Machine Learning

Russell Chap. 18, 19, 20 Luger Chap. 10

Machine Learning

Definition

 Changes in a system that enable it to perform better on repetition of same task

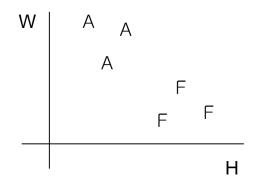
Types of learning

- Supervised learning
 - Given: cyamples
 Given: cyamples (labeled)
 - Learning: model rules, trees, neural nets to give the right answer
- Unsupervised learning
 - Given: cyroblem instanceexamples (unlabeled)
 - Learning: clusters, probability distributions
- Reinforcement learning
 - Given: <action, reward> experiences
 - Learning: rules for right action

Machine Learning

Supervised learning

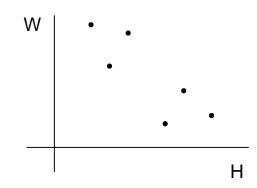
Н	W	Grade
185	65	F
162	80	Α
175	70	F
165	92	А



<187, 68> → ?

Unsupervised learning

Н	W
185	65
160	90
180	70
165	95



Group?

Supervised Learning

- Example: <x, f(x)>
 - X: input, f(X): output (f: target function)
- Learning
 - Given a set of examples
 - Find f (model or classifier)

Supervised Learning

- x = <size, color, shape>
- f(x) = Y/N (good obj?)
- <small, blue, cube> → N
- <large, blue, ball> → Y
- <large, red, cube> → N

✓ <large, red, ball> →

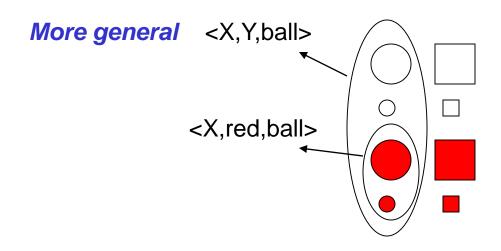
learning

If (shape = ball) then Y If (shape = cube) then N

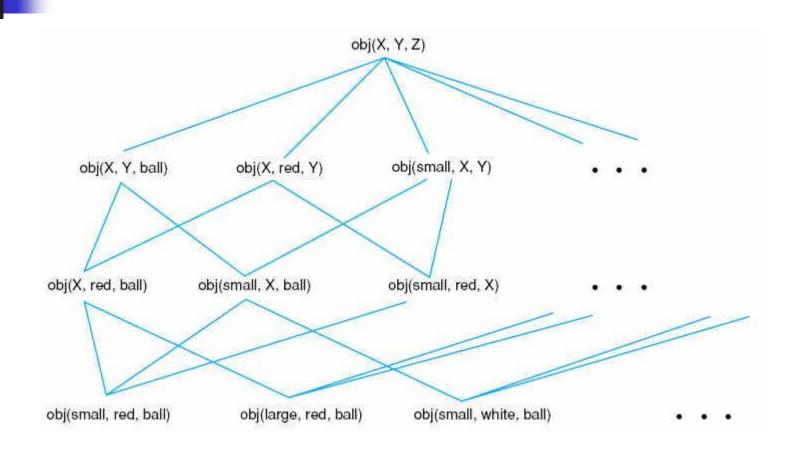
Learning Concepts

- Learning
 - Search through a concept space
- Concept representation
 - Conjunctive logical description
 ∀Y, color(Y, red) ∧ shape(Y, ball) → <X, red, ball>
- Concept space
 - a set of descriptions with a partial ordering by generality
 X, Y, ball> is more general than <X, red, ball>

Concept Representation



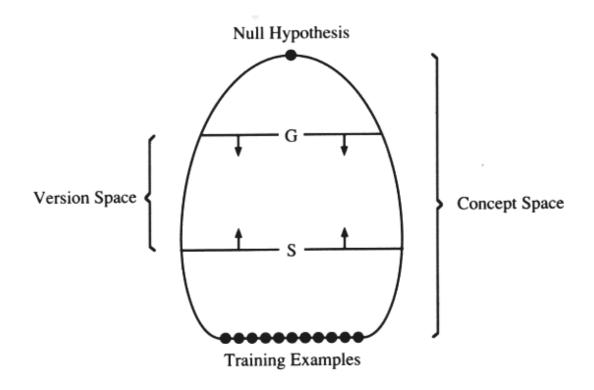
Concept Space



Version Space

- Version space
 - a set of descriptions consistent with example concepts
- Consistent concept example
 - Training examples
 - <small, red, ball> → Y
 - <large, red, ball> → Y
 - <small, red, cube> → N
 - Consistency
 - <X, red, ball>, <X, Y, ball>, ...: Consistent (gives correct answer)
 - <X, red, Z>, <small, red, Z>, ... : Inconsistent

Version Space Search



Version Space Search

Algorithm

- G: Most general description consistent with examples
- S: Most specific descriptions consistent with examples
 - Start with G = most general, S = ∅
 - For positive examples: Make S more general
 - For negative examples: Make G more specific
 - Until G = S



Version Space Search

Generalization by a positive example

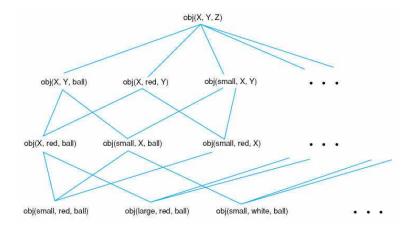
Specialization by a negative example

```
G: \langle X, Y, Z \rangle
S: Ø
                                                       +: <small, red, ball>
G: \langle X, Y, Z \rangle
S: <small, red, ball>
                                                       -: <small, blue, ball>
G: <a href="https://www.com/scales.com/">large, Y, Z> <X, red, Z> <X, Y, cube></a>
S: <small, red, ball>
                                                       +: <large, red, ball>
G: \langle X, \text{ red}, Z \rangle
S: <X, red, ball>
                                                       -: <large, red, cube>
G: <small, red, Z> <X, red, ball>
S: <X, red, ball>
```

Limitation

Binary function

- Learning Y(concept)/N(not concept) function only Ex> f(x): x → A or B or C?
- Conjunctive function description
 - Learning conjunctive description only Ex> f(x) = (a ∧ b) ∨ c ?



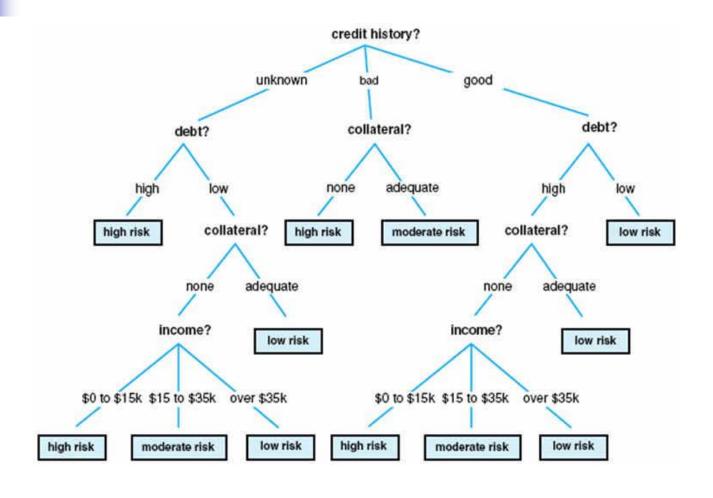
Decision Tree

Decision tree

- Representing the model(classifier) as a tree
 - $X : (A_1, A_2, ..., A_n), f(X) = C_1 \text{ or } C_2 \text{ or } ... C_m$
 - Internal nodes: attributes (A_i)
 - Edges: different attribute values
 - Leaves: answer (C_k)

$$X = \langle large, red, ball \rangle \longrightarrow \begin{cases} color? \\ blue \\ N \end{cases}$$
 $shape? \\ ball \\ Y \end{cases} N$

NO.	RISK	CREDIT HISTORY	DEBT	COLLATERAL	INCOME
1.	high	bad	high	none	\$0 to \$15k
2.	high	unknown	high	none	\$15 to \$35k
3.	moderate	unknown	low	none	\$15 to \$35k
4.	high	unknown	low	none	\$0 to \$15k
5,	low	unknown	low	none	over \$35k
6.	low	unknown	low	adequate	over \$35k
7.	high	bad	low	none	\$0 to \$15k
8.	moderate	bad	low	adequate	over \$35k
9,	low	good	low	none	over \$35k
10.	low	good	high	adequate	over \$35k
11.	high	good	high	none	\$0 to \$15k
12.	moderate	good	high	none	\$15 to \$35k
13.	low	good	high	none	over \$35k
14.	high	bad	high	none	\$15 to \$35k



Decision Tree Learning

Goal

Build the (smallest) decision tree consistent with examples

```
<small, red, ball> → Y
<small, blue, ball> → N
<large, red, ball> → Y
<large, red, cube> → N

color?
blue
red
shape?
ball
cube
Y
N
```

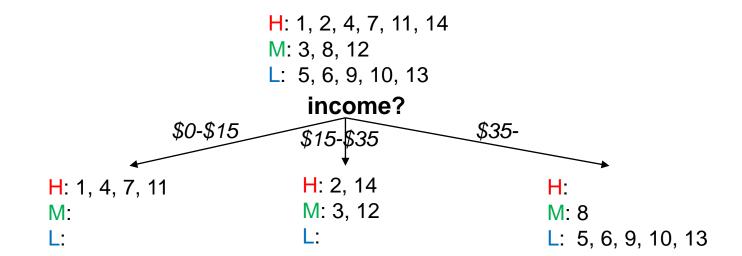
Method

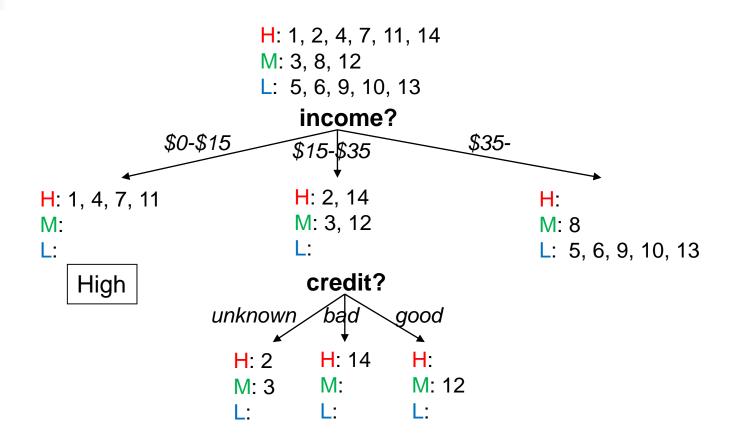
Recursively choose an attribute and split examples

Decision Tree Learning

```
function BuildTree (e: set of examples)
   if (all examples \in C_k) return a leaf node C_k
   if (no example left) return majority class from parent
   if (no attribute left) return majority class
                                                                 BuildTree(e)
   else
        root ← choose an attribute A
       for each value v<sub>i</sub> of A
           e_i \leftarrow examples with A = v_i
                                                     BuildTree(e<sub>1</sub>) BuildTree(e<sub>2</sub>)
           subtree ← BuildTree (e<sub>i</sub>)
            add branch v<sub>i</sub> and subtree
        return (root)
```

NO.	RISK	CREDIT HISTORY	DEBT	COLLATERAL	INCOME
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13.	low	good	high	none	over \$35k
14.	high	bad	high	none	\$15 to \$35k



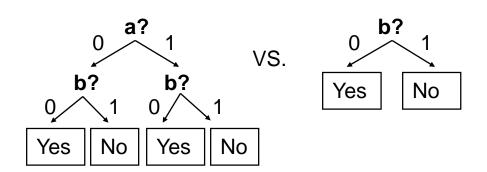


Selection of Attributes

■ Different selection → different tree

■
$$(a=0, b=0) \rightarrow Yes$$

 $(a=0, b=1) \rightarrow No$
 $(a=1, b=0) \rightarrow Yes$
 $(a=1, b=1) \rightarrow No$



Rule

- Select A that classifies most examples
- Selection based on information theory

- Amount of information
 - Depend on the probability
 - Example> Rolling a die
 Knowing that output is 2 (prob.=1/6) → most information
 Knowing that output is even (prob.=1/2)
 Knowing that output is 1~6 (prob.=1) → zero information
 - Low prob. → high info.
 - Prob. 1 → 0 info.

$$I(m) = \log_2(\frac{1}{p(m)}) = -\log_2(p(m))$$

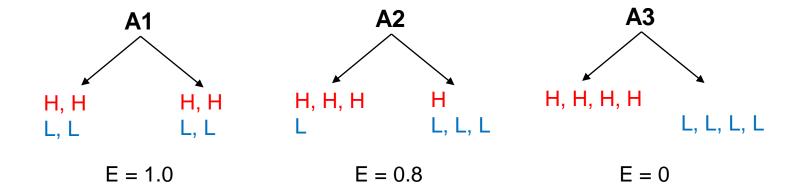
- Entropy of a set
 - $M = \{m_1, m_2, \dots, m_n\}, m_i \text{ has probability } p(m_i)$
 - E(M) = expected amount of information

$$E(M) = \sum p(m_i)/(m_i) = \sum -p(m_i)\log(p(m_i))$$

- Examples
 - M: {H(1,2), L(3,4)} $\rightarrow E(M) = \left(-\frac{1}{2}\log\frac{1}{2}\right) + \left(-\frac{1}{2}\log\frac{1}{2}\right) = 1.0$
 - M: {H(1,2,3), L(4)} $\rightarrow E(M) = \left(-\frac{3}{4}\log\frac{3}{4}\right) + \left(-\frac{1}{4}\log\frac{1}{4}\right) = 0.81$
 - M: {H(1,2,3,4), L()} $\rightarrow E(M) = \left(-\frac{4}{4}\log\frac{4}{4}\right) + \left(-\frac{0}{4}\log\frac{0}{4}\right) = 0.0$

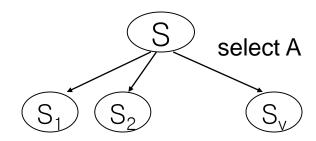
-

H, H, H, H
L, L, L, L
$$E = -1/2\log 1/2 - 1/2\log 1/2 = 1.0$$



- \rightarrow A1 < A2 < A3 reduces more entropy
- A1 < A2 < A3 has more information for H/L decision

- Attribute selection
 - Select A that reduces entropy most
 - Entropy = $0 \rightarrow$ all examples are in one category \rightarrow leaf
 - Gain = current entropy expected entropy after check A
 - Select A with largest gain



$$Gain(A) = E(S) - \sum \frac{|S_i|}{|S|} E(S_i)$$

$$S = \{H(1,2,4,7,11,14), M(3,8,12), L(5,6,9,10,13)\}$$

E(S) =
$$\left(-\frac{6}{14}\log\frac{6}{14}\right) + \left(-\frac{3}{14}\log\frac{3}{14}\right) + \left(-\frac{5}{14}\log\frac{5}{14}\right) = 1.53$$

If we select A = income,

$$E(S_1) = \left(-\frac{4}{4}\log\frac{4}{4}\right) + 0 + 0 = 0.0$$

E(S₂) =
$$\left(-\frac{2}{4}\log\frac{2}{4}\right) + \left(-\frac{2}{4}\log\frac{2}{4}\right) + 0 = 1.0$$

E(S₃) =
$$0 + \left(-\frac{1}{6}\log\frac{1}{6}\right) + \left(-\frac{5}{6}\log\frac{5}{6}\right) = 0.65$$

Gain(A=income) =
$$1.53 - \left(\frac{4}{14} \times 0.0 + \frac{4}{14} \times 1.0 + \frac{6}{14} \times 0.65\right) = 0.97$$

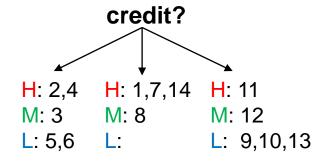
$$S = \{H(1,2,4,7,11,14), M(3,8,12), L(5,6,9,10,13)\}$$

Gain(A=income) = 0.97

Gain(A=credit) =0.27

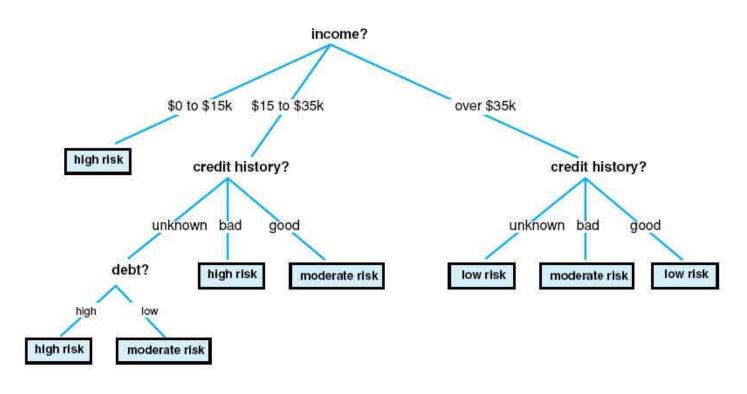
Gain(A=debt) = 0.58

Gain(A=collateral) = 0.76



Select 'income' for partition

Result tree



Gain Ratio

Problem

 Information gain measure is biased towards attributes with a large number of values

GainRatio

Normalization to information gain

$$SplitInfo_{A}(S) = -\sum_{j=1}^{\nu} \frac{|S_{j}|}{|S|} \times \log(\frac{|S_{j}|}{|S|})$$

 $GainRatio(A) = Gain(A) / SplitInfo_A$

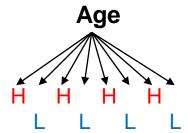
$$Gain = 0.46$$
 Sex
$$SplitInfo = 1.0$$

$$GainRatio = 0.46$$

$$H,H,H,H,H,H$$

$$L$$

$$L,L,L,L,L,L,L$$



Gain = 1.0 SplitInfo = 3.0GainRatio = 0.33

Gini Impurity

- CART (classification and regression tree) algorithm
 - Gini impurity is a measure of how often a randomly chosen element from the set would be incorrectly labeled
 - The Gini impurity can be computed by summing the probability p_i of an item with label i

Gini Index: $\sum_{k
eq i} p_k = 1 - p_i$

Gini Impurity

Attribute Selection

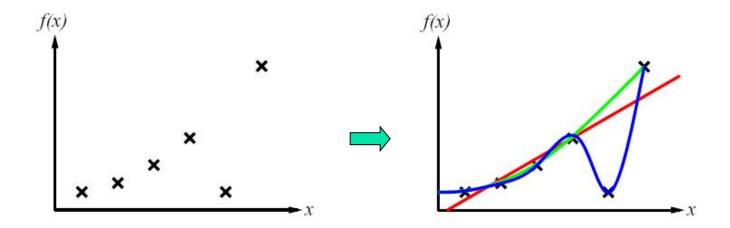
■ To compute Gini impurity for a set of items with J classes, suppose $i \in \{1, 2, ..., J\}$, and let p_i be the fraction of items labeled with class i in the set

$$I_G(p) = \sum_{i=1}^J p_i \sum_{k
eq i} p_k = \sum_{i=1}^J p_i (1-p_i) = \sum_{i=1}^J (p_i - p_i{}^2) = \sum_{i=1}^J p_i - \sum_{i=1}^J p_i{}^2 = 1 - \sum_{i=1}^J p_i{}^2$$

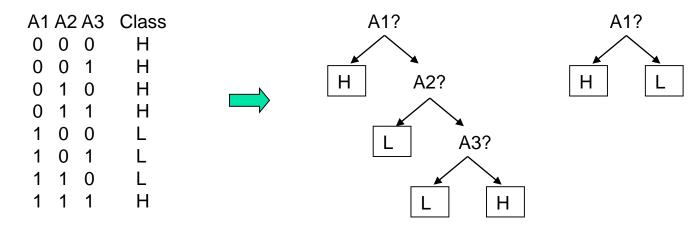
- Select A that reduces Impurity is most small
 - Impurity = 0 → all examples are in one category → leaf

Overfitting

- The generated model may overfit to the training data
 - Too many branches, some may reflect anomalies due to noise or outliers
 - Result is in poor accuracy for unseen samples



Pruning



Prepruning

- Halt tree construction early
- Do not split a node if this would result in the goodness measure falling below a threshold

Postpruning

- Remove branches from a "fully grown" tree
- If pruning a node lead to a smaller error rate (with test set), prune it

Performance of Learning

Performance measure

- 1. Collect set of examples
- 2. Divide it into training set / test set
- 3. Learning by using training set
- 4. Measure the % of correct answer on test set

K-fold cross-validation

- Divide the data set into k subsets
- Use k-1 subsets as training data and 1 subset as test data
- Repeat k times, and average the accuracy

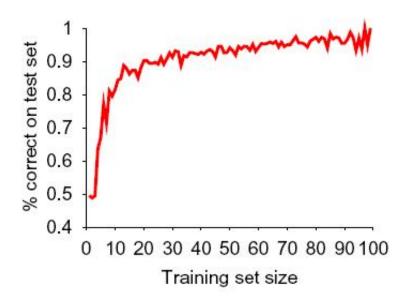
$$S_1, S_2, S_3, S_4, S_5$$

 S_1, S_2, S_3, S_4, S_5
 S_1, S_2, S_3, S_4, S_5

Performance of Learning

The learning curve

 Measure the % of correct classification with different size of randomly selected training sets



WEKA

Machine learning/data mining software written in Java

- http://www.cs.waikato.ac.nz/ml/weka
- Used for research, education, and applications
- Complements "Data Mining" by Witten & Frank

Main features

- Comprehensive set of data pre-processing tools, learning algorithms and evaluation methods
- Graphical user interfaces (incl. data visualization)
- Environment for comparing learning algorithms

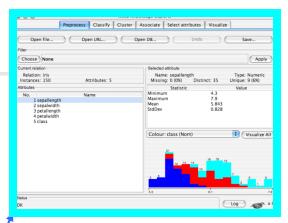
Data Files (ARFF)

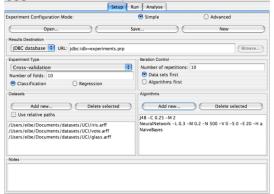
- @relation heart-disease-simplified
- @attribute age numeric
- @attribute sex {female, male}
- @attribute chest_pain_type {typ_angina, asympt, non_anginal, typ_angina}
- @attribute cholesterol numeric
- @attribute exercise_induced_angina {no, yes}
- @attribute class {present, not_present}
- @data
- 63,male,typ_angina,233,no,not_present
- 67,male,asympt,286,yes,present
- 67, male, asympt, 229, yes, present

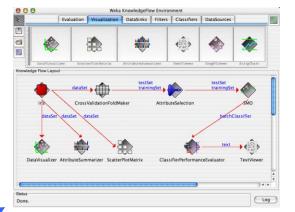
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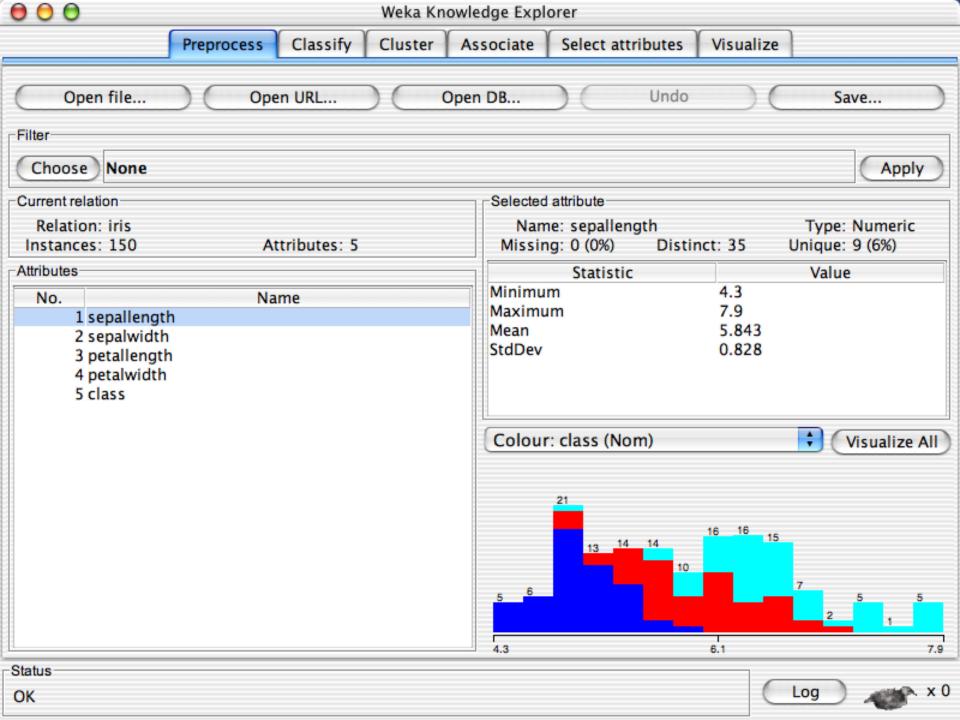


Source

- Data can be imported from a file in various formats: ARFF, CSV, C4.5, binary
- Data can also be read from a URL or from an SQL database (using JDBC)

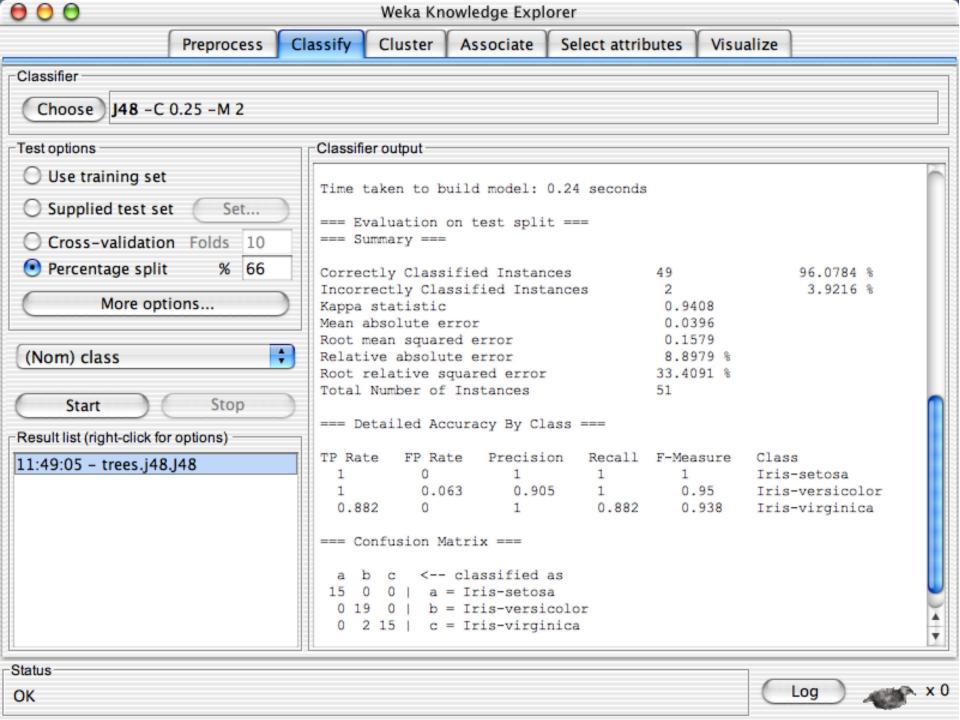
Pre-processing tools

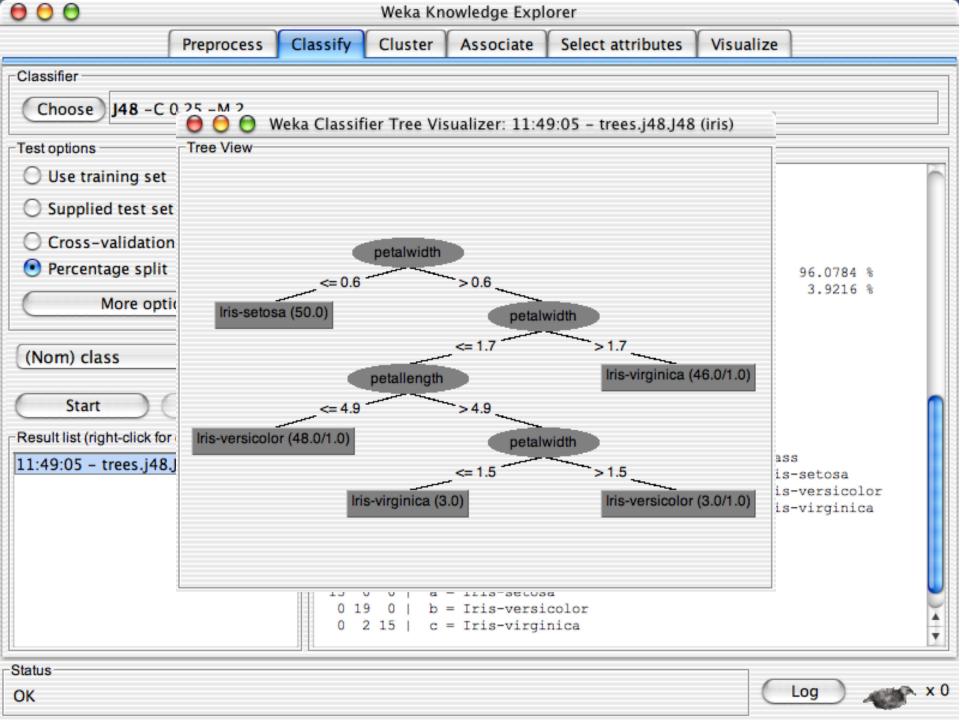
- Called "filters"
- Discretization, normalization, resampling, attribute selection, transforming and combining attributes, ...

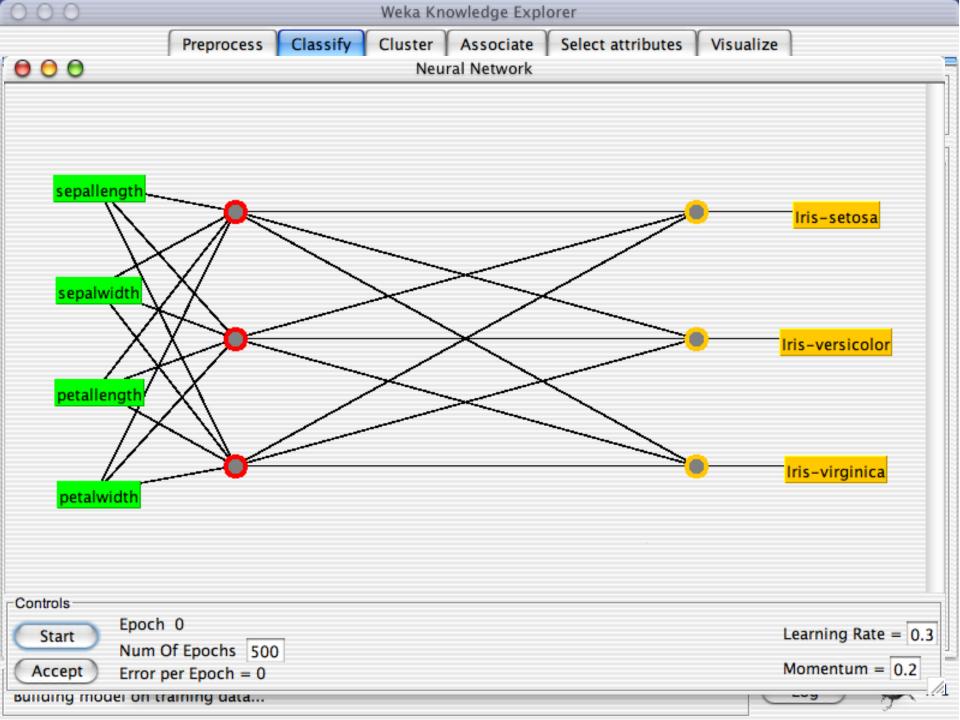


Explorer: building "classifiers"

- Classifiers in WEKA are models for predicting nominal or numeric quantities
- Implemented learning schemes include:
 - Decision trees and lists, instance-based classifiers, support vector machines, multi-layer perceptrons, logistic regression, Bayes' nets, ...
- "Meta"-classifiers include:
 - Bagging, boosting, stacking, error-correcting output codes, locally weighted learning, ...





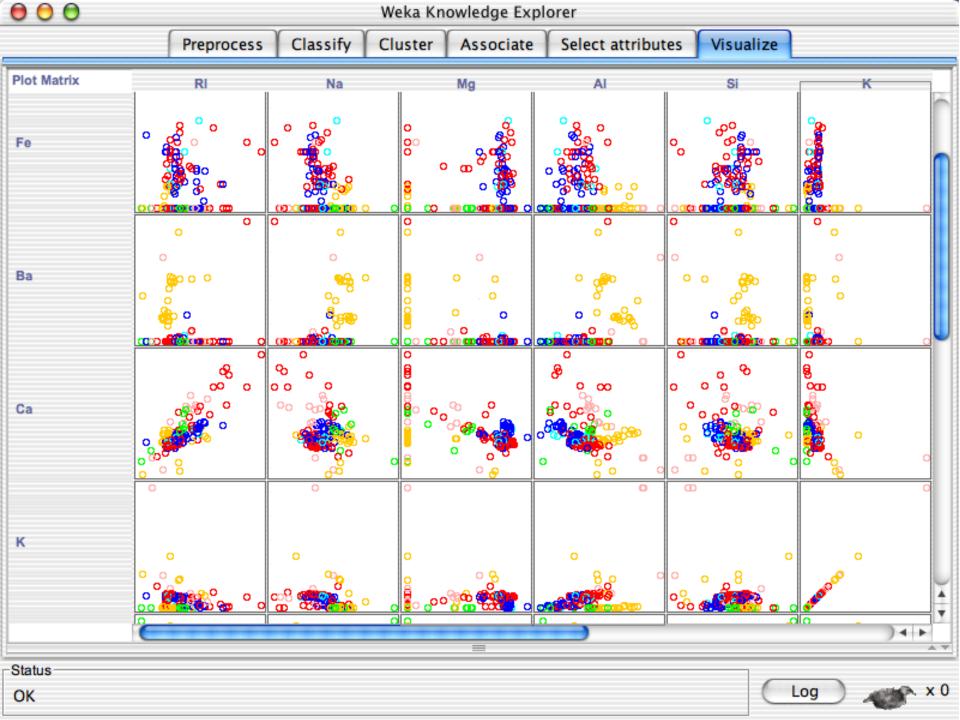


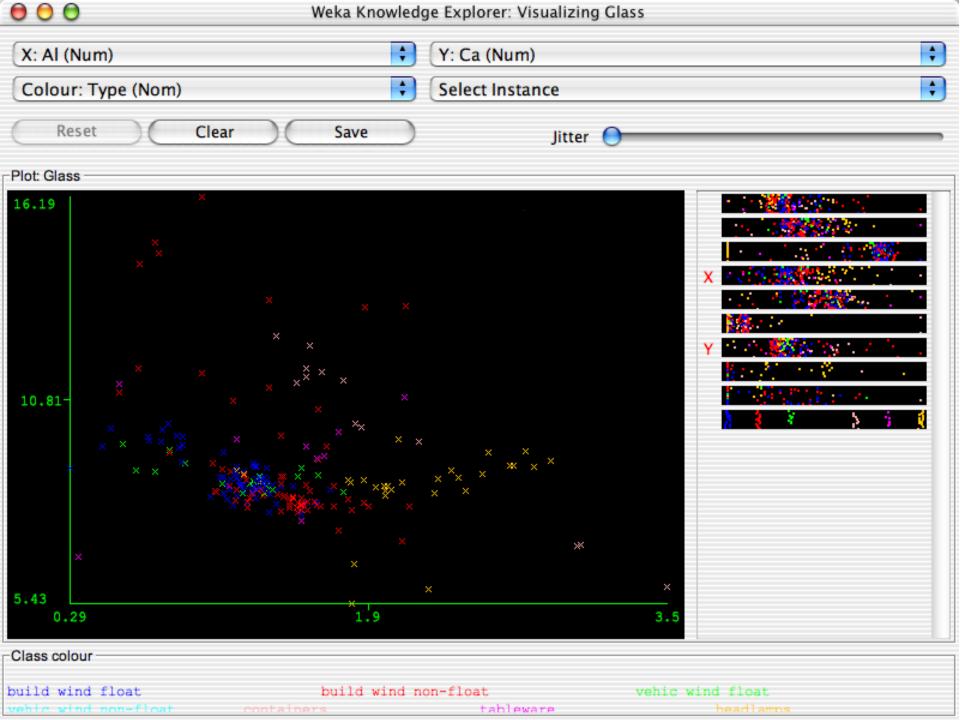


- WEKA contains "clusterers" for finding groups of similar instances in a dataset
- Implemented schemes are:
 - *k*-Means, EM, Cobweb, *X*-means, FarthestFirst
- Clusters can be visualized and compared to "true" clusters (if given)
- Evaluation based on loglikelihood if clustering scheme produces a probability distribution

Explorer: data visualization

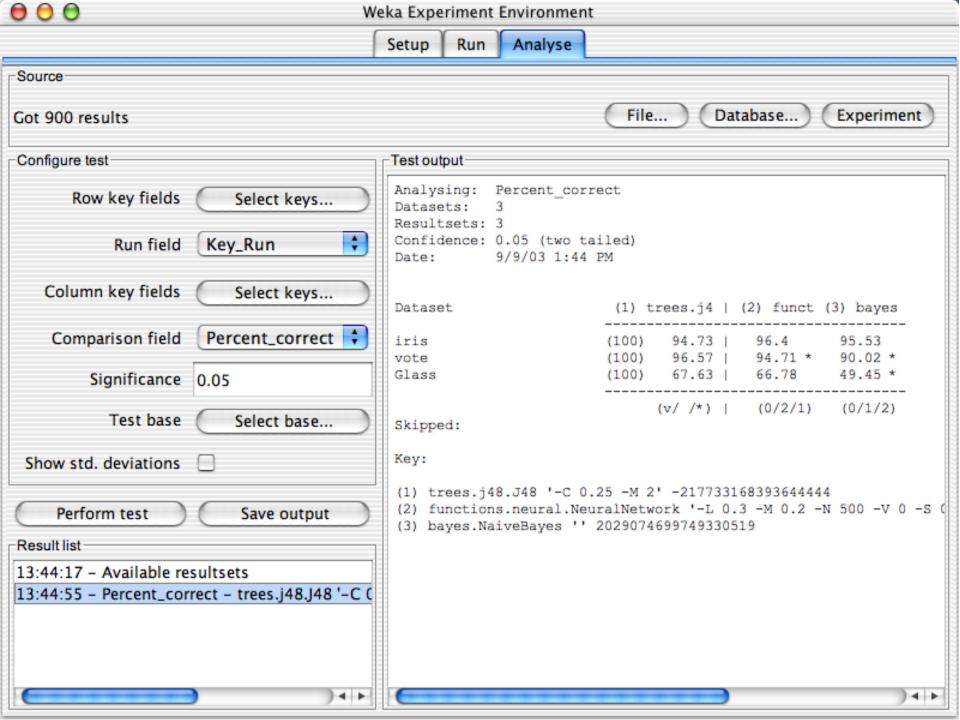
- Visualization very useful in practice: e.g. helps to determine difficulty of the learning problem
 - WEKA can visualize single attributes (1-d) and pairs of attributes (2-d)
 - Color-coded class values
 - "Jitter" option to deal with nominal attributes (and to detect "hidden" data points)
 - "Zoom-in" function





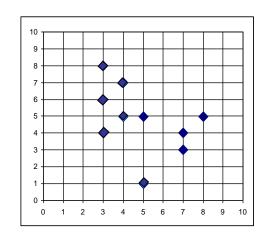


- Experimenter makes it easy to compare the performance of different learning schemes
 - For classification and regression problems
 - Results can be written into file or database
 - Evaluation options: cross-validation, learning curve, hold-out
 - Can also iterate over different parameter settings
 - Significance-testing built in!



Unsupervised Learning

Class labels are not provided



Clustering

K-Means Method

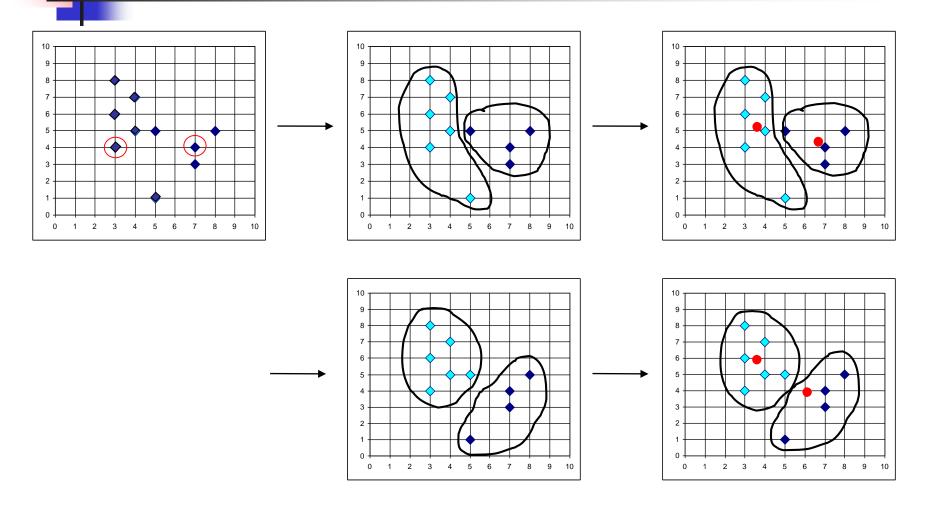
K-means

- Input: a set of unclassified data objects
- Output: k clusters

Algorithm

- Choose k objects as initial cluster centers
- 2. Assign each object to the cluster with the nearest center
- 3. Update cluster centers as the mean point of the cluster
- 4. Go back to Step 2, stop when there is no change

K-Means Method

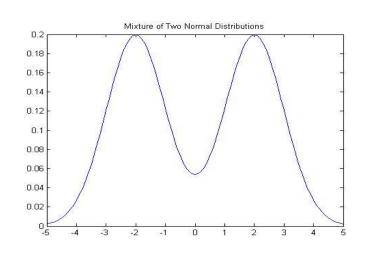


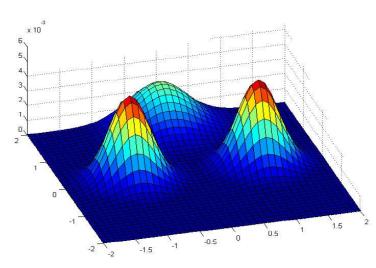
Assumption

 Data are generated from a mixture distribution with k components (C₁, ..., C_k)

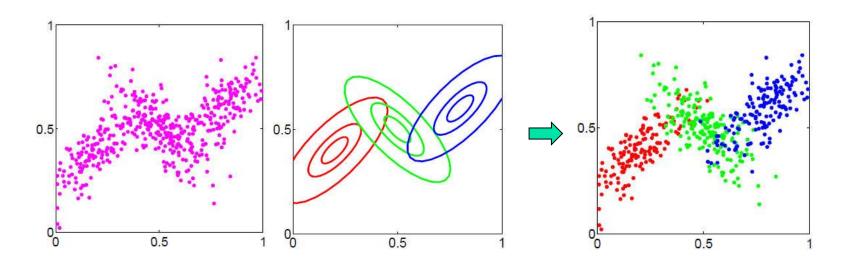
$$P(x) = \sum_{i} P(C_i) P(x \mid C_i)$$

EX> Mixture Gaussian





- Clustering = finding the unknown distribution
 - If we assume mixture Gaussian, find
 - $W_i : P(C_i)$
 - μ_i: mean of C_i
 - σ_i : variance of C_i



Finding C_i

- If we know C_i (w_i , μ_i , σ_i) \rightarrow We can find which C_i generate x
- If we know which C_i generate x \rightarrow We can find C_i (w_i, μ_i , σ_i)

Basic idea

- Assume C_i
- Repeat:
 - Assign cluster (according to $p(C_i | x)$)
 - Compute new C_i (w_i , μ_i , σ_i)

- Expectation
- **Maximization**

- Algorithm (Mixture Gaussian)
 - Initialize C_i (w_i, μ_i, σ_i) arbitrarily
 - Repeat:
 - E-step

$$p_{ij} = P(C_i \mid x_j) = \alpha P(x_j \mid C_i) P(C_i)$$

M-step

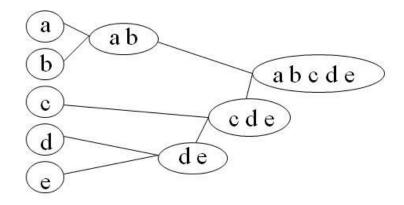
$$w_i = p_i = \sum_j p_{ij}$$

$$\mu_i = \sum_j \frac{p_{ij}}{p_i} x_j$$

$$\sigma_i = \sum_j \frac{p_{ij}}{p_i} (x_j - \mu_i)^2$$

Hierarchical Clustering

Find a hierarchical cluster structure



- Conceptual clustering
 - Input: a set of unclassified objects
 - Output: a hierarchy of classes (clusters)
 - Goal: maximize the similarity of objects in the same class

Hierarchical Clustering

COBWEB

- Use Category utility
 - $C = \{C_1 .. C_p\}$ categories
 - $A = \{A_1 ... A_n\}$ attributes, each A_i has $\{V_{i1} ... V_{im}\}$ values

$$CU(C) = \frac{1}{p} \sum_{k} P(C_{k}) \left[\sum_{i} \sum_{j} P(A_{i} = V_{ij} \mid C_{k})^{2} - \sum_{i} \sum_{j} P(A_{i} = V_{ij})^{2} \right]$$

P(A=V | C): prob. of correctly guessing the value when we know the category labels

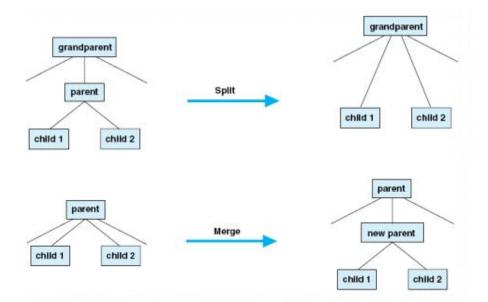
P(A=V) : prob. of correctly guessing the value without the knowledge of category structure

Hierarchical Clustering

COBWEB(C, i)

Compute CU of each case, and choose best

- 1. Put i in one subclass $C1 \rightarrow COBWEB(C1, i)$
- 2. Split a subclass C1 \rightarrow COBWEB(C, i)
- 3. Merge two subclass to $Cm \rightarrow COBWEB(Cm, i)$
- 4. Make a new subclass Cn





Category	C1	P(C1)=4/4
Feature	Value	p(vlc)
Tails	One	0.50
	Two	0.50
Color	Light Dark	0.50 0.50
Nudei	One Two Three	0.25 0.50 0.25

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Category	C2	P(C2)=1/4
Feature	Value	p(vlc)
Tails	One	1.0
	Two	0.0
Color	Light Dark	1.0 0.0
Nuclei	One Two Three	1.0 0.0 0.0

Category	Сз	P(C3)=2/4
Feature	Value	p(vlc)
Tails	One	0.0
	Two	1.0
Color	Light Dark	0.50 0.50
Nuclei	One Two Three	0.0 1.0 0.0
	$\sim$	

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Category	C4	P(C4)=1/4
Feature	Value	p(vlc)
Tails	One	1.0
	Two	0.0
Color	Light Dark	0.0 1.0
Nuclei	One Two Three	0.0 0.0 1.0

Category	C5	P(C5)=1/4
Feature	Value	p(vlc)
Tails	One	0.0
	Two	1.0
Color	Light	1.0
	Dark	0.0
Nuclei	One	0.0
Nuclei		1.0
	Two	
	Three	0.0

Category	C6	P(C6)=1/4
Feature	Value	p(vlc)
Tails	One	0.0
	Two	1.0
Color	Light	0.0
	Dark	1.0
Nuclei	One	0.0
	Two	1.0
	Three	0.0









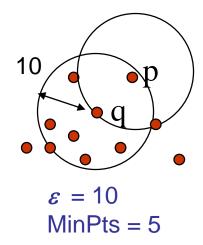
Density-Based Methods

- Group objects in dense region
 - Density parameters

Radius ε : distance to determine the neighborhood

MinPts: Minimum number of points in neighborhood

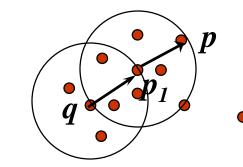
- Core object
 - *ε*-neighborhood contains *MinPts* objects
- Directly density-reachable
 - p is directly density-reachable from q
 if q is a core object, and
 p is ε-neighborhood of q





Density-reachable

• p is density-reachable from q if there are objects p₁(=q), p₂, ... p_n such that

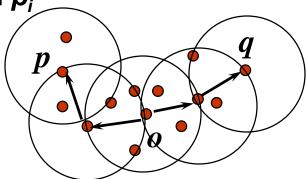


 p_{i+1} is directly density-reachable from p_i

Density-connected

p is density-connected to q if there is an object o such that

p and **q** are density-reachable from **o**





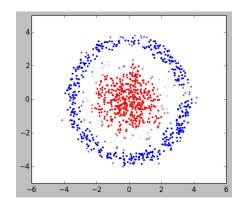
Density-Based Methods

DBSCAN

- Cluster a maximal set of density-connected points
 - Arbitrary select a point \boldsymbol{p} and retrieve all ε -neighborhood
 - 2. If **p** is a core object, a cluster is formed
 - From each core object **p**, iteratively collects directly density-reachable objects (may merge clusters)
 - 4. Continue the process until no new points can be added

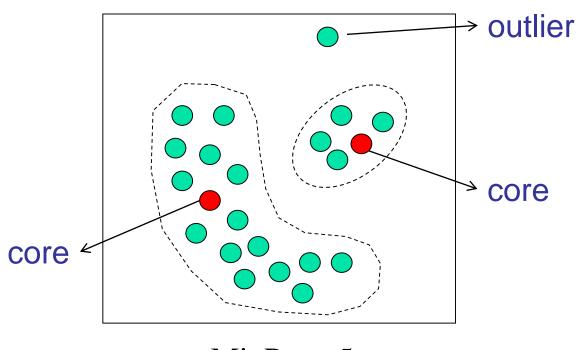
Major features

- Discover clusters of arbitrary shape
- Handle noise
- Problem: selecting parameters
 ε and MinPts



4

Density-Based Methods



MinPts = 5