Probabilistic Inference (CO-493)

Imperial College London

Graphical Models

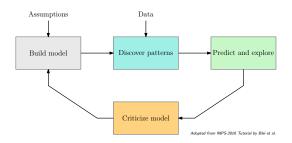
Marc Deisenroth

Department of Computing Imperial College London

m.deisenroth@imperial.ac.uk

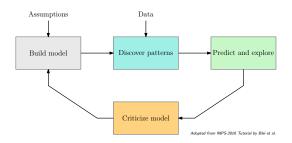
January 15, 2019

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

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
- ➤ 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)

Probabilistic Machine Learning

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

► **Inference**: Learning about the unknowns *z* through the posterior distribution

$$p(z|x) = \frac{p(x,z)}{p(x)}, \qquad p(x) = \int p(x|z)p(z)dz$$

Probabilistic Machine Learning

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

► **Inference**: Learning about the unknowns *z* through the posterior distribution

$$p(z|x) = \frac{p(x,z)}{p(x)}, \qquad p(x) = \int p(x|z)p(z)dz$$

- 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

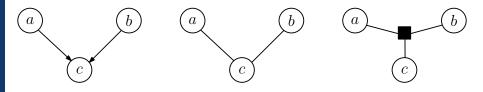
Probabilistic Models

- 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

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
- ▶ 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

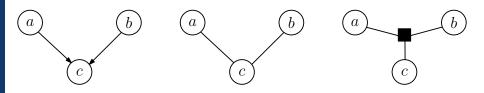
Probabilistic Graphical Models



Three types of probabilistic graphical models:

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

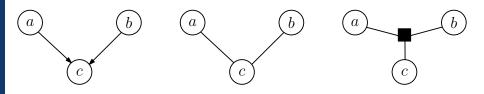
Probabilistic Graphical Models



Three types of probabilistic graphical models:

- Bayesian networks (directed graphical models)
- Markov random fields (undirected graphical models)
- Factor graphs
- ► **Nodes:** (Sets of) random variables
- ► Edges: Probabilistic/functional relations between variables

Probabilistic Graphical Models



Three types of probabilistic graphical models:

- 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

► Simple way to visualize the structure of a probabilistic model

- ► Simple way to visualize the structure of a probabilistic model
- ► Insights into properties of the model (e.g., conditional independence) by inspection of the graph

- ► Simple way to visualize the structure of a probabilistic model
- ► Insights into properties of the model (e.g., conditional independence) by inspection of the graph
- Can be used to design/motivate new models

- ► Simple way to visualize the structure of a probabilistic model
- ► 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

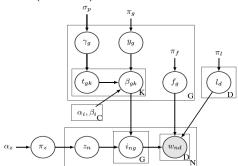
From Kim et al. (NIPS, 2015)

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

Importance of Visualization

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

From Kim et al. (NIPS, 2015)

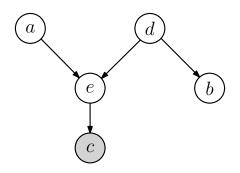


From Kim et al. (NIPS, 2015)



11

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).

12

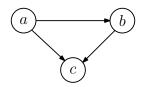
From Joints to Graphs

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



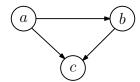
From Joints to Graphs

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
- 2. For each conditional distribution, we add a directed link (arrow) to the graph from the nodes corresponding to the variables on which the distribution is conditioned on



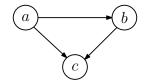
From Joints to Graphs

Consider the joint distribution

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

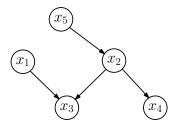
Building the corresponding graphical model:

- 1. Create a node for all random variables
- 2. For each conditional distribution, we add a directed link (arrow) to the graph from the nodes corresponding to the variables on which the distribution is conditioned on

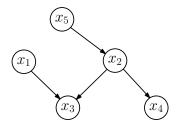


Graph layout depends on the choice of factorization

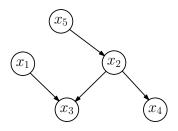
13



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



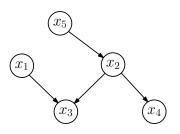
- Joint distribution is the product of a set of conditionals, one for each node in the graph
- Each conditional depends only on the parents of the corresponding node in the graph



- ► Joint distribution is the product of a set of conditionals, one for each node in the graph
- Each conditional depends only on the parents of the corresponding node in the graph

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

14



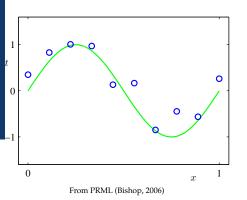
- ► Joint distribution is the product of a set of conditionals, one for each node in the graph
- Each conditional depends only on the parents of the corresponding node in the graph

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

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



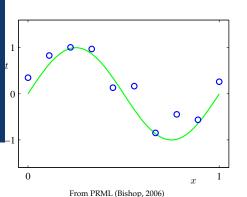
We are given a data set $(x_1, y_1), \dots, (x_N, y_N)$ where

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

with *f* unknown.

➤ Find a (regression) model that explains the data

Graphical Model for (Bayesian) Linear Regression



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

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

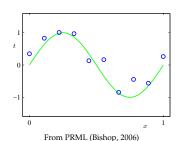
with *f* unknown.

➤ Find a (regression) model that explains the data

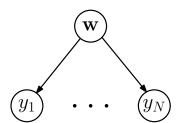
15

- 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: $p(w) = \mathcal{N}(\mathbf{0}, \alpha^2 \mathbf{I})$

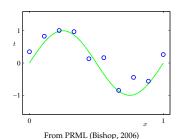
Graphical Model for Linear Regression



$$p(y|x) = \mathcal{N}(y | f(x), \sigma^2)$$
$$f(x) = \sum_{j=0}^{M} w_j x^j$$
$$p(w) = \mathcal{N}(\mathbf{0}, \alpha^2 \mathbf{I})$$

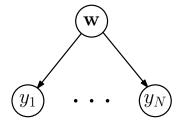


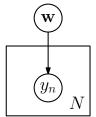
Graphical Model for Linear Regression



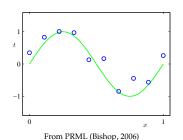
$$p(y|x) = \mathcal{N}(y | f(x), \sigma^{2})$$
$$f(x) = \sum_{j=0}^{M} w_{j}x^{j}$$
$$p(w) = \mathcal{N}(\mathbf{0}, \alpha^{2}\mathbf{I})$$

16

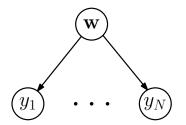


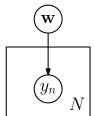


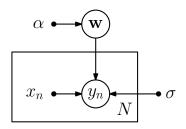
Graphical Model for Linear Regression



$$p(y|x) = \mathcal{N}(y | f(x), \sigma^2)$$
$$f(x) = \sum_{j=0}^{M} w_j x^j$$
$$p(w) = \mathcal{N}(\mathbf{0}, \alpha^2 \mathbf{I})$$

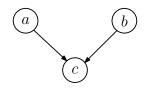






16

Conditional Independence

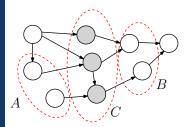


$$a \perp b|c \iff p(a|b,c) = p(a|c)$$

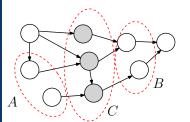
 $\iff p(a,b|c) = p(a|c)p(b|c)$

- ► (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)

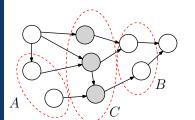


Directed, acyclic graph in which A, B, C are arbitrary, non-intersecting sets of nodes. Does $A \perp \!\!\!\perp B \mid C$ hold? Note: C is observed if we condition on it (and the nodes in the GM are shaded)



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)

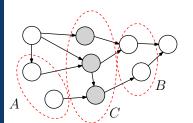
Consider all possible paths from any node in *A* to any node in *B*.



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)

➤ 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

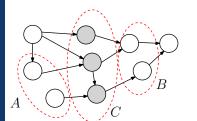
► Arrows on the path meet either head-to-tail or tail-to-tail at the node, <u>and</u> the node is in the set *C* or



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)

➤ 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

- ► Arrows on the path meet either head-to-tail or tail-to-tail at the node, and the node is in the set *C* or
 - Arrows meet head-to-head at the node and neither the node nor any of its descendants is in the set C



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)

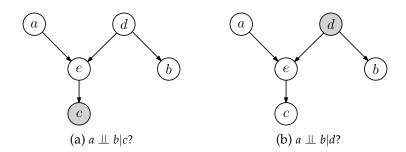
Consider all possible paths from any node in *A* to any node in *B*.

Any such path is blocked if it includes a node such that either

- Arrows on the path meet either head-to-tail or tail-to-tail at the node, <u>and</u> the node is in the set C or
- Arrows meet head-to-head at the node and neither the node nor any of its descendants is in the set C

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

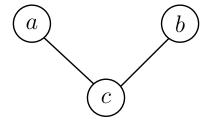


A path is **blocked** if it includes a node such that either

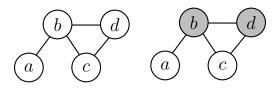
- ► The arrows on the path meet either head-to-tail or tail-to-tail at the node, and the node is in the set *C* (observed) or
- The arrows meet head-to-head at the node, and neither the node nor any of its descendants is in the set *C* (observed)



Markov Random Fields

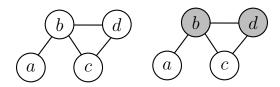


Joint Distribution



▶ Express joint distribution $p(x_1,...,x_n) =: p(x)$ as a product of functions defined on subsets of variables that are local to the graph

Joint Distribution



- ▶ Express joint distribution $p(x_1,...,x_n) =: p(x)$ as a product of functions defined on subsets of variables that are local to the graph
- ▶ 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)

Factorization of the Joint Distribution

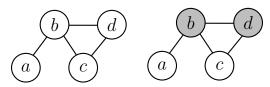
- ▶ If $x_i \perp \!\!\! \perp x_j | x \setminus \{x_i, x_j\}$ then x_i, x_j never appear in a common factor in the factorization of the joint
 - **▶** Joint distribution as a product of cliques (fully connected subgraphs)

Factorization of the Joint Distribution

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

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

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



Factorization of the Joint Distribution

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

- ► 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

Clique Potentials

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

Clique potentials $\psi_C(x_C)$:

- $\psi_C(\mathbf{x}_C) \geqslant 0$
- Unlike directed graphs, no probabilistic interpretation necessary (e.g., marginal or conditional)
 Greater flexibility but computational challenges
- If we convert a directed graph into an MRF, the clique potentials do have a probabilistic interpretation

Normalization Constant

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

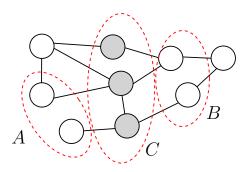
- ► Gives us flexibility in the definition the factorization in an MRF
- ▶ Normalization constant (also: partition function) *Z* is required for parameter learning (not covered in here) and model selection

Normalization Constant

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

- Gives us 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 $A \perp \!\!\! \perp B \mid C$ does not hold

Potentials as Energy Functions

- Look only at potential functions with $\psi_C(x_C) > 0$
 - \Rightarrow $\psi_C(x_C) = \exp(-E(x_C))$ 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

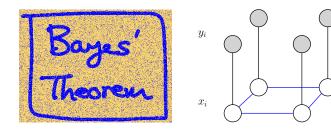
Example: Image De-Noising



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

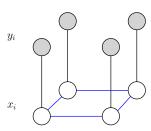
Example: Image De-Noising (2)



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

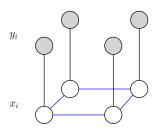
Example: Image De-Noising (2)





- 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

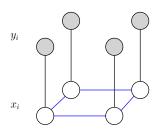
Clique Potentials



Two types of clique potentials:

- - ➤ Strong correlation between observed and latent variables

Clique Potentials



Two types of clique potentials:

- - ▶ 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:

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

- ▶ 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





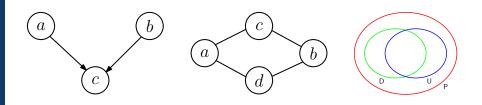


Noise-corrupted image, ICM, Graph-cut (From PRML (Bishop, 2006))

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: $a \perp \!\!\!\perp b | \varnothing$, $a \not\perp \!\!\!\perp b | c$ 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

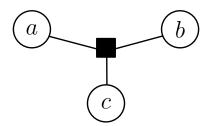
Factor Graphs

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

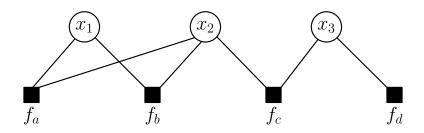
Factorizing the Joint

The joint distribution is a product of factors:

$$p(\mathbf{x}) = \prod_{s} f_s(\mathbf{x}_s)$$

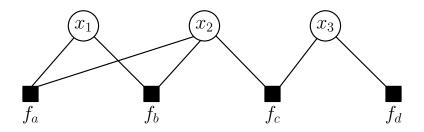
- $x = (x_1, ..., x_n)$
- x_s : Subset of variables
- f_s : Factor; non-negative function of the variables x_s
- ► Building a factor graph as a bipartite graph:
 - Nodes for all random variables (same as in (un)directed graphical models)
 - Additional nodes for factors (black squares) in the joint distribution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



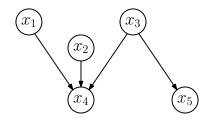
$$p(\mathbf{x}) = f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$$

➤ Efficient inference algorithms for factor graphs (e.g., sum-product algorithm, see Appendix for more information)

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

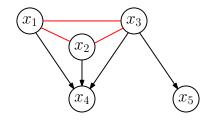


Directed Graph → MRF



1. Moralization:

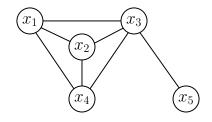
Directed Graph → MRF



1. Moralization:

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

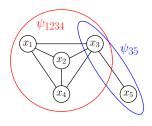
Directed Graph → MRF



1. Moralization:

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

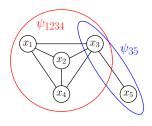
Directed Graph → MRF



1. Moralization:

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

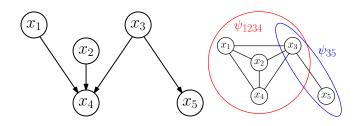
Directed Graph → MRF



1. Moralization:

- 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

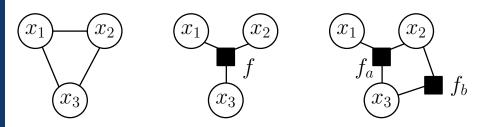
Directed Graph → MRF



1. Moralization:

- 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

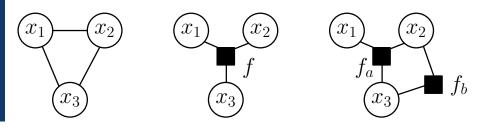
MRF → Factor Graph



- 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



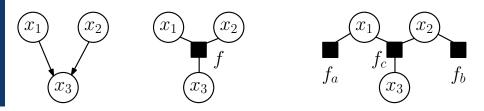
- MRF with clique potential $\psi(x_1, x_2, x_3)$
- ► Factor graph with factor $f(x_1, x_2, x_3) = \psi(x_1, x_2, x_3)$
- Factor graph with factors, such that $f_a(x_1, x_2, x_3) f_b(x_2, x_3) = \psi(x_1, x_2, x_3)$

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

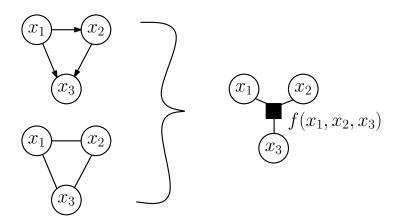
Not unique

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



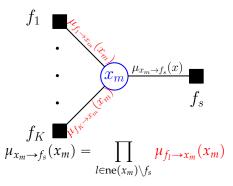
► Local cycles in an (un)directed graph (due to links connecting parents of a node) can be removed on conversion to a factor graph

Exact Inference in Factor Graphs

Sum-Product Algorithm for Factor Graphs

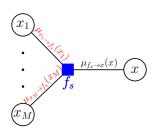
- Factor graphs give a uniform treatment to message passing, which is used for inference in graphs
- ► Inference: Find (marginal) posterior distributions
- ► Two different types of messages:
 - Messages $\mu_{x \to f}(x)$ from variable nodes to factors
 - ► Messages $\mu_{f \to x}(x)$ from factors to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

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



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

- ► 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 of the variables associated with the incoming messages

Initialization

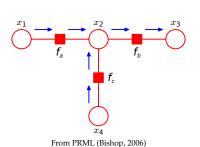
► If the leaf node is a variable nodes, initialize the corresponding messages to 1:

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

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

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

Example (1)



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

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

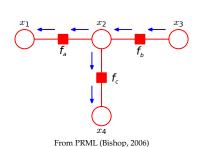
$$\mu_{x_4 \to f_c}(x_4) = 1$$

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

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

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

Example (2)



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

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

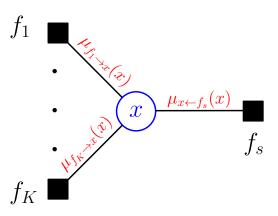
$$\mu_{x_2 \to f_a}(x_2) = \mu_{f_b \to x_2}(x_2) \mu_{f_c \to x_2}(x_2)$$

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

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

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

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
- $x = h \cup v$, 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 $p(h_i|v=\hat{v})$ via sum-product algorithm and some local computations

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

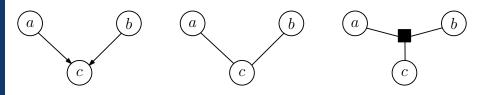






- ► Ranking: TrueSkill (Herbrich et al., 2007)
- Computer vision: de-noising, segmentation, semantic labeling, ...
 (e.g., Sucar & Gillies, 1994; Shotton et al., 2006; Szeliski et al., 2008)
- ► Coding theory: Low-density parity-check codes, turbo codes, ... (e.g., McEliece et al., 1998)
- ► Linear algebra: 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

References I

- D. Bickson, D. Dolev, O. Shental, P. H. Siegel, and J. K. Wolf. Linear Detection via Belief Propagation. In Proceedings of the Annual Allerton Conference on Communication, Control, and Computing, 2007.
- C. M. Bishop. Pattern Recognition and Machine Learning. Information Science and Statistics. Springer-Verlag, 2006.
- [3] M. P. Deisenroth and S. Mohamed. Expectation Propagation in Gaussian Process Dynamical Systems. In Advances in Neural Information Processing Systems, pages 2618–2626, 2012.
- [4] B. J. Frey and D. J. C. MacKay. A Revolution: Belief Propagation in Graphs with Cycles. In Advances in Neural Information Processing Systems, 1998.
- [5] R. Herbrich, T. Minka, and T. Graepel. TrueSkill(TM): A Bayesian Skill Rating System. In Advances in Neural Information Processing Systems, pages 569–576. MIT Press, 2007.
- [6] M. I. Jordan, Z. Ghahramani, T. S. Jaakkola, and L. K. Saul. An Introduction to Variational Methods for Graphical Models. Machine Learning, 37:183–233, 1999.
- [7] B. Kim, J. A. Shah, and F. Doshi-Velez. Mind the Gap: A Generative Approach to Interpretable Feature Selection and Extraction. In C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, editors, Advances in Neural Information Processing Systems, pages 2260–2268, 2015.
- [8] J. Kittler and J. Föglein. Contextual Classification of Multispectral Pixel Data. IMage and Vision Computing, 2(1):13–29, 1984.
- [9] F. R. Kschischang, B. J. Frey, and H.-A. Loeliger. Factor Graphs and the Sum-Product Algorithm. IEEE Transactions on Information Theory, 47:498–519, 2001.
- [10] S. L. Lauritzen and D. J. Spiegelhalter. Local Computations with Probabilities on Graphical Structures and their Application to Expert Systems. *Journal of the Royal Statistical Society*, 50:157–224, 1988.
- [11] H.-A. Loeliger. An Introduction to Factor Graphs. IEEE Signal Processing Magazine, 21(1):28–41, 2004.
- [12] R. J. McEliece, D. J. C. MacKay, and J.-F. Cheng. Turbo Decoding as an Instance of Pearl's "Belief Propagation" Algorithm. IEEE Journal on Selected Areas in Communications, 16(2):140–152, 1998.
- [13] T. P. Minka. A Family of Algorithms for Approximate Bayesian Inference. PhD thesis, Massachusetts Institute of Technology, Cambridge, MA, USA, Jan. 2001.

References II

- [14] J. Pearl. Probabilistic Reasoning in Intelligent Systems: Networks of Plausible Inference. Morgan Kaufmann, 1988.
- [15] O. Shental, D. Bickson, J. K. W. P. H. Siegel and, and D. Dolev. Gaussian Belief Propagatio Solver for Systems of Linear Equations. In *IEEE International Symposium on Information Theory*, 2008.
- [16] J. Shotton, J. Winn, C. Rother, and A. Criminisi. TextonBoost: Joint Appearance, Shape and Context Modeling for Mulit-Class Object Recognition and Segmentation. In Proceedings of the European Conference on Computer Vision, 2006.
- [17] L. E. Sucar and D. F. Gillies. Probabilistic Reasoning in High-Level Vision. Image and Vision Computing, 12(1):42-60, 1994.
- [18] R. Szeliski, R. Zabih, D. Scharstein, O. Veksler, A. A. Vladimir Kolmogorov, M. Tappen, and C. Rother. A Comparative Study of Energy Minimization Methods for Markov Random Fields with Smoothness-based Priors. IEEE Transactions on Pattern Analysis and Machine Intelligence, 30(6):1068–1080, 2008.