#### Bayesian Learning: An Introduction

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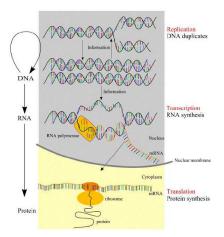


- Motivation: Information Processing
- 2 Introduction
- Bayesian Network Classifiers
- 4 k-Dependence Bayesian Classifiers
- **5** Links and References

#### Outline

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# Life as information processing:



**Experimental Cell** 

# Motivation: Micro Array



Fig. 13.2. Schematised experimental process of cDNA technique for microarray construction.

# Motivation: Supervised Learning Task

- Given:
  - a set of micro-array experiments, each done with mRNA from a different patient (same cell type from every patient)
  - Patient's expression values for each gene constitute the features, and
  - patient's disease constitutes the class
- Goal: Learn a model that accurately predicts class based on features

## Micro-array data: Data Points are Samples

Person	A28202_ac	AB00014_at	AB00015_at	
Person1	1144.0	321.0	2567.2	
Person2	105.2	586.1	759.2	
Person3	586.3	559.0	3210.2	
Person4	42.8	692.0	812.2	

# Supervision: Add Class Values

Person	A28202_ac	AB00014_at	AB00015_at	 Class
Person1	1144.0	321.0	2567.2	 normal
Person2	105.2	586.1	759.2	 cancer
Person3	586.3	559.0	3210.2	 normal
Person4	42.8	692.0	812.2	 cancer

#### Learning Problems:

- Find a function: Class = f(A28202\_ac, AB00014\_at, AB00015\_at, ...)
- Given the expression level of genes of a Person, predict if he has cancer or not.

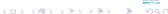


# Illustrative Example: patient monitoring in ICU ...

ALARM is a diagnostic application used to explore probabilistic reasoning techniques in belief networks. ALARM implements an alarm message system for patient monitoring; it calculates probabilities for a differential diagnosis based on available evidence. The medical knowledge is encoded in a graphical structure connecting 8 diagnoses, 16 finding and 13 intermediate variables.

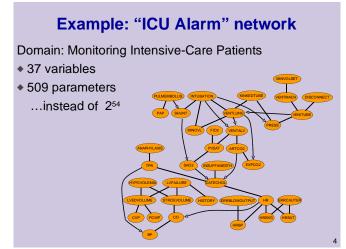
Three types of variables are represented in ALARM. Diagnoses and other qualitative information are at the top level of the network. These variables have no predecessors and they are assumed to be mutually independent a priori. All nodes are associated with a set of mutually exclusive and exhaustive values representing the presence or absence or the severity of a particular disease. Measurements represent any available quantitative information. All continuous variables are represented categorically with sets of discrete intervals dividing the value range. Depending on the necessary level of detail, three to five categories are used per node. Intermediate variables are inferred entities that cannot be measured directly.

The probabilities in a belief network can represent objective as well as subjective knowledge. ALARM contains statistical data on prior probabilities, logical conditional probabilities computed from equations relating variables, and a number of subjective assessments. It is necessary to obtain conditional probabilities for the states of a node, given all different states of the parent nodes.



#### Illustrative Example: Qualitative model ...

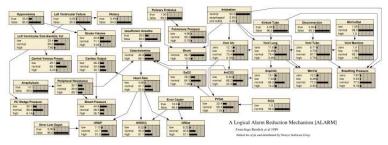
A DAG that reflects the conditional independence between variables.





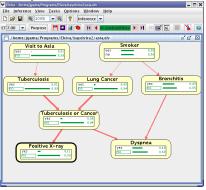
#### Illustrative Example: .. and Quantitative model

A set of contingency tables between dependent variables.

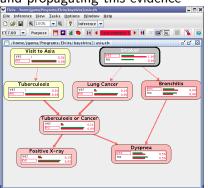


# Illustrative Example: Propagating Evidence ...

#### A Bayesian net:

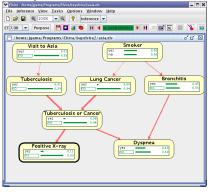


# Prediction: Observing Smoking and propagating this evidence

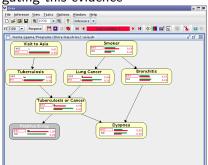


## Illustrative Example: Propagating Evidence ...

#### A Bayesian net:



Diagnosis: Observing Positive X-ray and propagating this evidence



# Why Learn Bayesian Networks?

- Join Probability Distribution of a set of Variables.
- Conditional independences & graphical language capture structure of many real-world distributions
- Graph structure provides much insight into domain
- Learned model can be used for many tasks:
  - Prediction: Given the Inputs: which Outputs?
  - Diagnosis: Given the Outputs: which Inputs?
  - Unsupervised: Given Inputs and Outputs: Which structure?



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## Bayes Theorem

What is the most probable hypothesis h, given training data D? A method to calculate the probability of a hypothesis based on

- its prior probability,
- the probability of observing the data given the hypothesis,
- The data itself

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

- 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









- The Win envelope has 1 dollar and four beads in it.
- The Lose envelope has three beads in it.

Someone draws an envelope at random and offers to sell it to you. Which one should we choose?





Before deciding, you are allowed to see one bead in one envelope.

- If it is black, Which one should we choose?
- And if it is red?



```
Prior Probabilities:

P(Win) =

P(Lose) =

P(red) =

P(black) =

P(black|Win) =

P(red|Win) =

After seeing the bead:

P(Win|black) =

P(Win|red) =
```





Prior Probabilities:

$$P(Win) = 1/2$$

$$P(Lose) = 1/2$$
  
 $P(red) = 3/7$ 

$$T(rea) = 3/T$$

$$P(black) = 4/7$$

$$P(black|Win) = 1/2$$
  
 $P(red|Win) = 1/2$ 

After seeing the bead:

If bead 
$$=$$
 black:

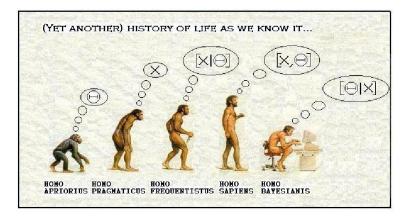
$$P(Win|black) = \frac{P(Win)P(black|Win)}{P(black)} = \frac{1/2*1/2}{4/7} = 0.4375$$

If bead = red: 
$$P(Win|red) = \frac{P(Win)P(red|Win)}{P(red)} = \frac{1/2*1/2}{3/7} = 0.583$$





#### Bayesians ...



## Bayesians ...

- The Homo apriorius establishes the probability of an hypothesis, no matter what data tell. Astronomical example: H0=25. What the data tell is uninteresting.
- The Homo pragamiticus establishes that it is interested by the data only.
   Astronomical example: In my experiment I found H0=66.6666666, full stop.
- The Homo frequentistus measures the probability of the data given the hypothesis. Astronomical example: if H0=66.666666, then the probability to get an observed value more different from the one I observed is given by an opportune expression. Don't ask me if my observed value is near the true one, I can only tell you that if my observed values is the true one, then the probability of observing data more extreme than mine is given by an opportune expression.
- The Homo sapients measures the probability of the data and of the hypothesis.
   Astronomical example: [missing]
- The Homo bayesianis measures the probability of the hypothesis, given the data.
   Astronomical example: the true value of H0 is near 72 with +-3 uncertainty.

Stefano Andreon Homepage



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#### An Illustrative Problem:

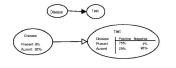
A patient takes a lab test and the result comes back positive.

- The test returns a correct positive result in only 75% of the cases in which the disease is actually present,
- and a correct negative result in only 96% of the cases in which the disease is not present.
- Furthermore, 8% of the entire population have this cancer.

How to represent that information?



#### Representation:



It is useful to represent this information in a graph.

- The graphical information is qualitative
- The nodes represent variables.
- Arcs specify the (in)dependence between variables. Direct arcs represent influence between variables.

The direction of the arc tell us that the value of the variable *disease* influences the value of the variable *test*.



#### Inference:

Inference using Bayes Theorem:

$$P(\textit{Disease}|\textit{Test} = '\textit{Positive}') =$$
 $= P(\textit{Disease})P(\textit{Test} = '\textit{Positive}'|\textit{Disease})$ 

## Naive Bayes Classifier

Assume target function  $f: X \to Y$ , where each instance x described by attributes  $\langle x_1, x_2 \dots x_n \rangle$ . Most probable value of f(x) is:

$$Y_{MAP} = \underset{y_j \in Y}{\operatorname{argmax}} P(y_j | x_1, x_2 \dots x_n)$$

$$Y_{MAP} = \underset{y_j \in Y}{\operatorname{argmax}} \frac{P(x_1, x_2 \dots x_n | y_j) P(y_j)}{P(x_1, x_2 \dots x_n)}$$

$$= \underset{y_i \in Y}{\operatorname{argmax}} P(x_1, x_2 \dots x_n | y_j) P(y_j)$$

# Naive Bayes Classifier

Naive Bayes assumption: Attributes are independent given the class.

 $P(x_1, x_2 ... x_n | y_j) = \prod_i P(x_i | y_j)$  which gives Naive Bayes classifier:

$$Y_{NB} = \operatorname*{argmax}_{y_j \in V} P(y_j) \prod_i P(x_i|y_j)$$

#### Naive Bayes

- Assume a decision problem with p variables.
- Each variable assume k values.
- The joint probability requires to estimate  $k^p$  probabilities.
- Assuming that variables are conditionally independent given the class, only requires to estimate  $k \times p$  probabilities.

## Naive Bayes Formulae

• Naive Bayes can be expressed in addictive form:

$$P(y_i|\vec{x}) \propto ln(P(y_i)) + \sum ln(P(x_j|y_i))$$

- Points out the contribution of each attribute to the decision.
- Two class problems:

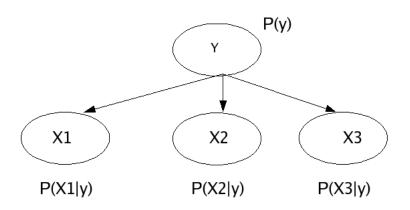
$$lnrac{P(y_{+}|\vec{x})}{P(y_{-}|\vec{x})} \propto lnrac{P(y_{+})}{P(y_{-})} + \sum lnrac{P(x_{j}|y_{+})}{P(x_{j}|y_{-})}$$
 $lnrac{P(y_{+}|\vec{x})}{P(y_{-}|\vec{x})} \propto lnrac{P(y_{+})}{1 - P(y_{+})} + \sum lnrac{P(x_{j}|y_{+})}{1 - P(x_{j}|y_{+})}$ 

The sign of each term indicates the class the attribute contributes to.





#### Naive Bayes as a Bayesian Net



p(Y|X1,X2,X3)=P(Y)P(X1|Y)P(X2|Y)P(X3|Y)



# Naive Bayes Algorithm

```
Naive_Bayes_Learn(examples)
Initialize all counts to zero
For each example \{X, y_j\}
Nr = Nr + 1
Count(y_j) = Count(y_j) + 1
For each attribute value x_i \in X
Count(x_i, y_j) = Count(x_i, y_j) + 1
```

 $Classify_New_Instance(x)$ 

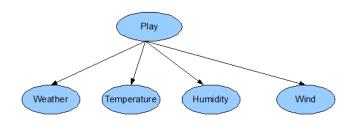
$$y_{NB} = \underset{y_j \in Y}{\operatorname{argmax}} \hat{P}(y_j) \prod_{x_i \in X} \hat{P}(x_i | y_j)$$



# Naive Bayes: Example

Weather	Temperature	Humidity	Wind	Play
Rainy	71	91	Yes	No
Sunny	69	70	No	Yes
Sunny	80	90	Yes	No
Overcast	83	86	No	Yes
Rainy	70	96	No	Yes
Rainy	65	70	Yes	No
Overcast	64	65	Yes	Yes
Overcast	72	90	Yes	Yes
Sunny	75	70	Yes	Yes
Rainy	68	80	No	Yes
Overcast	81	75	No	Yes
Sunny	85	85	No	No
Sunny	72	95	No	No
Rainy	75	80	No	Yes

#### Two representations:



P(play, weather, temperature, humidity, wind) =

= P(Play)P(Weather|Play)P(Temperature|Play)P(Humidity|Play)P(Wind|Play)



# Naive Bayes: Counts

Nr. examples: 14 *Play* =' *Yes*' : 9 *Play* =' *No*' : 5

Weather		Temperature			Humidity			Wind			
	Yes	No		Yes	No		Yes	No		Yes	No
Sunny	2	3	Mean	73	74.6	Mean	79.1	86.2	False	6	2
Overcast	4	0	SD	6.2	7.9	SD	10.2	9.3	True	3	3
Rainy	3	2									

## Naive Bayes: Distribution Tables

Nr. examples: 14

$$P(Play =' Yes') = 9/14$$
  
 $P(Play =' No') = 5/14$ 

Weather			Temperature			Humidity			Wind		
	Yes	No		Yes	No		Yes	No		Yes	No
Sunny	2/9	3/5	Mean	73	74.6	Mean	79.1	86.2	False	6/9	2/5
Overcast	4/9	0/5	SD	6.2	7.9	SD	10.2	9.3	True	3/9	3/5
Rainy	3/9	2/5									

Continuous attributes can be approximated using normal

distribution: 
$$N(x) = \frac{1}{\sqrt{2\pi\sigma}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$





# Naive Bayes: Test Example

Weather	Temperature	Humidity	Wind	Play
Sunny	66	90	Yes	?

```
P(Yes|Weather = `Sunny', Temperature = 66, Humidity = 90, Wind = `Yes') = \\ = P(Yes)P(Weather = `Sunny'|Yes)P(Temperature = 66|Yes)P(Humidity = \\ 90|Yes)P(Wind = `Yes'|Yes)
```

```
P(No|Weather = 'Sunny', Temperature = 66, Humidity = 90, Wind = 'Yes') = P(No)P(Weather = "Sunny"|No)P(Temperature = 66|No)P(Humidity = 90|No)P(Wind = "Yes"|No)
```



# Naive Bayes: Subtleties

• what if none of the training instances with target value  $y_j$  have attribute value  $x_i$ ? Then  $\hat{P}(x_i|y_j) = 0$  and  $\hat{P}(y_i) \prod_i \hat{P}(x_i|y_i) = 0$ 

Typical solution is Bayesian estimate for  $\hat{P}(x_i|y_j)$   $\hat{P}(x_i|y_j) \leftarrow \frac{n_c + mp}{n+m}$  where

- n is number of training examples for which  $y = y_j$ ,
- $n_c$  number of examples for which  $Y = y_j$  and  $X = x_i$
- p is prior estimate for  $\hat{P}(x_i|y_j)$
- m is weight given to prior (i.e. number of "virtual" examples)

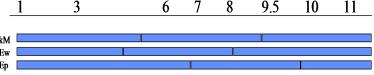
#### Discretization

Transform a continuous variable into a set of ordered intervals (bins). Two Main Problems:

- How many Intervals?
   Generic: Use 10 intervals or min(10, nr. of different values)
   Bioinformtics: few intervals (2, 3, ...)
- How to define to borders of each Interval?

#### Discretization: Basic Methods

- **Equal width discretization**. Divides the range of observed values for a feature into *k* equally sized bins. Pos: simplicity, Neg: the presence of outliers.
- Equal frequency discretization. Divides the range of observed values into k bins, where (considering n instances) each bin contains n/k values.
- k-means. An iterative method that begins with an equal-width discretization, iteratively adjust the boundaries to minimize a squared-error function and only stops when it can not change any value to improve the previous criteria.







# Naive Bayes: Analysis

Conditional independence assumption is often violated

$$P(x_1, x_2 \dots x_n | y_j) = \prod_i P(x_i | y_j)$$

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

$$\underset{y_j \in Y}{\operatorname{argmax}} \hat{P}(y_j) \prod_i \hat{P}(x_i|y_j) = \underset{y_j \in Y}{\operatorname{argmax}} P(y_j) P(x_1 \dots, x_n|y_j)$$

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

# Naive Bayes: Analysis

• Robust to the presence of irrelevant attributes. Suppose a two class problem, where  $X_i$  is an irrelevant attribute:  $p(x_i|y_1) = p(x_i|y_2)$ .  $p(Y|x_1,...,x_i,...,x_n) \propto p(Y)p(x_i|c) \prod_{l=1}^{i-1} p(x_l|Y) \prod_{l=i+1}^{n} p(x_l|Y)$  and

 $p(Y|x_1,...,x_i,...,x_n) \propto p(Y|x_1,...,x_{i-1},x_{i+1},...,x_n)$ 

• Redundant variables must be taken into account. Suppose that 
$$X_i = X_{i-1}$$
 then  $p(x_{i-1}|Y) = p(x_i|Y)$   $p(Y|x_1,...,x_{i-1},x_i,...,x_n) \propto p(Y)p(x_{i-1}|Y)p(x_i|Y)\prod_{l=1}^{i-2}p(x_l|Y)\prod_{l=i+1}^{n}p(x_l|Y)$  and  $p(Y|x_1,...,x_{i-1},x_i,...,x_n) \propto p(Y)p(x_i|Y)^2\prod_{l=1}^{i-2}p(x_l|Y)\prod_{l=i+1}^{n}p(x_l|Y)$ 



# Naive Bayes: Summary

- The variability of a dataset is summarized in contingency tables.
  - Requires a single scan over the dataset.
  - The algorithm is Incremental (incorporation of new examples) and decremental (forgetting old examples).
- The dimension of the decision model is independent of the number of examples.
  - Low variance: stable with respect to small perturbations of the training set.
  - High bias: the number of possible states is finite.

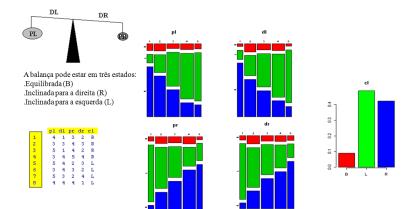
### Naive Bayes: Extensions

- Techniques that apply different naive Bayes classifiers to different regions of the input space. Recursive Bayes (Langley, 93), Naive Bayes Tree (Kohavi,96).
- Techniques that built new attributes that reflect interdependencies between original attributes. Semi-naive Bayes (Kononenko, 91).
- Processing continuous attributes: Flexible Bayes (G.John),
   Linear Bayes (Gama, 01)
- Search for better Parameters: Iterative Bayes (Gama, 99)

#### Successful Stories

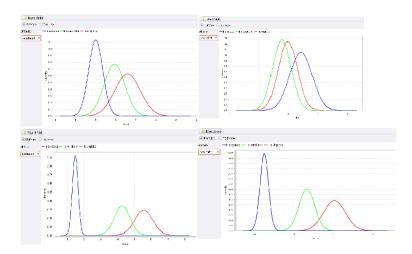
- KDDCup 1998: Winner Boosting naive Bayes;
- Coil 1999: Winner Simple naive Bayes;
- The most used classifier in Text Mining;

#### The Balance-scale Problem





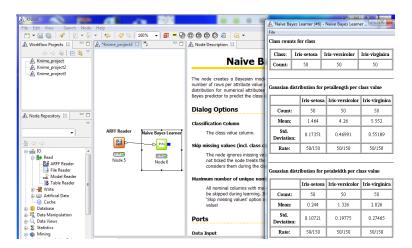
# Rapid Miner: Naive Bayes







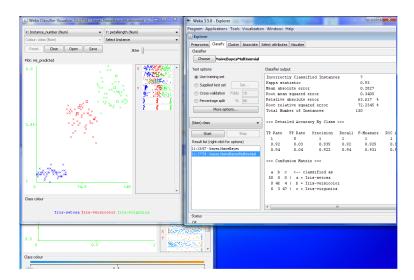
# Knimer: Naive Bayes







#### Weka: Naive Bayes



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#### Entropy

Entropy: measures the randomness of a random variable. Uncertainty of a random discrete variable (Entropy):

$$H(X) = -\sum P(x)log_2(P(x))$$

#### Conditional Entropy

conditional entropy quantifies the remaining entropy (i.e. uncertainty) of a random variable Y given that the value of a second random variable X is known.

Uncertainty about X after knowing Y:

$$H(X|Y) = -\sum_{y} P(y) \sum_{x} P(x|y) log P(x|Y)$$



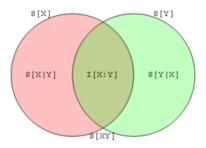
#### Mutual Information

Reduction in the uncertainty of X when Y is known:

$$I(X,Y) = H(X|Y) - H(X)$$

$$I(X,Y) = \sum_{i} \sum_{j} P(x_i, y_j) log \frac{P(x_i, y_j)}{P(x_i)p(x_j)}$$

- I(X, Y) = 0 if and only if X and Y are independent random variables;
- I(X,Y) increases with the increase of the degree of dependence between X and Y;
- nonnegative:  $I(X, Y) \ge 0$ ;
- symmetric: I(X, Y) = I(Y, X).



Individual (S[X],S[Y]), joint (S[XY]), & conditional entropies for a pair of correlated subsystems X,Y with mutual information I[X:Y].

# Example: TAN

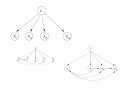
#### Tree augmented naive Bayes

 Compute the Mutual Information between all pairs of variables given the Class

$$I(X,Y|C) = \sum_{c} P(c)I(X,Y|C=c)$$

- Construct a spanning tree maximizing MI.
- All the variables depends on the class.

$$p(c|x_1,x_2,x_3) \propto p(c)p(x_1|c)p(x_2|x_1,c)p(x_3|x_1,c)$$



- All the attributes depends on the class
- Any attribute depends on k other attributes, at most.
- Restricted Bayesian Networks
- Decision Models of Increase Complexity

$$p(c|x_1,x_2,x_3) \propto p(c)p(x_1|c)p(x_2|x_1,c)p(x_3|x_1,c)$$

k-Dependency Bayesian Networks: a common framework for classifiers with increase (smooth) complexity.





- Compute  $I(X_i, C)$  and  $I(X_i, X_i | C)$  for all pairs of variables
- Iterate
  - Choose the variable  $X_{max}$  not yet in the model that maximizes  $I(X_i|C)$
  - Choose the k parents of  $X_{max}$ : those with greater  $I(X_j, X_{max} | C)$

#### Factorization:

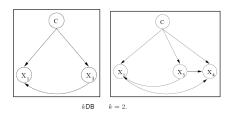
$$P(x_1,\ldots,x_n)=\prod_{i=1}^n P(x_i|Parents(X_i))$$

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



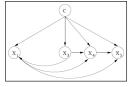
$$\begin{split} I(X_3,C) > I(X_1,C) > I(X_4,C) > I(X_5,C) > I(X_2,C) \\ I(X_3,X_4|C) > I(X_2,X_5|C) > I(X_1,X_3|C) > I(X_1,X_2|C) > I(X_2,X_4|C) > I(X_2,X_3|C) > I(X_1,X_4|C) > I(X_4,X_5|C) > I(X_1,X_5|C) > I(X_3,X_5|C) \end{split}$$

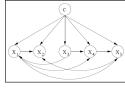




$$\begin{split} &I(X_3,C) > I(X_1,C) > I(X_4,C) > I(X_5,C) > I(X_2,C) \\ &I(X_3,X_4|C) > I(X_2,X_5|C) > I(X_1,X_3|C) > I(X_1,X_2|C) > I(X_2,X_4|C) > \\ &I(X_2,X_3|C) > I(X_1,X_4|C) > I(X_4,X_5|C) > I(X_1,X_5|C) > I(X_3,X_5|C) \\ &p(c|x_1,x_2,x_3,x_4,x_5) \end{split}$$





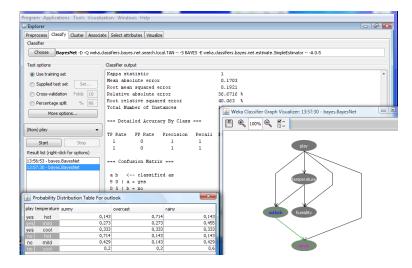


kDB k = 2.

$$\begin{split} &I(X_3,C) > I(X_1,C) > I(X_4,C) > I(X_5,C) > I(X_2,C) \\ &I(X_3,X_4|C) > I(X_2,X_5|C) > I(X_1,X_3|C) > I(X_1,X_2|C) > I(X_2,X_4|C) > \\ &I(X_2,X_3|C) > I(X_1,X_4|C) > I(X_4,X_5|C) > I(X_1,X_5|C) > I(X_3,X_5|C) \\ &p(c|x_1,x_2,x_3,x_4,x_5) & \\ &p(c)p(x_1|x_3,c)p(x_2|x_1,x_5,c)p(x_3|c)p(x_4|x_1,x_3,c)p(x_5|x_1,x_4,c) \end{split}$$



#### Weka: TAN



#### Outline

- Motivation: Information Processing
- 2 Introduction
- Bayesian Network Classifiers
- 4 k-Dependence Bayesian Classifiers
- 6 Links and References

#### Software Available

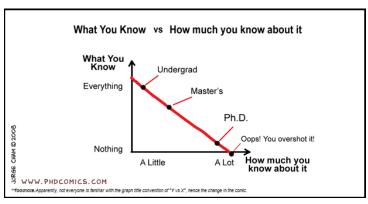
- R (package e1071)
- Weka (naive Bayes, TAN models, k-dependence Bayesian classifiers)
- Genie: Bayesian Networks, Influence Diagrams, Dynamic Bayesian Networks (http://genie.sis.pitt.edu/)
- Hugin (http://www.hugin.com/)
- Elvira (http://www.ia.uned.es/ elvira)
- Kevin Murphy's MATLAB toolbox supports dynamic BNs, decision networks, many exact and approximate inference algorithms, parameter estimation, and structure learning (http://www.ai.mit.edu/ murphyk/Software/BNT/bnt.html)
- Free Windows software for creation, assessment and evaluation of belief networks.
  - $(\mathsf{http://www.research.microsoft.com/dtas/msbn/default.htm})$
- Open source package for the technical computing language R, developed by Aalborg University (http://www.math.auc.dk/novo/deal)
- http://www.snn.ru.nl/nijmegen





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