Algorithms: The basic methods

Most of these slides (used with permission) are based on the book:

Data Mining: Practical Machine Learning Tools and Techniques
by I. H. Witten, E. Frank, M. A. Hall, and C. J. Pal

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Algorithms: The basic methods

- Inferring rudimentary rules
- Simple probabilistic modeling
- Constructing decision trees
- Constructing rules
- Association rule learning
- Linear models
- Clustering

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Simplicity first

- Simple algorithms often work very well!
- There are many kinds of simple structure, e.g.:
  - One attribute does all the work
  - All attributes contribute equally & independently
  - Logical structure with a few attributes suitable for tree
  - A set of simple logical rules
  - Relationships between groups of attributes
  - A weighted linear combination of the attributes
  - Strong neighborhood relationships based on distance
  - Clusters of data in unlabeled data
  - Bags of instances that can be aggregated
- Success of method depends on the domain

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Inferring rudimentary rules

- 1R rule learner: learns a 1-level decision tree
  - A set of rules that all test one particular attribute that has been identified as the one that yields the lowest classification error
- Basic version for finding the rule set from a given training set (assumes nominal attributes):
  - For each attribute
    - Make one branch for each value of the attribute
    - To each branch, assign the most frequent class value of the instances pertaining to that branch
    - Error rate: proportion of instances that do not belong to the majority class of their corresponding branch
  - Choose attribute with lowest error rate

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Pseudo-code for 1R

```
For each attribute,
For each value of the attribute, make a rule as follows:
  count how often each class appears
  find the most frequent class
  make the rule assign that class to this attribute-value
Calculate the error rate of the rules
Choose the rules with the smallest error rate
```

- 1R's handling of missing values: a missing value is treated as a separate attribute value

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Evaluating the weather attributes

Outlook	Temp	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

Attribute	Rules	Errors	Total errors
Outlook	Sunny → No	2/5	4/14
	Overcast → Yes	0/4	
	Rainy → Yes	2/5	
Temp	Hot → No	2/4	5/14
	Mild → Yes	2/6	
	Cool → Yes	1/4	
Humidity	High → No	3/7	4/14
	Normal → Yes	1/7	
Windy	False → Yes	2/8	5/14
	True → No	3/6	

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Dealing with numeric attributes

- Idea: discretize numeric attributes into sub ranges (intervals)
- **Discretization** is the process of putting values into buckets so that there are a limited number of possible states.
- How to divide each attribute's overall range into intervals?
  - Sort instances according to attribute's values
  - Place breakpoints where (majority) class changes
  - This minimizes the total classification error
- Example: *temperature* from weather data

```
64    65    68    69    70    71    72    72    75    75    80    81    83    85
Yes | No | Yes   Yes   Yes | No    No    Yes | Yes   Yes | No | Yes   Yes | No
```

Outlook	Temperature	Humidity	Windy	Play
Sunny	85	85	False	No
Sunny	80	90	True	No
Overcast	83	86	False	Yes
Rainy	75	80	False	Yes
…	…	…	…	…

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The problem of overfitting

- Discretization procedure is very sensitive to noise
  - A single instance with an incorrect class label will probably produce a separate interval
- Simple solution:
  enforce minimum number of instances in majority class per interval
- Example: *temperature* attribute with required minimum number of instances in majority class set to three:

```
64    65    68    69    70    71    72    72    75    75    80    81    83    85
Yes   No    Yes   Yes   Yes | No    No    Yes | Yes   Yes | No    Yes   Yes   No

64    65    68    69    70    71    72    72    75    75    80    81    83    85
Yes   No    Yes   Yes   Yes   No    No    Yes   Yes   Yes | No    Yes   Yes   No
```

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Results with overfitting avoidance

- Resulting rule sets for the four attributes in the weather data, with only two rules for the temperature attribute:

Attribute	Rules	Errors	Total errors
Outlook	Sunny → No	2/5	4/14
	Overcast → Yes	0/4	
	Rainy → Yes	2/5	
Temperature	≤ 77.5 → Yes	3/10	5/14
	> 77.5 → No*	2/4	
Humidity	≤ 82.5 → Yes	1/7	3/14
	> 82.5 and ≤ 95.5 → No	2/6	
	> 95.5 → Yes	0/1	
Windy	False → Yes	2/8	5/14
	True → No*	3/6	

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Discussion of 1R

- 1R was described in a paper by Holte (1993):

  Very Simple Classification Rules Perform Well on Most Commonly Used Datasets
  Robert C. Holte, Computer Science Department, University of Ottawa

  - Contains an experimental evaluation on 16 datasets (using *cross-validation* to estimate classification accuracy on fresh data)
  - Required minimum number of instances in majority class was set to 6 after some experimentation
  - 1R's simple rules performed not much worse than much more complex decision trees
- Lesson: simplicity first can pay off on practical datasets
- Note that 1R does not perform as well on more recent, more sophisticated benchmark datasets

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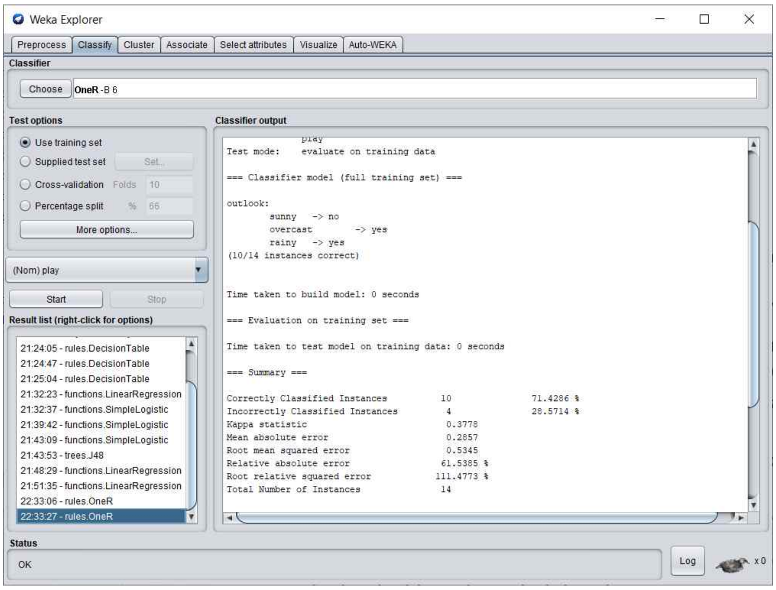
1R on weather data (numeric)



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Simple probabilistic modeling

- "Opposite" of 1R: use all the attributes
- Two assumptions: Attributes are
  - *equally important*
  - *statistically independent* (given the class value)
    - This means knowing the value of one attribute tells us nothing about the value of another takes on (if the class is known)
- Independence assumption is almost never correct!
- But … this scheme often works surprisingly well in practice
- The scheme is easy to implement in a program and very fast
- It is known as *naïve Bayes*

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Probabilities for weather data

Outlook			Temperature			Humidity			Windy			Play	
	Yes	*No*		*Yes*	*No*		*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3	Hot	2	2	High	3	4	False	6	2	9	5
Overcast	4	0	Mild	4	2	Normal	6	1	True	3	3		
Rainy	3	2	Cool	3	1								
Sunny	2/9	3/5	Hot	2/9	2/5	High	3/9	4/5	False	6/9	2/5	9/14	5/14
Overcast	4/9	0/5	Mild	4/9	2/5	Normal	6/9	1/5	True	3/9	3/5		
Rainy	3/9	2/5	Cool	3/9	1/5								

Outlook	Temp	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

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Probabilities for weather data

Outlook			Temperature			Humidity			Windy			Play	
	Yes	*No*		*Yes*	*No*		*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3	Hot	2	2	High	3	4	False	6	2	9	5
Overcast	4	0	Mild	4	2	Normal	6	1	True	3	3		
Rainy	3	2	Cool	3	1								
Sunny	2/9	3/5	Hot	2/9	2/5	High	3/9	4/5	False	6/9	2/5	9/14	5/14
Overcast	4/9	0/5	Mild	4/9	2/5	Normal	6/9	1/5	True	3/9	3/5		
Rainy	3/9	2/5	Cool	3/9	1/5								

- A new day:

Outlook	Temp.	Humidity	Windy	Play
Sunny	Cool	High	True	?

Likelihood of the two classes

For "yes" = 2/9 × 3/9 × 3/9 × 3/9 × 9/14 = 0.0053

For "no" = 3/5 × 1/5 × 4/5 × 3/5 × 5/14 = 0.0206

Conversion into a probability by normalization:

P("yes") = 0.0053 / (0.0053 + 0.0206) = 0.205

P("no") = 0.0206 / (0.0053 + 0.0206) = 0.795

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Naïve Bayes for classification

- Classification learning: what is the probability of the class given an instance?
  - Evidence *E* = instance's non-class attribute values
  - Event *H* = class value of instance
- Naïve assumption: evidence splits into parts (i.e., attributes) that are conditionally *independent*
- This means, given *n* attributes, we can write Bayes' rule using a product of per-attribute probabilities:

$$P(H \mid E) = P(E_1 \mid H) P(E_3 \mid H) \ast P(E_n \mid H) P(H) / P(E)$$

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Weather data example

Outlook	Temp.	Humidity	Windy	Play
Sunny	Cool	High	True	?

Evidence E

$$\begin{aligned} P(yes \mid E) = {} & P(Outlook = Sunny \mid yes) \\ & P(Temperature = Cool \mid yes) \\ & P(Humidity = High \mid yes) \\ & P(Windy = True \mid yes) \\ & P(yes) / P(E) \end{aligned}$$

Probability of class "yes"

$$P(yes)/P(E) = \frac{2/9 \times 3/9 \times 3/9 \times 3/9 \times 9/14}{P(E)}$$

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Missing values

- Training: instance is not included in frequency count for attribute value-class combination
- Classification: attribute will be omitted from calculation
- Example:

Outlook	Temp.	Humidity	Windy	Play
?	Cool	High	True	?

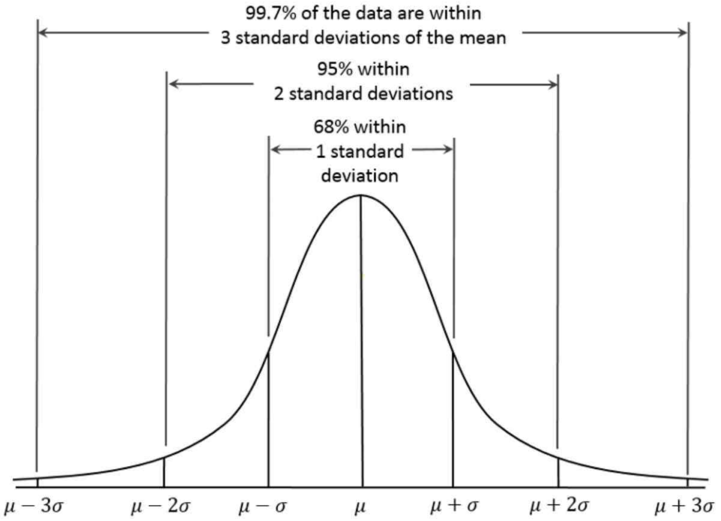
Likelihood of "yes" = 3/9 × 3/9 × 3/9 × 9/14 = 0.0238

Likelihood of "no" = 1/5 × 4/5 × 3/5 × 5/14 = 0.0343

P("yes") = 0.0238 / (0.0238 + 0.0343) = 41%

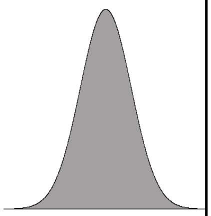
P("no") = 0.0343 / (0.0238 + 0.0343) = 59%

68-95-99.7 Rule of bell curve



Numeric attributes

- Usual assumption: attributes have a *normal* or *Gaussian* probability distribution (given the class)
- The *probability density function* for the normal distribution is defined by two parameters:
  - *Sample mean* $\mu = \frac{1}{N}\sum_{i=1}^{N} x_i$



  - *Standard deviation* $\sigma = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(x_i-\mu)^2}$
  - Then the density function *f(x) is* $f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

For density function refer to: https://towardsdatascience.com/probability-concepts-explained-probability-distributions-introduction-part-3-4a5db81858dc

In probability theory, a probability density function is a function whose value at any given sample in the sample space can be interpreted as providing a relative likelihood that the value of the random variable would equal that sample.

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Statistics for weather data

Outlook			Temperature		Humidity		Windy			Play	
	Yes	*No*	*Yes*	*No*	*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3	64, 68,	65,71,	65, 70,	70, 85,	False	6	2	9	5
Overcast	4	0	69, 70,	72,80,	70, 75,	90, 91,	True	3	3		
Rainy	3	2	72, …	85, …	80, …	95, …					
Sunny	2/9	3/5	μ =73	μ =75	μ =79	μ =86	False	6/9	2/5	9/ 14	5/ 14
Overcast	4/9	0/5	σ =6.2	σ =7.9	σ =10.2	σ =9.7	True	3/9	3/5		
Rainy	3/9	2/5									

- Example density value: $f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

$$f(temperature = 66|yes) = \frac{1}{\sqrt{2\pi}\cdot 6.2} e^{-\frac{(66-73)^2}{2\cdot 6.2^2}} = 0.0340$$

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Classifying a new day

- A new day:

Outlook	Temp.	Humidity	Windy	Play
Sunny	66	90	true	?

Likelihood of "yes" = 2/9 × 0.0340 × 0.0221 × 3/9 × 9/14 = 0.000036

Likelihood of "no" = 3/5 × 0.0221 × 0.0381 × 3/5 × 5/14 = 0.000108

P("yes") = 0.000036 / (0.000036 + 0. 000108) = 25%

P("no") = 0.000108 / (0.000036 + 0. 000108) = 75%

- Missing values during training are not included in calculation of mean and standard deviation

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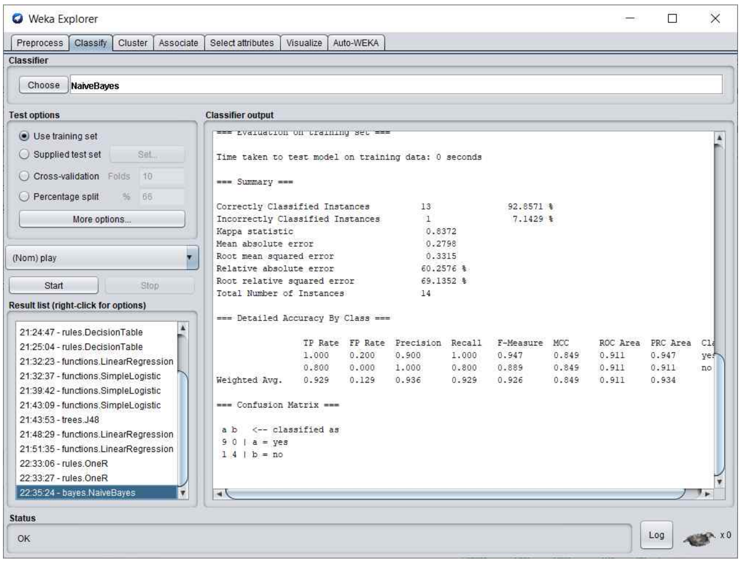
Naïve Bayes on Weather Data



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Naïve Bayes: discussion

- Naïve Bayes works surprisingly well even if independence assumption is clearly violated
- Why? Because classification does not require accurate probability estimates *as long as maximum probability is assigned to the correct class*
- However: adding too many redundant attributes will cause problems (e.g., identical attributes)

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Constructing decision trees

- Strategy: top down learning using recursive *divide-and-conquer* process
  - First: select attribute for root node
    Create branch for each possible attribute value
  - Then: split instances into subsets
    One for each branch extending from the node
  - Finally: repeat recursively for each branch, using only instances that reach the branch
- Stop if all instances have the same class

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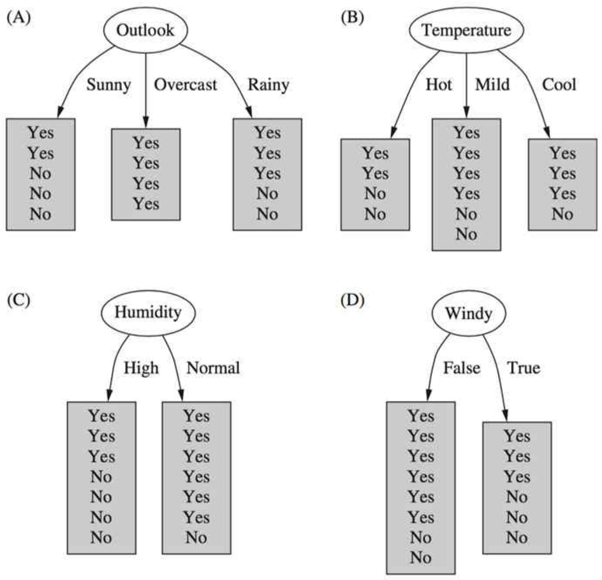
Which attribute to select?



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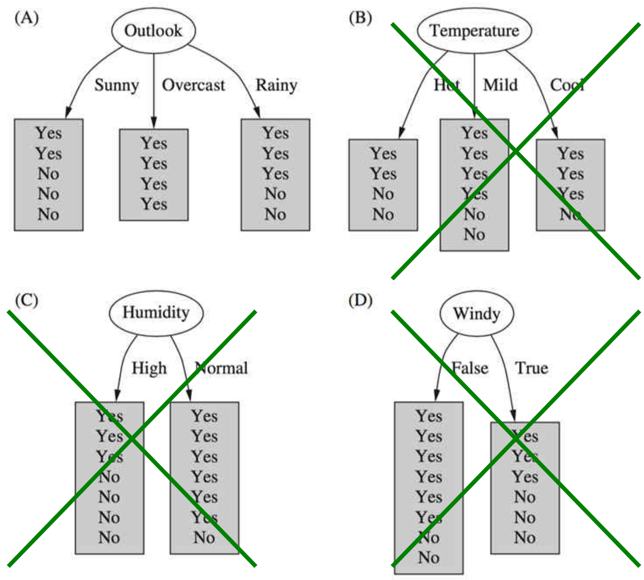
Which attribute to select?



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Criterion for attribute selection

- Which is the best attribute?
  - Want to get the smallest tree
  - Heuristic: choose the attribute that produces the "purest" nodes
- Popular selection criterion: *information gain*
  - Information gain increases with the average purity of the subsets
- Strategy: amongst attributes available for splitting, choose attribute that gives greatest information gain
- Information gain requires measure of *impurity*
- Impurity measure that it uses is the *entropy* of the class distribution, which is a measure from information theory

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Computing information

- We have a probability distribution: the class distribution in a subset of instances
- The expected information required to determine an outcome (i.e., class value), is the distribution's *entropy*
- Formula for computing the entropy:

$$\text{Entropy}(p_1, p_2, \ldots, p_n) = -p_1 \log p_1 - p_2 \log p_2 \ldots - p_n \log p_n$$

- Using base-2 logarithms, entropy gives the information required in expected *bits*
- Entropy is maximal when all classes are equally likely and minimal when one of the classes has probability 1

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A Fair Die Example

The Expected Value of a Random Variable or a Function of a Random Variable

Definition

$E(x)$: **expected value** of x, or μ $\qquad E(x) = \mu = \sum_x xp(x)$

Example: The probability distribution of random variable x:

x	0	1	2
$p(x)$	1/4	1/2	1/4

Find $E(x)$.

x	0	1	2	Total
$p(x)$	1/4	1/2	1/4	1
$xp(x)$	0	1/2	1/2	1=E(x)

The formula for Shannon entropy is as follows,

$$\text{Entropy}(S) = -\sum_i p_i \log_2 p_i$$

Thus, a fair six sided dice should have the entropy,

$$-\sum_{i=1}^{6} \frac{1}{6} \log_2 \frac{1}{6} = \log_2(6) = 2.5849\ldots$$

Example: Toss a die. x = number observed. Find $p(x)$.
$p(x)$ = 1/6 for x=1, 2, 3, 4, 5, 6.

Find $E(x)$.

x	1	2	3	4	5	6	Total
$p(x)$	1/6	1/6	1/6	1/6	1/6	1/6	1
$xp(x)$	1/6	2/6	3/6	4/6	5/6	6/6	21/6=3.5=E(x)

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Example: attribute *Outlook*

- *Outlook* = *Sunny* :

$$\text{Info}([2,3]) = 0.971 \text{ bits}$$

-0.4 * -1.32192809489 + -0.6 * -0.736965594166 = 0.9709

- *Outlook* = *Overcast* :

$$\text{Info}([4,0]) = 0.0 \text{ bits}$$

1 * 0 + 0 * 0 = 0

- *Outlook* = *Rainy* :

$$\text{Info}([3,2]) = 0.971 \text{ bits}$$

-0.6 * -0.736965594166 + -0.4 * -1.32192809489 = 0.9709

- Expected information for attribute:

$$\text{Info}([2,3],[4,0],[3,2]) = (5/14) \times 0.971 + (4/14) \times 0 + (5/14) \times 0.971$$
$$= 0.693 \text{ bits}$$

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Computing information gain

- Information gain: information before splitting – information after splitting

Gain(*Outlook*) = Info([9,5]) – info([2,3],[4,0],[3,2])
= 0.940 – 0.693
= 0.247 bits

- Information gain for attributes from weather data:

Gain(*Outlook*)	= 0.247 bits
Gain(*Temperature*)	= 0.029 bits
Gain(*Humidity*)	= 0.152 bits
Gain(*Windy*)	= 0.048 bits

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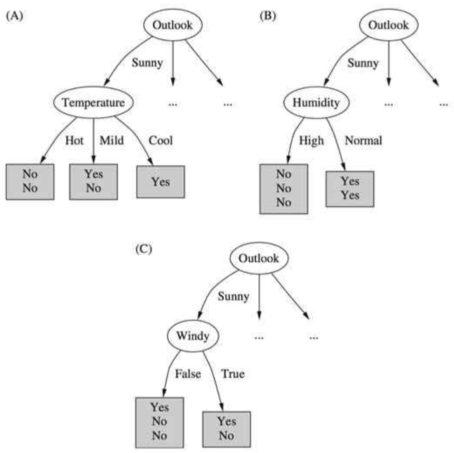
Continuing to split



Gain(*Temperature*)	= 0.571 bits
Gain(*Humidity*)	= 0.971 bits
Gain(*Windy*)	= 0.020 bits

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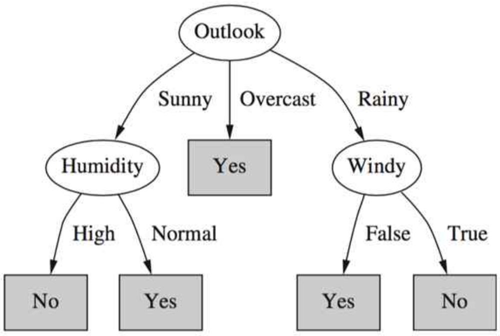
Final decision tree



- Note: not all leaves need to be pure; sometimes identical instances have different classes
  - Splitting stops when data cannot be split any further

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Discussion

- Top-down induction of decision trees: ID3, algorithm developed by Ross Quinlan
  - C4.5 tree learner deals with numeric attributes, missing values, noisy data
- Similar approach: CART tree learner
  - Uses Gini index rather than entropy to measure impurity
- There are many other attribute selection criteria! (But little difference in accuracy of result)

$$Gini = 1 - \sum_{i=1}^{n} p^2(c_i)$$

$$Entropy = \sum_{i=1}^{n} -p(c_i)log_2(p(c_i))$$

where $p(c_i)$ is the probability/percentage of class c_i in a node.

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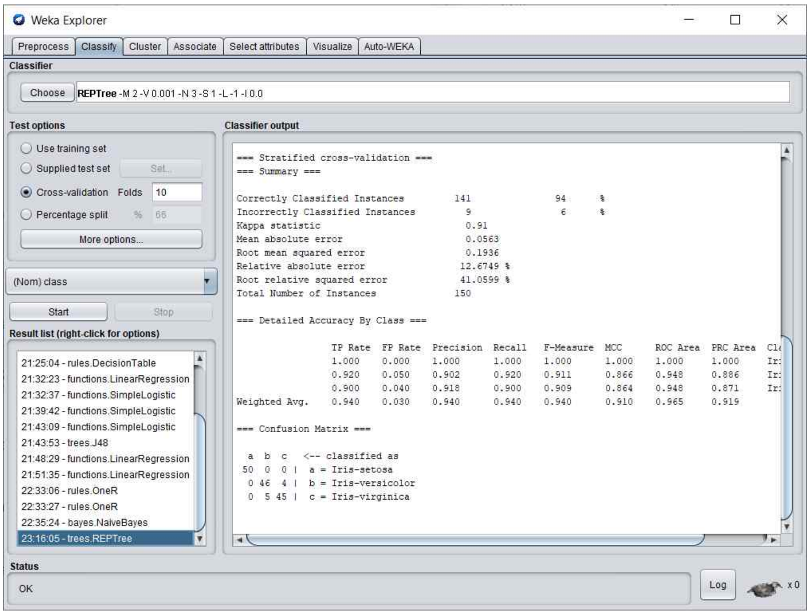
WEKA – REPTree (one of the CART algorithms)



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Covering algorithms

- Can convert decision tree into a rule set
  - Straightforward, but rule set overly complex
  - More effective conversions are not trivial and may incur a lot of computation
- Instead, we can generate rule set directly
  - One approach: for each class in turn, find rule set that covers all instances in it
    (excluding instances not in the class)
- Called a *covering* approach:
  - At each stage of the algorithm, a rule is identified that "covers" some of the instances

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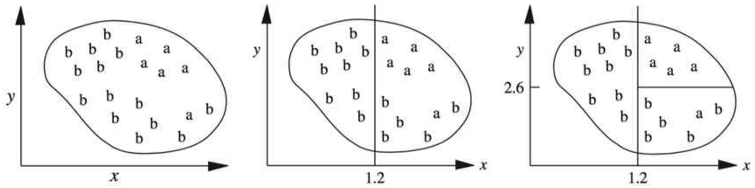
Example: generating a rule




```
If true
   then class = a
```

```
If x > 1.2
   then class = a
```

```
If x > 1.2 and y > 2.6
   then class = a
```

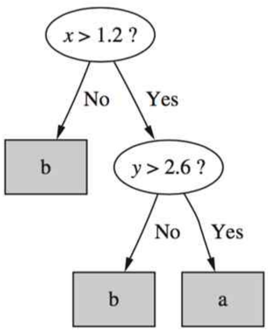
- Possible rule set for class “b”:

```
If x ≤ 1.2 then class = b
If x > 1.2 and y ≤ 2.6 then class = b
```

- Could add more rules, get “perfect” rule set

Rules vs. trees

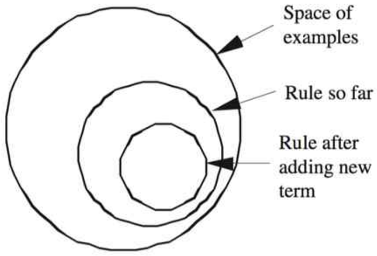
- Corresponding decision tree: (produces exactly the same predictions)



- But: rule sets *can* be more perspicuous (understandable) when decision trees suffer from replicated subtrees
- Also: in multiclass situations, covering algorithm concentrates on one class at a time whereas decision tree learner takes all classes into account

Simple covering algorithm

- Basic idea: generate a rule by adding tests that maximize the rule's accuracy
- Similar to situation in decision trees: problem of selecting an attribute to split on
  - But: decision tree inducer maximizes overall purity
- Each new test reduces rule's coverage:



Selecting a test

- Goal: maximize accuracy
  - *t* total number of instances covered by rule
  - *p* positive examples of the class covered by rule
  - *t – p* number of errors made by rule
  - Select test that maximizes the ratio *p/t*
- We are finished when *p/t* = 1 or the set of instances cannot be split any further

The contact lenses data

Age	Spectacle prescription	Astigmatism	Tear production rate	Recommended lenses
Young	Myope	No	Reduced	None
Young	Myope	No	Normal	Soft
Young	Myope	Yes	Reduced	None
Young	Myope	Yes	Normal	Hard
Young	Hypermetrope	No	Reduced	None
Young	Hypermetrope	No	Normal	Soft
Young	Hypermetrope	Yes	Reduced	None
Young	Hypermetrope	Yes	Normal	hard
Pre-presbyopic	Myope	No	Reduced	None
Pre-presbyopic	Myope	No	Normal	Soft
Pre-presbyopic	Myope	Yes	Reduced	None
Pre-presbyopic	Myope	Yes	Normal	Hard
Pre-presbyopic	Hypermetrope	No	Reduced	None
Pre-presbyopic	Hypermetrope	No	Normal	Soft
Pre-presbyopic	Hypermetrope	Yes	Reduced	None
Pre-presbyopic	Hypermetrope	Yes	Normal	None
Presbyopic	Myope	No	Reduced	None
Presbyopic	Myope	No	Normal	None
Presbyopic	Myope	Yes	Reduced	None
Presbyopic	Myope	Yes	Normal	Hard
Presbyopic	Hypermetrope	No	Reduced	None
Presbyopic	Hypermetrope	No	Normal	Soft
Presbyopic	Hypermetrope	Yes	Reduced	None
Presbyopic	Hypermetrope	Yes	Normal	None

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Example: contact lens data

- Rule we seek:

```
If ?
    then recommendation = hard
```

- Possible tests:

Age = Young	2/8
Age = Pre-presbyopic	1/8
Age = Presbyopic	1/8
Spectacle prescription = Myope	3/12
Spectacle prescription = Hypermetrope	1/12
Astigmatism = no	0/12
Astigmatism = yes	4/12
Tear production rate = Reduced	0/12
Tear production rate = Normal	4/12

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Modified rule and resulting data

- Rule with best test added:

```
If astigmatism = yes
    then recommendation = hard
```

- Instances covered by modified rule:

Age	Spectacle prescription	Astigmatism	Tear production rate	Recommended lenses
Young	Myope	Yes	Reduced	None
Young	Myope	Yes	Normal	Hard
Young	Hypermetrope	Yes	Reduced	None
Young	Hypermetrope	Yes	Normal	hard
Pre-presbyopic	Myope	Yes	Reduced	None
Pre-presbyopic	Myope	Yes	Normal	Hard
Pre-presbyopic	Hypermetrope	Yes	Reduced	None
Pre-presbyopic	Hypermetrope	Yes	Normal	None
Presbyopic	Myope	Yes	Reduced	None
Presbyopic	Myope	Yes	Normal	Hard
Presbyopic	Hypermetrope	Yes	Reduced	None
Presbyopic	Hypermetrope	Yes	Normal	None

Further refinement

- Current state:

```
If astigmatism = yes
    and ?
  then recommendation = hard
```

- Possible tests:

```
Age = Young                                 2/4
Age = Pre-presbyopic                        1/4
Age = Presbyopic                            1/4
Spectacle prescription = Myope              3/6
Spectacle prescription = Hypermetrope       1/6
Tear production rate = Reduced              0/6
Tear production rate = Normal               4/6
```

Modified rule and resulting data

- Rule with best test added:

```
If astigmatism = yes
    and tear production rate = normal
then recommendation = hard
```

- Instances covered by modified rule:

Age	Spectacle prescription	Astigmatism	Tear production rate	Recommended lenses
Young	Myope	Yes	Normal	Hard
Young	Hypermetrope	Yes	Normal	hard
Pre-presbyopic	Myope	Yes	Normal	Hard
Pre-presbyopic	Hypermetrope	Yes	Normal	None
Presbyopic	Myope	Yes	Normal	Hard
Presbyopic	Hypermetrope	Yes	Normal	None

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Further refinement

- Current state:

```
If astigmatism = yes
    and tear production rate = normal
    and ?
  then recommendation = hard
```

- Possible tests:

```
Age = Young                                 2/2
Age = Pre-presbyopic                        1/2
Age = Presbyopic                            1/2
Spectacle prescription = Myope              3/3
Spectacle prescription = Hypermetrope       1/3
```

- Tie between the first and the fourth test
  - We choose the one with greater coverage

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The final rule

- Final rule:

```
If astigmatism = yes
   and tear production rate = normal
   and spectacle prescription = myope
   then recommendation = hard
```

- Second rule for recommending "hard lenses":
  (built from instances not covered by first rule)

```
If age = young and astigmatism = yes
   and tear production rate = normal
   then recommendation = hard
```

- These two rules cover all "hard lenses":
  - Process is repeated with other two classes

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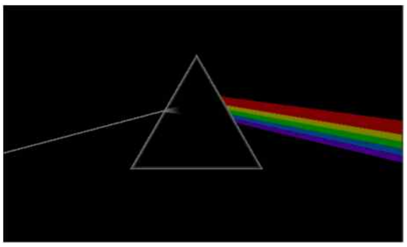
Pseudo-code for PRISM

```
For each class C
  Initialize E to the instance set
  While E contains instances in class C
    Create a rule R with an empty left-hand side that predicts class C
    Until R is perfect (or there are no more attributes to use) do
      For each attribute A not mentioned in R, and each value v,
        Consider adding the condition A = v to the left-hand side of R
        Select A and v to maximize the accuracy p/t
          (break ties by choosing the condition with the largest p)
      Add A = v to R
    Remove the instances covered by R from E
```



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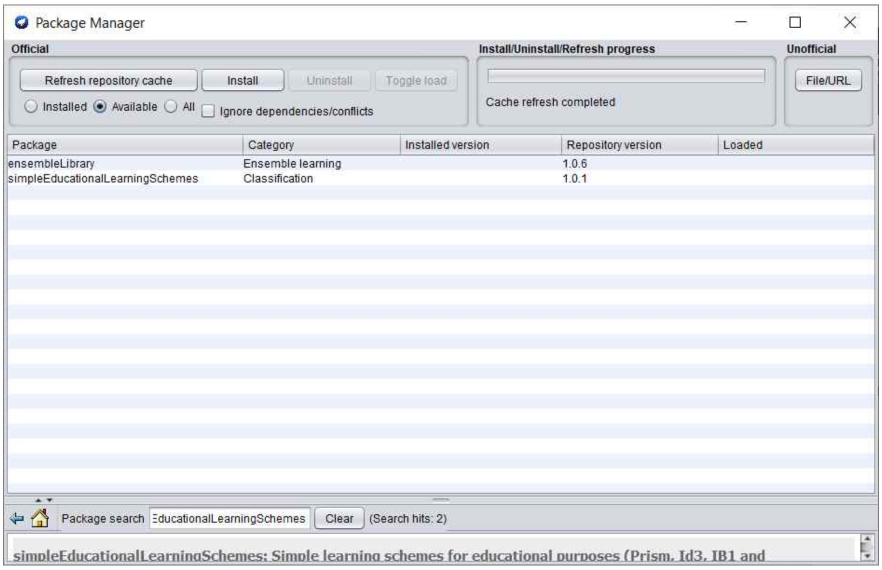
Installing PRISM in WEKA – Package Manager
SimpleEducationalLearningSchemes



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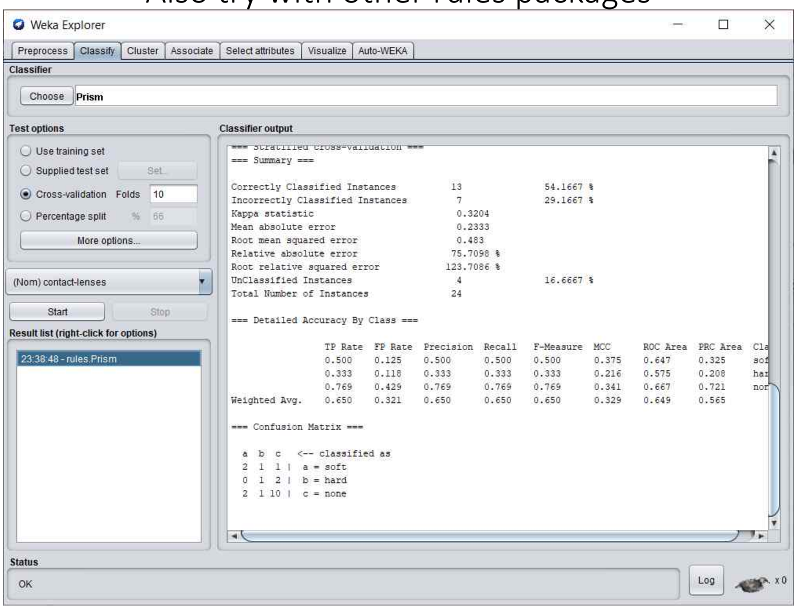
PRISM on Contact Lenses
Also try with other rules packages



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Separate and conquer rule learning

- Rule learning methods like the one PRISM employs (for each class) are called *separate-and-conquer* algorithms:
  - First, identify a useful rule
  - Then, separate out all the instances it covers
  - Finally, “conquer” the remaining instances
- Difference to divide-and-conquer methods:
  - Subset covered by a rule does not need to be explored any further

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Mining association rules

- Naïve method for finding association rules:
  - Use separate-and-conquer method
  - Treat every possible combination of attribute values as a separate class
- Two problems:
  - Computational complexity
  - Resulting number of rules (which would have to be pruned on the basis of support and confidence)
- It turns out that we can look for association rules with high support and accuracy directly

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Item sets: the basis for finding rules

- Support: number of instances correctly covered by association rule
  - The same as the number of instances covered by *all* tests in the rule (LHS and RHS!)
- *Item*: one test/attribute-value pair
- *Item set* : all items occurring in a rule
- Goal: find only rules that exceed pre-defined support
  - Do it by finding all item sets with the given minimum support and generating rules from them!

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Weather data

Outlook	Temp	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

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Item sets for weather data

One-item sets	Two-item sets	Three-item sets	Four-item sets
Outlook = Sunny (5)	Outlook = Sunny Temperature = Hot (2)	Outlook = Sunny Temperature = Hot Humidity = High (2)	Outlook = Sunny Temperature = Hot Humidity = High Play = No (2)
Temperature = Cool (4)	Outlook = Sunny Humidity = High (3)	Outlook = Sunny Humidity = High Windy = False (2)	Outlook = Rainy Temperature = Mild Windy = False Play = Yes (2)
…	…	…	…

- Total number of item sets with a minimum support of at least two instances: 12 one-item sets, 47 two-item sets, 39 three-item sets, 6 four-item sets and 0 five-item sets

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Generating rules from an item set

- Once all item sets with the required minimum support have been generated, we can turn them into rules
- Example 4-item set with a support of 4 instances:

```
Humidity = Normal, Windy = False, Play = Yes (4)
```

- Seven (2^N-1) potential rules:

```
If Humidity = Normal and Windy = False then Play = Yes     4/4
If Humidity = Normal and Play = Yes then Windy = False     4/6
If Windy = False and Play = Yes then Humidity = Normal     4/6
If Humidity = Normal then Windy = False and Play = Yes     4/7
If Windy = False then Humidity = Normal and Play = Yes     4/8
If Play = Yes then Humidity = Normal and Windy = False     4/9
If True then Humidity = Normal and Windy = False
   and Play = Yes                                          4/12
```

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Rules for weather data

- All rules with support > 1 and confidence = 100%:

	Association rule		Sup.	Conf.
1	Humidity=Normal Windy=False	⇒ Play=Yes	4	100%
2	Temperature=Cool	⇒ Humidity=Normal	4	100%
3	Outlook=Overcast	⇒ Play=Yes	4	100%
4	Temperature=Cold Play=Yes	⇒ Humidity=Normal	3	100%
	...	...	...	...
58	Outlook=Sunny Temperature=Hot	⇒ Humidity=High	2	100%

- In total:
  3 rules with support four
  5 with support three
  50 with support two

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Example rules from the same item set

- Item set:

```
Temperature = Cool, Humidity = Normal, Windy = False, Play = Yes (2)
```

- Resulting rules (all with 100% confidence):

```
Temperature = Cool, Windy = False ⇒ Humidity = Normal, Play = Yes
Temperature = Cool, Windy = False, Humidity = Normal ⇒ Play = Yes
Temperature = Cool, Windy = False, Play = Yes ⇒ Humidity = Normal
```

- We can establish their confidence due to the following "frequent" item sets:

```
Temperature = Cool, Windy = False                      (2)
Temperature = Cool, Humidity = Normal, Windy = False   (2)
Temperature = Cool, Windy = False, Play = Yes          (2)
```

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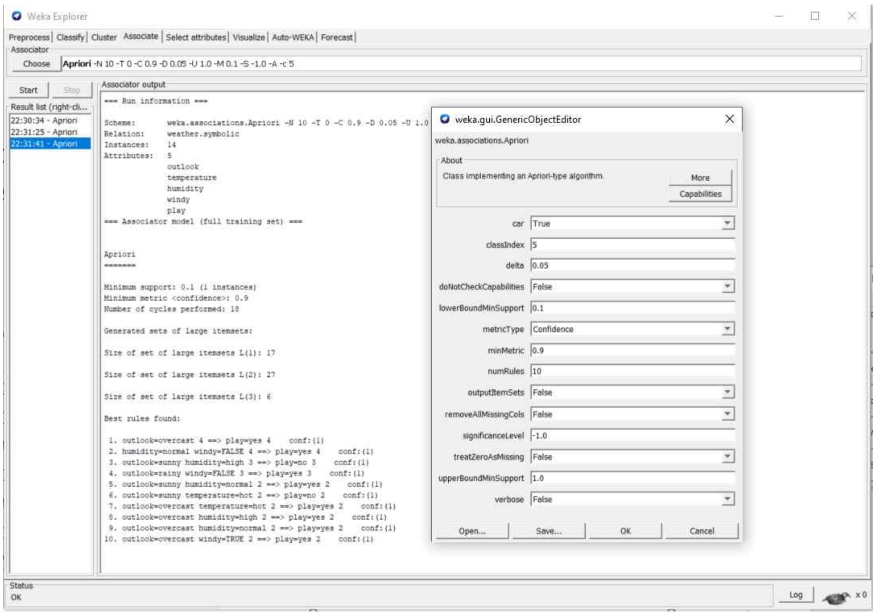
Weka Class Association Rules



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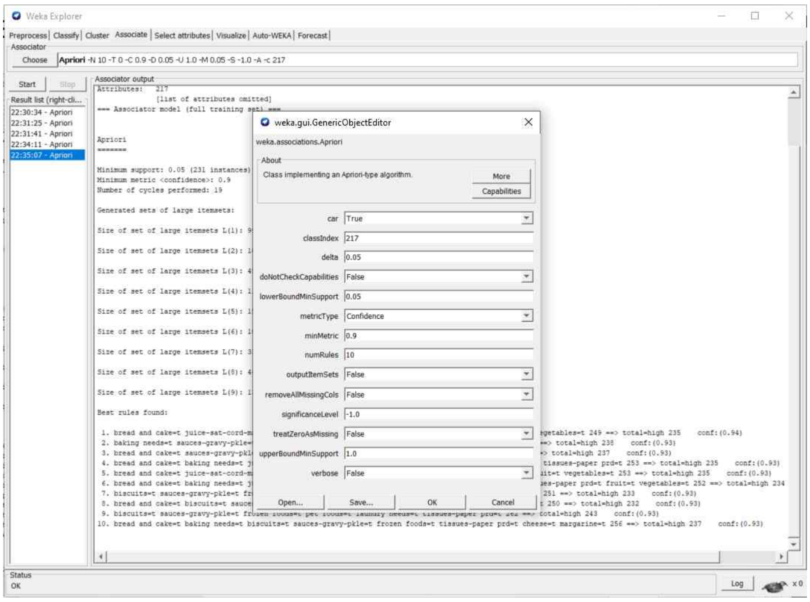
Weka Class Association Rules



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Generating item sets efficiently

- How can we efficiently find all frequent item sets?
- Finding one-item sets easy
- Idea: use one-item sets to generate two-item sets, two-item sets to generate three-item sets, …
  - If (A B) is a frequent item set, then (A) and (B) have to be frequent item sets as well!
  - In general: if X is a frequent k-item set, then all (k-1)-item subsets of X are also frequent
  - Compute k-item sets by merging (k-1)-item sets

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Example

- Given: five frequent three-item sets

  (A B C), (A B D), (A C D), (A C E), (B C D)
- Lexicographically ordered!
- Candidate four-item sets:

(A B C D)	**OK because of (A C D) (B C D) (A B C)**
(A C D E)	**Not OK because of (C D E)**

- To establish that these item sets are really frequent, we need to perform a final check by counting instances
- For fast look-up, the (k –1)-item sets are stored in a hash table

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Algorithm for finding item sets

```
Set k to 1
Find all k-item sets with sufficient coverage and store them in hash table #1
While some k-item sets with sufficient coverage have been found
    Increment k
    Find all pairs of (k-1)-item sets in hash table #(k-1) that differ only in
    their last item
    Create a k-item set for each pair by combining the two (k-1)-item sets
    that are paired
    Remove all k-item sets containing any (k-1)-item sets that are not in the
    #(k-1)hash table
    Scan the data and remove all remaining k-item sets that do not have
    sufficient coverage
    Store the remaining k-item sets and their coverage in hash table #k,
    sorting items in lexical order
```

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Association rules: discussion

- Above method makes one pass through the data for each different item set size
  - Another possibility: generate (k+2)-item sets just after (k+1)-item sets have been generated
  - Result: more candidate (k+2)-item sets than necessary will be generated but this requires less passes through the data
  - Makes sense if data too large for main memory
- Practical issue: support level for generating a certain minimum number of rules for a particular dataset
  - This can be done by running the whole algorithm multiple times with different minimum support levels
  - Support level is decreased until a sufficient number of rules has been found

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Linear models: linear regression

- Work most naturally with numeric attributes
- Standard technique for numeric prediction
  - Outcome is linear combination of attributes

  $x = w_0 + w_1 a_1 + w_2 a_2 + \cdots + w_k a_k$
- Weights are calculated from the training data
- Predicted value for first training instance $\mathbf{a}^{(1)}$

  $$w_0 a_0^{(1)} + w_1 a_1^{(1)} + w_2 a_2^{(1)} + \cdots + w_k a_k^{(1)} = \sum_{j=0}^{k} w_j a_j^{(1)}$$

(assuming each instance is extended with a constant attribute with value 1)

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Minimizing the squared error

- Choose k +1 coefficients to minimize the squared error on the training data
- Squared error: $$\sum_{i=1}^{n} \left(x^{(i)} - \sum_{j=0}^{k} w_j a_j^{(i)} \right)^2$$
- Coefficients can be derived using standard matrix operations
- Can be done if there are more instances than attributes (roughly speaking)
- Minimizing the *absolute error* is more difficult

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Classification

- *Any* regression technique can be used for classification
  - Training: perform a regression for each class, setting the output to 1 for training instances that belong to class, and 0 for those that don't
  - Prediction: predict class corresponding to model with largest output value (*membership value*)
- For linear regression this method is also known as *multi-response linear regression*
- Problem: membership values are not in the [0,1] range, so they cannot be considered proper probability estimates
  - In practice, they are often simply clipped into the [0,1] range and normalized to sum to 1

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Linear models: logistic regression

- Can we do better than using linear regression for classification?
- Yes, we can, by applying logistic regression
- Logistic regression builds a linear model for a transformed target variable
- Assume we have two classes
- Logistic regression replaces the target (probability)

$$\Pr[1|a_1, a_2, \ldots, a_k]$$

by this target (odds)

$$\log[\Pr[1|a_1, a_2, \ldots, a_k]/(1 - \Pr[1|a_1, a_2, \ldots, a_k])$$

- This *logit transformation* maps [0,1] to (-∞ , +∞), i.e., the new target values are no longer restricted to the [0,1] interval

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Logistic regression explained

TABLE 3.1: Current Use of Contraception Among Married Women by Age, Education and Desire for More Children Fiji Fertility Survey, 1975

Age	Education	Desires More Children?	Contraceptive Use No	Contraceptive Use Yes	Total
<25	Lower	Yes	53	6	59
		No	10	4	14
	Upper	Yes	212	52	264
		No	50	10	60
25–29	Lower	Yes	60	14	74
		No	19	10	29
	Upper	Yes	155	54	209
		No	65	27	92
30–39	Lower	Yes	112	33	145
		No	77	80	157
	Upper	Yes	118	46	164
		No	68	78	146
40–49	Lower	Yes	35	6	41
		No	46	48	94
	Upper	Yes	8	8	16
		No	12	31	43
Total			1100	507	1607

- In the contraceptive use data there are 507 users of contraception among 1607 women.
- So we estimate the probability as 507/1607 = 0.316.
- The odds are 507/1100 or 0.461 to one, so non-users outnumber users roughly two to one.
- The logit is log(0.461) = −0.775.

See for details: https://data.princeton.edu/wws509/notes/c3.pdf

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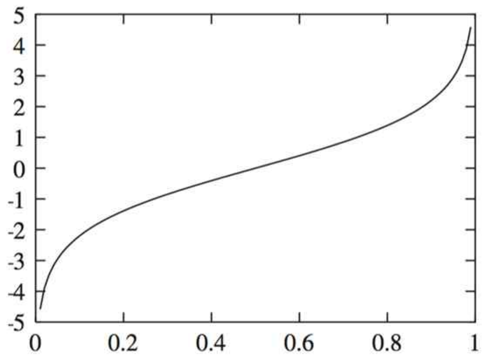
Logit transformation



- Resulting class probability model:

$$\Pr[1|a_1, a_2, \ldots, a_k] = 1/(1 + \exp(-w_0 - w_1 a_1 - \cdots - w_k a_k))$$

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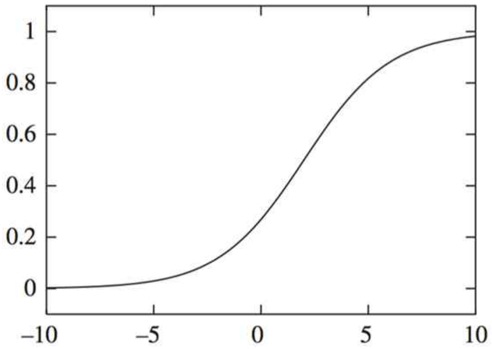
Example logistic regression model

- Model with w_0 = -1.25 and w_1 = 0.5:



- Parameters are found from training data using *maximum likelihood*

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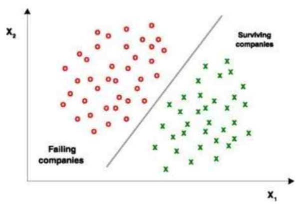
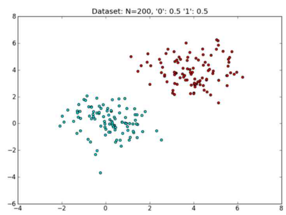
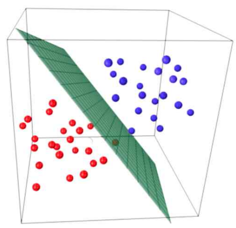
Linearly separable data

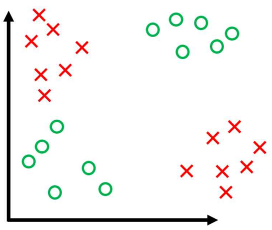
- A dataset is said to be linearly separable if it is possible to draw a line that can separate points belonging to different classes from each other.

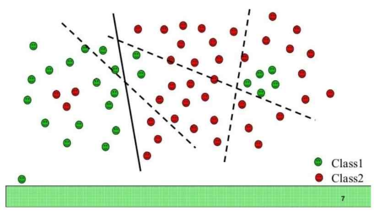






- Linearly non-separable data:





Illustrative figures taken from:
https://www.commonlounge.com/discussion/6caf49570d9c4d0789afbc544b32cdbf

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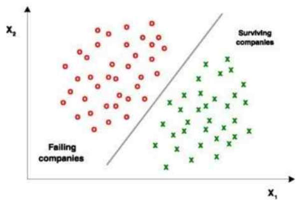
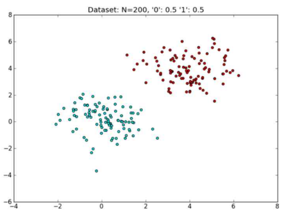
Linearly separable data

- A dataset is said to be linearly separable if it is possible to draw a line that can separate points belonging to different classes from each other.





Algebraic definition:

- Algebraically, the separator is a linear function, i.e. if data point x is given by (x1, x2), when the separator is a function f(x) = w1*x1 + w2*x2 + b
- All points for which f(x) = 0, are on the separator line. All points for which f(x) > 0 are on one side of the line, and all points for which f(x) < 0 are on the other side.

Illustrative figures taken from:
https://www.commonlounge.com/discussion/6caf49570d9c4d0789afbc544b32cdbf 73

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Linear models are hyperplanes

- Decision boundary for two-class logistic regression is where probability equals 0.5:

$$\Pr[1|a_1, a_2, \ldots, a_k] = 1/(1 + \exp(-w_0 - w_1a_1 - \cdots - w_ka_k)) = 0.5$$

  which occurs when $-w_0 - w_1a_1 - \cdots - w_ka_k = 0.$

- Thus logistic regression can only separate data that can be separated by a hyperplane

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Maximum likelihood

- Aim: maximize probability of observed training data with respect to final parameters of the logistic regression model
- We can use logarithms of probabilities and maximize conditional *log-likelihood* instead of product of probabilities:

$$\sum_{i=1}^{n}(1-x^{(i)})\log(1-\Pr[1|a_1^{(i)}, a_2^{(i)}, \ldots, a_k^{(i)}]) + x^{(i)}\log(\Pr[1|a_1^{(i)}, a_2^{(i)}, \ldots, a_k^{(i)}])$$

  where the class values $x^{(i)}$ are either 0 or 1
- Weights w_i need to be chosen to maximize log-likelihood
- A relatively simple method to do this is *iteratively re-weighted least squares* but other optimization methods can be used

Illustrative example: https://machinelearningmastery.com/logistic-regression-with-maximum-likelihood-estimation/
Also see: https://www.youtube.com/watch?v=inVuoCE3-Wk

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Linear models: the perceptron

- Observation: we do not actually need probability estimates if all we want to do is classification
- Different approach: learn separating hyperplane directly
- Let us assume the data is *linearly separable*
- In that case there is a simple algorithm for learning a separating hyperplane called the *perceptron learning rule*
- Hyperplane: $w_0a_0 + w_1a_1 + w_2a_2 + \cdots + w_ka_k = 0$
  where we again assume that there is a constant attribute with value 1 (*bias*)
- If the weighted sum is greater than zero we predict the first class, otherwise the second class

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The algorithm

```
Set all weights to zero
Until all instances in the training data are classified correctly
  For each instance I in the training data
    If I is classified incorrectly by the perceptron
      If I belongs to the first class add it to the weight vector
      else subtract it from the weight vector
```

- Why does this work?
  Consider a situation where an instance *a* pertaining to the first class has been added:

$$(w_0 + a_0)a_0 + (w_1 + a_1)a_1 + (w_2 + a_2)a_2 + \cdots + (w_k + a_k)a_k$$

  This means the output for *a* has increased by:

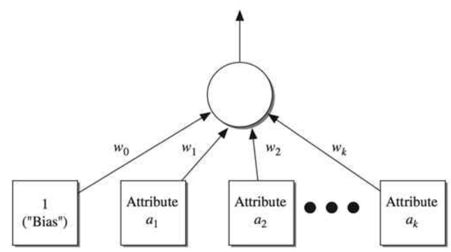
$$a_0 \times a_0 + a_1 \times a_1 + a_2 \times a_2 + \cdots + a_k \times a_k$$

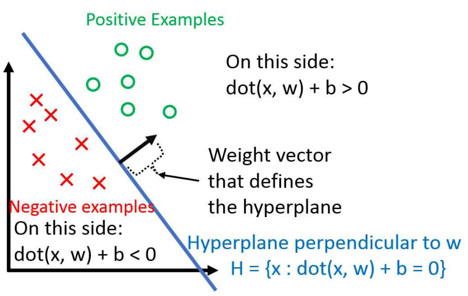
  This number is always positive, thus the hyperplane has moved into the correct direction (and we can show that output decreases for instances of other class)
- It can be shown that this process converges to a linear separator if the data is linearly separable

Perceptron as a neural network

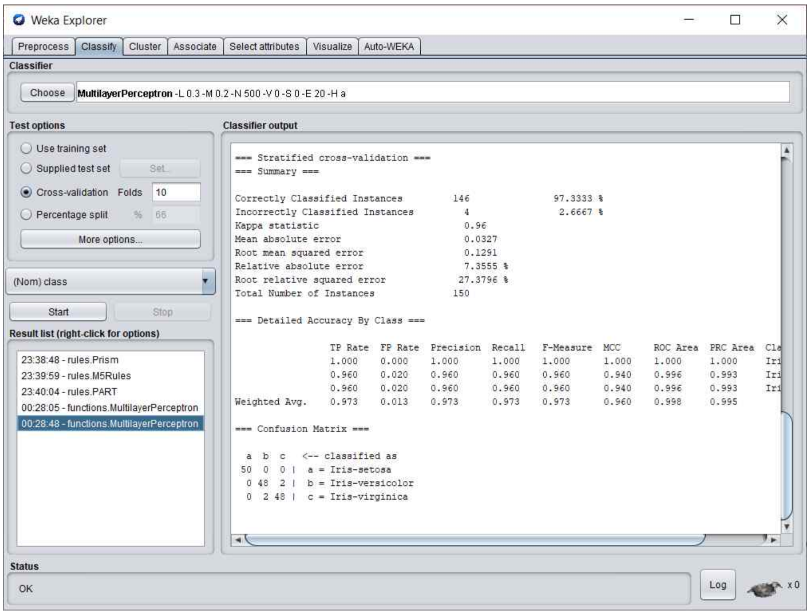
Output layer

Input layer





Multilayer Perceptron as a neural network – IRIS dataset



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Clustering

- Clustering techniques apply when there is no class to be predicted: they perform unsupervised learning
- Aim: divide instances into “natural” groups
- As we have seen, clusters can be:
  - disjoint vs. overlapping
  - deterministic vs. probabilistic
  - flat vs. hierarchical
- We will look at a classic clustering algorithm called *k-means*
- *k-means* clusters are disjoint, deterministic, and flat

Euclidian distance formula: $d_{euc}(x,y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$

Manhattan distance formula: $d_{man}(x,y) = \sum_{i=1}^{n}|(x_i - y_i)|$

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The *k*-means algorithm

- Step 1: Choose *k* random cluster centers
- Step 2: Assign each instance to its closest cluster center based on Euclidean distance
- Step 3: Recompute cluster centers by computing the average (aka *centroid*) of the instances pertaining to each cluster
- Step 4: If cluster centers have moved, go back to Step 2
- This algorithm minimizes the squared Euclidean distance of the instances from their corresponding cluster centers
  - Determines a solution that achieves a *local* minimum of the squared Euclidean distance
- Equivalent termination criterion: stop when assignment of instances to cluster centers has not changed

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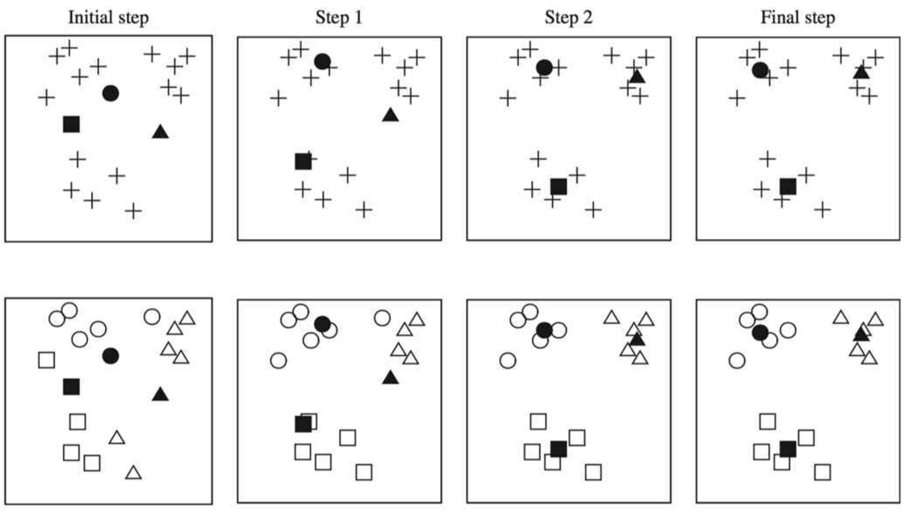
The *k*-means algorithm: example



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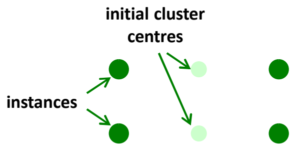
Discussion

- Algorithm minimizes squared distance to cluster centers
- Result can vary significantly
  - based on initial choice of seeds
- Can get trapped in local minimum
  - Example:



- To increase chance of finding global optimum: restart with different random seeds
- Can be applied recursively with *k* = 2

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Hierarchical clustering

- Bisecting *k*-means performs hierarchical clustering in a top-down manner
- Standard hierarchical clustering performs clustering in a bottom-up manner; it performs *agglomerative* clustering:
  - First, make each instance in the dataset into a trivial mini-cluster
  - Then, find the two closest clusters and merge them; repeat
  - Clustering stops when all clusters have been merged into a single cluster
- Outcome is determined by the distance function that is used:
  - *Single-linkage* clustering: distance of two clusters is measured by finding the two closest instances, one from each cluster, and taking their distance
  - *Complete-linkage* clustering*:* use the two most distant instances instead
  - *Average-linkage* clustering: take average distance between all instances
  - *Centroid-linkage* clustering: take distance of cluster centroids
  - *Group-average* clustering: take average distance in merged clusters
  - *Ward's method*: optimize *k-means* criterion (i.e., squared distance)

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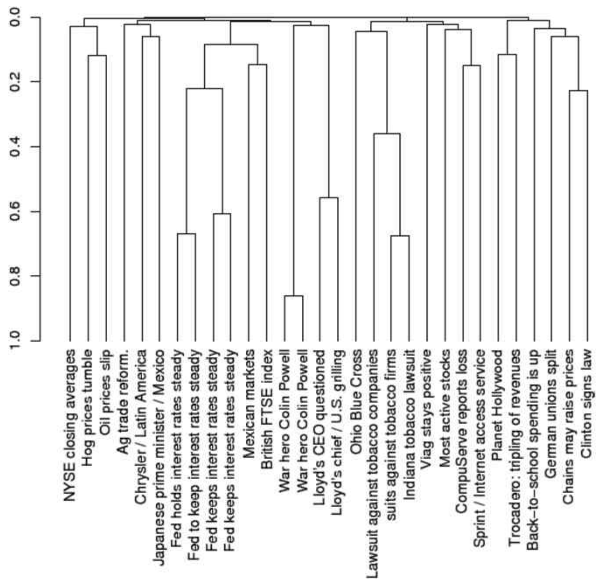
Example: hierarchical clustering



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Incremental clustering

- Heuristic approach (COBWEB/CLASSIT)
- Forms a hierarchy of clusters incrementally
- Start:
  - tree consists of empty root node
- Then:
  - add instances one by one
  - update tree appropriately at each stage
  - to update, find the right leaf for an instance
  - may involve restructuring the tree using *merging* or *splitting* of nodes
- Update decisions are based on a goodness measure called *category utility*

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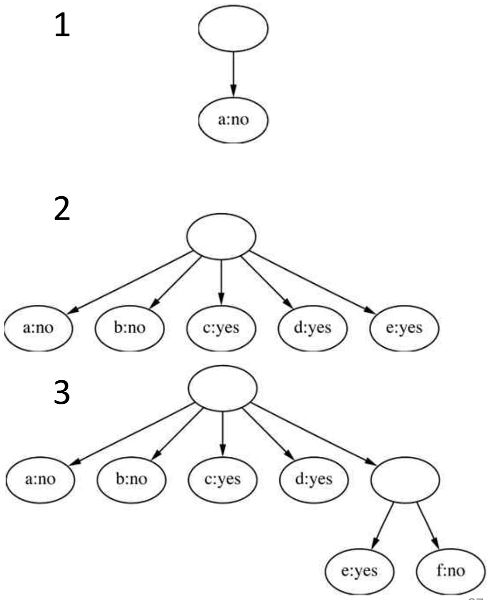
Clustering the weather data I

ID	Outlook	Temp.	Humidity	Windy
A	Sunny	Hot	High	False
B	Sunny	Hot	High	True
C	Overcast	Hot	High	False
D	Rainy	Mild	High	False
E	Rainy	Cool	Normal	False
F	Rainy	Cool	Normal	True
G	Overcast	Cool	Normal	True
H	Sunny	Mild	High	False
I	Sunny	Cool	Normal	False
J	Rainy	Mild	Normal	False
K	Sunny	Mild	Normal	True
L	Overcast	Mild	High	True
M	Overcast	Hot	Normal	False
N	Rainy	Mild	High	True



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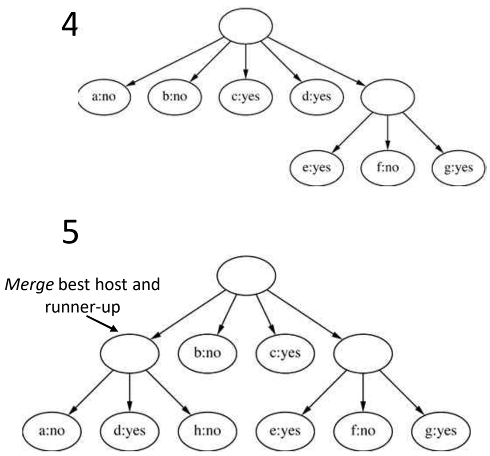
Clustering the weather data II

ID	Outlook	Temp.	Humidity	Windy
A	Sunny	Hot	High	False
B	Sunny	Hot	High	True
C	Overcast	Hot	High	False
D	Rainy	Mild	High	False
E	Rainy	Cool	Normal	False
F	Rainy	Cool	Normal	True
G	Overcast	Cool	Normal	True
H	Sunny	Mild	High	False
I	Sunny	Cool	Normal	False
J	Rainy	Mild	Normal	False
K	Sunny	Mild	Normal	True
L	Overcast	Mild	High	True
M	Overcast	Hot	Normal	False
N	Rainy	Mild	High	True



Consider *splitting* the best host if merging does not help

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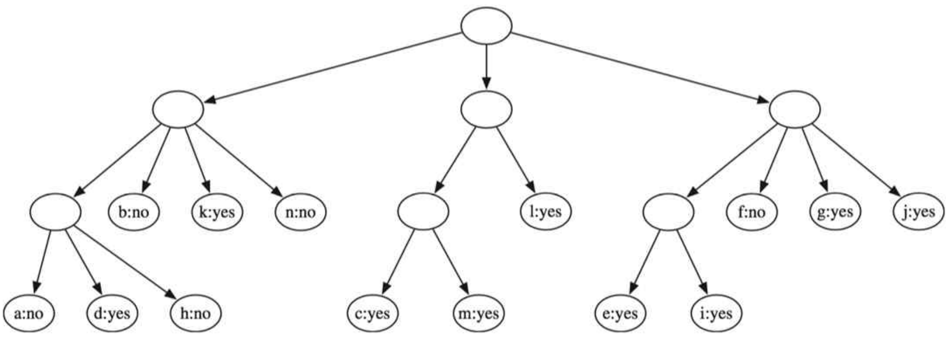
Final clustering



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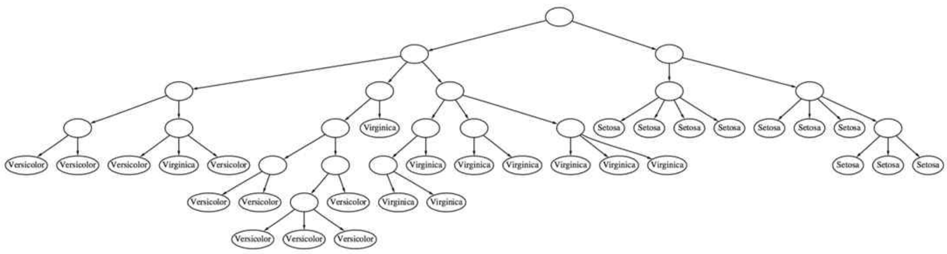
Example: clustering a subset of the iris data



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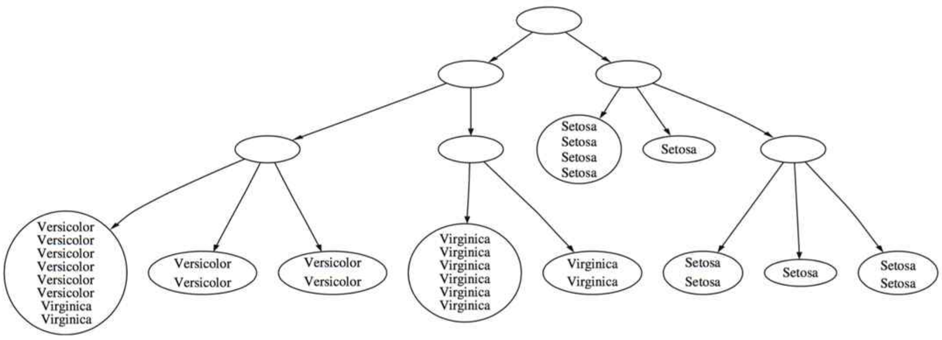
Example: iris data with cutoff



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Some final comments on the basic methods

- Bayes' rule stems from his "Essay towards solving a problem in the doctrine of chances" (1763)
  - Difficult bit in general: estimating prior probabilities (easy in the case of naïve Bayes)
- Extension of naïve Bayes: Bayesian networks (which we will discuss later)
- The algorithm for association rules we discussed is called APRIORI; many other algorithms exist
- Minsky and Papert (1969) showed that linear classifiers have limitations, e.g., can't learn a logical XOR of two attributes
  - But: combinations of them can (this yields multi-layer neural nets)

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