Graphical Models

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Probabilistic Models

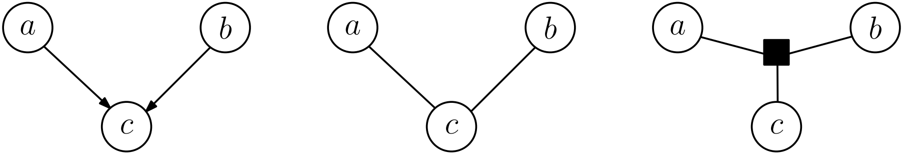
Previously we saw:

- Probabilistic model is a **joint distribution** $p(\mathbf{x}, \mathbf{z})$.
- We make factorisation assumptions to specify the model.
- Factorisation assumptions help simplify the posterior.

Graphical models help us to:

- visualise (conditional) independence,
- specify models with the right structure,
- find (conditional) independence when conditioning,
- do inference automatically and efficiently.

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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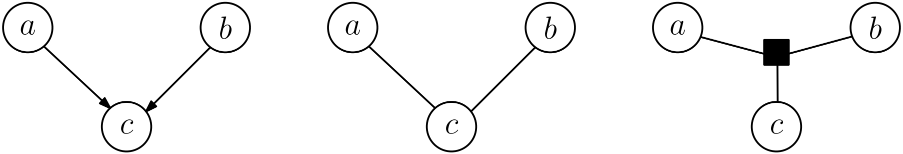

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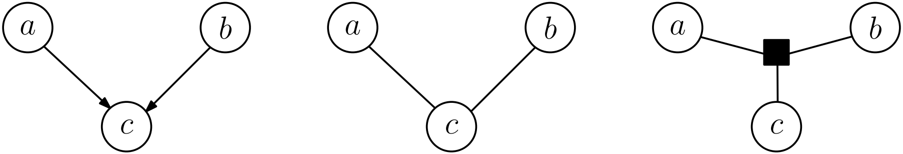

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▶▶ Graph captures the way in which the joint distribution over all random variables can be decomposed into a product of factors depending only on a subset of these variables

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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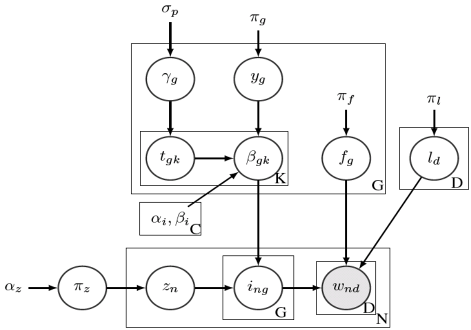

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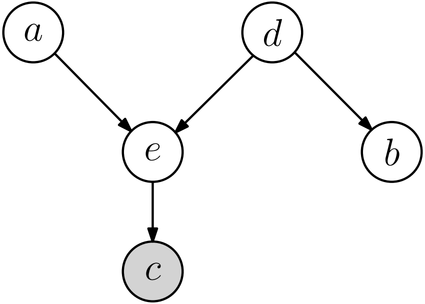
Expressing Factorisations as Graphs

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 $p(b|a)$.

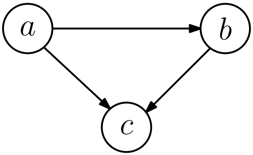
Skill: From Joints to Graphs

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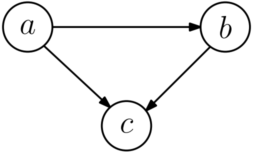
2. For each conditional distribution, we add a directed link (arrow) to the graph from the nodes corresponding to the variables on which the distribution is conditioned on



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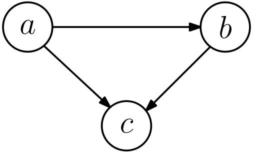

▸▸ Graph layout depends on the choice of factorization

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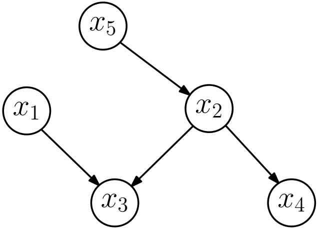

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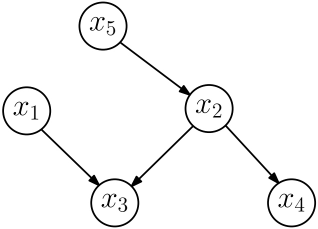

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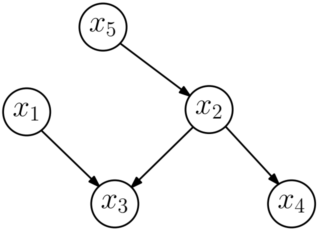

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$$p(x_1, x_2, x_3, x_4, x_5) = p(x_1)p(x_5)p(x_2|x_5)p(x_3|x_1, x_2)p(x_4|x_2)$$

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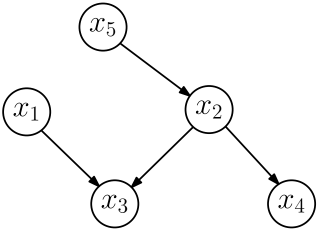

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In general: $p(\boldsymbol{x}) = p(x_1, \ldots, x_K) = \prod_{k=1}^{K} p(x_k|\text{parents}(x_k))$

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Remember, a model is defined simply by its joint distribution, which often is just between data and a latent variable:

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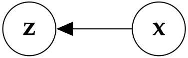

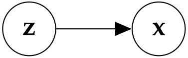

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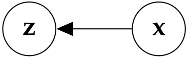
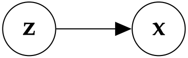
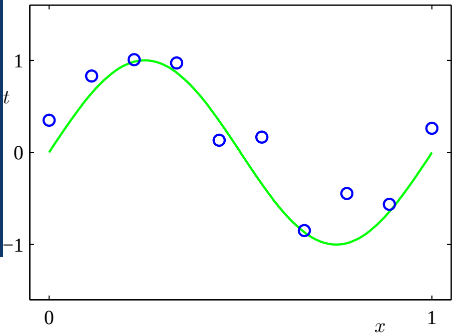




Which one is correct? Depends on which conditional you specified!

$$p(\mathbf{x}, \mathbf{z}) = p(\mathbf{x}|\mathbf{z})\, p(\mathbf{z}) = p(\mathbf{x})\, p(\mathbf{z}|\mathbf{x}) \tag{3}$$

Graphical Model for (Bayesian) Linear Regression



From PRML (Bishop, 2006)

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

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

with f unknown.

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

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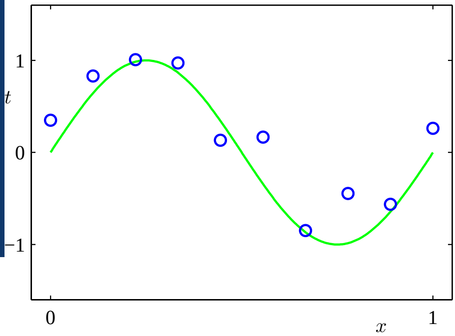

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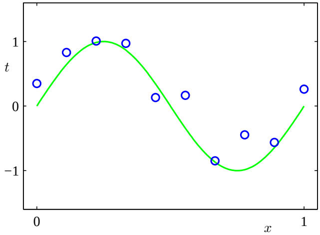
- Consider polynomials $f(x) = \sum_{j=0}^{M} w_j x^j$ with parameters $\boldsymbol{w} = [w_0, \ldots, w_M]^\top$.
- Bayesian linear regression: Place a conjugate Gaussian prior on the parameters: $p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{0}, \alpha^2 \boldsymbol{I})$

Graphical Model for Linear Regression



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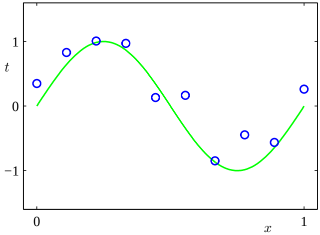

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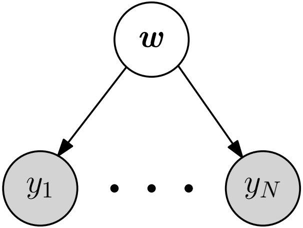

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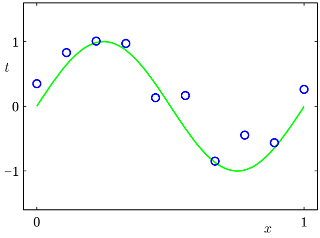

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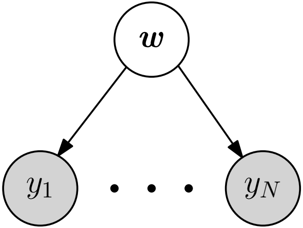

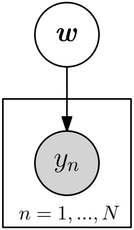

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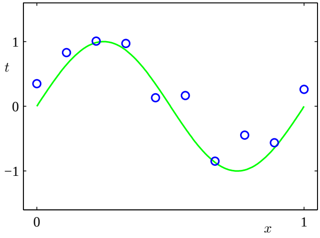

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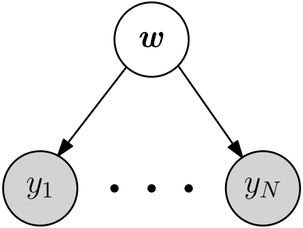
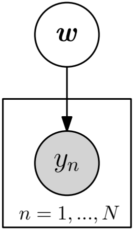
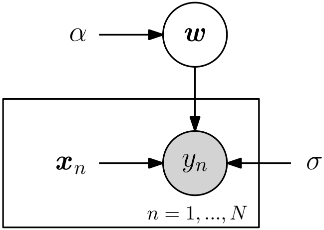
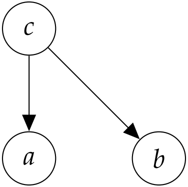






Finding Conditional Independence

Conditional Independence



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

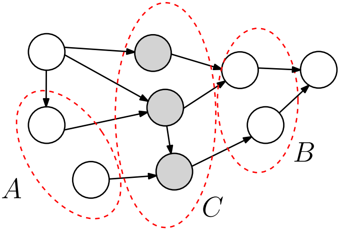
- (Conditional) independence allows for a factorization of the joint distribution ⏩ More efficient inference

$$\mathbb{E}_{p(a,b|c)}[f(a)g(b)] = \mathbb{E}_{p(a|c)}[f(a)] \cdot \mathbb{E}_{p(b|c)}[g(b)] \tag{4}$$

- Conditional independence properties of the joint distribution can be read directly from the graph without analytical manipulations!

⏩ **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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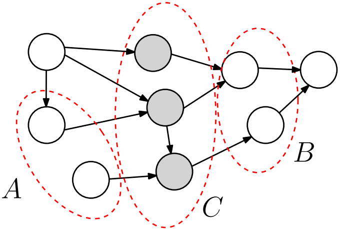

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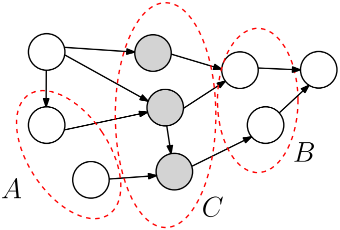

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Any such **path is blocked** if it includes a node such that either

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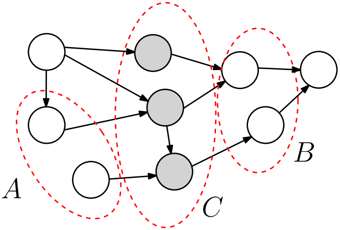

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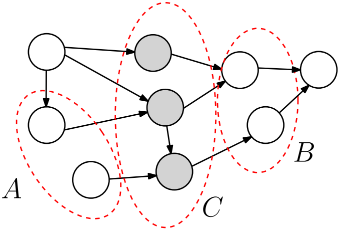

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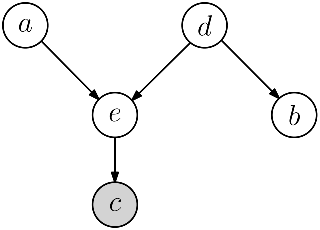
If all paths are blocked, then A is d-separated (conditionally indep.) from B by C, and the joint distribution satisfies $A \perp\!\!\!\perp B | C$.

Exam skill: Find conditional independencies



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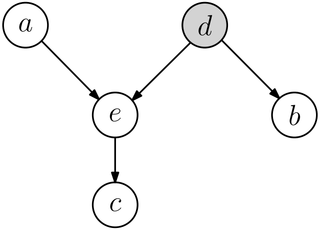

(b) $a \perp\!\!\!\perp b | d$?

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
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(Hidden) Markov Models

- Models of time-varying phenomena (time series)
- Conditional Independencies are crucial

Time-series models

Many phenomena vary over time:

- Dynamical systems
  - motion of stars in the sky, that you want to understand
  - motion of a robot arm, that you want to control
- Audio signals
- Communication signals
- Price of assets over time

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More generally, we can think about **sequence** models:

- DNA sequences
- Language

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- To simplify the specification of the model, we can **assume** that x_t is the **state** of the dynamical system.
- The state is a variable that, if known, determines **everything** there is to know about future states.

Time-series models

What are the relevant random variables?
At the very least, we have one observation for each time point, and a joint over all:

$$p(x_1, x_2, x_3, x_4, \ldots, x_T) \tag{5}$$

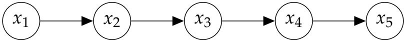
- To simplify the specification of the model, we can **assume** that x_t is the **state** of the dynamical system.
- The state is a variable that, if known, determines **everything** there is to know about future states.
- In other words, $x_{t+T} \perp\!\!\!\perp x_{t-\tau} | x_t$ for $t, T > 0$.

Markov Chains

We can express this assumption with the factorisation:

$$p(x_1, \ldots, x_5) = p(x_1) \prod_{t=2}^{5} p(x_t | x_{t-1}) \tag{6}$$

With the corresponding graphical model:



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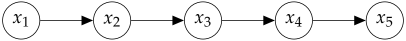

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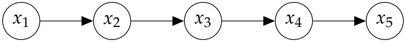

Exercise: Show that $x_4 \perp\!\!\!\perp x_1 | x_3$.

▶▶ Single path from x_4 to x_3, blocked by rule 1 since x_3 is observed.

Hidden Markov Models

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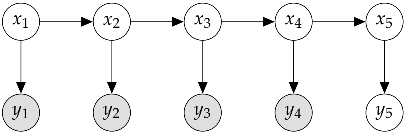

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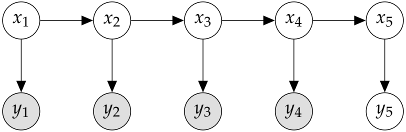
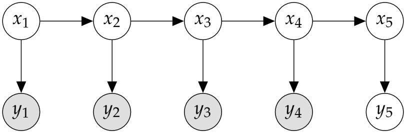


$$p(\{x_t\}_{t=1}^5, \{y_t\}_{t=1}^5) = p(x_1)\left[\prod_{t=2}^5 p(x_t|x_{t-1})\right]\left[\prod_{t=1}^5 p(y_t|x_t)\right] \tag{7}$$

Hidden Markov Models



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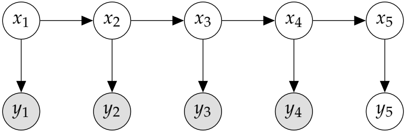
Hidden Markov Models



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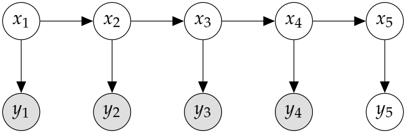
Hidden Markov Models



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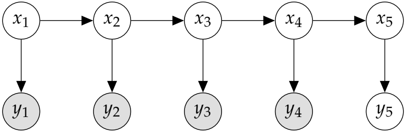
Hidden Markov Models



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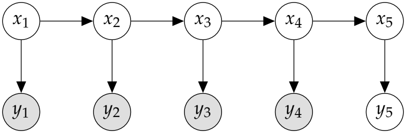
$$p(y_1, \ldots, y_T) \stackrel{\text{AT}}{=} p(y_1)p(y_2|y_1)p(y_3|y_2, y_1)\prod_{t=4}^{T} p(y_t|y_1, \ldots, y_{t-1}) \quad (8)$$

Hidden Markov Models



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- We never needed to specify a function on more than 2 variables! ($p(x_t|x_{t-1})$ vs e.g. $p(y_t|y_1, \dots, y_{t-1})$).

Hidden Markov Models: Example Applications

- Figuring out the trajectory of a projectile from RADAR observations (e.g. spacecraft).
  - State is the location and speed of a projectile
  - $p(x_t|x_{t-1})$ is determined by Newton's laws, plus uncertainty form unknown forces acting on the object.
  - This is an example of physics-inspired model, where latent variables have physical interpretation.
- Stock market models
  - Posit some hypothetical "market state", which *if you knew it* would predict the future well.
  - No "real" way in which the state "exists", but it can help with prediction!

Hidden Markov Models: Two Questions

- Given all observations, what is our belief on the latent at time t?
  I.e. find $p(x_t|y_{1:t})$.
- How can we predict into the future?
  I.e. find $p(y_{t+1}|y_{1:t})$.

Filtering Distribution

Systematic method: Probability of Everything

$$p(x_t|y_{1:t}) \overset{\text{AT}}{=} \int \frac{p(x_1, \dots, x_t, y_1, \dots, y_t)}{p(y_1, \dots, y_t)} \mathrm{d}x_1 \dots x_{t-1}$$

$$\overset{\text{MA}}{=} \int \frac{p(x_1)\left[\prod_{t=2}^{t} p(x_t|x_{t-1})\right]\left[\prod_{t=1}^{t} p(y_t|x_t)\right]}{p(y_1, \dots, y_t)} \mathrm{d}x_1 \dots x_{t-1}$$

$$p(y_1, \dots, y_t) = \int p(x_1)\left[\prod_{t=2}^{t} p(x_t|x_{t-1})\right]\left[\prod_{t=1}^{t} p(y_t|x_t)\right] \mathrm{d}x_1 \dots x_t$$

- In principle, we could compute this (everything is specified in a density from the model specification!)
- Lots of sums/integrals though! Very slow to compute!
- Could rearrange the sums to speed things up?

Recursive Filtering

You can actually get a recursive equation to solve this problem, which is much easier to compute:

$$\text{Step 1:} \qquad p(x_t|y_1,\ldots,y_{t-1}) = \int p(x_t|x_{t-1})p(x_{t-1}|y_1,\ldots,y_{t-1})\mathrm{d}y_{1:t-1}$$

$$\text{Step 2:} \qquad p(x_t|y_1,\ldots,y_t) = \frac{p(y_t|x_t)p(x_t|y_{1:t-1})}{p(y_t|y_{1:t-1})}$$

- Only needs one sum/integral.
- See `exercises.pdf` (question 9) for full derivation.
- Look at `hmm-demo.ipynb` for alternative derivation and code demonstrating the model.

HMM Demo

Demo `hmm-demo.ipynb`. TODO: Save figures from ipynb and put in slides.

Algorithms on Graphs

- It took some effort to derive the recursive algorithm for efficient filtering.
- Algorithms on graphs can discover these **efficient** algorithms **automatically**!
- ⏩ Belief Propagation (not examinable)

Conclusion

- Skill: Conditionals to Graphical Model
- Skill: Graphical model to Conditionals
- Skill: Conditional Independence from Graphical Model
- Skill: Simplification of Posteriors using Conditional Independencies

Further Reading

Bishop: Pattern Recognition and Machine Learning, Chapter 8
Directed graphical models

References I

[1] C. M. Bishop. *Pattern Recognition and Machine Learning*. Information Science and Statistics. Springer-Verlag, 2006.

[2] 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.

[3] J. Pearl. *Probabilistic Reasoning in Intelligent Systems: Networks of Plausible Inference*. Morgan Kaufmann, 1988.

Not examinable from here

Factor Graphs

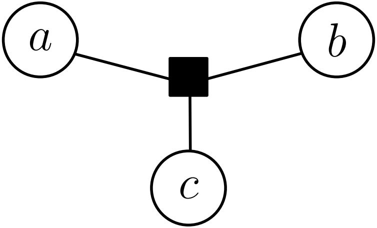
A different graphical representation

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 $\boldsymbol{x}_s$

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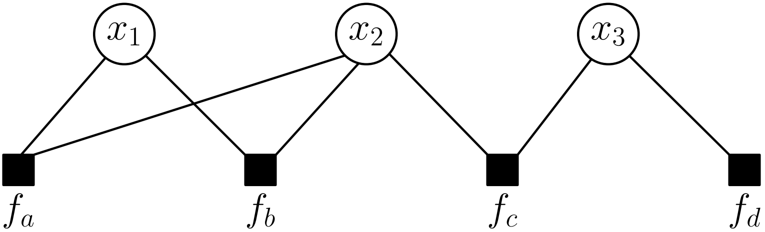
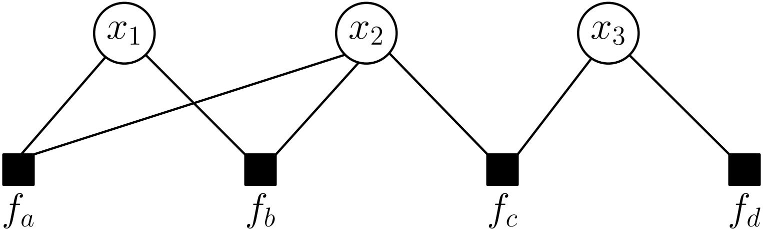
- $\boldsymbol{x}_s$: Subset of variables
- f_s: Factor; non-negative function of the variables $\boldsymbol{x}_s$
- Building a factor graph as a bipartite graph:
  - Nodes for all random variables (same as in (un)directed graphical models)
  - Additional nodes for factors (black squares) in the joint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



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

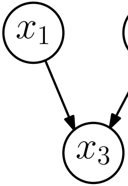
- Efficient inference algorithms for factor graphs (e.g., sum-product algorithm)

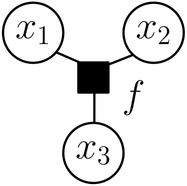
Directed Graphical Model → Factor Graph

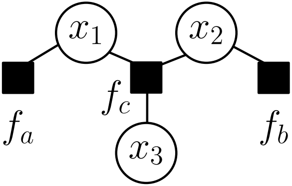
1. Take variable nodes from Bayesian network
2. Create additional factor nodes corresponding to the conditional distributions
3. Add appropriate links

Not unique

Example: Directed Graph → Factor Graph

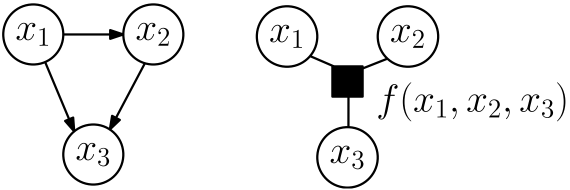






- Directed graph with factorization $p(x_1)p(x_2)p(x_3|x_1, x_2)$
- Factor graph with factor $f(x_1, x_2, x_3) = p(x_1)p(x_2)p(x_3|x_1, x_2)$
- Factor graph with factors $f_a = p(x_1),\ f_b = p(x_2),\ f_c = p(x_3|x_1, x_2)$

Removing Cycles



$$p(x_3|x_2, x_1)p(x_2|x_1)p(x_1) = f_a(x_1, x_2, x_3)f_b(x_1, x_2)f_c(x_2) = f(x_1, x_2, x_3) \tag{9}$$

- 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

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- 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

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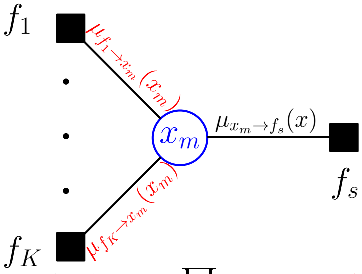
- Two different types of messages:
  - Messages $\mu_{x\to f}(x)$ from variable nodes to factors
  - Messages $\mu_{f\to x}(x)$ from factors to variable nodes
- Repeated sending of these messages through the graph converges
- Factors transform messages into evidence for the receiving node

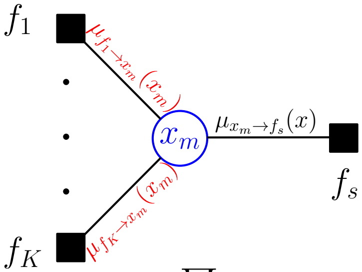
Variable-to-Factor Message



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

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

Variable-to-Factor Message



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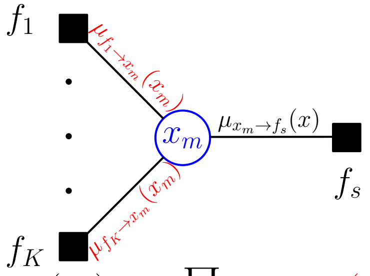
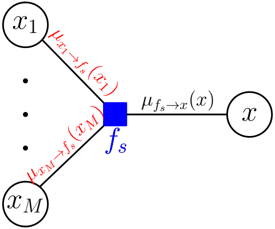


$$\mu_{x_m \to f_s}(x_m) = \prod_{l \in \text{ne}(x_m) \setminus f_s} \mu_{f_l \to x_m}(x_m)$$

- 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.

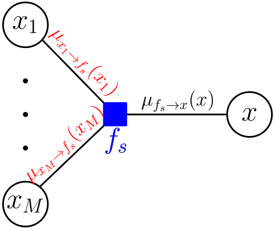
Factor-to-Variable Message



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

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

Factor-to-Variable Message



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

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

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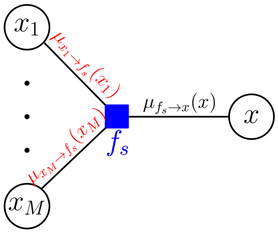


$$\mu_{f_s \to x}(x) = \sum_{x_1} \cdots \sum_{x_M} f_s(x, x_1, \ldots, x_M) \prod_{m \in \mathrm{ne}(f_s) \setminus x} \mu_{x_m \to f_s}(x_m)$$

- 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

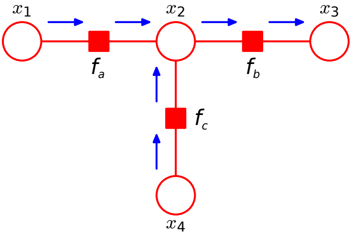
- If the leaf node is a variable node, initialize the corresponding messages to 1:

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

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

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

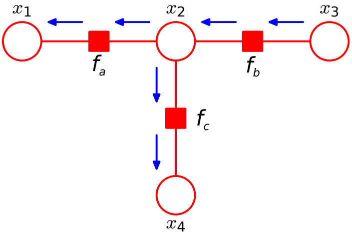
Example (1)



From PRML (Bishop, 2006)

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

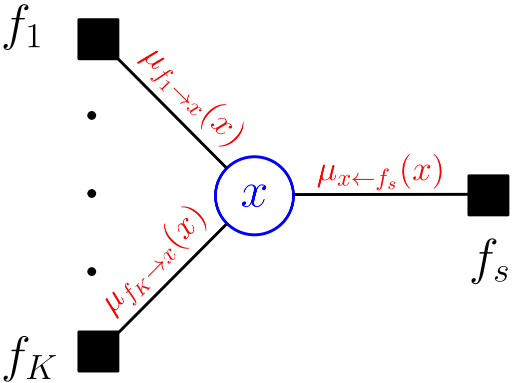
Example (2)



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:

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

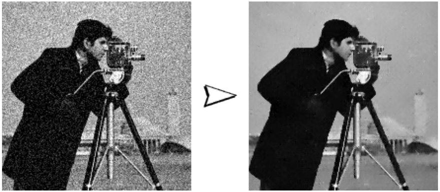
Observed Variables ⏩ Posterior

- Thus far, we have focused on the case where all variables are unobserved.
- Posterior is always conditioned on observations
- Partition $\boldsymbol{x} = \boldsymbol{h} \cup \boldsymbol{v}$, $\boldsymbol{h}$: hidden variables, $\boldsymbol{v}$: visible variables with observations $\hat{\boldsymbol{v}}$
- $p(\boldsymbol{v} = \hat{\boldsymbol{v}}) = \prod_i I(v_i = \hat{v}_i)$
- $p(\boldsymbol{x})p(\boldsymbol{v} = \hat{\boldsymbol{v}}) = p(\boldsymbol{h}, \boldsymbol{v} = \hat{\boldsymbol{v}}) \propto p(\boldsymbol{h}|\boldsymbol{v} = \hat{\boldsymbol{v}})$
- Marginal posteriors $p(h_i|\boldsymbol{v} = \hat{\boldsymbol{v}})$ 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)