Graphical Models - Part II

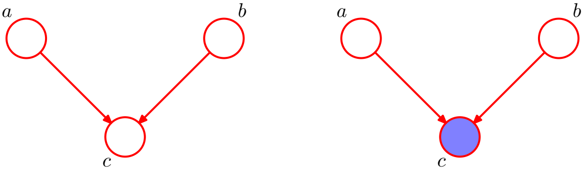
Greg Mori - CMPT 419/726

Bishop PRML Ch. 8

Outline

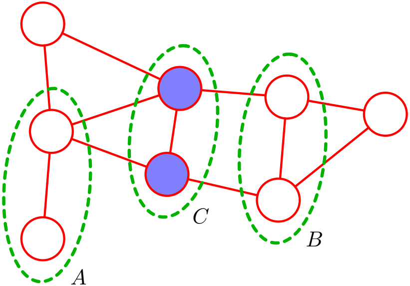
Outline

Conditional Independence in Graphs



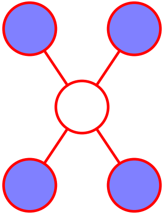
- Recall that for Bayesian Networks, conditional independence was a bit complicated
  - d-separation with head-to-head links
- We would like to construct a graphical representation such that conditional independence is straight-forward path checking

Markov Random Fields



- Markov random fields (MRFs) contain one node per variable
- Undirected graph over these nodes
- Conditional independence will be given by simple separation, blockage by observing a node on a path
  - e.g. in above graph, $A \perp\!\!\!\perp B|C$

Markov Blanket Markov



- With this simple check for conditional independence, Markov blanket is also simple
  - Recall Markov blanket MB of x_i is set of nodes such that x_i conditionally independent from rest of graph given MB
- Markov blanket is neighbours

MRF Factorization

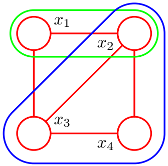
- Remember that graphical models define a factorization of the joint distribution
- What should be the factorization so that we end up with the simple conditional independence check?
- For x_i and x_j not connected by an edge in graph:

$$x_i \perp\!\!\!\perp x_j | \boldsymbol{x}_{\setminus\{i,j\}}$$

- So there should not be any factor $\psi(x_i, x_j)$ in the factorized form of the joint

Cliques

- A clique in a graph is a subset of nodes such that there is a link between every pair of nodes in the subset
- A maximal clique is a clique for which one cannot add another node and have the set remain a clique



MRF Joint Distribution

- Note that nodes in a clique cannot be made conditionally independent from each other
  - So defining factors $\psi(\cdot)$ on nodes in a clique is "safe"
- The joint distribution for a Markov random field is:

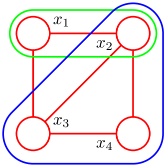
$$p(x_1, \dots, x_K) = \frac{1}{Z} \prod_C \psi_C(\boldsymbol{x}_C)$$

  where $\boldsymbol{x}_C$ is the set of nodes in clique C, and the product runs over all maximal cliques
- Each $\psi_C(\boldsymbol{x}_C) \geq 0$
- Z is a normalization constant

MRF Joint Distribution Example

- The joint distribution for a Markov random field is:

$$
\begin{aligned}
p(x_1, \ldots, x_4) &= \frac{1}{Z} \prod_C \psi_C(\boldsymbol{x}_C) \\
&= \frac{1}{Z} \psi_{123}(x_1, x_2, x_3) \psi_{234}(x_2, x_3, x_4)
\end{aligned}
$$



- Note that maximal cliques subsume smaller ones: $\psi_{123}(x_1, x_2, x_3)$ could include $\psi_{12}(x_1, x_2)$, though sometimes smaller cliques are explicitly used for clarity

MRF Joint - Terminology

- The joint distribution for a Markov random field is:

$$p(x_1, \ldots, x_K) = \frac{1}{Z} \prod_C \psi_C(\boldsymbol{x}_C)$$

- Each $\psi_C(\boldsymbol{x}_C)$ is called a potential function
- Z, the normalization constant, is called the partition function:

$$Z = \sum_{\boldsymbol{x}} \prod_C \psi_C(\boldsymbol{x}_C)$$

  - Z is very costly to compute, since it is a sum/integral over all possible states for all variables in $\boldsymbol{x}$
  - Don't always need to evaluate it though, will cancel for computing conditional probabilities

Hammersley-Clifford

- The definition of the joint:

$$p(x_1, \dots, x_K) = \frac{1}{Z} \prod_C \psi_C(\boldsymbol{x}_C)$$

- Note that we started with particular conditional independences
- We then formulated the factorization based on clique potentials
  - This formulation resulted in the right conditional independences
- The converse is true as well, any distribution with the conditional independences given by the undirected graph can be represented using a product of clique potentials
- This is the Hammersley-Clifford theorem

Energy Functions

- Often use exponential, which is non-negative, to define potential functions:

$$\psi_C(\boldsymbol{x}_C) = \exp\{-E_C(\boldsymbol{x}_C)\}$$

- Minus sign $-$ by convention
- $E_C(\boldsymbol{x}_C)$ is called an energy function
  - From physics, low energy = high probability
- This exponential representation is known as the Boltzmann distribution

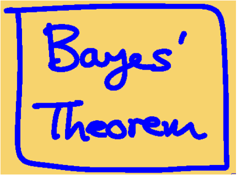
Energy Functions - Intuition

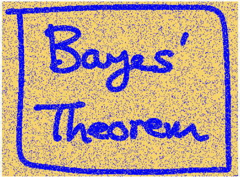
- Joint distribution nicely rearranges as

$$
\begin{aligned}
p(x_1, \ldots, x_K) &= \frac{1}{Z} \prod_C \psi_C(\boldsymbol{x}_C) \\
&= \frac{1}{Z} \exp\{-\sum_C E_C(\boldsymbol{x}_C)\}
\end{aligned}
$$

- Intuition about potential functions: ψ_C are describing good (low energy) sets of states for adjacent nodes
- An example of this is next

Image Denoising





- Consider the problem of trying to correct (denoise) an image that has been corrupted
- Assume image is binary
- Observed (noisy) pixel values $y_i \in \{-1, +1\}$
- Unobserved true pixel values $x_i \in \{-1, +1\}$

Image Denoising - Graphical Model

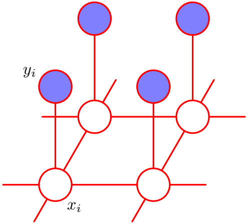
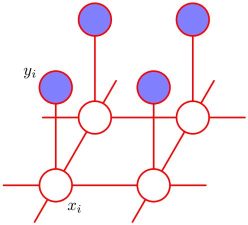
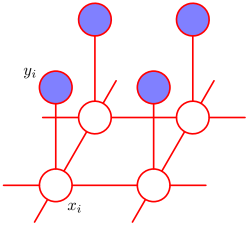


Image Denoising - Graphical Model



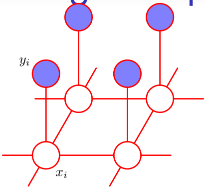
- Cliques containing each true pixel value $x_i \in \{-1, +1\}$ and observed value $y_i \in \{-1, +1\}$
  - Observed pixel value is usually same as true pixel value
  - Energy function $-\eta x_i y_i$, $\eta > 0$, lower energy (better) if $x_i = y_i$

Image Denoising - Graphical Model



- Cliques containing each true pixel value $x_i \in \{-1, +1\}$ and observed value $y_i \in \{-1, +1\}$
  - Observed pixel value is usually same as true pixel value
  - Energy function $-\eta x_i y_i$, $\eta > 0$, lower energy (better) if $x_i = y_i$
- Cliques containing adjacent true pixel values x_i, x_j
  - Nearby pixel values are usually the same
  - Energy function $-\beta x_i x_j$, $\beta > 0$, lower energy (better) if $x_i = x_j$

Image Denoising - Graphical Model



- Complete energy function:

$$E(\boldsymbol{x},\boldsymbol{y}) = -\beta \sum_{\{i,j\}} x_i x_j - \eta \sum_i x_i y_i$$

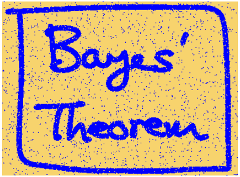
- Joint distribution:

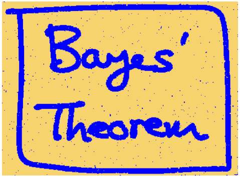
$$p(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{Z} \exp\{-E(\boldsymbol{x},\boldsymbol{y})\}$$

- Or, as potential functions $\psi_n(x_i, x_j) = \exp(\beta x_i x_j)$, $\psi_p(x_i, y_i) = \exp(\eta x_i y_i)$:

$$p(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{Z} \prod_{i,j} \psi_n(x_i, x_j) \prod_i \psi_p(x_i, y_i)$$

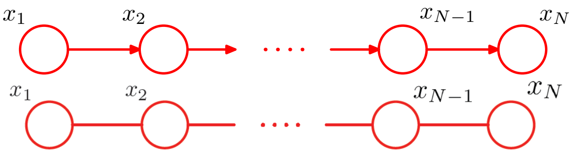
Image Denoising - Inference





- The denoising query is $\arg\max_{\boldsymbol{x}} p(\boldsymbol{x}|\boldsymbol{y})$
- Two approaches:
  - Iterated conditional modes (ICM): hill climbing in $\boldsymbol{x}$, one variable x_i at a time
    - Simple to compute, Markov blanket is just observation plus neighbouring pixels
  - Graph cuts: formulate as max-flow/min-cut problem, exact inference (for this graph)

Converting Directed Graphs into Undirected Graphs

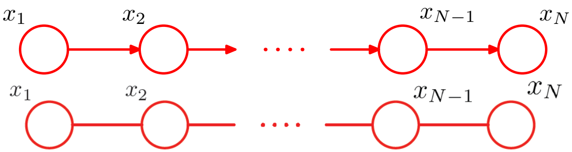


- Consider a simple directed chain graph:

$$p(\boldsymbol{x}) = p(x_1)p(x_2|x_1)p(x_3|x_2)\dots p(x_N|x_{N-1})$$

- Can convert to undirected graph

Converting Directed Graphs into Undirected Graphs



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$$p(\boldsymbol{x}) = p(x_1)p(x_2|x_1)p(x_3|x_2)\dots p(x_N|x_{N-1})$$

- Can convert to undirected graph

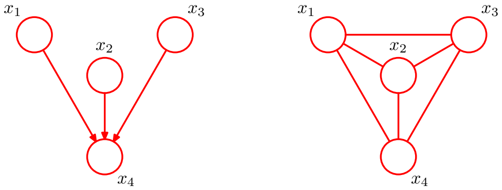
$$p(\boldsymbol{x}) = \frac{1}{Z}\psi_{1,2}(x_1, x_2)\psi_{2,3}(x_2, x_3)\dots\psi_{N-1,N}(x_{N-1}, x_N)$$

where $\psi_{1,2} = p(x_1)p(x_2|x_1)$, all other $\psi_{k-1,k} = p(x_k|x_{k-1})$, $Z = 1$

Converting Directed Graphs into Undirected Graphs

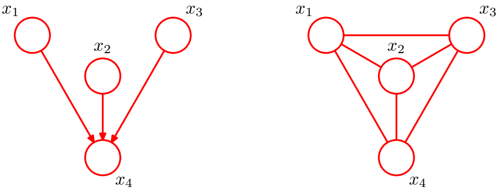
- The chain was straight-forward because for each conditional $p(x_i|pa_i)$, nodes $x_i \cup pa_i$ were contained in one clique
  - Hence we could define that clique potential to include that conditional
- For a general undirected graph we can force this to occur by "marrying" the parents
  - Add links between all parents in pa_i
  - This process known as moralization, creating a moral graph

Strong Morals



- Start with directed graph on left
- Add undirected edges between all parents of each node
- Remove directionality from original edges

Constructing Potential Functions



- Initialize all potential functions to be 1
- With moral graph, for each $p(x_i|pa_i)$, there is at least one clique which contains all of $x_i \cup pa_i$
  - Multiply $p(x_i|pa_i)$ into potential function for one of these cliques
- $Z = 1$ again since:

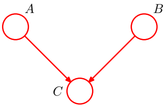
$$p(\boldsymbol{x}) = \prod_C \psi_C(\boldsymbol{x}_C) = \prod_i p(x_i|pa_i)$$

which is already normalized

Equivalence Between Graph Types

- Note that the moralized undirected graph loses some of the conditional independence statements of the directed graph
- Further, there are certain conditional independence assumptions which can be represented by directed graphs which cannot be represented by undirected graphs, and vice versa

Equivalence Between Graph Types



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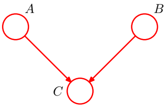

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- Directed graph: $A \perp\!\!\!\perp B|\emptyset$, $A \not\!\perp\!\!\!\perp B|C$, cannot be represented using undirected graph

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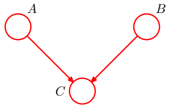

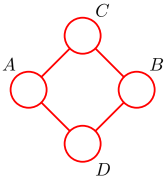

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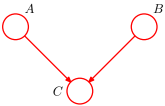

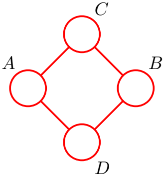

- Note that the moralized undirected graph loses some of the conditional independence statements of the directed graph
- Further, there are certain conditional independence assumptions which can be represented by directed graphs which cannot be represented by undirected graphs, and vice versa
- Directed graph: $A \perp\!\!\!\perp B | \emptyset$, $A \top\!\!\!\top B | C$, cannot be represented using undirected graph
- Undirected graph: $A \top\!\!\!\top B | \emptyset$, $A \perp\!\!\!\perp B | C \cup D$, $C \perp\!\!\!\perp D | A \cup B$ cannot be represented using directed graph

Outline

Inference

- Inference is the process of answering queries such as $p(x_n|\boldsymbol{x}_e = \boldsymbol{e})$
- We will focus on computing marginal posterior distributions over single variables x_n using

$$p(x_n|\boldsymbol{x}_e = \boldsymbol{e}) \propto p(x_n, \boldsymbol{x}_e = \boldsymbol{e})$$

- The proportionality constant can be obtained by enforcing $\sum_{x_n} p(x_n|\boldsymbol{x}_e = \boldsymbol{e}) = 1$

Inference on a Chain

- Consider a simple undirected chain
- For inference, we want to compute $p(x_n, \boldsymbol{x}_e = \boldsymbol{e})$
- First, we'll show how to compute $p(x_n)$
    - $p(x_n, \boldsymbol{x}_e = \boldsymbol{e})$ will be a simple modification of this

Inference on a Chain

- The naive method of computing the marginal $p(x_n)$ is to write down the factored form of the joint, and marginalize (sum out) all other variables:

$$
\begin{aligned}
p(x_n) &= \sum_{x_1} \cdots \sum_{x_{n-1}} \sum_{x_{n+1}} \cdots \sum_{x_N} p(\boldsymbol{x}) \\
&= \sum_{x_1} \cdots \sum_{x_{n-1}} \sum_{x_{n+1}} \cdots \sum_{x_N} \frac{1}{Z} \prod_C \psi_C(\boldsymbol{x}_C)
\end{aligned}
$$

- This would be slow – $O(K^N)$ work if each variable could take K values

Inference on a Chain

- However, due to the factorization terms in this summation can be rearranged nicely
- This will lead to efficient algorithms

Simple Algebra

- This efficiency comes from a very simple distributivity

$$ab + ac = a(b + c)$$

- Or more complicated version

$$\begin{aligned} \sum_{i=1}^{n} \sum_{j=1}^{n} a_i b_j &= a_1 b_1 + a_1 b_2 + \ldots + a_n b_n \\ &= (a_1 + \ldots + a_n)(b_1 + \ldots + b_n) \end{aligned}$$

- Much faster to do right hand side ($2(n-1)$ additions, 1 multiplication) than left hand side (n^2 multiplications, $n^2 - 1$ additions)

A Simple Chain

- First consider a chain with 3 nodes, and computing $p(x_3)$:

$$
\begin{aligned}
p(x_3) &= \sum_{x_1}\sum_{x_2} \psi_{12}(x_1,x_2)\psi_{23}(x_2,x_3) \\
&= \sum_{x_2} \psi_{23}(x_2,x_3) \left[\sum_{x_1} \psi_{12}(x_1,x_2) \right]
\end{aligned}
$$

Performing the sums

$$p(x_3) = \sum_{x_2} \psi_{23}(x_2, x_3) \left[\sum_{x_1} \psi_{12}(x_1, x_2) \right]$$

- For example, if x_i are binary:

$$\psi_{12}(x_1, x_2) = x_1 \underbrace{\begin{bmatrix} a & b \\ c & d \end{bmatrix}}_{x_2} \qquad \psi_{23}(x_2, x_3) = x_2 \underbrace{\begin{bmatrix} s & t \\ u & v \end{bmatrix}}_{x_3}$$

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$$\sum_{x_1} \psi_{12}(x_1, x_2) = \underbrace{\begin{bmatrix} a+c & b+d \end{bmatrix}}_{x_2} \equiv \mu_{12}(x_2)$$

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$$\psi_{23}(x_2, x_3) \times \mu_{12}(x_2) = x_2 \underbrace{\begin{bmatrix} s(a+c) & t(a+c) \\ u(b+d) & v(b+d) \end{bmatrix}}_{x_3}$$

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$$p(x_3) = \begin{bmatrix} s(a+c) + u(b+d) & t(a+c) + v(b+d) \end{bmatrix}$$

Complexity of Inference

- There were two types of operations
  - Summation
    $$\sum_{x_1} \psi_{12}(x_1, x_2)$$
    $K \times K$ numbers in ψ_{12}, takes $O(K^2)$ time
  - Multiplication
    $$\psi_{23}(x_2, x_3) \times \mu_{12}(x_2)$$
    Again $O(K^2)$ work
- For a chain of length N, we repeat these operations $N - 1$ times each
  - $O(NK^2)$ work, versus $O(K^N)$ for naive evaluation

More complicated chain

- Now consider a 5 node chain, again asking for $p(x_3)$

$$p(x_3) = \sum_{x_1}\sum_{x_2}\sum_{x_4}\sum_{x_5} \psi_{12}(x_1, x_2)\psi_{23}(x_2, x_3)\psi_{34}(x_3, x_4)\psi_{45}(x_4, x_5)$$

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&= \left[\sum_{x_2}\sum_{x_1} \psi_{12}(x_1,x_2)\psi_{23}(x_2,x_3)\right]\left[\sum_{x_4}\sum_{x_5} \psi_{34}(x_3,x_4)\psi_{45}(x_4,x_5)\right]
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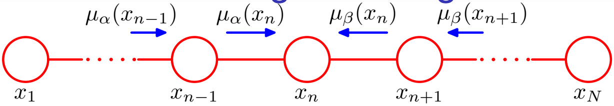
p(x_3) &= \sum_{x_1}\sum_{x_2}\sum_{x_4}\sum_{x_5} \psi_{12}(x_1,x_2)\psi_{23}(x_2,x_3)\psi_{34}(x_3,x_4)\psi_{45}(x_4,x_5) \\
&= \sum_{x_2}\sum_{x_1} \psi_{12}(x_1,x_2)\psi_{23}(x_2,x_3) \sum_{x_4}\sum_{x_5} \psi_{34}(x_3,x_4)\psi_{45}(x_4,x_5) \\
&= \left[\sum_{x_2}\sum_{x_1} \psi_{12}(x_1,x_2)\psi_{23}(x_2,x_3)\right]\left[\sum_{x_4}\sum_{x_5} \psi_{34}(x_3,x_4)\psi_{45}(x_4,x_5)\right]
\end{aligned}
$$

- Each of these factors resembles the previous, and can be computed efficiently
  - Again $O(NK^2)$ work

Message Passing



- The factors can be thought of as messages being passed between nodes in the graph

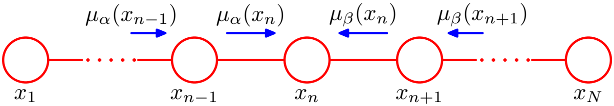
$$\mu_{12}(x_2) \equiv \sum_{x_1} \psi_{12}(x_1, x_2)$$

  is a message passed from node x_1 to node x_2 containing all information in node x_1
- In general,

$$\mu_{k-1,k}(x_k) = \sum_{x_{k-1}} \psi_{k-1,k}(x_{k-1}, x_k)\mu_{k-2,k-1}(x_{k-1})$$

- Possible to do so because of conditional independence

Computing All Marginals



- Computing one marginal $p(x_n)$ takes $O(NK^2)$ time
- Naively running same algorithms for all nodes in a chain would take $O(N^2K^2)$ time
- But this isn't necessary, same messages can be reused at all nodes in the chain
- Pass all messages from one end of the chain to the other, pass all messages in the other direction too
- Can compute marginal at any node by multiplying the two messages delivered to the node
    - $2(N-1)K^2$ work, twice as much as for just one node

Including Evidence

- If a node $x_{k-1} = e$ is observed, simply clamp to observed value rather than summing:

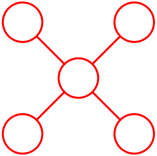
$$\mu_{k-1,k}(x_k) = \sum_{x_{k-1}} \psi_{k-1,k}(x_{k-1}, x_k)\mu_{k-2,k-1}(x_{k-1})$$

becomes

$$\mu_{k-1,k}(x_k) = \psi_{k-1,k}(x_{k-1} = e, x_k)\mu_{k-2,k-1}(x_{k-1} = e)$$

Trees

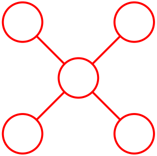
- The algorithm for a tree-structured graph is very similar to that for chains
- Formulation in PRML uses factor graphs, we'll just give the intuition here
- Consider calcuating the marginal $p(x_n)$ for the center node of the graph at right
- Treat x_n as root of tree, pass messages from leaf nodes up to root



Trees

- Message passing similar to that in chains, but possibly multiple messages reaching a node
- With multiple messages, multiply them together
- As before, sum out variables

$$\mu_{k-1,k}(x_k) = \sum_{x_{k-1}} \psi_{k-1,k}(x_{k-1}, x_k)\mu_{k-2,k-1}(x_{k-1})$$



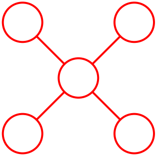
- Known as sum-product algorithm
- Complexity still $O(NK^2)$

Most Likely Configuration

- A similar algorithm exists for finding

$$\arg\max_{x_1,\ldots,x_N} p(x_1,\ldots,x_N)$$

- Replace summation operations with maximize operations
- Maximum of products at each node
- Known as max-sum, since often take log-probability to avoid underflow errors



General Graphs

- Junction tree algorithm is an exact inference method for arbitrary graphs
    - A particular tree structure defined over cliques of variables
    - Inference ends up being exponential in maximum clique size
    - Therefore slow in many cases
- Approximate inference techniques
    - Loopy belief propagation: run message passing scheme (sum-product) for a while
        - Sometimes works
        - Not guaranteed to converge
    - Variational methods: approximate desired distribution using analytically simple forms, find parameters to make these forms similar to actual desired distribution (Ch. 10, we won't cover)
    - Sampling methods: represent desired distribuion with a set of samples, as more samples are used, obtain more accurate representation (Ch. 11, we will cover)

Conclusion

- Readings: Ch. 8
- Graphical models depict conditional independence assumptions
- Directed graphs (Bayesian networks)
  - Factorization of joint distribution as conditional on node given parents
- Undirected graphs (Markov random fields)
  - Factorization of joint distribution as clique potential functions
- Inference algorithm sum-product, based on local message passing
  - Works for tree-structured graphs
  - Non-tree-structured graphs, either slow exact or approximate inference