# Classification II

- More Classification Models
  - Bayes classifier, Association-based classifier, k-nearest neighbor (kNN), Neural network (shallow and deep models), etc.
- Classification Measures
- Ensemble Methods
  - Ideas and Examples
  - Bagging: Random Forest
  - Boosting: Adaboost
- Take-home messages

# More Classification Models

# Bayesian Classification: Why?

- Probabilistic learning: Calculate explicit probabilities for hypothesis, among the most practical approaches to certain types of learning problems
- Incremental: Each training example can incrementally increase/decrease the probability that a hypothesis is correct. Prior knowledge can be combined with observed data.
- Probabilistic prediction: Predict multiple hypotheses, weighted by their probabilities
- Standard: Even when Bayesian methods are computationally intractable, they can provide a standard of optimal decision making against which other methods can be measured

# Bayesian Theorem

- Given training data *D, posteriori probability of a hypothesis h, P(h|D)* follows the Bayes theorem

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)} \qquad \text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}$$

- MAP (maximum a-posteriori) hypothesis

$$h_{MAP} \equiv \arg\max_{h \in H} P(h|D) = \arg\max_{h \in H} P(D|h)P(h).$$

- Practical difficulty: require initial knowledge of many probabilities, significant computational cost

# Bayesian classification

- The classification problem may be formalized using a-posteriori probabilities:
- P(C|X) = probability that the sample tuple $X=<x_1,\ldots,x_k>$ is of class C.

  e.g. P(buys_computer=Yes |Age≤30, Income=high, Student=no, Credit_rating=fair)

  e.g. P(class=N |outlook=sunny,windy=true,…)
- Idea: assign to sample X the class label C such that P(C|X) is maximal

# Estimating a-posteriori probabilities

- Bayes theorem:

$$P(C|X) = P(X|C) \cdot P(C) / P(X)$$

- P(X) is constant for all classes
- P(C) = relative freq. of class C samples
- choose C such that P(C|X) is maximum =

  choose C such that P(X|C)·P(C) is maximum
- Problem: computing P(X|C) is unfeasible!

X is multidimensional
(multiple attributes)!

# Naïve Bayes Classifier

- A simplified assumption: attributes are conditionally independent:

$$P(C_j|X) \propto P(C_j)\prod_{i=1}^{n} P(x_i|C_j)$$

- Greatly reduces the computation cost, only count the class distribution.

# Naïve Bayesian Classification

- Naïve assumption: attribute independence

$$P(x_1,\ldots,x_k|C) = P(x_1|C)\cdot\ldots\cdot P(x_k|C)$$

- If i-th attribute is categorical:
  $P(x_i|C)$ is estimated as the relative freq of samples having value $x_i$ as i-th attribute in class C
- If i-th attribute is continuous:
  $P(x_i|C)$ is estimated thru a Gaussian density function
- Computationally easy in both cases

# Play-tennis example: estimating $P(x_i|C)$

| Outlook | Temperature | Humidity | Windy | Class |
|---|---|---|---|---|
| sunny | hot | high | false | n |
| sunny | hot | high | true | n |
| overcast | hot | high | false | p |
| rain | mild | high | false | p |
| rain | cool | normal | false | p |
| rain | cool | normal | true | n |
| overcast | cool | normal | true | p |
| sunny | mild | high | false | n |
| sunny | cool | normal | false | p |
| rain | mild | normal | false | p |
| sunny | mild | normal | true | p |
| overcast | mild | high | true | p |
| overcast | hot | normal | false | p |
| rain | mild | high | true | n |

| |
|---|
| **P(p) = 9/14** |
| **P(n) = 5/14** |

| **outlook** | |
|---|---|
| **P(sunny\|p) = 2/9** | **P(sunny\|n) = 3/5** |
| **P(overcast\|p) = 4/9** | **P(overcast\|n) = 0** |
| **P(rain\|p) = 3/9** | **P(rain\|n) = 2/5** |
| **temperature** | |
| **P(hot\|p) = 2/9** | **P(hot\|n) = 2/5** |
| **P(mild\|p) = 4/9** | **P(mild\|n) = 2/5** |
| **P(cool\|p) = 3/9** | **P(cool\|n) = 1/5** |
| **humidity** | |
| **P(high\|p) = 3/9** | **P(high\|n) = 4/5** |
| **P(normal\|p) = 6/9** | **P(normal\|n) = 1/5** |
| **windy** | |
| **P(true\|p) = 3/9** | **P(true\|n) = 3/5** |
| **P(false\|p) = 6/9** | **P(false\|n) = 2/5** |

# Play-tennis example: Classifying X

- An unseen sample X = <rain, hot, high, false>
- P(X|p)·P(p) =
  P(rain|p)·P(hot|p)·P(high|p)·P(false|p)·P(p) =
  3/9·2/9·3/9·6/9·9/14 = 0.010582
- P(X|n)·P(n) =
  P(rain|n)·P(hot|n)·P(high|n)·P(false|n)·P(n) =
  2/5·2/5·4/5·2/5·5/14 = 0.018286
- Sample X is classified as class n (don't play tennis)

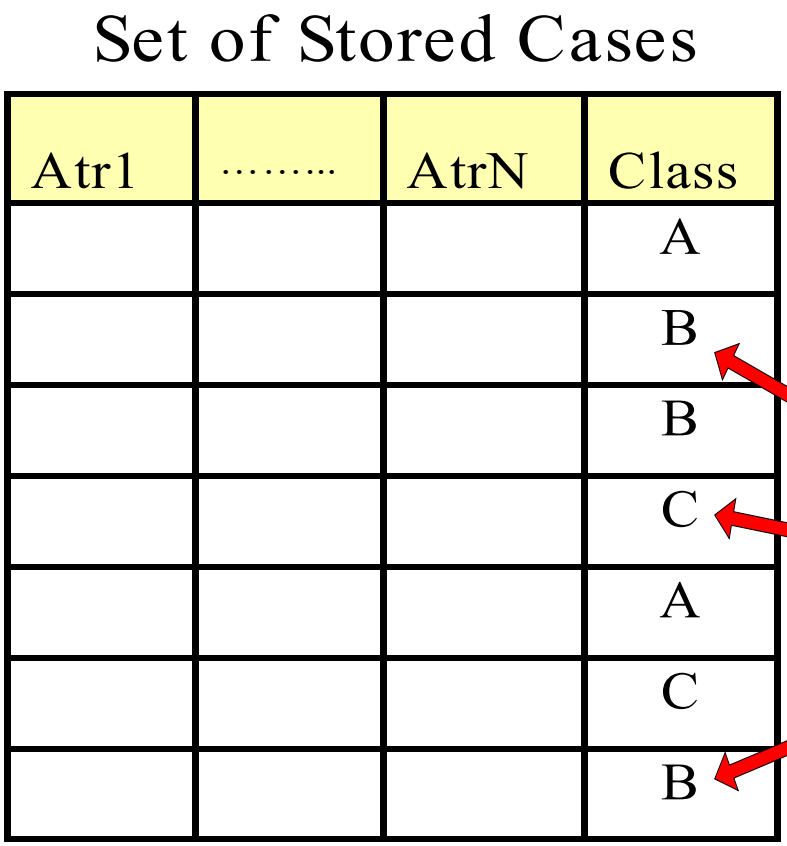
# Association-Based Classification

- Several methods for association-based classification
  - Associative classification: (Liu et al'98)
    - It mines high support and high confidence rules in the form of "cond_set => y", where y is a class label
  - ARCS: Quantitative association mining and clustering of association rules (Lent et al'97)
    - It beats C4.5 in (mainly) scalability and also accuracy
  - CAEP (Classification by aggregating emerging patterns) (Dong et al'99)
    - Emerging patterns (EPs): the itemsets whose support increases significantly from one class to another
    - Mine EPs based on minimum support and growth rate

# Eager learning vs lazy learning

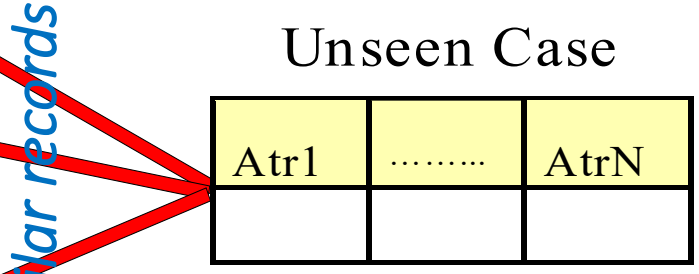
- Decision tree is a representative eager learning approach which takes proactive steps to build up a hypothesis of the learning task.
- It has an explicit description of target function on the whole training set
- Let's take a look at a more "relaxed" supervised learning approach, i.e. lazy learning, which can be mostly manifested by the so-called instance-based models.

# Instance-Based Classifiers




Basic idea:

- Store the training records/cases
- Use training records to predict the class label of unseen cases, typically with majority rule applied.




*Similar records*

Got 2 votes of class B and 1 vote of class C, so classify the unseen case as class B.

# k-Nearest Neighbor (kNN) Classification

| ID | Food | Chat | Fast | Price | Bar | BigTip |
|---|---|---|---|---|---|---|
| 1 | great | yes | yes | normal | no | yes |
| 2 | great | no | yes | normal | no | yes |
| 3 | mediocre | yes | no | high | no | no |
| 4 | great | yes | yes | normal | yes | yes |

Stored Records For BigTip Classification

Similarity metric: Number of matching attributes

Number of nearest neighbors: k=2

Classifying new data:

- New data (x, great, no, no, normal, no)

  → most similar: ID=2 (1 mismatch, 4 match) → yes

  → Second most similar example: ID=1 (2 mismatch, 3 match) → yes

  So, classify it as "Yes".

- New data (y, mediocre, yes, no, normal, no)

  → Most similar: ID=3 (1 mismatch, 4 match) → no

  → Second most similar example: ID=1 (2 mismatch, 3 match) → yes

  So, classify it as "Yes/No"?!

# Classification by Neural Networks

- Advantages
  - prediction accuracy is generally high
  - robust, works when training examples contain errors
  - output may be discrete, real-valued, or a vector of several discrete or real-valued attributes
  - fast evaluation of the learned target function
- Criticisms
  - long training time (model construction time)
  - difficult to understand the learned function (weights)
  - not easy to incorporate domain knowledge

# Classification by Neural Networks

- Shallow models:
  - Perceptron
  - Multilayer Perceptron (MLP)
  - Support Vector Machine (SVM)…
- Deep models:
  - Convolutional Neural Network (CNN)
  - Recurrent Neural Network (RNN), e.g. Long Short-Term Memory (LSTM)
  - Graph Neural Network (GNN)
  - Transformer…

# Classification Measures

# Measuring Error

| | Predicted class | |
|---|---|---|
| True Class | Yes | No |
| Yes | TP: True Positive | FN: False Negative |
| No | FP: False Positive | TN: True Negative |

- Error rate = # of errors / # of instances = (FN+FP) / N
- Recall = # of found positives / # of positives
  = TP / (TP+FN) = sensitivity = hit rate
- Precision = # of found positives / # of found
  = TP / (TP+FP)
- Specificity = TN / (TN+FP)
- False alarm rate = FP / (FP+TN) = 1 - Specificity

## Classification Accuracy:
# Estimating Error Rates

- Partition: Training-and-testing
  - use two independent data sets, e.g., training set (2/3), test set(1/3)
  - used for data set with large number of samples
- Cross-validation
  - divide the data set into *k* subsamples
  - use *k-1* subsamples as training data and one sub-sample as test data --- *k*-fold cross-validation
  - for data set with moderate size

Classification Accuracy:

# Estimating Error Rates

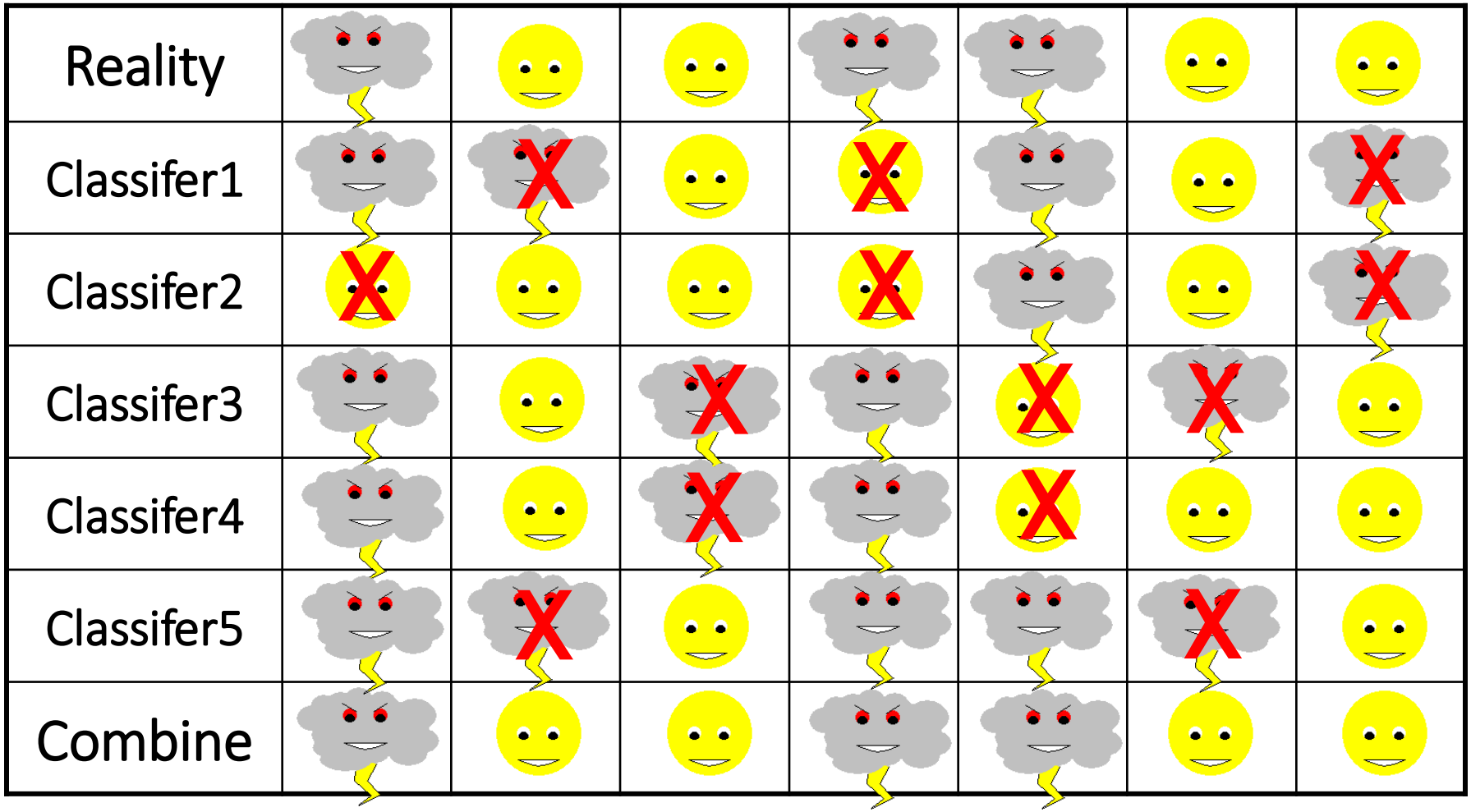
- k-fold cross-validation


- Leave-one-out (n-fold cross validation)

# Ensemble Methods

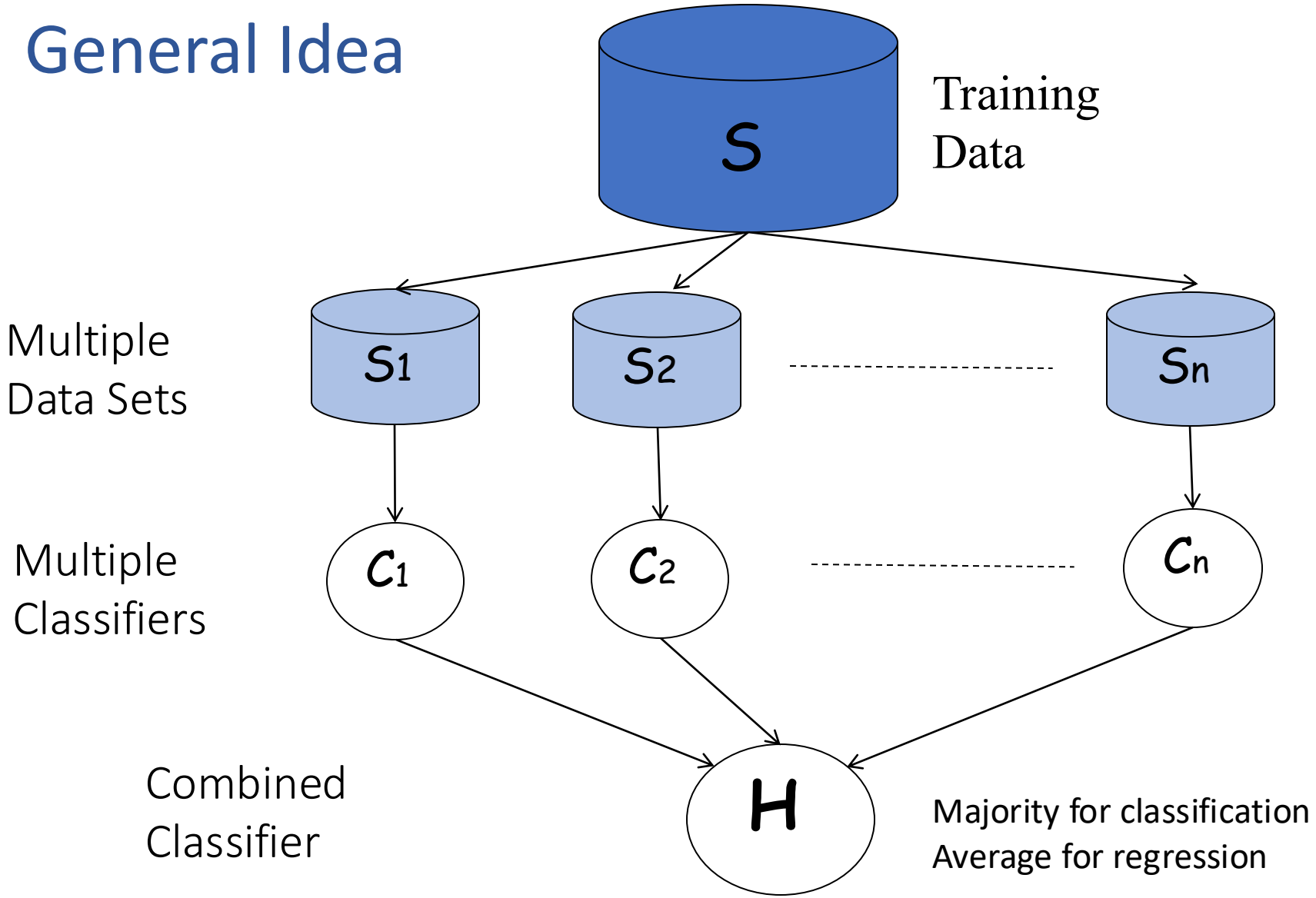
# Collective wisdom

## An illustrative example: Weather forecasting




Collective wisdom ——> better performance!!

# Collective Wisdom: General Idea



# Why does it 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:

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

# Building Ensemble Classifiers

- Basic idea:
  Build different "experts", and let them vote
- Advantages:
  Improve predictive performance
  Easy to implement
  No too much *parameter tuning*
- Disadvantages:
  The combined classifier is not so transparent (black box; low interpretability)
  Not a compact representation
- Two approaches: Bagging (Bootstrap Aggregating) and Boosting

## Bagging Ensemble Methods:
# Random Forest (RF)

- A single decision tree does not perform well
- But, it is super fast
- What if we learn multiple trees?

We need to make sure they do not all just learn the same

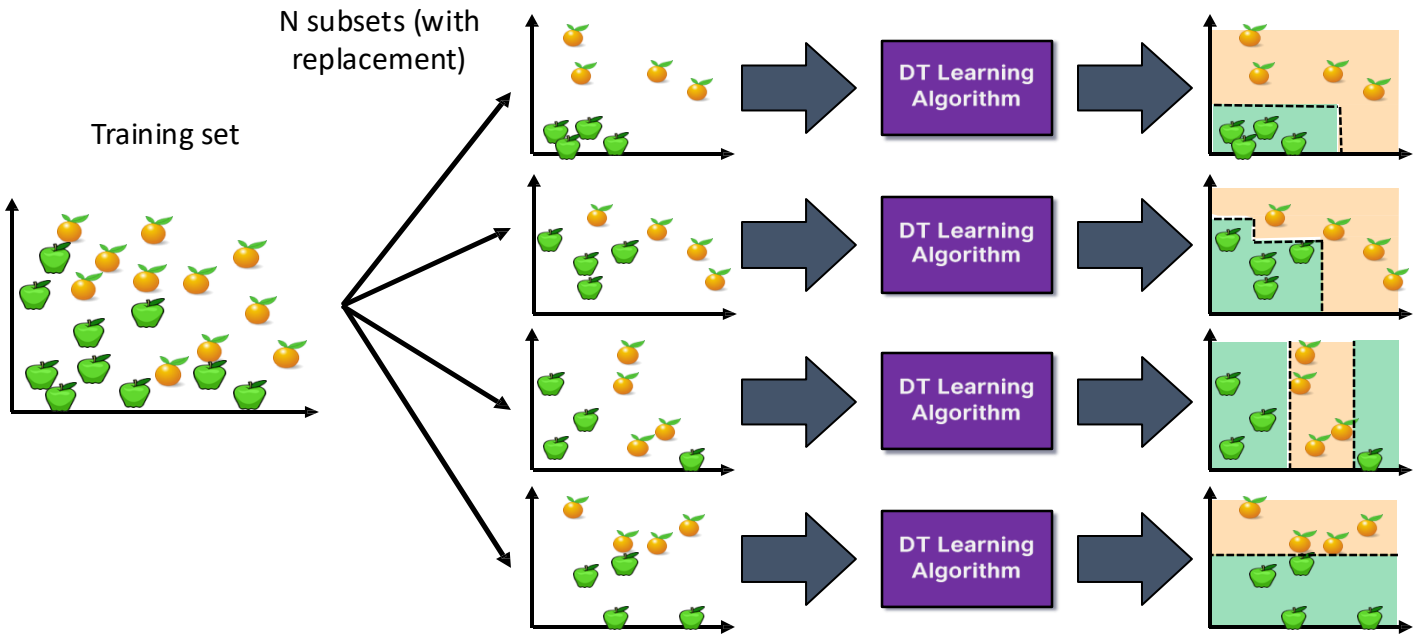
# What is a Random Forest?

*Definition 1.1.* A random forest is a classifier consisting of a collection of tree-structured classifiers $\{h(\mathbf{x}, \Theta_k),\ k = 1, \ldots\}$ where the $\{\Theta_k\}$ are independent identically distributed random vectors and each tree casts a unit vote for the most popular class at input $\mathbf{x}$.

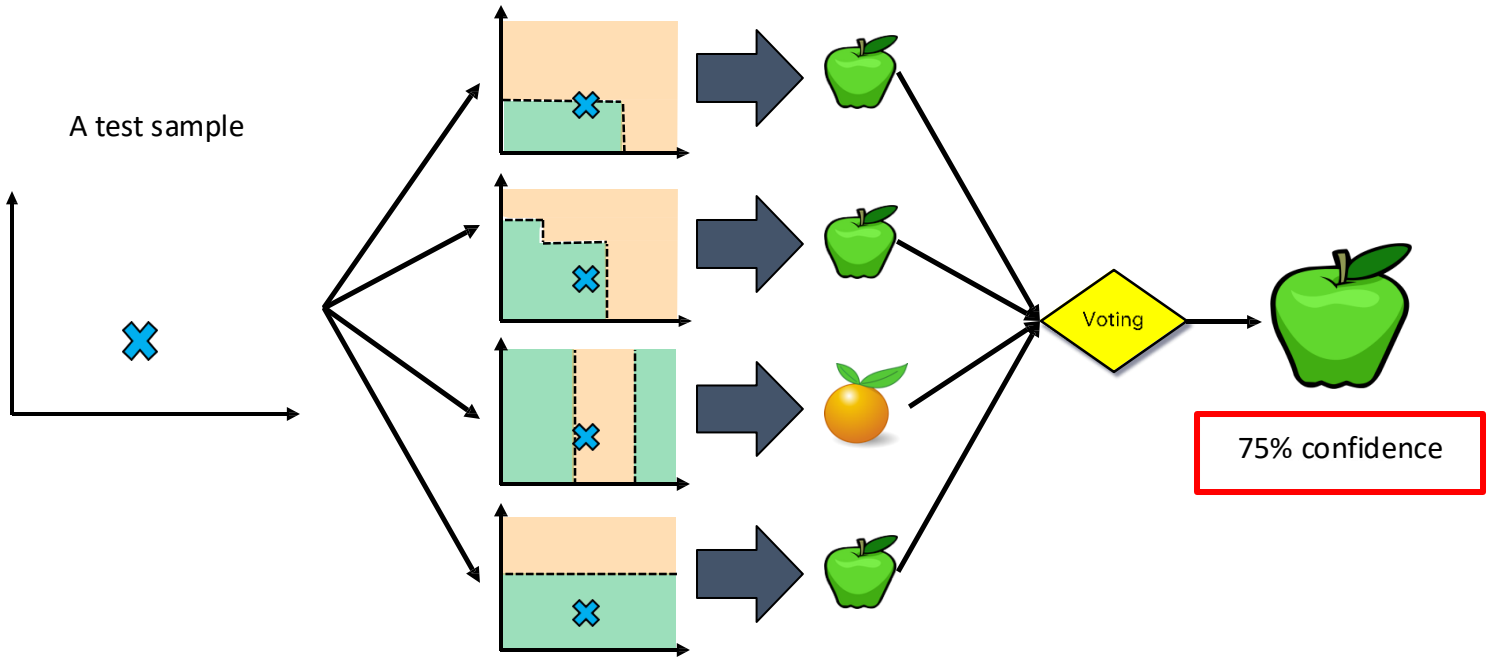
- Suppose we have a single data set, so how do we obtain slightly different trees?

  1. Basic Bagging:
     - Take random subsets of data points from the training set to create N smaller data sets
     - Fit a decision tree on each subset
  2. Feature Bagging:
     - Fit N different decision trees by constraining each one to operate on a random subset of features

# Basic bagging at training time (model construction)



# Basic bagging at inference time (model usage)



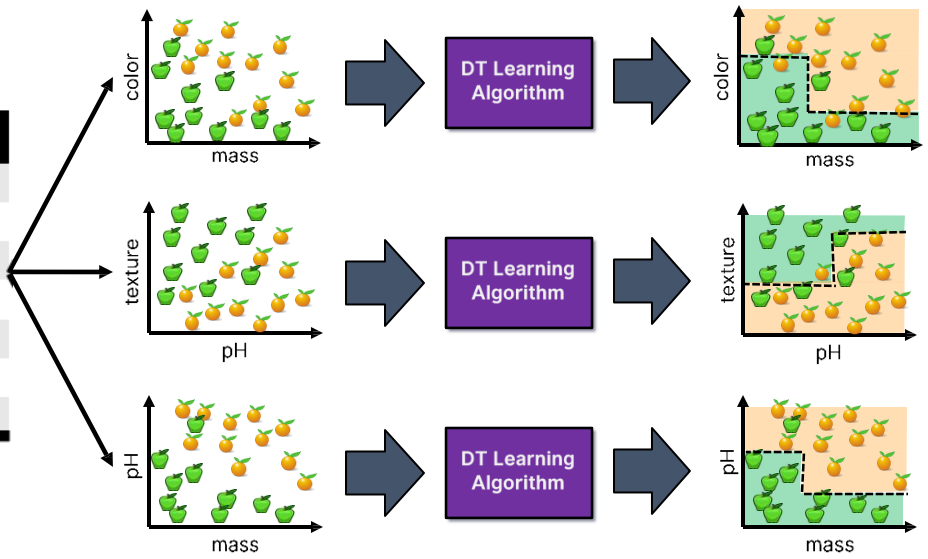
# Feature bagging at training time (model construction)

Training data

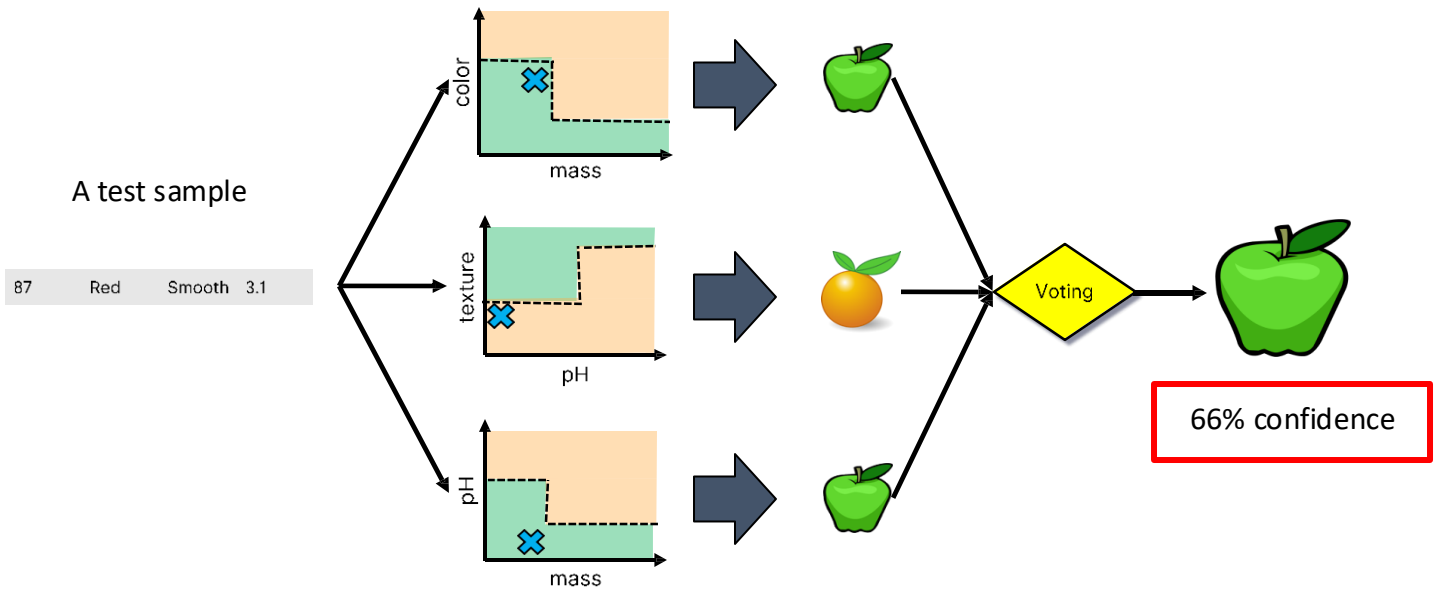
| Mass (g) | Color | Texture | pH | Label |
|---|---|---|---|---|
| 84 | Green | Smooth | 3.5 | **Apple** |
| 121 | Orange | Rough | 3.9 | **Orange** |
| 85 | Red | Smooth | 3.3 | **Apple** |
| 101 | Orange | Smooth | 3.7 | **Orange** |
| 111 | Green | Rough | 3.5 | **Apple** |
| ... | | | | |
| 117 | Red | Rough | 3.4 | **Orange** |

4-D Data

(4 features: Mass, Color, Texture, pH)



# Feature bagging at inference time (model usage)



# Random Forests

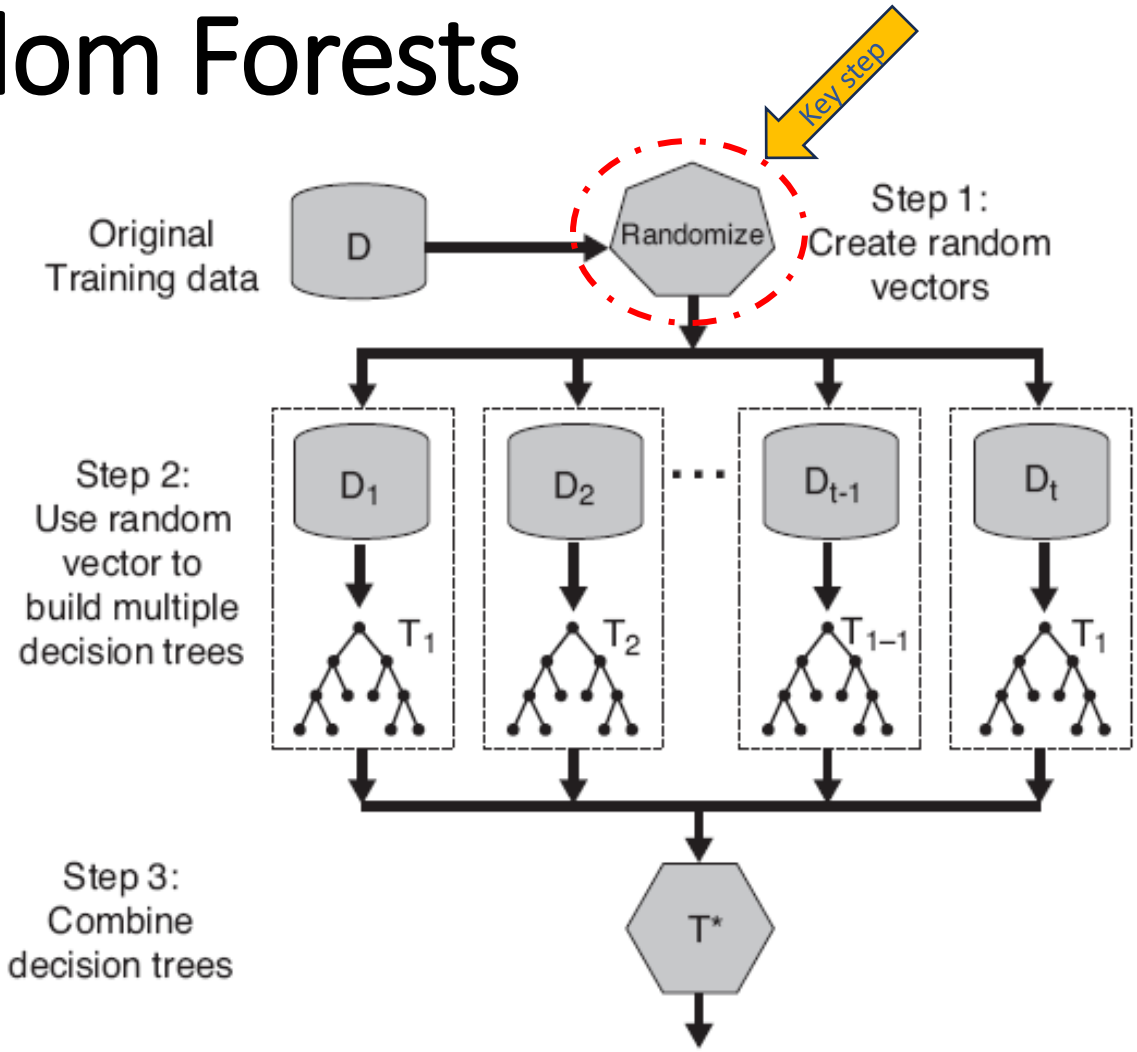



**Figure 5.40.** Random forests.

# Random Forests

Random forests are popular. Leo Breiman's and Adele Cutler maintains a random forest website where the software is freely available, and of course it is included in every ML/STAT package

http://www.stat.berkeley.edu/~breiman/RandomForests/

# Boosting Ensemble Methods:
# Adaboost

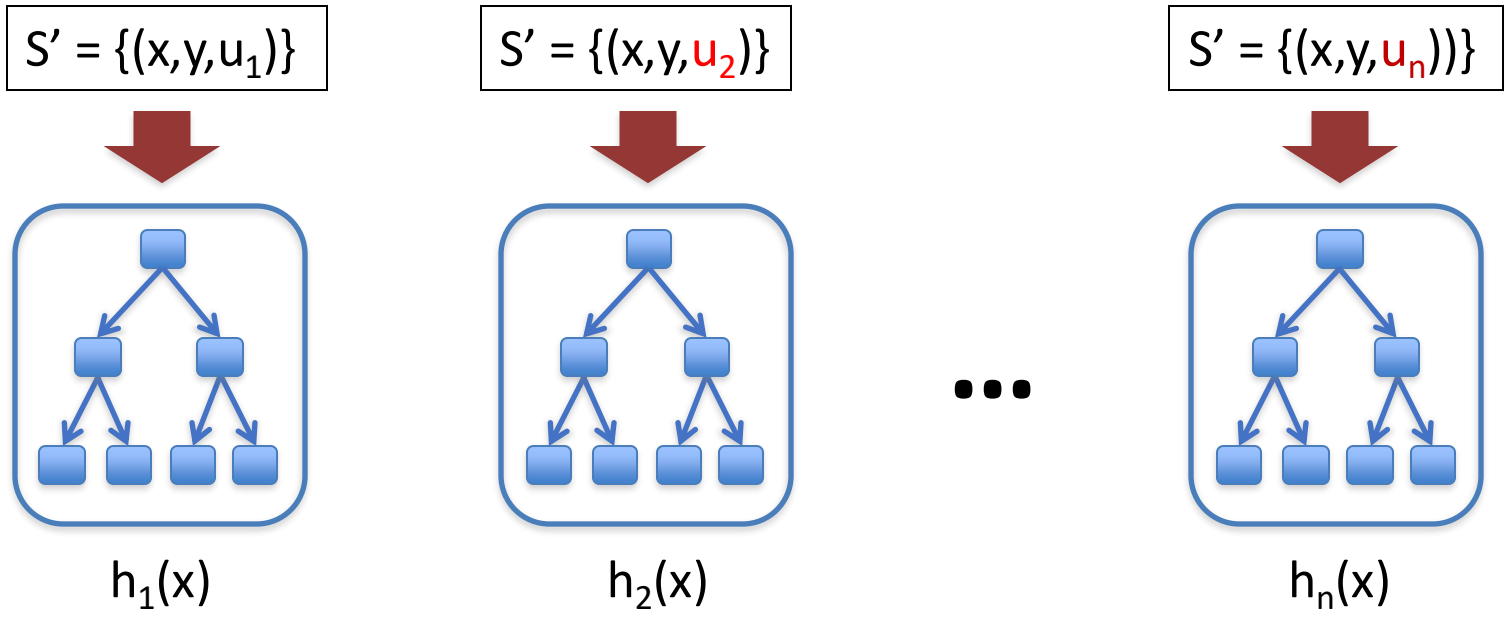
Most boosting algorithms follow these steps:

1. Train a weak model on some training data
2. Compute the error of the model on each training example
3. Give higher importance to examples on which the model made mistakes
4. Re-train the model using “importance weighted” training examples
5. Go back to step 2

# Boosting (AdaBoost)

https://towardsdatascience.com/a-comprehensive-mathematical-approach-to-understand-adaboost-f185104edced

$$h(x) = a_1h_1(x) + a_2h_2(x) + \ldots + a_nh_n(x)$$




u – weighting on data points
a – weight of linear combination

Stop when validation performance plateaus

# AdaBoost (Adaptive Boosting): Algorithm

- Given: Training data $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$ with $y_n \in \{-1, +1\}$, $\forall n$
- Initialize weight of each example $(\boldsymbol{x}_n, y_n)$: $D_1(n) = 1/N$, $\forall n$
- For round $t = 1 : T$
  - Learn a weak $h_t(\boldsymbol{x}) \rightarrow \{-1, +1\}$ using training data weighted as per $D_t$
  - Compute the weighted fraction of errors of $h_t$ on this training data

$$\epsilon_t = \sum_{n=1}^{N} D_t(n) \mathbb{1}[h_t(\boldsymbol{x}_n) \neq y_n]$$

  - Set "importance" of $h_t$: $\alpha_t = \frac{1}{2} \log(\frac{1-\epsilon_t}{\epsilon_t})$(gets larger as $\epsilon_t$ gets smaller)
  - Update the weight of each example

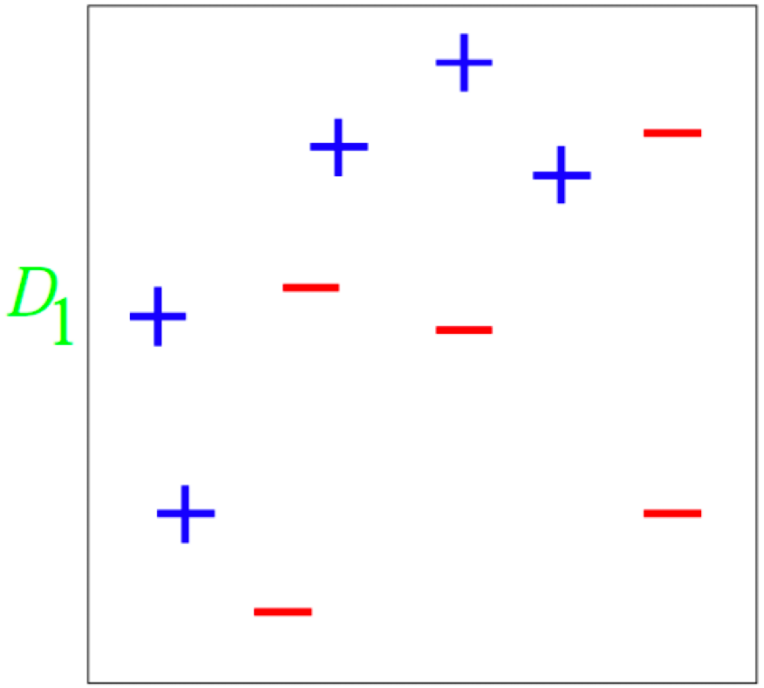
$$\begin{aligned} D_{t+1}(n) &\propto \begin{cases} D_t(n) \times \exp(-\alpha_t) & \text{if } h_t(\boldsymbol{x}_n) = y_n \quad \text{(correct prediction: decrease weight)} \\ D_t(n) \times \exp(\alpha_t) & \text{if } h_t(\boldsymbol{x}_n) \neq y_n \quad \text{(incorrect prediction: increase weight)} \end{cases} \\ &= D_t(n) \exp(-\alpha_t y_n h_t(\boldsymbol{x}_n)) \end{aligned}$$

  - Normalize $D_{t+1}$ so that it sums to 1: $D_{t+1}(n) = \frac{D_{t+1}(n)}{\sum_{m=1}^{N} D_{t+1}(m)}$
- Output the "boosted" final hypothesis $H(\boldsymbol{x}) = \text{sign}(\sum_{t=1}^{T} \alpha_t h_t(\boldsymbol{x}))$

# AdaBoost: An Example

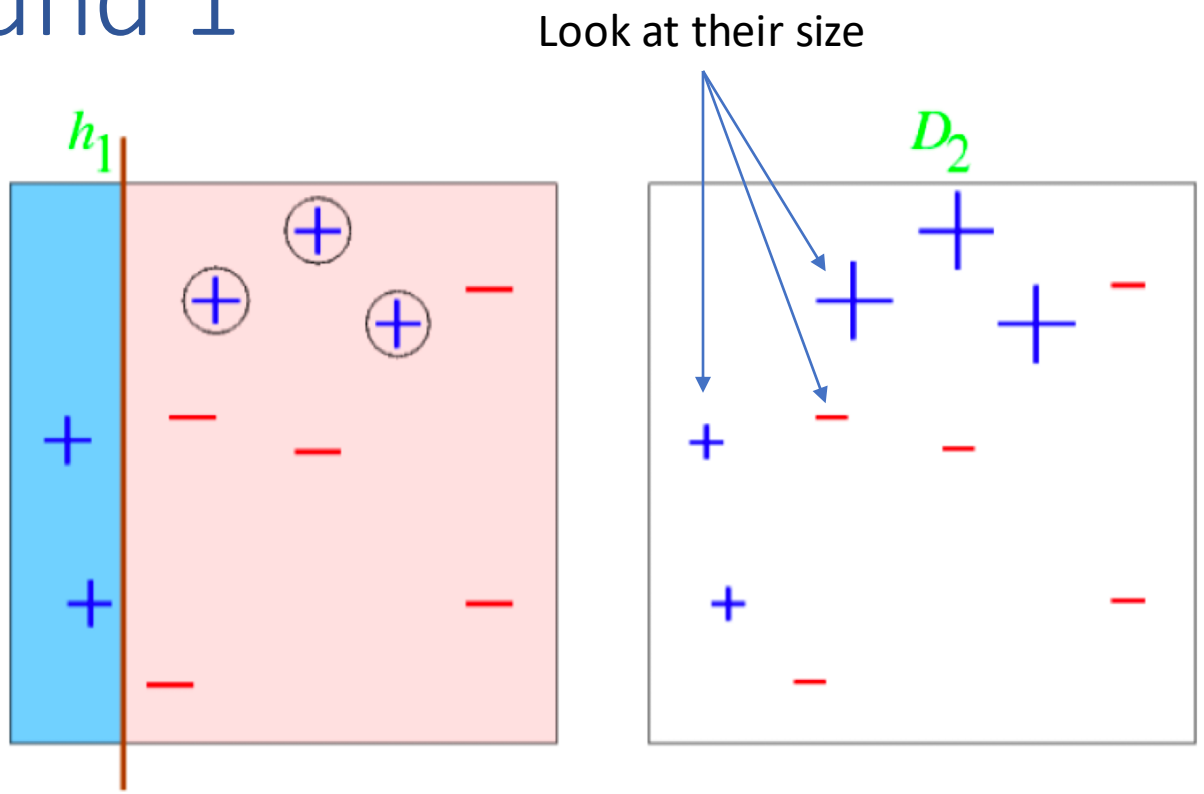
Consider binary classification with 10 training examples

Initial weight distribution $D_1$ is uniform (each point has equal weight $= 1/10$)



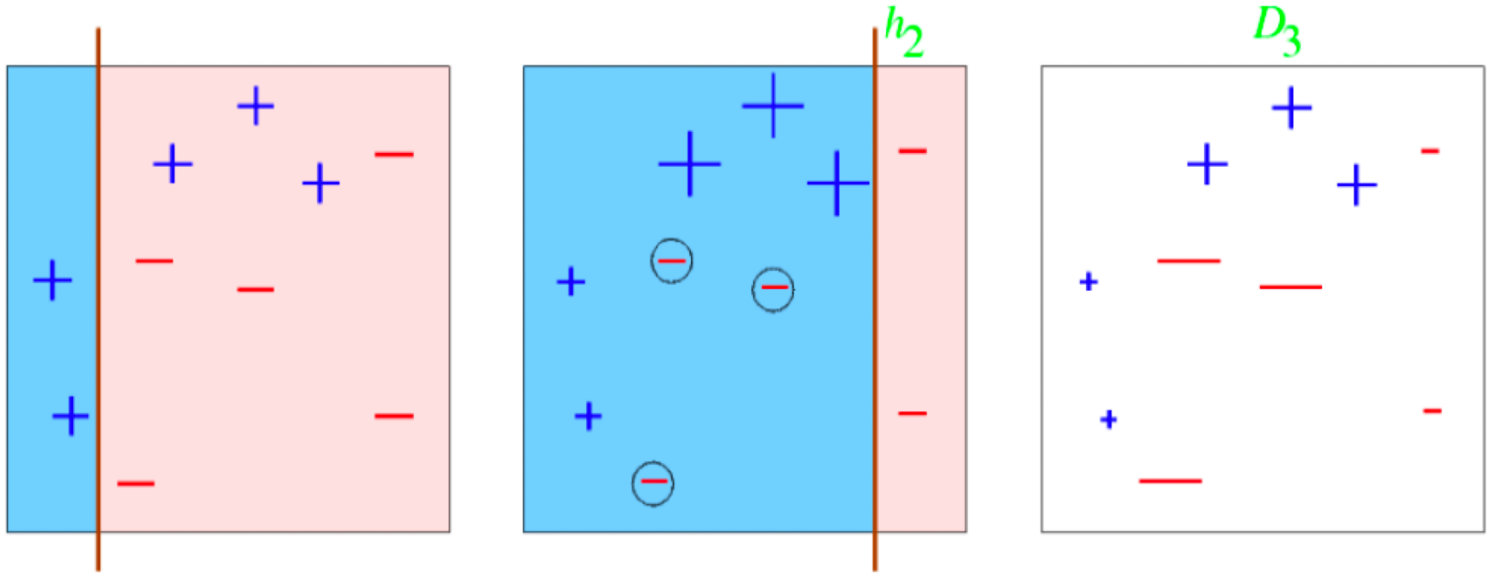

Each of our weak classifers will be an **axis-parallel linear classifier**

# After Round 1



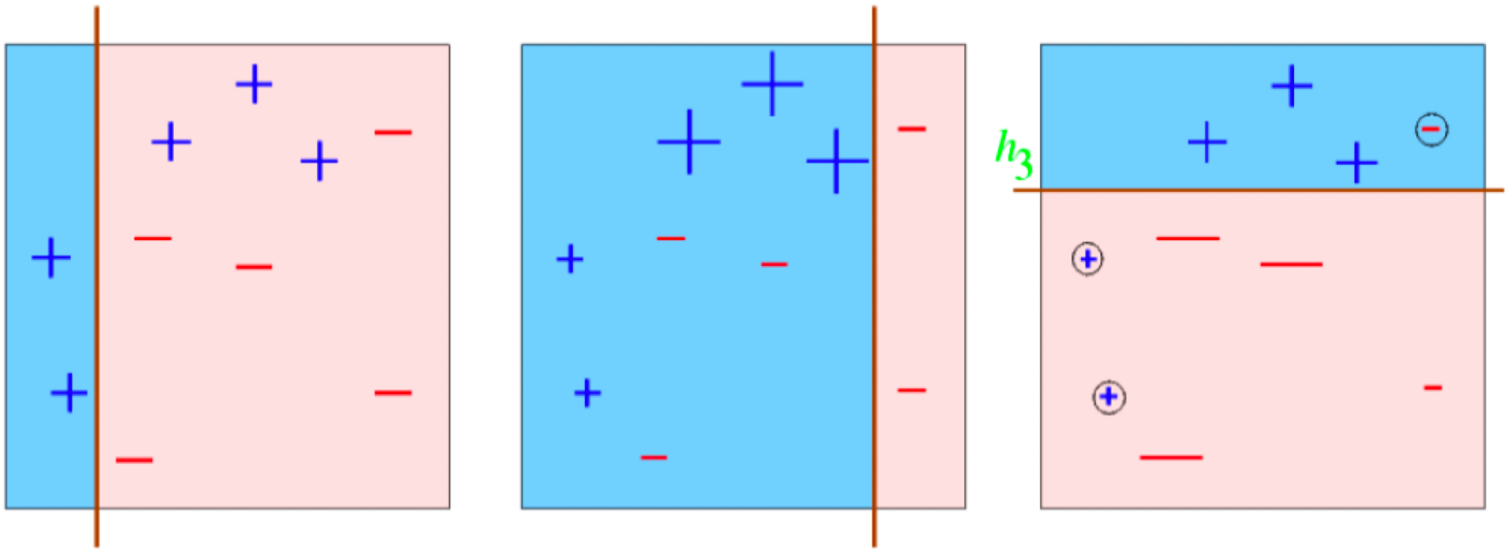

- Error rate of $h_1$: $\epsilon_1 = 0.3$; weight of $h_1$: $\alpha_1 = \frac{1}{2}\ln((1-\epsilon_1)/\epsilon_1) = 0.42$
- Each misclassified point upweighted (weight multiplied by $\exp(\alpha_2)$)
- Each correctly classified point downweighted (weight multiplied by $\exp(-\alpha_2)$)

# After Round 2




- Error rate of $h_2$: $\epsilon_2 = 0.21$; weight of $h_2$: $\alpha_2 = \frac{1}{2}\ln((1-\epsilon_2)/\epsilon_2) = 0.65$
- Each misclassified point upweighted (weight multiplied by $\exp(\alpha_2)$)
- Each correctly classified point downweighted (weight multiplied by $\exp(-\alpha_2)$)

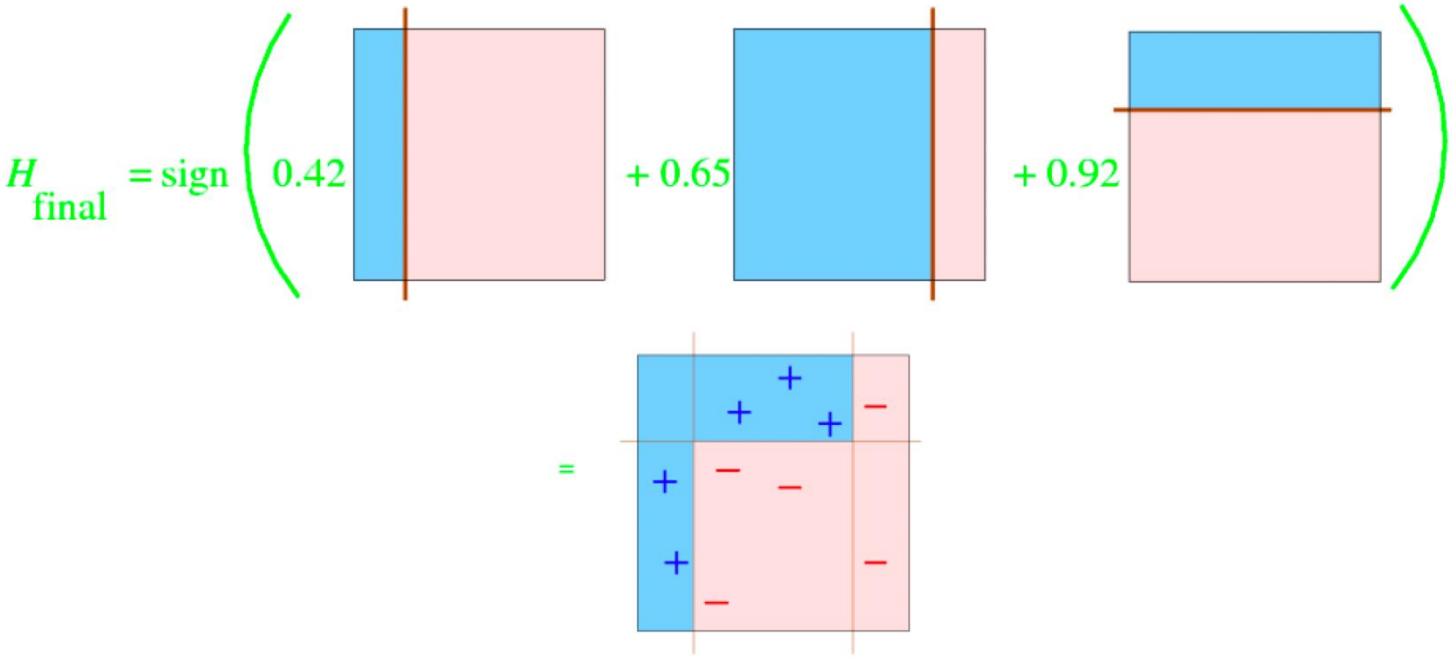
# After Round 3




- Error rate of $h_3$: $\epsilon_3 = 0.14$; weight of $h_3$: $\alpha_3 = \frac{1}{2}\ln((1-\epsilon_3)/\epsilon_3) = 0.92$
- Suppose we decide to stop after round 3
- Our ensemble now consists of 3 classifiers: $h_1, h_2, h_3$

# Finally, we have

- Final classifier is a weighted linear combination of all the classifiers
- Classifier $h_i$ gets a weight $\alpha_i$




- Multiple weak, linear classifiers **combined** to give a strong, nonlinear classifier

## A bit more … XGBoost

# Why use XGBoost?

- All of the advantages of gradient boosting (a kind of learning tree ensembles), plus more.
- Frequent Kaggle data competition champion.
- Utilizes CPU Parallel Processing by default.
- Two main reasons for use:
  1. Low Runtime
  2. High Model Performance

# Remarks

- Competitor-LightGBM (Microsoft)
  - Very similar, not as mature and feature rich
  - Slightly faster than XGBoost – much faster when it was published
- Hardly find an example where Random Forest outperforms XGBoost
- XGBoost Github: https://github.com/dmlc/xgboost
- XGBoost documentation: http://xgboost.readthedocs.io

# Take-home Messages

- Classification is an extensively studied problem (mainly in statistics, machine learning & neural networks)
- Scalability is still an important issue for database applications: thus combining classification with database techniques should be a promising topic
- Research directions: classification of non-relational data, e.g., text, spatial, multimedia, etc..
- Ensemble methods are effective approaches to boost the performance of ML/DM system.
- One particular advantage is that they typically do not involve too many parameters and too involved tuning.

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