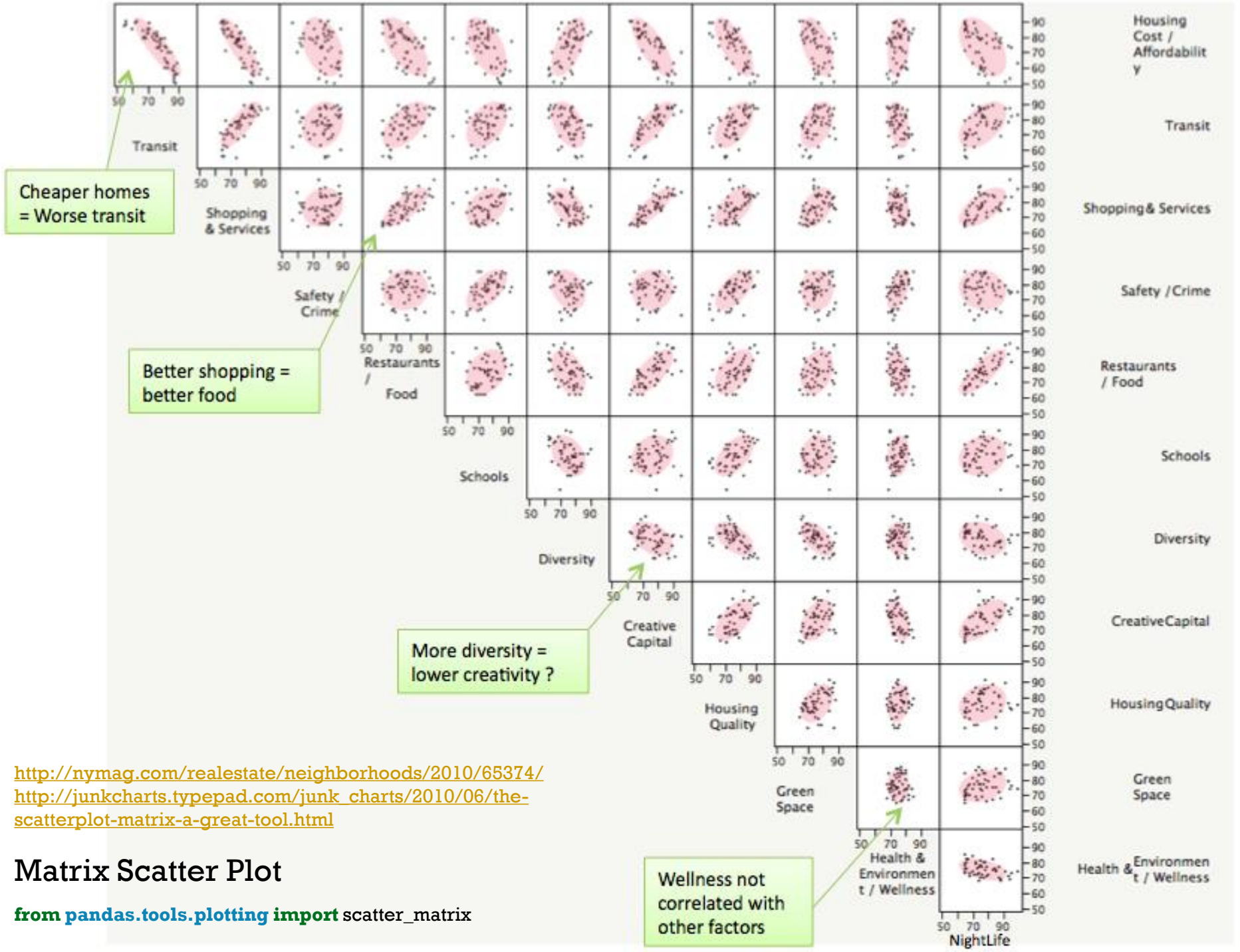
# ENSEMBLE METHODS

INTRODUCTION TO DATA SCIENCE

TIM KRASKA



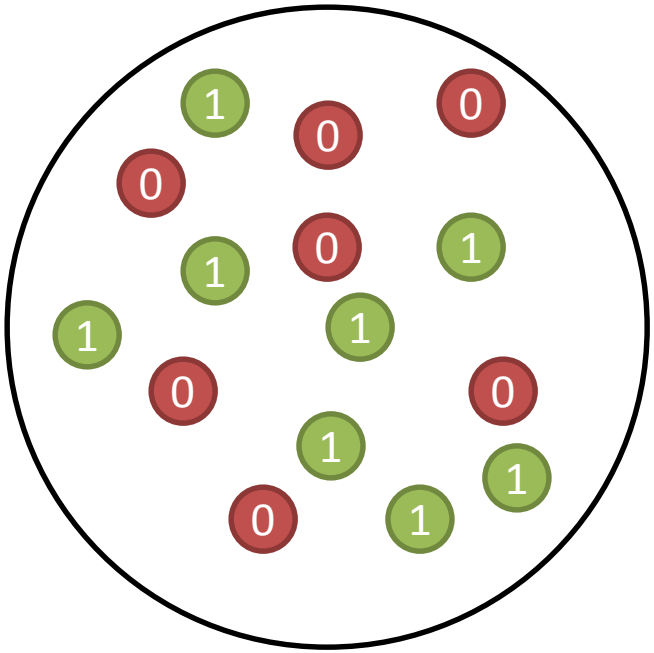

http://nymag.com/realestate/neighborhoods/2010/65374/
http://junkcharts.typepad.com/junk_charts/2010/06/the-scatterplot-matrix-a-great-tool.html

# Matrix Scatter Plot

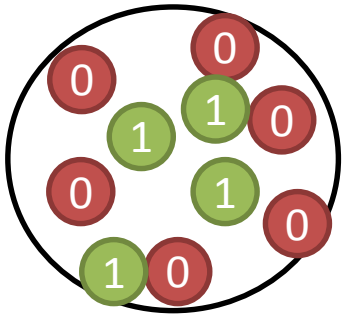
```
from pandas.tools.plotting import scatter_matrix
```

# Recap: Information Gain

Titanic Entropy = 0.96

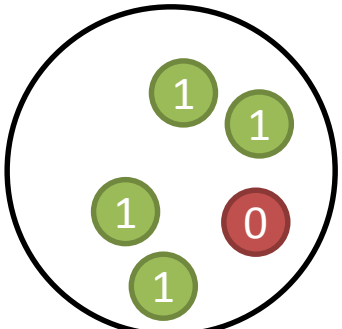


male



Entropy= - 682/843 log(682/843 )
- 161/843 log(161/843 )
= 0.21

female



Entropy= - 127/466 log(127/466)
- 339/466 log(339/466)
= 0.25

Weighted Entropy: 466/1309 * 0.25 + 843 / 1309 * 0.21 = 0.22
Information Gain for split: 0.96 – 0.22 = 0.74

| outlook | temperature | humidity | windy | play |
|---|---|---|---|---|
| overcast | cool | normal | TRUE | yes |
| overcast | hot | high | FALSE | yes |
| overcast | hot | normal | FALSE | yes |
| overcast | mild | high | TRUE | yes |
| rainy | cool | normal | TRUE | no |
| rainy | mild | high | TRUE | no |
| rainy | cool | normal | FALSE | yes |
| rainy | mild | high | FALSE | yes |
| rainy | mild | normal | FALSE | yes |
| sunny | hot | high | FALSE | no |
| sunny | hot | high | TRUE | no |
| sunny | mild | high | FALSE | no |
| sunny | cool | normal | FALSE | yes |
| sunny | mild | normal | TRUE | yes |

Before: 14 records, 9 are “yes”

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

If we choose **outlook**:

overcast : 4 records, 4 are “yes”

$$-\left(\frac{4}{4}\log_2\frac{4}{4}\right)=0$$

rainy : 5 records, 3 are “yes”

$$-\left(\frac{3}{5}\log_2\frac{3}{5}+\frac{2}{5}\log_2\frac{2}{5}\right)=0.97$$

sunny : 5 records, 2 are “yes”

$$-\left(\frac{2}{5}\log_2\frac{2}{5}+\frac{3}{5}\log_2\frac{3}{5}\right)=0.97$$

Expected new entropy:

$$\frac{4}{14}\times 0.0+\frac{5}{14}\times 0.97+\frac{5}{14}\times 0.97$$

= 0.69

| outlook | temperature | humidity | windy | play |
|---|---|---|---|---|
| overcast | cool | normal | TRUE | yes |
| overcast | hot | high | FALSE | yes |
| overcast | hot | normal | FALSE | yes |
| overcast | mild | high | TRUE | yes |
| rainy | cool | normal | TRUE | no |
| rainy | mild | high | TRUE | no |
| rainy | cool | normal | FALSE | yes |
| rainy | mild | high | FALSE | yes |
| rainy | mild | normal | FALSE | yes |
| sunny | hot | high | FALSE | no |
| sunny | hot | high | TRUE | no |
| sunny | mild | high | FALSE | no |
| sunny | cool | normal | FALSE | yes |
| sunny | mild | normal | TRUE | yes |

Before: 14 records, 9 are “yes”

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

If we choose **windy**:

FALSE: 8 records, 6 are “yes”

0.81 = -(6/8*log(6/8)+2/8*log(2/8))

TRUE: 6 records, 3 are “yes”

1

Expected new entropy:

0.81(8/14) + 1 (6/14)

= 0.89

| outlook | temperature | humidity | windy | play |
|---|---|---|---|---|
| overcast | cool | normal | TRUE | yes |
| overcast | hot | high | FALSE | yes |
| overcast | hot | normal | FALSE | yes |
| overcast | mild | high | TRUE | yes |
| rainy | cool | normal | TRUE | no |
| rainy | mild | high | TRUE | no |
| rainy | cool | normal | FALSE | yes |
| rainy | mild | high | FALSE | yes |
| rainy | mild | normal | FALSE | yes |
| sunny | hot | high | FALSE | no |
| sunny | hot | high | TRUE | no |
| sunny | mild | high | FALSE | no |
| sunny | cool | normal | FALSE | yes |
| sunny | mild | normal | TRUE | yes |

Before: 14 records, 9 are “yes”

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

If we choose **temperature**:

cool : 4 records, 3 are “yes”

0.81

rainy : 4 records, 2 are “yes”

1.0

sunny : 6 records, 4 are “yes”

0.92

Expected new entropy:

0.81(4/14) + 1.0(4/14) + 0.92(6/14)

= 0.91

| outlook | temperature | humidity | windy | play |
|---|---|---|---|---|
| overcast | cool | normal | TRUE | yes |
| overcast | hot | high | FALSE | yes |
| overcast | hot | normal | FALSE | yes |
| overcast | mild | high | TRUE | yes |
| rainy | cool | normal | TRUE | no |
| rainy | mild | high | TRUE | no |
| rainy | cool | normal | FALSE | yes |
| rainy | mild | high | FALSE | yes |
| rainy | mild | normal | FALSE | yes |
| sunny | hot | high | FALSE | no |
| sunny | hot | high | TRUE | no |
| sunny | mild | high | FALSE | no |
| sunny | cool | normal | FALSE | yes |
| sunny | mild | normal | TRUE | yes |

Before: 14 records, 9 are “yes”

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

If we choose **humidity**:

normal : 7 records, 6 are “yes”

0.59

high : 7 records, 2 are “yes”

0.86

Expected new entropy:

0.59(7/14) + 0.86(7/14)

= 0.725

| outlook | temperature | humidity | windy | play |
|---|---|---|---|---|
| overcast | cool | normal | TRUE | yes |
| overcast | hot | high | FALSE | yes |
| overcast | hot | normal | FALSE | yes |
| overcast | mild | high | TRUE | yes |
| rainy | cool | normal | TRUE | no |
| rainy | mild | high | TRUE | no |
| rainy | cool | normal | FALSE | yes |
| rainy | mild | high | FALSE | yes |
| rainy | mild | normal | FALSE | yes |
| sunny | hot | high | FALSE | no |
| sunny | hot | high | TRUE | no |
| sunny | mild | high | FALSE | no |
| sunny | cool | normal | FALSE | yes |
| sunny | mild | normal | TRUE | yes |

Before: 14 records, 9 are “yes”

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

outlook

0.94 – 0.69 = 0.25 highest gain

temperature

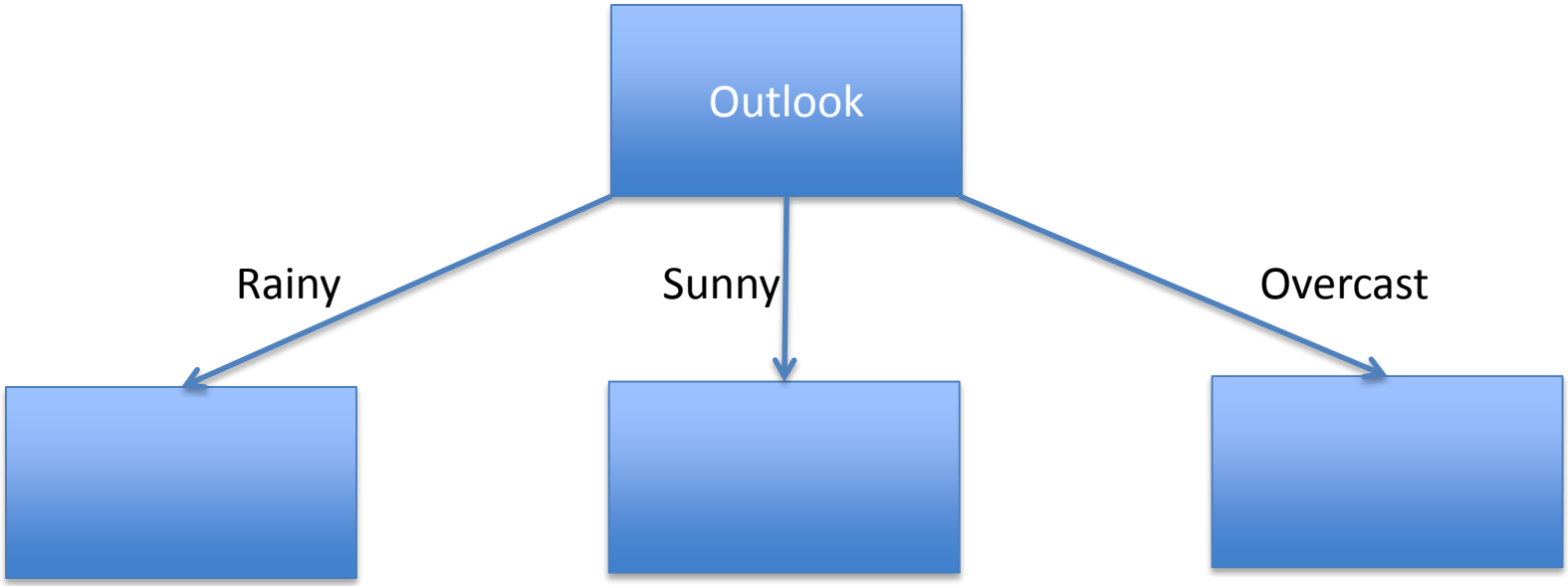
0.94 – 0.91 = 0.03

humidity

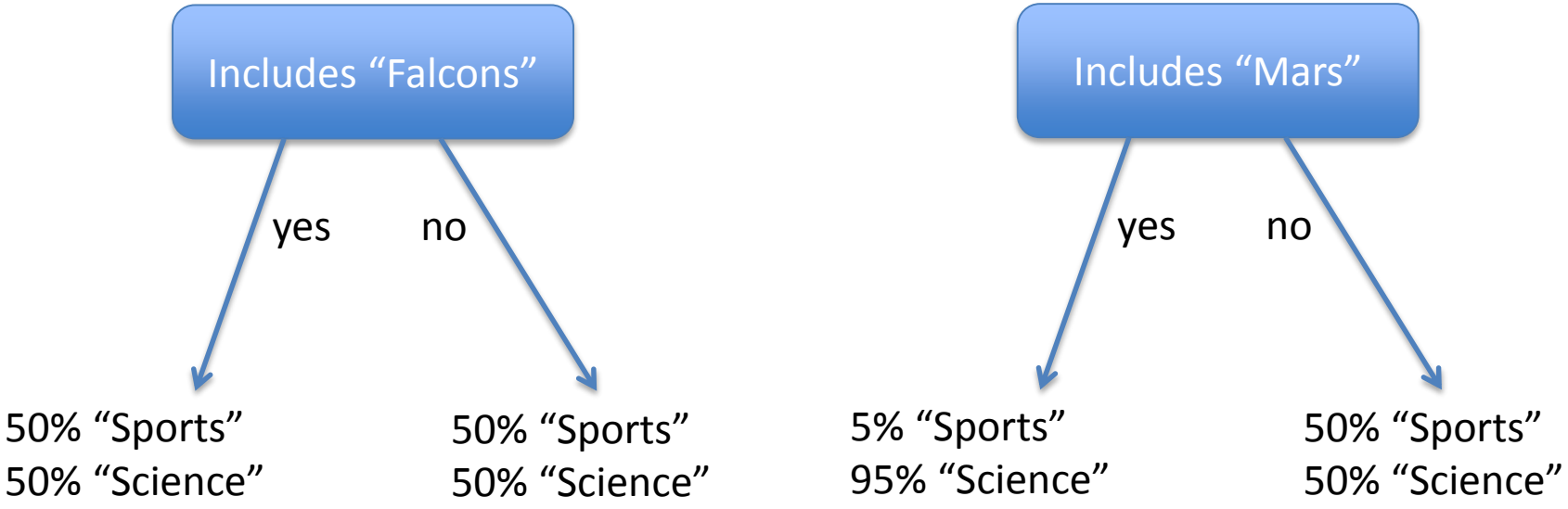
0.94 – 0.725 = 0.215

windy

0.94 – 0.87 = 0.07


Outlook
Rainy
Sunny
Overcast

# Clicker: Document Classification




**Question (assuming equal size splits):**
**a) Falcon’s Information Gain is higher**
**b) Mars’ Information Gain is higher**

# Building a Decision Tree (ID3 Algorithm)

- Assume attributes are discrete
  - Discretize continuous attributes
- Choose the attribute with the highest Information Gain
- Create branches for each value of attribute
- Examples partitioned based on selected attributes
- Repeat with remaining attributes
- Stopping conditions
  - All examples assigned the same label
  - No examples left

# Problems

- Expensive to train
- Prone to overfitting
  - Drive to perfection on training data, bad on test data
  - Pruning can help: remove or aggregate subtrees that provide little discriminatory power (C45)

# C4.5 Extensions

- Continuous Attributes

| outlook | temperature | humidity | windy | play |
|---|---|---|---|---|
| overcast | cool | 60 | TRUE | yes |
| overcast | hot | 80 | FALSE | yes |
| overcast | hot | 63 | FALSE | yes |
| overcast | mild | 81 | TRUE | yes |
| rainy | cool | 58 | TRUE | no |
| rainy | mild | 90 | TRUE | no |
| rainy | cool | 54 | FALSE | yes |
| rainy | mild | 92 | FALSE | yes |
| rainy | mild | 59 | FALSE | yes |
| sunny | hot | 90 | FALSE | no |
| sunny | hot | 89 | TRUE | no |
| sunny | mild | 90 | FALSE | no |
| sunny | cool | 60 | FALSE | yes |
| sunny | mild | 62 | TRUE | yes |

Consider every possible binary partition; choose the partition with the highest gain

| outlook | temperature | humidity | windy | play |
|---|---|---|---|---|
| rainy | mild | 54 | FALSE | yes |
| overcast | hot | 58 | FALSE | yes |
| overcast | cool | 59 | TRUE | yes |
| rainy | cool | 60 | FALSE | yes |
| overcast | mild | 60 | TRUE | yes |
| overcast | hot | 62 | FALSE | yes |
| rainy | mild | 63 | TRUE | no |
| sunny | cool | 80 | FALSE | yes |
| rainy | mild | 81 | FALSE | yes |
| sunny | mild | 89 | TRUE | yes |
| sunny | hot | 90 | FALSE | no |
| rainy | cool | 90 | TRUE | no |
| sunny | hot | 90 | TRUE | no |
| sunny | mild | 92 | FALSE | no |

E(6/6)

= 0.0

E(3/8) + E(5/8)

= 0.95

E(9/10)+ E(1/10)

= 0.47

E(4/4)

= 0.0

Expect = 8/14*0.95 + 6/14*0

= 0.54

Expect = 10/14*0.47 + 4/14*0

= 0.33

# Ensemble Methods

Some slides are due to Zhuowen Tu, Robert Schapire and Pier Luca Lnzi

# Ensemble Methods

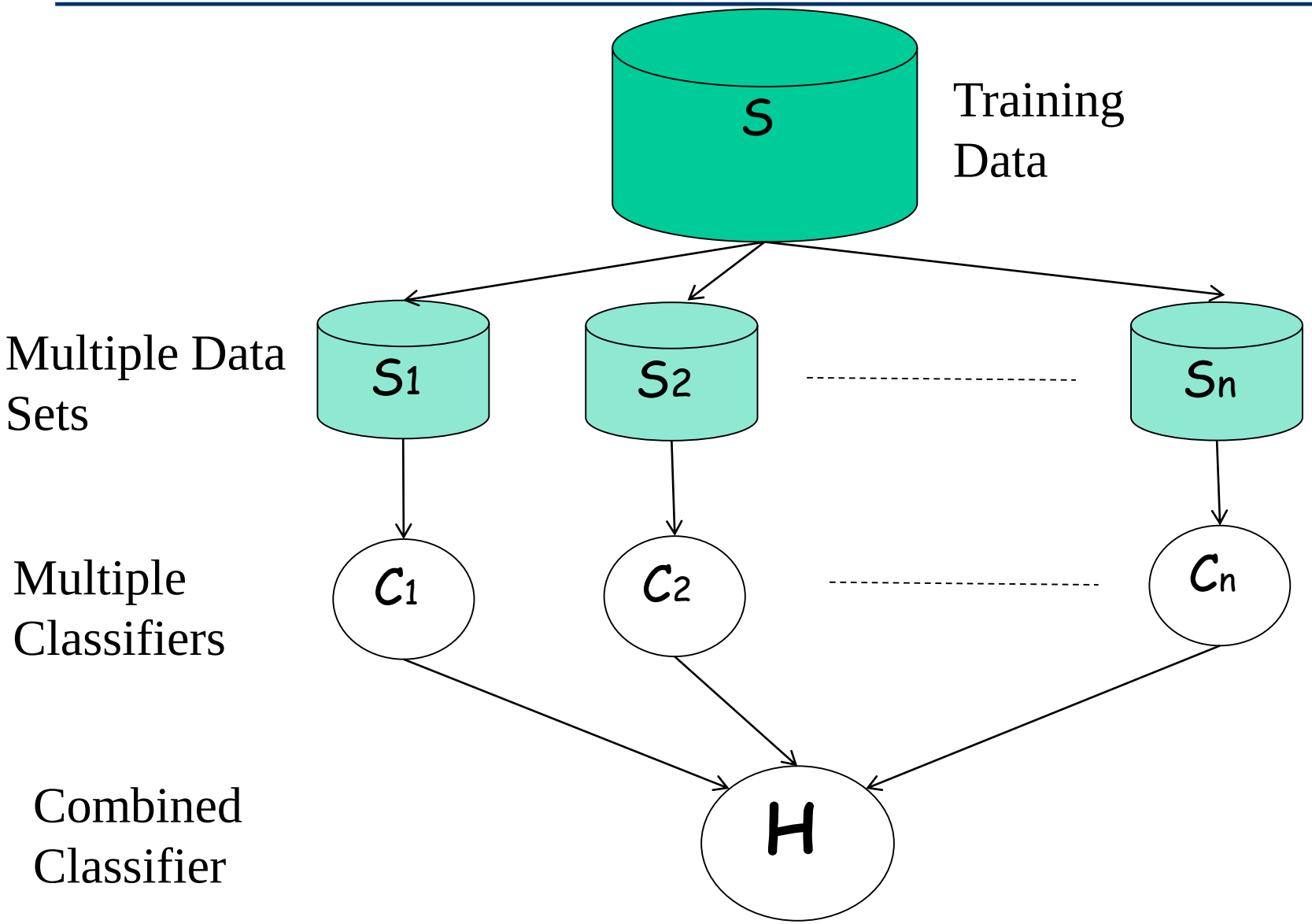
Bagging (Breiman 1994,…)

Boosting (Freund and Schapire 1995, Friedman et al. 1998,…)

Random forests (Breiman 2001,…)

Predict class label for unseen data by aggregating a set of predictions (classifiers learned from the training data).

# General Idea



# Build Ensemble Classifiers

- Basic idea:

  Build different “experts”, and let them vote

- Advantages:

  Improve predictive performance

  Other types of classifiers can be directly included

  Easy to implement

  No too much parameter tuning

- Disadvantages:

  The combined classifier is not so transparent (black box)

  Not a compact representation

# Why do they work?

- Suppose there are 25 base classifiers
- Each classifier has error rate, $\varepsilon = 0.35$
- Assume independence among classifiers
- Probability that the ensemble classifier makes a wrong prediction:

$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^{i} (1-\varepsilon)^{25-i} = 0.06$$

# Bagging

- Training
  - Given a dataset S, at each iteration i, a training set $s_i$ is sampled with replacement from S (i.e. bootstraping)
  - A classifier $c_i$ is learned for each $s_i$
- Classification: given an unseen sample x,
  - Each classifier $c_i$ returns its class prediction
  - The bagged classifier h counts the votes and assigns the class with the most votes to x
- Regression: can be applied to the prediction of continuous values by taking the average value of each prediction.

# Bagging

- Bagging works because it reduces variance by voting/averaging
  - In some pathological hypothetical situations the overall error might increase
  - Usually, the more classifiers the better
- Problem: we only have one dataset.
- Solution: generate new ones of size n by bootstrapping, i.e. sampling it with replacement
- Can help a lot if data is noisy.

# When does Bagging work?

- Learning algorithm is unstable: if small changes to the training set cause large changes in the learned classifier.
- If the learning algorithm is unstable, then Bagging almost always improves performance
- Some candidates:

  Decision tree, linear regression, SVMs, decision stump, regression tree,

  Questions: Why are decision trees or SVMs unstable?

# Randomization

- Can randomize learning algorithms instead of inputs
- Some algorithms already have random component: e.g. random initialization
- Most algorithms can be randomized
  - Pick from the N best options at random instead of always picking the best one
  - Split rule in decision tree
- Random projection in kNN (Freund and Dasgupta 08)

# Ensemble Methods

Bagging (Breiman 1994,…)

Boosting (Freund and Schapire 1995, Friedman et al. 1998,…)

Random forests (Breiman 2001,…)

# Boosting

- Idea: Build a classifier based on many weak learners

# Boosting

- Idea: Build a classifier based on many weak learners
- Defines a classifier using an additive model:

$$F(x) = \alpha_1 f_1(x) + \alpha_2 f_2(x) + \alpha_3 f_3(x) + \ldots$$

Strong classifier

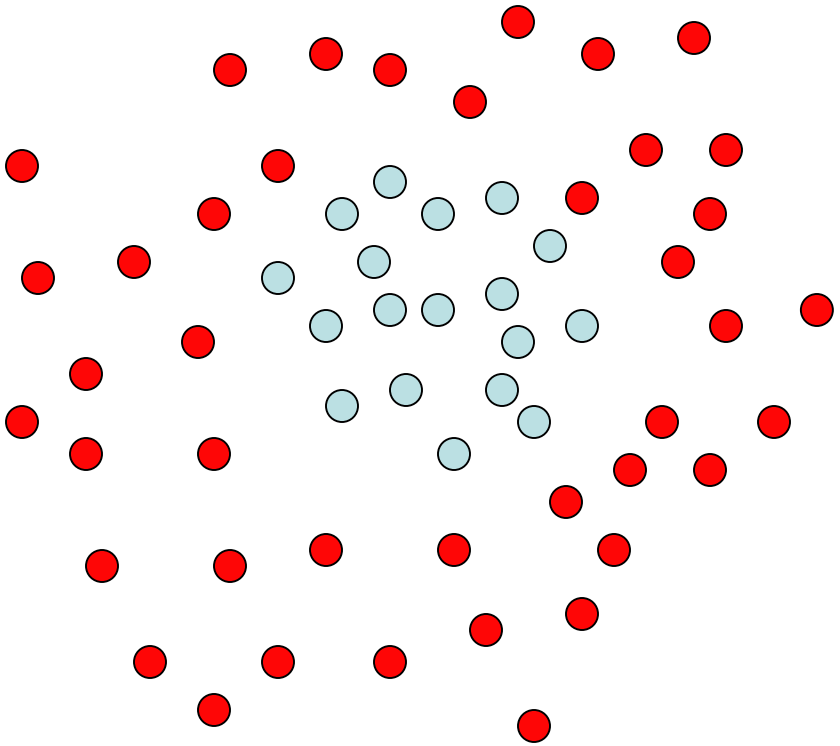
Features vector

Weight

Weak classifier

# Boosting

It is a sequential procedure:



Each data point has

a class label:

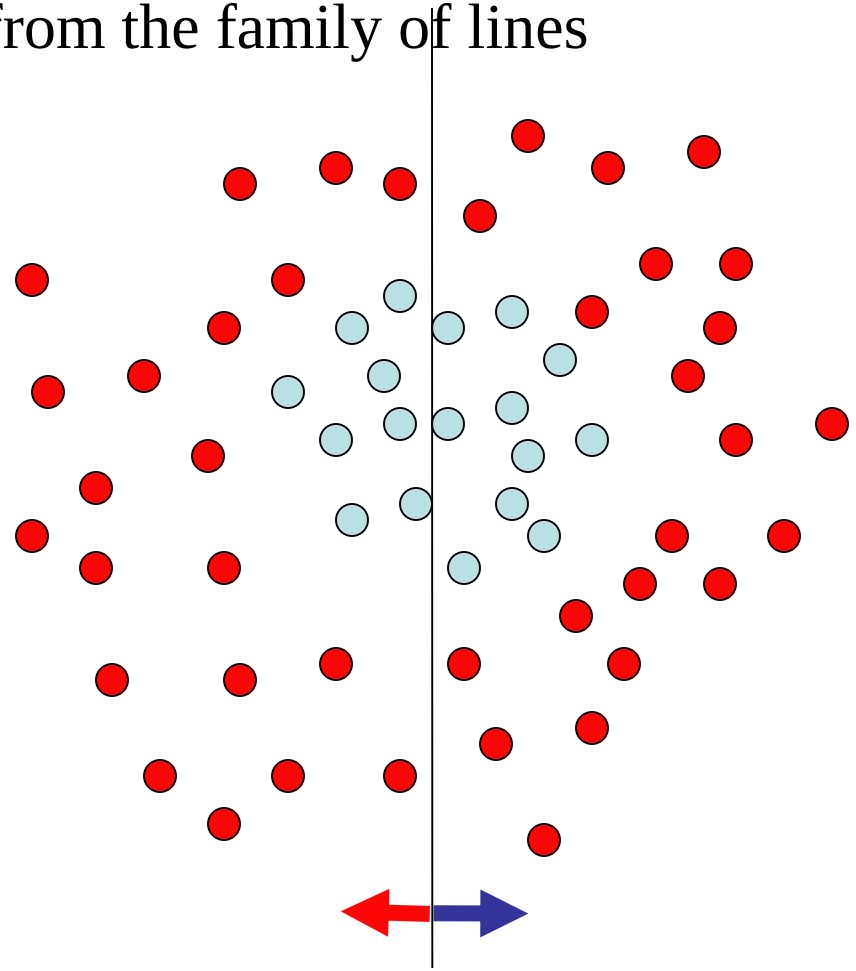
$$y_t = \begin{cases} +1 \ (\bullet) \\ -1 \ (\circ) \end{cases}$$

and a weight:

$$w_t = 1$$

# Toy example

Weak learners from the family of lines



Each data point has

a class label:

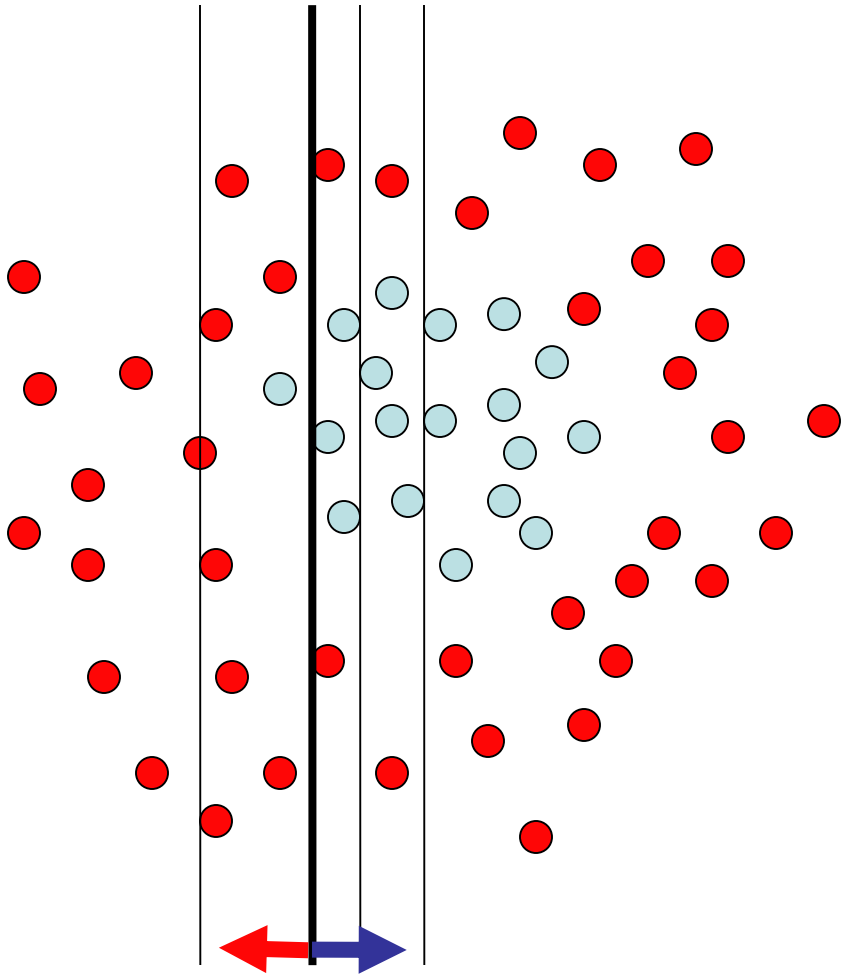
$$y_t = \begin{cases} +1 \ (\bullet) \\ -1 \ (\circ) \end{cases}$$

and a weight:

$$w_t = 1$$

h => p(error) = 0.5 it is at chance

# Toy example



Each data point has

a class label:

$$y_t = \begin{cases} +1 & (\bullet) \\ -1 & (\circ) \end{cases}$$

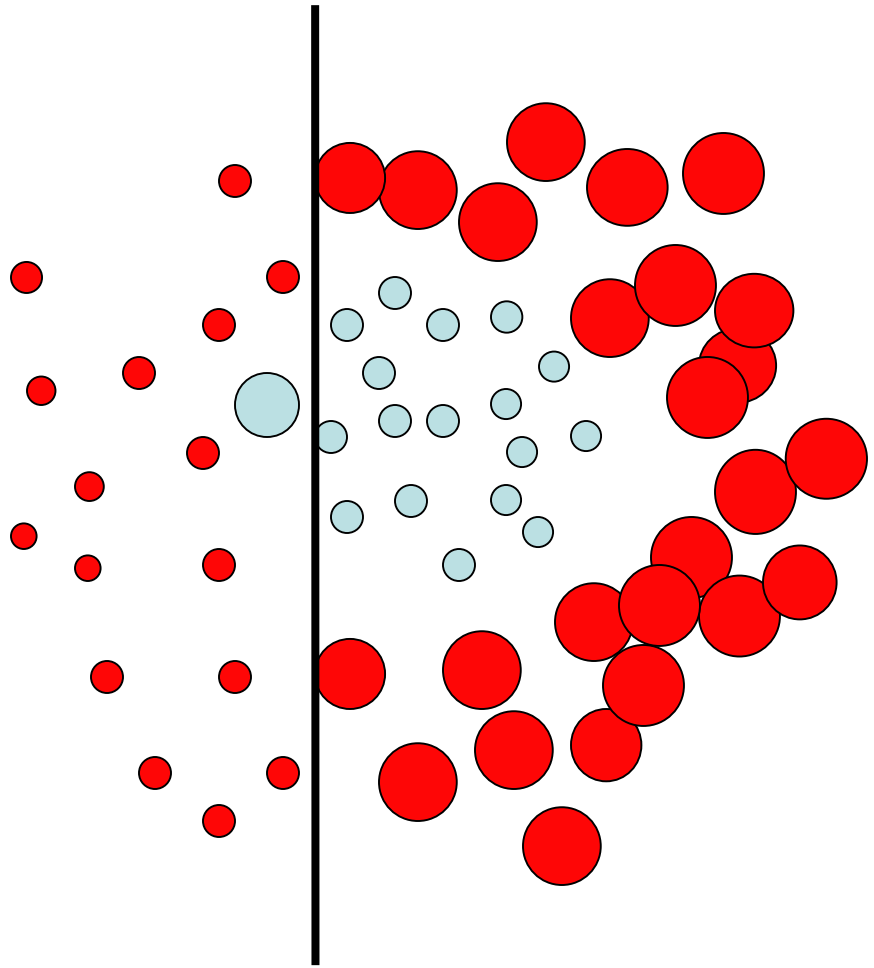
and a weight:

$$w_t = 1$$

This one seems to be the best

This is a '**weak classifier**': It performs slightly better than chance.

# Toy example



Each data point has a class label:

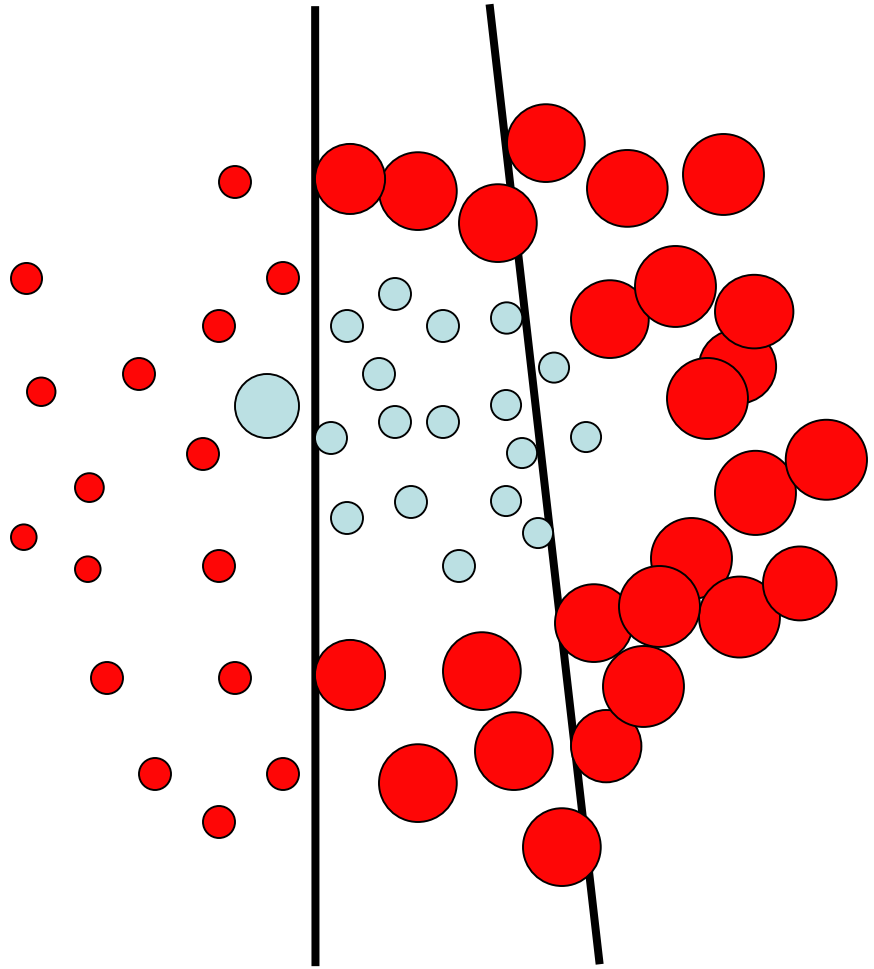
$$y_t = \begin{cases} +1 & (\bullet) \\ -1 & (\circ) \end{cases}$$

**We update the weights:**

$$w_t \leftarrow w_t \exp\{-y_t H_t\}$$

We set a new problem for which the previous weak classifier performs at chance again

# Toy example



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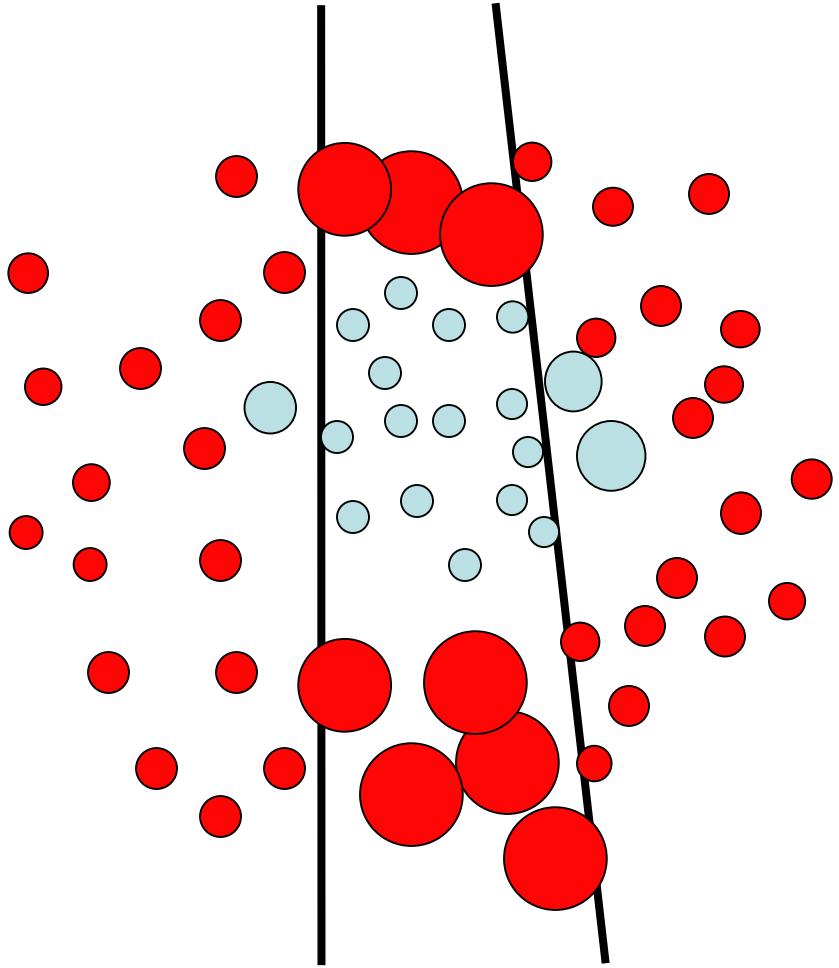
# Toy example



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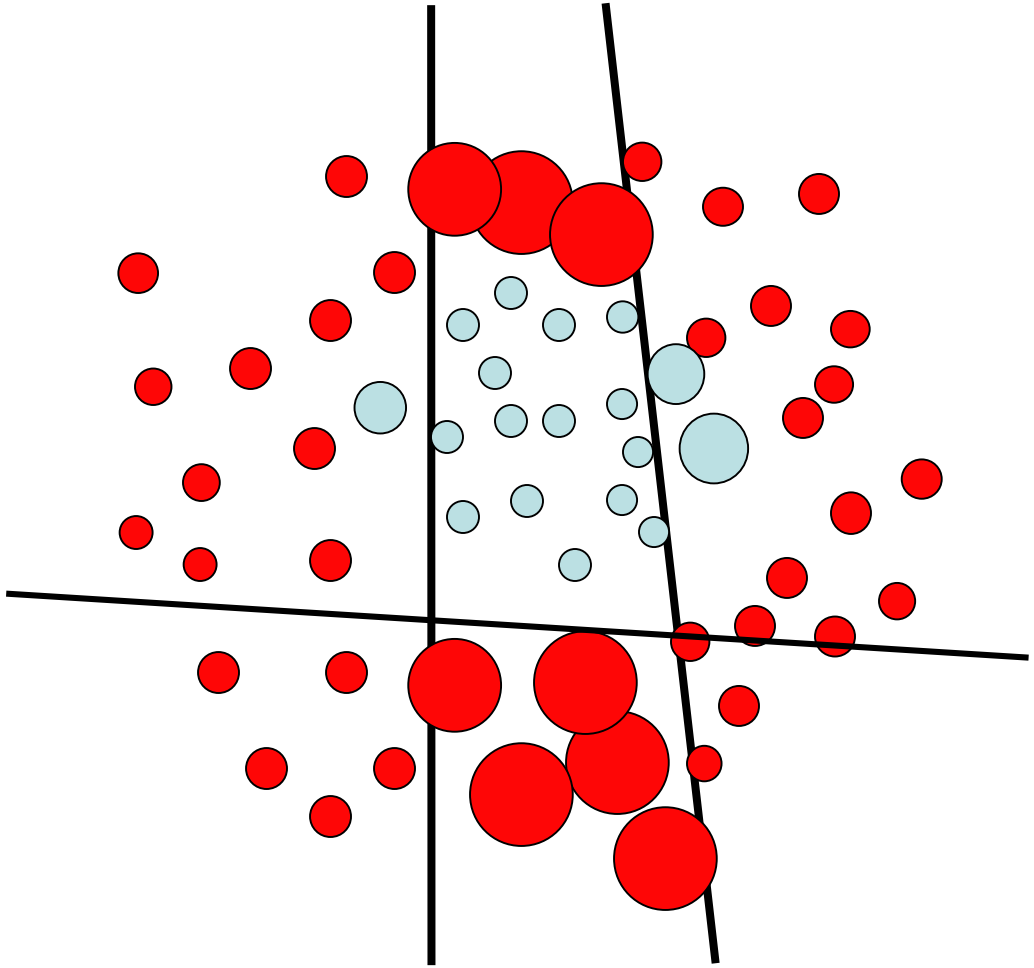
# Toy example



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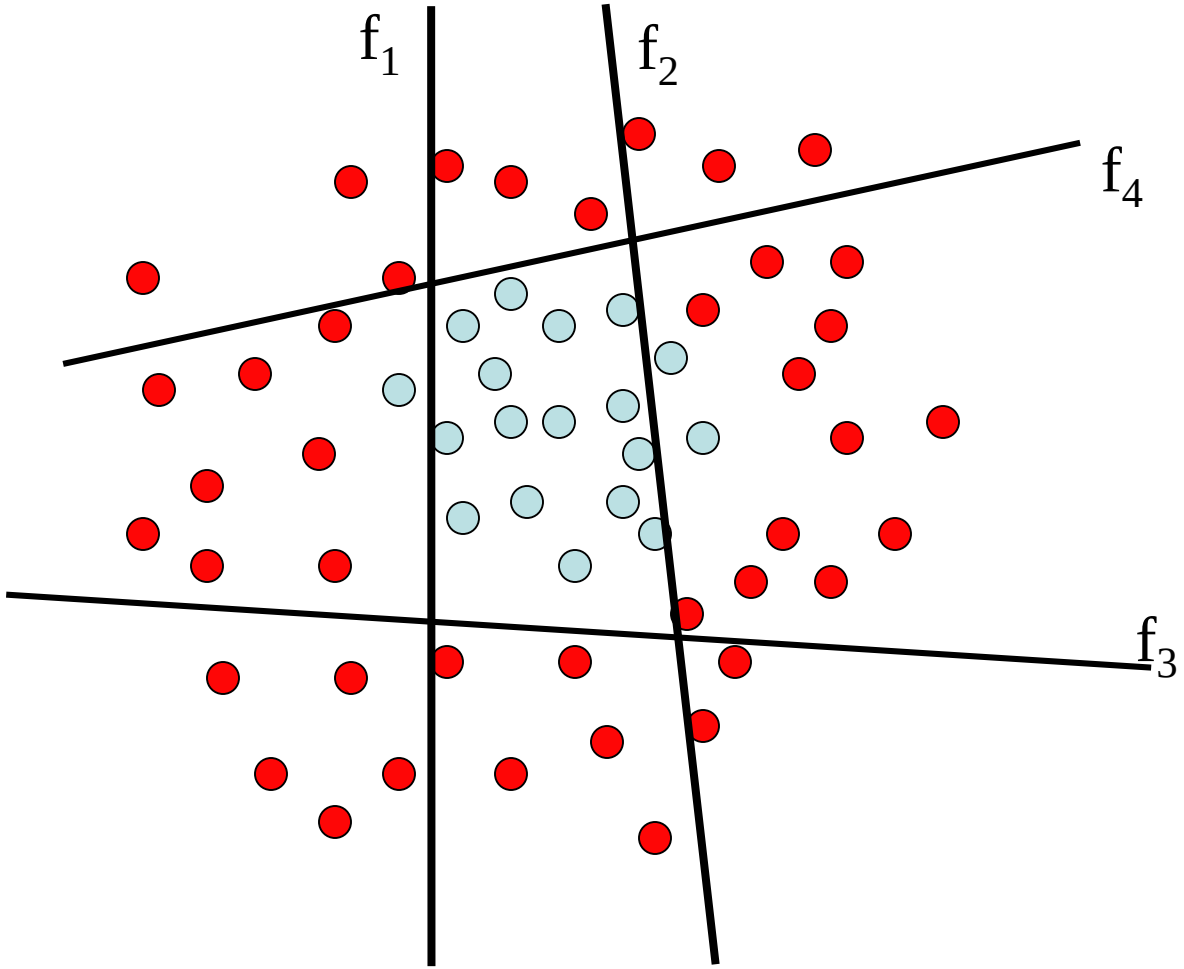
$$y_t = \begin{cases} +1 & (\bullet) \\ -1 & (\circ) \end{cases}$$

**We update the weights:**

$$w_t \leftarrow w_t \exp\{-y_t H_t\}$$

We set a new problem for which the previous weak classifier performs at chance again

# Toy example




The strong (non- linear) classifier is built as the combination of all the weak (linear) classifiers.

# AdaBoost Algorithm

Given: m examples $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in X$, $y_i \in Y = \{-1, +1\}$

Initialize $D_1(i) = 1/m$

For t = 1 to T

1. Train learner $\boldsymbol{h_t}$ with min error $\varepsilon_t = \Pr_{i \sim D_t}[h_t(x_i) \neq y_i]$
2. Compute the hypothesis weight $\alpha_t = \frac{1}{2} \ln\left(\frac{1-\varepsilon_t}{\varepsilon_t}\right)$
3. For each example $i$ = 1 to m

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(x_i) = y_i \\ e^{\alpha_t} & \text{if } h_t(x_i) \neq y_i \end{cases}$$

Output

$$H(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$$

The goodness of $h_t$ is calculated over $D_t$ and the bad guesses.

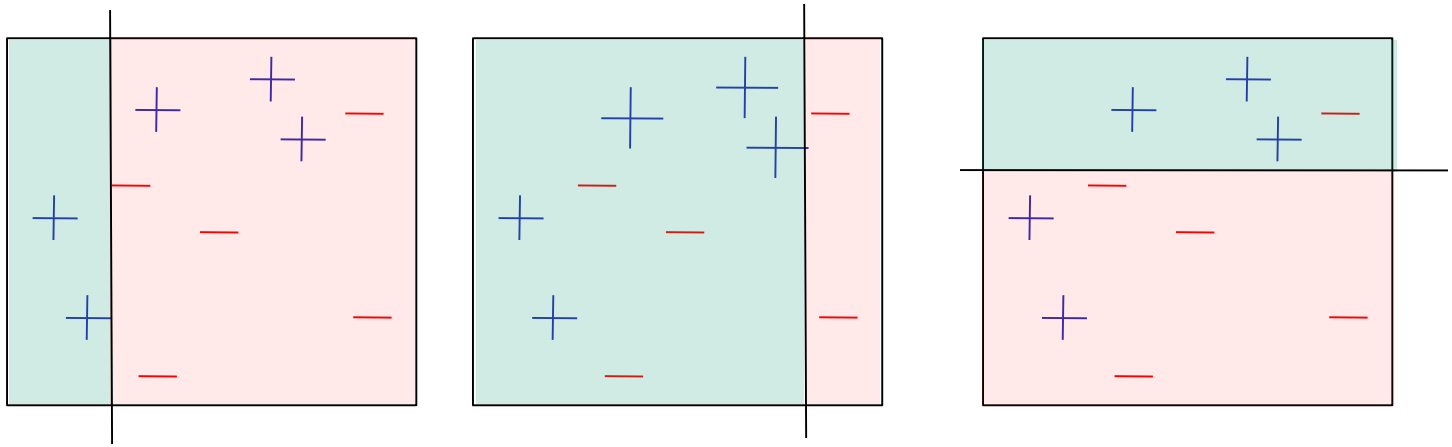
The weight **Ada**pts. The bigger $\varepsilon_t$ becomes the smaller $\alpha_t$ becomes.

Boost example if incorrectly predicted.

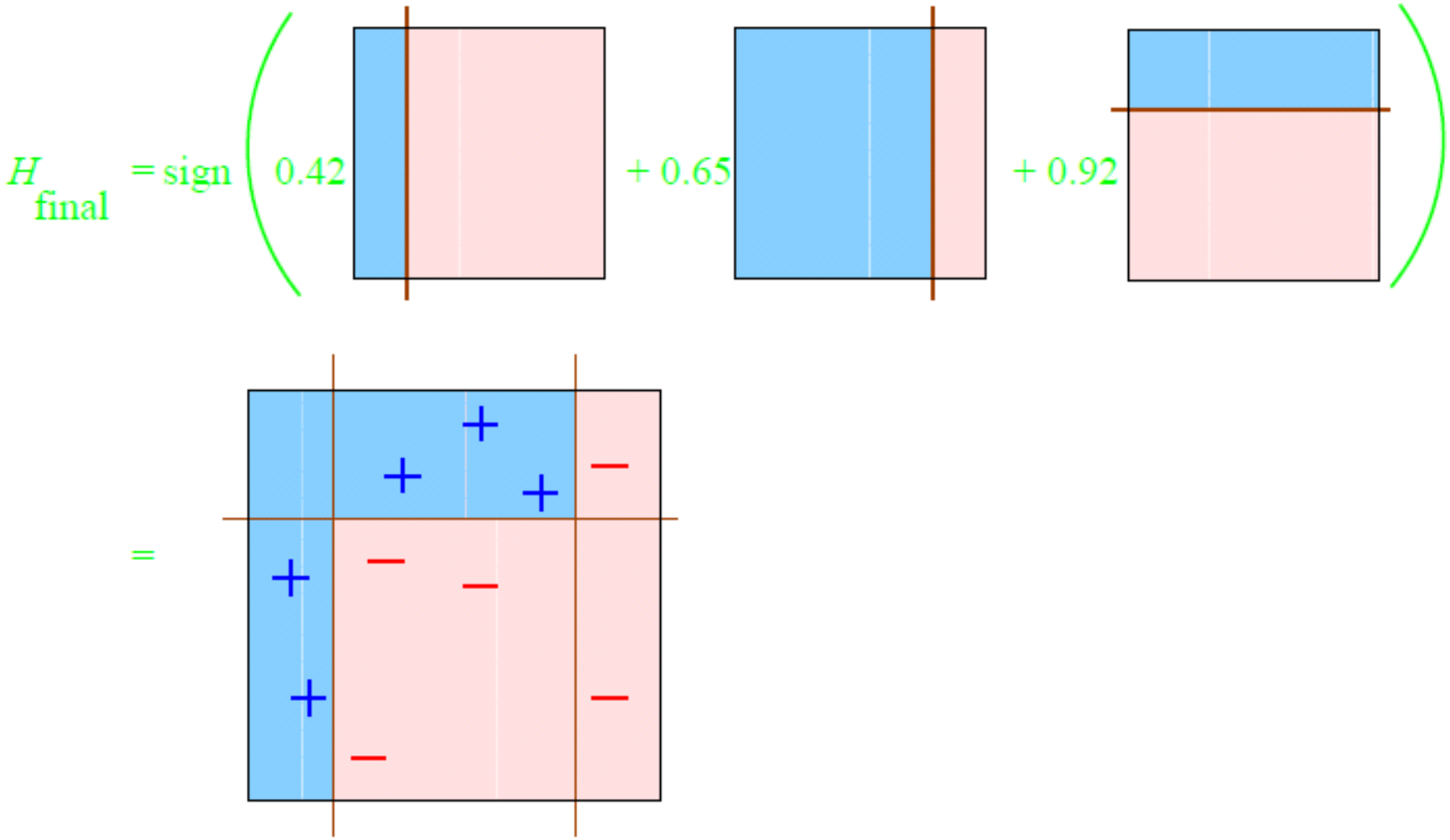
$Z_t$ is a normalization factor.

Linear combination of models.

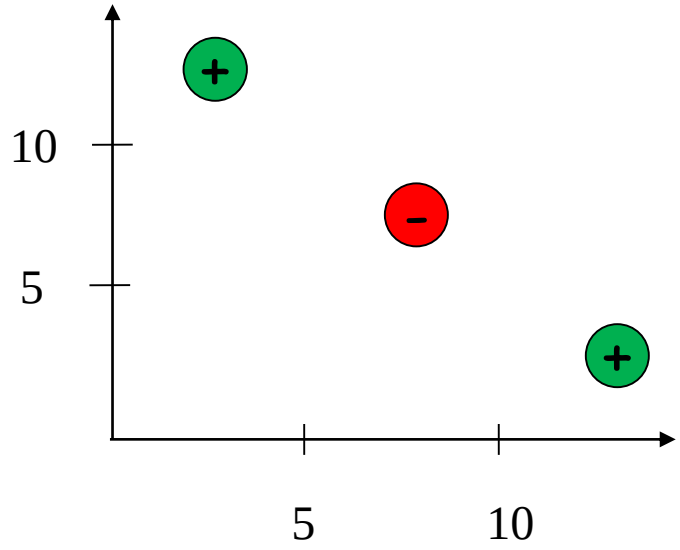
# Toy Example



# Final Classifier



# Clicker




Assume a weak classifier can only use one feature (e.g., { $x \leq 5$ → +1 and $x > 5$ → -1})
How many weak classifiers are needed to correctly identify all data items in the example above

A) One weak classifier
B) Two weak classifiers with equal weights
C) Two weak classifiers with unequal weights
D) Three weak classifiers with equal weights
E) Three weak classifiers with unequal weights

# Advantages of Boosting

- Simple and easy to implement
- Flexible– can combine with any learning algorithm
- No requirement on data metric– data features don't need to be normalized, like in kNN and SVMs (this has been a central problem in machine learning)
- Feature selection and fusion are naturally combined with the same goal for minimizing an objective error function
- No parameters to tune
- No prior knowledge needed about weak learner
- Provably effective
- Versatile– can be applied on a wide variety of problems
- Non-parametric

# Caveats

- Performance of AdaBoost depends on data and weak learner
- Consistent with theory, AdaBoost can fail if
  - weak classifier too complex– overfitting
  - weak classifier too weak -- underfitting
- Empirically, AdaBoost seems especially susceptible to uniform noise

# Ensemble Methods

Bagging (Breiman 1994,…)

Boosting (Freund and Schapire 1995, Friedman et al. 1998,…)

Random forests (Breiman 2001,…)

# Motivation: You have To Hire A New Expert

Willow is one of the interviewers

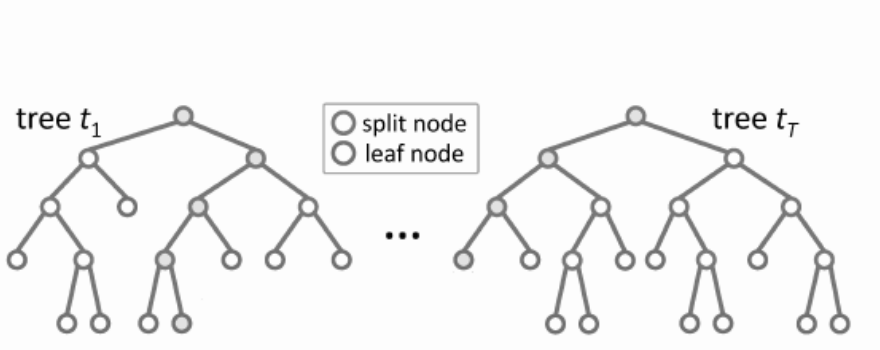
But he is not really good in interviewing (yet)

# So We Need More Interviewers

# Setting I

# Setting 2

# Random Forests




- Random forests (RF) are a combination of tree predictors
- Each tree depends on the values of a random vector sampled in dependently
- The generalization error depends on the strength of the individual trees and the correlation between them

# The Random Forests Algorithm

Given a training set S

For i = 1 to k do:

Build subset $s_i$ by sampling with replacement from S

Learn tree $t_i$ from $s_i$

At each node:

Choose best split from random subset of F features

Each tree grows to the largest extend, and no pruning

Make predictions according to majority vote of the set of k trees.

# Features of Random Forests

- Boosting-decision tree (C4.5) often works very well.
- It runs efficiently on large data bases.
- It can handle thousands of input variables without variable deletion.
- It gives estimates of what variables are important in the classification.
- It generates an internal unbiased estimate of the generalization error as the forest building progresses.
- It has an effective method for estimating missing data and maintains accuracy when a large proportion of the data are missing.
- It has methods for balancing error in class population unbalanced data sets.

# Compared with Boosting

Pros:

- It is more robust.
- It is faster to train (no reweighting, each split is on a small subset of data and feature).
- Can handle missing/partial data.
- Is easier to extend to online version.

Cons:

- The feature selection process is not explicit.
- Feature fusion is also less obvious.
- Has weaker performance on small size training data.

# Ensemble Methods

- Random forests (also true for many machine learning algorithms) is an example of a tool that is useful in doing analyses of scientific data.
- But the cleverest algorithms are no substitute for human intelligence and knowledge of the data in the problem.
- Take the output of random forests not as absolute truth, but as smart computer generated guesses that may be helpful in leading to a deeper understanding of the problem.

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