Graphical Models

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Contents

Introduction to graphical models

- This presentation concentrates on *probabilistic graphical models*, they have several benefits
  - They provide a simple, clear way to visualize the probabilistic model, this helps e.g. designing new models
  - Different properties of the probabilistic model, like conditional independence can be seen from the graphical model
  - Complex computations in sophisticated models can be expressed in terms of graphical manipulations

Introduction to graphical models

- A graph consists of nodes (vertices) that are connected by edges (links, arcs)
- The graph can be directed (edges have arrows to indicate the direction) or undirected (edges do not have arrows)
- In probabilistic graphical models each node in a graph represents a random variable and the edges of the graph represent probabilistic relationships between these variables

Bayesian networks

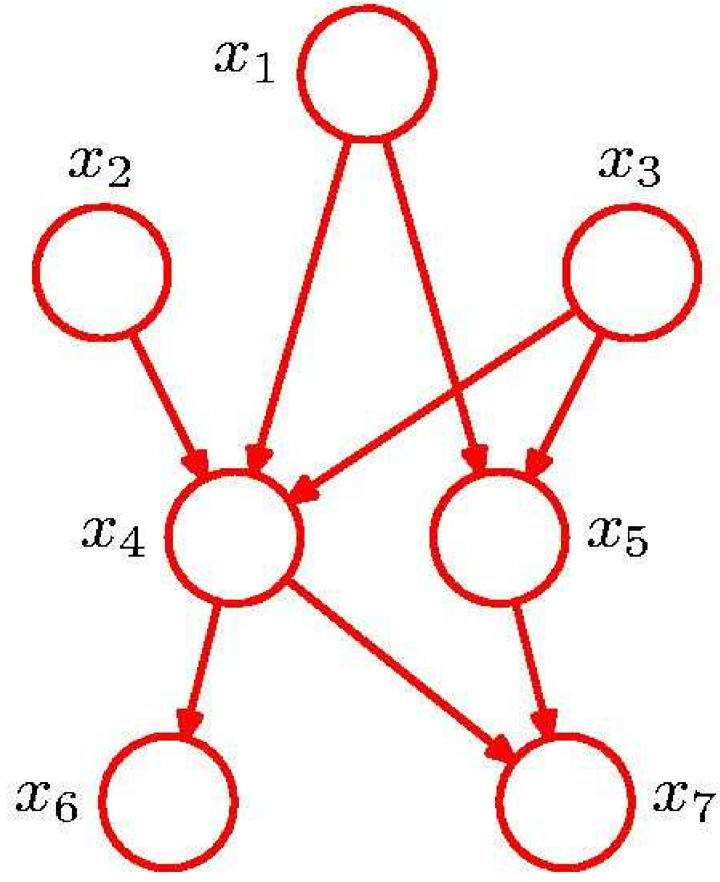
- Also known as directed graphical models
- Each node is associated with a random variable or with a group of variables
- Edges describe conditional relationships between variables
  - For example, if the distribution is $p(b|a)$ then the corresponding graphical model will have a directed edge from a to b

Bayesian networks: example

- Let the distribution be:

$$p(x_1)\,p(x_2)\,p(x_3)\,p(x_4 \mid x_1, x_2, x_3)\,p(x_5 \mid x_1, x_3)\,p(x_6 \mid x_4)\,p(x_7 \mid x_4, x_5)$$

- Then the corresponding graphical model is:



Bayesian networks: polynomial regression

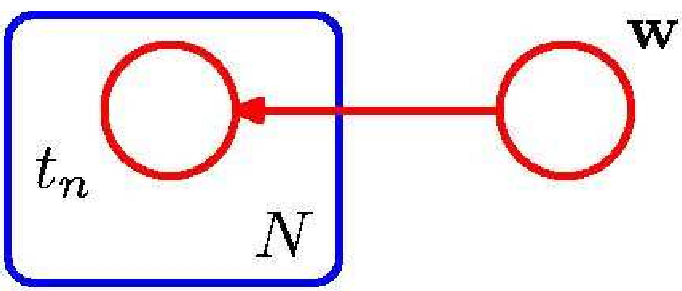
- Lets build a graphical model for polynomial regression
- The polynomial regression model contains
  - Vector of polynomial coefficients **w**
  - Observed data $\mathbf{t} = (t_1, \ldots, t_N)^T$
  - Input data $\mathbf{x} = (x_1, \ldots, x_N)^T$
  - Noise variance σ^2
  - Hyperparameter α

Bayesian networks: polynomial regression

- Lets concentrate first on random variables, their distribution can be expressed as

$$p(\mathbf{t}, w) = p(w)\prod_{n=1}^{N} p(t_n \mid w)$$

- The corresponding graphical model (the box denotes that there are *N* values inside) is:



Bayesian networks: polynomial regression

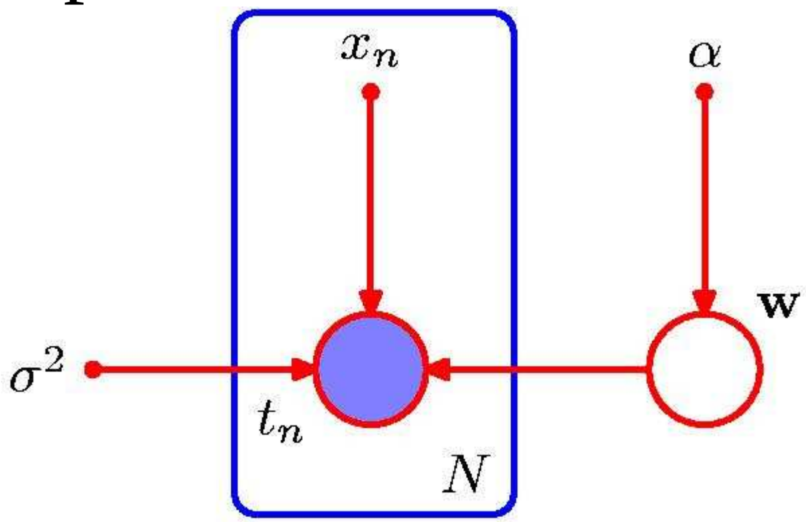
- Machine learning problems usually have a training set
  - In graphical models these observed variables are denoted by shading
- Sometimes it is better to show parameters of a model explicitly
  - In graphical models deterministic parameters are denoted by small, solid circles (variables are denoted by larger, open circles)

Bayesian networks: polynomial regression

- With parameters the distribution becomes:

$$p(\mathbf{t}, w \mid \mathbf{x}, \alpha, \sigma^2) = p(w \mid \alpha) \prod_{n=1}^{N} p(t_n \mid w, x_n, \sigma^2)$$

- And the graphical model:



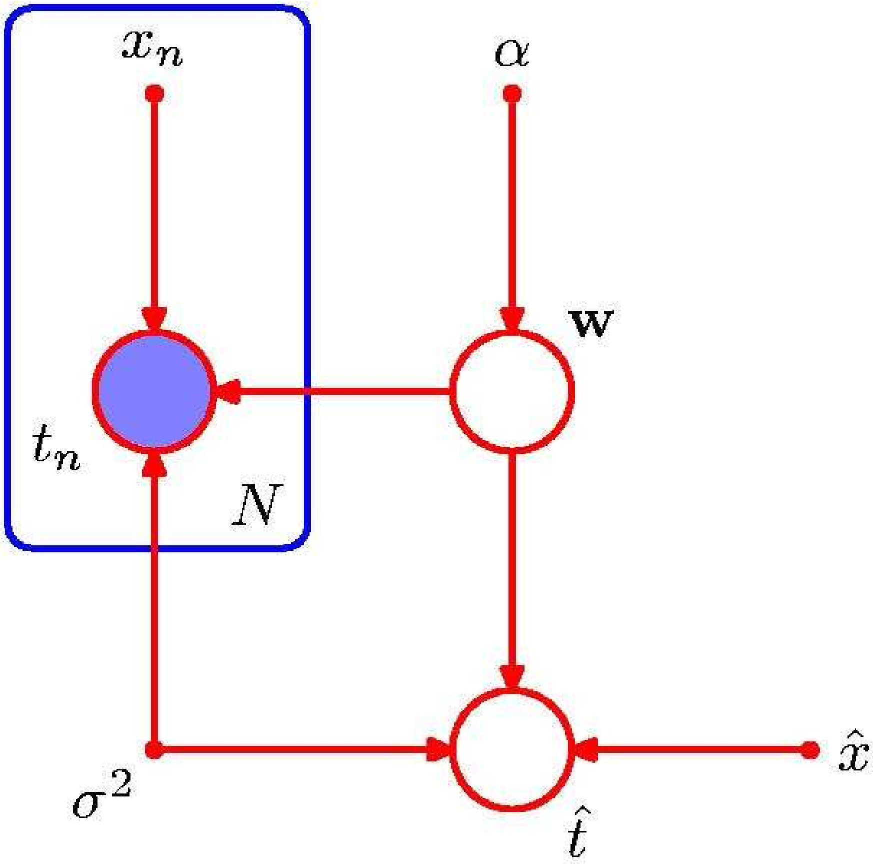
Bayesian networks: polynomial regression

- The aim of the polynomial regression model is: given a new input value $\hat{x}$ find the corresponding probability distribution $\hat{t}$ conditioned on the observed data
- Thus, the final form of the model is:

$$p(\hat{t}, \mathbf{t}, w \mid \hat{x}, \mathbf{x}, \alpha, \sigma^2) = \left[\prod_{n=1}^{N} p(t_n \mid w, x_n, \sigma^2) \right] p(w \mid \alpha) p(\hat{t} \mid \hat{x}, w, \sigma^2)$$

Bayesian networks: polynomial regression

- The corresponding final graphical model is:



Conditional independence

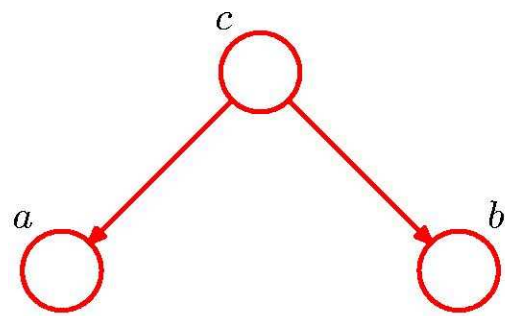
- If p(a|b,c) = p(a|c) then a is conditionally independent of b given c: $a \perp\!\!\!\perp b \mid c$
- We can write above as:

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

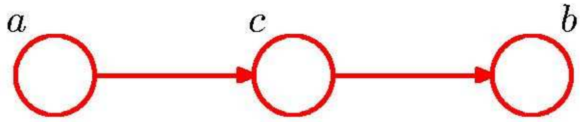
  – Now the joint distribution factorises into the product of marginal distribution of a and b, both of these marginal distributions are conditioned on c

Conditional independence: d-separation

- D-separation can be used to determine wherever of not there exist a conditional independence in the underlying model
- Some concepts
  - Node c is a tail-to-tail node:

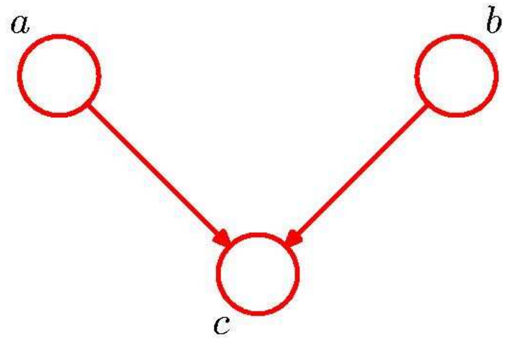


  - Node c is a head-to-tail node:



Conditional independence: d-separation

– Node c is a head-to-head node:

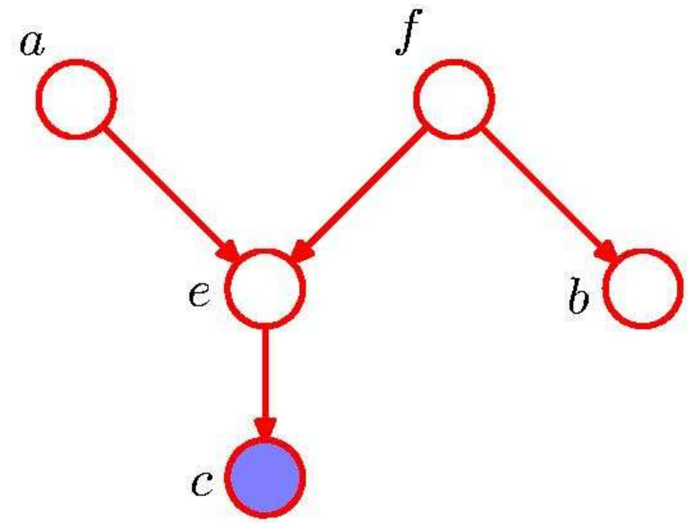


– Node y is a descendant of node x if there is a path from x to y in which each step of the path follows the directions of the arrows

Conditional independence: d-separation

- Let A, B and C be nonintersecting sets of nodes
- Lets consider all possible paths from any node in A to any node in B, the 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, or
  - the 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 from B by C and thus condition $A \perp\!\!\!\perp B \mid C$ is satisfied

Conditional independence: example

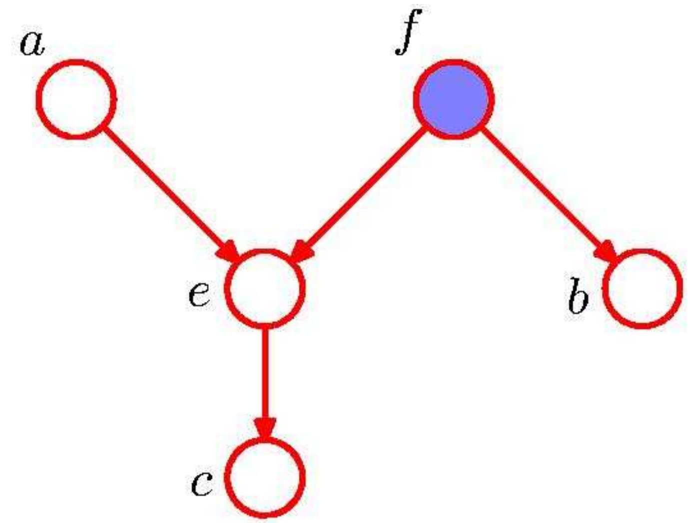


- Node *f* does not block the path between *a* and *b* because it is a tail-to-tail node and is not observed
- Node *e* does not block the path because it has a descendant *c*
- Thus, *a* and *b* are **not** conditionally independent given *c*

Conditional independence: second example

- Node *f* blocks the path between *a* and *b* because it is a tail-to-tail node that is observed, thus there exist a conditional independence:

  $a \perp\!\!\!\perp b \mid f$



- In this case, also node *e* blocks the path, because *e* does not have descendants in the conditioned set

Markov random fields

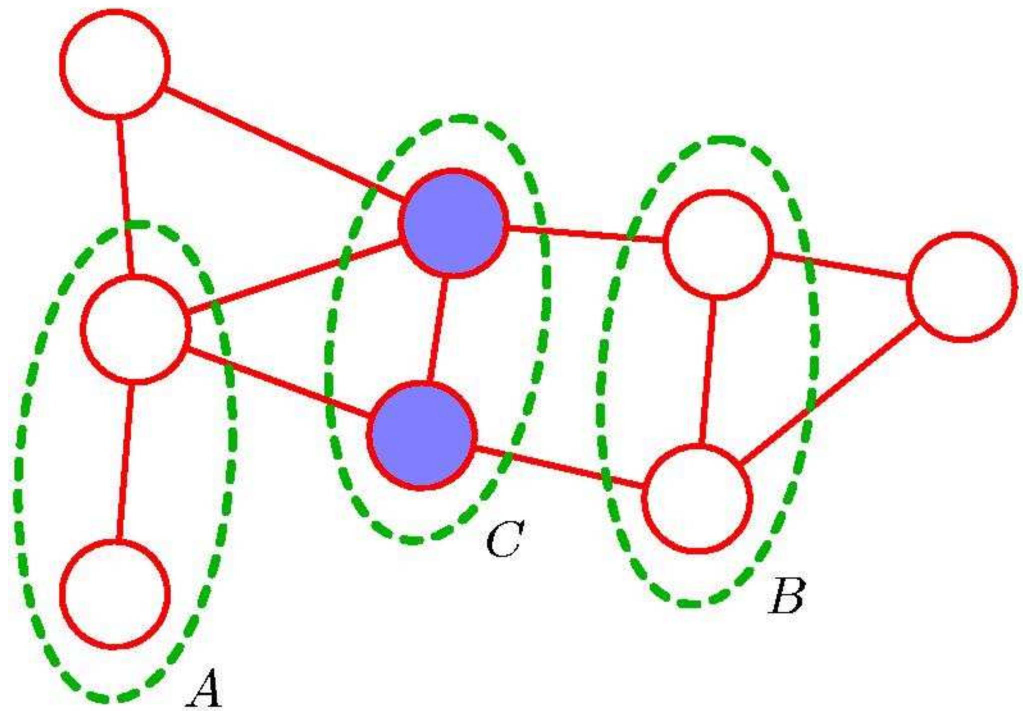
- Also known as Markov networks or undirected graphical models
- In Markov random fields each node corresponds to a variable or to a group of variables just like in the Bayesian networks
- However, edges between nodes are undirected in Markov random fields

Markov random fields: conditional independence

- Let A, B and C be nonintersecting sets of nodes
- Lets consider all possible paths from any node in A to any node in B, the path is blocked if it includes a node from C
- If all such paths are blocked, then A and B are conditionally independent give C: $A \perp\!\!\!\perp B \mid C$

Markov random fields: conditional independence

- In this example A and B are conditionally independent because all paths between A and B go through C



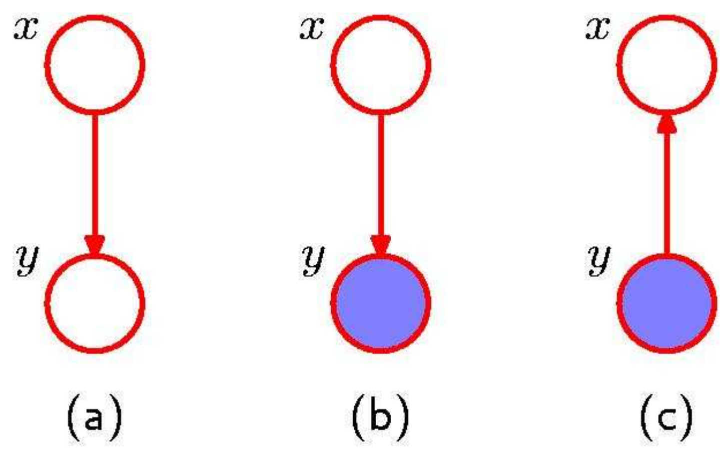
Inference in graphical models

- Lets look at the Bayes' theorem's rule: p(x,y)=p(x)p(y|x) , this rule can be represented by a graph (a) on the next slide
- If the y is observed (graph (b)), then it is possible to infer corresponding posterior distribution of x: $p(y) = \sum_{x'} p(y \mid x')\, p(x')$

$$p(x \mid y) = \frac{p(y \mid x)\, p(x)}{p(y)}$$

Inference in graphical models

- Now the joint distribution p(x,y) can be expressed in terms of p(y) and p(x|y) as graph (c) shows: p(x,y) = p(y)p(x|y)
- This is a simple example of inference problem in graphical models



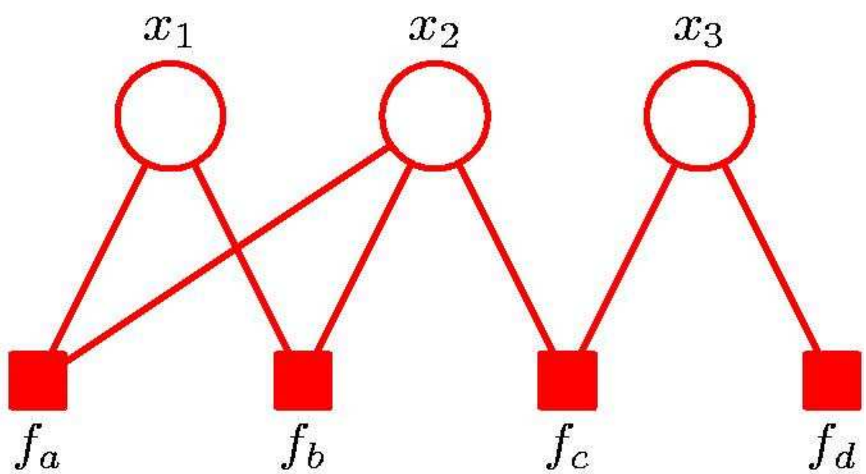
Inference in graphical models: factor graphs

- Graphical models allow a function of several variables to be expressed a product of factors over subsets of those variables
- Factor graphs make this separation explicit by introducing additional nodes for factors
- Lets write the joint distribution in the form of a product of factors (x_s denotes a subset of variables)

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

Inference in graphical models: factor graphs, example

- Let the distribution be
  $p(x) = f_a(x_1, x_2)\, f_b(x_1, x_2)\, f_c(x_2, x_3)\, f_d(x_3)$
- The corresponding factor graph is



Inference in graphical models: factor graphs

- Factor graphs are bipartite graphs, because they consist of two different kinds of nodes, and all edges go between nodes of opposite type
- Factor graphs are useful for building more complex models that are not covered here