to arbitrary overlapping subset of variables in a UDGM. Example = edge potentials in a grid graph. iterative solution as in the case of learning with shared parameters Discussed later.

Easy case: fully observed, decoupled potentials, table potentials

1. Potentials in a Bayesian network $P(\mathbf{x}) = \prod_i \Pr(x_i|Pa(x_i))$
2. potentials attached to maximal cliques in UDGM.

$$\Pr(\mathbf{x}) = \frac{\prod_{C \in \text{Cliques}} \Pr(\mathbf{x}_c)}{\prod_{S \in Separators} \Pr(\mathbf{x}_s)}$$

Maximum likelihood estimation with constraints on potentials to make them behave like probabilities:

$$\Pr(\mathbf{x}_C) = \frac{\sum_{i=1}^{N} [[\mathbf{x}_C^i == \mathbf{x}_c]]}{N}$$

$$\Pr(x_j|pa(x_j)) = \frac{\sum_{i=1}^{N} [[x_j^i == x_j, \mathbf{x}_{Pa(j)}^i = pa(x_j)]]}{\sum_{i=1}^{N} [[\mathbf{x}_{Pa(j)}^i = pa(x_j)]]}$$

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The framework

- Conditional distribution $\Pr(\mathbf{y}|\mathbf{x}, \theta)$, potentials are function of $\mathbf{x}$ and parameters θ to be learned.
- $\mathbf{y} = y_1, \ldots, y_n$ forms a graphical model: directed or undirected.
- Undirected:

$$\Pr(y_1, \ldots, y_n|\mathbf{x}, \theta) = \frac{\prod_C \psi_c(\mathbf{y}_c, \mathbf{x}, \theta)}{Z_\theta(\mathbf{x})}$$
$$= \frac{1}{Z_\theta(\mathbf{x})} \exp(\sum_c F_\theta(\mathbf{y}_c, c, \mathbf{x}))$$

where $Z_\theta(\mathbf{x}) = \sum_{\mathbf{y}'} \exp(\sum_c F_\theta(\mathbf{y}'_c, c, \mathbf{x}))$
clique potential $\psi_c(\mathbf{y}_c, \mathbf{x}) = \exp(F_\theta(\mathbf{y}_c, c, \mathbf{x}))$

Local conditional probability for BN

$$\Pr(y_1, \ldots, y_n | \mathbf{x}, \theta) = \prod_j \Pr(y_j | \mathbf{y}_{\mathrm{Pa}(j)}, \mathbf{x}, \theta)$$

$$= \prod_j \frac{\exp(F_\theta(\mathbf{y}_{\mathrm{Pa}(j)}, y, j, \mathbf{x}))}{\sum_{y'=1}^{m} \exp(F_\theta(\mathbf{y}_{\mathrm{Pa}(j)}, y', j, \mathbf{x}))}$$

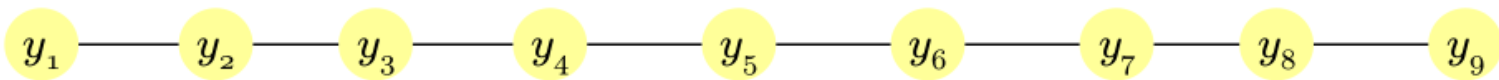
Forms of $F_\theta(\mathbf{y}_c, c, \mathbf{x})$

- Log-linear model over user-defined features. E.g. CRFs, Maxent models, etc.
  Let K be number of features. Denote a feature as $f_k(\mathbf{y}_c, c, \mathbf{x})$.
  Then,
$$F_\theta(\mathbf{y}_c, c, \mathbf{x}) = \sum_{k=1}^{K} \theta_k f_k(\mathbf{y}_c, c, \mathbf{x})$$
- Arbitrary function, e.g. a neural network that takes as input $\mathbf{y}_c, c, \mathbf{x}$ and transforms them possibly non-linearly into a real value. θ are the parameters of the network.

Example: Named Entity Recognition

My review of Fermat's last theorem by S. Singh

t	1	2	3	4	5	6	7	8	9
x	My	review	of	Fermat's	last	theorem	by	S.	Singh
y	**Other**	**Other**	**Other**	**Title**	**Title**	**Title**	**other**	**Author**	**Author**



$$\mathbf{f}(y_i, y_{i-1}, i, \mathbf{x})$$

Features decompose over adjacent labels.

$$\mathbf{f}(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{|\mathbf{x}|} \mathbf{f}(y_i, y_{i-1}, i, \mathbf{x})$$

Named Entity Recognition: Features

- Feature vector for each position

$$\mathbf{f}(y_i, \mathbf{x}, i, y_{i-1})$$

User provided

i-th label

Word i & neighbors

previous label

- Examples

$$f_2(y_i, \mathbf{x}, i, y_{i-1}) = 1 \text{ if } y_i \text{ is Person \& } x_i \text{ is Douglas}$$

$$f_3(y_i, \mathbf{x}, i, y_{i-1}) = 1 \text{ if } y_i \text{ is Person \& } y_{i-1} \text{ is Other}$$

Training

Given

- N input output pairs $D = \{(\mathbf{x}^1, \mathbf{y}^1), (\mathbf{x}^2, \mathbf{y}^2), \ldots, (\mathbf{x}^N, \mathbf{y}^N)\}$
- Form of F_θ
- Learn parameters θ by maximum likelihood.

$$\max_\theta LL(\theta, D) = \max_\theta \sum_{i=1}^{N} \log \Pr(\mathbf{y}^i | \mathbf{x}^i, \theta)$$

Training for BN

$$
\begin{aligned}
LL(\theta, D) &= \sum_{i=1}^{N} \log \Pr(\mathbf{y}^i | \mathbf{x}^i, \theta) \\
&= \sum_{i=1}^{N} \log \prod_j \Pr(y_j^i | \mathbf{y}_{\mathrm{Pa}}^i(j), \mathbf{x}^i, \theta) \\
&= \sum_i \sum_j \log \Pr(y_j^i | \mathbf{y}_{\mathrm{Pa}}^i(j), \mathbf{x}^i, \theta) \\
&= \sum_i \sum_j F_\theta(\mathbf{y}_{\mathrm{Pa}(j)}^i, y_j^i, j, \mathbf{x}^i)) - \log \sum_{y'=1}^{m} \exp(F_\theta(\mathbf{y}_{\mathrm{Pa}(j)}^i, y', j, \mathbf{x}^i))
\end{aligned}
$$

Like normal classification task. No challenge arising during training because of graphical model. Normalizer is easy to compute.

Training undirected graphical model

$$
\begin{aligned}
LL(\theta, D) &= \sum_{i=1}^{N} \log \Pr(\mathbf{y}^i | \mathbf{x}^i, \theta) \\
&= \sum_{i=1}^{N} \log \frac{1}{Z_\theta(\mathbf{x}^i)} \exp(\sum_c F_\theta(\mathbf{y}^i_c, c, \mathbf{x}^i)) \\
&= \sum_i [\sum_c F_\theta(\mathbf{y}^i_c, c, \mathbf{x}^i) - \log Z_\theta(\mathbf{x}^i)
\end{aligned}
$$

The first part is easy to compute but the second term requires to invoke an inference algorithm to compute $Z_\theta(\mathbf{x}^i)$ for each i. Computing the gradient of the above objective with respect to θ also requires inference.

Training via gradient descent

Assume log-linear models like in CRFs where $F_\theta(\mathbf{y}^i_c, c, \mathbf{x}^i) = \theta \cdot \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i_c, c)$ Also, for brevity write $\mathbf{f}(\mathbf{x}^i, \mathbf{y}^i) = \sum_c \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i_c, c)$

$$LL(\theta) = \sum_i \log \Pr(\mathbf{y}^i | \mathbf{x}^i, \theta) = \sum_i (\theta \cdot \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i) - \log Z_\theta(\mathbf{x}^i))$$

Add a regularizer to prevent over-fitting.

$$\max_\theta \sum_i (\theta \cdot \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i) - \log Z_\theta(\mathbf{x}^i)) - \|\theta\|^2 / C$$

Concave in $\theta \implies$ gradient descent methods will work.

Gradient of the training objective

$$
\begin{aligned}
\nabla L(\theta) &= \sum_i \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i) - \frac{\sum_{\mathbf{y}'} \mathbf{f}(\mathbf{y}', \mathbf{x}^i) \exp \theta \cdot \mathbf{f}(\mathbf{x}^i, \mathbf{y}')}{Z_\theta(\mathbf{x}^i)} - 2\theta/C \\
&= \sum_i \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i) - \sum_{\mathbf{y}'} \mathbf{f}(\mathbf{x}^i, \mathbf{y}') \Pr(\mathbf{y}'|\theta, \mathbf{x}^i) - 2\theta/C \\
&= \sum_i \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i) - E_{\Pr(\mathbf{y}'|\theta, \mathbf{x}^i)} \mathbf{f}(\mathbf{x}^i, \mathbf{y}') - 2\theta/C
\end{aligned}
$$

$$
\begin{aligned}
E_{\Pr(\mathbf{y}'|\theta, \mathbf{x}^i)} f_k(\mathbf{x}^i, \mathbf{y}') &= \sum_{\mathbf{y}'} f_k(\mathbf{x}^i, \mathbf{y}') \Pr(\mathbf{y}'|\theta, \mathbf{x}^i) \\
&= \sum_{\mathbf{y}'} \sum_c f_k(\mathbf{x}^i, \mathbf{y}'_c, c) \Pr(\mathbf{y}'|\theta, \mathbf{x}^i) \\
&= \sum_c \sum_{\mathbf{y}'_c} f_k(\mathbf{x}^i, \mathbf{y}'_c, c) \Pr(\mathbf{y}'_c|\theta, \mathbf{x}^i)
\end{aligned}
$$

Computing $E_{\Pr(\mathbf{y}|\theta^t,\mathbf{x}^i)} f_k(\mathbf{x}^i, \mathbf{y})$

Three steps:

1. $\Pr(\mathbf{y}|\theta^t, \mathbf{x}^i)$ is represented as an undirected model where nodes are the different components of $\mathbf{y}$, that is $y_1, \ldots, y_n$.
   The potential $\psi_c(\mathbf{y}_c, \mathbf{x}, \theta)$ on clique c is $\exp(\theta^t \cdot \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i_c, c))$
2. Run a sum-product inference algorithm on above UGM and compute for each $c, \mathbf{y}_c$ marginal probability $\mu(\mathbf{y}_c, c, \mathbf{x}^i)$.
3. Using these μs we compute
   $E_{\Pr(\mathbf{y}|\theta^t,\mathbf{x}^i)} f_k(\mathbf{x}^i, \mathbf{y}) = \sum_c \sum_{\mathbf{y}_c} \mu(\mathbf{y}_c, c, \mathbf{x}^i) f_k(\mathbf{x}^i, c, \mathbf{y}_c)$

Training algorithm

1: Initialize $\theta^0 = \mathbf{0}$

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2: **for** $t = 1 \ldots \mathrm{T}$ **do**
3: **for** $i = 1 \ldots N$ **do**
4: $g_{k,i} = f_k(\mathbf{x}^i, \mathbf{y}^i) - E_{\Pr(\mathbf{y}'|\theta^t, \mathbf{x}^i)} f_k(\mathbf{x}^i, \mathbf{y}') \quad k = 1 \ldots K$
5: **end for**
6: $g_k = \sum_i g_{k,i} \quad k = 1 \ldots K$

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5: **end for**
6: $g_k = \sum_i g_{k,i} \quad k = 1 \ldots K$
7: $\theta_k^t = \theta_k^{t-1} + \gamma_t(g_k - 2\theta_k^{t-1}/C)$
8: **Exit** if $\|\mathbf{g}\| \approx$ *zero*
9: **end for**

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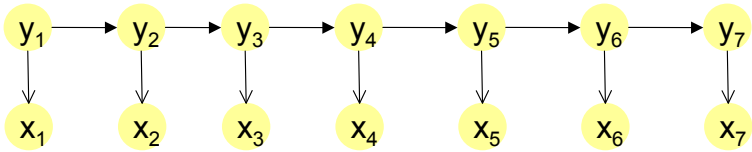
9: **end for**

Running time of the algorithm is $O(INn(m^2 + K))$ where I is the total number of iterations.

Partially observed, decoupled potentials



EM Algorithm

Input: Graph G, Data D with observed subset of variables $\mathbf{x}$ and hidden variables $\mathbf{z}$.

Initially ($t = 0$): Assign random variables of parameters $\Pr(x_j|pa(x_j))^t$

for $= 1, \ldots, T$ **do**

E-step

for $i = 1, \ldots, N$ **do**

Use inference in G to estimate conditionals $\Pr_i(\mathbf{z}_c|\mathbf{x}^i)^t$ for all variable subsets $(i, pa(i))$ involving any hidden variable.

end for

M-step

$$\Pr(x_j|pa(x_j) = \mathbf{z}_c)^t = \frac{\sum_{i=1}^{N} \Pr_i(\mathbf{z}_c|\mathbf{x}^i)[[x_j^i == x_j]]}{\sum_{i=1}^{N} \Pr_i(\mathbf{z}_c|\mathbf{x}^i)^t}$$

end for

Part I: Outline

1. Representation
   - Directed graphical models: Bayesian networks
   - Undirected graphical models
2. Inference Queries
   - Exact inference on chains
   - Variable elimination on general graphs
   - Junction trees
3. Approximate inference
   - Generalized belief propagation
   - Sampling: Gibbs, Particle filters
4. Constructing a graphical model
   - Graph Structure
   - Parameters in Potentials
5. General framework for Parameter learning in graphical models
6. References

More on graphical models

- Koller and Friedman, Probabilistic Graphical Models: Principles and Techniques. MIT Press, 2009.
- Wainwright's article in FnT for Machine Learning. 2009.
- Kevin Murphy's brief online introduction (`http://www.cs.ubc.ca/~murphyk/Bayes/bnintro.html`)
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  - R. G. Cowell, A. P. Dawid, S. L. Lauritzen and D. J. Spiegelhalter. "Probabilistic Networks and Expert Systems". Springer-Verlag. 1999.
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