Foundations of Machine Learning
African Masters in Machine Intelligence

Graphical Models

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Reading Material

Bishop: Pattern Recognition and Machine Learning, Chapter 8

Probabilistic Models

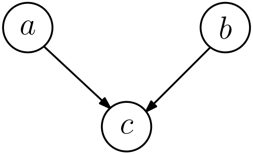
- Quantity of interest: Joint distribution of all observed and unobserved (latent) random variables
  ⏩ Probabilistic model
- Comprises information about the prior, the likelihood and the posterior

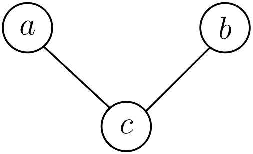
Probabilistic Models

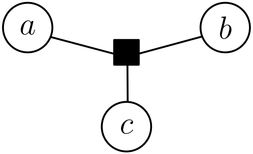
- Quantity of interest: Joint distribution of all observed and unobserved (latent) random variables
  ⏩ Probabilistic model
- Comprises information about the prior, the likelihood and the posterior
- Joint distribution itself can be complicated
- Does not tell us anything about structural properties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

⏩ **Probabilistic graphical models**

Probabilistic Graphical Models



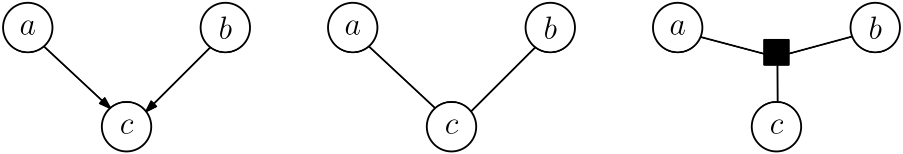




Three types of probabilistic graphical models:

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

Probabilistic Graphical Models



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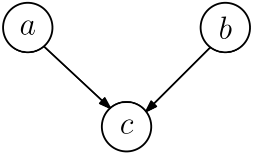
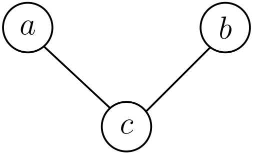
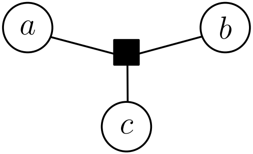
- **Nodes:** (Sets of) random variables
- **Edges:** Probabilistic/functional relations between variables

Probabilistic Graphical Models







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- **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

Why are they useful?

- 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

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

From Kim et al. (NIPS, 2015)

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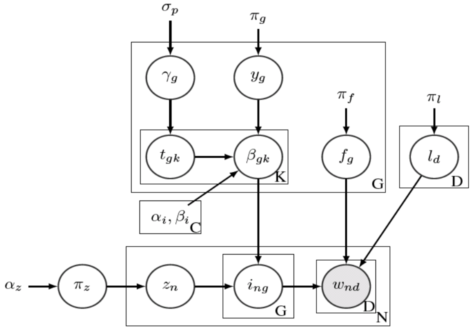

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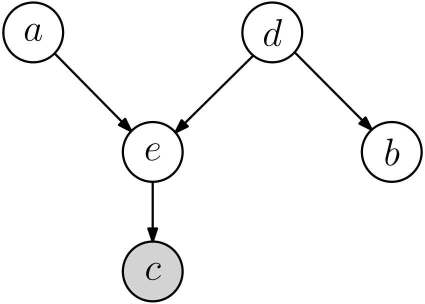
Bayesian Networks (Directed Graphical Models)

Directed Graphical Models



- Nodes: Random variables
- Shaded nodes: Observed
- Unshaded nodes: Unobserved (latent)
- Directed arrows from a to b: Conditional distribution $p(b|a)$.

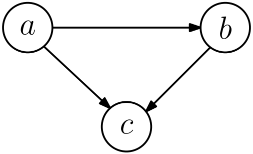
From Joints to Graphs

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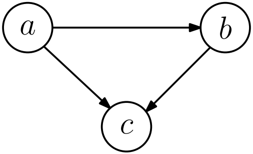
2. For each conditional distribution, we add a directed link (arrow) to the graph from the nodes corresponding to the variables on which the distribution is conditioned on



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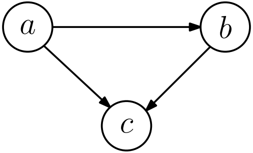
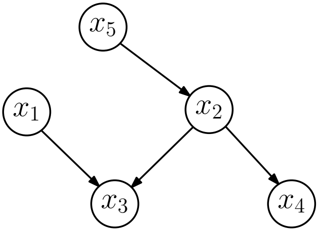


▶▶ Graph layout depends on the choice of factorization

From Graphs to Joints

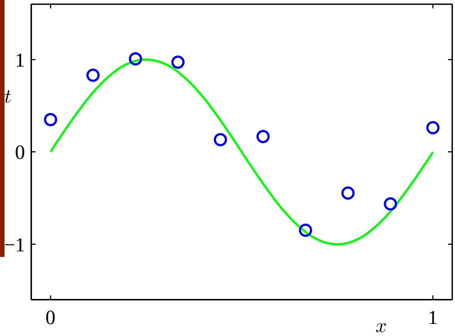


- Joint distribution is the product of a set of conditionals, one for each node in the graph
- Each conditional is conditioned only on the parents of the corresponding node in the graph

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

In general: $p(\boldsymbol{x}) = p(x_1, \ldots, x_K) = \prod_{k=1}^{K} p(x_k|\text{parents}(x_k))$

Graphical Model for Linear Regression



From PRML (Bishop, 2006)

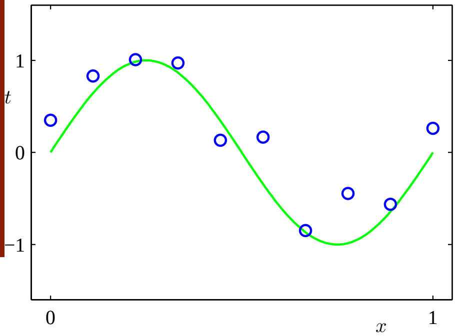
We are given a data set $(x_1, y_1), \ldots, (x_N, y_N)$ where

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

with f unknown.

▶▶ Find a (regression) model that explains the data

Graphical Model for Linear Regression



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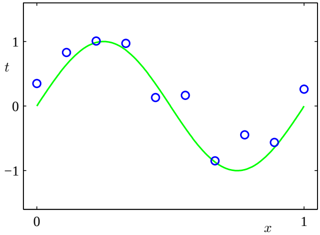
▶▶ Find a (regression) model that explains the data

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

Graphical Model for Linear Regression



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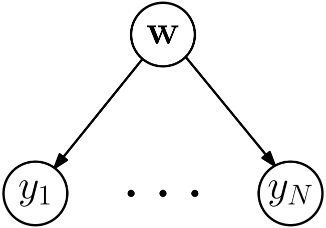

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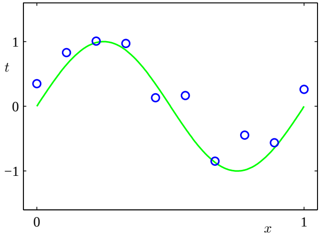

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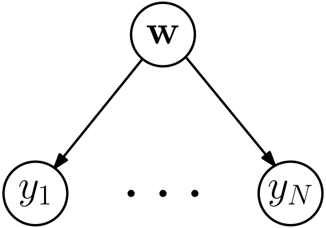

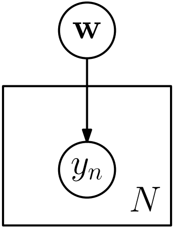

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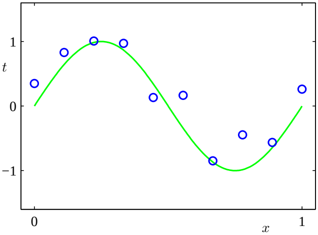

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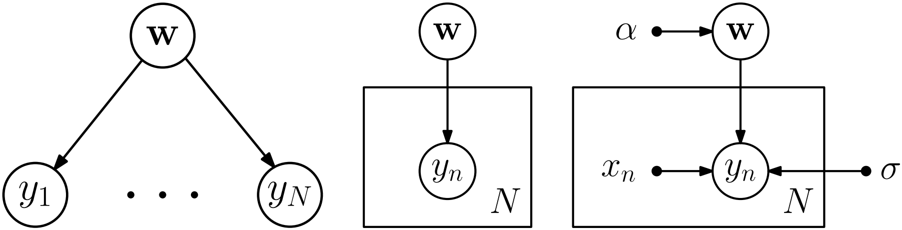
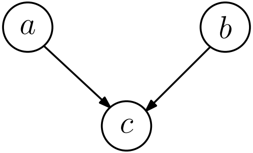


Conditional Independence

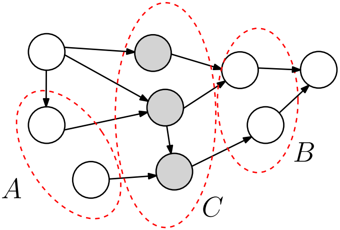


$$a \perp\!\!\!\perp b|c \iff p(a|b,c) = p(a|c)$$
$$\iff p(a,b|c) = p(a|c)p(b|c)$$

- (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 $A \perp\!\!\!\perp B | C$ hold?
Note: C is observed if we condition on it (and the nodes in the GM are shaded)

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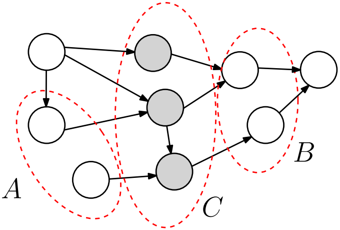

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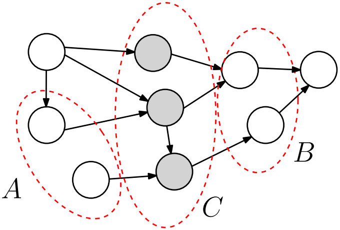
▶▶ Consider all possible paths from any node in A to any node in B.

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

- 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

D-Separation (Directed Graphs)



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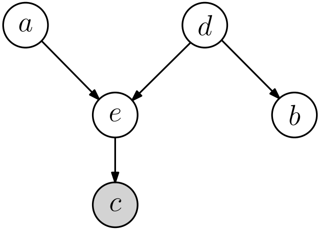
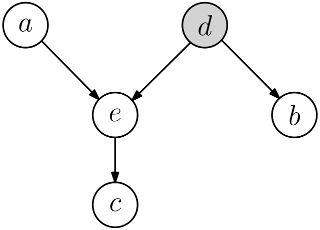
If all paths are blocked, then A is d-separated from B by C, and the joint distribution satisfies $A \perp\!\!\!\perp B | C$.

Example



(a) $a \perp\!\!\!\perp b | c$?



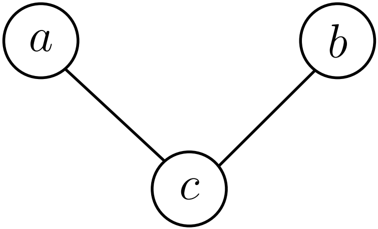
(b) $a \perp\!\!\!\perp b | d$?

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

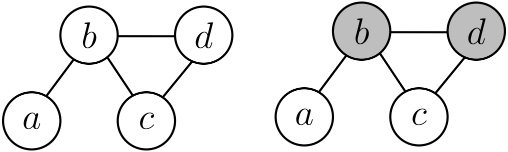
- The arrows on the path meet either head-to-tail or tail-to-tail at the node, and the node is in the set C (observed) or
- The arrows meet head-to-head at the node, and neither the node nor any of its descendants is in the set C (observed)

Markov Random Fields (Undirected Graphical Models)

Markov Random Fields

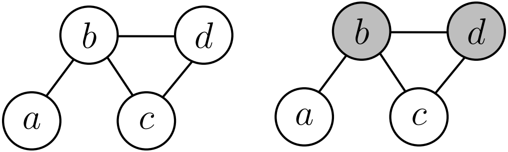


Joint Distribution



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

Joint Distribution



- Express joint distribution $p(x_1, \ldots, x_n) =: p(\boldsymbol{x})$ 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 $x_i \perp\!\!\!\perp x_j | \boldsymbol{x} \backslash \{x_i, x_j\}$ (conditionally independent given everything else)

Factorization of the Joint Distribution

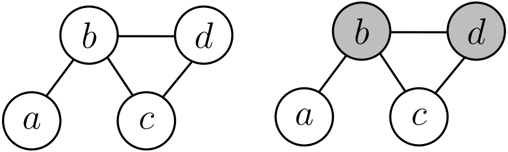
- If $x_i \perp\!\!\!\perp x_j | \boldsymbol{x} \backslash \{x_i, x_j\}$ then x_i, x_j never appear in a common factor in the factorization of the joint

  ⏩ 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:

$$p(\boldsymbol{x}) \propto \prod_C \psi_C(\boldsymbol{x}_C)$$

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



Factorization of the Joint Distribution

$$p(\boldsymbol{x}) = \frac{1}{Z} \prod_{C} \psi_C(\boldsymbol{x}_C)$$

- C: maximal clique
- $\boldsymbol{x}_C$: all variables in this clique
- $\psi_C(\boldsymbol{x}_C)$: clique potential
- $Z = \sum_x \prod_C \psi_C(\boldsymbol{x}_C)$: normalization constant

Clique Potentials

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

Clique potentials $\psi_C(\boldsymbol{x}_C)$:

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

Normalization Constant

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

- 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)

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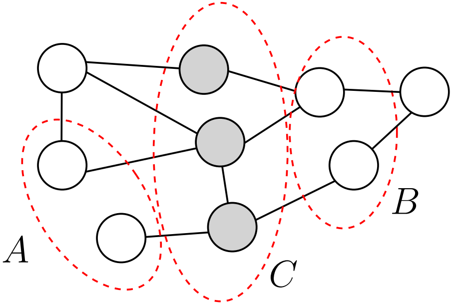
- Gives us flexibility in the definition the factorization in an MRF
- Normalization constant (also: partition function) Z is required for parameter learning (not covered in here)
- In a discrete model with M discrete nodes each having K states, the evaluation Z requires summing over K^M states
  ▶▶ Exponential in the size of the model
- In a continuous model, we need to solve integrals
  ▶▶ Intractable in many cases

▶▶ Major limitation of MRFs

Conditional Independence



Two easy checks for conditional independence:

- $A \perp\!\!\!\perp B|C$ 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 $\psi_C(\boldsymbol{x}_C) > 0$
  - $\psi_C(\boldsymbol{x}_C) = \exp(-E(\boldsymbol{x}_C))$ for some energy function E

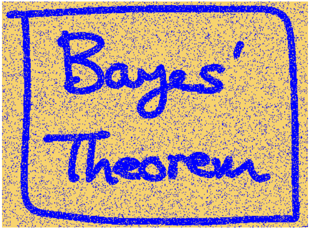
Potentials as Energy Functions

- Look only at potential functions with $\psi_C(\boldsymbol{x}_C) > 0$

  ⏩ $\psi_C(\boldsymbol{x}_C) = \exp(-E(\boldsymbol{x}_C))$ 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 Restoration

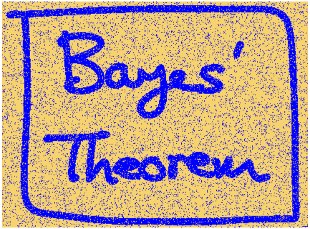


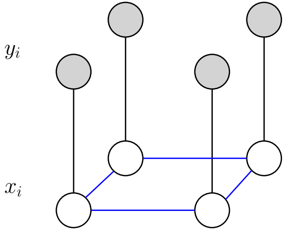
From PRML (Bishop, 2006)

- 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

Image Restoration (2)





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

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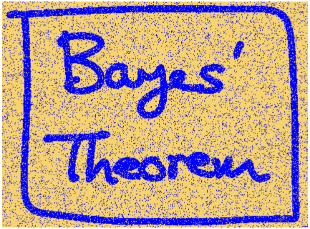
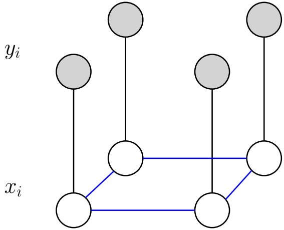
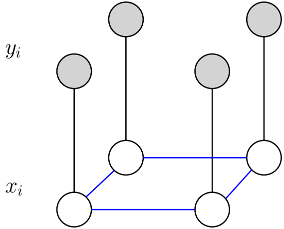




- MRF-based approach
- Latent variables $x_i \in \{-1, +1\}$ are the binary noise-free pixel values that we wish to recover
- Observed variables $y_i \in \{-1, +1\}$ are the noise-corrupted pixel values

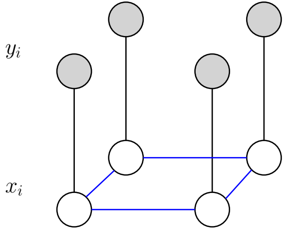
Clique Potentials



Two types of clique potentials:

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

Clique Potentials



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
- $\log \psi_{xx}(x_i, x_j) = E(x_i, x_j) = -\beta x_i x_j\,, \quad \beta > 0$
  for neighboring pixels x_i, x_j
  ⏩ Favor similar labels for neighboring pixels (smoothness prior)

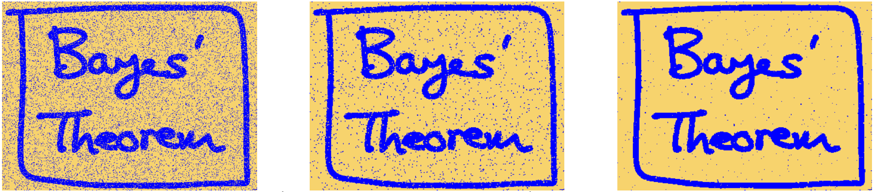
Energy Function

Total energy:

$$E(\boldsymbol{x}, \boldsymbol{y}) = \underbrace{-\eta \sum_i x_i y_i}_{\text{latent-observed}} \underbrace{-\beta \sum_{\{i,j\}} x_i x_j}_{\text{latent-latent}} + \underbrace{\gamma \sum_i x_i}_{\text{bias}}$$

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

ICM Algorithm for Image Restoration



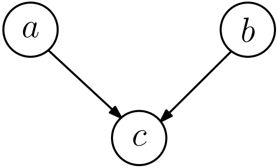
Noise-corrupted image, ICM, Graph-cut (From PRML (Bishop, 2006))

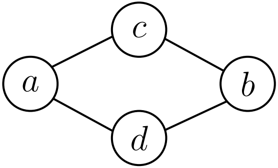
Iterated Conditional Modes (ICM, Kittler & Föglein, 1984)

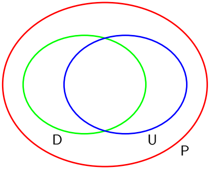
1. Initialize all $x_i = y_i$
2. Pick any x_j: Evaluate total energy
   $E(\boldsymbol{x}^{\setminus j} \cup \{+1\}, \boldsymbol{y}), \quad E(\boldsymbol{x}^{\setminus j} \cup \{-1\}, \boldsymbol{y})$
3. Set x_j to whichever state (± 1) has the lower energy
4. Repeat

▸▸ Local optimum

Relation to Directed Graphs







- Directed and undirected graphs express different conditional independence properties
- Left: $a \perp\!\!\!\perp b | \emptyset$, $a \not\perp\!\!\!\perp b | c$ has no MRF equivalent
- Center: $a \not\perp\!\!\!\perp b | \emptyset$, $c \perp\!\!\!\perp d | a \cup b$, $a \perp\!\!\!\perp b | c \cup d$ has no Bayesnet equivalent

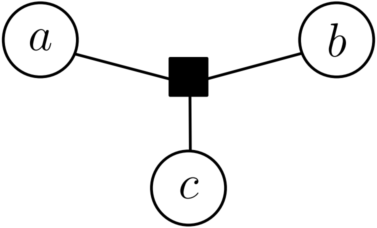
Factor Graphs

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:

$$p(\boldsymbol{x}) = \prod_s f_s(\boldsymbol{x}_s)$$

- $\boldsymbol{x} = (x_1, \ldots, x_n)$
- $\boldsymbol{x}_s$: Subset of variables
- f_s: Factor; non-negative function of the variables $\boldsymbol{x}_s$

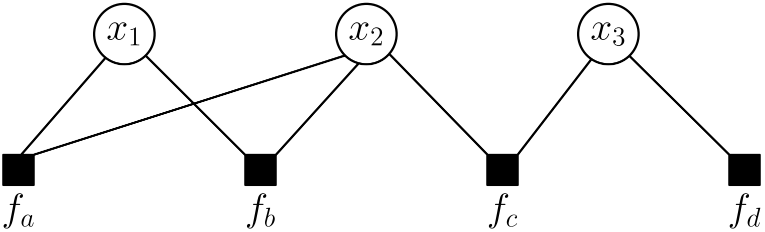
Factorizing the Joint

The joint distribution is a product of factors:

$$p(\boldsymbol{x}) = \prod_s f_s(\boldsymbol{x}_s)$$

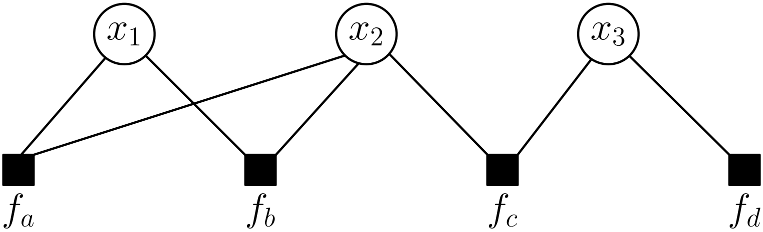
- $\boldsymbol{x} = (x_1, \dots, x_n)$
- $\boldsymbol{x}_s$: Subset of variables
- f_s: Factor; non-negative function of the variables $\boldsymbol{x}_s$
- Building a factor graph as a bipartite graph:
  - Nodes for all random variables (same as in (un)directed graphical models)
  - Additional nodes 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



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

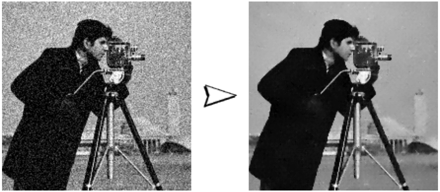
Example



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

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

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)

Appendix

MRF → Factor Graph

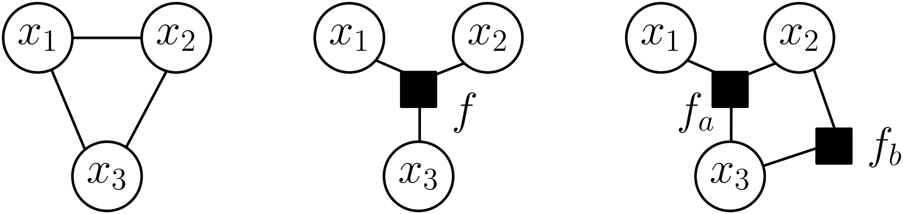
1. Take variable nodes from MRF
2. Create additional factor nodes corresponding to the maximal cliques $\boldsymbol{x}_s$
3. The factors $f_s(\boldsymbol{x}_s)$ equal the clique potentials
4. Add appropriate links

Not unique

Directed Graph → MRF

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

Example: MRF → Factor Graph



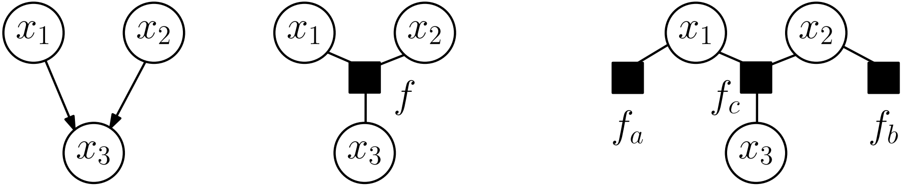
- MRF with clique potential $\psi(x_1, x_2, x_3)$
- Factor graph with factor $f(x_1, x_2, x_3) = \psi(x_1, x_2, x_3)$
- Factor graph with factors, such that $f_a(x_1, x_2, x_3) f_b(x_2, x_3) = \psi(x_1, x_2, x_3)$

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

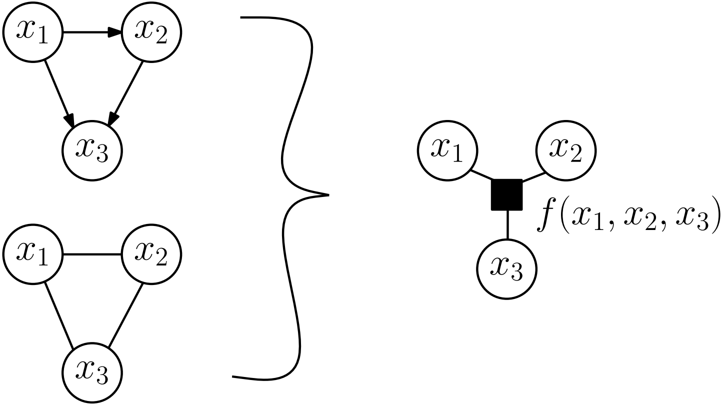
Not unique

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

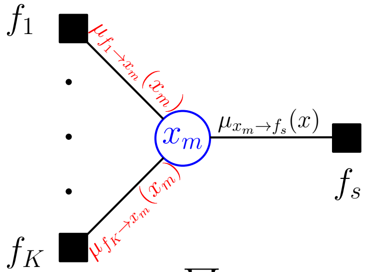


- Local cycles in an (un)directed graph (due to links connecting parents of a node) can be removed on conversion to a factor graph

Sum-Product Algorithm for Factor Graphs

- Factor graphs give a uniform treatment to message passing
- 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.

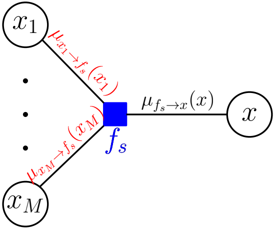
Variable-to-Factor Message



$$\mu_{x_m \to f_s}(x_m) = \prod_{l \in \text{ne}(x_m) \backslash f_s} \mu_{f_l \to x_m}(x_m)$$

- 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



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

- 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

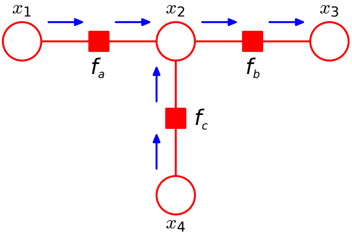
- If the leaf node is a variable nodes, initialize the corresponding messages to 1:

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

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

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

Example (1)



From PRML (Bishop, 2006)

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

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

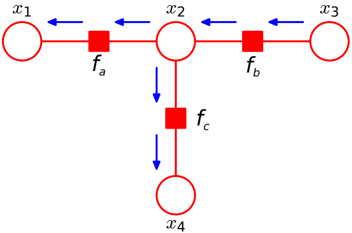
$$\mu_{x_4 \to f_c}(x_4) = 1$$

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

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

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

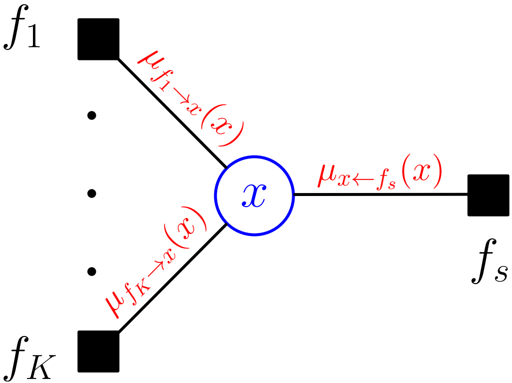
Example (2)



From PRML (Bishop, 2006)

$$
\begin{aligned}
\mu_{x_3 \to f_b}(x_3) &= 1 \\
\mu_{f_b \to x_2}(x_2) &= \sum_{x_3} f_b(x_2, x_3) \cdot 1 \\
\mu_{x_2 \to f_a}(x_2) &= \mu_{f_b \to x_2}(x_2) \mu_{f_c \to x_2}(x_2) \\
\mu_{f_a \to x_1}(x_1) &= \sum_{x_2} f_a(x_1, x_2) \mu_{x_2 \to f_a}(x_2) \\
\mu_{x_2 \to f_c}(x_2) &= \mu_{f_a \to x_2}(x_2) \mu_{f_b \to x_2}(x_2) \\
\mu_{f_c \to x_4}(x_4) &= \sum_{x_2} f_c(x_2, x_4) \mu_{x_2 \to f_c}(x_2)
\end{aligned}
$$

Marginals



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

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

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