

# Data Science

Deriving Knowledge from Data at Scale

Valentine N. Fontama

July 30<sup>th</sup>, 2015

Deriving Knowledge from Data at Scale



# PREDICTIVE ANALYTICS



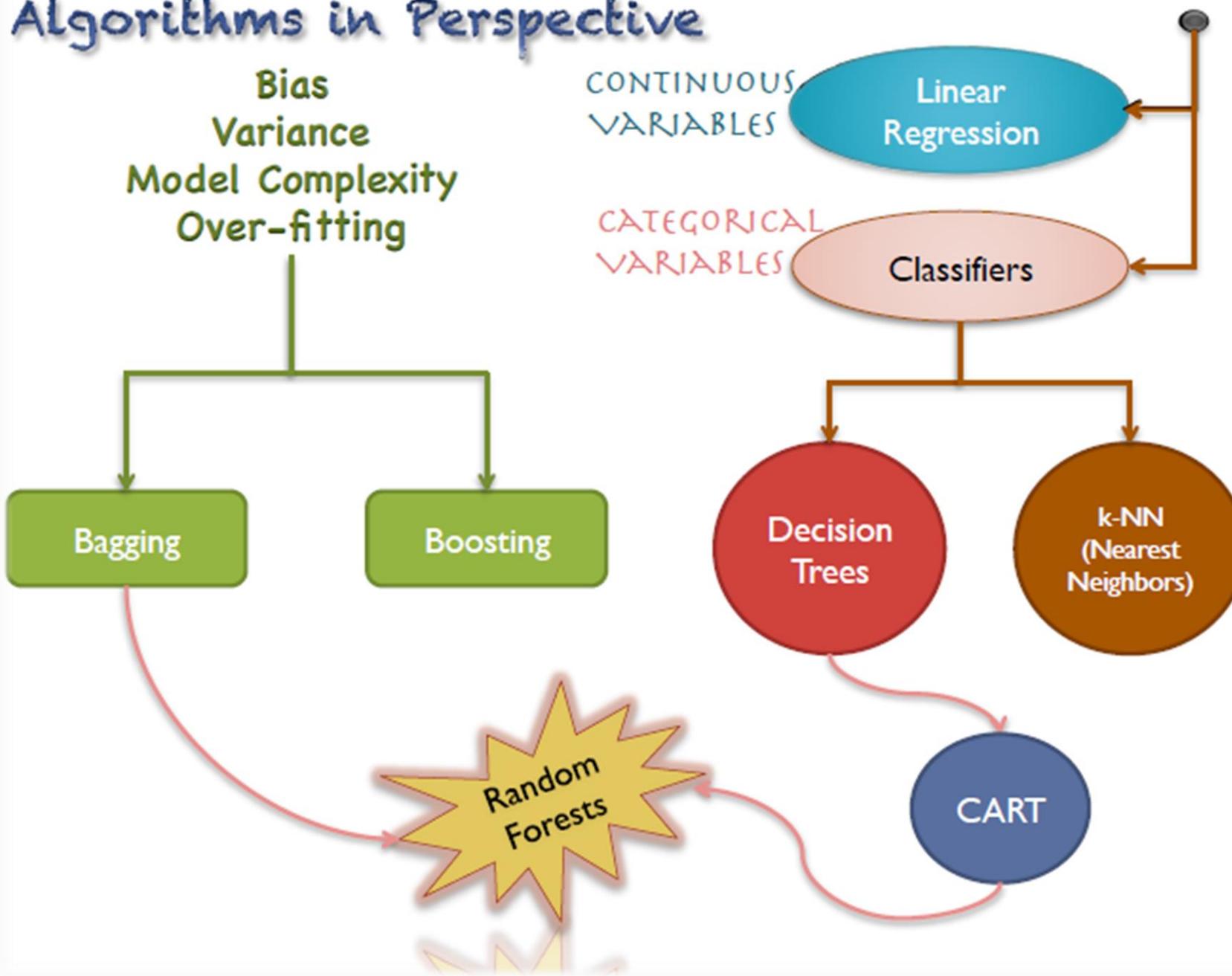
THE POWER TO PREDICT WHO WILL  
CLICK, BUY, LIE, OR DIE

ERIC SIEGEL

Read this... A brilliant read that offers an accessible overview of predictive analytics, technical but at the same time a recreational read with ample practical examples, and it provides footnotes for further study...

*I highly recommend it...*

# An Amateur Data Scientist's Algorithms in Perspective



## Review of Course Plan...

- W5: Clustering Review  
Clustering Assignment
- W6: Feature Select/Create  
SVMs & Regression  
Data Prep Assignment  
Kaggle Contest HW
- W7: SVMs Cont'd

# Lecture Outline

- Opening Discussion  
*Review Discussion...* 30 minutes
- Data Science Hands On 60 minutes
- Break 5 minutes
- Data Science Modelling  
*Model performance evaluation...* 30 minutes
- Machine Learning Boot Camp  
*Clustering, k-Means...* ~60 minutes
- Close

# Lecture 4 Homework

## Assignment: Decisions Trees and Classification

Due Date: July 30, 2015

### 1. Targeted Marketing Campaign

In this problem we will use historical data from past customer responses to build a classification model. In class next week we will apply the trained model to a new set of prospects to whom we may want extend an offer for a PEP. Rather than doing a mass marketing campaign to all new prospects, we would like to target those that are likely to respond positively to our offer (according to our classification model).

There is one data sets available, comma delimited, and the first row contains the field names):

- [bank-data.csv](#) - Preclassified training data Set for Building a Model



# Clustering

**Fundamental Concepts:** Calculating similarity of objects described by data; Using similarity for prediction; Clustering as similarity-based segmentation.

**Exemplary Techniques:** Searching for similar entities; Nearest neighbor methods; Clustering methods; Distance metrics for calculating similarity.

# Clustering

- Cluster images based on key features most useful for identification
- Use Cluster ID as index over images for exact match & retrieval



# Clustering

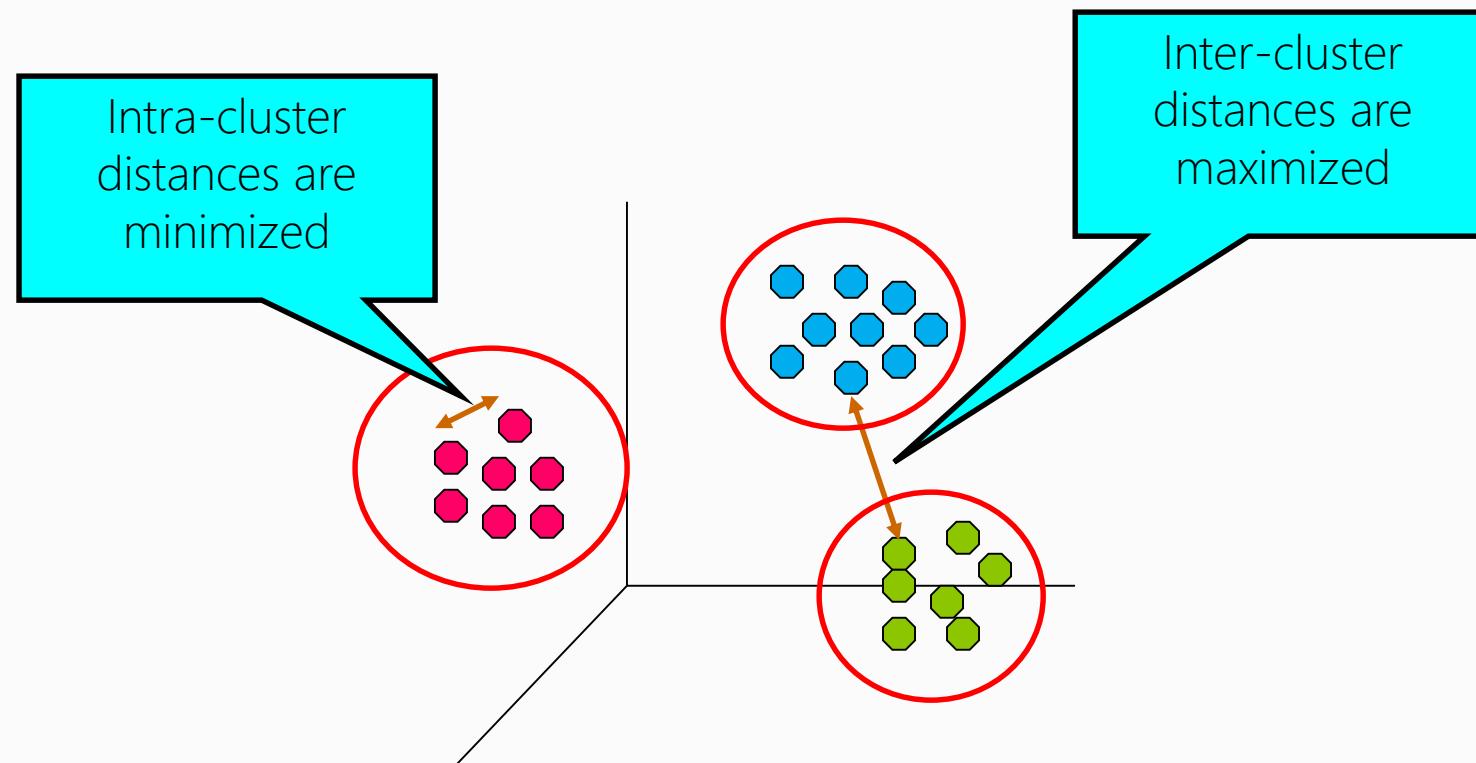
We may want to *retrieve* similar things directly. For example, IBM wants to find companies that are *similar to their best business customers*, in order to have sales staff look at them as prospects. Hewlett-Packard maintains many high performance servers for clients; this maintenance is aided by a tool that, given a server configuration, *retrieves information on other similarly configured servers*.

We may want to group similar items together into clusters, for example to see whether our *customer base contains groups of similar customers* and what these groups have in common.

Reasoning from similar cases of course extends beyond business applications; it is natural to fields such as medicine and law. A doctor may *reason about a new difficult case by recalling a similar case and its diagnosis*. A lawyer often argues cases by citing legal precedents, which are *similar historical cases whose dispositions were previously judged and entered into the legal casebook*.

# What is clustering?

A **grouping** of data objects such that the objects **within a group are similar** (or related) to one another **and different from** (or unrelated to) the objects in other groups

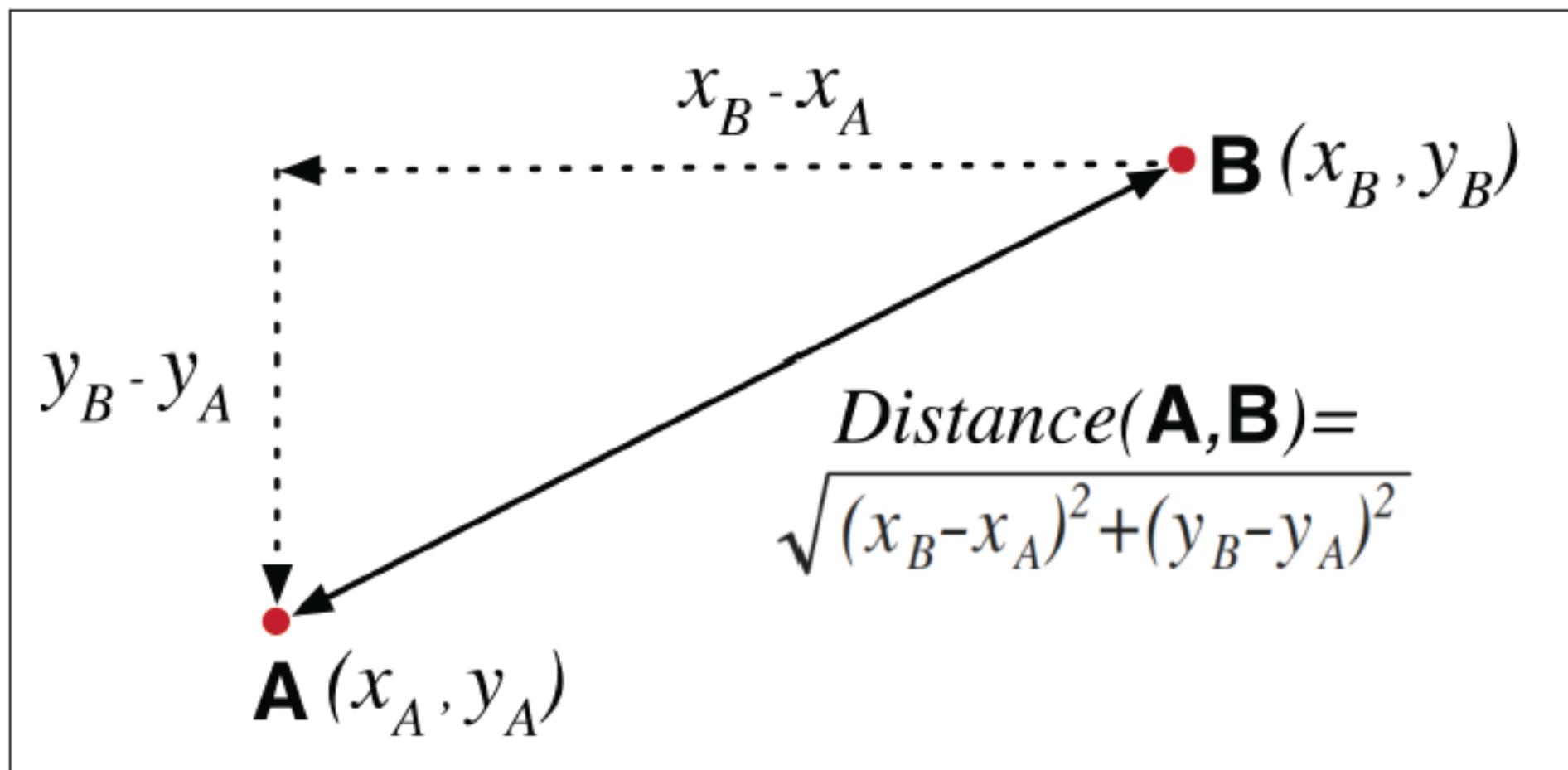


# How do we define “similarity”?

- Goal is to group together “similar” data – but what does this mean?
- No single answer, it depends on what we want to find or emphasize in the data; this is one reason why clustering is an “art”
- The similarity measure is often more important than the clustering algorithm used – don’t overlook this choice!
- There is no golden standard, depends on goal: data reduction, “natural clusters”, “useful” clusters, outlier detection, etc.

# Similarity Measures

- Euclidean Distance



# Similarity Measures

## Manhattan Distance

$$d_{\text{Manhattan}}(X, Y) = \| X - Y \|_1 = |x_1 - y_1| + |x_2 - y_2| + \dots$$

## Jaccard Distance

$$d_{\text{Jaccard}}(X, Y) = 1 - \frac{|X \cap Y|}{|X \cup Y|}$$

## Edit Distance

- |                     |                            |
|---------------------|----------------------------|
| 1. 1113 Bleaker St. | 1. Delete a 1,             |
| 2. 113 Bleecker St. | 2. Insert a c, and         |
|                     | 3. Replace an a with an e. |

# Lecture Outline

- Opening Discussion  
*Review Discussion...* 30 minutes
- **Data ScienceHands On** 60 minutes
- Break 5 minutes
- Data Science Modelling  
*Model performance evaluation...* 30 minutes
- Machine Learning Boot Camp  
*Clustering, k-Means...* ~60 minutes
- Close

# WEKA Explorer: clustering data

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);

# WEKA Explorer: clustering data (optional reading)



**International Journal of Emerging Technology and Advanced Engineering**  
Website: [www.ijetae.com](http://www.ijetae.com) (ISSN 2250-2459, Volume 2, Issue 5, May 2012)

## Comparison the various clustering algorithms of weka tools

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**Abstract—** Generally, data mining (sometimes called data or knowledge discovery) is the process of analyzing data from different perspectives and summarizing it into useful information. Data mining software is one of a number of analytical tools for analyzing data. It allows users to analyze data from many different dimensions or angles, categorize it, and summarize the relationships identified. Weka is a data mining tools. It is contain the many machine leaning algorithms. It is provide the facility to classify our data through various algorithms. In this paper we are studying the various clustering algorithms. Cluster analysis or clustering is the task of assigning a set of objects into groups (called clusters) so that the objects in the same cluster are more similar (in some sense or another) to each other than to

The main thing, why I am chooses WEKA, because we can work in weka easily without having the deep knowledge of data mining techniques.

### II. WHAT IS CLUSTER ANALYSIS?

Cluster analysis[1] groups objects (observations, events) based on the information found in the data describing the objects or their relationships. The goal is that the objects in a group will be similar (or related) to one other and different from (or unrelated to) the objects in other groups. The greater the likeness (or homogeneity) within a group, and the greater the disparity between groups, the “better” or

# Weka Explorer

Preprocess Classify **Cluster** Associate Select attributes Visualize

Open file... Open URL... Open DB... Generate... Undo Edit... Save...

Filter Choose None Apply

Current relation  
Relation: iris Instances: 150 Attributes: 5

Attributes  
All None Invert Pattern

No.	Name
1	<input checked="" type="checkbox"/> sepal length
2	<input type="checkbox"/> sepal width
3	<input type="checkbox"/> petal length
4	<input type="checkbox"/> petal width
5	<input type="checkbox"/> class

Remove

Status OK

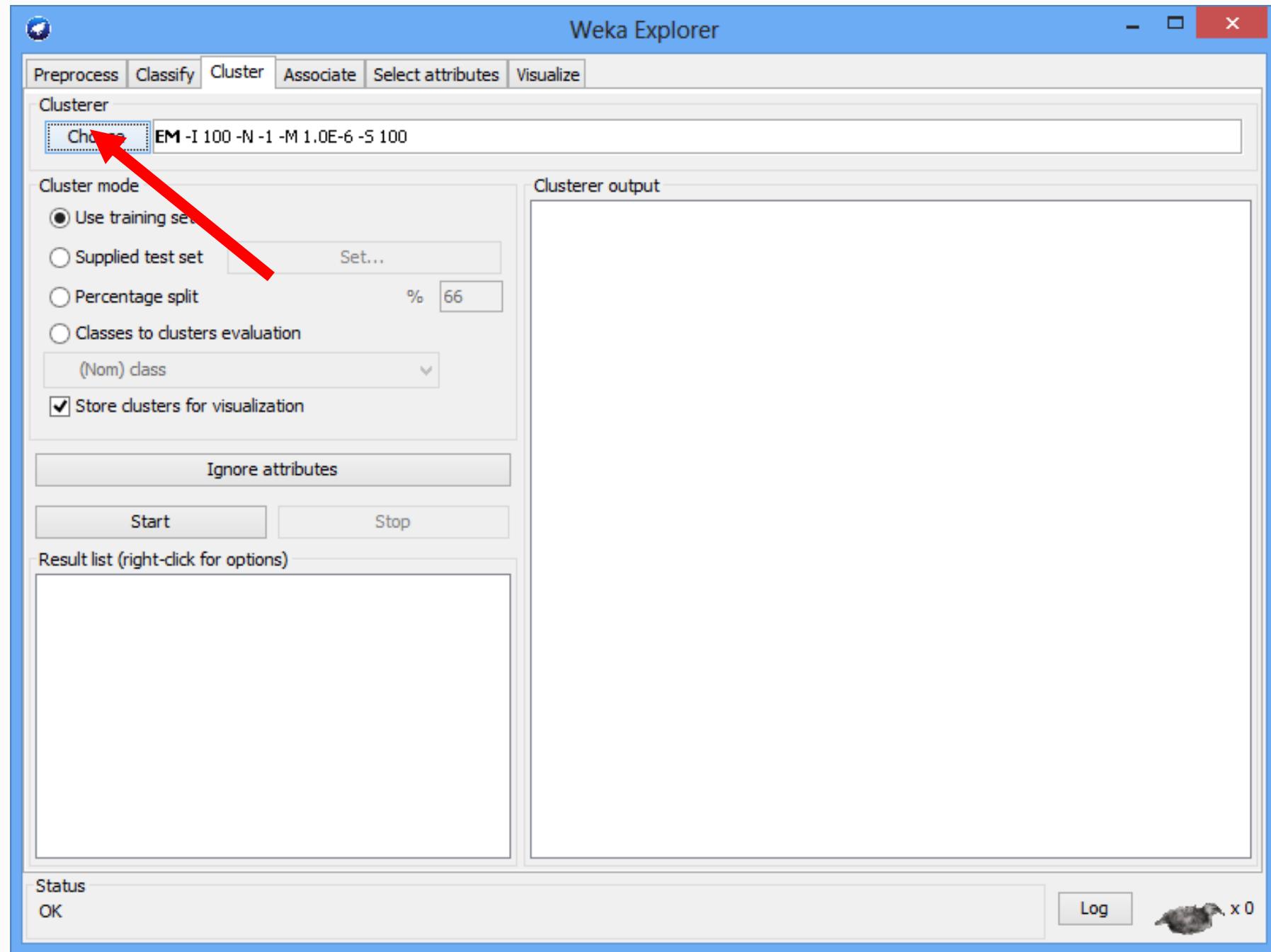
Selected attribute  
Name: sepal length Type: Numeric  
Missing: 0 (0%) Distinct: 35 Unique: 9 (6%)

Statistic	Value
Minimum	4.3
Maximum	7.9
Mean	5.843
StdDev	0.828

Class: class (Nom) Visualize All

4.3 6.1 7.9

Log  x 0



Preprocess

Classify

Cluster

Associate

Select attributes

Visualize

## Clusterer

- weka
- clusterers
  - EM
  - SimpleKMeans
  - Cobweb
  - FarthestFirst
  - XMeans

77387815

## Clusterer output

## Status

OK

Log



x 0



Preprocess

Classify

Cluster

Associate

Select attributes

Visualize

## Clusterer

Choose

Cobweb -A 1.0 -C 0.0028209479177387815

## Cluster mode

 Use training set Supplied test set

Set...

 Percentage split

% 66

 Classes to clusters evaluation

(Nom) class

 Store clusters for visualization

Ignore attributes

Start

Stop

## Result list (right-click for options)

## Clusterer output

## Status

OK

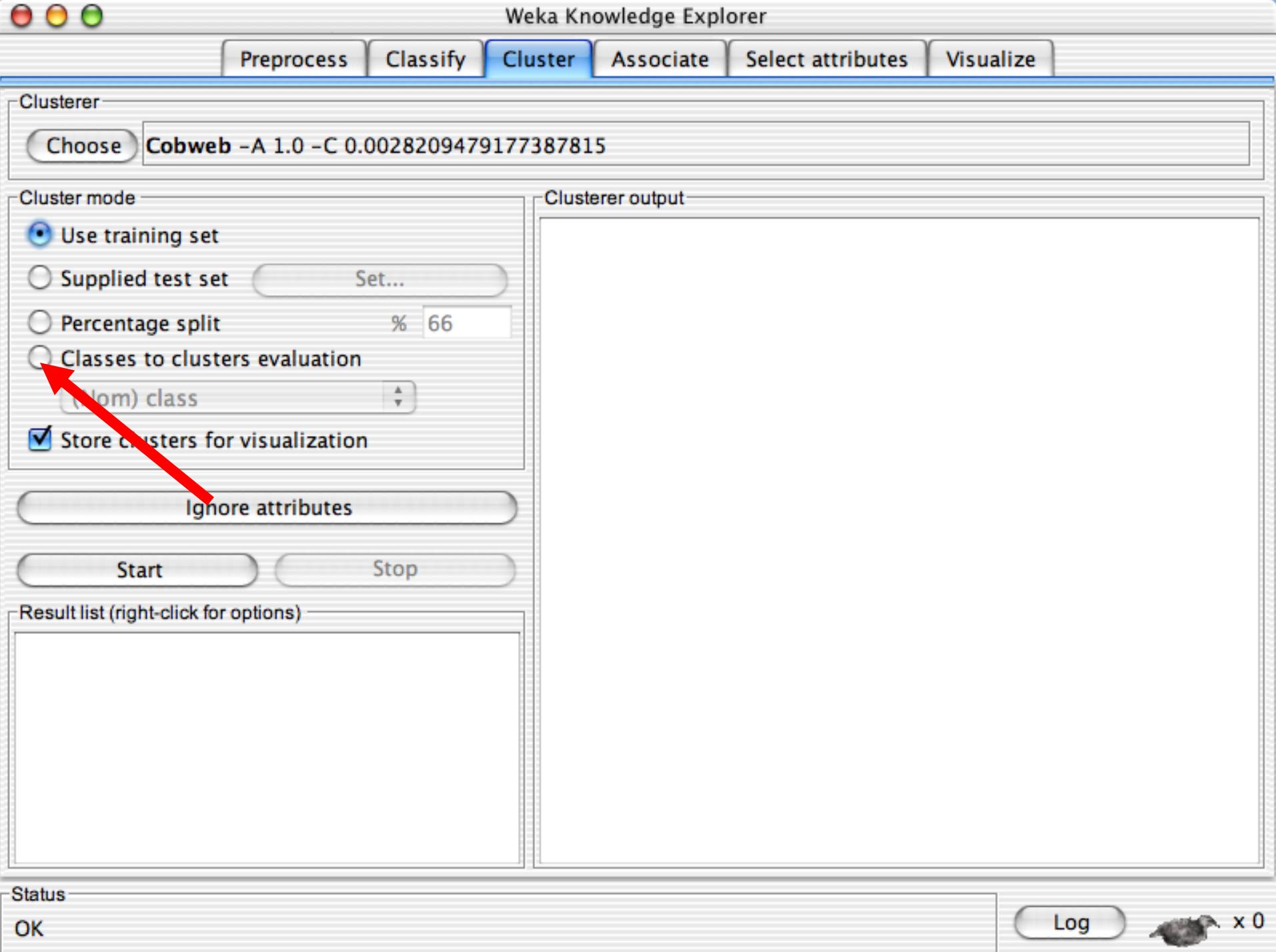
Log



x 0

Data at Scale





# Evaluation in WEKA

The way Weka **evaluates** clusterings depends on the cluster mode you select. Four different cluster modes are available (as buttons in the Cluster mode panel):

- **Use training set** (default). After generating the clustering Weka classifies the training instances into clusters according to the cluster representation and computes the percentage of instances falling in each cluster.
- In **Supplied test** set or **Percentage split** Weka can evaluate clusterings on separate test data.
- **Classes to clusters** evaluation. In this mode Weka first ignores the class attribute and generates the clustering. Then during the test phase it assigns classes to the clusters, based on the majority value of the class attribute within each cluster. Then it computes the classification error, based on this assignment and also shows the corresponding confusion matrix.



Preprocess

Classify

Cluster

Associate

Select attributes

Visualize

## Clusterer

Choose

Cobweb -A 1.0 -C 0.0028209479177387815

## Cluster mode

 Use training set Supplied test set [Set...](#) Percentage split % 66 Classes to clusters evaluation(Nom) class [▼](#) Store clusters for visualization

Ignore attributes

[Start](#)[Stop](#)

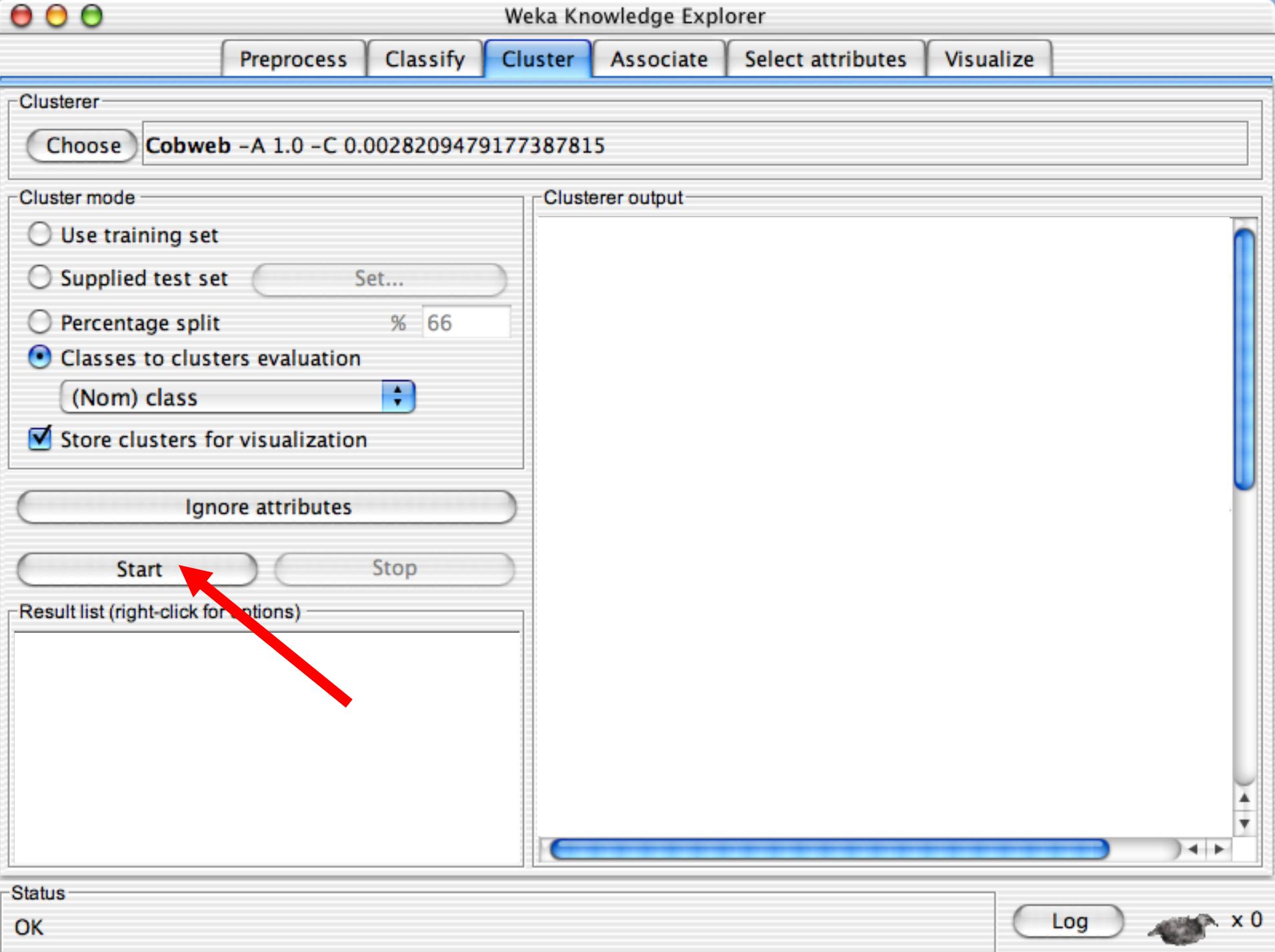
## Result list (right-click for options)

## Status

OK

Log





Weka Knowledge Explorer

Preprocess Classify Cluster Associate Select attributes Visualize

**Clusterer**

**Choose** Cobweb -A 1.0 -C 0.0028209479177387815

**Cluster mode**

Use training set

Supplied test set Set...

Percentage split % 66

Classes to clusters evaluation  
(Nom) class

Store clusters for visualization

**Ignore attributes**

**Start** **Stop**

**Result list (right-click for options)**

16:05:58 - Cobweb

**Status**

OK

**Clusterer output**

```
==== Run information ====
Scheme: weka.clusterers.Cobweb -A 1.0 -C 0.0028209479177387815
Relation: iris
Instances: 150
Attributes: 5
sepallength
sepalwidth
petallength
petalwidth
Ignored:
class
Test mode: Classes to clusters evaluation on training data
==== Clustering model (full training set) ====
Number of merges: 0
Number of splits: 0
Number of clusters: 3
node 0 [ 150]
| leaf 1 [ 96]
node 0 [ 150]
| leaf 2 [ 54]
==== Evaluation on training set ====

```

**Log** x 0

Weka Knowledge Explorer

Preprocess Classify Cluster Associate Select attributes Visualize

**Clusterer**

**Choose** Cobweb -A 1.0 -C 0.0028209479177387815

**Cluster mode**

Use training set

Supplied test set Set...

Percentage split % 66

Classes to clusters evaluation  
(Nom) class

Store clusters for visualization

**Ignore attributes**

**Start** **Stop**

**Result list (right-click for options)**

16:05:58 - Cobweb

**Clusterer output**

==== Run information ====  
Scheme: weka.clusterers.Cobweb -A 1.0 -C 0.0028209479177387815  
Relation: iris  
Instances: 150  
Attributes: 5  
sepallength  
sepalwidth  
petallength  
petalwidth  
Ignored:  
class  
Test mode: Classes to clusters evaluation on training data

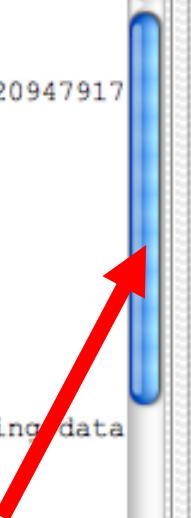
==== Clustering model (full training set) ====  
Number of merges: 0  
Number of splits: 0  
Number of clusters: 3  
  
node 0 [ 150]  
| leaf 1 [ 96]  
node 0 [ 150]  
| leaf 2 [ 54]

==== Evaluation on training set ====

**Status**

OK

**Log** x 0



Weka Knowledge Explorer

Preprocess Classify Cluster Associate Select attributes Visualize

**Clusterer**

**Choose Cobweb -A 1.0 -C 0.0028209479177387815**

**Cluster mode**

Use training set

Supplied test set Set...

Percentage split % 66

Classes to clusters evaluation

(Nom) class

Store clusters for visualization

**Ignore attributes**

Start Stop

**Result list (right-click for options)**

16:05:58 - Cobweb

**Clusterer output**

Number of clusters: 3

node 0 [ 150]  
| leaf 1 [ 96]  
node 0 [ 150]  
| leaf 2 [ 54]

Clustered Instances

1 100 ( 67%)  
2 50 ( 33%)

Class attribute: class  
Classes to Clusters:

1 2 <-- assigned to cluster  
0 50 | Iris-setosa  
50 0 | Iris-versicolor  
50 0 | Iris-virginica

Cluster 1 <-- Iris-versicolor  
Cluster 2 <-- Iris-setosa

Incorrectly clustered instances : 50.0 33.3333 %

Status

OK Log x 0

Weka Knowledge Explorer

Preprocess Classify Cluster Associate Select attributes Visualize

Clusterer

Choose Cobweb -A 1.0 -C 0.0028209479177387815

Cluster mode

Use training set

Supplied test set Set...

Percentage split % 66

Classes to clusters evaluation (Nom) class

Store clusters for visualization

Ignore attributes

Start Stop

Result list (right-click for options)

16:05:58 - Cobweb

Clusterer output

Number of clusters: 3

node 0 [ 150]  
| leaf 1 [ 96]  
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Cluster 1 <-- Iris-versicolor  
Cluster 2 <-- Iris-setosa

Incorrectly clustered instances : 50.0 33.3333 %

Status

OK Log x 0



Weka Knowledge Explorer

Preprocess Classify Cluster Associate Select attributes Visualize

**Clusterer**

**Choose Cobweb -A 1.0 -C 0.0028209479177387815**

**Cluster mode**

Use training set

Supplied test set Set...

Percentage split % 66

Classes to clusters evaluation  
(Nom) class

Store clusters for visualization

**Ignore attributes**

**Start** **Stop**

**Result list (right-click for options)**

16:05:58 - Cobweb

- [View in main window](#)
- [View in separate window](#)
- [Save result buffer](#)
- [Load model](#)
- [Save model](#)
- [Re-evaluate model on current test set](#)

**Status**

OK

**Clusterer output**

```
==== Run information ====
Scheme: weka.clusterers.Cobweb -A 1.0 -C 0.0028209479177387815
Relation: iris
Instances: 150
Attributes: 5
sepallength
sepalwidth
petallength
petalwidth
Ignored:
class
Test mode: Classes to clusters evaluation on training data
==== Clustering model (full training set) ====
Number of merges: 0
Number of splits: 0
Number of clusters: 3
```

**training set ===**

**Log** x 0

 Data at Scale

Weka Knowledge Explorer

Preprocess Classify Cluster Associate Select attributes Visualize

Clusterer

Choose Cobweb -A 1.0 -C 0.0028209479177387815

Cluster mode

- Use training set
- Supplied test se
- Percentage split
- Classes to cluster

(Nom) class

Store clusters for later

Ignore misclassified instances

Start

Result list (right-click for details)

16:05:58 - Cobweb

Clusterer output

Weka Classifier Tree Visualizer: 16:05:58 - Cobweb (iris)

Tree View

0 -C 0.0028209479177387815

on on training data

==

Status

OK

Log x 0

Data at Scale W

Weka Knowledge Explorer

Preprocess Classify Cluster Associate Select attributes Visualize

**Clusterer**

**Choose Cobweb -A 1.0 -C 0.0028209479177387815**

**Cluster mode**

Use training set

Supplied test set Set...

Percentage split % 66

Classes to clusters evaluation  
(Nom) class

Store clusters for visualization

**Ignore attributes**

**Start** **Stop**

**Result list (right-click for options)**

16:05:58 - Cobweb

- [View in main window](#)
- [View in separate window](#)
- [Save result buffer](#)
- [Load model](#)
- [Save model](#)
- [Re-evaluate model on current test set](#)

**Clusterer output**

```
==== Run information ====
Scheme: weka.clusterers.Cobweb -A 1.0 -C 0.0028209479177387815
Relation: iris
Instances: 150
Attributes: 5
sepallength
sepalwidth
petallength
petalwidth
Ignored:
class
Test mode: Classes to clusters evaluation on training data
==== Clustering model (full training set) ====
Number of merges: 0
Number of splits: 0
Number of clusters: 3
```

**Status**

OK

**Visualize cluster assignments**

**Visualize tree**

**Log** x 0

The screenshot shows the Weka Knowledge Explorer interface with the 'Cluster' tab selected. In the 'Clusterer' panel, 'Cobweb' is chosen with parameters '-A 1.0 -C 0.0028209479177387815'. The 'Cluster mode' section is set to 'Classes to clusters evaluation' for the 'iris' dataset, with 66% of instances used for training. The 'Clusterer output' panel displays run information, clustering model details, and a summary of the full training set. The 'Result list' shows a recent entry for 'Cobweb' with options to view it in the main window or save the result buffer. The 'Status' bar at the bottom indicates an 'OK' status.

## Clusterer

Choose

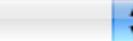
**Cobweb -A 1.0 -C 0.0028209479177387815**

Weka Clusterer Visualize: 16:05:58 – Cobweb (iris)

## Cluster mode

 Use training se

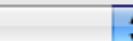
X: petallength (Num)



Y: petalwidth (Num)

 Supplied test s

Colour: Cluster (Nom)



Select Instance

 Percentage spli

Reset

Clear

Save

Jitter

 Classes to clus

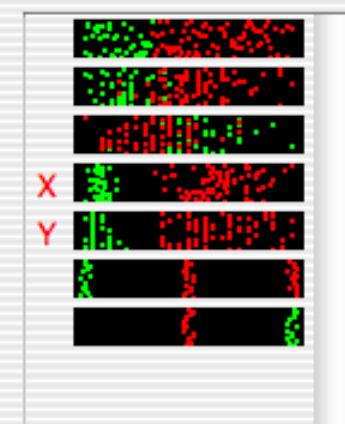
(Nom) class

 Store clusters f Ignore class Start

## Result list (right-click for details)

16:05:58 – Cobweb

Plot: iris\_clustered



Class colour

cluster0

cluster1

cluster2

==== Evaluation on training set ====

## Status

OK

Log



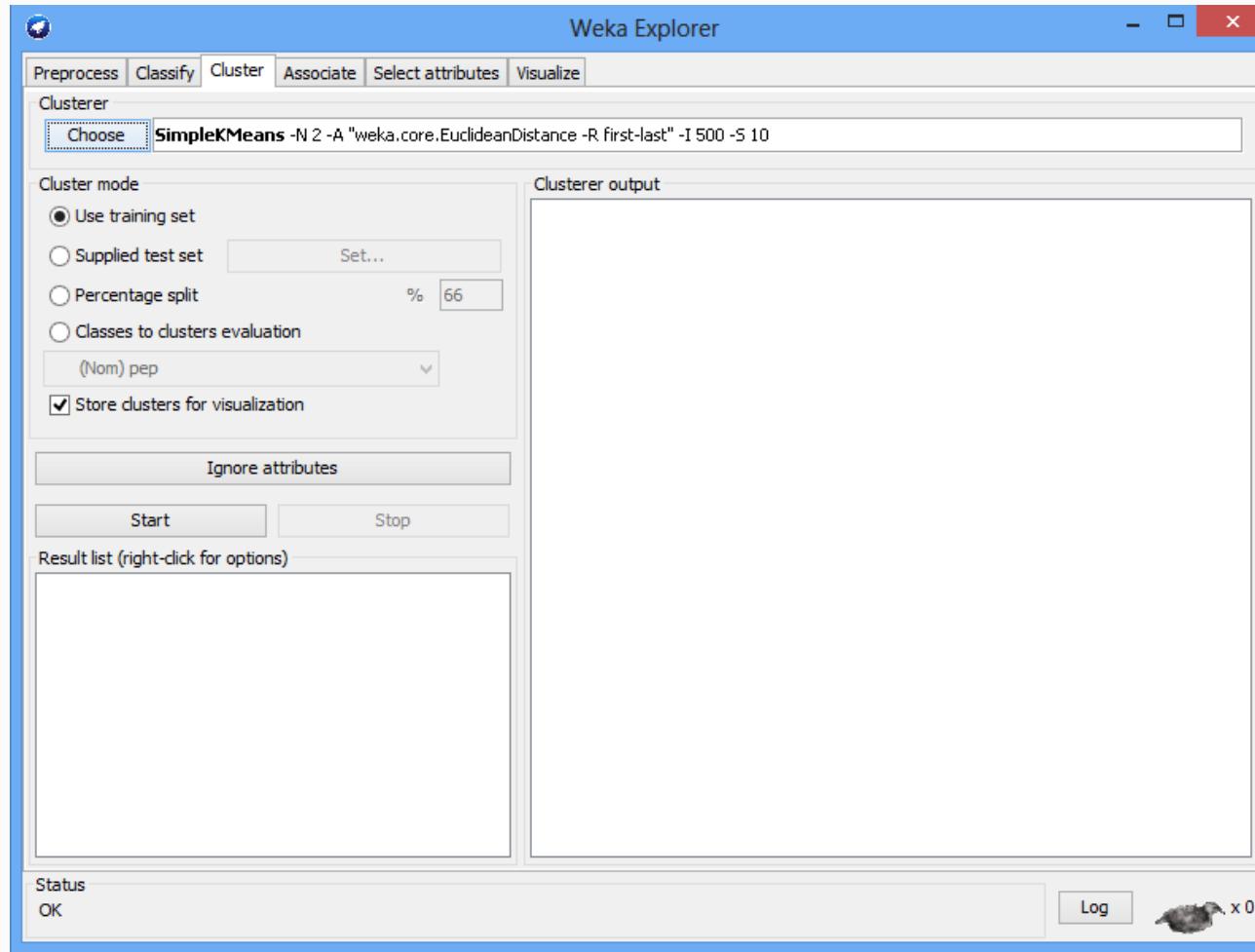
x 0

Data at Scale



# K-Means in WEKA

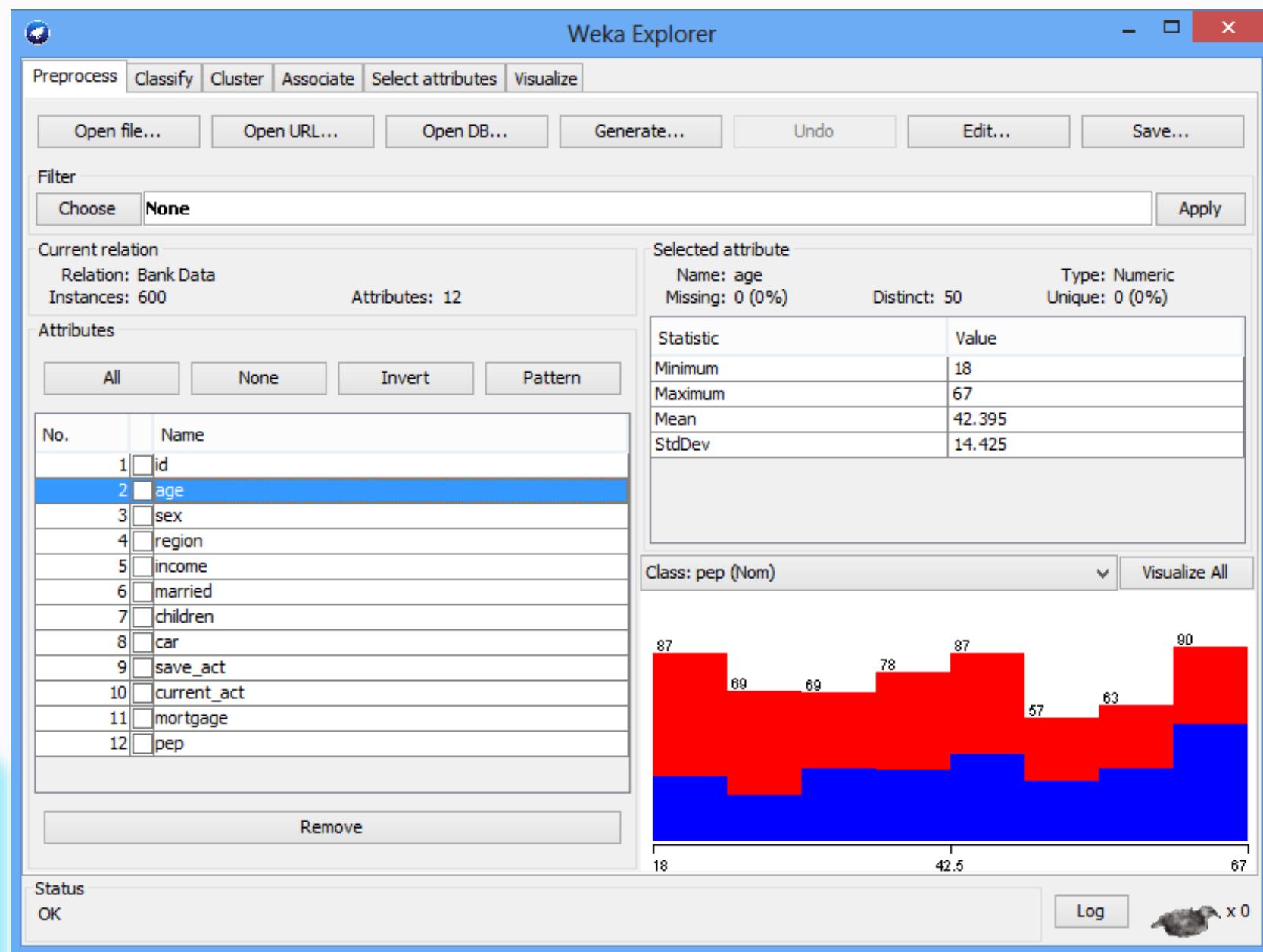
- WEKA automatically handles mixture of categorical and numerical variables;
- Algorithm automatically normalizes numerical attributes, replaces missing;
- Uses Euclidean distance to compute distance between instance and cluster;



# K-Means in WEKA Bank Data

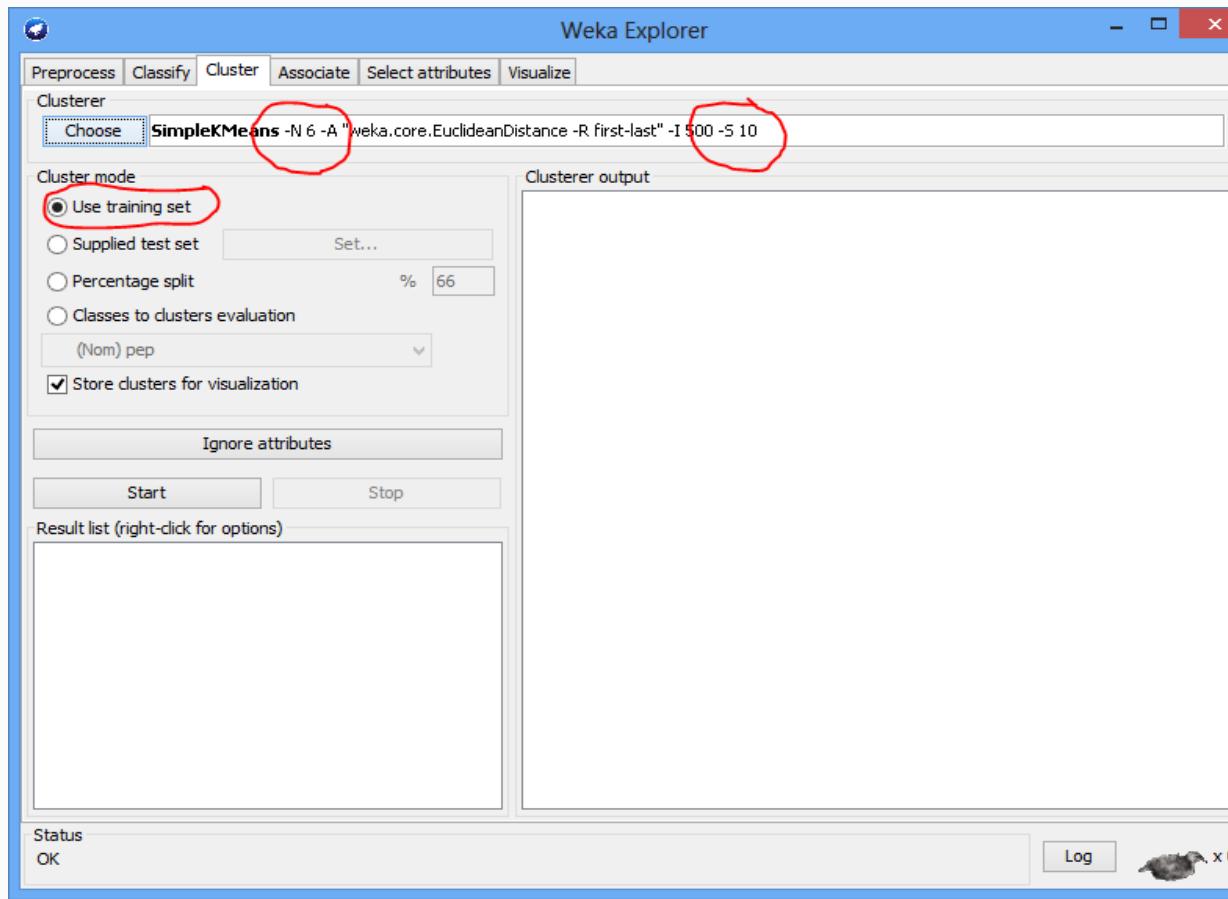
Note, some implementations of K-means only allow numerical values so it may be necessary to convert categorical to binary.

Also, normalize attributes on very differently scales (age and income).



# K-Means in WEKA

- Select 'cluster' tab, click on 'choose' and select 'SimpleKMeans' from dropdown.
- Enter 6 as the number of clusters, leave seed 'as is';
- Note Kmeans can be sensitive to initial placement of clusters, play with seed;
- Select 'Use training set' option, click start...



# K-Means in WEKA, let's analyze the results...

- Right click the result set in the "Results List" panel

```
Number of iterations: 18
Within cluster sum of squared errors: 1955.4146634784236
Missing values globally replaced with mean/mode

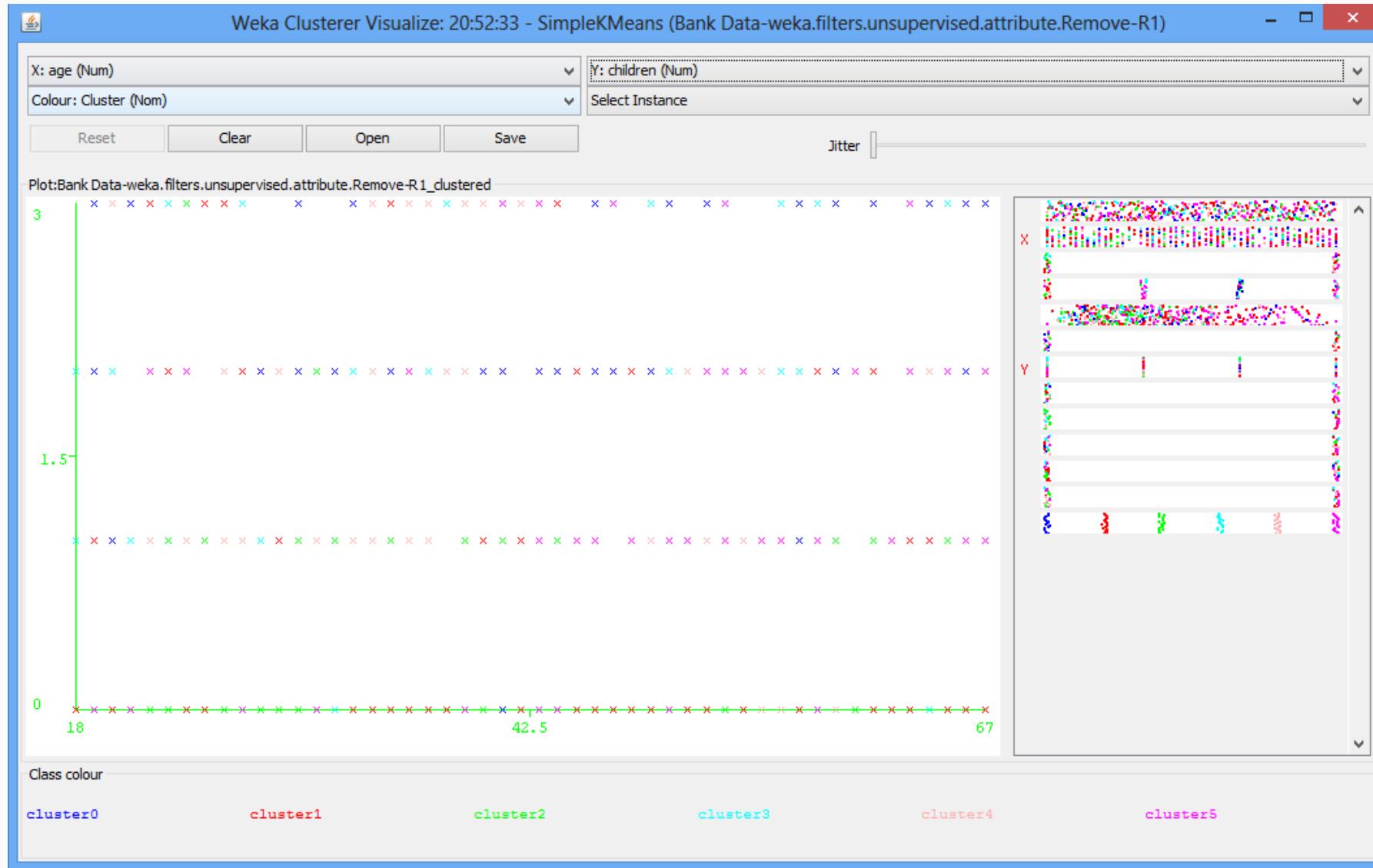
Cluster centroids:

          Cluster#
Attribute   Full Data      0       1       2       3       4       5
           (600)  (74)  (164)  (71)  (58)  (99)  (134)
=====
id          ID12101  ID12107  ID12103  ID12101  ID12104  ID12102  ID12108
age         42.395  42.9324  43.7744  39.0282  37.3103  38.404  47.3433
sex        FEMALE  FEMALE  FEMALE  FEMALE  FEMALE  MALE   MALE
region     INNER_CITY  RURAL  INNER_CITY  INNER_CITY  TOWN  INNER_CITY  TOWN
income    27524.0312 28838.7605 28586.4063 20463.1273 20600.8528 25720.037 33568.3929
married    YES      NO      YES      YES      YES      YES      NO
children   1.0117  1.973  0.628  0.6901  1.6207  0.899  0.9403
car         NO      NO      NO      NO      NO      YES      YES
save_act   YES      YES      YES      NO      NO      NO      YES
current_act YES      YES      YES      YES      YES      YES      YES
mortgage   NO      NO      NO      NO      NO      YES      NO
pep        NO      NO      NO      YES      NO      YES      YES

Time taken to build model (full training data) : 0.14 seconds
```

# K-Means in WEKA

- Right click 'visualize cluster assignments' in the "Results List" panel



# Clustering

Some final takeaways from this model: The power of clustering and Nearest Neighbor becomes obvious when we talk about data sets like Netflix and Amazon. Amazon with their ~100 million users and Netflix with their 4 Billion streamed moves, their algorithms are very accurate since there are likely many potential customers in their databases with similar buying/viewing habits to you. Thus, the nearest neighbor to yourself is likely very similar. This creates an accurate and effective model.

Contrarily, the model breaks down quickly and becomes inaccurate when you have few data points for comparison. In the early stages of an online e-commerce store for example, when there are only 50 customers, a product recommendation feature will likely not be accurate at all, as the nearest neighbor may in fact be very distant from yourself.

# Lecture 5 Homework 5b

## Homework Lecture 5, mandatory

An online shopping site has the following primary pages or sections: **Home, Products, Search, Prod\_A, Prod\_B, Prod\_C, Cart, Purchase**. A user may browse from "Home" to "Products" and then to one of the individual products. The user may also search for a specific product by using the "Search" function. A visit to "Cart" implies that the user has placed an item in the shopping cart, and "Purchase" indicates the user completed the purchase of items in the shopping cart. The site has collected the hypothetical session data for 100 sessions. This data is available in **CSV** format, Sessions.CSV, on course website.

Use WEKA's K-means clustering algorithm to cluster these user sessions into segments. Try different clustering runs with various numbers of clusters (e.g., between 4 and 8), and select the result set(s) that seem to best answer as many of the following questions as possible.

- o If a new user is observed to access the following pages: **Home => Search => Prod\_B**, according to your clusters, what other product should be recommended to this user? Explain your answer based on your clustering results. What if the new user has accessed the following sequence instead: **Products => Prod\_C**?
- o Can clustering help us identify casual browsers ("window shoppers"), focused browsers (those who seem to know what products they are looking for), and searchers (those using the search function to find items they want)? If so, are any of these groups show a higher or lower propensity to make a purchase?
- o Do any of the segments show particular interest in one or more products, and if so, can we identify any special characteristics about their navigational behavior or their purchase propensity?
- o If we know that, during the time of data collection, independent banner ads had been placed on some popular sites pointing to products A and B, can we identify segments corresponding to visitors that respond to the ads? If so, can we determine if either of these promotional campaigns are having any success?

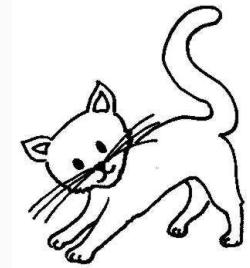
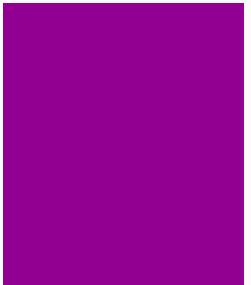
# Distributions Matter...

Sometimes two wrongs do make a right...



# Distributions Matter...

Because the Internet is all about cute kittens



*Resulting in highly skewed distribution in training set...*

# The Class Imbalance Problem I

- Data sets are said to be balanced if there are, approximately, as many positive examples of the concept as there are negative ones.
- Many domains that do not have a balanced data set.

## Examples:

- Helicopter Gearbox Fault Monitoring
- Discrimination between Earthquakes and Nuclear Explosions
- Document Filtering
- Detection of Oil Spills
- Detection of Fraudulent Telephone Calls

# The Class Imbalance Problem II

- The problem with class imbalances is that standard learners are often biased towards the majority class.
- That is because these classifiers attempt to reduce global quantities such as the error rate, not taking the data distribution into consideration.
- As a result examples from the overwhelming class are well-classified whereas examples from the minority class tend to be misclassified.

# Some Generalities

- Evaluating performance of a model on a class imbalance problem is not done appropriately with standard accuracy/error rate.
  - ROC Analysis is typically used, instead.
- There are three main ways to deal with class imbalances: re-sampling, re-weighing, and one-class learning (cover in SVMs)
- Re-sampling provides a simple way of biasing generalization process.
- It can do so by:
  - Generating synthetic samples accordingly biased
  - Controlling the amount and placement of the new samples

**Weka GUI Chooser**

Program Visualization Tools Help

Applications

Package Manager

Official

Refresh repository cache Install Uninstall

Installed  Available  All  Ignore dependencies / conflicts

Unofficial File/URL

Waikato En Version 3.7. (c) 1999 - 2011 The University of Waikato, N

Print Partner Program Workload Review WSSC Thresholds Predictive Analytics Recycle Bin

Install/Uninstall/Refresh progress

Package	Category	Installed version	Repository version	Loaded
classAssociationRules	Associations	1.0.1	1.0.1	
generalizedSequentialPatterns	Associations	1.0.1	1.0.1	
hotSpot	Associations	1.0.5	1.0.5	
predictiveApriori	Associations	1.0.1	1.0.1	
tertius	Associations	1.0.1	1.0.1	
SSF	Attribute Selection	1.0.0	1.0.0	
probabilisticSignificanceAE	Attribute Selection	1.0.1	1.0.1	
raceSearch	Attribute Selection	1.0.1	1.0.1	
EvolutionarySearch	Attribute selection	1.0.0	1.0.0	Yes
IWSS	Attribute selection	1.0.0	1.0.0	

Weka 3: Data Mining Software in Java

Weka is a collection of machine learning algorithms for data mining tasks. The algorithms can either be applied directly to a dataset or called from your own Java code. Weka contains tools for data pre-processing, classification, regression, clustering, association rules, and visualization. It is also well-suited for developing new machine learning schemes.

Weka is open source software issued under the [GNU General Public License](#).

---

**Pentaho's live forum for Weka**

The open-source BI software company Pentaho is a major sponsor of Weka development and provides a live [forum](#) for interaction among Weka project community members.

---

**The Weka mailing list**

Please post Weka-related questions, comments, and bug reports to the [Weka mailing list](#). There is also the searchable mailing list [archive](#) (Mirrors: [news.gmane.org](#), [Nabble](#)). Please do not email individual members of our research group about Weka problems.

---

**IRC channel for discussing Weka**

#weka on freenode.

---

If you have any comments about these pages then please contact: [mhall at cs.waikato.ac.nz](mailto:mhall@cs.waikato.ac.nz)

Package Manager

Official

Refresh repository cache    Install    Uninstall

Installed    Available    All    Ignore dependencies/conflicts

Install/Uninstall/Refresh progress

Package	Category	Installed version	Repository version	Loaded
multiInstanceLearning	Multi-instance learning		1.0.7	
isolationForest	Outlier		1.0.1	
localOutlierFactor	Outlier		1.0.4	
ArabicStemmers_LightStemmers	Preprocessing		1.0.0	
DistributionBasedBalance	Preprocessing		1.0.0	
EMImputer	Preprocessing	1.0.1	1.0.1	Yes
SMOTE	Preprocessing	1.0.3	1.0.3	Yes
anonymizationPackage	Preprocessing		1.0.1	
denormalize	Preprocessing		1.0.1	
latentSemanticAnalysis	Preprocessing		1.0.2	

Back Home !

## Weka 3: Data Mining Software in Java

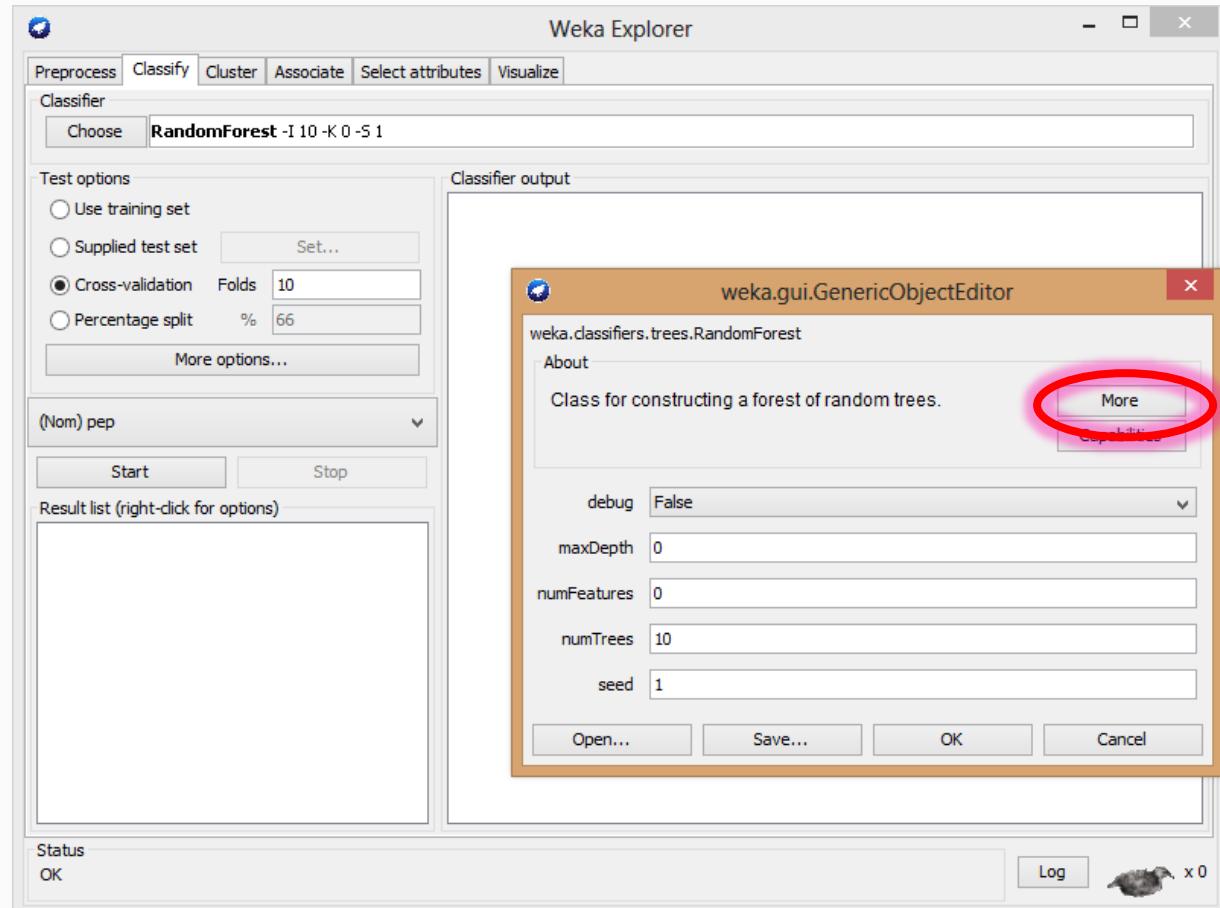
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Weka is open source software issued under the [GNU General Public License](#).

[Dontcho's live forum for Weka](#)

# Improve Your Modelling Skills

## Explore a bit, both in WEKA and online (references in WEKA notes)



Machine Learning, 54, 255–273, 2004  
© 2004 Kluwer Academic Publishers. Manufactured in The Netherlands.

### Is Combining Classifiers with Stacking Better than Selecting the Best One?

SASO DŽEROSKI [saso.dzeroski@jjs.si](mailto:saso.dzeroski@jjs.si)

#### How to Make Stacking Better and Faster While Also Taking Care of an Unknown Weakness

Alexander K. Seewald [ALEX@SEEWALD.AT; ALEXSEE@AI.UNIVIE.AC.AU](mailto:ALEX@SEEWALD.AT; ALEXSEE@AI.UNIVIE.AC.AU)  
Austrian Research Institute for Artificial Intelligence, Schottengasse 3, A-1010 Wien, Austria

#### Abstract

We investigated performance differences between multi-class and two-class datasets for ensemble learning schemes. We were surprised to find that Stacking, the best-known such scheme, performs worse on multi-class datasets. In this paper we will present results concerning this heretofore unknown weakness of Stacking. In addition we will present a new variant of Stacking which is able to compensate for this weakness, improving Stacking significantly on some multi-class datasets. The dimensionality of the meta-data set is reduced by a factor equal to the number of classes, which leads to faster learning. In comparison to other ensemble learning methods this improves Stacking's lead further, making it the most successful system by a variety of measures.

#### 1. Introduction

When faced with the decision "Which algorithm will be most accurate on my classification problem?", the first, we will present the basic concept behind Stack-

# SMOTE: A State-of-the-Art Resampling Approach

- SMOTE stands for Synthetic Minority Oversampling Technique.
  - Technique designed by Chawla, Hall, & Kegelmeyer in 2002.
- It combines Informed **oversampling** of the **minority class** with **random undersampling** of the **majority class**.
- SMOTE currently yields the best results as far as re-sampling and modifying the probabilistic estimate techniques go (Chawla, 2003).

# SMOTE's Informed Oversampling Procedure II

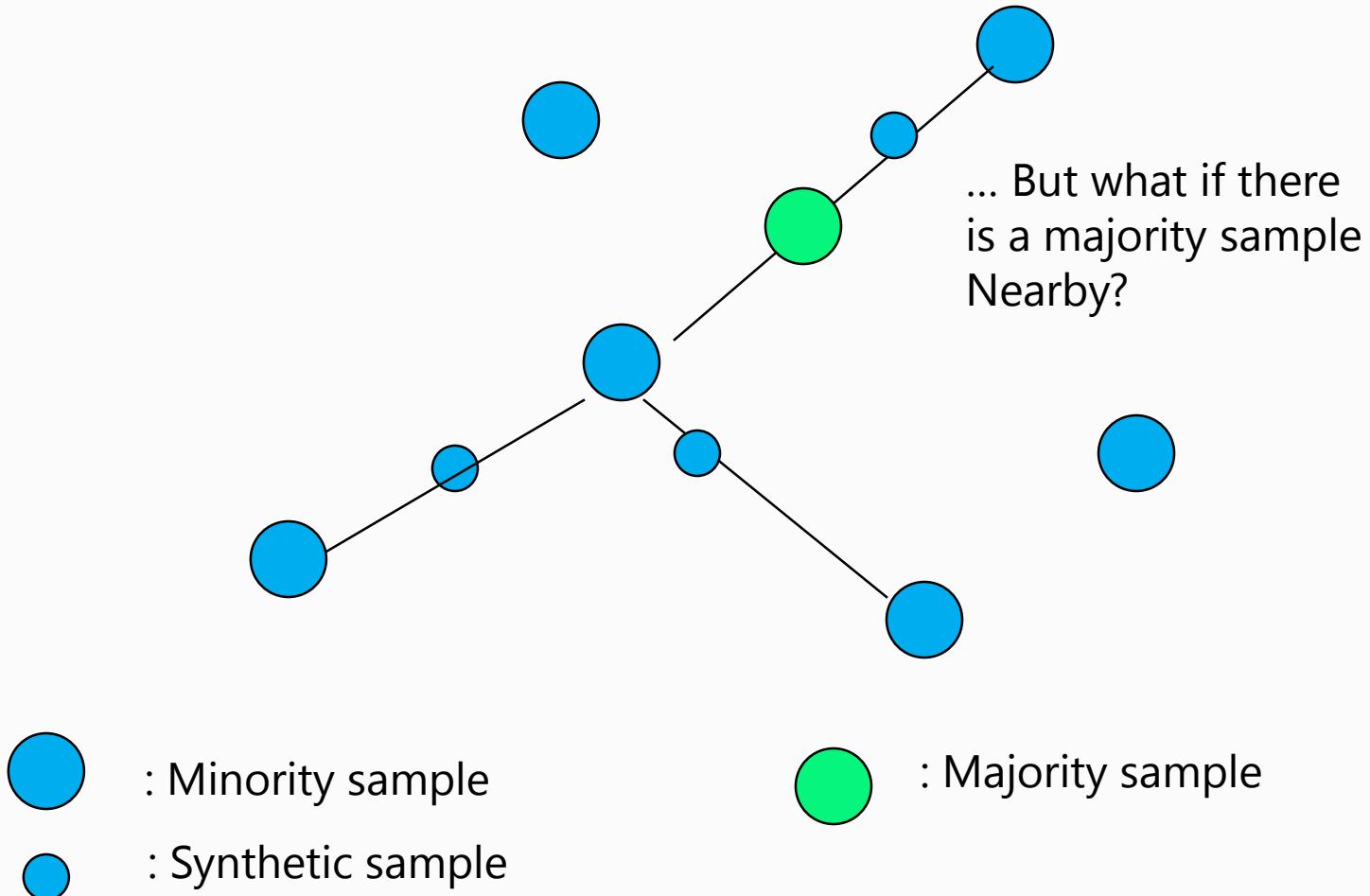
For each minority Sample

- Find its k-nearest minority neighbors
- Randomly select j of these neighbors
- Randomly generate synthetic samples along the lines joining the minority sample and its j selected neighbors  
(j depends on the amount of oversampling desired)

# SMOTE's Informed vs. Random Oversampling

- Random Oversampling (with replacement) of the minority class has the effect of making the decision region for the minority class very specific.
- In a decision tree, it would cause a new split and often leads to overfitting.
- SMOTE's informed oversampling generalizes the decision region for the minority class.
- As a result, larger and less specific regions are learned, thus, paying attention to minority class samples without causing overfitting.

# SMOTE's Informed Oversampling Procedure I



# SMOTE's Shortcomings

- Overgeneralization
  - SMOTE's procedure can be dangerous since it blindly generalizes the minority area without regard to the majority class.
  - This strategy is problematic in the case of highly skewed class distributions since, in such cases, the minority class is very sparse with respect to the majority class, thus resulting in a greater chance of class mixture.
- Lack of Flexibility
  - The number of synthetic samples generated by SMOTE is fixed in advance, thus not allowing for any flexibility in the re-balancing rate.

**Weka Explorer**

Preprocess Classify Cluster Associate Select attributes Visualize Forecast

Open file... Open URL... Open DB... Generate... Undo Edit... Save...

Filter Choose **None** Apply

Current relation  
Relation: survival-imbalanced-fold0 Attributes: 4  
Instances: 204 Sum of weights: 204

Selected attribute  
Name: class Type: Nominal  
Missing: 0 (0%) Distinct: 2 Unique: 0 (0%)

No.	Label	Count	Weight
1	0	150	150.0
2	1	54	54.0

Attributes  
All None Invert Pattern

No.	Name
1	attribute1
2	attribute2
3	attribute3
4	<b>class</b>

Class: class (Nom) Visualize All

Remove

Status OK Log x 0

The chart shows two horizontal bars. The left bar is blue and labeled '150' above it, representing the count for class 0. The right bar is red and labeled '54' above it, representing the count for class 1.

*Let's try it:* open the file example\_imbalanced.arff...



If your model is 98% accurate, so what?  
Or right 1 time in 35



# Cross Validation

- In cross validation, you break your training data up into  $K$  equally-sized partitions. You train a learning algorithm on  $K-1$  of them and test it on the remaining 1. You do this  $K$  times, each time holding out a different partition as the “development” part. You can then average your performance over  $K$  runs.
- Suppose that you’ve presented a machine learning solution to your boss that achieves 7% error on cross validation. Your nemesis, Gabe, gives a solution to your boss that achieves 6.9% error on cross validation. How impressed should your boss be?
- **It depends.** If this 0.1% improvement was measured over 1000 examples, perhaps not too impressed. It would mean that Gabe got exactly *one more example right than you did*. (In fact, he probably got 15 more right and 14 more wrong.) If this 0.1% improvement was measured over 1,000,000 examples, perhaps this is more impressive.

# How can you evaluate models?

## Type I and Type II errors

- Different types of error losing different types of money...
- What is the cost (opportunity and actual) of a false positive?
- What is the cost of a false negative?

## Gain Curves

## Don't forget the user

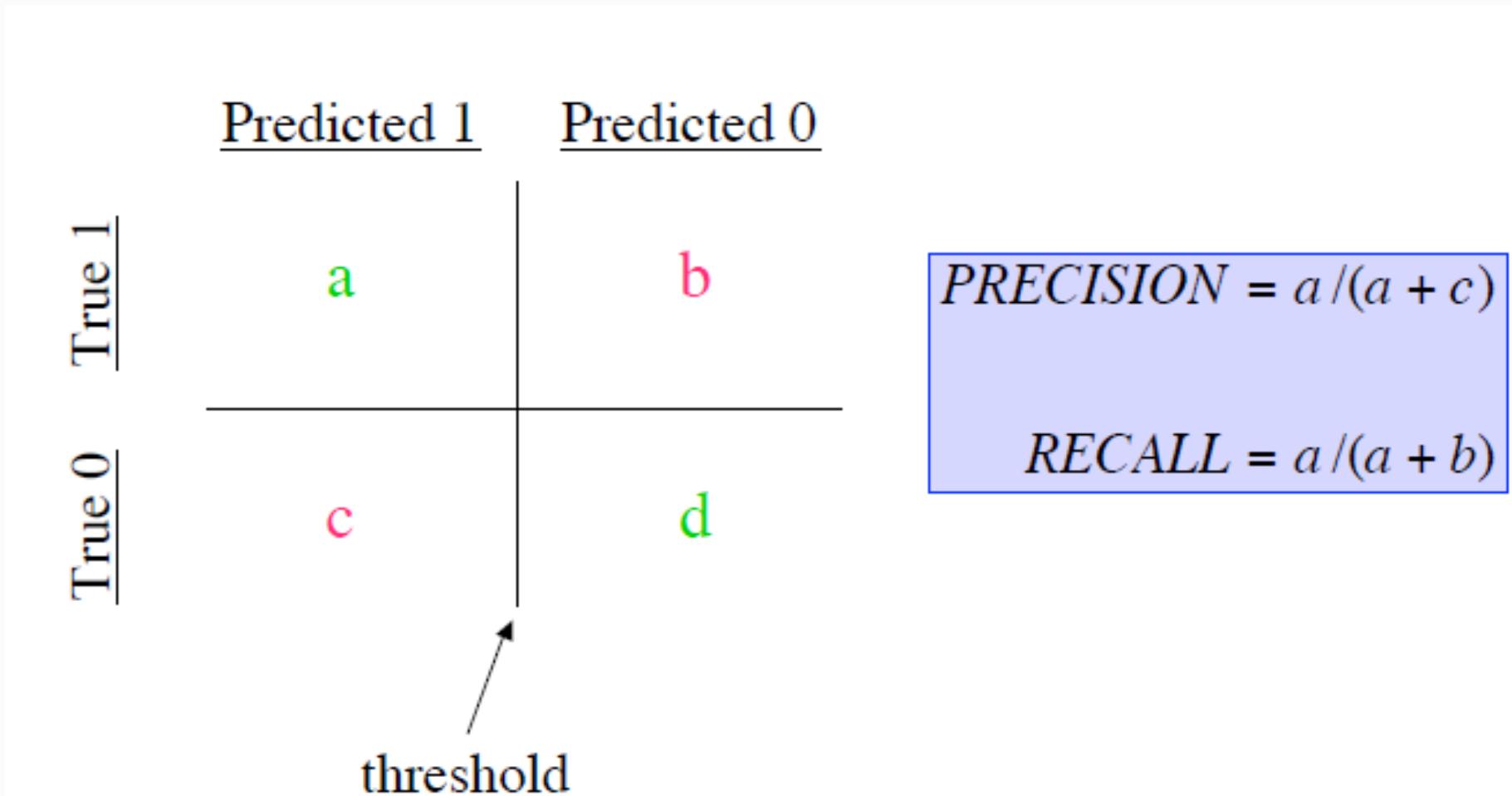
- They may need to be able to explain (or justify) their decision
- Decision trees fight back

# Cost Considerations

- Cost / Profit Matrix
- Example: decide whether to offer Personal Equity Plan (PEP)
  - True Positive: Payoff is \$1000/customer
  - True Negative: \$0
  - False Positive: -\$10/customer
  - False negative: -\$1000/customer (opp. Cost)

# Precision/Recall Curves

## Precision and Recall



# Precision/Recall Curves

Once you can compute precision and recall, you are often able to produce precision/recall curves. Suppose that you are attempting to identify spam. You run a learning algorithm to make predictions on a test set. But instead of just taking a “yes/no” answer, you allow your algorithm to produce its confidence. For instance, using a perceptron, you might use the distance from the hyperplane as a confidence measure. You can then sort all of your test emails according to this ranking. You may put the most spam-like emails at the top and the least spam-like emails at the bottom

# Precision/Recall Curves

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Once you have this sorted list, you can choose how aggressively you want your spam filter to be by setting a threshold anywhere on this list. One would hope that if you set the threshold very high, you are likely to have high precision (but low recall). If you set the threshold very low, you'll have high recall (but low precision). By considering every possible place you could put this threshold, you can trace out a curve of precision/recall values. This allows us to ask the question: for some fixed precision, what sort of recall can I get...

# F Score

Sometimes we want a single number that informs us of the quality of the solution. A popular way to combine precision and recall into a single number is by taking their harmonic mean. This is known as the balanced f-measure:

$$F = \frac{2 \times P \times R}{P + R}$$

The reason to use a harmonic mean rather than an arithmetic mean is that it favors systems that achieve roughly equal precision and recall. In the extreme case where  $P = R$ , then  $F = P = R$ . But in the imbalanced case, for instance  $P = 0.1$  and  $R = 0.9$ , the overall f-measure is a modest 0.18.

	0.0	0.2	0.4	0.6	0.8	1.0
0.0	0.00	0.00	0.00	0.00	0.00	0.00
0.2	0.00	0.20	0.26	0.30	0.32	0.33
0.4	0.00	0.26	0.40	0.48	0.53	0.57
0.6	0.00	0.30	0.48	0.60	0.68	0.74
0.8	0.00	0.32	0.53	0.68	0.80	0.88
1.0	0.00	0.33	0.57	0.74	0.88	1.00

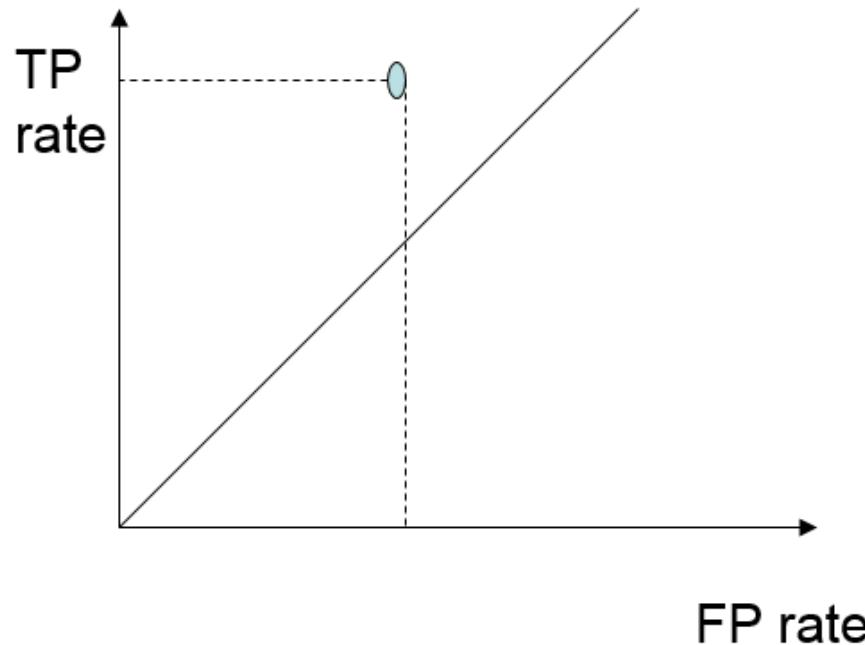
# Note...

One thing to keep in mind is that precision and recall (and hence f-measure) ***depend crucially on which class is considered*** the thing you wish to find. In particular, if you take a binary data set and flip what it means to be a positive or negative example, you will end up with completely different precision and recall values.

It is ***not the case that precision on the flipped task is equal to recall on the original task*** (nor vice versa). Consequently, f-measure is also not the same. For some tasks where you are less sure about what you want, report two sets of precision/recall/f-measure numbers, which vary based on which class is considered the thing to spot.

# Point in ROC Space

		TRUE CLASS	
		YES	NO
PREDICTED CLASS	YES	TP	FP
	NO	FN	TN
Total:		P	N



FP rate:  $FP/N$

TP rate:  $TP/P$  (recall)

FN rate:  $FN/N$

TN rate:  $TN/P$

Classifier accuracy:  $(TP+TN)/(P+N)$

Shows how good is classifier in discriminating positive instances from negative ones

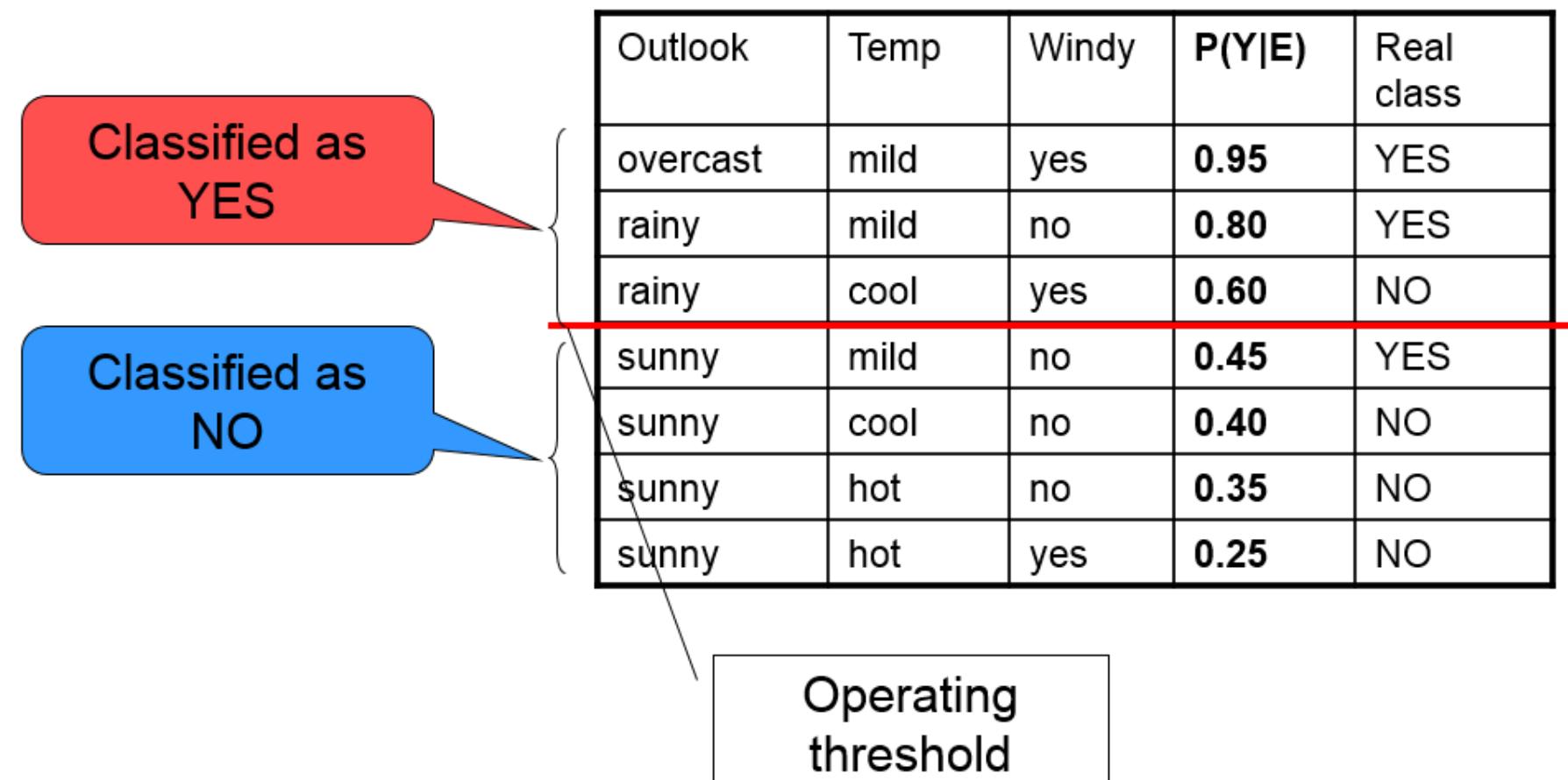
# ROC Curve of a Probabilistic Classifier

Naïve Bayes, for example, outputs the probability of an instance in a testing set to be classified as YES

Outlook	Temp	Windy	$P(Y E)$	Real class
overcast	mild	yes	<b>0.95</b>	YES
rainy	mild	no	<b>0.80</b>	YES
rainy	cool	yes	<b>0.60</b>	NO
sunny	mild	no	<b>0.45</b>	YES
sunny	cool	no	<b>0.40</b>	NO
sunny	hot	no	<b>0.35</b>	NO
sunny	hot	yes	<b>0.25</b>	NO

# ROC Curve of a Probabilistic Classifier

In a general case, we classify an instance as YES if the probability is more than 50%



# ROC Curve of a Probabilistic Classifier

We compute the confusion matrix

		TRUE CLASS	
		YES	NO
PREDICTED CLASS	YES	2 (TP)	1 (FP)
	NO	1 (FN)	3 (TN)
Total:		3 (P)	4 (N)

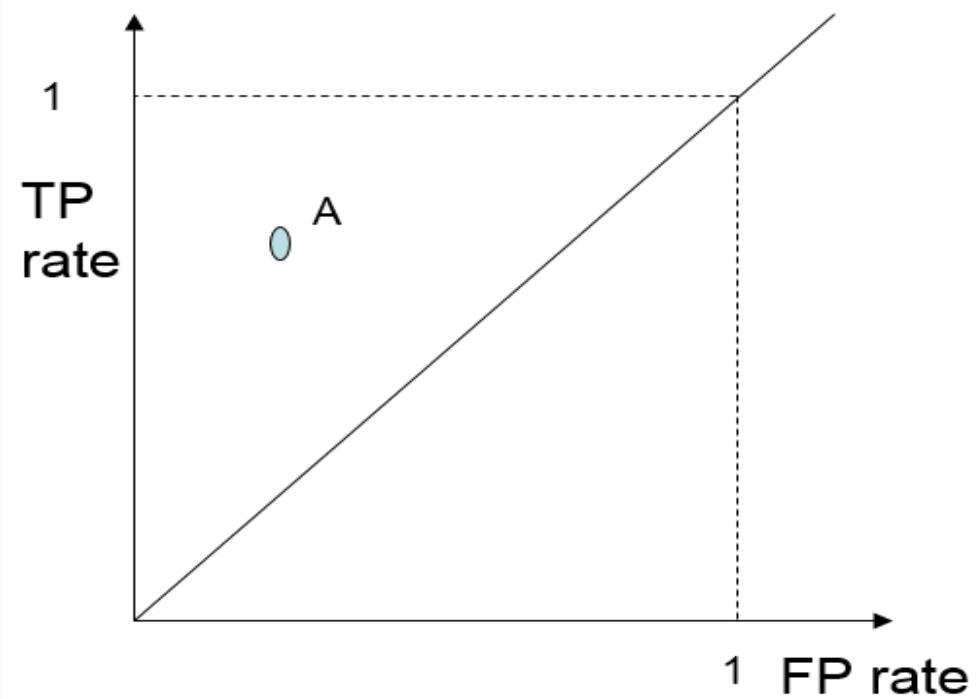
Outlook	Temp	Windy	P(Y E)	Predicted class	Real class
overcast	mild	yes	0.95	YES	YES
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rainy	cool	yes	0.60	YES	NO
sunny	mild	no	0.45	NO	YES
sunny	cool	no	0.40	NO	NO
sunny	hot	no	0.35	NO	NO
sunny	hot	yes	0.25	NO	NO

And the TP and FP rates:

TP rate:  $TP/P=2/3 \approx 0.7$

FP rate:  $FP/N=1/4=0.25$

# ROC Curve of a Probabilistic Classifier



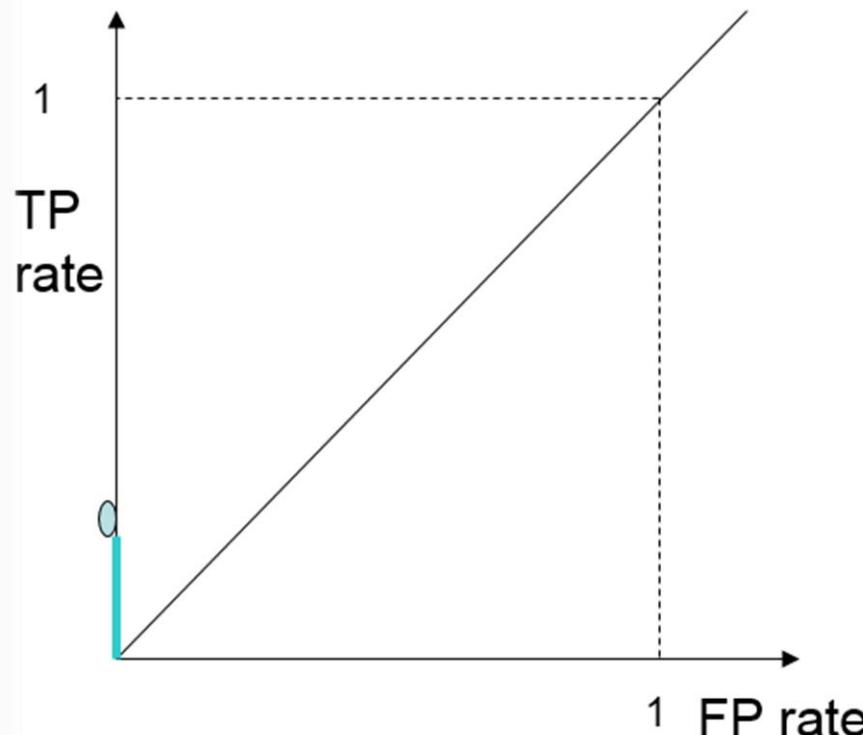
This corresponds to point A  
in a ROC space

FP rate:  $FP/N=1/4=0.25$

TP rate:  $TP/P=2/3\approx0.7$

Outlook	Temp	Windy	$P(Y E)$	Predicted class	Real class
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# ROC Curve of a Probabilistic Classifier



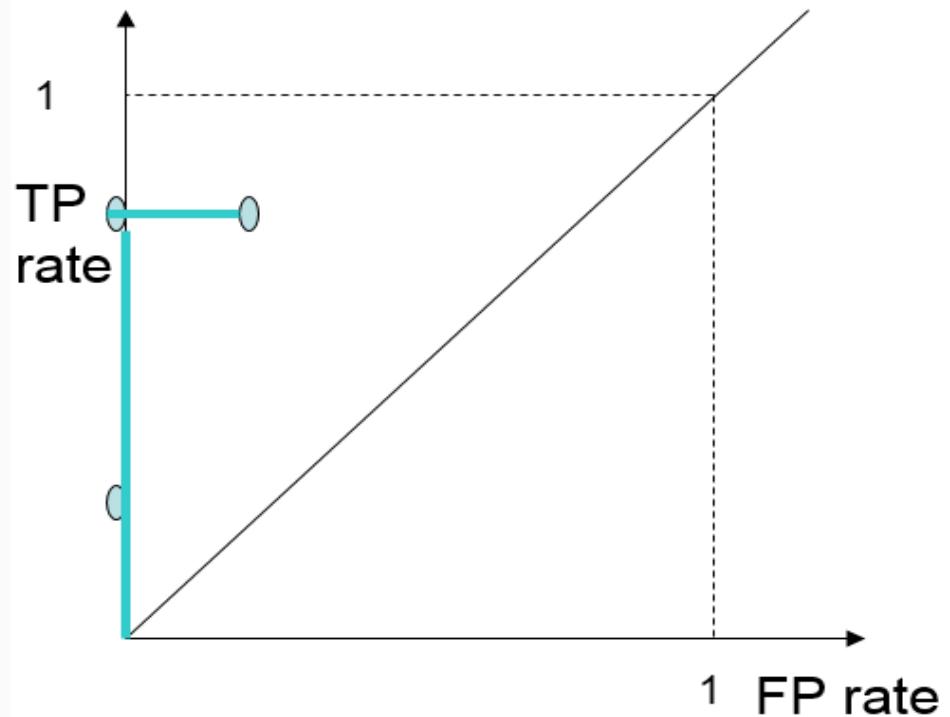
For different threshold values we get different points in a ROC space

Outlook	Temp	Windy	P(Y E)	Predicted class	Real class
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sunny	cool	no	0.40	NO	NO
sunny	hot	no	0.35	NO	NO
sunny	hot	yes	0.25	NO	NO

FP rate:  $FP/N=0/4=0$

TP rate:  $TP/P=1/3 \approx 0.3$

# ROC Curve of a Probabilistic Classifier



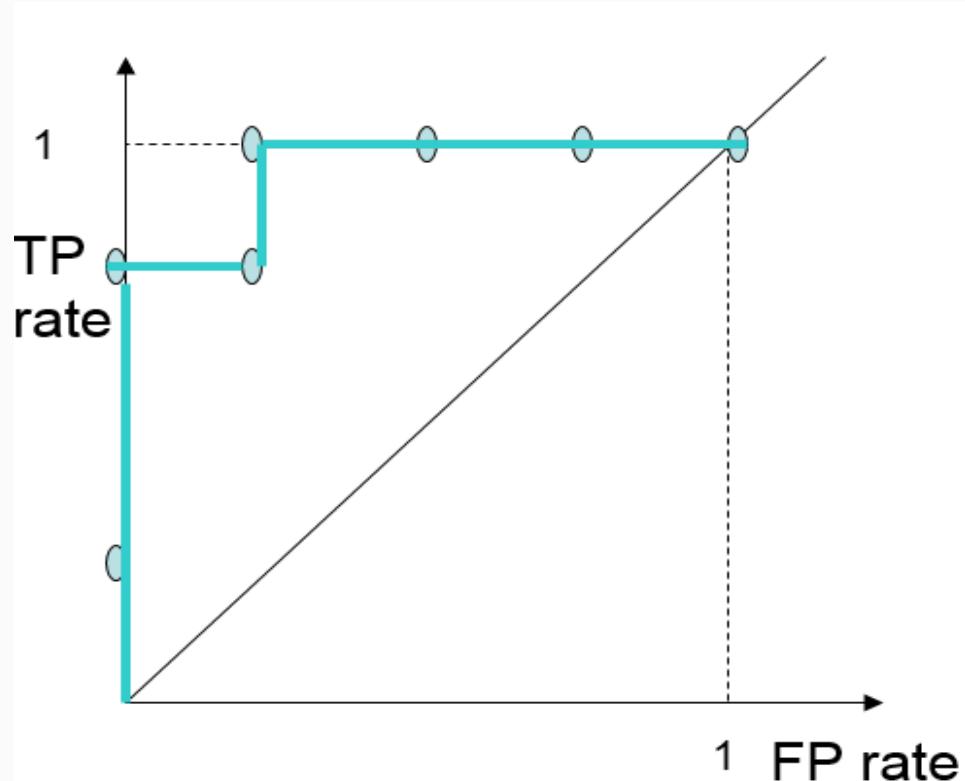
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# ROC Curve of a Probabilistic Classifier



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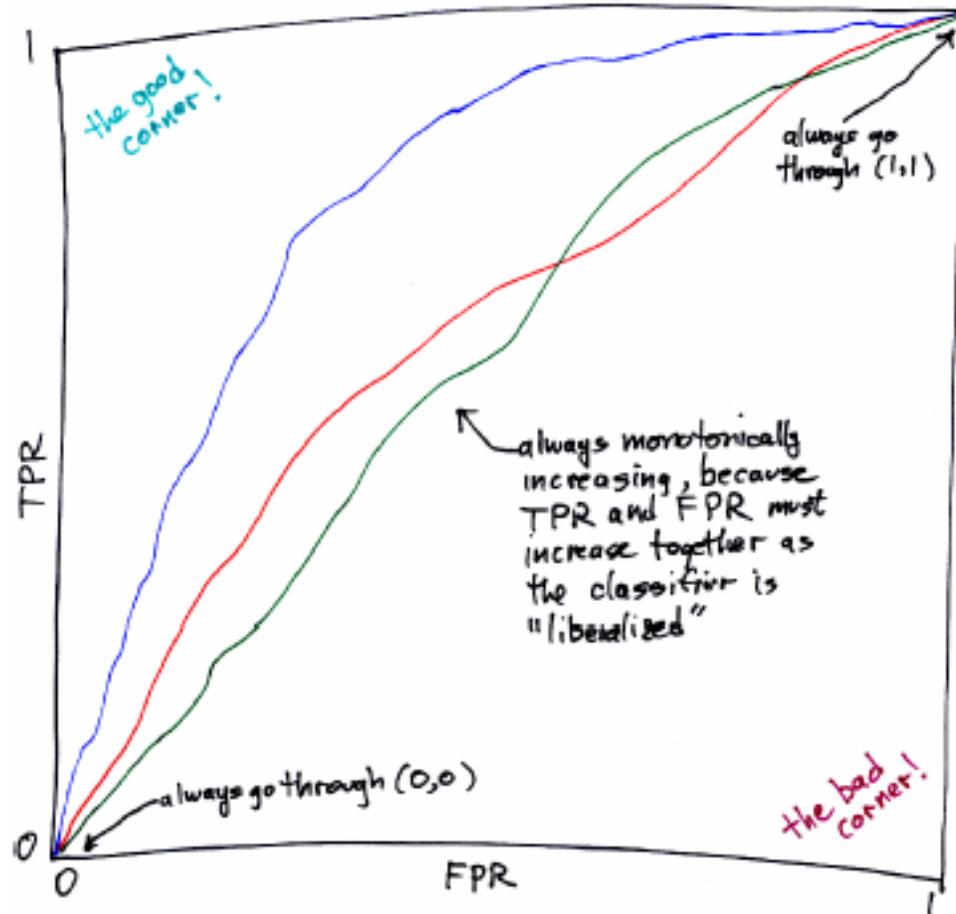
FP rate:  $FP/N=1/4=0.25$

TP rate:  $TP/P=3/3=1.0$ , etc...

# Performance Metrics

## Receiver operating characteristic (ROC) curve

- True positive rate vs. False positive rate for various operating points, as the classifier goes from “conservative” to “liberal”



		actual	
classifier	+	+	-
		TP	FP
	-	FN	TN

true pos rate (TPR)  
≡ sensitivity  
≡ recall

		actual	
classifier	+	+	-
		TP	FP
	-	FN	TN

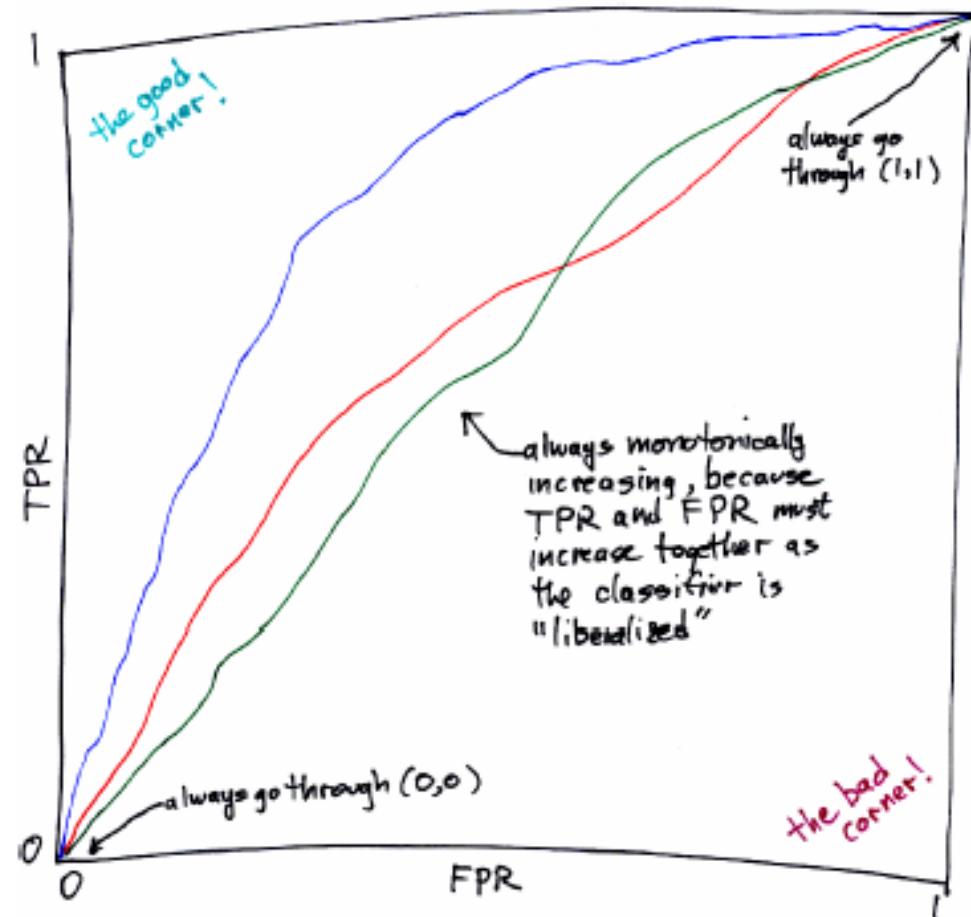
false pos rate (FPR)

ROC curve

# Performance Metrics

## Receiver operating characteristic (ROC) curve

- True positive rate vs. False positive rate for various operating points, as the classifier goes from “conservative” to “liberal”



blue dominates red and green  
neither red nor green dominate the other

You could get the best of the red and green curves by making a hybrid classifier that switches between strategies at the cross-over points.

# Performance Metrics

Since ROC curves don't explicitly show any dependence on the constant P/N (ratio of actual + to - in the sample) they can be misleading if you care about FP versus TP.

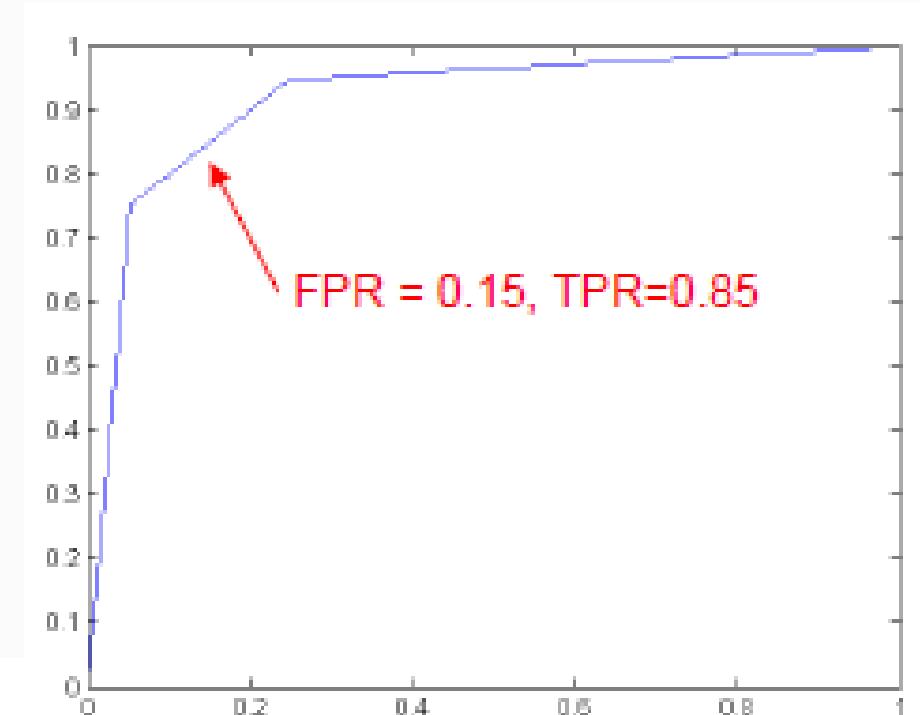
*Suppose you have a test for Alzheimer's whose false positive rate can be varied from 5% to 25% as the false negative rate varies from 25% to 5% (suppose linear dependences on both):*

*You try the test on a population of 10,000 people, 1% of whom actually are Alzheimer's positive:*

		actual	
classifier	+	-	
	+	85	1485
	-	15	8415

FP swamps TP by ~17:1. You'll be telling 17 people that they might have Alzheimer's for every one who actually does. It is unlikely that your test will be used.

In a case like this, ROC, while correct, somewhat misses the point.

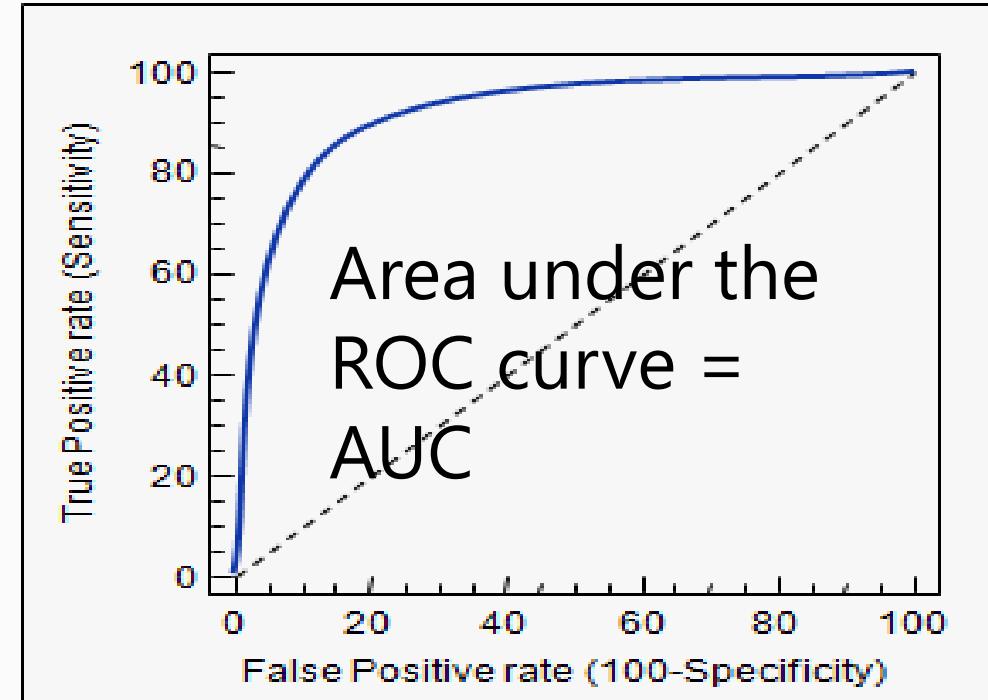


# ROC Curve

- Area under the ROC curve (AUC) is a measure of the model performance

$0.5 \text{ (random model)} < AUC < 1 \text{ (perfect model)}$

- Larger the AUC, better is the model



# Performance Metrics

Receiver operating characteristic (ROC) curve, AUC metric...

- 1.0: perfect prediction
- 0.9: excellent prediction
- 0.8: good prediction
- 0.7: mediocre prediction
- 0.6: poor prediction
- 0.5: random prediction
- <0.5: something wrong!

# Lecture 5 Homework 5a

## Targeted Marketing Campaign

In this problem we will use historical data from past customer responses to build a classification model. The model will then be applied to a new set of prospects to whom we may want extend an offer for a PEP. Rather than doing a mass marketing campaign to all new prospects, we would like to target those that are likely to respond positively to our offer (according to our classification model).

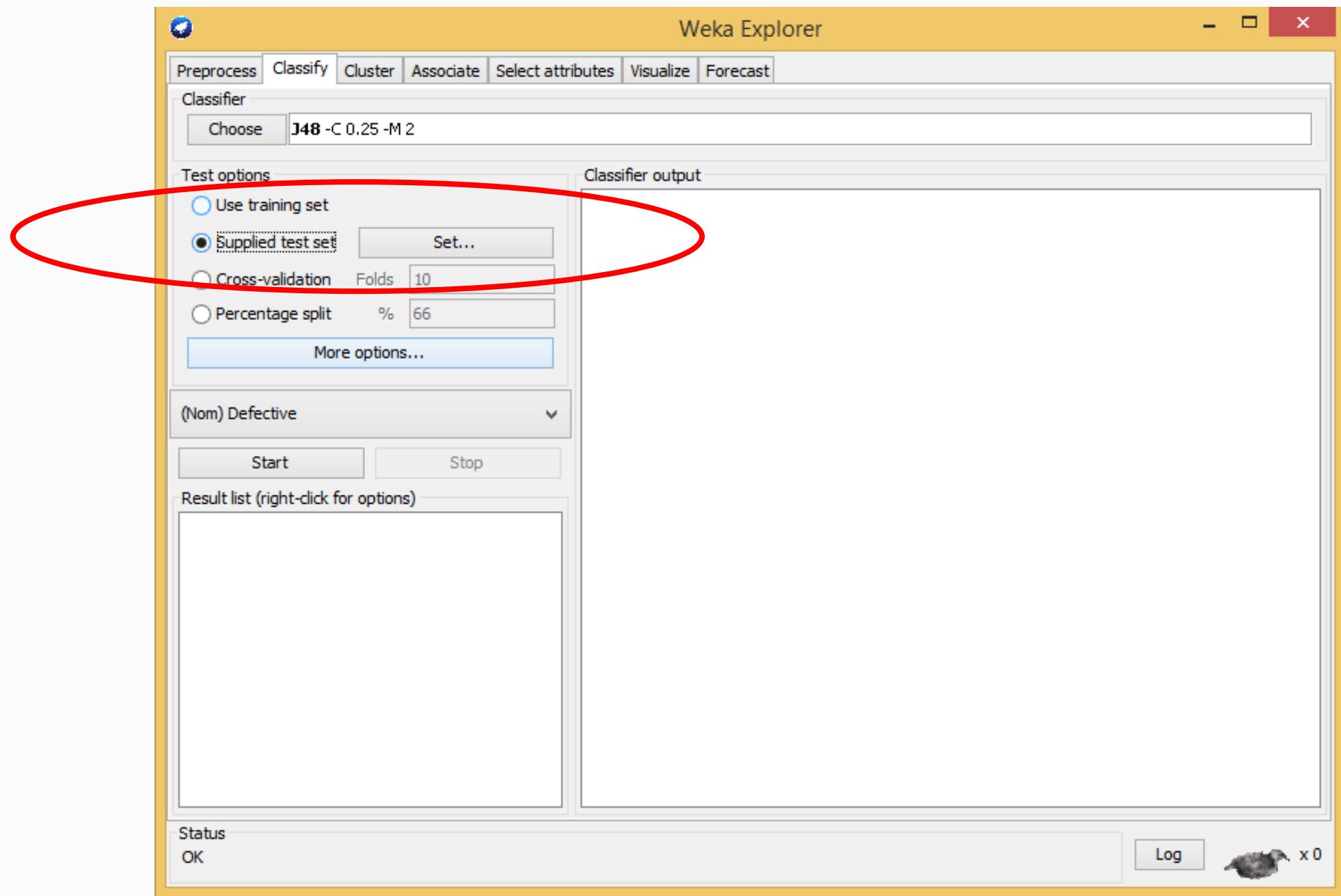
There are two data sets available (the data sets are comma delimited, and the first row contains the field names):

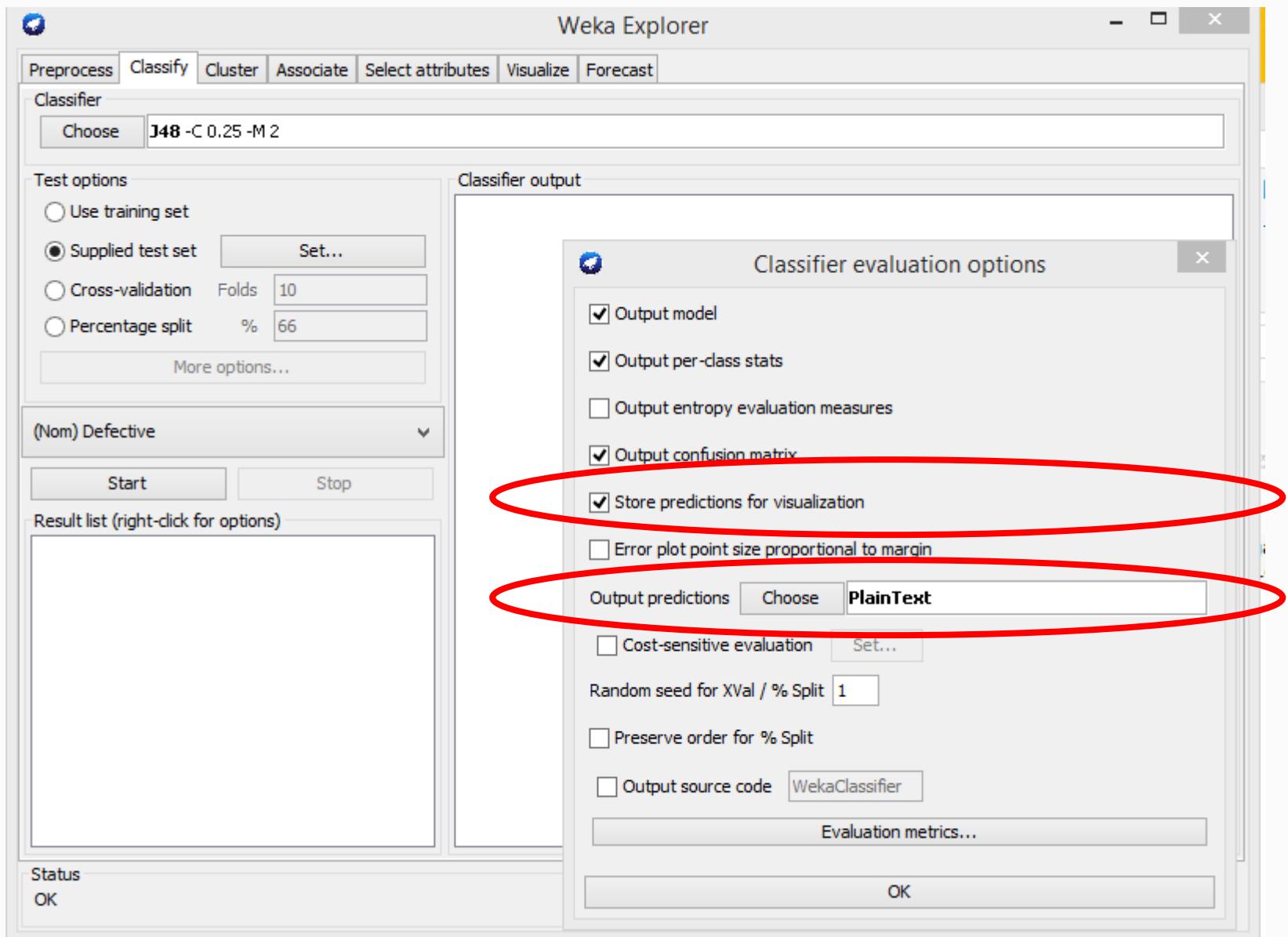
- [bank-data.csv](#) - Labelled training data set for Building a Model
- [bank-new.csv](#) - A set of new customers from which to find the "hot prospects" for the next mailing, using the profiles built from the training set.

- Decision Tree, 10-fold cross validation;
- Make predictions with the model against test data set;
- False Positive costs \$10, False Negative results in a \$1000 loss;
- Lift charts over predictive data;

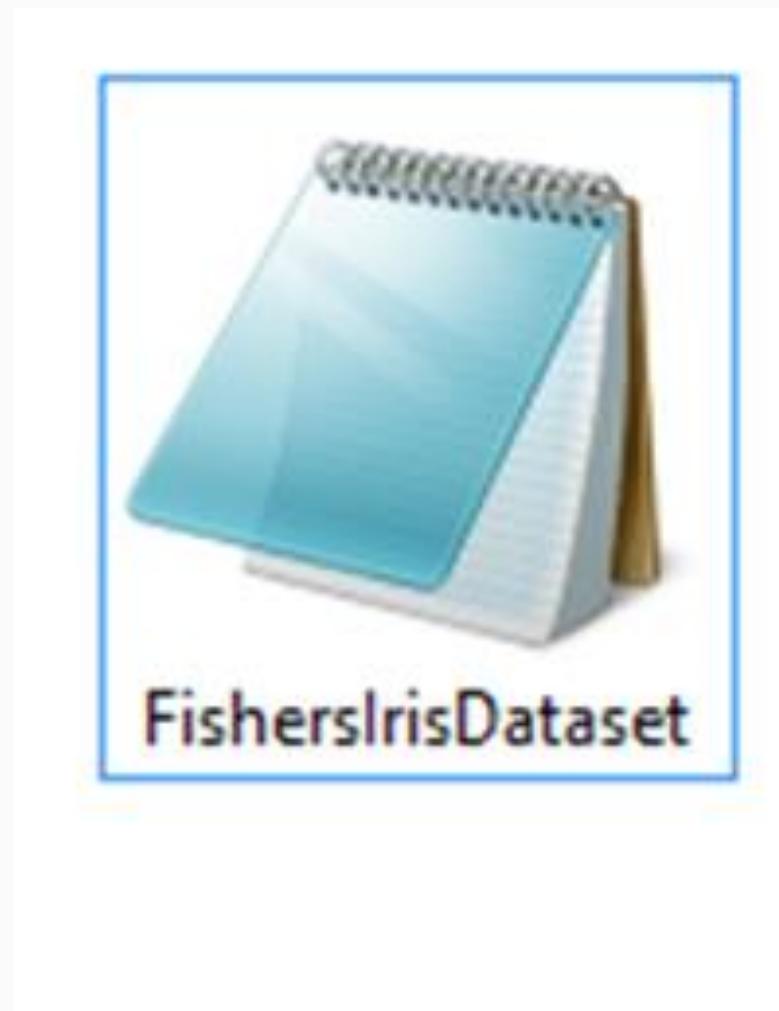
# From model construction to prediction **to impact...**

1. **Build** our predictive model in WEKA Explorer;
2. Use our model to **score (predict)** which new customers to target in our upcoming advertising campaign;
  - **ARFF file manipulation** (hacking), all too common pita...
  - **Excel manipulation** to join model output with our customers list
3. Compute the **lift chart** to assess business impact of our predictive model on the advertising campaign
  - How are Lift charts built, of all the charts and/or performance measures from a model this one is 'on you' to construct;
  - Where is the business 'bang for the buck'?





# How to avoid a time suck...



# Ensemble Methods

## Bagging

- Select many independent samples from training data, *with replacement...*
- Learn one model on each sample (training set), can be done in parallel
- Classifier: Majority voting of the various models

## Boosting

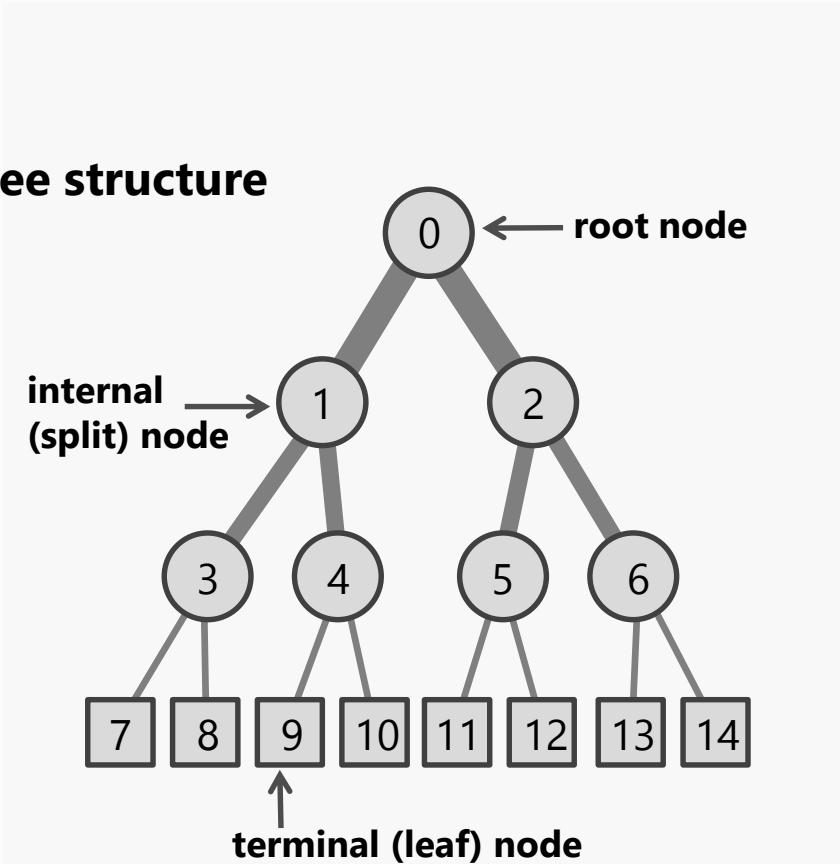
- Learns a sequence of models
- Each model focuses on examples that previous models did badly on
- Learns a weighting of the models

## Decision Trees:

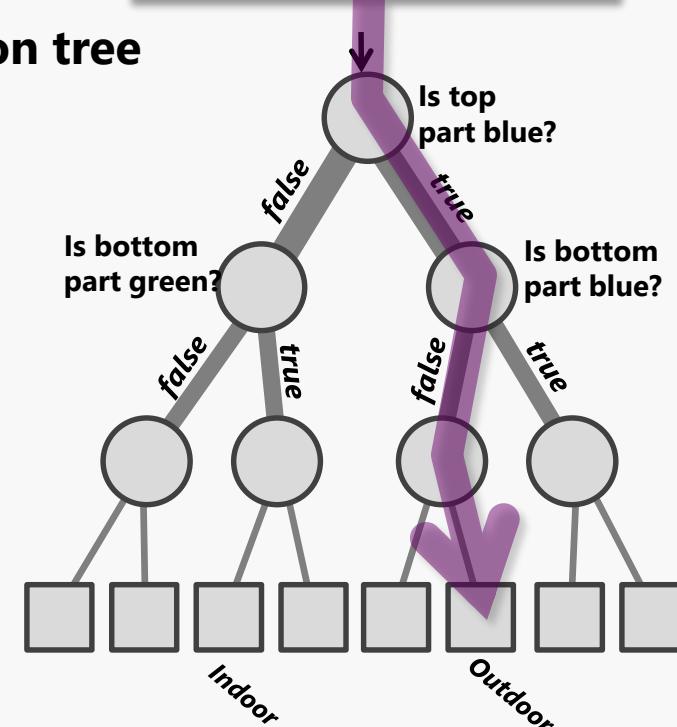
- With **bagging** (+random selection of  $m$  features to use with each node):  
Random Forest
- With **boosting**: Boosted Decision Trees (Bing ranking of search results)

# Decision Trees and Decision Forests

A general tree structure



A decision tree



A forest is an ensemble of trees. The trees are all slightly different from one another.

# Decision Forest Model: the randomness model

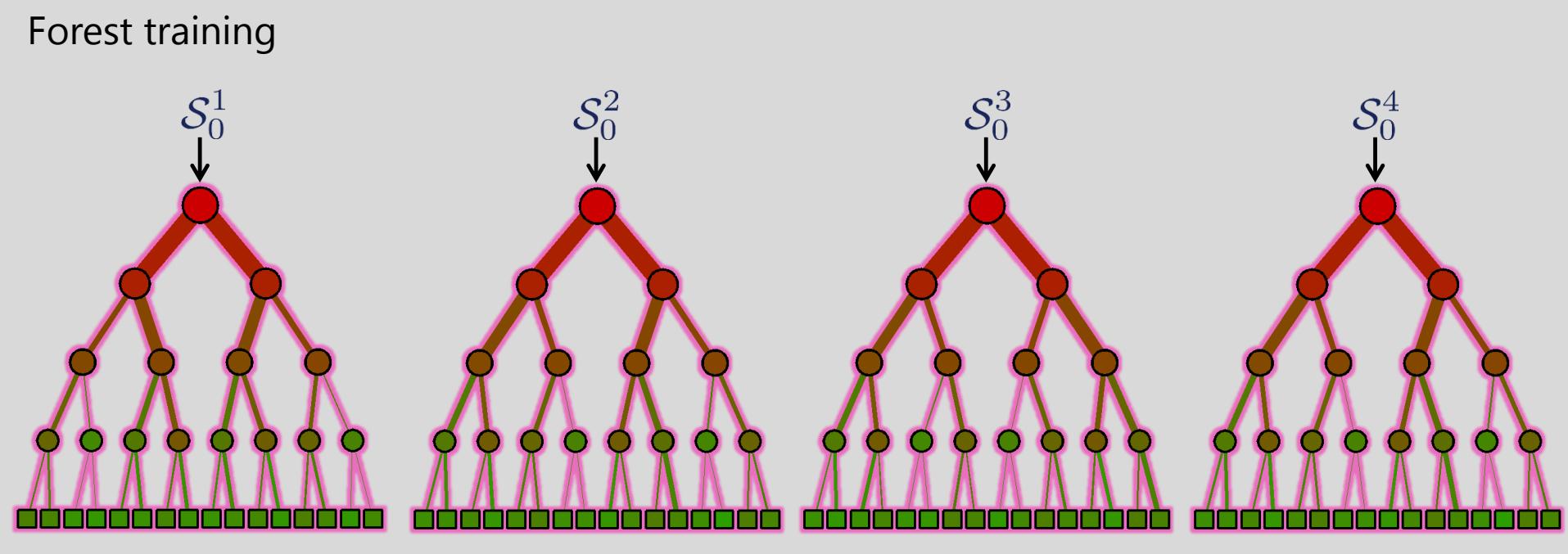
## 1) Bagging (randomizing the training set)

$\mathcal{S}_0$

The full training set

$\mathcal{S}_0^t \subset \mathcal{S}_0$

The randomly sampled subset of training data made available for the tree  $t$



# Decision Forest Model: the randomness model

## 2) Randomized node optimization (RNO)

 $\mathcal{T}$ 

The full set of all possible node test parameters

 $\mathcal{T}_j \subset \mathcal{T}$ 

For each node the set of randomly sampled features

 $\rho = |\mathcal{T}_j|$ 

Randomness control parameter.

For  $\rho = |\mathcal{T}|$  no randomness and maximum tree correlation.

For  $\rho = 1$  max randomness and minimum tree correlation.

### Node training

Node weak learner

$$h(\mathbf{v}, \boldsymbol{\theta}_j)$$

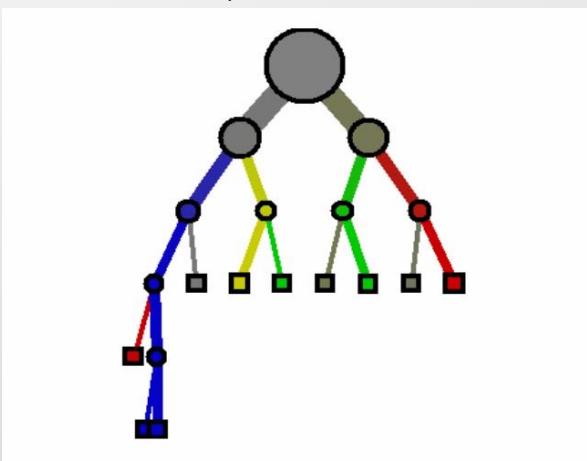
Node test params

$$\boldsymbol{\theta} \in \mathcal{T}_j$$

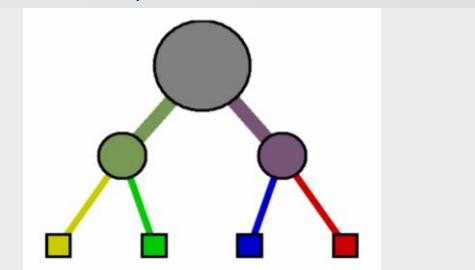


### The effect of $\rho$

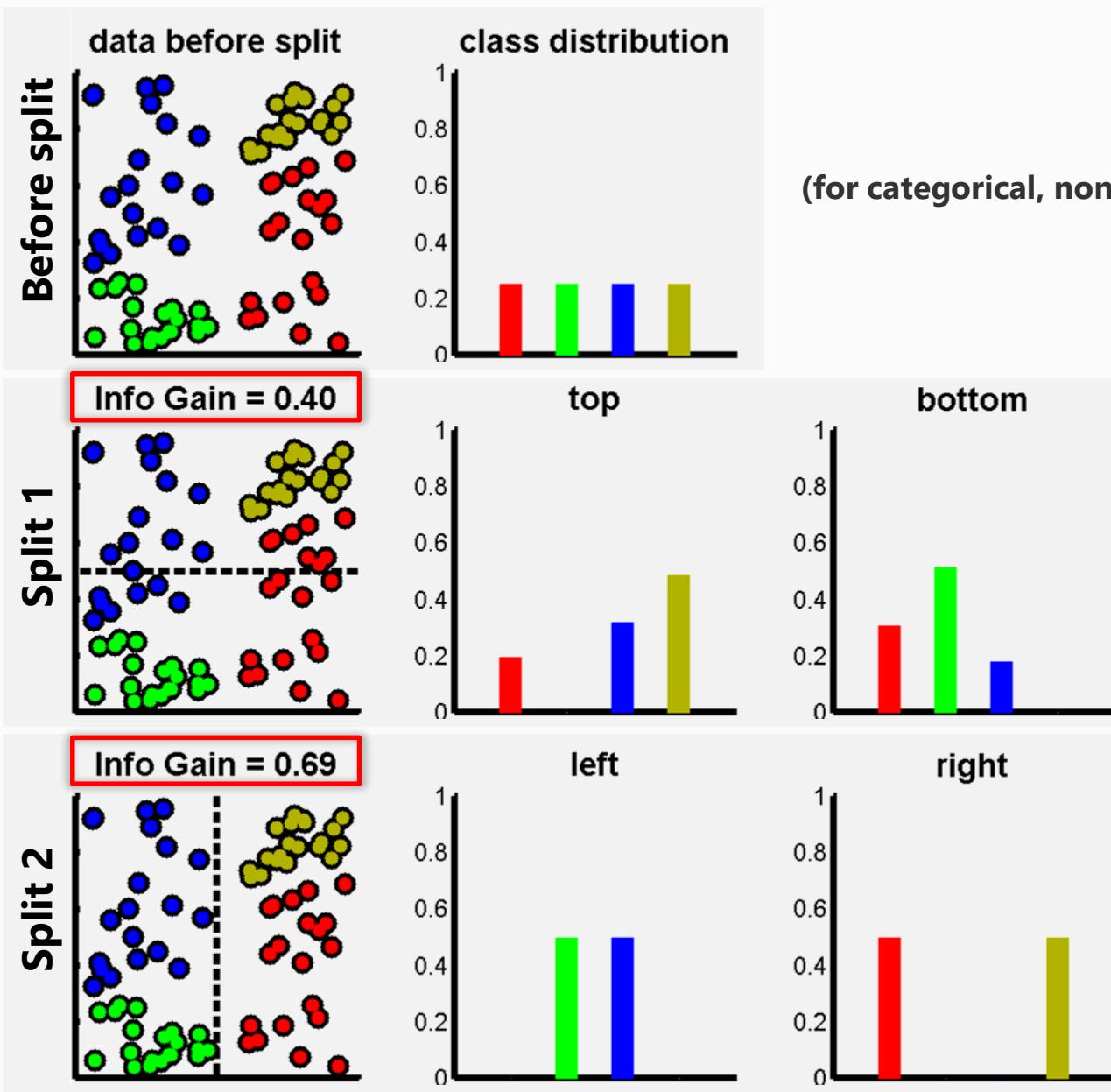
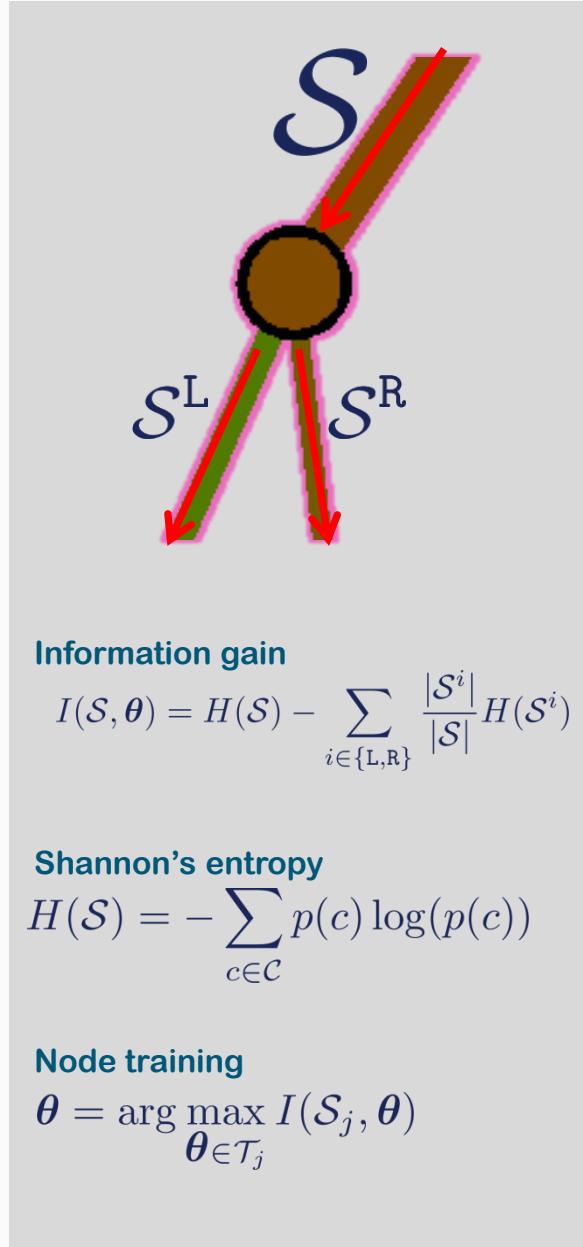
Small value of  $\rho$ ; little tree correlation.



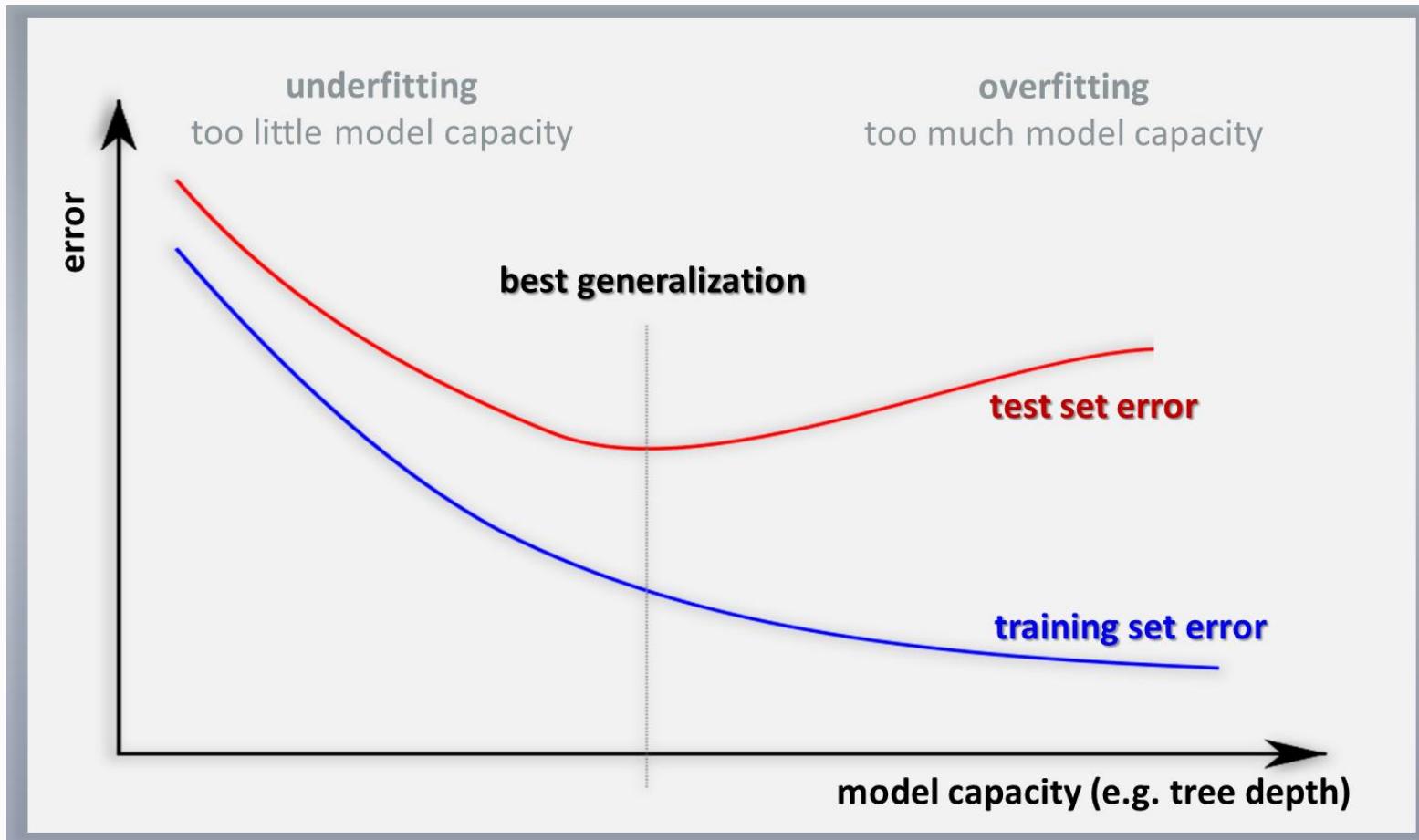
Large value of  $\rho$ ; large tree correlation.



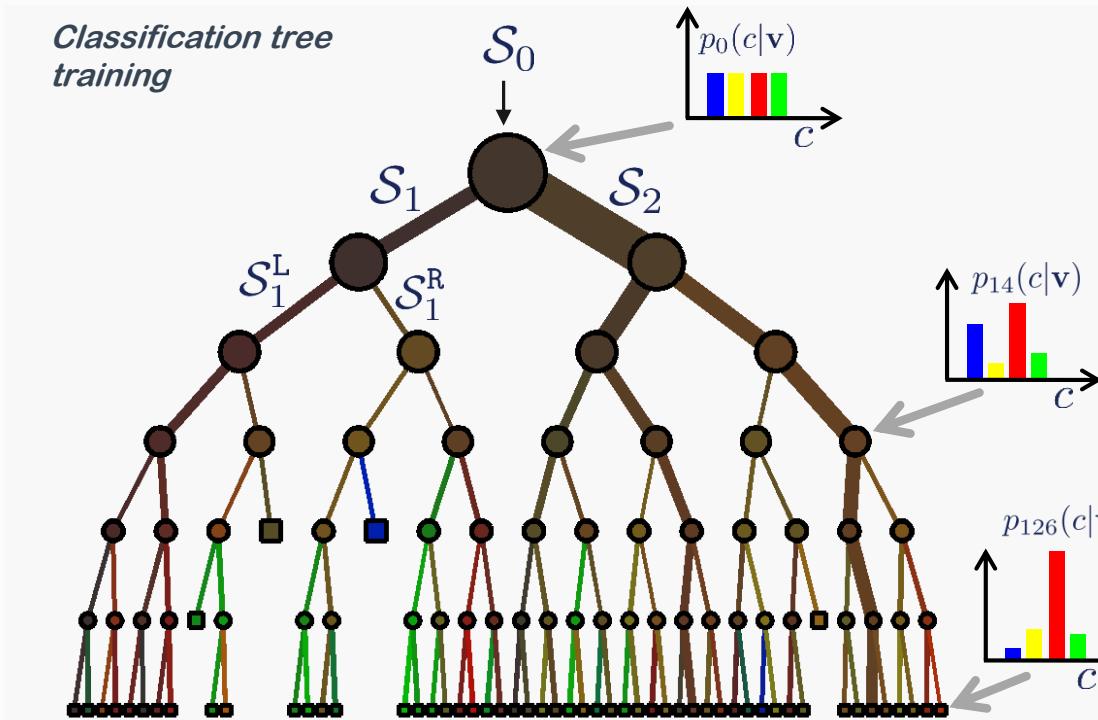
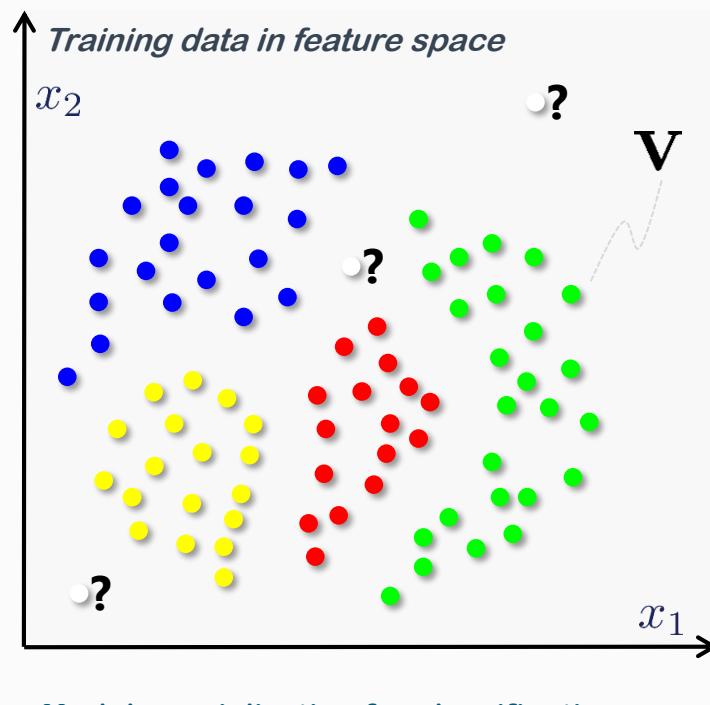
# Decision Forest Model: training and information gain



# Why we prune...



# Classification Forest



## Model specialization for classification

**Input data point**  $\mathbf{v} = (x_1, \dots, x_d) \in \mathbb{R}^d$  ( $x_i$  is feature response)

**Output is categorical**  $c \in \mathcal{C}$  with  $\mathcal{C} = \{c_k\}$  (discrete set)

**Node weak learner**  $h(\mathbf{v}, \theta) \in \{\text{true, false}\}$

**Obj. funct. for node j**  $I = H(S_j) - \sum_{i=L,R} \frac{|S_j^i|}{|S_j|} H(S_j^i)$  (information gain)

**Training node j**  $\theta_j = \arg \max_{\theta \in \mathcal{T}_j} I(S_j, \theta)$

**Predictor model**  $p(c|\mathbf{v}) = \sum_j p(c|j)p(j|\mathbf{v})$  (class posterior)

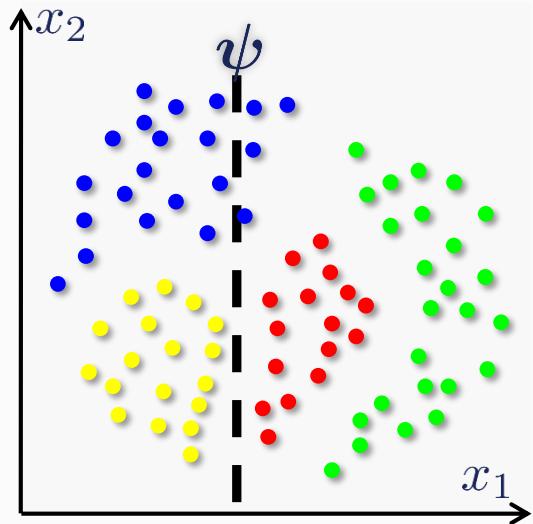
## Entropy of a discrete distribution

$$H(\mathcal{S}) = - \sum_{c \in \mathcal{C}} p(c) \log(p(c))$$

$$\text{with } c(\mathbf{v}) : \mathbb{R}^d \rightarrow \mathcal{C}$$

# Classification Forest: the weak learner model

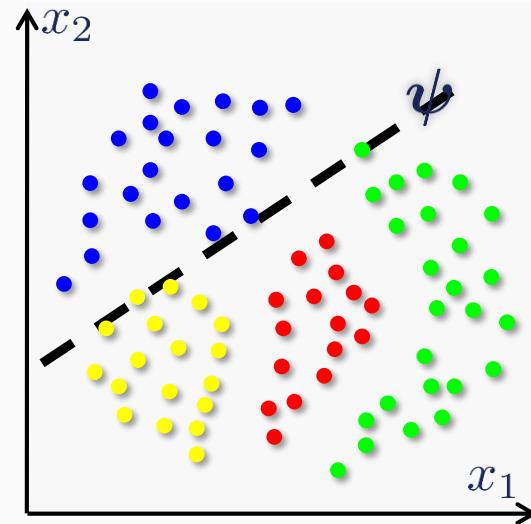
Examples of weak learners



Weak learner: axis aligned

$$h(\mathbf{v}, \theta) = [\tau_1 > \phi(\mathbf{v}) \cdot \psi > \tau_2]$$

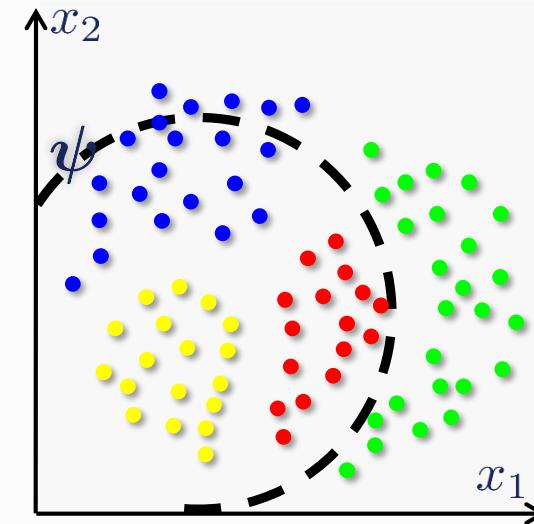
Feature response  
for 2D example.  
With  $\psi = (1 \ 0 \ \psi_3)$  or  $\psi = (0 \ 1 \ \psi_3)$

$$\phi(\mathbf{v}) = (x_1 \ x_2 \ 1)^\top$$


Weak learner: oriented line

$$h(\mathbf{v}, \theta) = [\tau_1 > \phi(\mathbf{v}) \cdot \psi > \tau_2]$$

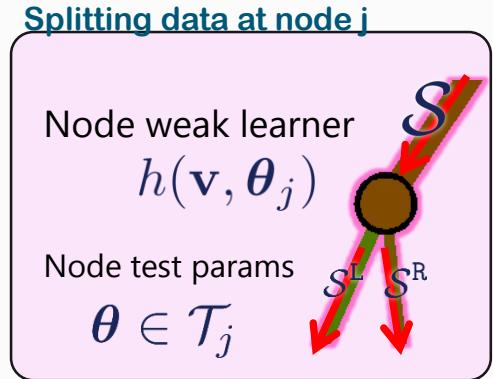
Feature response  
for 2D example.  
With  $\psi \in \mathbb{R}^3$  a generic line in homog. coordinates.

$$\phi(\mathbf{v}) = (x_1 \ x_2 \ 1)^\top$$


Weak learner: conic section

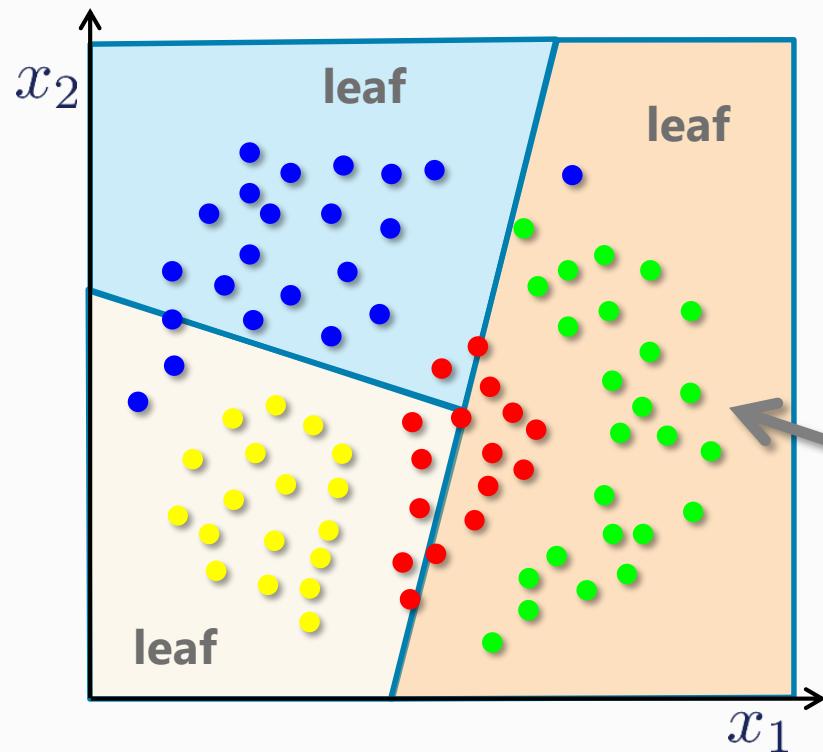
$$h(\mathbf{v}, \theta) = [\tau_1 > \phi^\top(\mathbf{v}) \psi \phi(\mathbf{v}) > \tau_2]$$

Feature response  
for 2D example.  
With  $\psi \in \mathbb{R}^{3 \times 3}$  a matrix representing a conic.

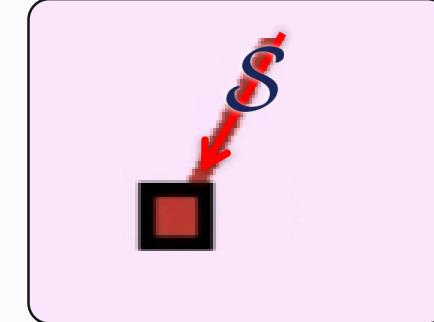
$$\phi(\mathbf{v}) = (x_1 \ x_2 \ 1)^\top$$


In general  $\phi$  may select only a very small subset of features  $\phi(\mathbf{v}) : \mathbb{R}^d \rightarrow \mathbb{R}^{d'+1}, d' \ll d$

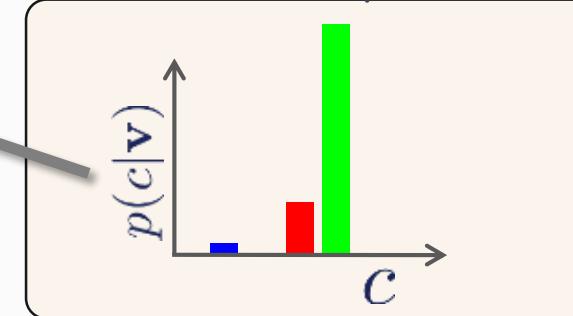
# Classification Forest: the prediction model



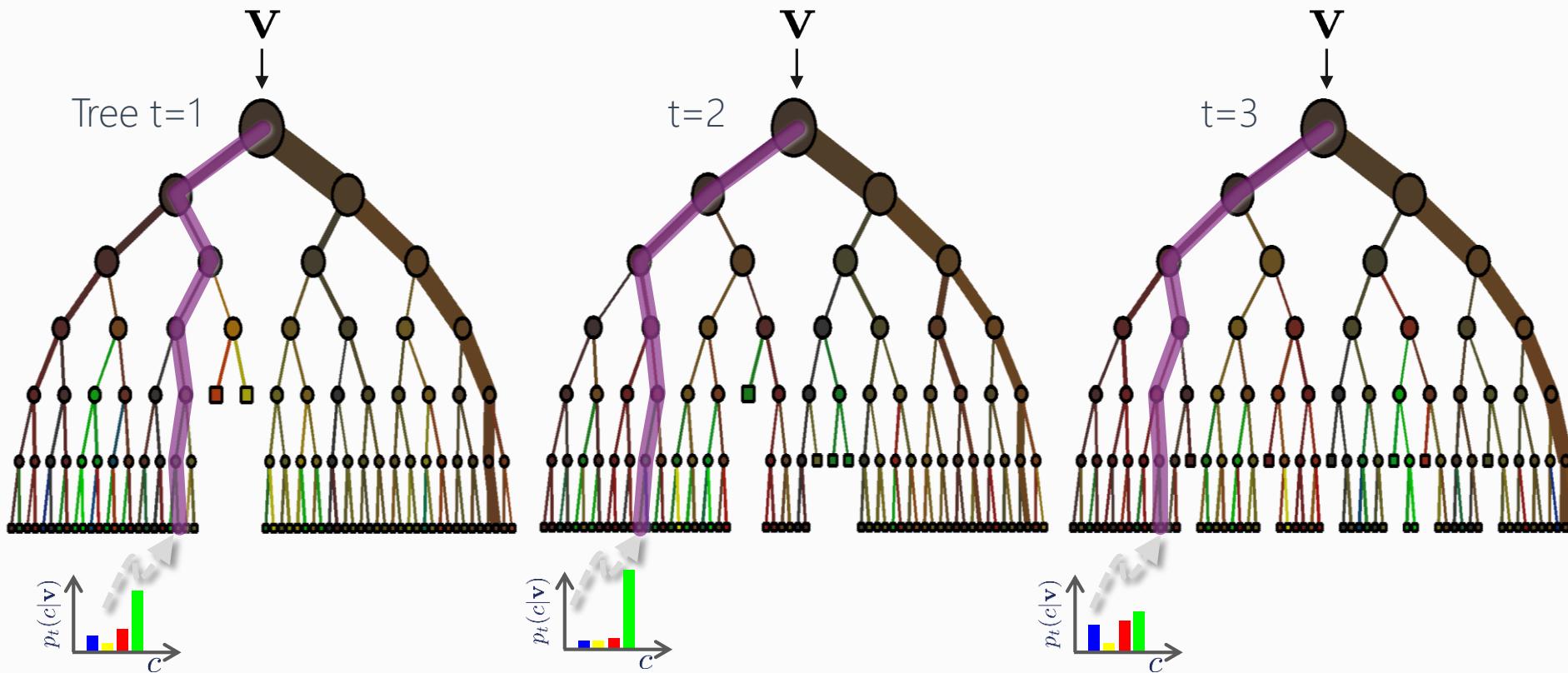
What do we do at the leaf?



Prediction model: probabilistic

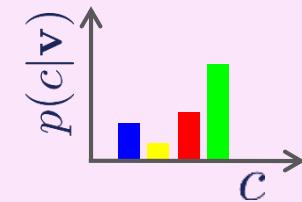


# Classification Forest: the ensemble model

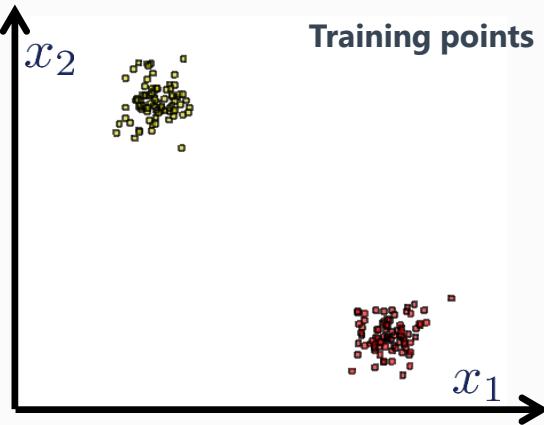


## The ensemble model

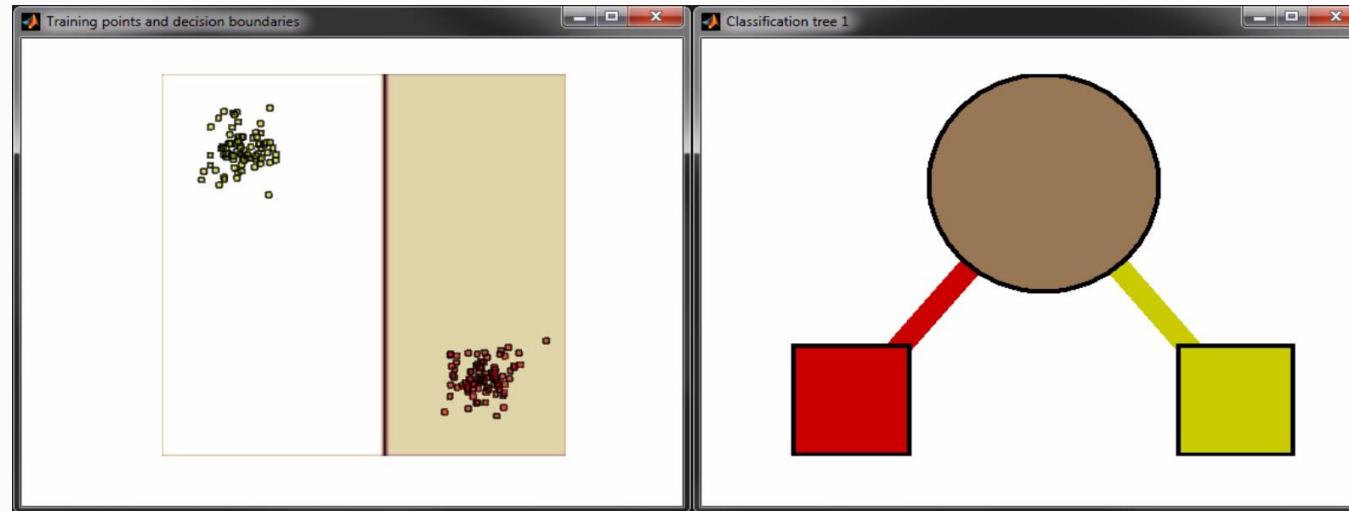
$$\text{Forest output probability} \quad p(c|\mathbf{v}) = \frac{1}{T} \sum_t p_t(c|\mathbf{v})$$



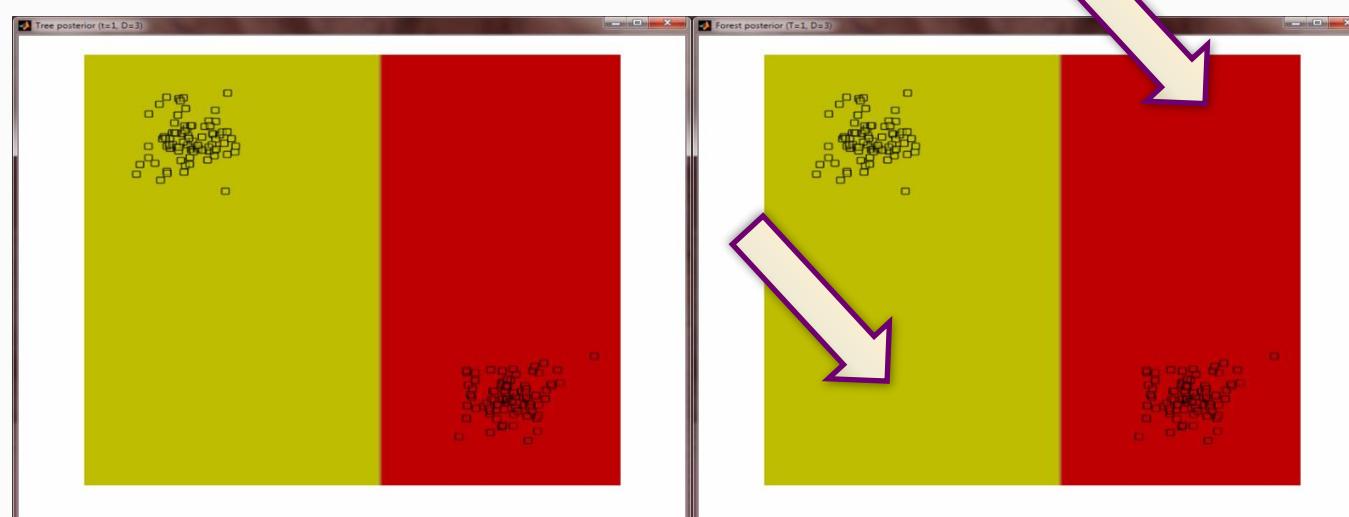
# Classification Forest: effect of the weak learner model



Training different trees in the forest



Testing different trees in the forest



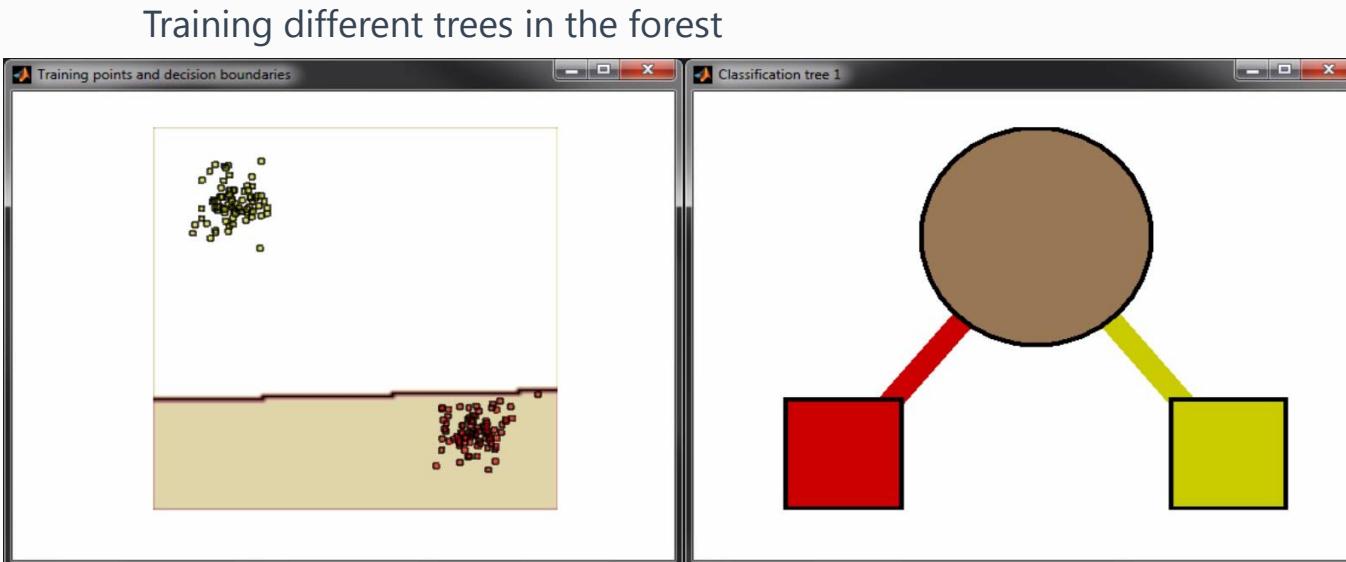
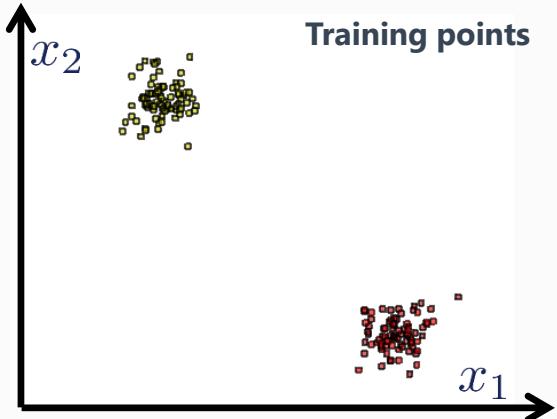
Three concepts to keep in mind:

- "Accuracy of prediction"
- "Quality of confidence"
- "Generalization"

(2 videos in this page)

Parameters: T=200, D=2, weak learner = aligned, leaf model = probabilistic

# Classification Forest: effect of the weak learner model

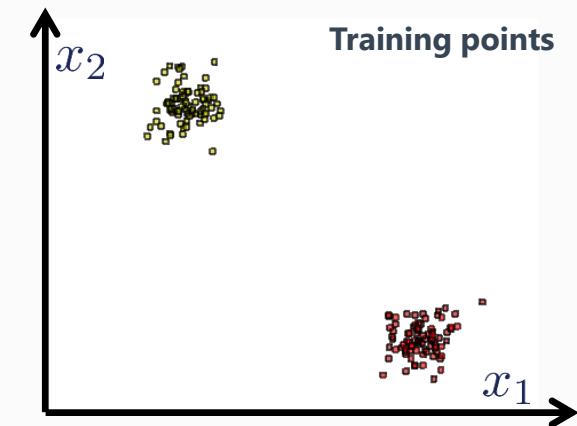


Parameters: T=200, D=2, weak learner = linear, leaf model = probabilistic

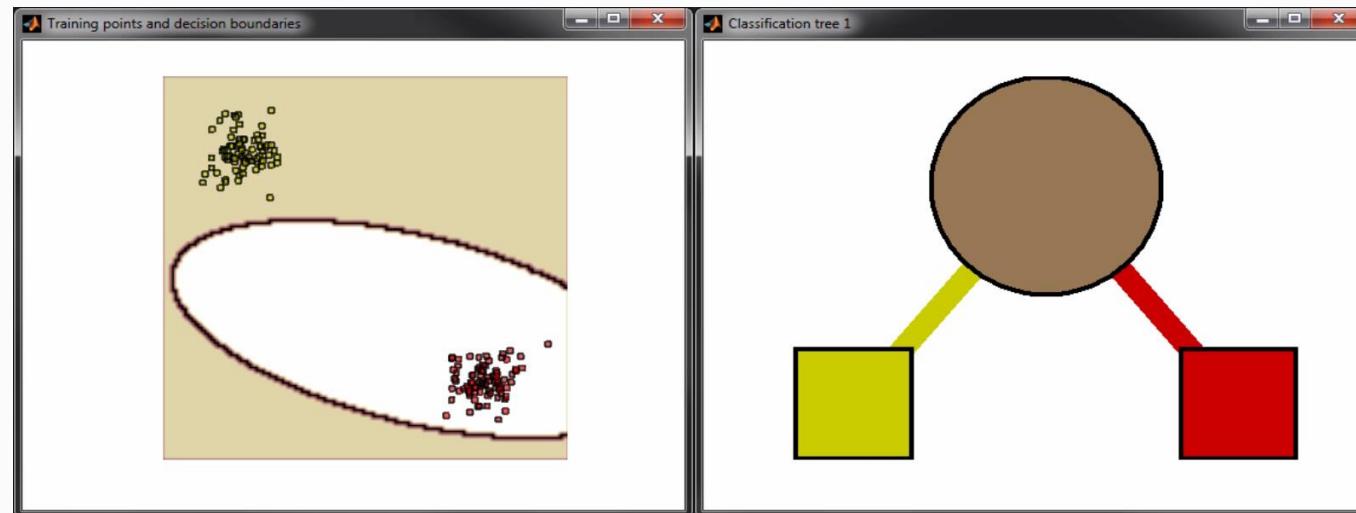
Deriving Knowledge from Data at Scale



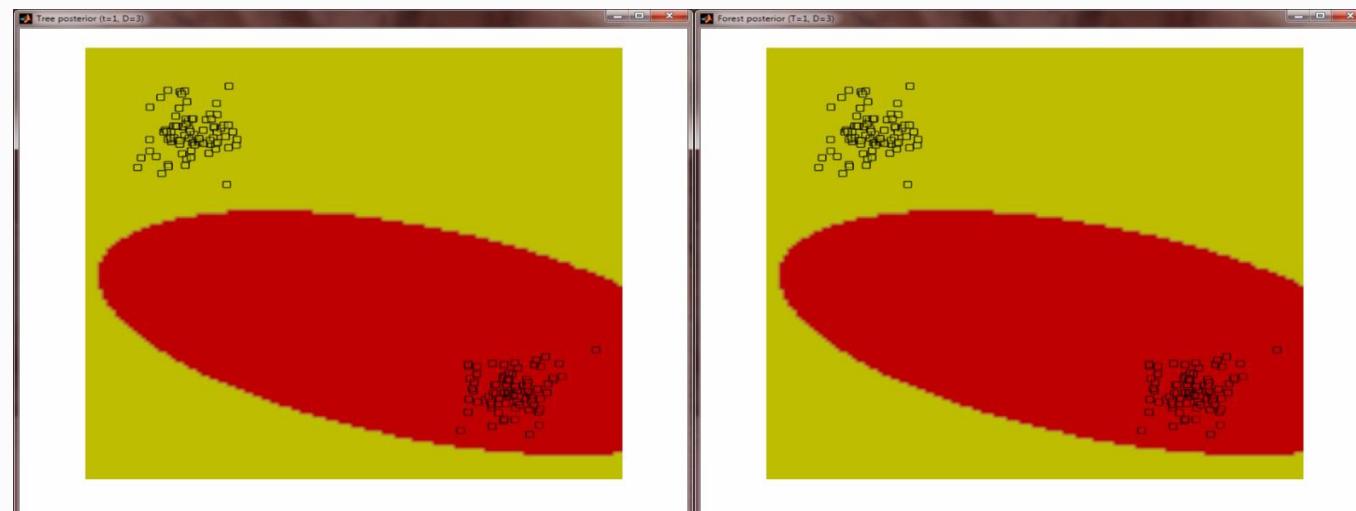
# Classification Forest: effect of the weak learner model



Training different trees in the forest



Testing different trees in the forest



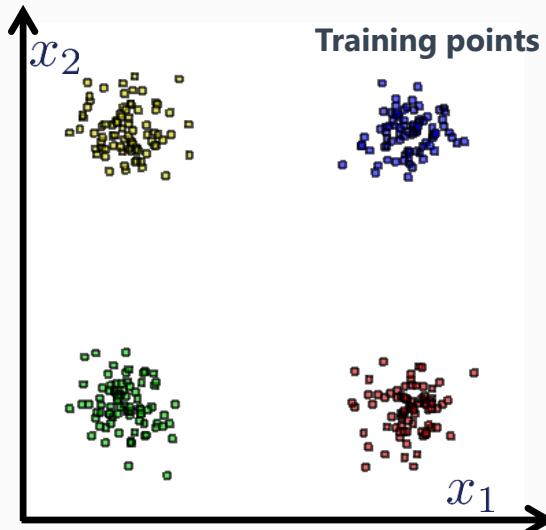
Parameters: T=200, D=2, weak learner = conic, leaf model = probabilistic

(2 videos in this page)

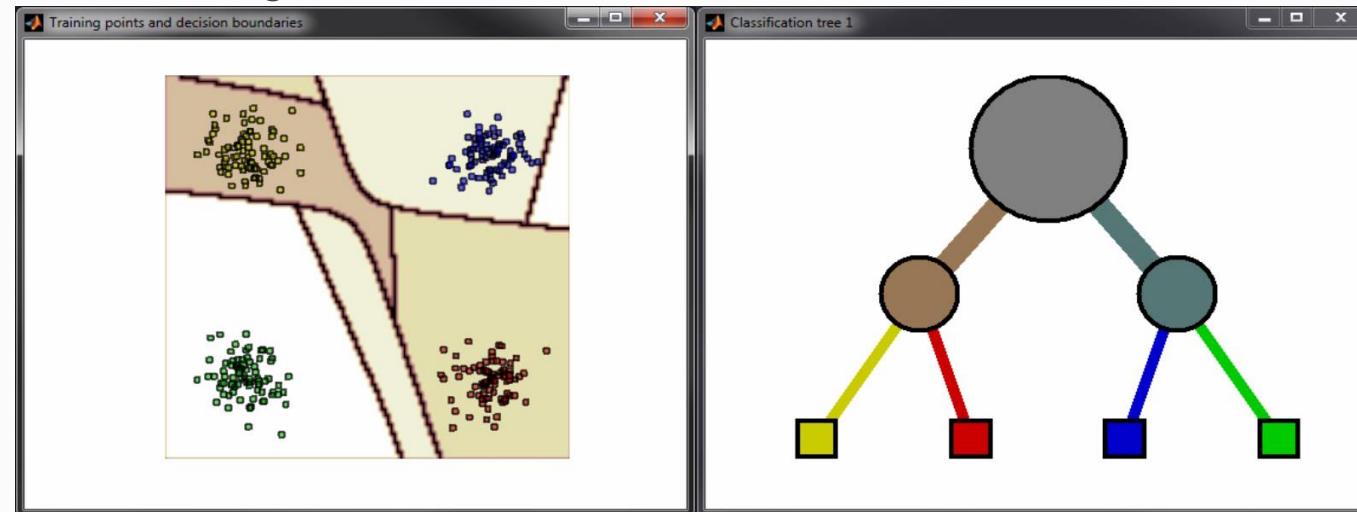
Deriving Knowledge from Data at Scale



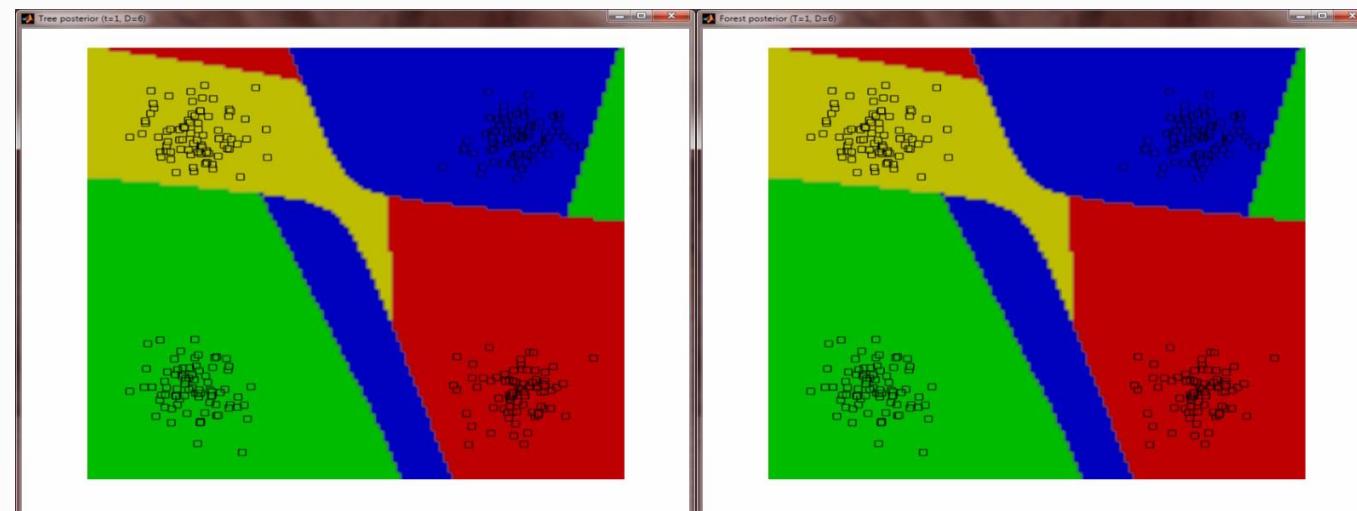
# Classification Forest: with >2 classes



Training different trees in the forest



Testing different trees in the forest



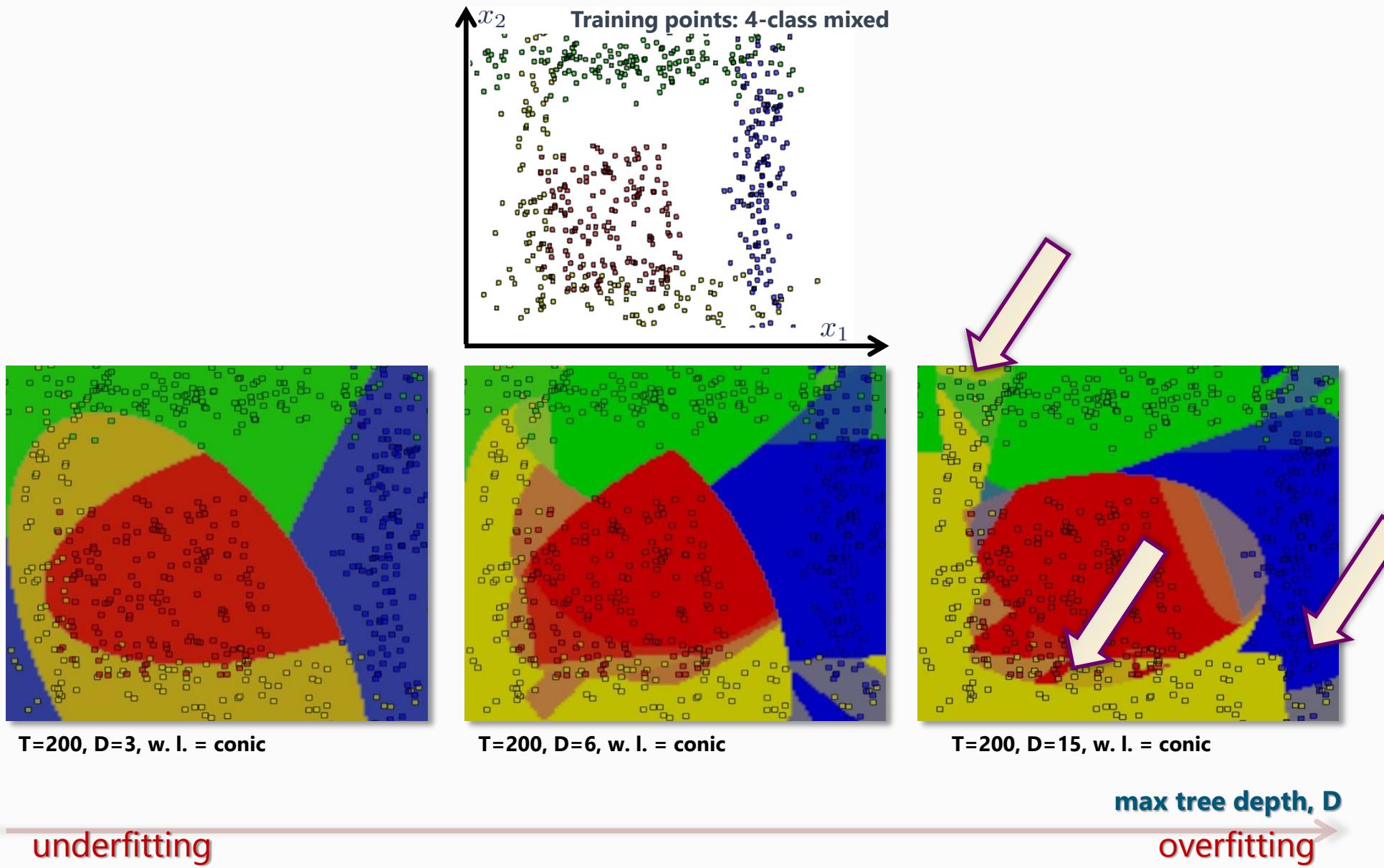
Parameters: T=200, D=3, weak learner = conic, leaf model = probabilistic

(2 videos in this page)

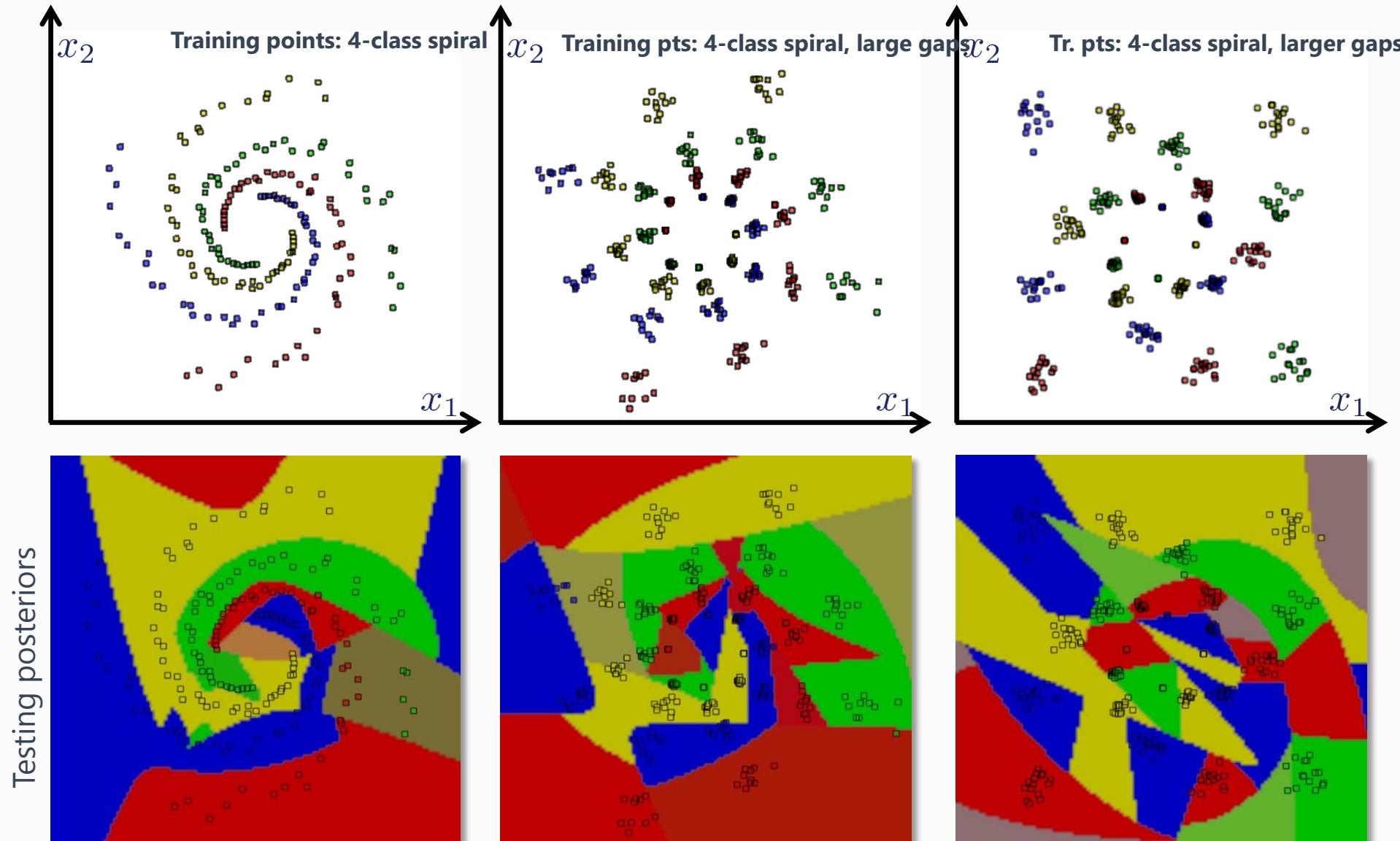
Deriving Knowledge from Data at Scale



# Classification Forest: effect of tree depth



# Classification Forest: analysing generalization



(3 videos in this page)

Parameters: T=200, D=13, w. l. = conic, predictor = prob.

# Data Science

Deriving Knowledge from Data at Scale

*Feature extraction and selection are the **most important** but underrated step of machine learning. Better features are better than better algorithms...*

better than better algorithms...

underrated step of machine learning. Better features are  
feature extraction and selection are the most important part



# Data Science

Deriving Knowledge from Data at Scale

*That's all for tonight...*

Valentine N. Fontama

July 30<sup>th</sup>, 2015

Deriving Knowledge from Data at Scale

