Maskinlæring (IT-3704) - vår 2004.

Forelesning 4 - Guest lecturer: Professor Keith Downing

Bayesian methods

- Background - probability
- Naive Bayes
- Bayesian Networks

Bayesian Learning

[Read Ch. 6]
[Suggested exercises: 6.1, 6.2, 6.6]

- Bayes Theorem
- MAP, ML hypotheses
- MAP learners
- Minimum description length principle
- Bayes optimal classifier
- Naive Bayes learner
- Example: Learning over text data
- Bayesian belief networks
- Expectation Maximization algorithm

Two Roles for Bayesian Methods

Provides practical learning algorithms:

- Naive Bayes learning
- Bayesian belief network learning
- Combine prior knowledge (prior probabilities) with observed data
- Requires prior probabilities

Provides useful conceptual framework

- Provides "gold standard" for evaluating other learning algorithms
- Additional insight into Occam's razor

Bayes Theorem

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

- $P(h)$ = prior probability of hypothesis h
- $P(D)$ = prior probability of training data D
- $P(h|D)$ = probability of h given D
- $P(D|h)$ = probability of D given h

Choosing Hypotheses

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

Generally want the most probable hypothesis given the training data
Maximum a posteriori hypothesis h_{MAP}:

$$\begin{aligned} h_{MAP} &= \arg\max_{h \in H} P(h|D) \\ &= \arg\max_{h \in H} \frac{P(D|h)P(h)}{P(D)} \\ &= \arg\max_{h \in H} P(D|h)P(h) \end{aligned}$$

If assume $P(h_i) = P(h_j)$ then can further simplify, and choose the *Maximum likelihood* (ML) hypothesis

$$h_{ML} = \arg\max_{h_i \in H} P(D|h_i)$$

Bayes Theorem

Does patient have cancer or not?

A patient takes a lab test and the result comes back positive. The test returns a correct positive result in only 98% of the cases in which the disease is actually present, and a correct negative result in only 97% of the cases in which the disease is not present. Furthermore, .008 of the entire population have this cancer.

$$P(cancer) = \qquad P(\neg cancer) =$$
$$P(+|cancer) = \qquad P(-|cancer) =$$
$$P(+|\neg cancer) = \qquad P(-|\neg cancer) =$$

Basic Formulas for Probabilities

- *Product Rule*: probability $P(A \wedge B)$ of a conjunction of two events A and B:

$$P(A \wedge B) = P(A|B)P(B) = P(B|A)P(A)$$

- *Sum Rule*: probability of a disjunction of two events A and B:

$$P(A \vee B) = P(A) + P(B) - P(A \wedge B)$$

- *Theorem of total probability*: if events $A_1, \ldots, A_n$ are mutually exclusive with $\Sigma_{i=1}^{n} P(A_i) = 1$, then

$$P(B) = \sum_{i=1}^{n} P(B|A_i)P(A_i)$$

Brute Force MAP Hypothesis Learner

1. For each hypothesis h in H, calculate the posterior probability

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

2. Output the hypothesis h_{MAP} with the highest posterior probability

$$h_{MAP} = \underset{h \in H}{\operatorname{argmax}} P(h|D)$$

Relation to Concept Learning

Consider our usual concept learning task

- instance space X, hypothesis space H, training examples D
- consider the FindS learning algorithm (outputs most specific hypothesis from the version space $VS_{H,D}$)

What would Bayes rule produce as the MAP hypothesis?

Does $FindS$ output a MAP hypothesis??

Relation to Concept Learning

Assume fixed set of instances $\langle x_1, \ldots, x_m \rangle$
Assume D is the set of classifications
$D = \langle c(x_1), \ldots, c(x_m) \rangle$

Choose $P(D|h)$:

Relation to Concept Learning

Assume fixed set of instances $\langle x_1, \ldots, x_m \rangle$
Assume D is the set of classifications
$D = \langle c(x_1), \ldots, c(x_m) \rangle$
Choose $P(D|h)$

- $P(D|h) = 1$ if h consistent with D
- $P(D|h) = 0$ otherwise

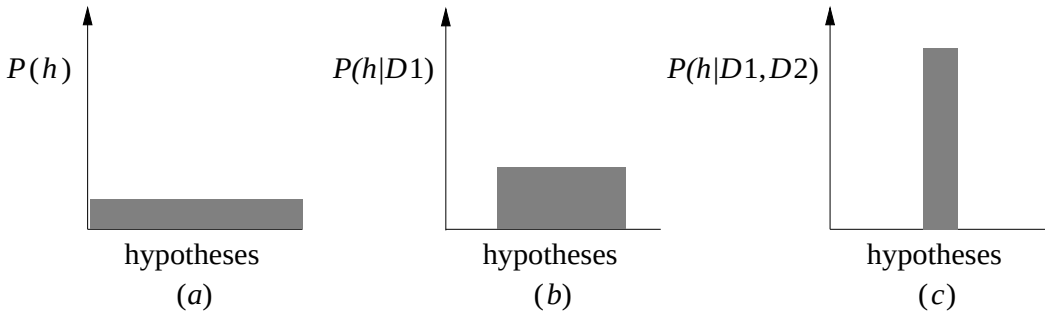
Choose $P(h)$ to be *uniform* distribution

- $P(h) = \frac{1}{|H|}$ for all h in H

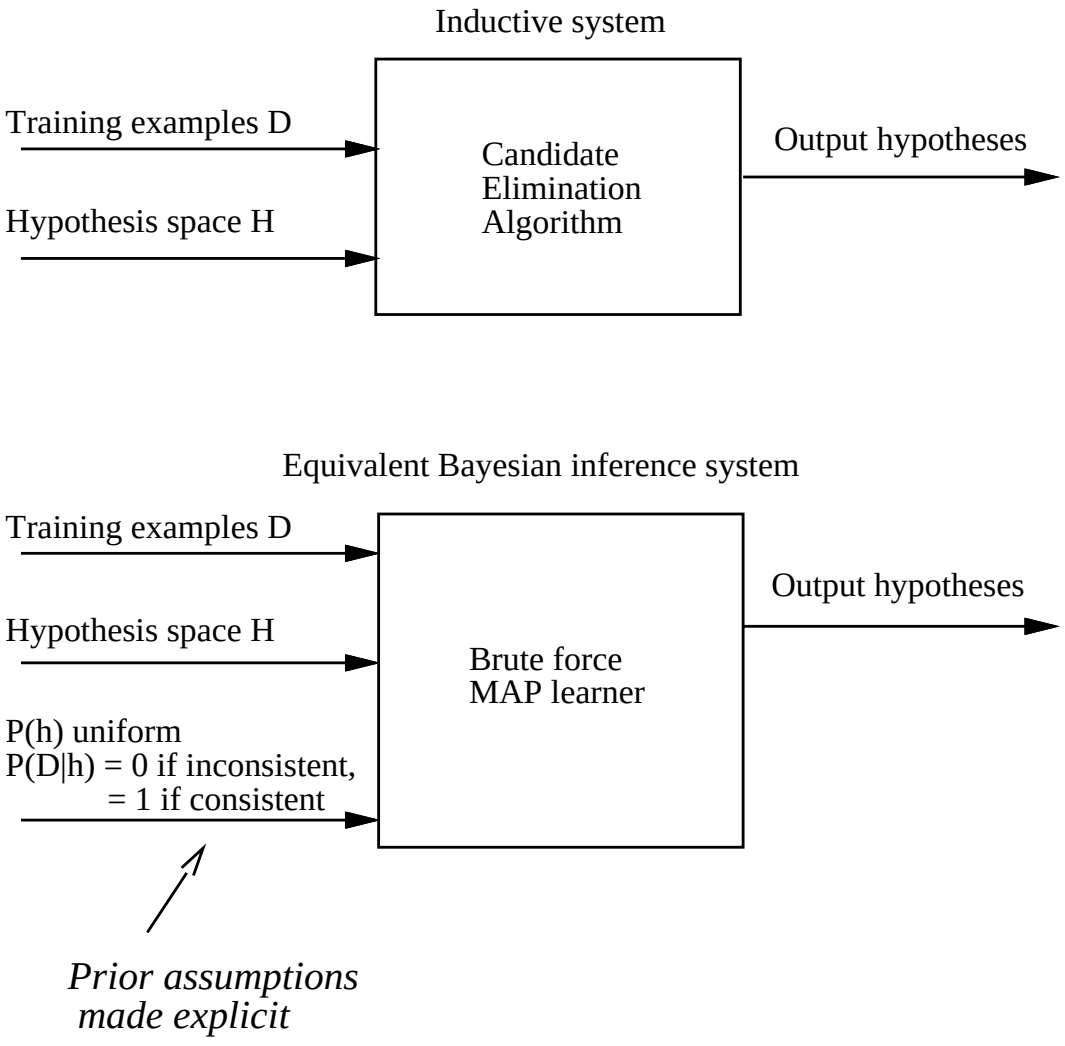
Then,

$$P(h|D) = \begin{cases} \frac{1}{|VS_{H,D}|} & \text{if } h \text{ is consistent with } D \\ 0 & \text{otherwise} \end{cases}$$

Evolution of Posterior Probabilities



Characterizing Learning Algorithms by Equivalent MAP Learners



Learning to Predict Probabilities

Consider predicting survival probability from patient data

Training examples $\langle x_i, d_i \rangle$, where d_i is 1 or 0

Want to train neural network to output a *probability* given x_i (not a 0 or 1)

In this case can show

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} d_i \ln h(x_i) + (1 - d_i) \ln(1 - h(x_i))$$

Weight update rule for a sigmoid unit:

$$w_{jk} \leftarrow w_{jk} + \Delta w_{jk}$$

where

$$\Delta w_{jk} = \eta \sum_{i=1}^{m} (d_i - h(x_i))\ x_{ijk}$$

Minimum Description Length Principle

Occam's razor: prefer the shortest hypothesis

MDL: prefer the hypothesis h that minimizes

$$h_{MDL} = \underset{h \in H}{\operatorname{argmin}} L_{C_1}(h) + L_{C_2}(D|h)$$

where $L_C(x)$ is the description length of x under encoding C

Example: H = decision trees, D = training data labels

- $L_{C_1}(h)$ is # bits to describe tree h
- $L_{C_2}(D|h)$ is # bits to describe D given h
  - Note $L_{C_2}(D|h) = 0$ if examples classified perfectly by h. Need only describe exceptions
- Hence h_{MDL} trades off tree size for training errors

Minimum Description Length Principle

$$\begin{aligned} h_{MAP} &= \arg\max_{h \in H} P(D|h)P(h) \\ &= \arg\max_{h \in H} \log_2 P(D|h) + \log_2 P(h) \\ &= \arg\min_{h \in H} -\log_2 P(D|h) - \log_2 P(h) \quad (1) \end{aligned}$$

Interesting fact from information theory:

> The optimal (shortest expected coding length) code for an event with probability p is $-\log_2 p$ bits.

So interpret (1):

- $-\log_2 P(h)$ is length of h under optimal code
- $-\log_2 P(D|h)$ is length of D given h under optimal code

$\rightarrow$ prefer the hypothesis that minimizes

$$length(h) + length(misclassifications)$$

Most Probable Classification of New Instances

So far we've sought the most probable *hypothesis* given the data D (i.e., h_{MAP})

Given new instance x, what is its most probable *classification*?

- $h_{MAP}(x)$ is not the most probable classification!

Consider:

- Three possible hypotheses:

  $$P(h_1|D) = .4,\ P(h_2|D) = .3,\ P(h_3|D) = .3$$

- Given new instance x,

  $$h_1(x) = +,\ h_2(x) = -,\ h_3(x) = -$$

- What's most probable classification of x?

Bayes Optimal Classifier

Bayes optimal classification:

$$\arg\max_{v_j \in V} \sum_{h_i \in H} P(v_j|h_i)P(h_i|D)$$

Example:

$$P(h_1|D) = .4,\ P(-|h_1) = 0,\ P(+|h_1) = 1$$
$$P(h_2|D) = .3,\ P(-|h_2) = 1,\ P(+|h_2) = 0$$
$$P(h_3|D) = .3,\ P(-|h_3) = 1,\ P(+|h_3) = 0$$

therefore

$$\sum_{h_i \in H} P(+|h_i)P(h_i|D) = .4$$
$$\sum_{h_i \in H} P(-|h_i)P(h_i|D) = .6$$

and

$$\arg\max_{v_j \in V} \sum_{h_i \in H} P(v_j|h_i)P(h_i|D) = -$$

Gibbs Classifier

Bayes optimal classifier provides best result, but can be expensive if many hypotheses.
Gibbs algorithm:

1. Choose one hypothesis at random, according to $P(h|D)$
2. Use this to classify new instance

Surprising fact: Assume target concepts are drawn at random from H according to priors on H. Then:

$$E[error_{Gibbs}] \leq 2E[error_{BayesOptimal}]$$

Suppose correct, uniform prior distribution over H, then

- Pick any hypothesis from VS, with uniform probability
- Its expected error no worse than twice Bayes optimal

Naive Bayes Classifier

Along with decision trees, neural networks, nearest nbr, one of the most practical learning methods.

When to use

- Moderate or large training set available
- Attributes that describe instances are conditionally independent given classification

Successful applications:

- Diagnosis
- Classifying text documents

Naive Bayes Classifier

Assume target function $f : X \to V$, where each instance x described by attributes $\langle a_1, a_2 \ldots a_n \rangle$. Most probable value of $f(x)$ is:

$$\begin{aligned} v_{MAP} &= \underset{v_j \in V}{\operatorname{argmax}} P(v_j | a_1, a_2 \ldots a_n) \\ v_{MAP} &= \underset{v_j \in V}{\operatorname{argmax}} \frac{P(a_1, a_2 \ldots a_n | v_j) P(v_j)}{P(a_1, a_2 \ldots a_n)} \\ &= \underset{v_j \in V}{\operatorname{argmax}} P(a_1, a_2 \ldots a_n | v_j) P(v_j) \end{aligned}$$

Naive Bayes assumption:

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

which gives

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

Naive Bayes Algorithm

Naive_Bayes_Learn($examples$)

For each target value v_j

$\hat{P}(v_j) \leftarrow$ estimate $P(v_j)$

For each attribute value a_i of each attribute a

$\hat{P}(a_i|v_j) \leftarrow$ estimate $P(a_i|v_j)$

Classify_New_Instance(x)

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

Naive Bayes: Example

Consider *PlayTennis* again, and new instance

$\langle Outlk = sun, Temp = cool, Humid = high, Wind = strong$

Want to compute:

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

$P(y)\ P(sun|y)\ P(cool|y)\ P(high|y)\ P(strong|y) = .005$

$P(n)\ P(sun|n)\ P(cool|n)\ P(high|n)\ P(strong|n) = .021$

$$\rightarrow v_{NB} = n$$

Naive Bayes: Subtleties

1. Conditional independence assumption is often violated

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

   - ...but it works surprisingly well anyway. Note don't need estimated posteriors $\hat{P}(v_j|x)$ to be correct; need only that

$$\underset{v_j \in V}{\text{argmax}}\, \hat{P}(v_j) \prod_i \hat{P}(a_i|v_j) = \underset{v_j \in V}{\text{argmax}}\, P(v_j) P(a_1 \ldots, a_n | v_j)$$

   - see [Domingos & Pazzani, 1996] for analysis
   - Naive Bayes posteriors often unrealistically close to 1 or 0

Naive Bayes: Subtleties

2. what if none of the training instances with target value v_j have attribute value a_i? Then

$$\hat{P}(a_i|v_j) = 0, \text{ and...}$$

$$\hat{P}(v_j) \prod_i \hat{P}(a_i|v_j) = 0$$

Typical solution is Bayesian estimate for $\hat{P}(a_i|v_j)$

$$\hat{P}(a_i|v_j) \leftarrow \frac{n_c + mp}{n + m}$$

where

- n is number of training examples for which $v = v_j$,
- n_c number of examples for which $v = v_j$ and $a = a_i$
- p is prior estimate for $\hat{P}(a_i|v_j)$
- m is weight given to prior (i.e. number of "virtual" examples)

Learning to Classify Text

Why?

- Learn which news articles are of interest
- Learn to classify web pages by topic

Naive Bayes is among most effective algorithms

What attributes shall we use to represent text documents??

Learning to Classify Text

Target concept $Interesting? : Document \rightarrow \{+, -\}$

1. Represent each document by vector of words
   - one attribute per word position in document
2. Learning: Use training examples to estimate
   - $P(+)$
   - $P(-)$
   - $P(doc|+)$
   - $P(doc|-)$

Naive Bayes conditional independence assumption

$$P(doc|v_j) = \prod_{i=1}^{length(doc)} P(a_i = w_k|v_j)$$

where $P(a_i = w_k|v_j)$ is probability that word in position i is w_k, given v_j

one more assumption:
$P(a_i = w_k|v_j) = P(a_m = w_k|v_j), \forall i, m$

LEARN_NAIVE_BAYES_TEXT($Examples, V$)

1. collect all words and other tokens that occur in Examples

- $Vocabulary \leftarrow$ all distinct words and other tokens in $Examples$

2. calculate the required $P(v_j)$ and $P(w_k|v_j)$ probability terms

- For each target value v_j in V do
  - $docs_j \leftarrow$ subset of $Examples$ for which the target value is v_j
  - $P(v_j) \leftarrow \frac{|docs_j|}{|Examples|}$
  - $Text_j \leftarrow$ a single document created by concatenating all members of $docs_j$
  - $n \leftarrow$ total number of words in $Text_j$ (counting duplicate words multiple times)
  - for each word w_k in $Vocabulary$
    - $n_k \leftarrow$ number of times word w_k occurs in $Text_j$
    - $P(w_k|v_j) \leftarrow \frac{n_k+1}{n+|Vocabulary|}$

CLASSIFY_NAIVE_BAYES_TEXT(Doc)

- $positions \leftarrow$ all word positions in Doc that contain tokens found in $Vocabulary$
- Return v_{NB}, where

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

Twenty NewsGroups

Given 1000 training documents from each group
Learn to classify new documents according to
which newsgroup it came from

comp.graphics	misc.forsale
comp.os.ms-windows.misc	rec.autos
comp.sys.ibm.pc.hardware	rec.motorcycles
comp.sys.mac.hardware	rec.sport.baseball
comp.windows.x	rec.sport.hockey
alt.atheism	sci.space
soc.religion.christian	sci.crypt
talk.religion.misc	sci.electronics
talk.politics.mideast	sci.med
talk.politics.misc	
talk.politics.guns	

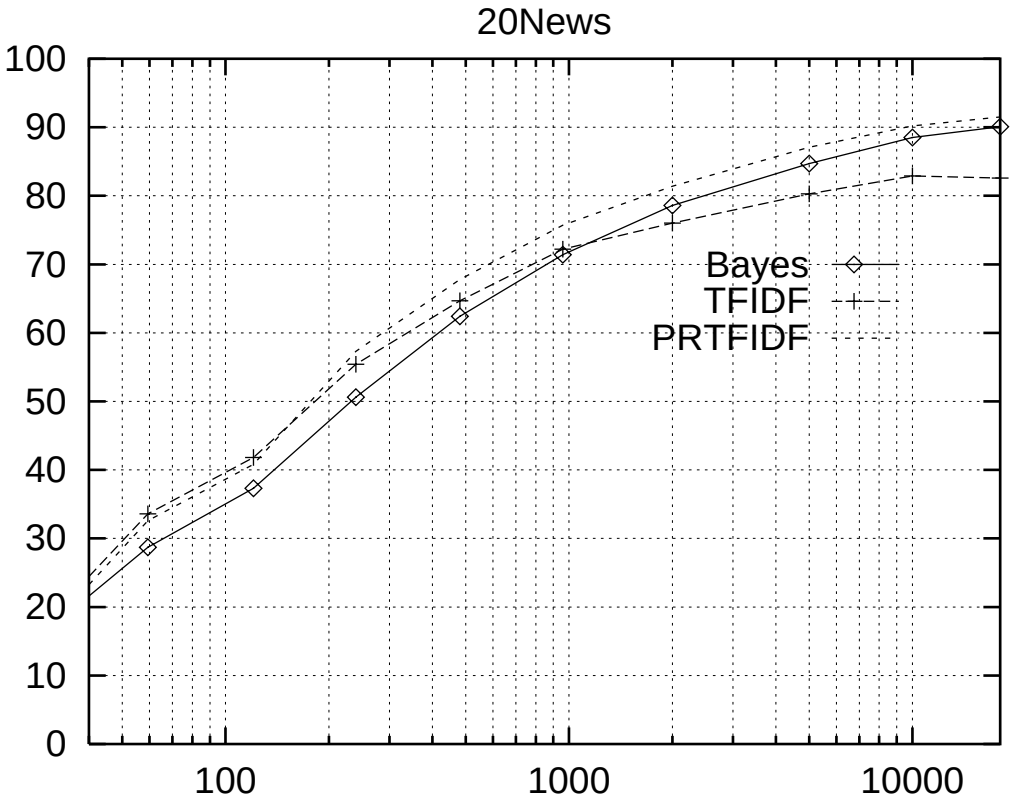
Naive Bayes: 89% classification accuracy

Article from rec.sport.hockey

Path: cantaloupe.srv.cs.cmu.edu!das-news.harvard.e
From: xxx@yyy.zzz.edu (John Doe)
Subject: Re: This year's biggest and worst (opinio
Date: 5 Apr 93 09:53:39 GMT

I can only comment on the Kings, but the most obvious candidate for pleasant surprise is Alex Zhitnik. He came highly touted as a defensive defenseman, but he's clearly much more than that. Great skater and hard shot (though wish he were more accurate). In fact, he pretty much allowed the Kings to trade away that huge defensive liability Paul Coffey. Kelly Hrudey is only the biggest disappointment if you thought he was any good to begin with. But, at best, he's only a mediocre goaltender. A better choice would be Tomas Sandstrom, though not through any fault of his own, but because some thugs in Toronto decided

Learning Curve for 20 Newsgroups



Accuracy vs. Training set size (1/3 withheld for test)

Bayesian Belief Networks

Interesting because:

- Naive Bayes assumption of conditional independence too restrictive
- But it's intractable without some such assumptions...
- Bayesian Belief networks describe conditional independence among *subsets* of variables

$\rightarrow$ allows combining prior knowledge about (in)dependencies among variables with observed training data

(also called Bayes Nets)

Conditional Independence

Definition: X is *conditionally independent* of Y given Z if the probability distribution governing X is independent of the value of Y given the value of Z; that is, if

$$(\forall x_i, y_j, z_k)\ P(X = x_i | Y = y_j, Z = z_k) = P(X = x_i | Z = z_k$$

more compactly, we write

$$P(X|Y,Z) = P(X|Z)$$

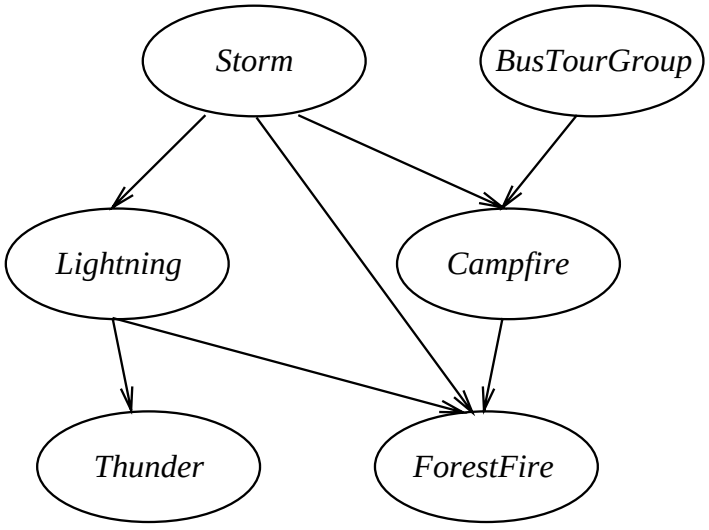
Example: $Thunder$ is conditionally independent of $Rain$, given $Lightning$

$$P(Thunder|Rain, Lightning) = P(Thunder|Lightning)$$

Naive Bayes uses cond. indep. to justify

$$\begin{aligned} P(X,Y|Z) &= P(X|Y,Z)P(Y|Z) \\ &= P(X|Z)P(Y|Z) \end{aligned}$$

Bayesian Belief Network



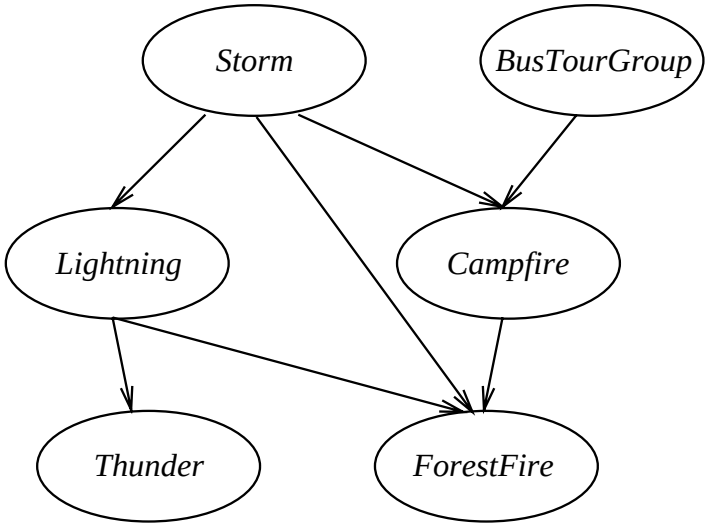
	S,B	$S,\neg B$	$\neg S,B$	$\neg S,\neg B$
C	0.4	0.1	0.8	0.2
$\neg C$	0.6	0.9	0.2	0.8

Campfire

Network represents a set of conditional independence assertions:

- Each node is asserted to be conditionally independent of its nondescendants, given its immediate predecessors.
- Directed acyclic graph

Bayesian Belief Network



	S,B	*S,¬B*	*¬S,B*	*¬S,¬B*
C	0.4	0.1	0.8	0.2
¬C	0.6	0.9	0.2	0.8

Campfire

Represents joint probability distribution over all variables

- e.g., $P(Storm, BusTourGroup, \ldots, ForestFire)$
- in general,

$$P(y_1, \ldots, y_n) = \prod_{i=1}^{n} P(y_i | Parents(Y_i))$$

  where $Parents(Y_i)$ denotes immediate predecessors of Y_i in graph

- so, joint distribution is fully defined by graph, plus the $P(y_i|Parents(Y_i))$

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

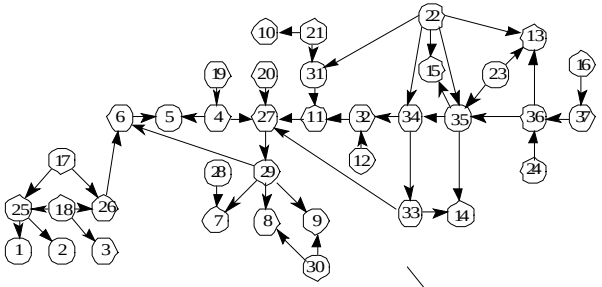
Learning of Bayesian Networks

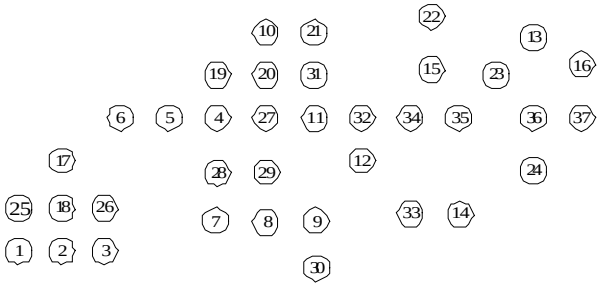
Several variants of this learning task

- Network structure might be *known* or *unknown*
- Training examples might provide values of *all* network variables, or just *some*

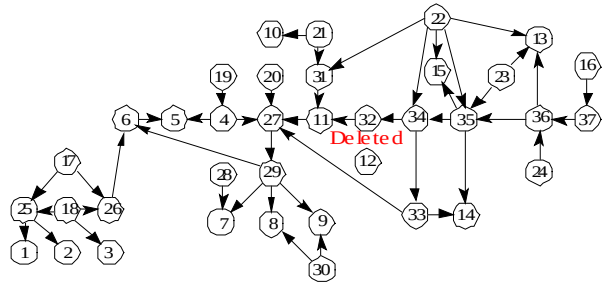
If structure known and observe all variables

- Then it's easy as training a Naive Bayes classifier





case#	1	2	3	37
1	3	3	2	4
2	2	2	2	3
3	1	3	3	3
4	3	2	3	1
10,000	2	2	2	3



Generating Networks:

- **Initialize Network**

repeat

- **Propose some Change to the structure**
- **Fit Parameters to the new structure**
- **Evaluate the new network according to some measure (like BIC, AIC, MDL)**
- **If the New network is Better than the previous, then Keep the Change**

until Finished

Learning Bayes Nets

Suppose structure known, variables partially observable

e.g., observe *ForestFire*, *Storm*, *BusTourGroup*, *Thunder*, but not *Lightning*, *Campfire*...

- Similar to training neural network with hidden units
- In fact, can learn network conditional probability tables using gradient ascent!
- Converge to network h that (locally) maximizes $P(D|h)$

Gradient Ascent for Bayes Nets

Let w_{ijk} denote one entry in the conditional probability table for variable Y_i in the network

$w_{ijk} = P(Y_i = y_{ij} | Parents(Y_i) = \text{the list } u_{ik} \text{ of values})$

e.g., if $Y_i = Campfire$, then u_{ik} might be $\langle Storm = T, BusTourGroup = F \rangle$

Perform gradient ascent by repeatedly

1. update all w_{ijk} using training data D

$$w_{ijk} \leftarrow w_{ijk} + \eta \sum_{d \in D} \frac{P_h(y_{ij}, u_{ik} | d)}{w_{ijk}}$$

2. then, renormalize the w_{ijk} to assure
   - $\Sigma_j w_{ijk} = 1$
   - $0 \leq w_{ijk} \leq 1$

More on Learning Bayes Nets

EM algorithm can also be used. Repeatedly:

1. Calculate probabilities of unobserved variables, assuming h
2. Calculate new w_{ijk} to maximize $E[\ln P(D|h)]$ where D now includes both observed and (calculated probabilities of) unobserved variables

When structure unknown...

- Algorithms use greedy search to add/substract edges and nodes
- Active research topic

Expectation Maximization (EM)

When to use:

- Data is only partially observable
- Unsupervised clustering (target value unobservable)
- Supervised learning (some instance attributes unobservable)

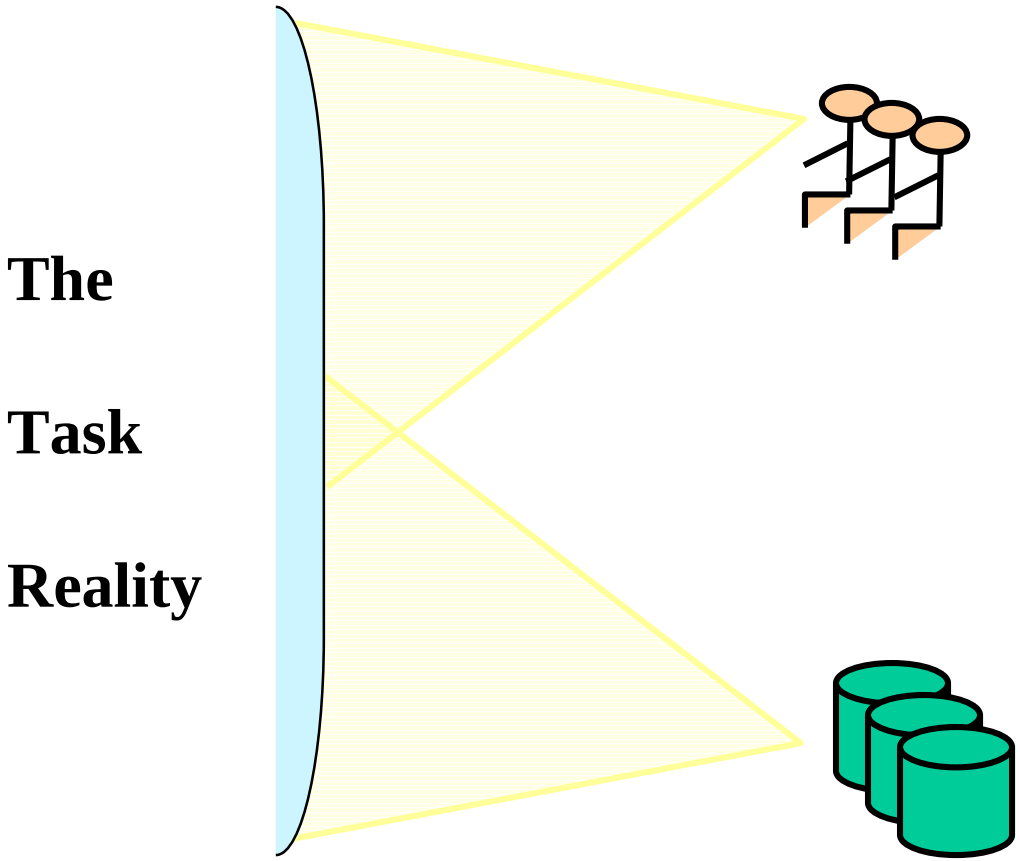
Some uses:

- Train Bayesian Belief Networks
- Unsupervised clustering (AUTOCLASS)
- Learning Hidden Markov Models

Summary: Bayesian Belief Networks

- Combine prior knowledge with observed data
- Impact of prior knowledge (when correct!) is to lower the sample complexity
- Active research area
  - Extend from boolean to real-valued variables
  - Parameterized distributions instead of tables
  - Extend to first-order instead of propositional systems
  - More effective inference methods
  - ...

Data and User views



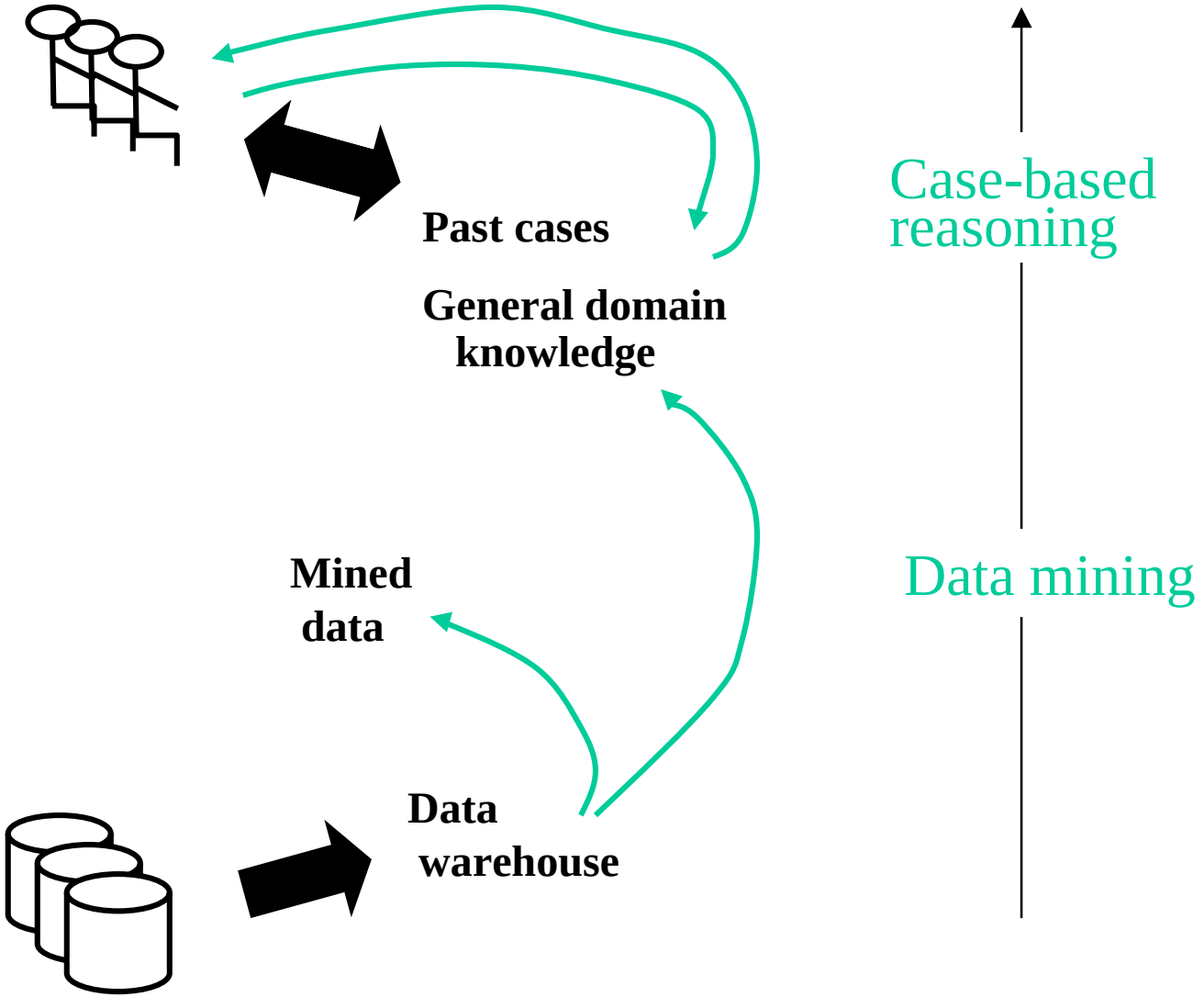
NOEMIE

‘An Environment for Improving the Industrial Feedback Process’

Expected Result: A tool, A methodology, A demonstrator

Core method: Combining CBR and DM

DB → DW → DM → CBR → RAMS → UI


Past cases
General domain knowledge
Mined data
Data warehouse
Case-based reasoning
Data mining

Study of the task reality