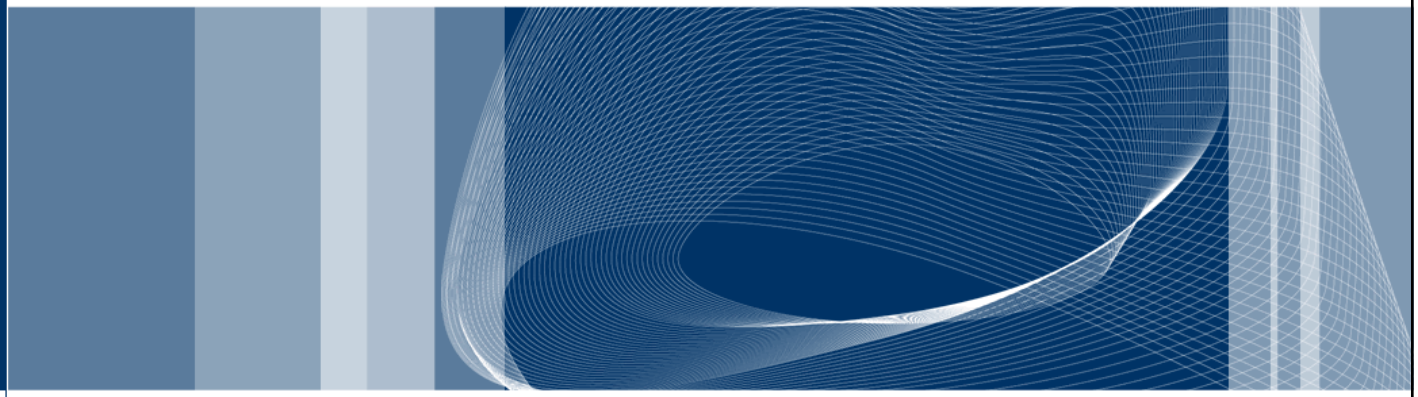
POLITECNICO DI MILANO



Naïve Bayes, KNN, and Other Approaches

Data Mining and Text Mining (UIC 583 @ Politecnico di Milano)

Prof. Pier Luca Lanzi

Study Material

- Mining of Massive Datasets Section 12.3, 12.4
- Data Mining and Analysis: Fundamental Concepts and Algorithms - Chapter 18 & 19
- Chapter 4 of Data Mining, Fourth Edition: Practical Machine Learning Tools and Techniques - Ian H. Witten et al.

Naïve Bayes

Bayes Probability

- Conditional Probability:

$$P(C|A) = \frac{P(A \wedge C)}{P(A)} \qquad P(A|C) = \frac{P(A \wedge C)}{P(C)}$$

- Bayes theorem,

$$P(C|A) = \frac{P(A|C)P(C)}{P(A)}$$

- A priori probability of C, P(C), is the probability of event before evidence is seen
- A posteriori probability of C, P(C|A), is the probability of event after evidence is seen

Naïve Bayes Classifiers

- What's the probability of the class given an example?
- An example is represented as a tuple of attributes

$$\vec{x} = \langle x_1, \ldots, x_n \rangle$$

- Given the target y (identifying the class value for the instance) we are looking for the class with the highest probability for X

$$class = \arg\max_y P(y|\vec{x})$$

Naïve Bayes Classifiers

- Given the target y and the example x described by n attributes, Bayes Theorem says that

$$P(y|\vec{x}) = \frac{P(\vec{x}|y)P(y)}{P(\vec{x})}$$

- Naïve Bayes classifiers assume that attributes are statistically independent

- Thus, evidence splits into parts that are independent

$$P(y|\vec{x}) = \frac{P(x_1|y)\cdots P(x_n|y)P(y)}{P(\vec{x})}$$

Naïve Bayes for Classification

- Training
  - Computes the class probability P(H) and the conditional probability $P(e_i|H)$ for each attribute value e_i and each class value H
- Testing
  - Given an example E, computes the class as

$$class = \arg\max_y P(y|\vec{x})$$

$$= \arg\max_y \frac{P(x_1|y)\cdots P(x_n|y)P(y)}{P(\vec{x})}$$

$$= \arg\max_y P(x_1|y)\cdots P(x_n|y)P(y)$$

Naïve Bayes Classifier

- Two assumptions
  - Attributes are equally important
  - Attribute are statistically independent

- Statistically independent means that knowing the value of one attribute says nothing about the value of another (if the class is known)

- Independence assumption is almost never correct! But the scheme works well in practice

The Weather Dataset

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

Computing Probabilities

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	Cool	High	True	?

What is the assigned class?

Using the Probabilities for Classification

Outlook	Temp.	Humidity	Windy	Play
Sunny	Cool	High	True	?

$$
\begin{aligned}
P(yes|E) &= P(Sunny|yes)P(Cool|yes)P(High|yes)P(True|yes)P(yes) \\
&= \frac{2}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{9}{14} \\
&= 0.0053
\end{aligned}
$$

$$
\begin{aligned}
P(no|E) &= P(Sunny|no)P(Cool|no)P(High|no)P(True|no)P(no) \\
&= \frac{3}{5} \times \frac{1}{5} \times \frac{4}{5} \times \frac{3}{5} \times \frac{5}{14} \\
&= 0.0206
\end{aligned}
$$

- Conversion into a probability by normalization:

$$
\begin{aligned}
P(yes) &= 0.0053/(0.0053 + 0.0206) = 0.205 \\
P(no) &= 0.0206/(0.0053 + 0.0206) = 0.795
\end{aligned}
$$

The "Zero-Frequency Problem"

- What if an attribute value does not occur with every class value? (for instance, "Humidity = high" for class "yes")
- The corresponding probability will be zero,

$$P(Humidity = high|yes) = 0$$

- A posteriori probability will also be zero!
(No matter how likely the other values are!)

$$P(yes|\langle \ldots,\ Humidity = high,\ \ldots\rangle) = 0$$

- The typical remedy is to add 1 to the count for every attribute value-class combination (Laplace estimator)
- The probabilities will never be zero! (also: stabilizes probability estimates)

Modified Probability Estimates

- Sometimes, adding a constant different from one might be more appropriate; for example, we can add the same μ/3 to each count

$$\frac{2+\mu/3}{9+\mu} \qquad \frac{4+\mu/3}{9+\mu} \qquad \frac{3+\mu/3}{9+\mu}$$

Sunny Overcast Rainy

- Or different weights to each count

$$\frac{2+\mu p_1}{9+\mu} \qquad \frac{4+\mu p_2}{9+\mu} \qquad \frac{3+\mu p_3}{9+\mu}$$

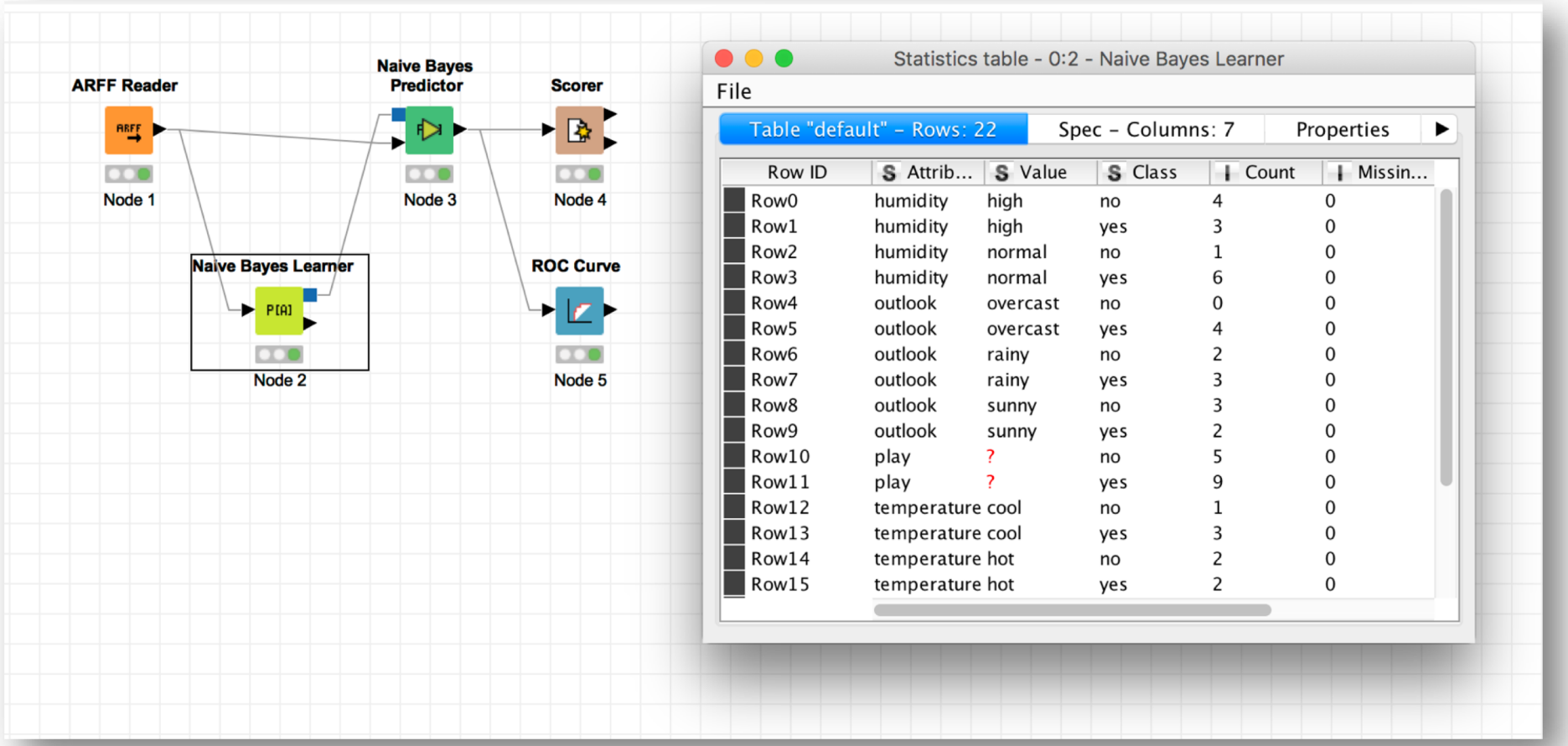
- Weights don't need to be equal (but they must sum to 1)

Missing Values

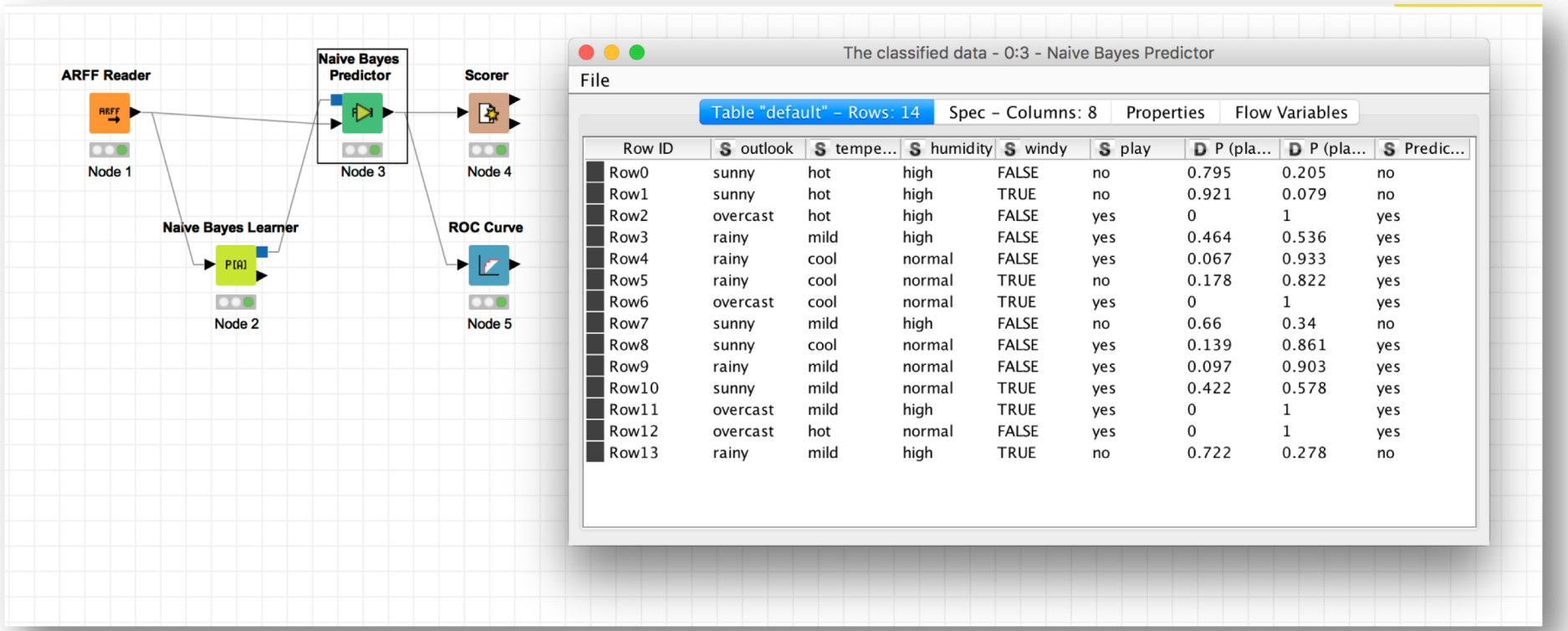
- Training
  - Instance is not included in frequency count for attribute value-class combination
- Testing
  - The attribute will be omitted from calculation

Outlook	Temperature	Humidity	Windy	Play
?	Cool	High	True	?

Likelihood of "yes" = 3/9 x 3/9 x 3/9 x 9/14 = 0.0238
Likelihood of "no" = 1/5 x 4/5 x 3/5 x 5/14 = 0.0343
P("yes") = 0.0238 / (0.0238 + 0.0343) = 41%
P("no") = 0.0343 / (0.0238 + 0.0343) = 59%



Example of Naïve Bayes using KNIME



Row ID	outlook	tempe...	humidity	windy	play	P (pla...	P (pla...	Predic...
Row0	sunny	hot	high	FALSE	no	0.795	0.205	no
Row1	sunny	hot	high	TRUE	no	0.921	0.079	no
Row2	overcast	hot	high	FALSE	yes	0	1	yes
Row3	rainy	mild	high	FALSE	yes	0.464	0.536	yes
Row4	rainy	cool	normal	FALSE	yes	0.067	0.933	yes
Row5	rainy	cool	normal	TRUE	no	0.178	0.822	yes
Row6	overcast	cool	normal	TRUE	yes	0	1	yes
Row7	sunny	mild	high	FALSE	no	0.66	0.34	no
Row8	sunny	cool	normal	FALSE	yes	0.139	0.861	yes
Row9	rainy	mild	normal	FALSE	yes	0.097	0.903	yes
Row10	sunny	mild	normal	TRUE	yes	0.422	0.578	yes
Row11	overcast	mild	high	TRUE	yes	0	1	yes
Row12	overcast	hot	normal	FALSE	yes	0	1	yes
Row13	rainy	mild	high	TRUE	no	0.722	0.278	no

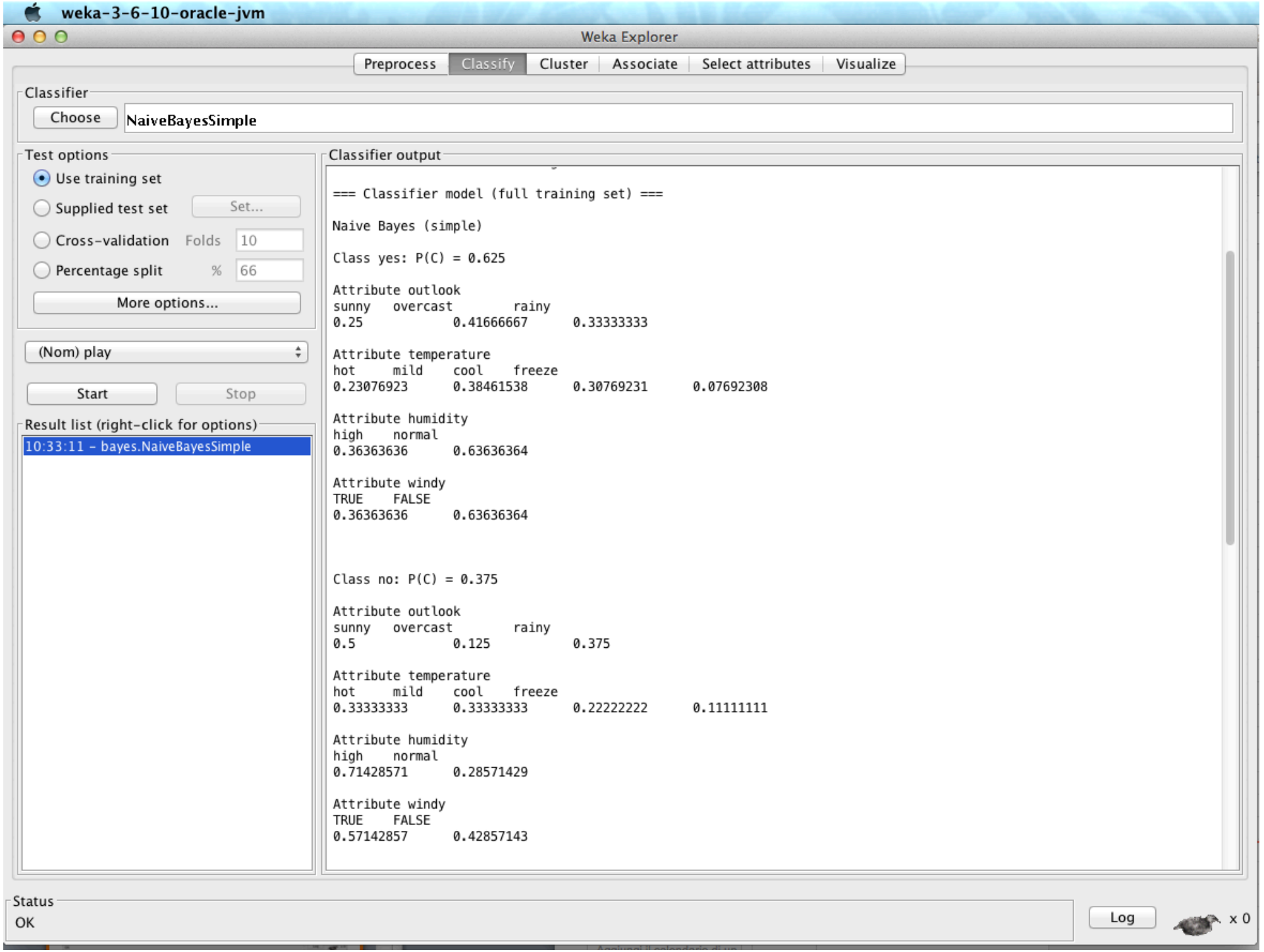
Example of Naïve Bayes using KNIME

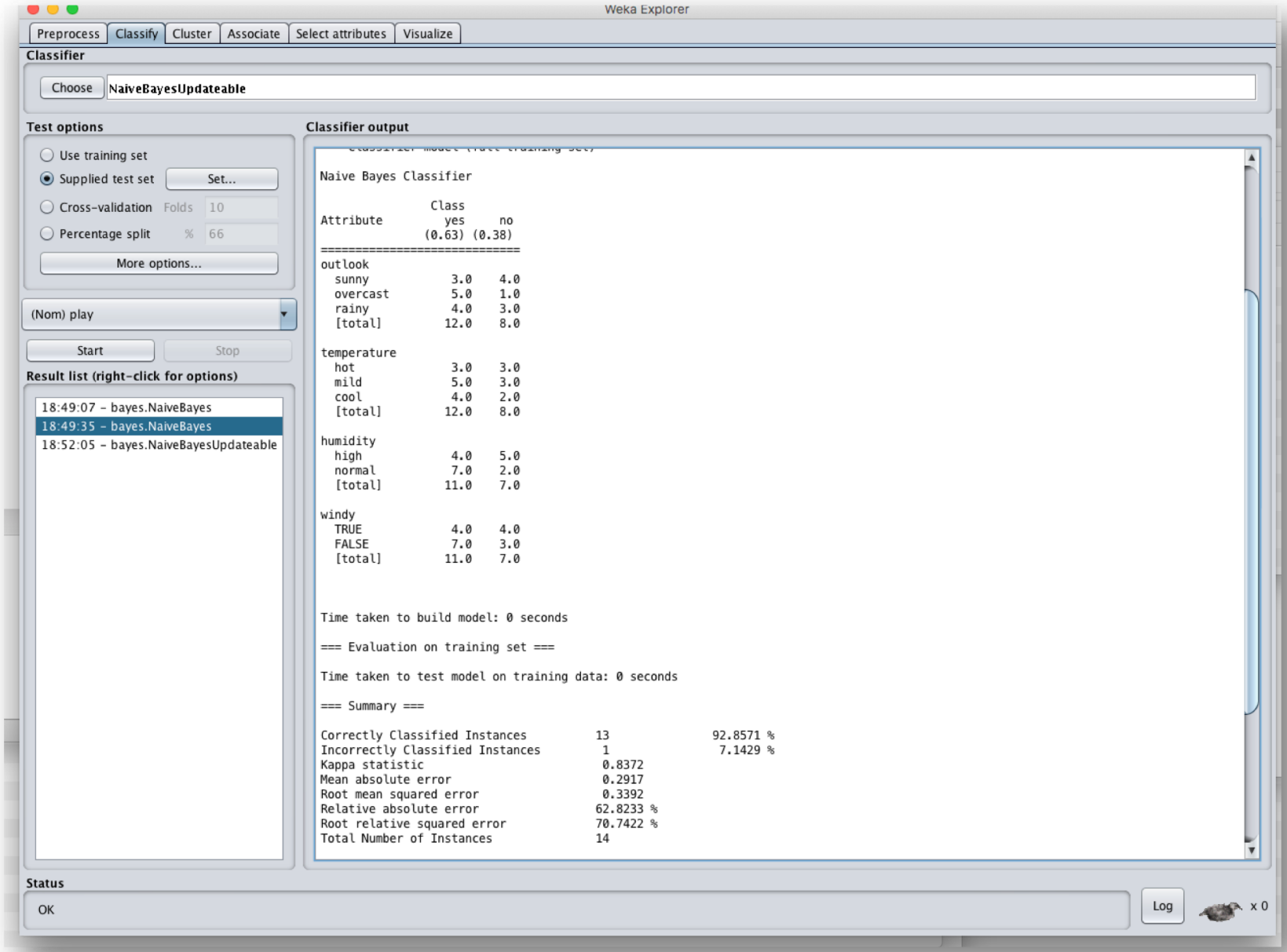
Another Version of the Weather Data


```
@relation weather.symbolic

@attribute outlook {sunny, overcast, rainy}
@attribute temperature {hot, mild, cool, freeze}
@attribute humidity {high, normal}
@attribute windy {TRUE, FALSE}
@attribute play {yes, no}

@data
sunny,hot,high,FALSE,no
sunny,hot,high,TRUE,no
...
```


weka-3-6-10-oracle-jvm
Weka Explorer
Preprocess
Classify
Cluster
Associate
Select attributes
Visualize
Classifier
Choose
NaiveBayesSimple
Test options
Use training set
Supplied test set
Set...
Cross-validation
Folds
10
Percentage split
%
66
More options...
(Nom) play
Start
Stop
Result list (right-click for options)
10:33:11 - bayes.NaiveBayesSimple
Classifier output
=== Classifier model (full training set) ===
Naive Bayes (simple)
Class yes: P(C) = 0.625
Attribute outlook
sunny overcast rainy
0.25 0.41666667 0.33333333
Attribute temperature
hot mild cool freeze
0.23076923 0.38461538 0.30769231 0.07692308
Attribute humidity
high normal
0.36363636 0.63636364
Attribute windy
TRUE FALSE
0.36363636 0.63636364
Class no: P(C) = 0.375
Attribute outlook
sunny overcast rainy
0.5 0.125 0.375
Attribute temperature
hot mild cool freeze
0.33333333 0.33333333 0.22222222 0.11111111
Attribute humidity
high normal
0.71428571 0.28571429
Attribute windy
TRUE FALSE
0.57142857 0.42857143
Status
OK
Log
x 0



Example of Naïve Bayes with Laplace Estimator

Numeric Attributes

- We assume that the attributes have a normal or Gaussian probability distribution (given the class)
- The probability density function for the normal distribution is defined by two parameters, the mean and the standard deviation
- Sample mean,

$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$$

- Standard deviation,

$$\sigma = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \mu)^2$$

- Then the density function f(x) is

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

Statistics for Weather data with numeric temperature

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									

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

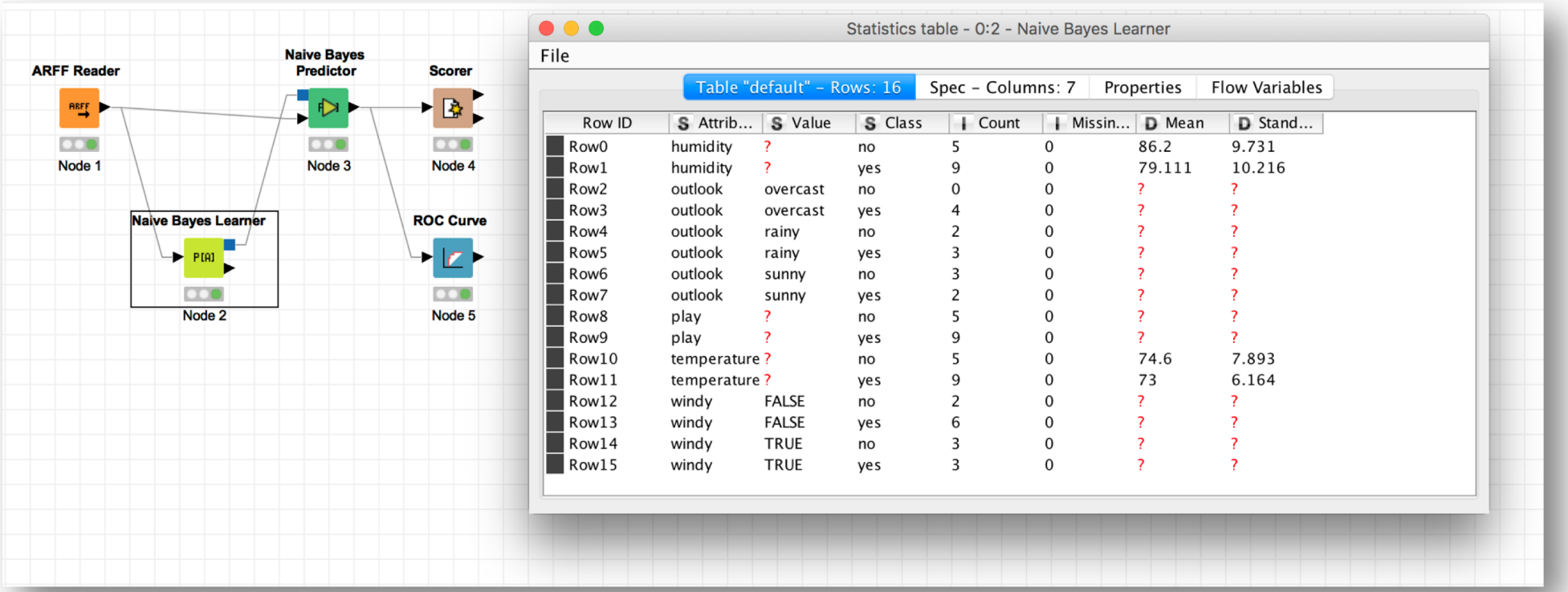
Classifying a new day

- A new day,

Outlook	Temperature	Humidity	Windy	Play
Sunny	66	90	true	?

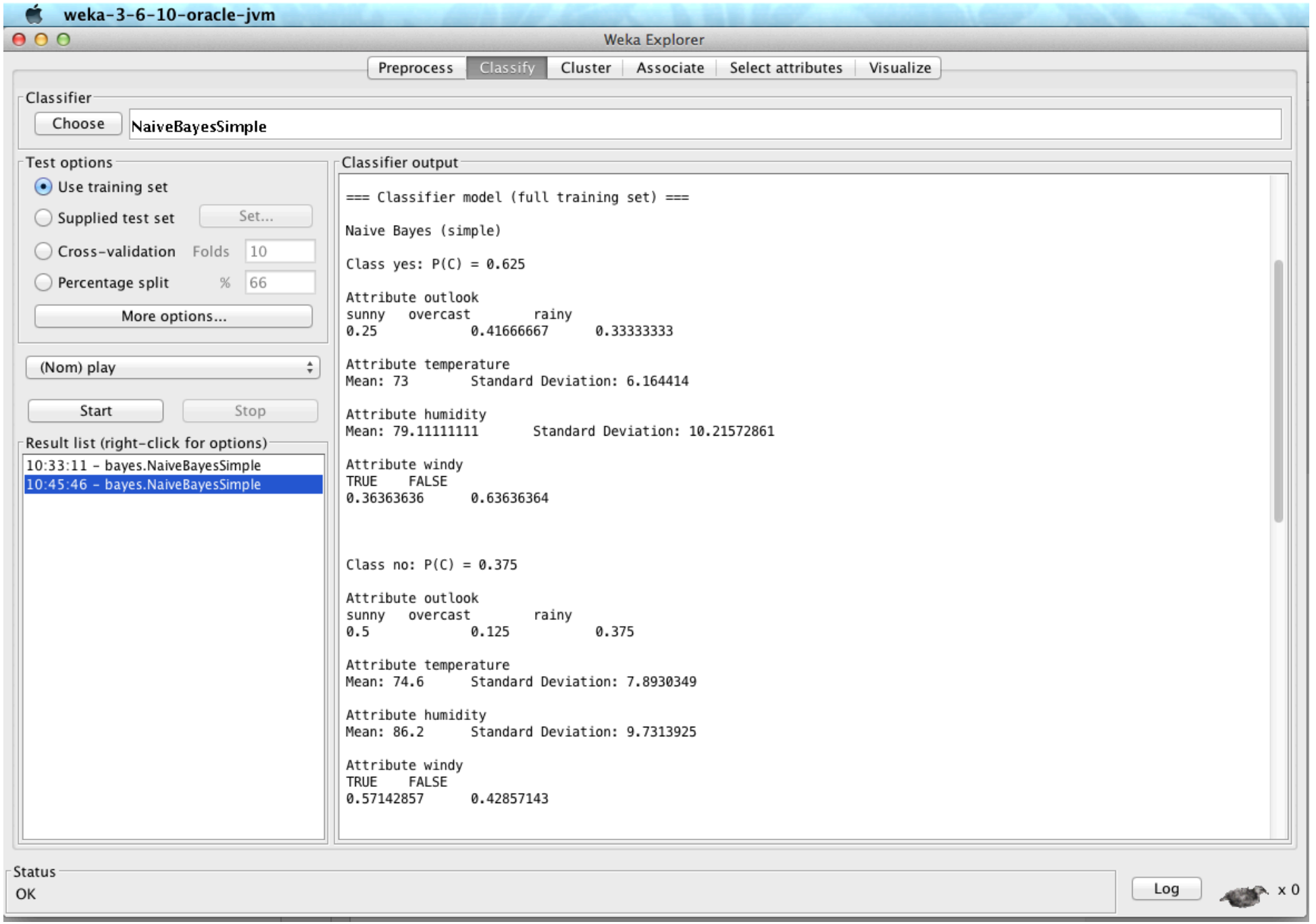
- Missing values during training are not included in calculation of mean and standard deviation

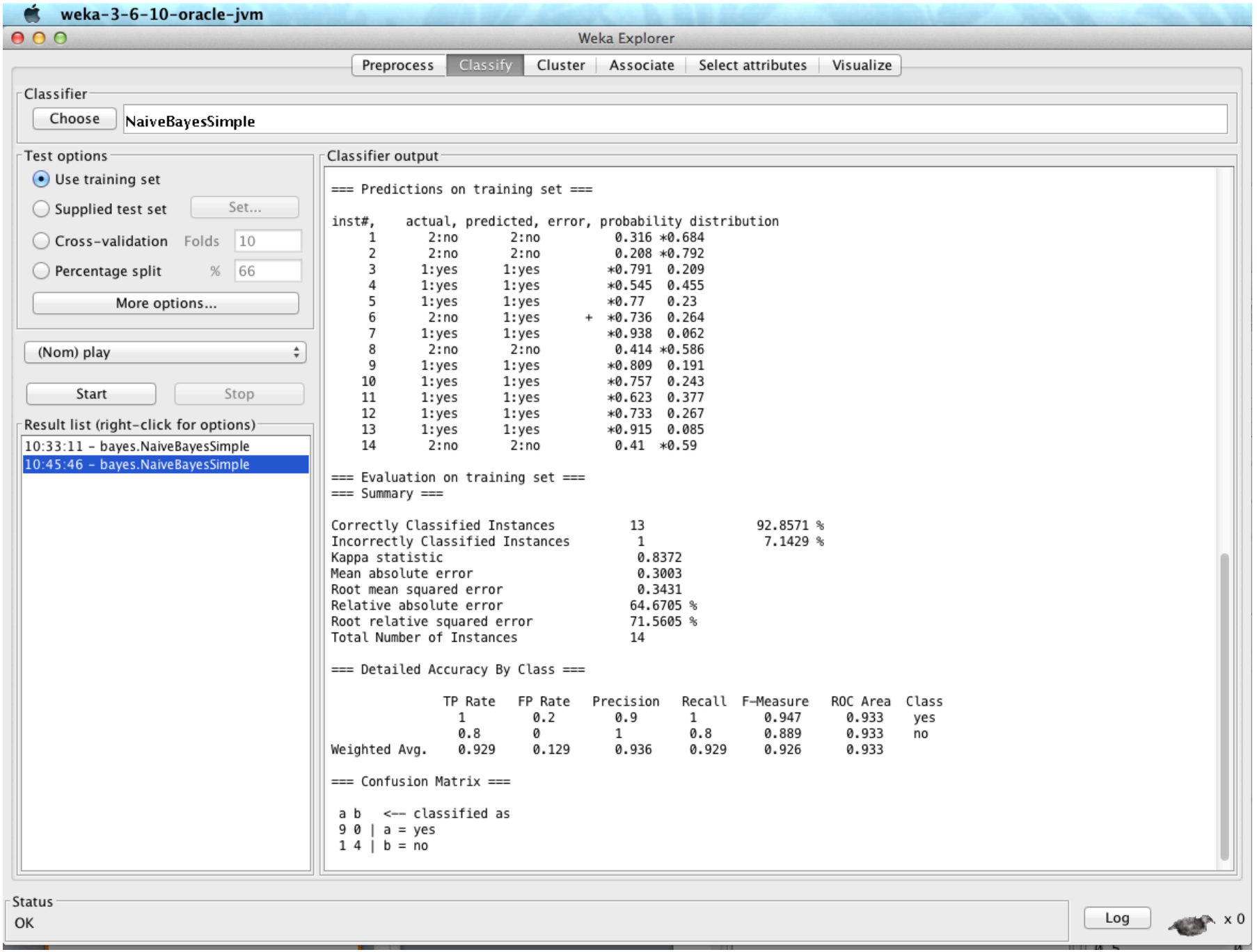
Likelihood of "yes" = 2/9 x 0.0340 x 0.0221 x 3/9 x 9/14 = 0.000036
Likelihood of "no" = 3/5 x 0.0291 x 0.0380 x 3/5 x 5/14 = 0.000136
P("yes") = 0.000036 / (0.000036 + 0. 000136) = 20.9%
P("no") = 0.000136 / (0.000036 + 0. 000136) = 79.1%



Row ID	Attrib...	Value	Class	Count	Missin...	Mean	Stand...
Row0	humidity	?	no	5	0	86.2	9.731
Row1	humidity	?	yes	9	0	79.111	10.216
Row2	outlook	overcast	no	0	0	?	?
Row3	outlook	overcast	yes	4	0	?	?
Row4	outlook	rainy	no	2	0	?	?
Row5	outlook	rainy	yes	3	0	?	?
Row6	outlook	sunny	no	3	0	?	?
Row7	outlook	sunny	yes	2	0	?	?
Row8	play	?	no	5	0	?	?
Row9	play	?	yes	9	0	?	?
Row10	temperature	?	no	5	0	74.6	7.893
Row11	temperature	?	yes	9	0	73	6.164
Row12	windy	FALSE	no	2	0	?	?
Row13	windy	FALSE	yes	6	0	?	?
Row14	windy	TRUE	no	3	0	?	?
Row15	windy	TRUE	yes	3	0	?	?

Example of Naïve Bayes with nominal and continuous attributes using KNIME

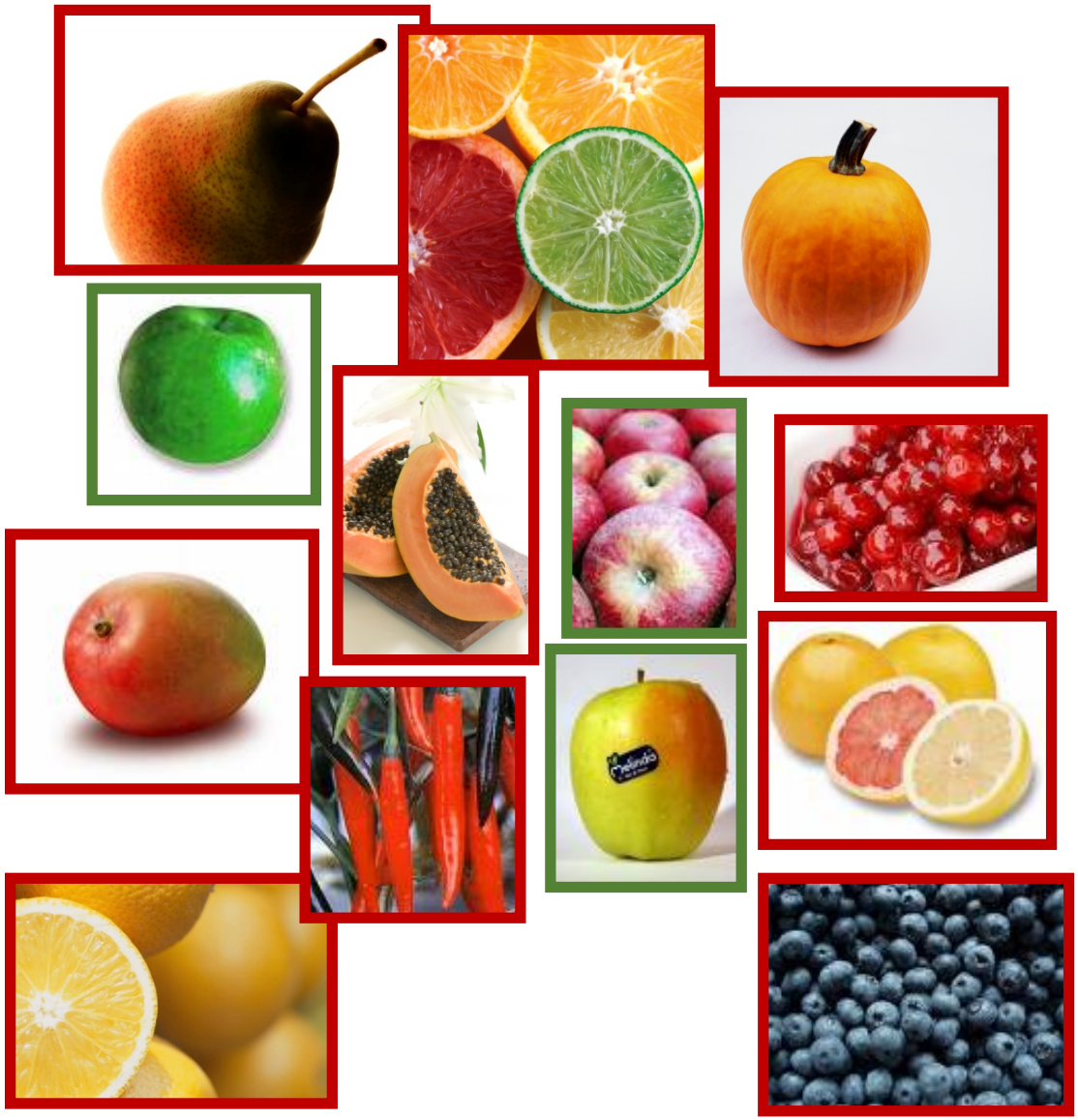

weka-3-6-10-oracle-jvm
Weka Explorer
Preprocess
Classify
Cluster
Associate
Select attributes
Visualize
Classifier
Choose
NaiveBayesSimple
Test options
Use training set
Supplied test set
Set...
Cross-validation
Folds
10
Percentage split
%
66
More options...
(Nom) play
Start
Stop
Result list (right-click for options)
10:33:11 - bayes.NaiveBayesSimple
10:45:46 - bayes.NaiveBayesSimple
Classifier output
=== Classifier model (full training set) ===
Naive Bayes (simple)
Class yes: P(C) = 0.625
Attribute outlook
sunny overcast rainy
0.25 0.41666667 0.33333333
Attribute temperature
Mean: 73 Standard Deviation: 6.164414
Attribute humidity
Mean: 79.11111111 Standard Deviation: 10.21572861
Attribute windy
TRUE FALSE
0.36363636 0.63636364
Class no: P(C) = 0.375
Attribute outlook
sunny overcast rainy
0.5 0.125 0.375
Attribute temperature
Mean: 74.6 Standard Deviation: 7.8930349
Attribute humidity
Mean: 86.2 Standard Deviation: 9.7313925
Attribute windy
TRUE FALSE
0.57142857 0.42857143
Status
OK
Log
x 0


weka-3-6-10-oracle-jvm
Weka Explorer
Preprocess
Classify
Cluster
Associate
Select attributes
Visualize
Classifier
Choose
NaiveBayesSimple
Test options
Use training set
Supplied test set
Set...
Cross-validation
Folds
10
Percentage split
%
66
More options...
(Nom) play
Start
Stop
Result list (right-click for options)
10:33:11 - bayes.NaiveBayesSimple
10:45:46 - bayes.NaiveBayesSimple
Classifier output
=== Predictions on training set ===
inst#, actual, predicted, error, probability distribution
1 2:no 2:no 0.316 *0.684
2 2:no 2:no 0.208 *0.792
3 1:yes 1:yes *0.791 0.209
4 1:yes 1:yes *0.545 0.455
5 1:yes 1:yes *0.77 0.23
6 2:no 1:yes + *0.736 0.264
7 1:yes 1:yes *0.938 0.062
8 2:no 2:no 0.414 *0.586
9 1:yes 1:yes *0.809 0.191
10 1:yes 1:yes *0.757 0.243
11 1:yes 1:yes *0.623 0.377
12 1:yes 1:yes *0.733 0.267
13 1:yes 1:yes *0.915 0.085
14 2:no 2:no 0.41 *0.59
=== Evaluation on training set ===
=== Summary ===
Correctly Classified Instances 13 92.8571 %
Incorrectly Classified Instances 1 7.1429 %
Kappa statistic 0.8372
Mean absolute error 0.3003
Root mean squared error 0.3431
Relative absolute error 64.6705 %
Root relative squared error 71.5605 %
Total Number of Instances 14
=== Detailed Accuracy By Class ===
TP Rate FP Rate Precision Recall F-Measure ROC Area Class
1 0.2 0.9 1 0.947 0.933 yes
0.8 0 1 0.8 0.889 0.933 no
Weighted Avg. 0.929 0.129 0.936 0.929 0.926 0.933
=== Confusion Matrix ===
a b <-- classified as
9 0 | a = yes
1 4 | b = no
Status
OK
Log
x 0

Discussion

- Naïve Bayes works surprisingly well, even if independence assumption is clearly violated
- Why? Because classification doesn't require accurate probability estimates as long as maximum probability is assigned to correct class
- However, adding too many redundant attributes will cause problems (e.g. identical attributes)
- Also, many numeric attributes are not normally distributed

Nearest Neighbors (Instance-Based Learning)



is this an apple?

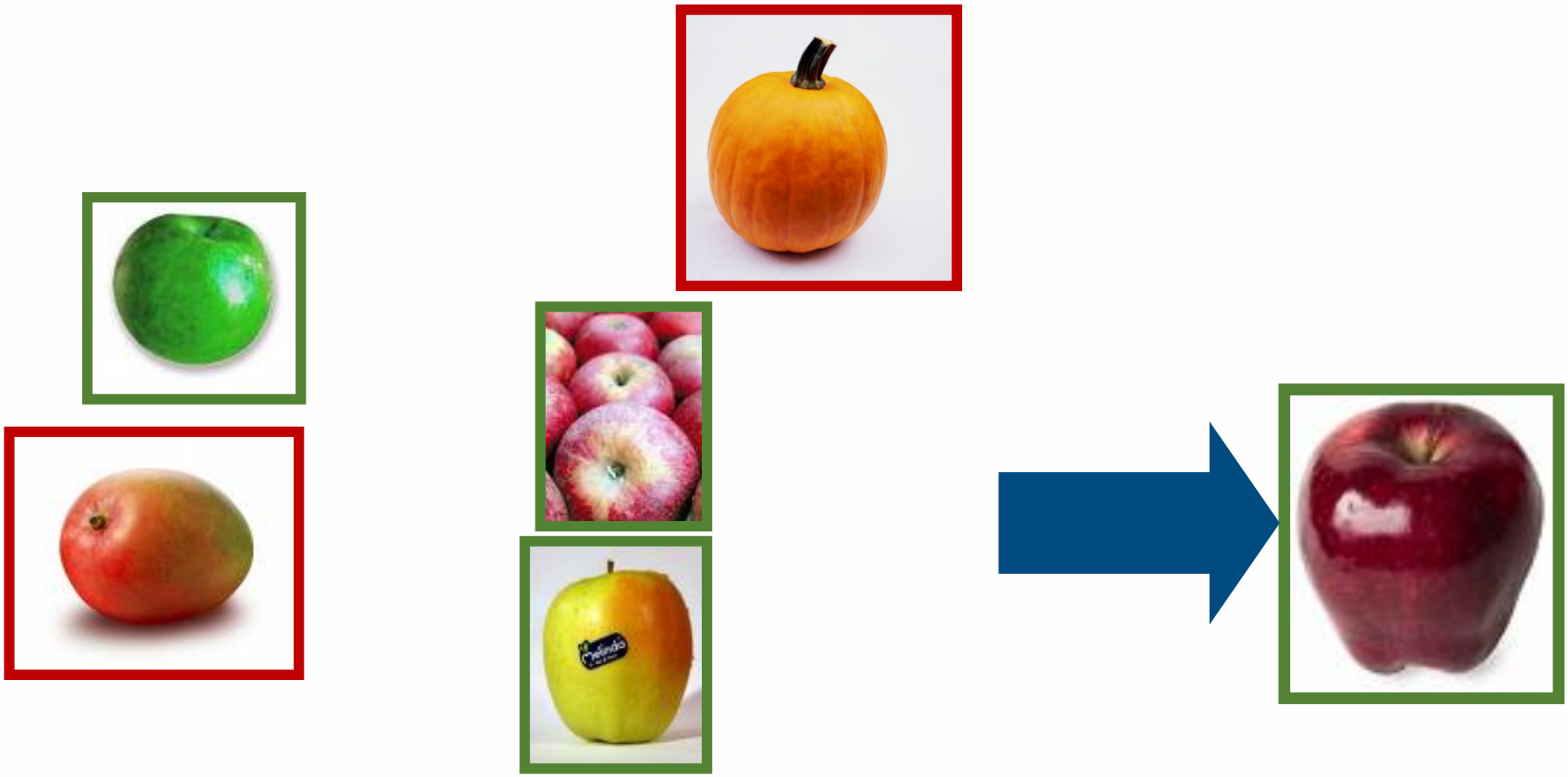
Nearest Neighbors

- To decide the label for an unseen example, consider the k examples from the training data that are more similar to the unknown one

- Classify the unknown example using the most frequent class

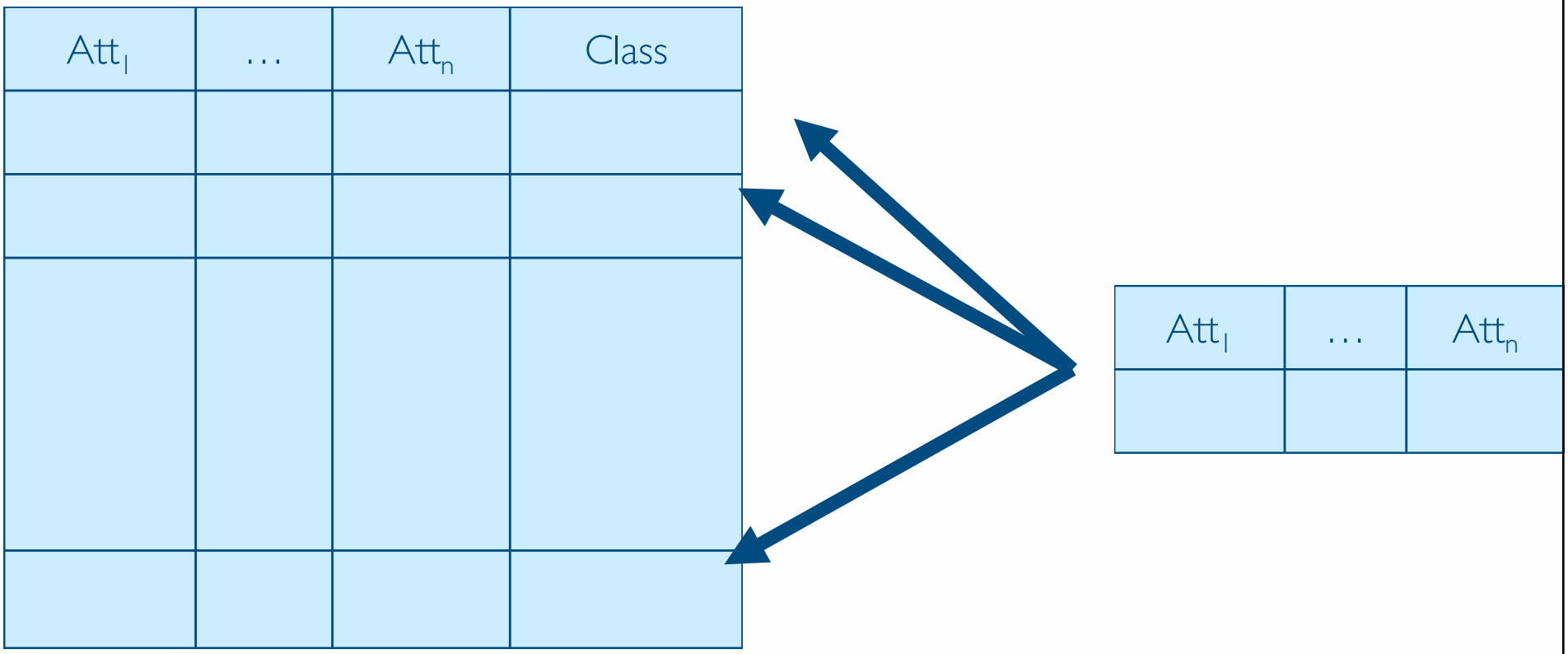
Nearest Neighbor in Action

- If k=5, these 5 fruits are the most similar ones to the unclassified example
- Since, the majority of the fruits are labeled as positive examples, we decide that the unknown fruit is an apple



Instance-Based Learning in General

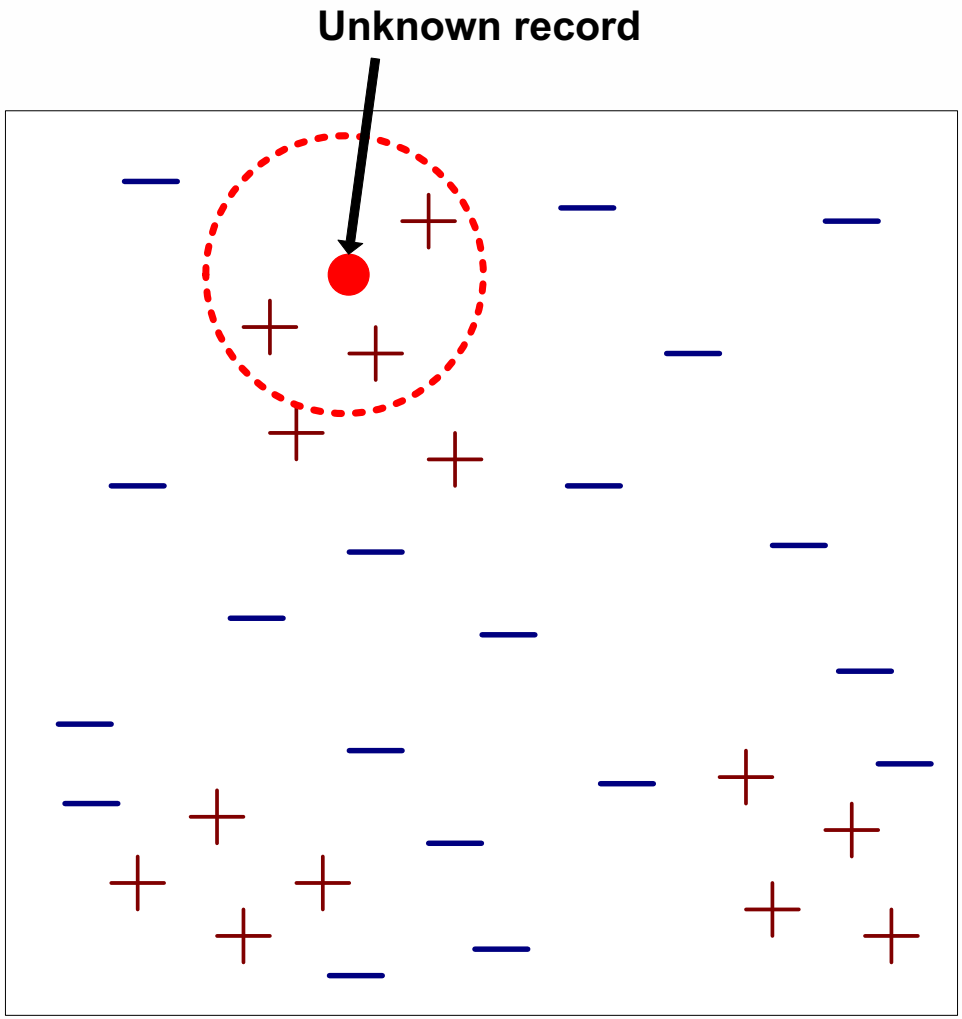
- Store the training records only, no model is computed
- Use the training records to predict an unknown class label



Instance-Based Methods

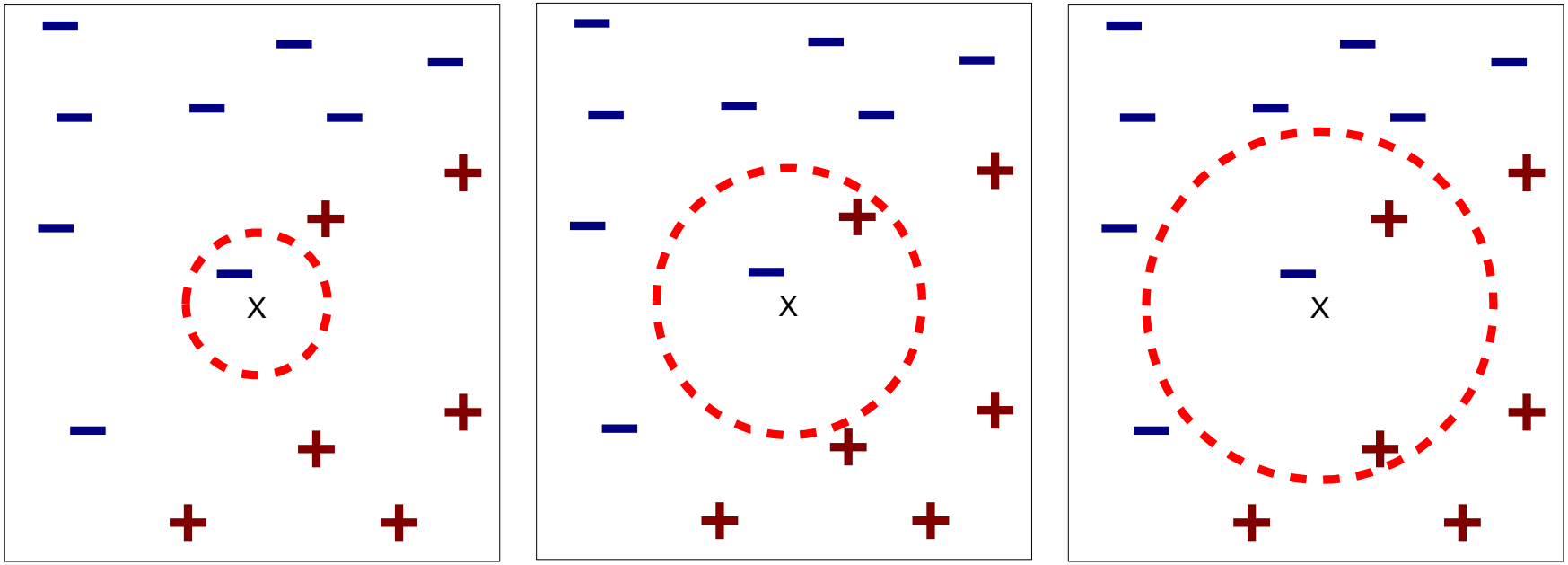
- They are the simplest form of learning
- The training dataset is searched for the instances that are more similar to the unlabeled instance
- The training dataset is the model itself, it is the knowledge
- The similarity function defines what's "learned"
- They implement a "lazy evaluation" (or lazy learning) scheme, nothing happens until a new unlabeled instance must be classified
- Known methods include "Rote Learning", "Case Base Reasoning", "k-Nearest Neighbors"

K-Nearest-Neighbors Classifier



- Three elements
  - The training dataset
  - Similarity function (or distance metric)
  - The value of k, the number of nearest neighbors to retrieve
- Classification
  - Compute distance to other training records
  - Identify the k nearest neighbors
  - Use class labels of nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

How Many Neighbors?



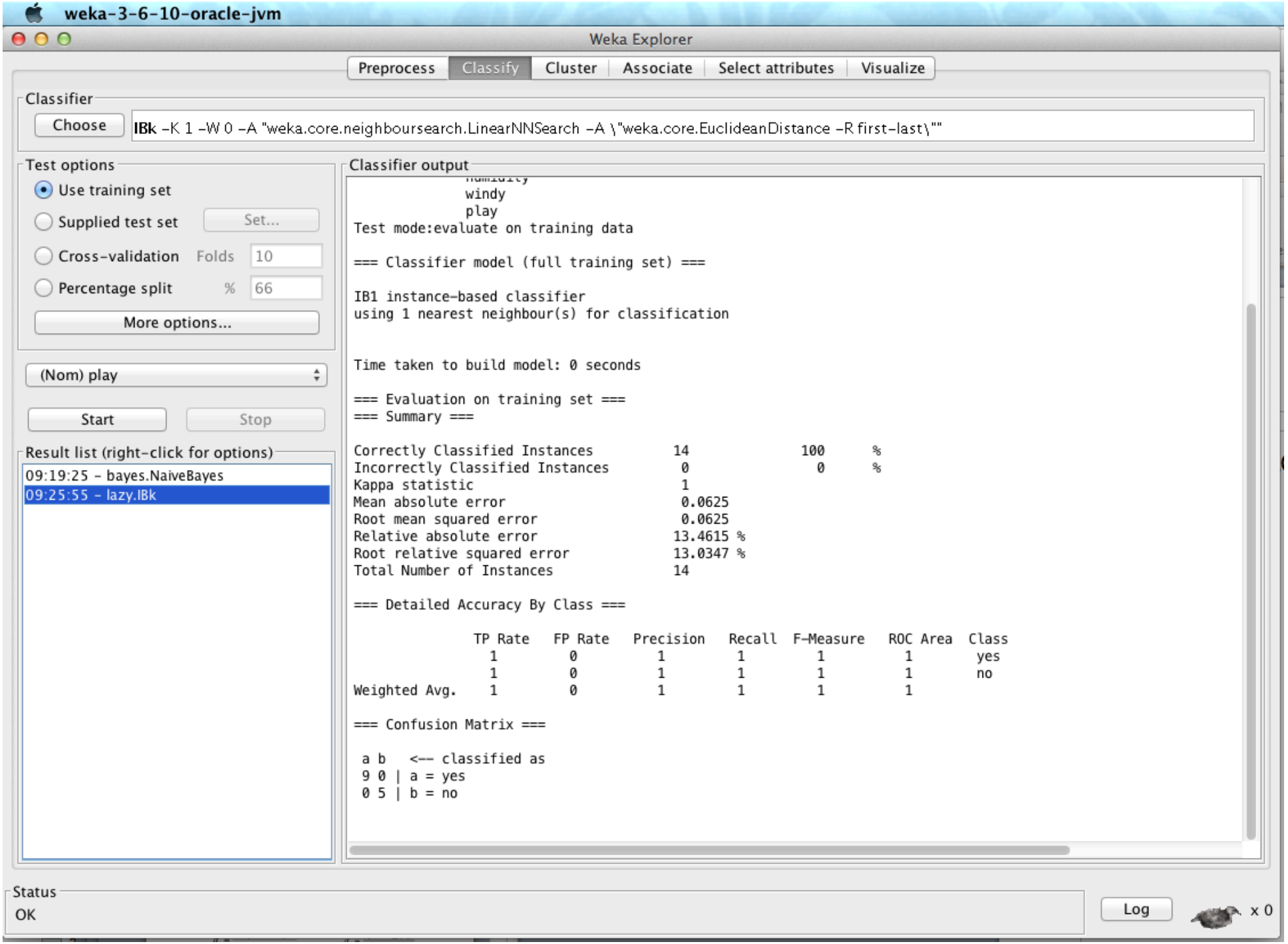
(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

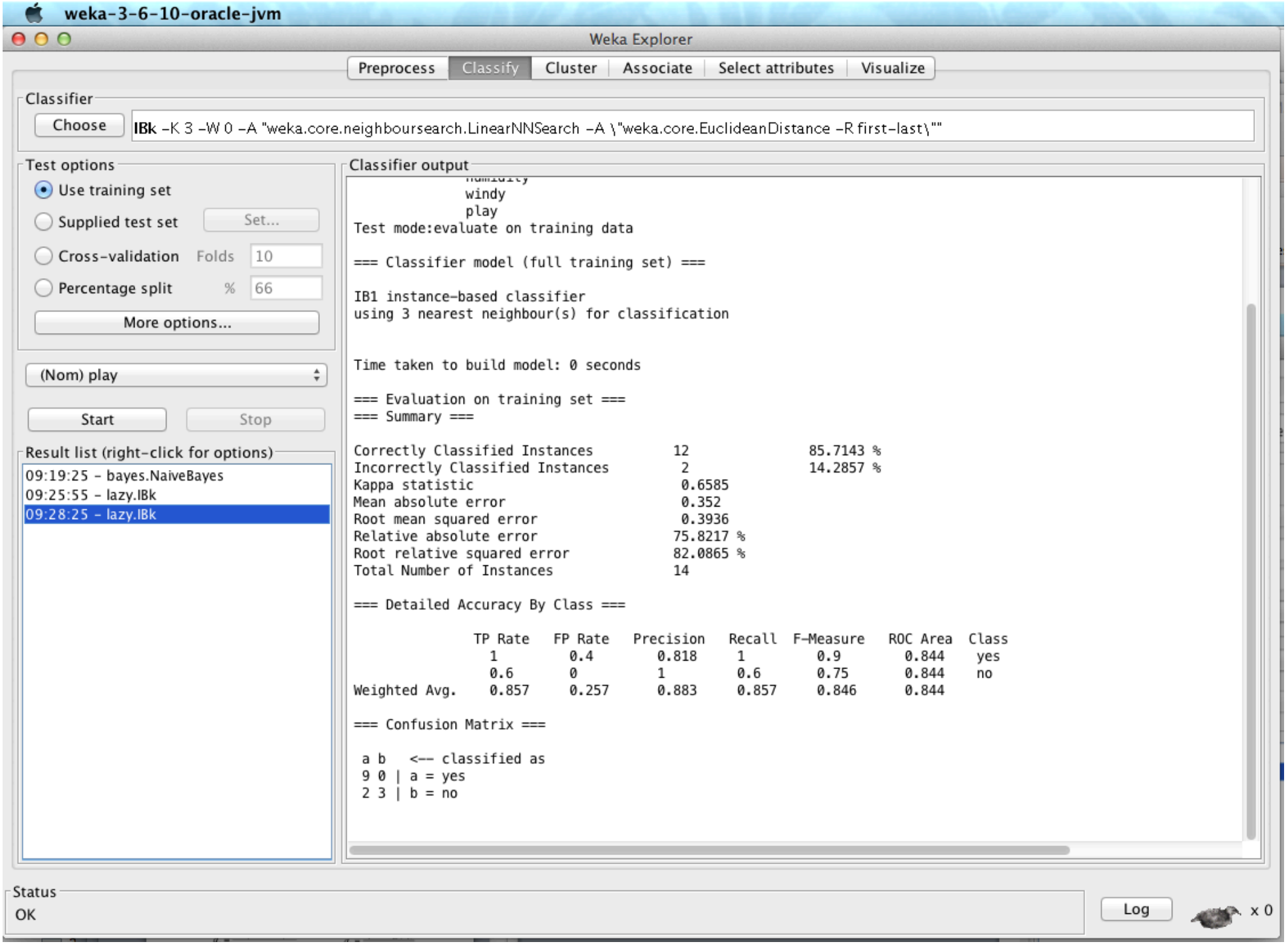
K-nearest neighbors of a record x are data points that have the k smallest distance to x

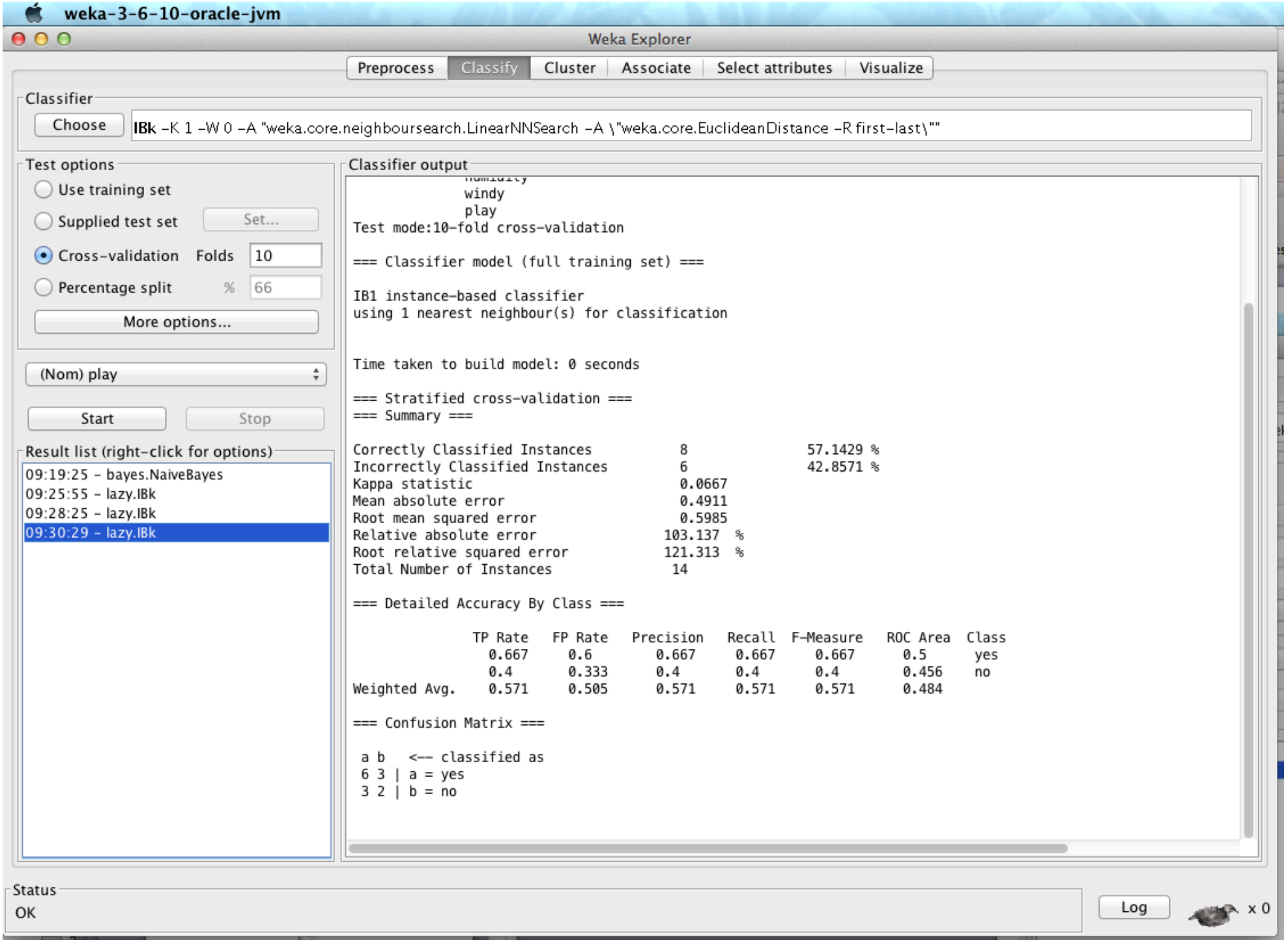
How many neighbors?

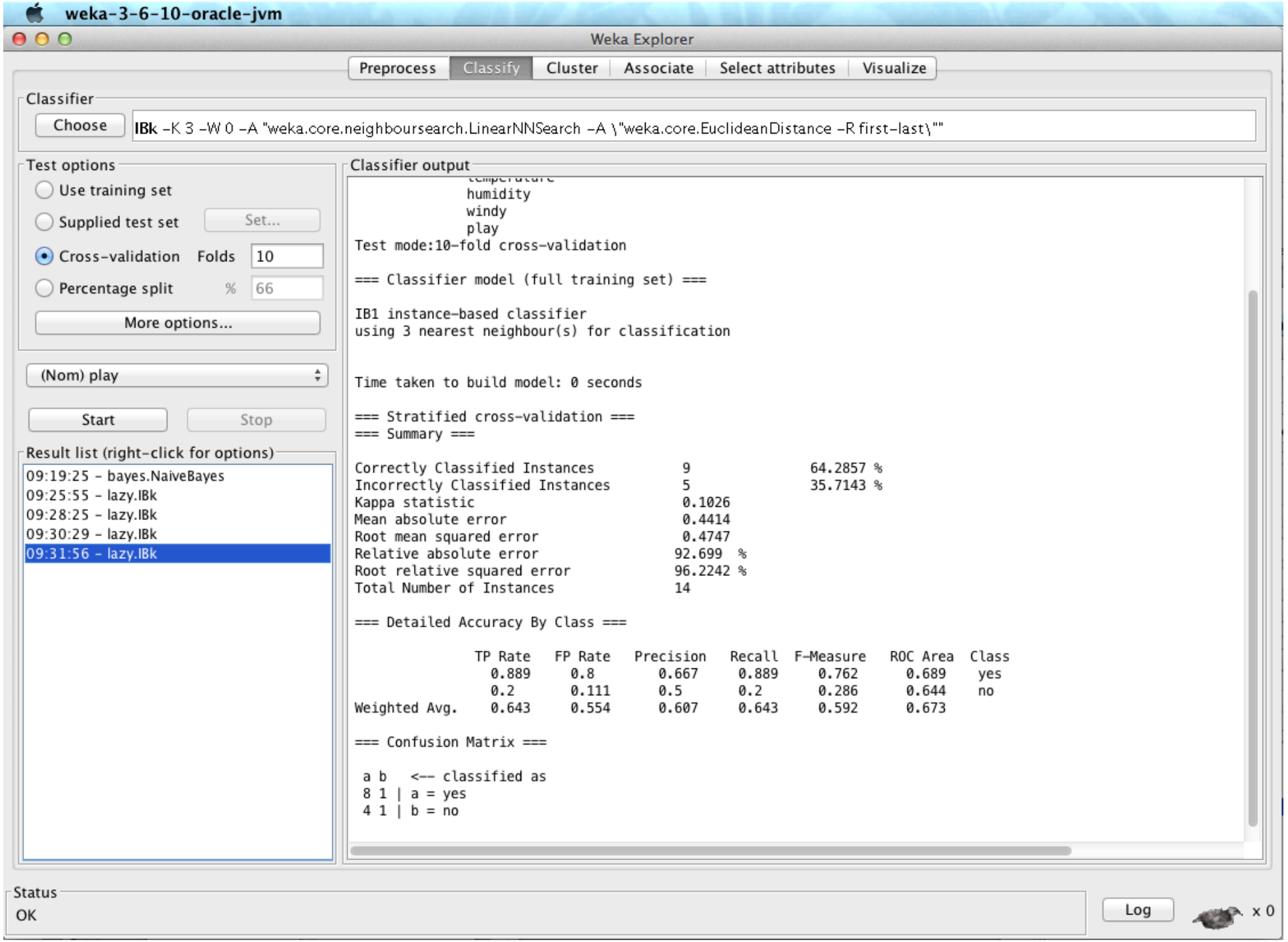
If k is too small, classification might be sensitive to noise points

If k is too large, neighborhood may include quite dissimilar examples


weka-3-6-10-oracle-jvm
Weka Explorer
Preprocess
Classify
Cluster
Associate
Select attributes
Visualize
Classifier
Choose
IBk -K 1 -W 0 -A "weka.core.neighboursearch.LinearNNSearch -A \"weka.core.EuclideanDistance -R first-last\""
Test options
Use training set
Supplied test set
Set...
Cross-validation
Folds
10
Percentage split
%
66
More options...
(Nom) play
Start
Stop
Result list (right-click for options)
09:19:25 - bayes.NaiveBayes
09:25:55 - lazy.IBk
Classifier output
windy
play
Test mode:evaluate on training data
=== Classifier model (full training set) ===
IB1 instance-based classifier
using 1 nearest neighbour(s) for classification
Time taken to build model: 0 seconds
=== Evaluation on training set ===
=== Summary ===
Correctly Classified Instances 14 100 %
Incorrectly Classified Instances 0 0 %
Kappa statistic 1
Mean absolute error 0.0625
Root mean squared error 0.0625
Relative absolute error 13.4615 %
Root relative squared error 13.0347 %
Total Number of Instances 14
=== Detailed Accuracy By Class ===
TP Rate FP Rate Precision Recall F-Measure ROC Area Class
1 0 1 1 1 1 yes
1 0 1 1 1 1 no
Weighted Avg. 1 0 1 1 1 1
=== Confusion Matrix ===
a b <-- classified as
9 0 | a = yes
0 5 | b = no
Status
OK
Log
x 0


weka-3-6-10-oracle-jvm
Weka Explorer
Preprocess
Classify
Cluster
Associate
Select attributes
Visualize
Classifier
Choose
IBk -K 3 -W 0 -A "weka.core.neighboursearch.LinearNNSearch -A \"weka.core.EuclideanDistance -R first-last\""
Test options
Use training set
Supplied test set
Set...
Cross-validation
Folds
10
Percentage split
%
66
More options...
(Nom) play
Start
Stop
Result list (right-click for options)
09:19:25 - bayes.NaiveBayes
09:25:55 - lazy.IBk
09:28:25 - lazy.IBk
Classifier output
windy
play
Test mode:evaluate on training data
=== Classifier model (full training set) ===
IB1 instance-based classifier
using 3 nearest neighbour(s) for classification
Time taken to build model: 0 seconds
=== Evaluation on training set ===
=== Summary ===
Correctly Classified Instances 12 85.7143 %
Incorrectly Classified Instances 2 14.2857 %
Kappa statistic 0.6585
Mean absolute error 0.352
Root mean squared error 0.3936
Relative absolute error 75.8217 %
Root relative squared error 82.0865 %
Total Number of Instances 14
=== Detailed Accuracy By Class ===
TP Rate FP Rate Precision Recall F-Measure ROC Area Class
1 0.4 0.818 1 0.9 0.844 yes
0.6 0 1 0.6 0.75 0.844 no
Weighted Avg. 0.857 0.257 0.883 0.857 0.846 0.844
=== Confusion Matrix ===
a b <-- classified as
9 0 | a = yes
2 3 | b = no
Status
OK
Log
x 0


weka-3-6-10-oracle-jvm
Weka Explorer
Preprocess
Classify
Cluster
Associate
Select attributes
Visualize
Classifier
Choose
IBk -K 1 -W 0 -A "weka.core.neighboursearch.LinearNNSearch -A \"weka.core.EuclideanDistance -R first-last\""
Test options
Use training set
Supplied test set
Set...
Cross-validation
Folds
10
Percentage split
%
66
More options...
(Nom) play
Start
Stop
Result list (right-click for options)
09:19:25 - bayes.NaiveBayes
09:25:55 - lazy.IBk
09:28:25 - lazy.IBk
09:30:29 - lazy.IBk
Classifier output
windy
play
Test mode:10-fold cross-validation
=== Classifier model (full training set) ===
IB1 instance-based classifier
using 1 nearest neighbour(s) for classification
Time taken to build model: 0 seconds
=== Stratified cross-validation ===
=== Summary ===
Correctly Classified Instances 8 57.1429 %
Incorrectly Classified Instances 6 42.8571 %
Kappa statistic 0.0667
Mean absolute error 0.4911
Root mean squared error 0.5985
Relative absolute error 103.137 %
Root relative squared error 121.313 %
Total Number of Instances 14
=== Detailed Accuracy By Class ===
TP Rate FP Rate Precision Recall F-Measure ROC Area Class
0.667 0.6 0.667 0.667 0.667 0.5 yes
0.4 0.333 0.4 0.4 0.4 0.456 no
Weighted Avg. 0.571 0.505 0.571 0.571 0.571 0.484
=== Confusion Matrix ===
a b <-- classified as
6 3 | a = yes
3 2 | b = no
Status
OK
Log
x 0


weka-3-6-10-oracle-jvm
Weka Explorer
Preprocess
Classify
Cluster
Associate
Select attributes
Visualize
Classifier
Choose
IBk -K 3 -W 0 -A "weka.core.neighboursearch.LinearNNSearch -A \"weka.core.EuclideanDistance -R first-last\""
Test options
Use training set
Supplied test set
Set...
Cross-validation
Folds
10
Percentage split
%
66
More options...
(Nom) play
Start
Stop
Result list (right-click for options)
09:19:25 - bayes.NaiveBayes
09:25:55 - lazy.IBk
09:28:25 - lazy.IBk
09:30:29 - lazy.IBk
09:31:56 - lazy.IBk
Classifier output
humidity
windy
play
Test mode:10-fold cross-validation
=== Classifier model (full training set) ===
IB1 instance-based classifier
using 3 nearest neighbour(s) for classification
Time taken to build model: 0 seconds
=== Stratified cross-validation ===
=== Summary ===
Correctly Classified Instances 9 64.2857 %
Incorrectly Classified Instances 5 35.7143 %
Kappa statistic 0.1026
Mean absolute error 0.4414
Root mean squared error 0.4747
Relative absolute error 92.699 %
Root relative squared error 96.2242 %
Total Number of Instances 14
=== Detailed Accuracy By Class ===
TP Rate FP Rate Precision Recall F-Measure ROC Area Class
0.889 0.8 0.667 0.889 0.762 0.689 yes
0.2 0.111 0.5 0.2 0.286 0.644 no
Weighted Avg. 0.643 0.554 0.607 0.643 0.592 0.673
=== Confusion Matrix ===
a b <-- classified as
8 1 | a = yes
4 1 | b = no
Status
OK
Log
x 0

What similarity measures?

Distance and similarity identify orthogonal yet related concepts

When distance is larger similarity is smaller

Viceversa, when similarity is larger, distance is smaller

What Similarity Measure?

- Euclidian distance is the typical function used to compute the similarity between two examples

$$d(p,q) = \sqrt{\sum_i (p_i - q_i)^2}$$

- To determine the class from nearest neighbor list
  - Take the majority vote of class labels among the k neighbors
  - Or weight the vote according to distance (e.g., $w = 1/d^2$)

- Another popular metric is city-block (Manhattan) metric, distance is the sum of absolute differences

Euclidean Distances

- L_r-norm

$$d([x_1, x_2, \ldots, x_n],\ [y_1, y_2, \ldots, y_n]) = (\sum_{i=1}^{n} |x_i - y_i|^r)^{1/r}$$

- Euclidean distance (r=2)

$$d([x_1, x_2, \ldots, x_n],\ [y_1, y_2, \ldots, y_n]) = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

- Manhattan distance (r=1)

$$d([x_1, x_2, \ldots, x_n], [y_1, y_2, \ldots, y_n]) = \sum_{i=1}^{n} |x_i - y_i|$$

- L_∞-norm

$$d([x_1, x_2, \ldots, x_n], [y_1, y_2, \ldots, y_n]) = \max_{i=1}^{n} |x_i - y_i|$$

Cosine Distance

- The cosine distance between x, y is the angle that the vectors to those points make

$$d(\vec{x}, \vec{y}) = \arccos \frac{\sum_1^n x_i y_i}{\sqrt{\sum_i^n x_i^2} \sqrt{\sum_i^n y_i^2}}$$

- This angle will be in the range 0 to 180 degrees, regardless of how many dimensions the space has.

- Example: given x = (1,2,-1) and y = (2,1,1) the angle between the two vectors is 60

Jaccard Distance

- Jaccard distance is a measure of how dissimilar two sets are. Examples are represented by binary variables and are viewed as representations of set
- Jaccard distance is defined as

$$d(\vec{x}, \vec{y}) = 1 - J(\vec{x}, \vec{y})$$

- J is the Jaccard similarity which is computed as the number of

$$J(\vec{x}, \vec{y}) = \frac{|\vec{x} \cap \vec{y}|}{|\vec{x} \cup \vec{y}|}$$

- Which can also be interpreted as the percentage of identical attributes

Hamming Distance

- Hamming distance between two vectors is the number of components in which they differ
- Or equivalently, given the number of variables n, and the number m of matching components, we define

$$d(\vec{x}, \vec{y}) = \frac{n - m}{n}$$

- Example: the Hamming distance between the vectors 10101 and 11110 is 3/5.

Normalization and Other Issues

- Different attributes are measured on different scales, thus we often need to normalize them, using for instance range normalization o standard score normalization

$$x'_i = \frac{x_i - \min_i x_i}{\max_i x_i - \min_i x_i} \qquad x'_i = \frac{x_i - \mu}{\sigma}$$

- For nominal attributes, the distance either 0 (the value is the same) or 1 (the value is different)

- Missing values are usually assumed to be maximally distant (given normalized attributes)

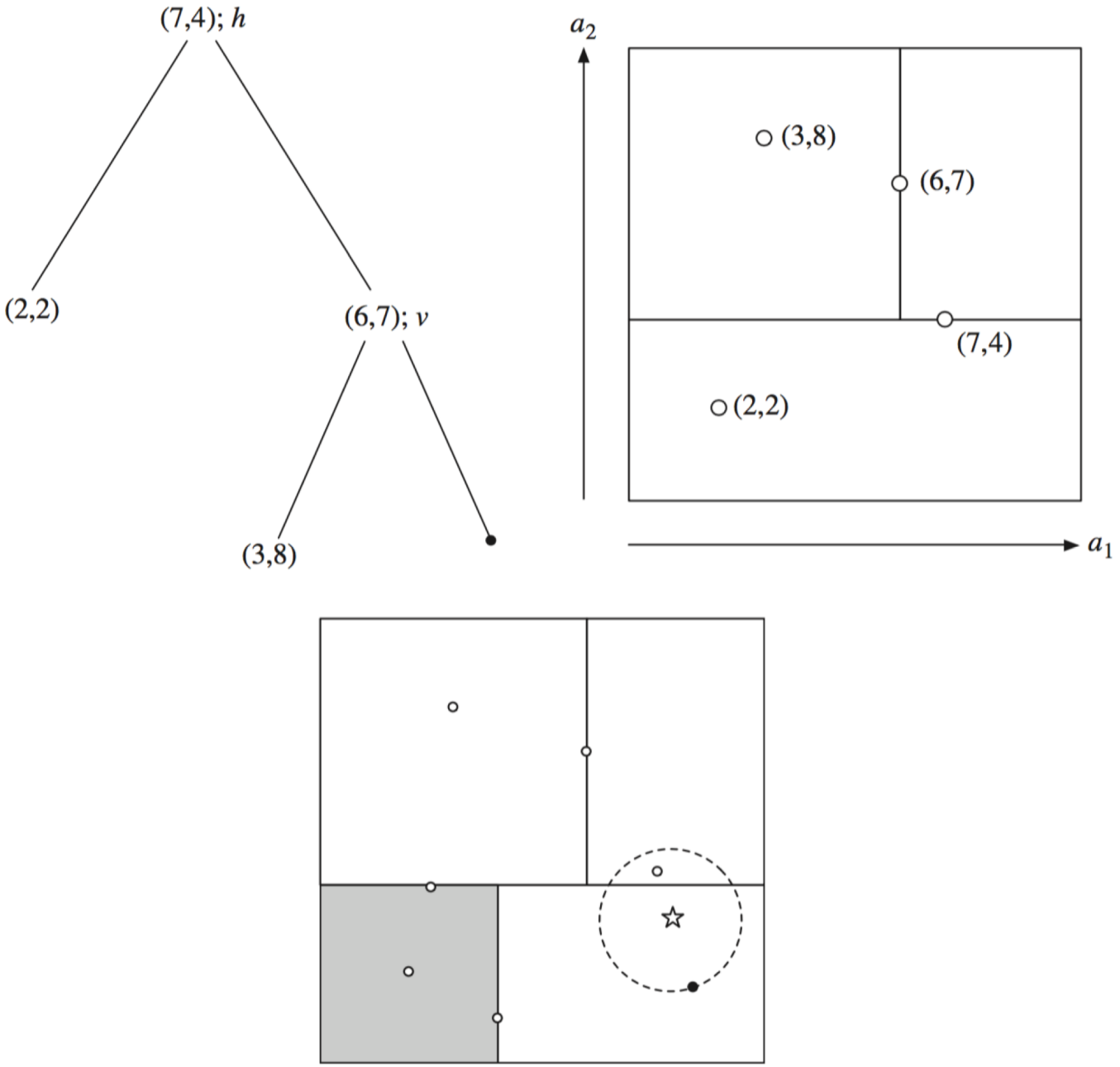
Finding Nearest Neighbors Efficiently

- Basic Approach
  - Linear scan of the data
  - Classification time is proportional to the product of the number of instances in training and test sets (and the
- Nearest-neighbor search can be speeded up by using
  - KD-Trees
  - Ball-Trees
  - …

KD-Trees

Split the space hierarchically using
a tree generated from the data

To find the neighbor of a specific example,
navigate the tree using the example



Example of KD-tree. The tree works like a decision tree and splits the space in a hierarchy. When the class of one example is needed, the tree is navigated until a leaf is reached and only the nearby areas are actually checked by backtracking on the tree.

More on kD-trees

- Complexity depends on depth of the tree, given by the logarithm of number of nodes for a balanced tree
- Amount of backtracking required depends on quality of tree ("square" vs. "skinny" nodes)
- How to build a good tree?
  - Need to find good split point and split direction
  - Possible split direction: direction with greatest variance
  - Possible split point: median value along that direction
- Using value closest to mean (rather than median) can be better if data is skewed
- Can apply this split selection strategy recursively just like in the case of decision tree learning

Example using the loan dataset

Evaluation using 10-fold crossvalidation

kd-tree

t=11.163 Accuracy=0.806 Std=0.00

Brute force

t=567.895 Accuracy=0.806 Std=0.001

Run the Python notebooks for k-Nearest-Neighbor

k-Nearest Neighbor Regression

- The regression methods we previously discussed are parametric
  - They assume an approximation function parametrized by a weight vector
  - The regression algorithm search for the best weight vector
  - E.g., linear regression assumes that the target is computed as a linear combination of the weight vector w and the feature vector h(x)
- Nearest Neighbor regression fits each point locally
- Basic Algorithm
  - Given a dataset $(x_1,y_1) \ldots (x_N,y_N)$
  - Given a query point x_q
  - The value y_q associated to x_q is computed as a local interpolation of the targets associated to neighbor points
- Prediction can use the plain average of the k nearest targets or a weighted average of the same targets
- Prediction can use kernel functions that take the distance as input and return a weight (e.g., a Gaussian function of the distance)

Discussion

- K-Nearest Neighbor is often very accurate but slow, since simple version scans entire training data to derive a prediction
- Assumes all attributes are equally important, thus may need attribute selection or weights
- Possible remedies against noisy instances:
  - Take a majority vote over the k nearest neighbors
  - Remove noisy instances from dataset (difficult!)
- Statisticians have used k-NN since early 1950s,
  If $n \rightarrow \infty$ and $k/n \rightarrow 0$, error approaches minimum
- Data Structures
  - kD-trees can become inefficient when the number of attributes is too large
  - Ball trees are may help

Bayesian Belief Networks

Bayesian Belief Networks

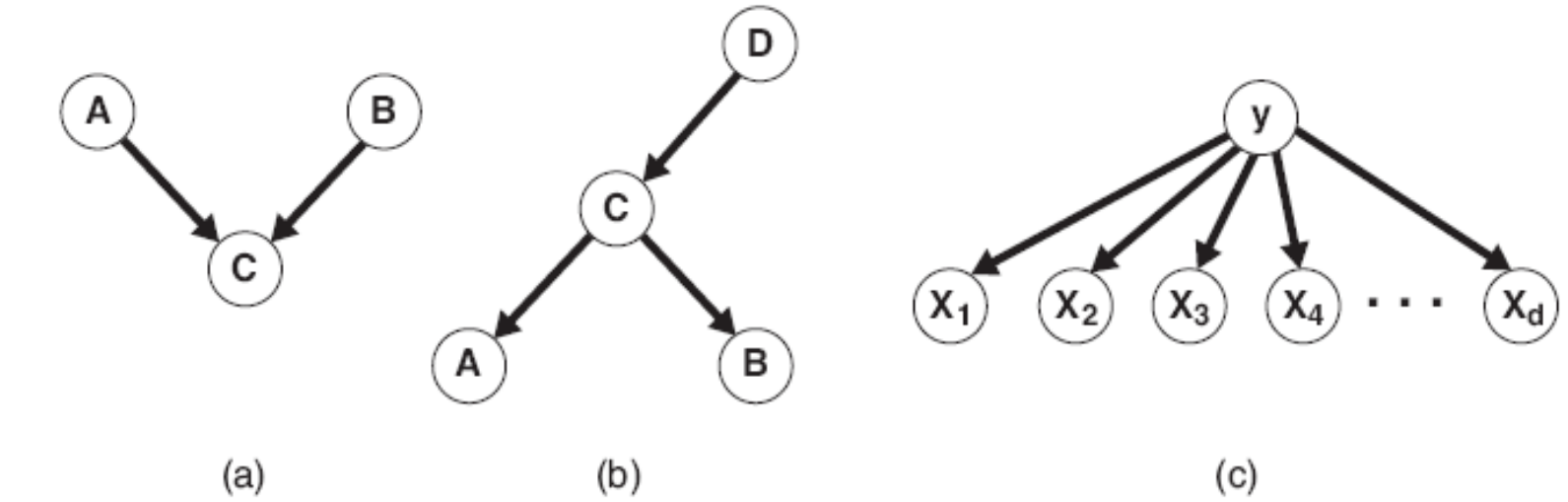
- The conditional independence assumption,
  - makes computation possible
  - yields optimal classifiers when satisfied
  - but is seldom satisfied in practice, as attributes (variables) are often correlated
- Bayesian Belief Networks (BBN) allows us to specify which pair of attributes are conditionally independent
- They provide a graphical representation of probabilistic relationships among a set of random variables

- Describe the probability distribution governing a set of variables by specifying
  - Conditional independence assumptions that apply on subsets of the variables
  - A set of conditional probabilities

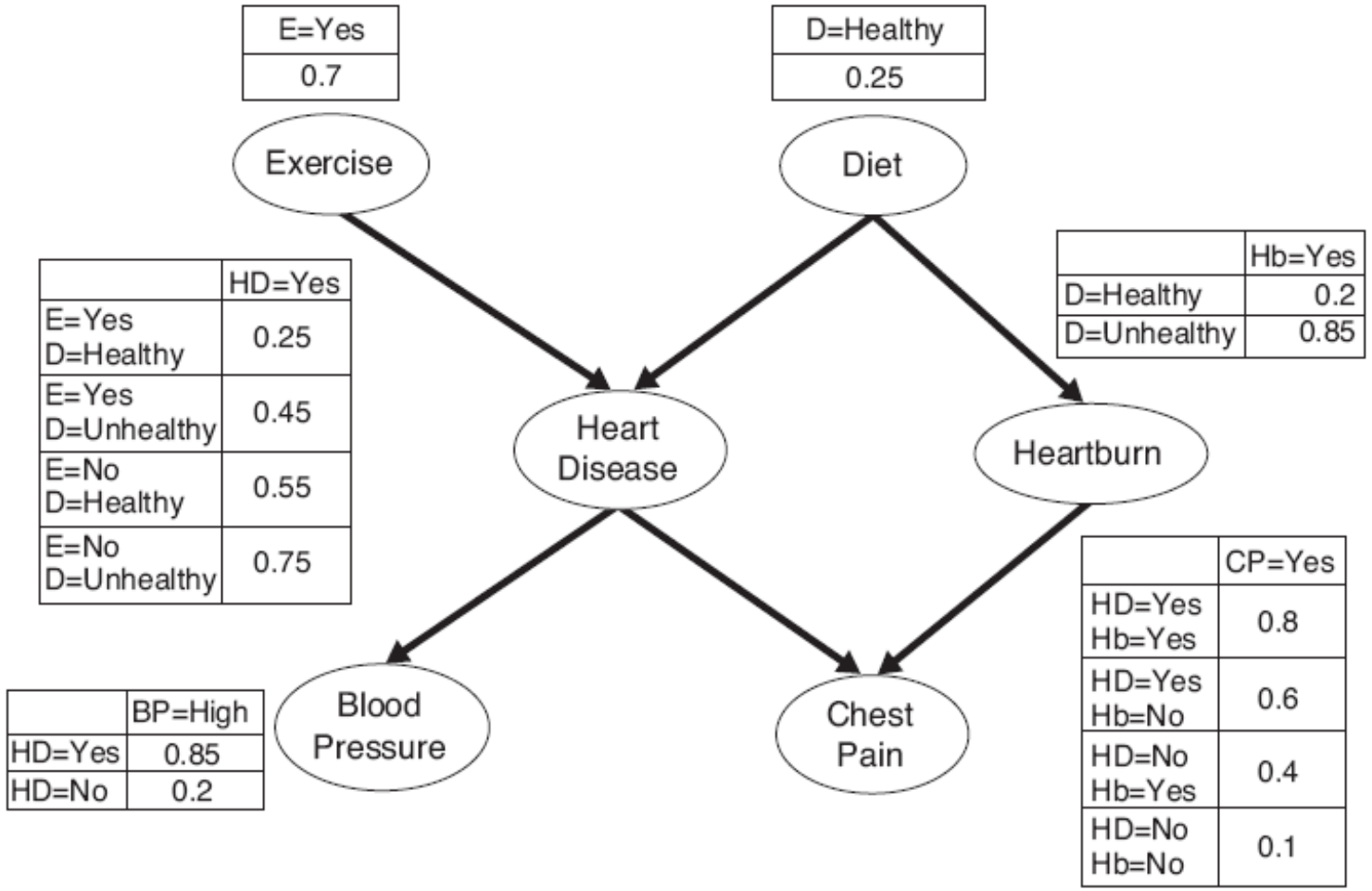
- Two key elements
  - A direct acyclic graph, encoding the dependence relationships among variables
  - A probability table associating each node to its immediate parents node

Examples of Bayesian Belief Networks

- Variable A and B are independent, but each one of them has an influence on the variable A
- A is conditionally independent of both B and D, given C
- The configuration of the typical naïve Bayes classifier



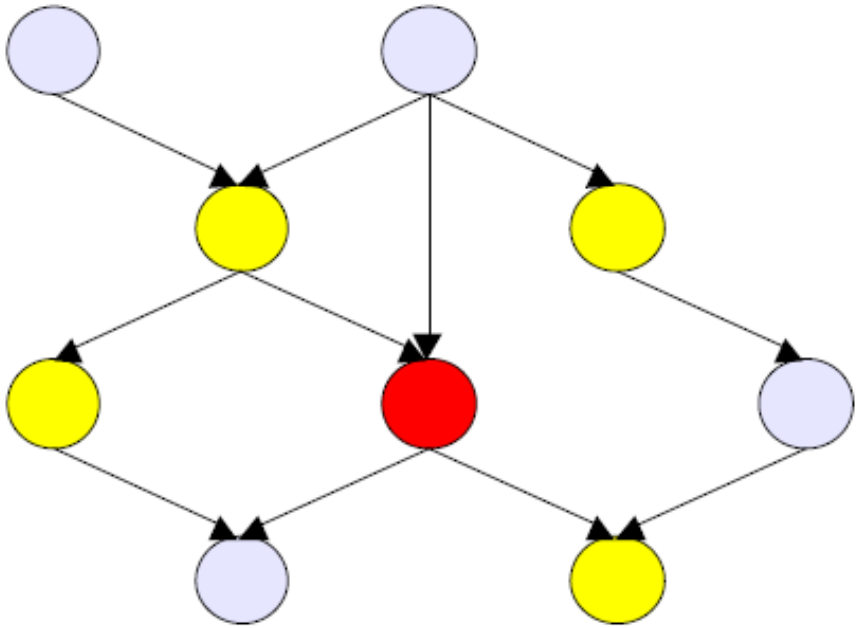
An Example of Bayesian Belief Network

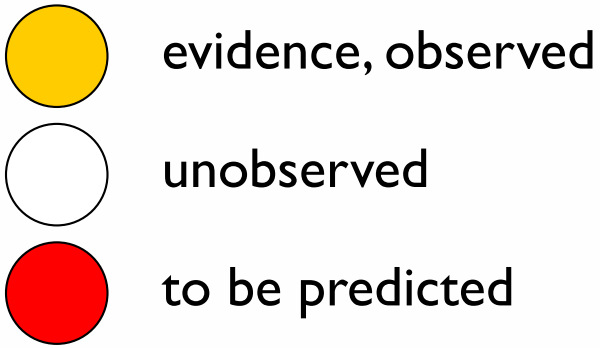


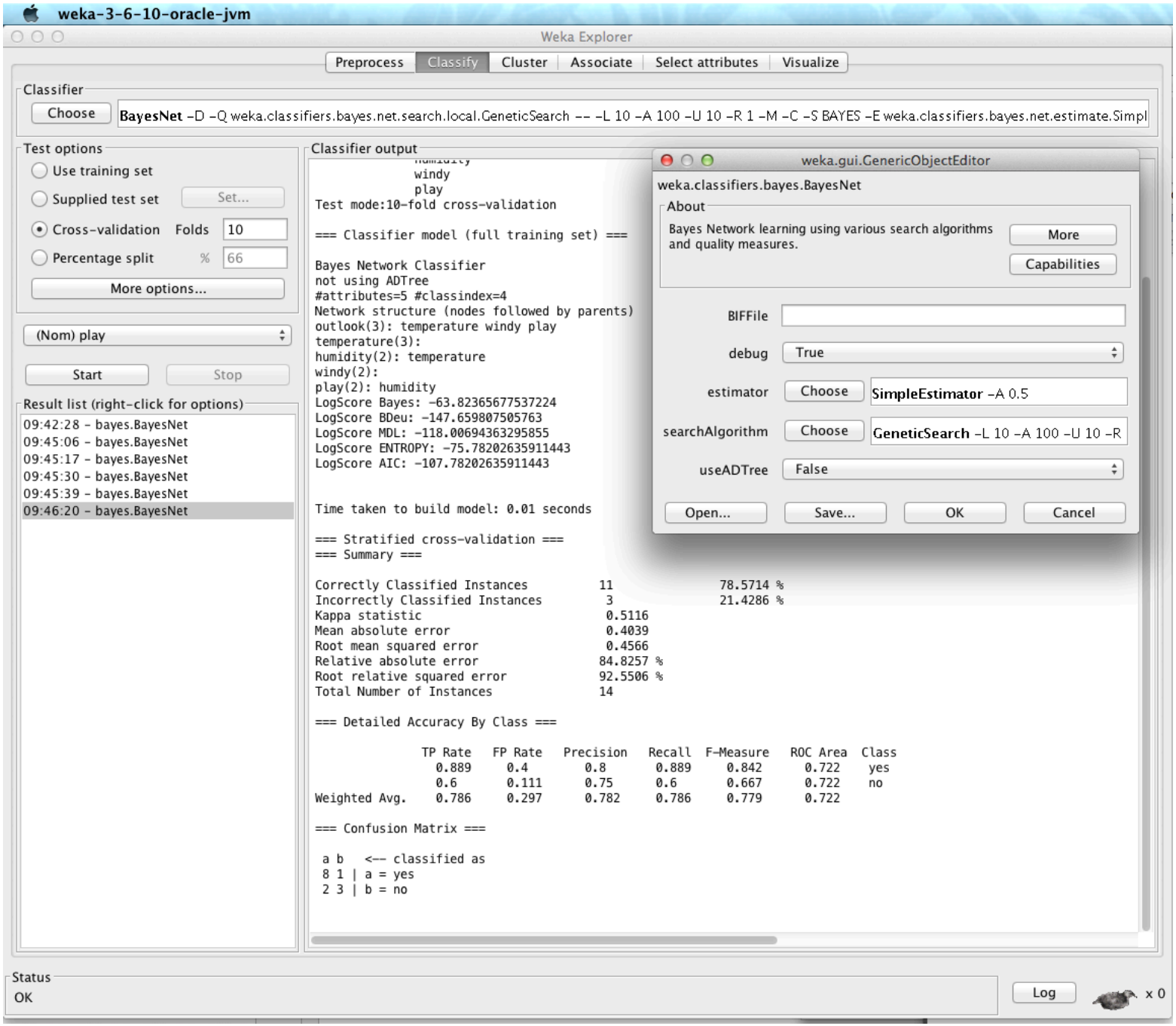
Probability Tables

- The network topology imposes conditions regarding the variable conditional independence
- Each node is associated with a probability table
  - If a node X does not have any parents, then the table contains only the prior probability P(X)
  - If a node X has only one any parent Y, then the table contains only the conditional probability P(X|Y)
  - If a node X has multiple parents, $Y_1, \ldots, Y_k$ the the table contains the conditional probability $P(X|Y_1 \ldots Y_k)$

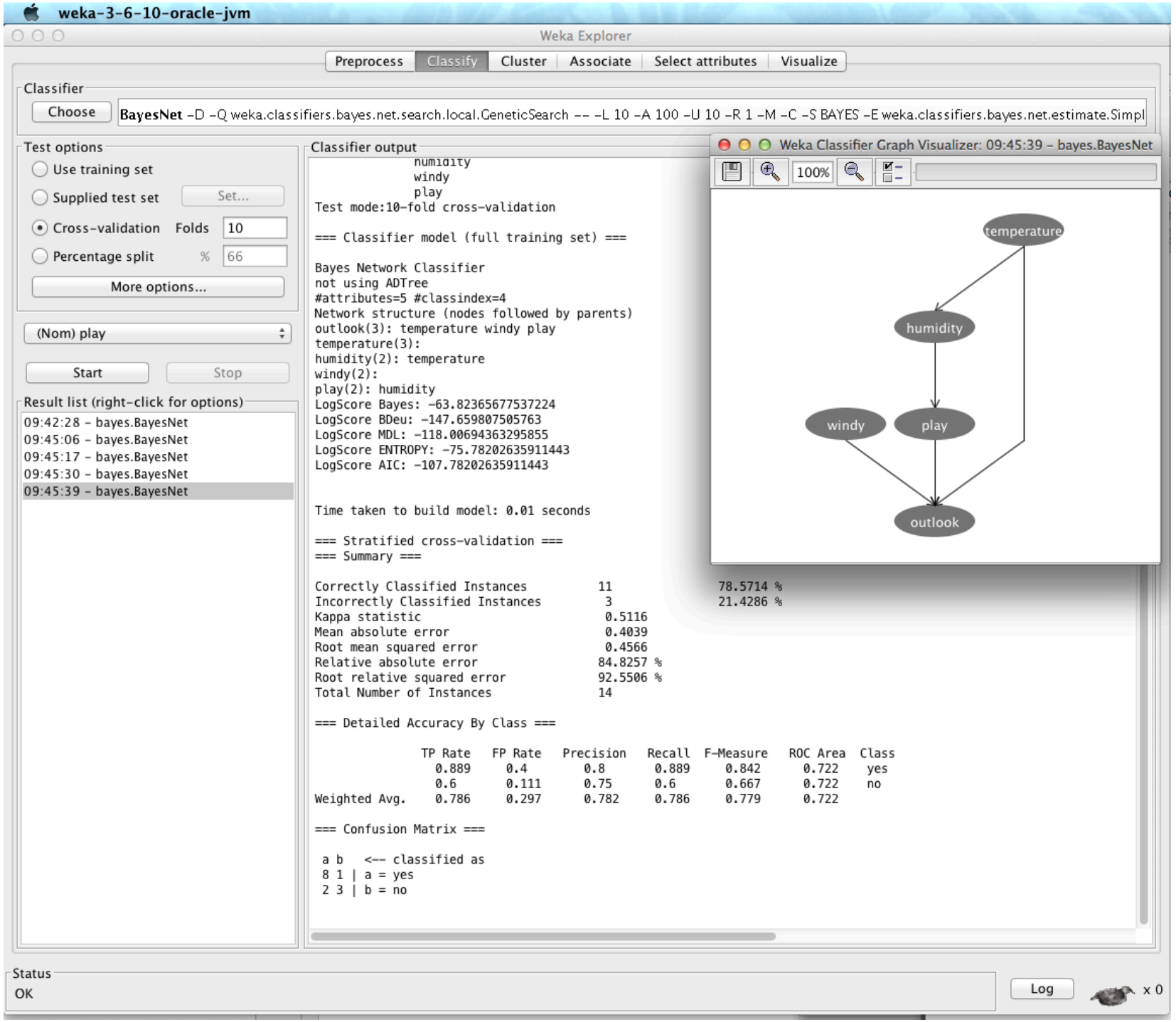
- In general the inference is NP-complete but there are approximating methods, e.g. Monte-Carlo







http://www.cs.waikato.ac.nz/~remco/weka.bn.pdf


weka-3-6-10-oracle-jvm
Weka Explorer
Preprocess
Classify
Cluster
Associate
Select attributes
Visualize
Classifier
Choose
BayesNet -D -Q weka.classifiers.bayes.net.search.local.GeneticSearch -- -L 10 -A 100 -U 10 -R 1 -M -C -S BAYES -E weka.classifiers.bayes.net.estimate.Simpl
Test options
Use training set
Supplied test set
Set...
Cross-validation
Folds
10
Percentage split
%
66
More options...
(Nom) play
Start
Stop
Result list (right-click for options)
09:42:28 - bayes.BayesNet
09:45:06 - bayes.BayesNet
09:45:17 - bayes.BayesNet
09:45:30 - bayes.BayesNet
09:45:39 - bayes.BayesNet
Classifier output
humidity
windy
play
Test mode:10-fold cross-validation
=== Classifier model (full training set) ===
Bayes Network Classifier
not using ADTree
#attributes=5 #classindex=4
Network structure (nodes followed by parents)
outlook(3): temperature windy play
temperature(3):
humidity(2): temperature
windy(2):
play(2): humidity
LogScore Bayes: -63.82365677537224
LogScore BDeu: -147.659807505763
LogScore MDL: -118.00694363295855
LogScore ENTROPY: -75.78202635911443
LogScore AIC: -107.78202635911443
Time taken to build model: 0.01 seconds
=== Stratified cross-validation ===
=== Summary ===
Correctly Classified Instances 11 78.5714 %
Incorrectly Classified Instances 3 21.4286 %
Kappa statistic 0.5116
Mean absolute error 0.4039
Root mean squared error 0.4566
Relative absolute error 84.8257 %
Root relative squared error 92.5506 %
Total Number of Instances 14
=== Detailed Accuracy By Class ===
TP Rate FP Rate Precision Recall F-Measure ROC Area Class
0.889 0.4 0.8 0.889 0.842 0.722 yes
0.6 0.111 0.75 0.6 0.667 0.722 no
Weighted Avg. 0.786 0.297 0.782 0.786 0.779 0.722
=== Confusion Matrix ===
a b <-- classified as
8 1 | a = yes
2 3 | b = no
Weka Classifier Graph Visualizer: 09:45:39 - bayes.BayesNet
100%
temperature
humidity
windy
play
outlook
Status
OK
Log
x 0

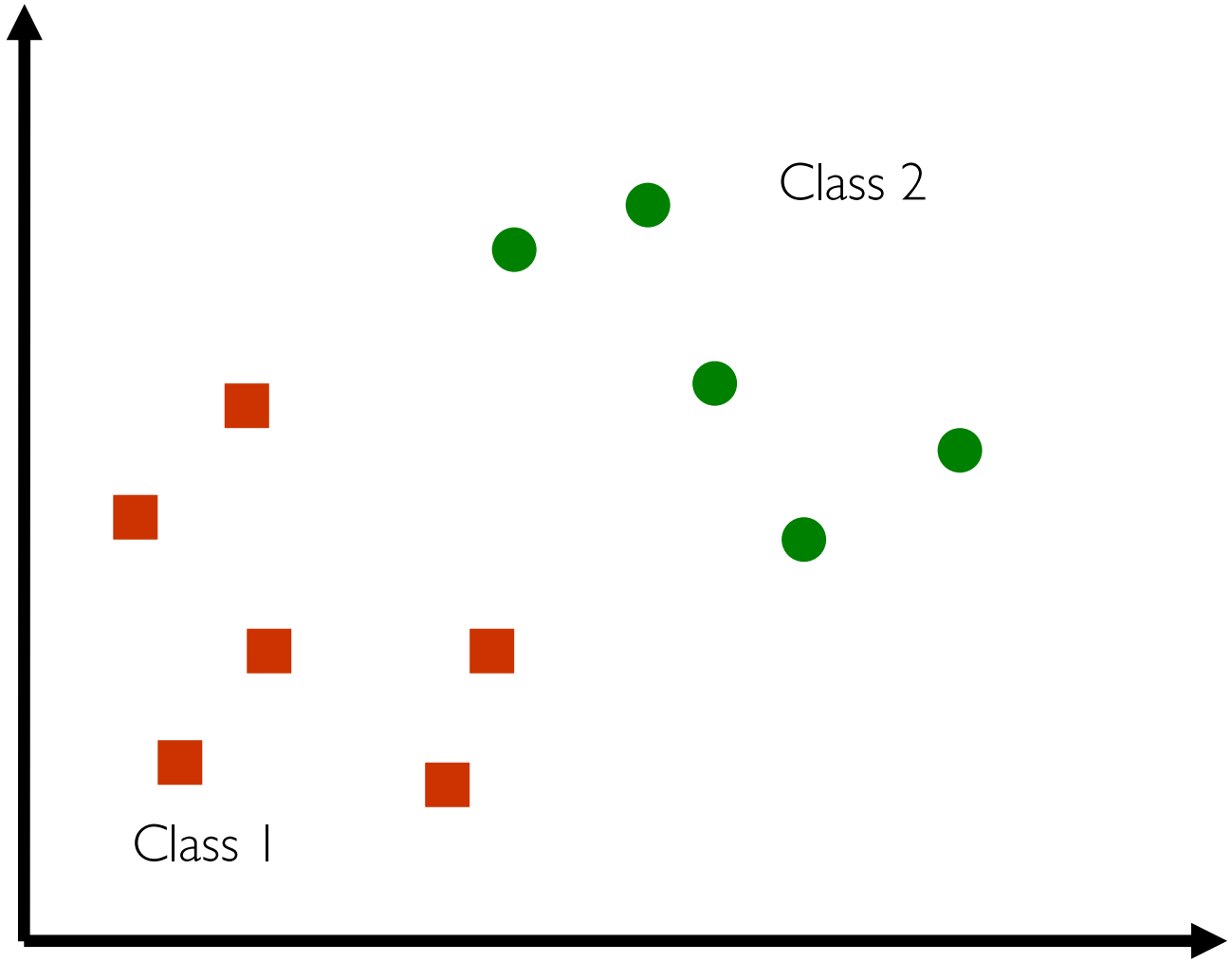
Bayesian Belief Networks

- Bayesian belief network allows a subset of the variables conditionally independent
- A graphical model of causal relationships
- Several cases of learning Bayesian belief networks
  - Given both network structure and all the variables is easy
  - Given network structure but only some variables
  - When the network structure is not known in advance

Bayesian Belief Networks

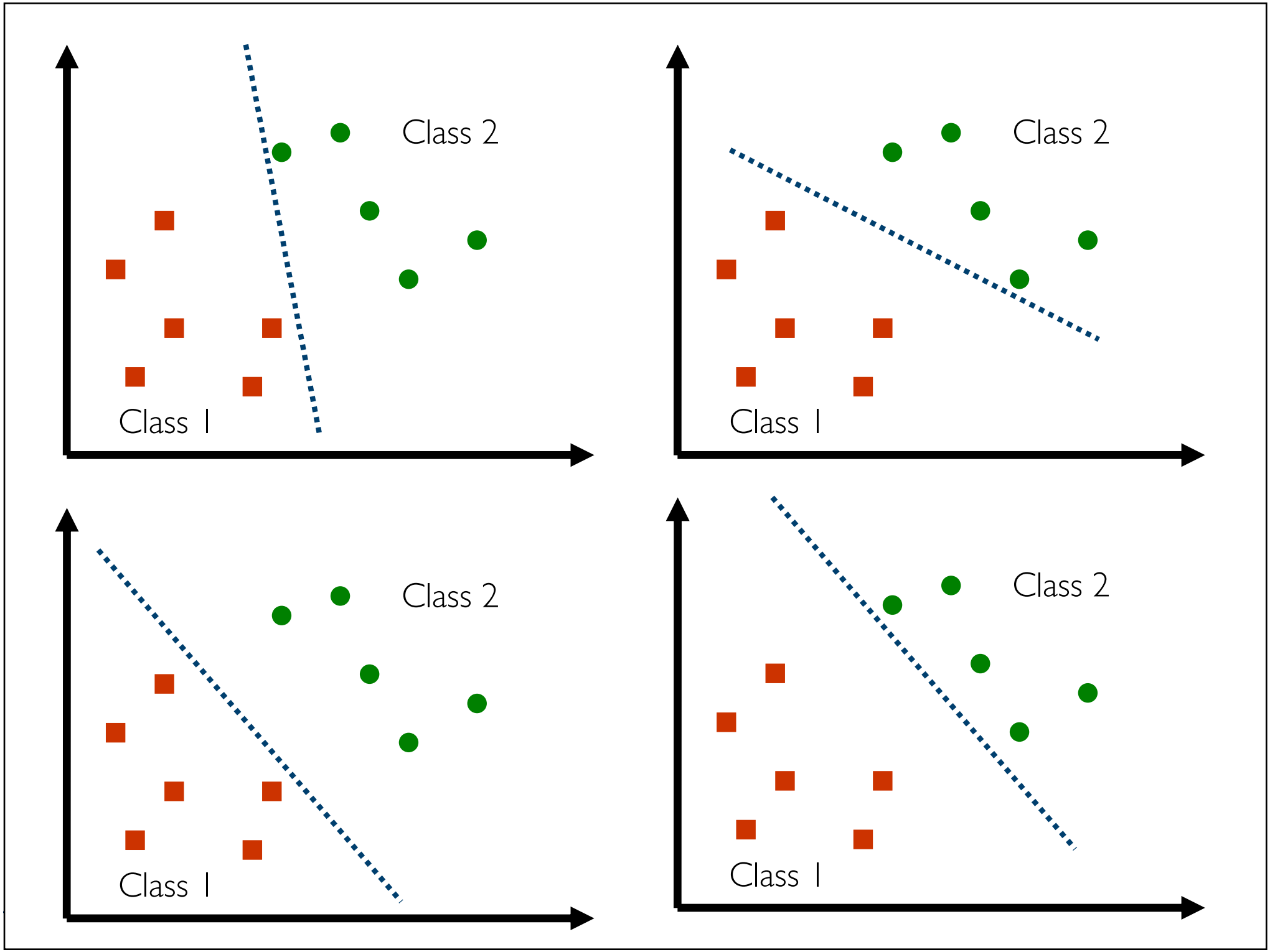
- They provide an approach for capturing prior knowledge of a particular domain using a graphical model
- Building the network is time consuming, but adding variables to a network is straightforward
- They can encode causal dependencies among variables
- They are well suited to dealing with incomplete data
- They are robust to overfitting

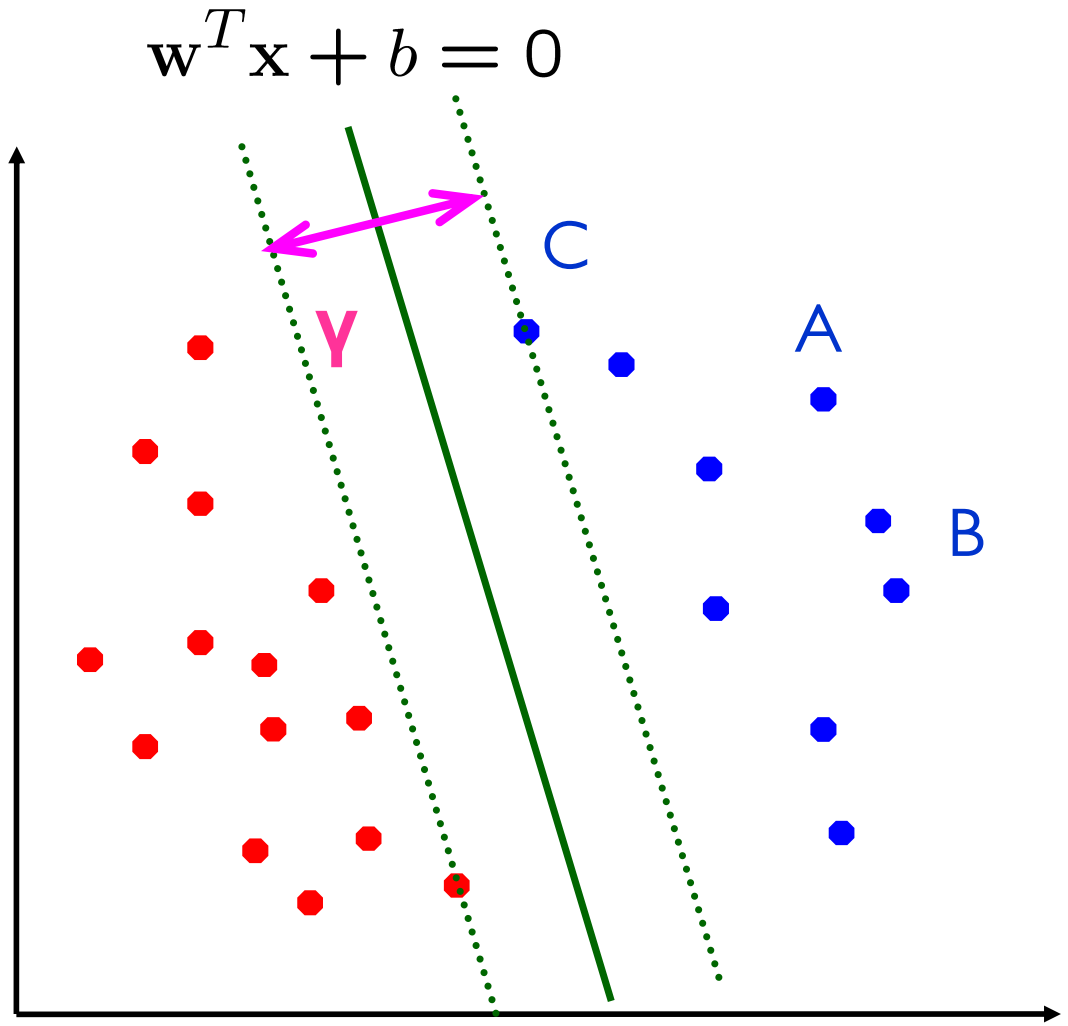
Support Vector Machines



Many decision boundaries can separate these two classes

Which one should we choose?


Class 2
Class 1
Class 2
Class 1
Class 2
Class 1
Class 2
Class 1



SVMs work by searching for the hyperplane that maximizes the margin or the largest γ such that

$$\forall i, y_i(wx_i + b) \geq \gamma$$