Probabilistic Inference (CO-493)

Imperial College London

Graphical Models

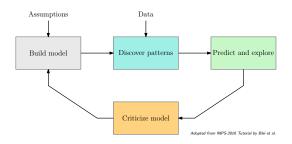
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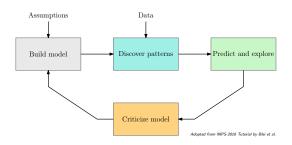
January 15, 2019

Probabilistic Pipeline



- Use knowledge and assumptions about the data to build a model
- Use model and data to discover patterns
- Predict and explore
- Criticize/revise the model

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- Use knowledge and assumptions about the data to build a model
- Use model and data to discover patterns
- Predict and explore
- Criticize/revise the model
- ➤ Inference is the key algorithmic problem: What does the model say about the data?
- **▶** Goal: general and scalable approaches to inference

Probabilistic Machine Learning

▶ **Probabilistic model:** Joint distribution of latent variables *z* and observed variables *x* (data):

p(x, z)

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- Normally: Denominator (marginal likelihood/evidence) intractable (i.e., we cannot compute the integral analytically)
 - **▶** Approximate inference to get the posterior

Some Options for Posterior Inference

- Exact inference (in some cases)
 - ► Conjugate models (see CO-496 for some examples)
 - Belief propagation and sum-product algorithm (Lauritzen & Spiegelhalter, 1988; Kschischang et al., 2001)
- Approximate inference
 - Sampling and Markov Chain Monte Carlo (to sample from the posterior)
 - Laplace approximation
 - Expectation propagation (Minka, 2001)
 - ► Variational inference (Jordan et al., 1999)

Graphical Models

Reading Material

Bishop: Pattern Recognition and Machine Learning, Chapter 8

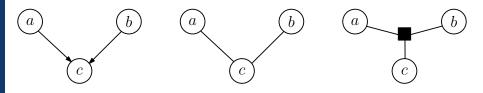
Probabilistic Models

- Quantity of interest: Joint distribution p(x, z) = p(z)p(x|z) of all observed x and unobserved (latent) z random variables
 - ▶ Probabilistic model
- Comprises information about the prior, the likelihood and the posterior

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- Quantity of interest: Joint distribution p(x, z) = p(z)p(x|z) of all observed x and unobserved (latent) z random variables
 - ▶ Probabilistic model
- Comprises information about the prior, the likelihood and the posterior
- ▶ Joint distribution p(x, z) itself can be complicated
- Does not tell us anything about structural properties of the probabilistic model (e.g., factorization, independence)
- >> Probabilistic graphical models

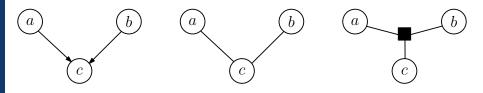
Probabilistic Graphical Models



Three types of probabilistic graphical models:

- Bayesian networks (directed graphical models)
- Markov random fields (undirected graphical models)
- Factor graphs

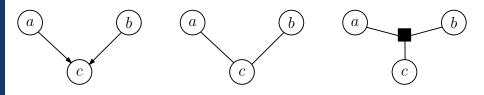
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- Bayesian networks (directed graphical models)
- Markov random fields (undirected graphical models)
- Factor graphs
- ► Nodes: (Sets of) random variables
- ► Edges: Probabilistic/functional relations between variables
- ➤ Graph captures the way in which the joint distribution over all random variables can be decomposed into a product of factors depending only on a subset of these variables

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- ► Insights into properties of the model (e.g., conditional independence) by inspection of the graph
- ► Can be used to design/motivate new models
- Complex computations for inference and learning can be expressed in terms of graphical manipulations

Importance of Visualization

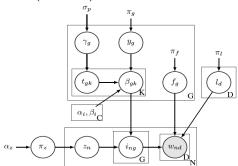
From Kim et al. (NIPS, 2015)

$$\begin{split} Pr(\{y_g,\gamma_g,t_{gk},\beta_{gk},l_d,f_g,z_n,i_{ng}\}|\{w_{nd}\}) &= \prod_g p(y_g|\rho)p(\gamma_g|\sigma)p(f_g|\alpha) \cdot \\ & [\prod_k^K p(t_{gk}|\gamma_g)p(\beta_{gk}|t_{gk},y_g)]p(\kappa|\alpha) \prod_d^D p(l_d|\kappa)p(\pi|\alpha) \prod_n^N p(z_n|\pi) \\ & \prod_n^N \prod_g^G p(i_{ng}|\beta,z_n) \prod_n^N \prod_d^D p(w_{nd}|i_{ng},f,l_d)] \end{split}$$

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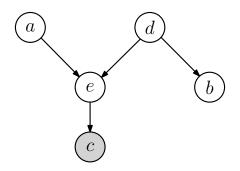


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Directed Graphical Models



- ▶ Nodes: Random variables
- ► Shaded nodes: Observed random variables
- Unshaded nodes: Unobserved (latent) random variables
- ▶ Directed arrow from a to b: Conditional distribution p(b|a).

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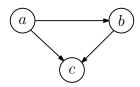
From Joints to Graphs

Consider the joint distribution

$$p(a,b,c) = p(c|a,b)p(b|a)p(a)$$

Building the corresponding graphical model:

1. Create a node for all random variables



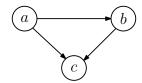
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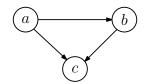
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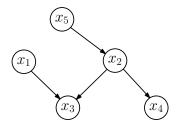
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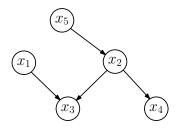


Graph layout depends on the choice of factorization

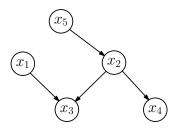
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 Joint distribution is the product of a set of conditionals, one for each node in the graph



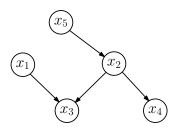
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$$p(x_1, x_2, x_3, x_4, x_5) = p(x_1)p(x_5)p(x_2|x_5)p(x_3|x_1, x_2)p(x_4|x_2)$$

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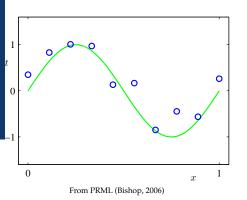
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$$p(x_1, x_2, x_3, x_4, x_5) = p(x_1)p(x_5)p(x_2|x_5)p(x_3|x_1, x_2)p(x_4|x_2)$$

In general:

$$p(x) = p(x_1, \dots, x_K) = \prod_{k=1}^K p(x_k | \text{parents}(x_k))$$

Graphical Model for (Bayesian) Linear Regression



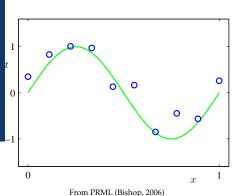
We are given a data set $(x_1, y_1), \dots, (x_N, y_N)$ where

$$y_i = f(x_i) + \varepsilon$$
, $\varepsilon \sim \mathcal{N}(0, \sigma^2)$

with *f* unknown.

➤ Find a (regression) model that explains the data

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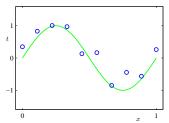
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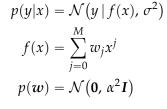
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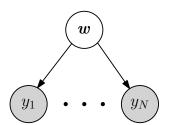
- Consider polynomials $f(x) = \sum_{j=0}^{M} w_j x^j$ with parameters $\mathbf{w} = [w_0, \dots, w_M]^{\top}$.
- ► Bayesian linear regression: Place a conjugate Gaussian prior on the parameters: $p(w) = \mathcal{N}(\mathbf{0}, \alpha^2 \mathbf{I})$

Graphical Model for Linear Regression

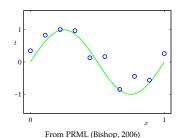


From PRML (Bishop, 2006)

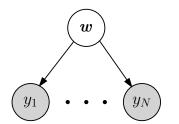


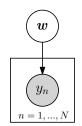


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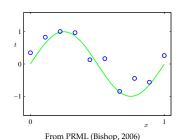


$$p(y|x) = \mathcal{N}(y | f(x), \sigma^2)$$
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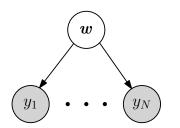


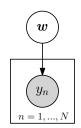


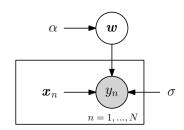
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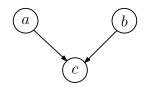
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Conditional Independence

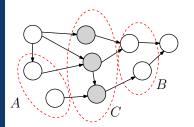


$$a \perp b|c \iff p(a|b,c) = p(a|c)$$

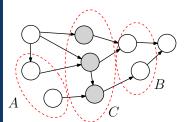
 $\iff p(a,b|c) = p(a|c)p(b|c)$

- ► (Conditional) independence allows for a factorization of the joint distribution ➤ More efficient inference
- Conditional independence properties of the joint distribution can be read directly from the graph
- ▶ No analytical manipulations required.
- **▶ d-separation** (Pearl, 1988)

D-Separation (Directed Graphs)

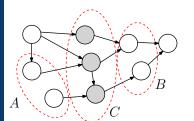


Directed, acyclic graph in which A, B, C are arbitrary, non-intersecting sets of nodes. Does $A \perp \!\!\!\perp B \mid C$ hold? Note: C is observed if we condition on it (and the nodes in the GM are shaded)



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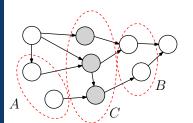
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➤ Consider all possible paths from any node in *A* to any node in *B*. Any such **path is blocked** if it includes a node such that either

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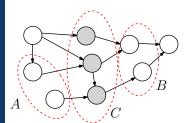


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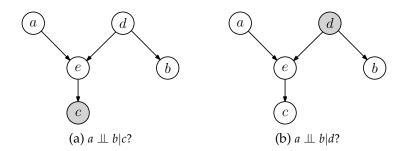
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If all paths are blocked, then A is d-separated (conditionally indep.) from B by C, and the joint distribution satisfies $A \perp \!\!\! \perp B \mid C$.

Example

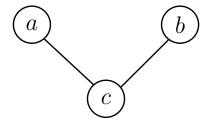


A path is **blocked** if it includes a node such that either

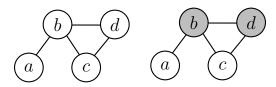
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Markov Random Fields

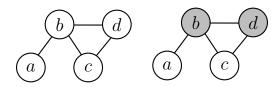


Joint Distribution



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- ▶ If x_i , x_j are not connected directly by a link then $x_i \perp \!\!\! \perp x_j | x \setminus \{x_i, x_j\}$ (conditionally independent given everything else)

- ▶ If $x_i \perp \!\!\! \perp x_j | x \setminus \{x_i, x_j\}$ then x_i, x_j never appear in a common factor in the factorization of the joint
 - **▶** Joint distribution as a product of cliques (fully connected subgraphs)

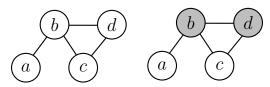
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- Define factors in the decomposition of the joint to be functions of the variables in (maximum) cliques:

$$p(\mathbf{x}) \propto \prod_{C} \psi_{C}(\mathbf{x}_{C})$$

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Example: $p(a,b,c,d) \propto \psi_1(a,b)\psi_2(b,c,d)$



More generally:

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{C} \psi_{C}(\mathbf{x}_{C})$$

- C: maximal clique
- x_C : all variables in this clique
- $\psi_C(x_C)$: clique potential
- $Z = \sum_{x} \prod_{C} \psi_{C}(x_{C})$: normalization constant

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{C} \psi_{C}(\mathbf{x}_{C})$$

Clique potentials $\psi_C(x_C)$:

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 - ▶ Greater flexibility but computational challenges

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Clique potentials $\psi_C(x_C)$:

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 - **▶** Greater flexibility but computational challenges
- If we convert a directed graph into an MRF, the clique potentials do have a probabilistic interpretation

Normalization Constant

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{C} \psi_{C}(\mathbf{x}_{C})$$

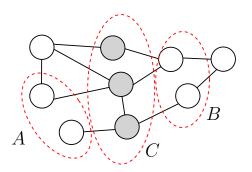
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- Flexibility in the definition the factorization in an MRF
- ▶ Normalization constant (also: partition function) *Z* is required for parameter learning (not covered in here) and model selection
- ▶ In a <u>discrete model</u> with M discrete nodes each having K states, the evaluation Z requires summing over K^M states
 - **▶** Exponential in the size of the model
- In a <u>continuous model</u>, we need to solve integrals
 - **▶** Intractable in many cases
- ▶ Major limitation of MRFs

Conditional Independence



Two easy checks for conditional independence:

- ▶ $A \perp \!\!\!\perp B \mid C$ if and only if all paths from A to B pass through C. (Then, all paths are blocked)
- ▶ Alternative: Remove all nodes in *C* from the graph. If there is a path from *A* to *B* then $A \perp\!\!\!\perp B|C$ does not hold

Potentials as Energy Functions

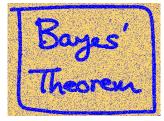
- ▶ Look only at potential functions with $\psi_C(x_C) > 0$
 - $\psi_C(x_C) = \exp(-E(x_C))$ for some energy function *E*

Potentials as Energy Functions

- Look only at potential functions with $\psi_C(x_C) > 0$
 - $\psi_C(x_C) = \exp(-E(x_C))$ for some energy function E
- ▶ Joint distribution is the product of clique potentials
 - Total energy is the sum of the energies of the clique potentials

$$-\log p(x) = -\log \prod_{C} \underbrace{\exp(-E(x_C))}_{=\psi_C(x_C)} = \sum_{C} E(x_C)$$

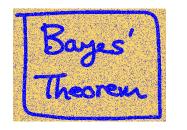
Example: Image De-Noising

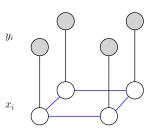


From PRML (Bishop, 2006)

- ▶ Binary image, corrupted by 10% binary noise (pixel values flip with probability 0.1).
- ► Objective: Restore noise-free image
- ▶ Pairwise MRF that has all its variables joined in cliques of size 2

Example: Image De-Noising (2)

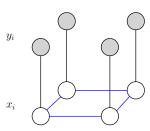




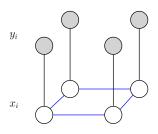
- MRF-based approach
- ▶ Latent variables $x_i \in \{-1, +1\}$ are the binary noise-free pixel values that we wish to recover

Example: Image De-Noising (2)



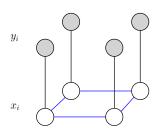


- MRF-based approach
- ▶ Latent variables $x_i \in \{-1, +1\}$ are the binary noise-free pixel values that we wish to recover
- ▶ Observed variables $y_i \in \{-1, +1\}$ are the noise-corrupted pixel values



Two types of clique potentials:

- $-\log \psi_{xy}(x_i,y_i) = E(x_i,y_i) = -\eta x_i y_i, \quad \eta > 0$
 - ➤ Strong correlation between observed and latent variables



Two types of clique potentials:

- $-\log \psi_{xy}(x_i,y_i) = E(x_i,y_i) = -\eta x_i y_i, \quad \eta > 0$
 - ➤ Strong correlation between observed and latent variables
- ► $-\log \psi_{xx}(x_i, x_j) = E(x_i, x_j) = -\beta x_i x_j$, $\beta > 0$ for neighboring pixels x_i, x_j
 - ➤ Favor similar labels for neighboring pixels (smoothness prior)

Energy Function

Total energy:

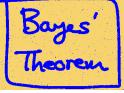
$$E(x,y) = -\eta \sum_{i} x_{i}y_{i} -\beta \sum_{\{i,j\}} x_{i}x_{j} + \gamma \sum_{i} x_{i}$$
latent-observed latent-latent

- ▶ Bias term places a prior on the latent pixel values, e.g., +1.
- ▶ Joint distribution $p(x, y) = \frac{1}{Z} \exp(-E(x, y))$
- ► Fix *y*-values to the observed ones \blacktriangleright Implicitly define p(x|y)
- ► Example of an Ising model ➤ Statistical physics

ICM Algorithm for Image De-Noising





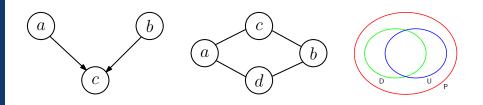


Noise-corrupted image, ICM, Graph-cut (From PRML (Bishop, 2006))

Iterated Conditional Modes (ICM, Kittler & Föglein, 1984)

- 1. Initialize all $x_i = y_i$
- 2. Pick any x_j : Evaluate total energy $E(\mathbf{x}^{\setminus j} \cup \{+1\}, \mathbf{y}), \quad E(\mathbf{x}^{\setminus j} \cup \{-1\}, \mathbf{y})$
- 3. Set x_i to whichever state (± 1) has the lower energy
- 4. Repeat
- ▶ Local optimum

Relation to Directed Graphs



- Directed and undirected graphs express different conditional independence properties
- ▶ Left: $a \perp \!\!\!\perp b | \varnothing$, $a \perp \!\!\!\!\perp b | c$ has no MRF equivalent
- ► Center: $a \perp b \mid \emptyset$, $c \perp d \mid a \cup b$, $a \perp b \mid c \cup d$ has no Bayesnet equivalent

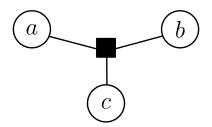
Factor Graphs

Good references:

Kschischang et al.: Factor Graphs and the Sum-Product Algorithm. IEEE Transactions on Information Theory (2001)

Loeliger: An Introduction to Factor Graphs. IEEE Signal Processing Magazine, (2004)

Factor Graphs



- (Un)directed graphical models express a global function of several variables as a product of factors over subsets of those variables
- Factor graphs make this decomposition explicit by introducing additional nodes for the factors themselves

Factorizing the Joint

The joint distribution is a product of factors:

$$p(\mathbf{x}) = \prod_{s} f_{s}(\mathbf{x}_{s})$$

- \bullet $x = (x_1, \ldots, x_n)$
- x_s : Subset of variables
- f_s : Factor; non-negative function of the variables x_s

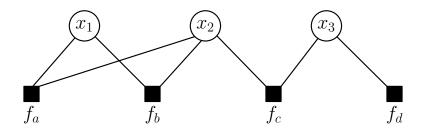
Factorizing the Joint

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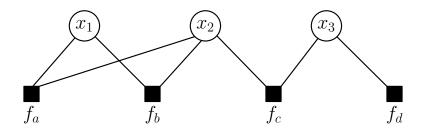
- $x = (x_1, ..., x_n)$
- x_s : Subset of variables
- f_s : Factor; non-negative function of the variables x_s
- ► Building a factor graph as a bipartite graph:
 - Nodes for all random variables (same as in (un)directed graphical models)
 - Additional nodes for factors (black squares) in the joint distribution
- Undirected links connecting each factor node to all of the variable nodes the factor depends on

Example



$$p(x) = f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$$

Example

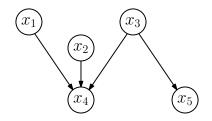


$$p(\mathbf{x}) = f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$$

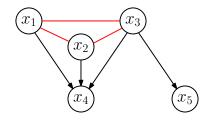
▶ Efficient inference algorithms for factor graphs (e.g., sum-product algorithm)

Graphical Models Marc Deisenroth @Imperial College London, January 15, 2019



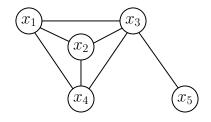


1. Moralization:

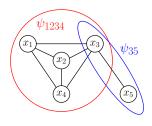


1. Moralization:

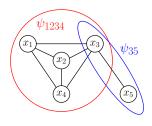
 Add additional undirected links between all pairs of parents for each node in the graph



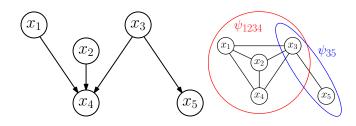
- Add additional undirected links between all pairs of parents for each node in the graph
- ► Drop arrows on original links



- Add additional undirected links between all pairs of parents for each node in the graph
- ▶ Drop arrows on original links
- 2. Identify (maximum) cliques

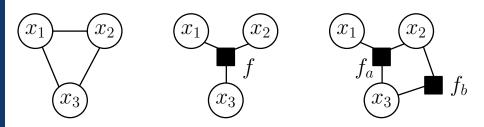


- Add additional undirected links between all pairs of parents for each node in the graph
- Drop arrows on original links
- 2. Identify (maximum) cliques
- 3. Initialize all clique potentials to 1



- Add additional undirected links between all pairs of parents for each node in the graph
- Drop arrows on original links
- 2. Identify (maximum) cliques
- 3. Initialize all clique potentials to 1
- 4. Take each conditional distribution factor in the directed graph, multiply it into one of the clique potentials

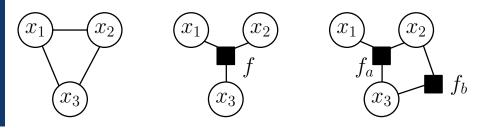
MRF → Factor Graph



- 1. Take variable nodes from MRF
- 2. Create additional factor nodes corresponding to the maximal cliques x_s
- 3. The factors $f_s(x_s)$ equal the clique potentials
- 4. Add appropriate links

Multiple factor graphs may correspond to the same undirected graph

Example: MRF → Factor Graph



Multiple factor graphs may correspond to the same undirected graph

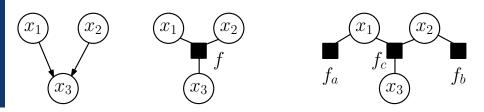
- ▶ MRF with clique potential $\psi(x_1, x_2, x_3)$
- ► Factor graph with factor $f(x_1, x_2, x_3) = \psi(x_1, x_2, x_3)$
- ► Factor graph with factors, such that $f_a(x_1, x_2, x_3) f_b(x_2, x_3) = \psi(x_1, x_2, x_3)$

Directed Graphical Model → Factor Graph

- 1. Take variable nodes from Bayesian network
- 2. Create additional factor nodes corresponding to the conditional distributions
- 3. Add appropriate links

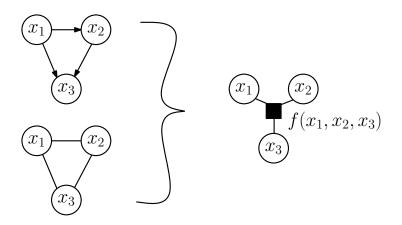
Not unique

Example: Directed Graph → Factor Graph



- ▶ Directed graph with factorization $p(x_1)p(x_2)p(x_3|x_1,x_2)$
- ► Factor graph with factor $f(x_1, x_2, x_3) = p(x_1)p(x_2)p(x_3|x_1, x_2)$
- Factor graph with factors $f_a = p(x_1)$, $f_b = p(x_2)$, $f_c = p(x_3|x_1,x_2)$

Removing Cycles



► Local cycles in an (un)directed graph (due to links connecting parents of a node) can be removed on conversion to a factor graph

Exact Inference in Factor Graphs

Sum-Product Algorithm for Factor Graphs

- Factor graphs give a uniform treatment to message passing, which is used for inference in graphs
- ► Inference: Find (marginal) posterior distributions

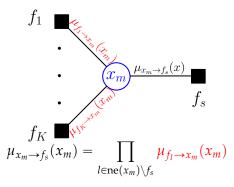
Sum-Product Algorithm for Factor Graphs

- Factor graphs give a uniform treatment to message passing, which is used for inference in graphs
- ► Inference: Find (marginal) posterior distributions
- ► Idea: Local message passing between nodes and factors
- ► Two different types of messages:
 - Messages $\mu_{x \to f}(x)$ from variable nodes to factors
 - ► Messages $\mu_{f \to x}(x)$ from factors to variable nodes

Sum-Product Algorithm for Factor Graphs

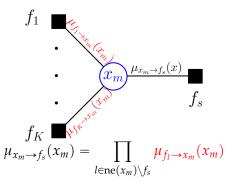
- Factor graphs give a uniform treatment to message passing, which is used for inference in graphs
- ► Inference: Find (marginal) posterior distributions
- ► Idea: Local message passing between nodes and factors
- ► Two different types of messages:
 - ► Messages $\mu_{x \to f}(x)$ from variable nodes to factors
 - ► Messages $\mu_{f \to x}(x)$ from factors to variable nodes
- Repeated sending of these messages through the graph converges
- ► Factors transform messages into evidence for the receiving node

Variable-to-Factor Message



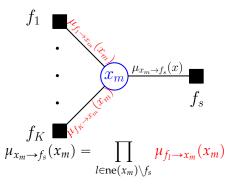
► Take the product of all incoming messages along all other links

Variable-to-Factor Message



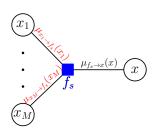
- ► Take the product of all incoming messages along all other links
- ► A variable node can send a message to a factor node once it has received messages from all other neighboring factors

Variable-to-Factor Message



- ► Take the product of all incoming messages along all other links
- ► A variable node can send a message to a factor node once it has received messages from all other neighboring factors
- ► The message that a node sends to a factor is made up of the messages that it receives from all other factors.

Factor-to-Variable Message

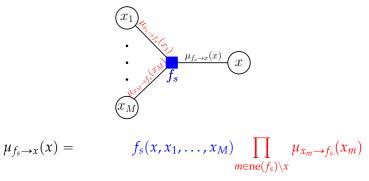


$$\mu_{f_s \to x}(x) =$$

$$\prod_{m\in \mathrm{ne}(f_s)\backslash x}\mu_{x_m\to f_s}(x_m)$$

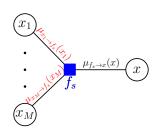
► Take the product of the incoming messages along all other links coming into the factor node

Factor-to-Variable Message



- ► Take the product of the incoming messages along all other links coming into the factor node
- Multiply by the factor associated with that node

Factor-to-Variable Message



$$\mu_{f_s \to x}(x) = \sum_{x_1} \cdots \sum_{x_M} f_s(x, x_1, \dots, x_M) \prod_{m \in ne(f_s) \setminus x} \mu_{x_m \to f_s}(x_m)$$

- ► Take the product of the incoming messages along all other links coming into the factor node
- Multiply by the factor associated with that node
- Marginalize over all variables associated with the incoming messages

Initialization

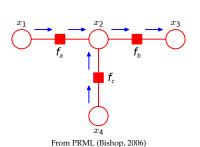
► If the leaf node is a variable node, initialize the corresponding messages to 1:

$$\mu_{x \to f}(x) = 1$$

▶ If the leaf node is a factor node, the message should be

$$\mu_{f \to x}(x) = f(x)$$

Example (1)



$$\mu_{x_1 \to f_a}(x_1) = 1$$

$$\mu_{f_a \to x_2}(x_2) = \sum_{x_1} f_a(x_1, x_2) \cdot 1$$

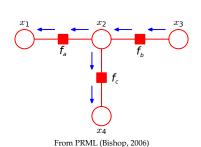
$$\mu_{x_4 \to f_c}(x_4) = 1$$

$$\mu_{f_c \to x_2}(x_2) = \sum_{x_4} f_c(x_2, x_4) \cdot 1$$

$$\mu_{x_2 \to f_b}(x_2) = \mu_{f_a \to x_2}(x_2) \mu_{f_c \to x_2}(x_2)$$

$$\mu_{f_b \to x_3}(x_3) = \sum_{x_2} f_b(x_2, x_3) \mu_{x_2 \to f_b}(x_2)$$

Example (2)



$$\mu_{x_3 \to f_b}(x_3) = 1$$

$$\mu_{f_b \to x_2}(x_2) = \sum_{x_3} f_b(x_2, x_3) \cdot 1$$

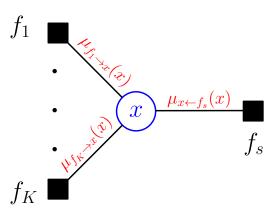
$$\mu_{x_2 \to f_a}(x_2) = \mu_{f_b \to x_2}(x_2) \mu_{f_c \to x_2}(x_2)$$

$$\mu_{f_a \to x_1}(x_1) = \sum_{x_2} f_a(x_1, x_2) \mu_{x_2 \to f_a}(x_2)$$

$$\mu_{x_2 \to f_c}(x_2) = \mu_{f_a \to x_2}(x_2) \mu_{f_b \to x_2}(x_2)$$

$$\mu_{f_c \to x_4}(x_4) = \sum_{x_2} f_c(x_2, x_4) \mu_{x_2 \to f_c}(x_2)$$

Marginals



For a single variable node the marginal is given as the product of all incoming messages:

$$p(x) = \prod_{f_i \in ne(x)} \mu_{f_i \to x}(x)$$

Observed Variables **▶** Posterior

- ► Thus far, we have focused on the case where all variables are unobserved.
- Posterior is always conditioned on observations
- ▶ Partition $x = h \cup v$, h: hidden variables, v: visible variables with observations \hat{v}
- $p(v = \hat{v}) = \prod_i I(v_i = \hat{v}_i)$
- $p(x)p(v=\hat{v}) = p(h,v=\hat{v}) \propto p(h|v=\hat{v})$
- ▶ Marginal posteriors $p(h_i|v=\hat{v})$ can be obtained via sum-product algorithm and some local computations
 - ▶ (Koller & Friedman, 2009)

Exact Inference in (Un)Directed Graphical Models

- ► Loops are possible ➤ Junction Tree Algorithm (Lauritzen & Spiegelhalter, 1988)
- ► Alternative: **Loopy Belief Propagation** (Frey & MacKay 1998)

Applications of Inference in Graphical Models

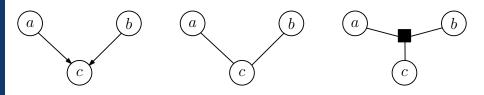






- ► Ranking: TrueSkill (Herbrich et al., 2007)
- Computer vision: de-noising, segmentation, semantic labeling, ...
 (e.g., Sucar & Gillies, 1994; Shotton et al., 2006; Szeliski et al., 2008)
- ► Coding theory: Low-density parity-check codes, turbo codes, ... (e.g., McEliece et al., 1998)
- ► Linear algebra: Solve linear equation systems (Shental et al., 2008)
- Signal processing: Iterative state estimation (e.g., Bickson et al., 2007; Deisenroth & Mohamed, 2012)

Summary



- ► Three types of graphical models: directed, undirected, factor graphs
- Conditional independence
- ► Sum-product algorithm for exact inference in factor graphs

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