Machine Learning

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Acknowledgements

- Eibe Frank
- Ian Witten
- Tom Mitchell

Outline

- Bayesian learning and Naive Bayes
- Brief introduction to Bayesian Networks
- Linear regression

Bayesian Theorem

likelihood

posterior

$$P(h \mid D) = \frac{P(D \mid h)P(h)}{P(D)}$$

prior(s)

P(h) = prior probability of hypothesis h

P(D) = prior probability of training data D

P(h|D) = conditional probability of h given D

P(D|h) = conditional probability of D given h

Naive Bayes Classifier

- Assume target function f: X → V, where each instance x is described by attributes $\{a_1, \ldots, a_n\}$
- Most probable value of f(x) is:

$$v_{MAP} = \operatorname*{argmax}_{v_j \in V} P(v_j | a_1, a_2 \ldots a_n)$$

$$v_{MAP} = \operatorname*{argmax}_{v_j \in V} \frac{P(a_1, a_2 \ldots a_n | v_j) P(v_j)}{P(a_1, a_2 \ldots a_n)}$$

$$= \operatorname*{argmax}_{v_j \in V} P(a_1, a_2 \ldots a_n | v_j) P(v_j)$$

- The Naive Bayes assumption of conditional independence

$$P(a_1, a_2 \ldots a_n | v_j) = \prod_i P(a_i | v_j)$$

gives the *Naive Bayes classifier*:

$$v_{NB} = \operatorname*{argmax}_{v_j \in V} P(v_j) \prod_i P(a_i | v_j)$$

Naive Bayes Example

- Consider PlayTennis again, and a new instance (Outlook=sunny, Temp=cool, Humid=high, Wind=strong)
- Want to compute:

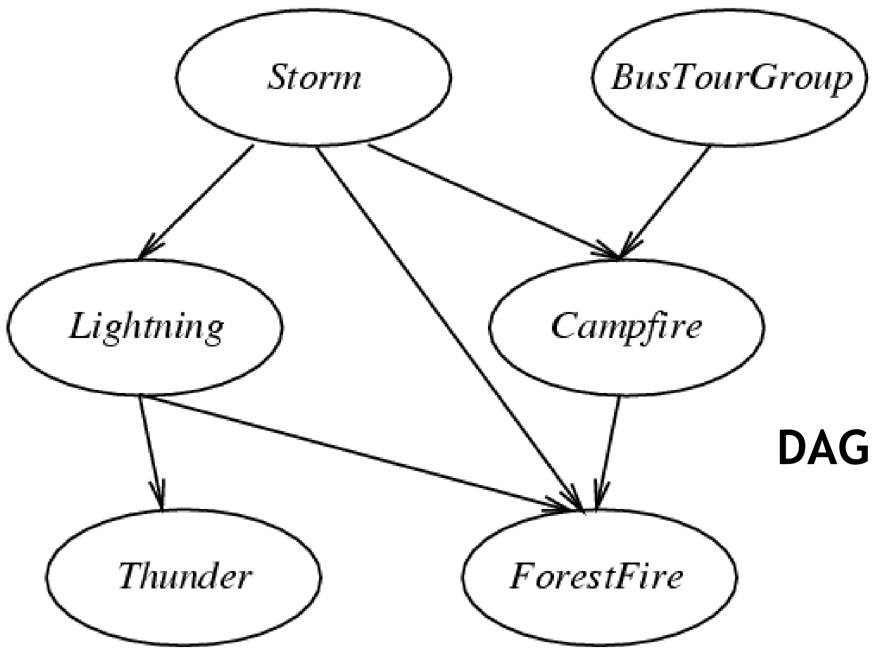
$$v_{NB} = \underset{v_j \in V}{\operatorname{argmax}} P(v_j) \prod_i P(a_i|v_j)$$

- P(y) P(sunny|y) P(cool|y) P(high|y) P(strong|y) = 0.005
- P(n) P(sunny|n) P(cool|n) P(high|n) P(strong|n) = 0.021

Bayesian Networks

Bayesian Networks

- Each node is asserted to be *conditionally independent* of its *non-descendants*, *given* its immediate *predecessors*
- Represents *joint probability distribution* over all variables, e.g., P(Storm, BusTourGroup, ..., ForestFire)



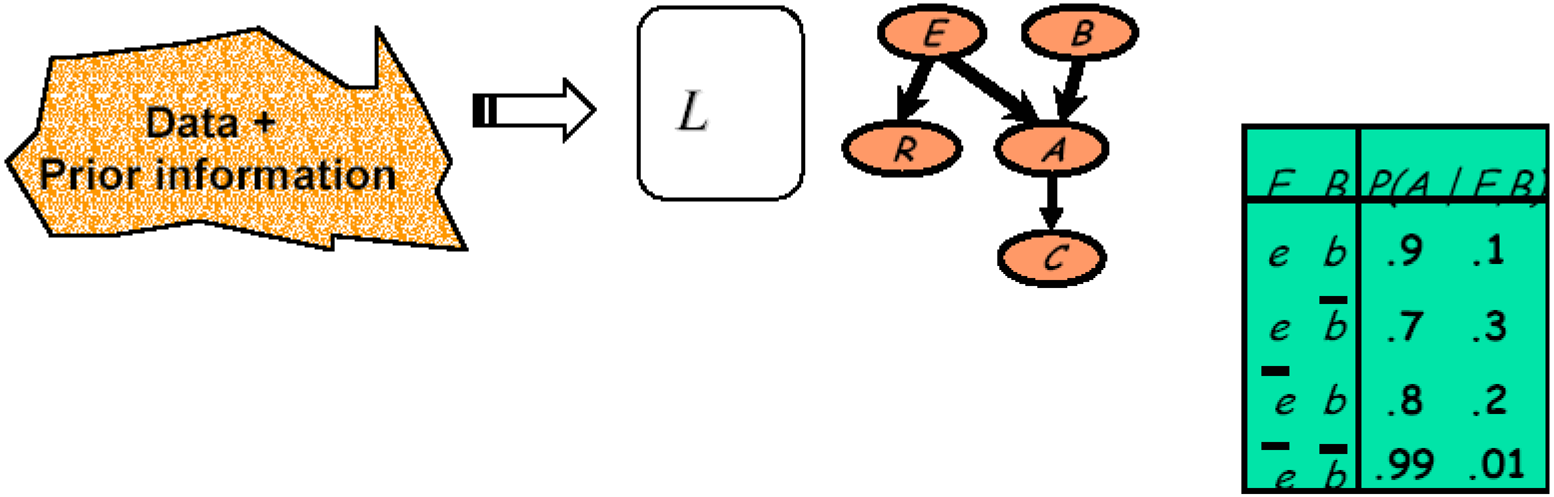
DAG

	S,B	$S,\neg B$	$\neg S,B$	$\neg S,\neg B$
C	0.4	0.1	0.8	0.2
$\neg C$	0.6	0.9	0.2	0.8

Inference in Bayesian Networks

- How can one infer the (probabilities of) values of one or more network variables, given observed values of others?
  - Bayes net contains all information needed for this inference
  - if only one variable with unknown value, easy to infer it
  - in general case, problem is *NP hard*
- In practice, can succeed in many cases
  - exact inference methods work well for some network structures
  - Monte Carlo methods “simulate” the network randomly to calculate approximate solutions

Learning in Bayesian Networks



Learning Problems

	Known Structure	Unknown Structure
Complete Data	Statistical parametric estimation (closed-form eq.)	Discrete optimization over structures (discrete search)
Incomplete Data	Parametric optimization (EM, gradient descent...)	Combined (Structural EM, mixture models…)

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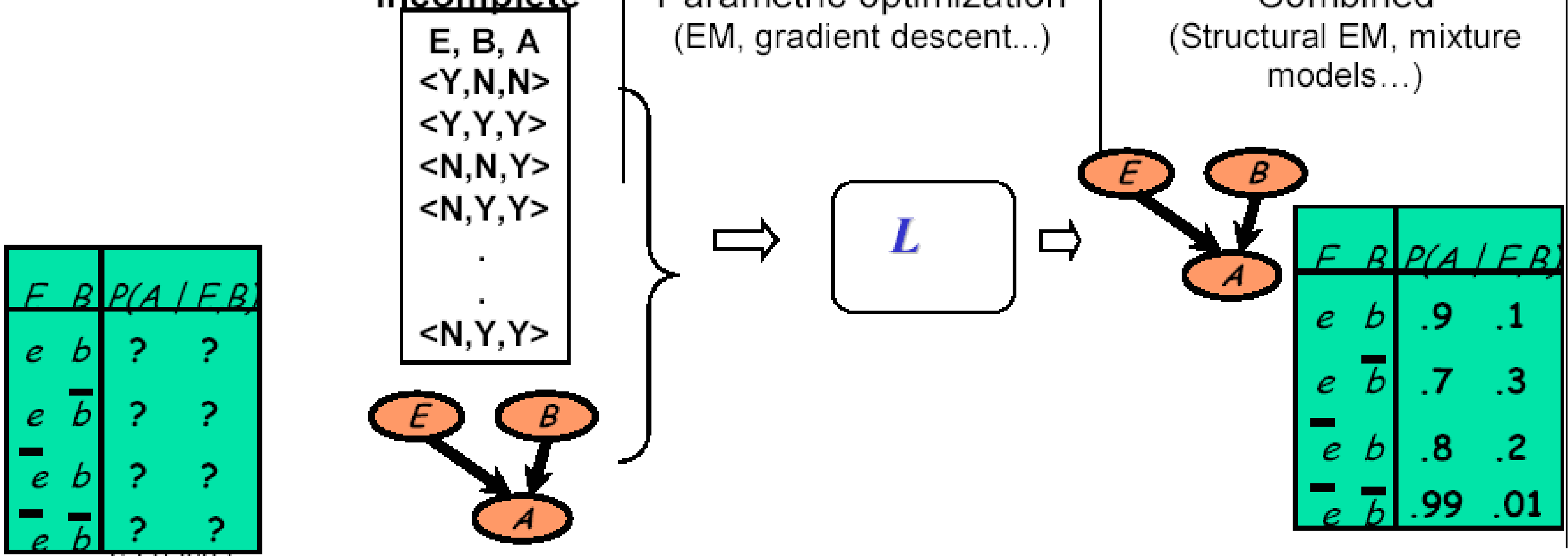

Learning Parameters

- Estimate of parameters relies on *sufficient statistics*, i.e., functions summarizing the data / relevant information for calculating likelihood
  - e.g., N_H and N_T are sufficient statistics for the binomial distribution
- One option: choose parameters maximizing the likelihood function (*maximum likelihood estimation*)

Bayesian Approach

- „Imaginary counts“ / choice of priors?
- *Conjugate families*: posterior distribution follows the same parametric form as prior distribution
- *Dirichlet prior* is the conjugate family for the multinomial likelihood
- Parameter estimation: MLE and Bayesian

$$\hat{\theta}_{x_i|pa_i} = \frac{N(x_i, pa_i)}{N(pa_i)} \qquad \tilde{\theta}_{x_i|pa_i} = \frac{\alpha(x_i, pa_i) + N(x_i, pa_i)}{\alpha(pa_i) + N(pa_i)}$$

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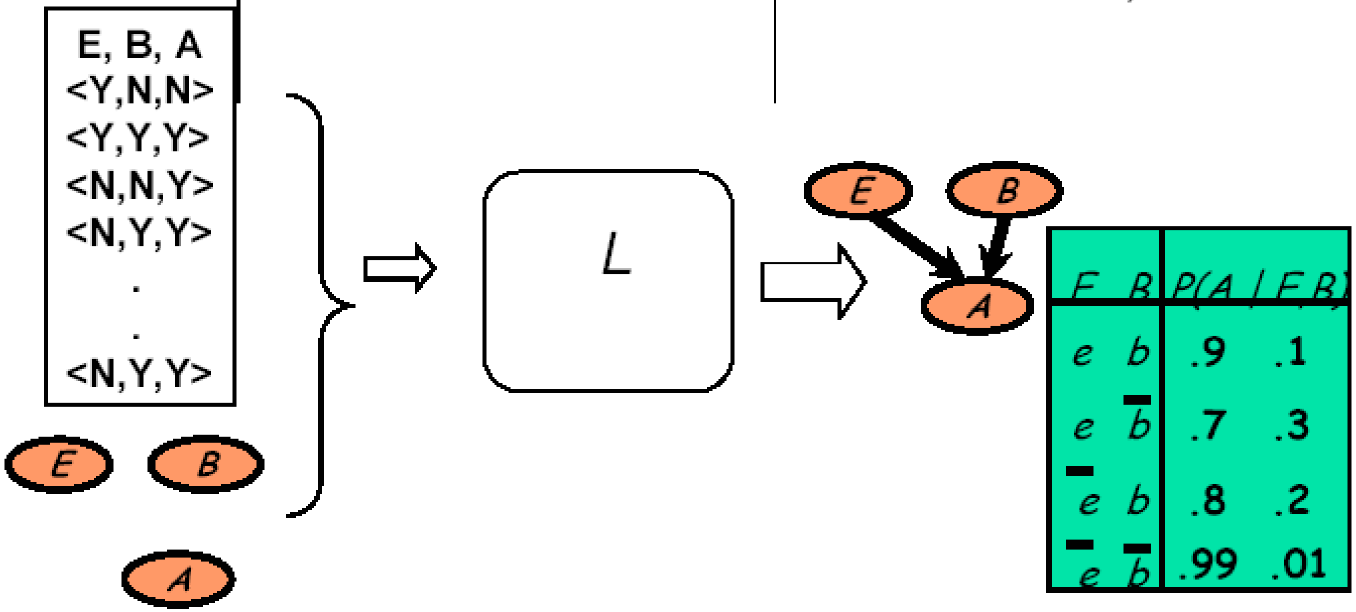
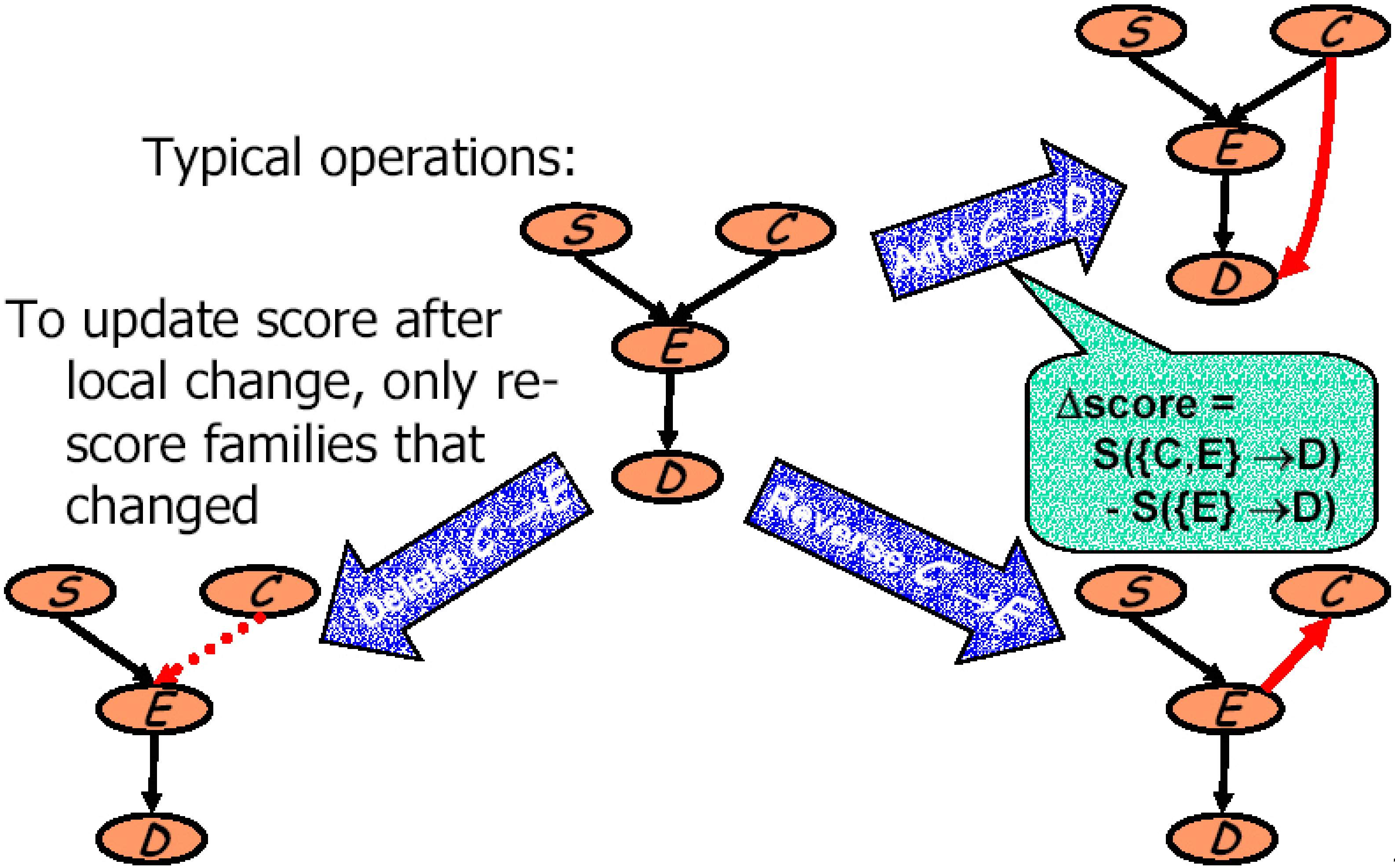


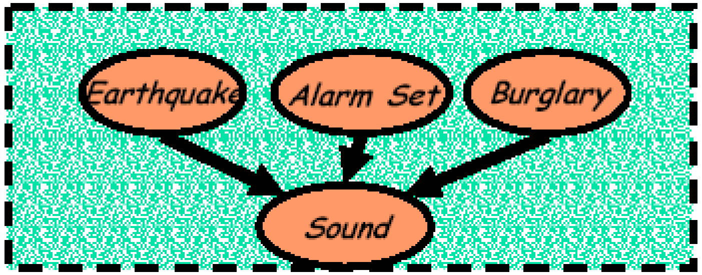
Heuristic Search

Typical operations:

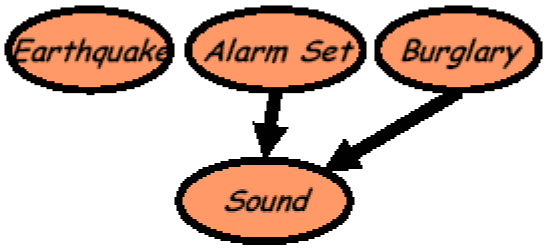
To update score after local change, only re-score families that changed



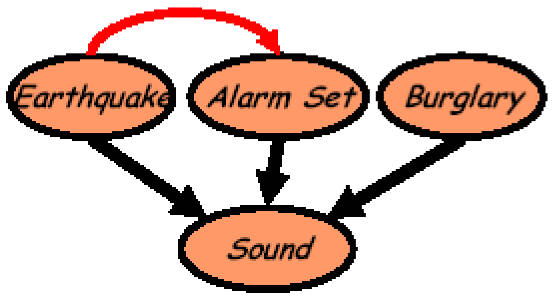
Why Do We Need Accurate Structure?



Missing an arc



Extraneous arc



- *Missing arc* cannot be compensated for
- *Extraneous arc* increases number of parameters to be estimated
- *Wrong assumptions about domain structure*

Learning Problem

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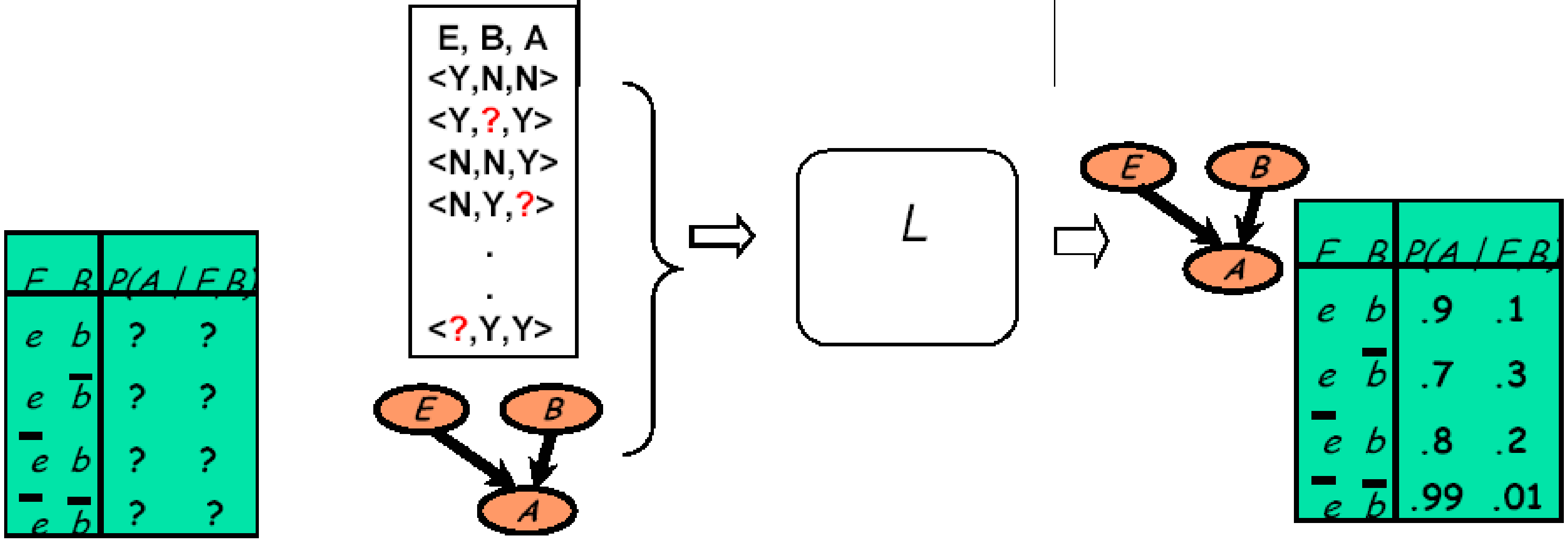
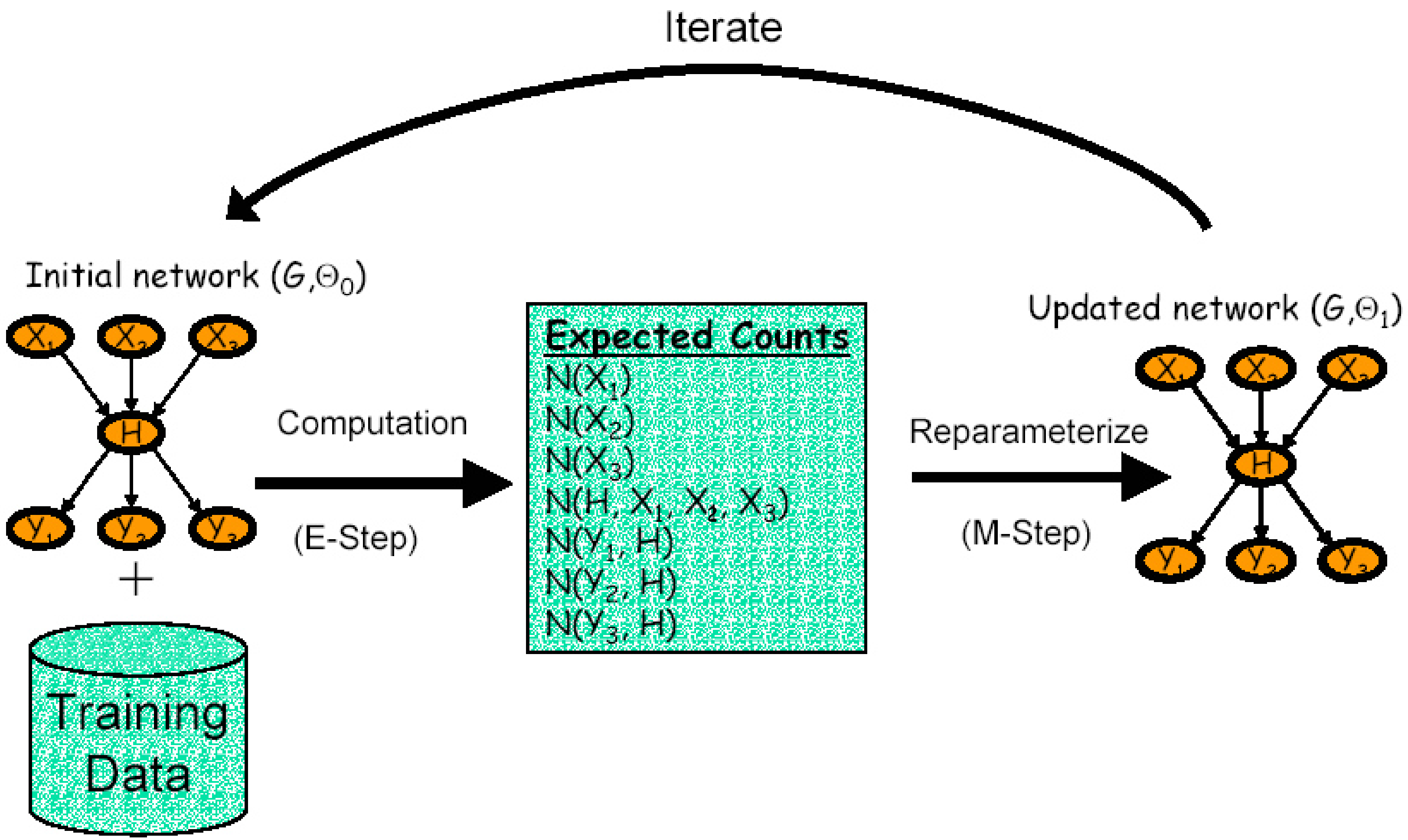


Incomplete Data

- Data are often incomplete
  - some variables of interest are not assigned values
- This phenomenon occurs when we have *missing values*
- Some *variables unobserved* in some instances
  - hidden variables
  - some variables may *never be observed*
  - *we might not even* know *they exist*

Expectation Maximization (EM)



Expectation Maximization (EM)

- Computational bottleneck: computation of expected counts in E-Step
  - need to compute posterior *for each unobserved variable in each instance of training set*
  - *all posteriors for an instance can be derived from one pass of standard BN inference*

Learning Problem

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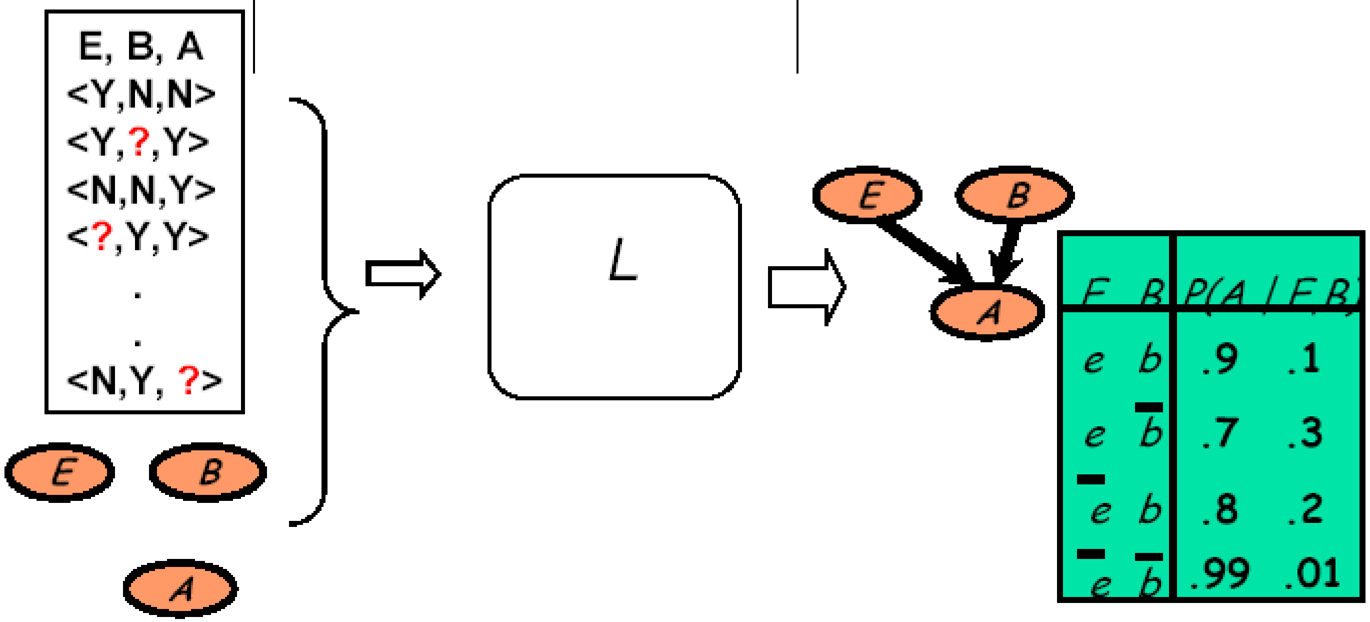
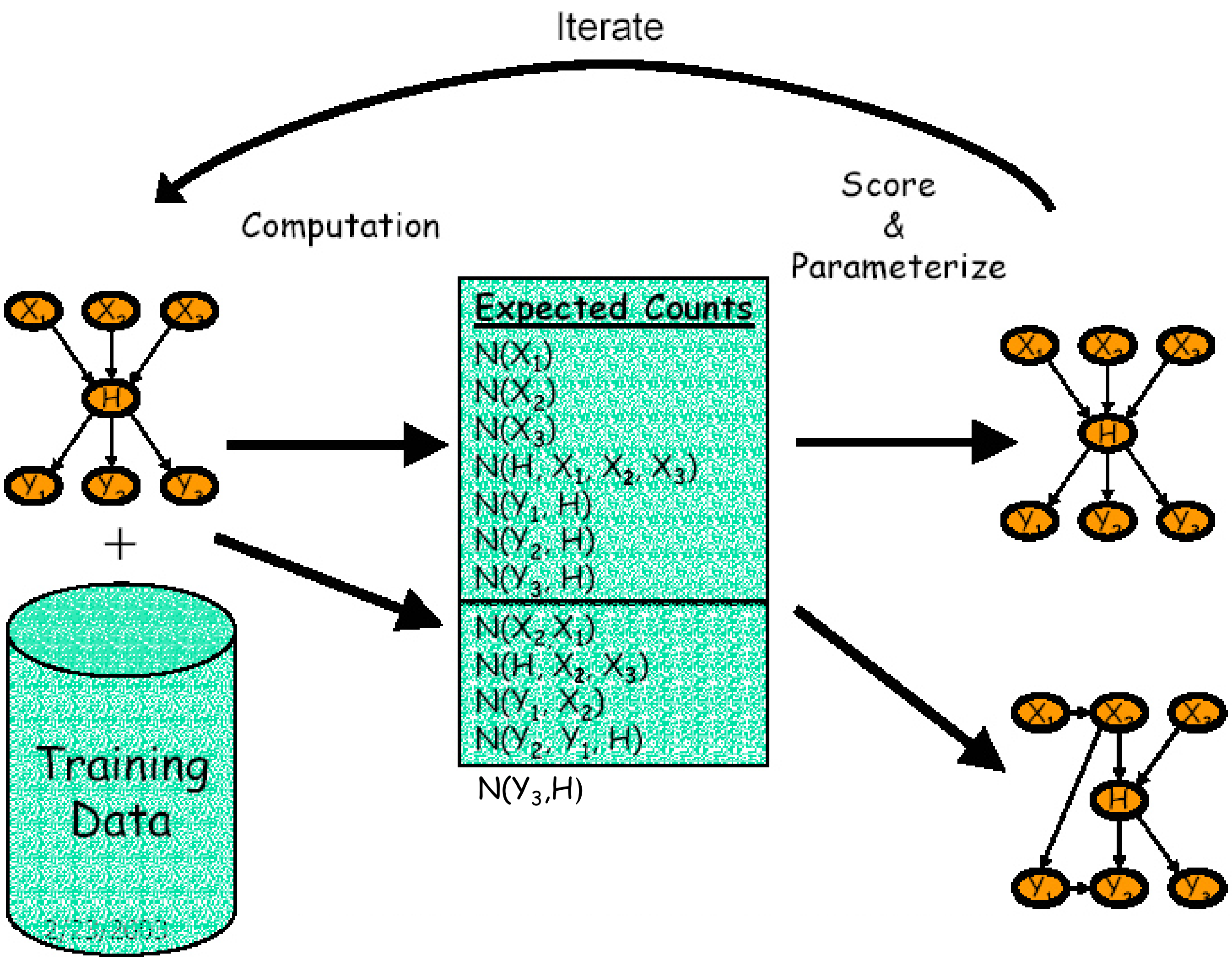


Structural EM

- Idea: use current model to help evaluate new structures
- Outline: perform search in (Structure, Parameters) space
- At each iteration, use current model for finding either
  - better scoring parameters: “parametric” EM step, or
  - better scoring structure: “structural” EM step

Structural EM



Conclusion

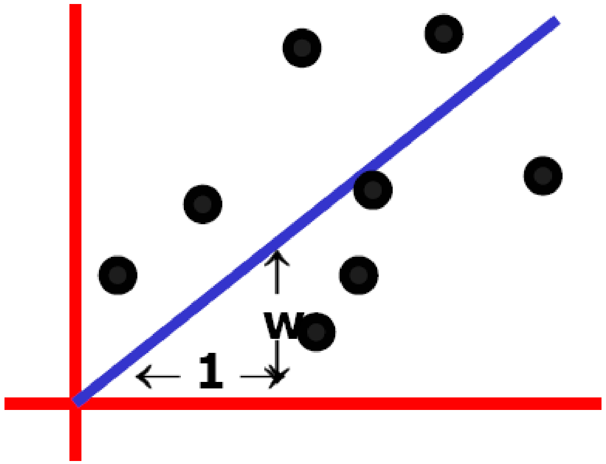
- Learning in Bayesian networks
- Four cases
- From simple counting (easy) to learning both structure and parameters (extremely hard)

Linear Regression

Linear Models

- Work most naturally with numeric attributes
- Standard technique for numeric prediction: *linear regression*
- Outcome is linear combination of attributes:
  $y = w_0 + w_1 x_1 + \ldots + w_m x_m$
- Weights are calculated from the training data
- *Predicted value* for first training instance $\mathbf{x}^{(1)}$:
  $w_0 + w_1 x_1^{(1)} + \ldots + w_m x_m^{(1)}$

Linear Regression



DATASET

inputs	outputs
$x_1 = 1$	$y_1 = 1$
$x_2 = 3$	$y_2 = 2.2$
$x_3 = 2$	$y_3 = 2$
$x_4 = 1.5$	$y_4 = 1.9$
$x_5 = 4$	$y_5 = 3.1$

- Linear regression assumes that the expected value of the output given an input, E[y|x], is linear.
- Simplest case: Out(x) = wx for some unknown w.
- Given the data, we can estimate w.

1-Parameter Linear Regression

Assume that the data is formed by

$$y_i = wx_i + \text{noise}_i$$

where

- the noise signals are independent
- the noise has normal distribution with mean 0 and unknown variance σ^2

$p(y|w,x)$ has normal distribution with

- mean wx
- variance σ^2

Bayesian Linear Regression

$p(y|w,x)$ = Normal(mean wx, var σ^2)

We have a set of data points $(x_1,y_1), (x_2, y_2), \ldots, (x_n, y_n)$, which are evidence about w.

We want to infer w from the data.

$$p(w|x_1, \ldots, x_n, y_1, \ldots, y_n)$$

- You can use Bayes rule to work out a posterior distribution for w given the data
- Or you could do Maximum Likelihood Estimation

MLE of w

Ask the question: „For which value of w is the data most likely to have happened?“

$\Leftrightarrow$

For what w is

$$p(y_1, \ldots, y_n | x_1, \ldots, x_n, w) \text{ maximized?}$$

$\Leftrightarrow$

For what w is

$$\prod_{i=1}^{n} p(y_i | w, x_i) \text{ maximized?}$$

Derivation (cf. Lecture on Bayesian Learning)

For what w is

$$\prod_{i=1}^{n} p(y_i | w, x_i) \text{ maximized?}$$

For what w is

$$\prod_{i=1}^{n} \exp\left(-\frac{1}{2}\left(\frac{y_i - wx_i}{\sigma}\right)^2\right) \text{ maximized?}$$

For what w is

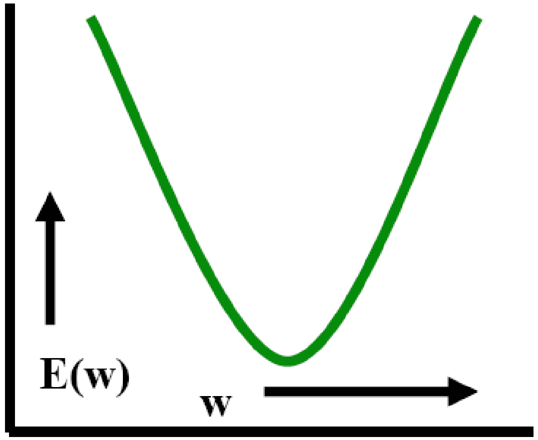
$$\sum_{i=1}^{n} -\frac{1}{2}\left(\frac{y_i - wx_i}{\sigma}\right)^2 \text{ maximized?}$$

For what w is

$$\sum_{i=1}^{n} \left(y_i - wx_i\right)^2 \text{ minimized?}$$

Linear Regression

The maximum likelihood w is the one that minimizes the sum-of-square residuals.



$$E = \sum_i (y_i - wx_i)^2$$

$$= \sum_i y_i^2 - \left(2\sum x_i y_i\right)w + \left(\sum x_i^2\right)w^2$$

We want to minimize a quadratic function of w.

Linear Regression

- Easy to show the sum of squares is minimized when

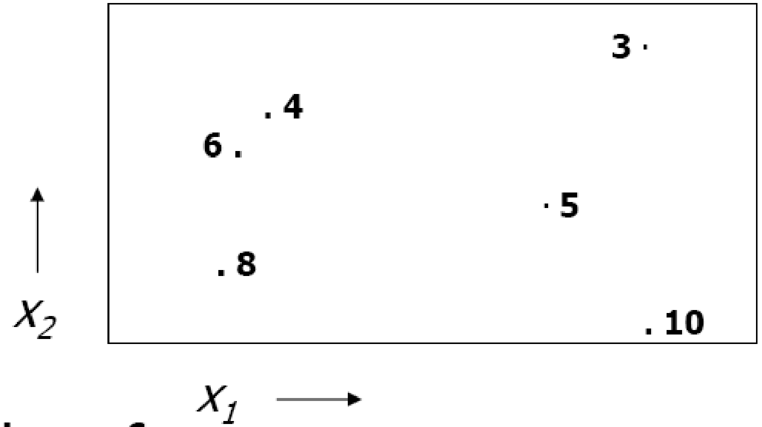
$$w = \frac{\sum x_i y_i}{\sum x_i^{\ 2}}$$

- The maximum likelihood model is Out(x) = wx

- We can use that for prediction.

Multivariate Regression

What if the inputs are vectors?



2-d input example

Dataset has form

$\mathbf{x}_1$	y_1
$\mathbf{x}_2$	y_2
$\mathbf{x}_3$	y_3
$\vdots$	$\vdots$
$\mathbf{x}_R$	y_R

Multivariate Regression

$$\mathbf{x} = \begin{bmatrix} \cdots\cdots\mathbf{x}_1\cdots\cdots \\ \cdots\cdots\mathbf{x}_2\cdots\cdots \\ \vdots \\ \cdots\cdots\mathbf{x}_R\cdots\cdots \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ & & \vdots & \\ x_{R1} & x_{R2} & \cdots & x_{Rm} \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_R \end{bmatrix}$$

Matrix **X** and **y**: R data points, inputs consisting of m components

The linear regression model assumes a vector ***w*** such that

$$\mathrm{Out}(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} = w_1 x[1] + w_2 x[2] + \ldots . w_m x[D]$$

The max. likelihood ***w*** is $\boldsymbol{w} = (X^T X)^{-1}(X^T Y)$

Multivariate Regression

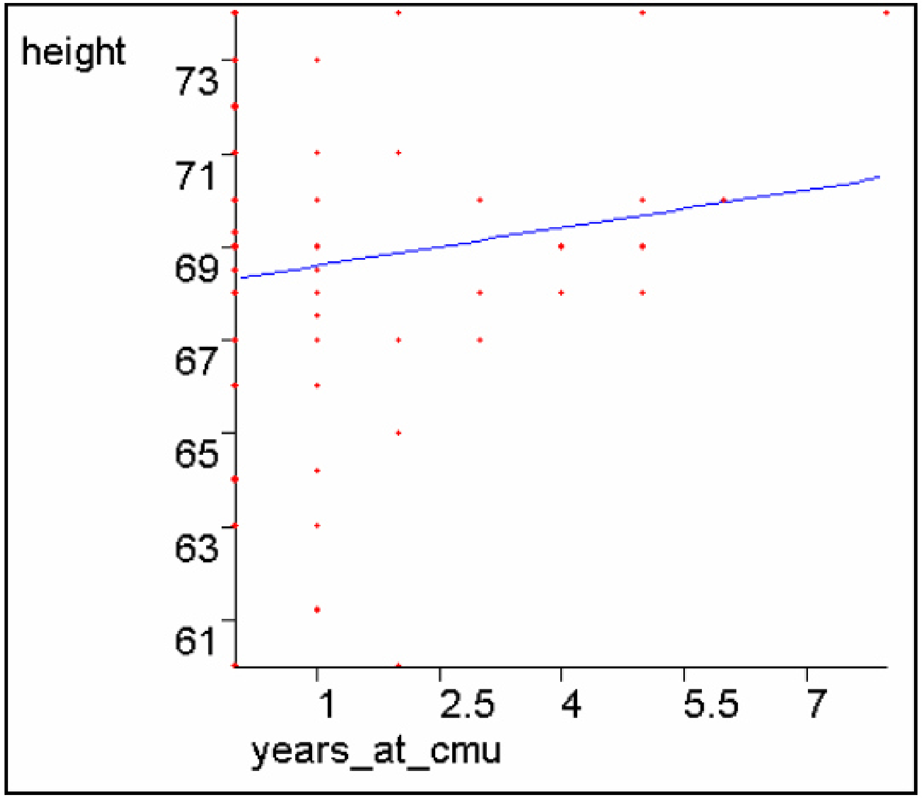
The max. likelihood $\boldsymbol{w}$ is $\boldsymbol{w} = (X^T X)^{-1}(X^T Y)$

$X^T X$ is an m x m matrix: i,j'th elt is $\sum_{k=1}^{R} x_{ki} x_{kj}$

$X^T Y$ is an m-element vector: i'th elt $\sum_{k=1}^{R} x_{ki} y_k$

Constant Term?

- We may expect linear data that does not go through the origin.
- Statisticians and neural net folks all agree on a simple obvious hack.
- *Can you guess?*



Use of Constant Term

The trick is to create a fake input X_0 *that always takes the value 1!*

X_1	X_2	Y
2	4	16
3	4	17
5	5	20

Before:

$Y = w_1 X_1 + w_2 X_2$

…has to be a poor model

X_0	X_1	X_2	Y
1	2	4	16
1	3	4	17
1	5	5	20

After:

$Y = w_0 X_0 + w_1 X_1 + w_2 X_2$

$= w_0 + w_1 X_1 + w_2 X_2$

…has a fine constant term

In this example, You should be able to see the MLE w_0, w_1 and w_2 by inspection

Ridge Regression

- Problem: if independent variables (features) are strongly correlated (near collinearity), then the estimated regression coefficients are unstable (high variance)
- Possible solution: e.g., *ridge regression*
  - Regression coefficients stabilized by mathematical trick ($X^T X$ is artificially modified by adding λI)
  - Not least squares (LS) solution anymore (no unbiased estimates)
  - Ridge parameter λ (e.g., set by cross-validation) determines how much ridge regression deviates from LS regression (if too small, it cannot fight collinearity, if too large, bias too strong)