# DS 4400

## Machine Learning and Data Mining I
## Spring 2021

Alina Oprea
Associate Professor
Khoury College of Computer Science
Northeastern University

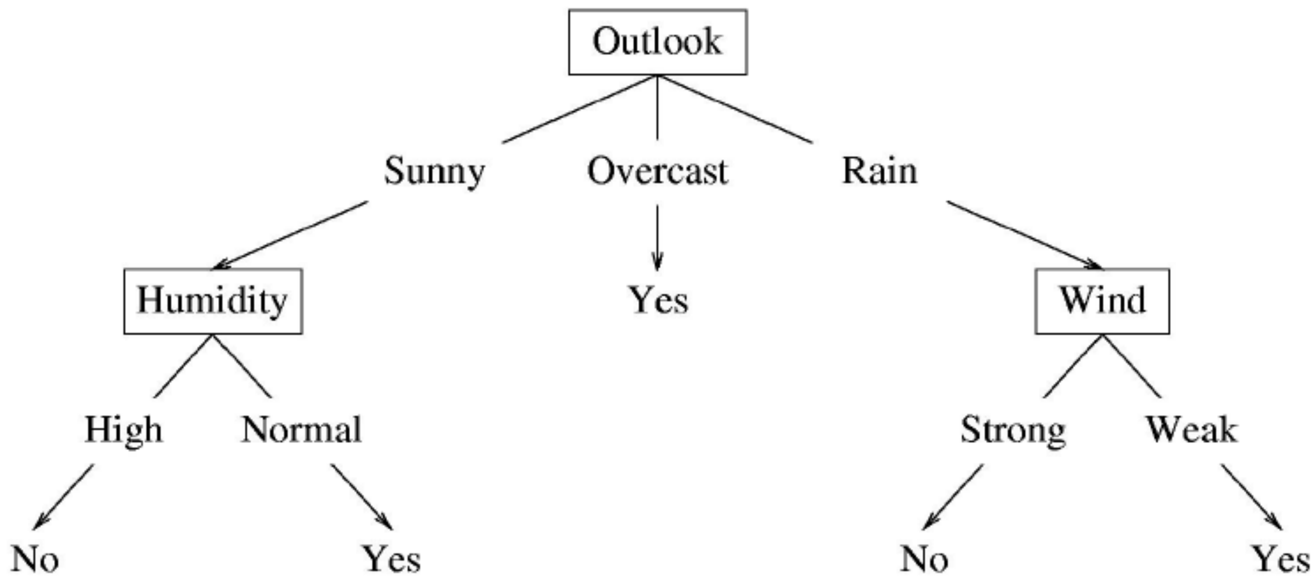
March 9 2021

# Outline

- Decision Trees
  - Regression trees
- Ensemble models
  - Majority vote over multiple models
- Bagging
  - Bootstrap samples
  - Random forest
- Boosting
  - AdaBoost

# Decision Tree

- A possible decision tree for the data:




- Each internal node: test one attribute $X_i$
- Each branch from a node: selects one value for $X_i$
- Each leaf node: predict $Y$ (or $p(Y \mid x \in \mathrm{leaf})$ )

# Learning Decision Trees

- Start from empty decision tree
- Split on **next best attribute (feature)**
  - Use, for example, information gain to select attribute:

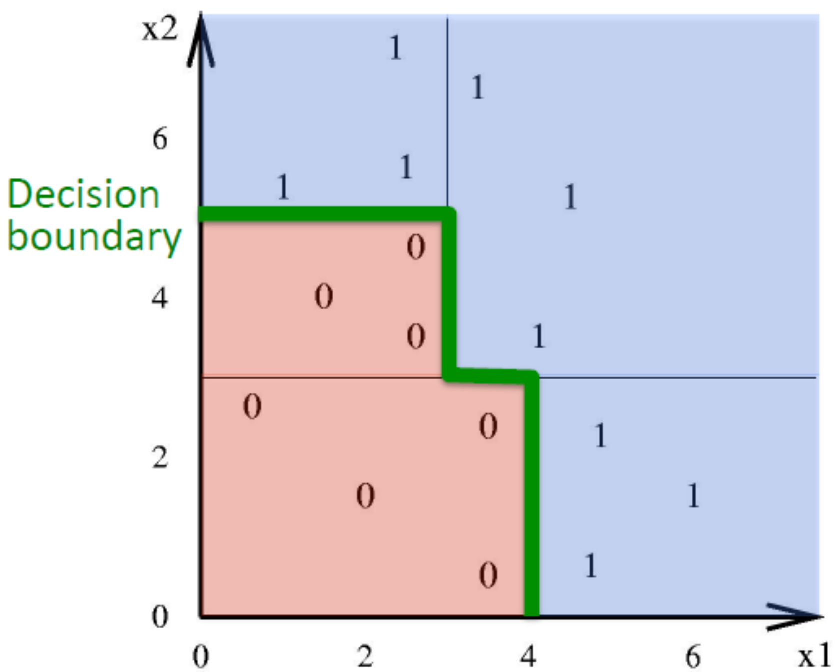
$$\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$$

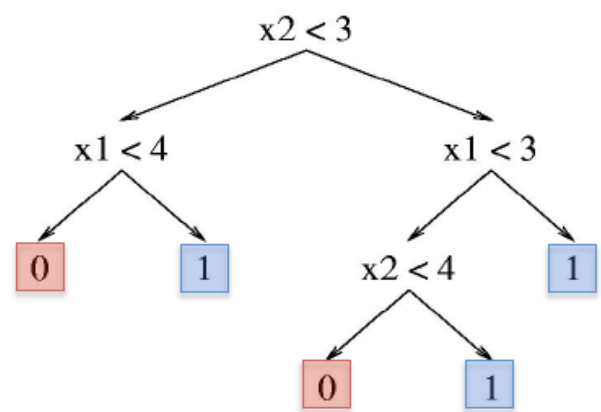
- Recurse

ID3 algorithm uses Information Gain
Information Gain reduces uncertainty on Y

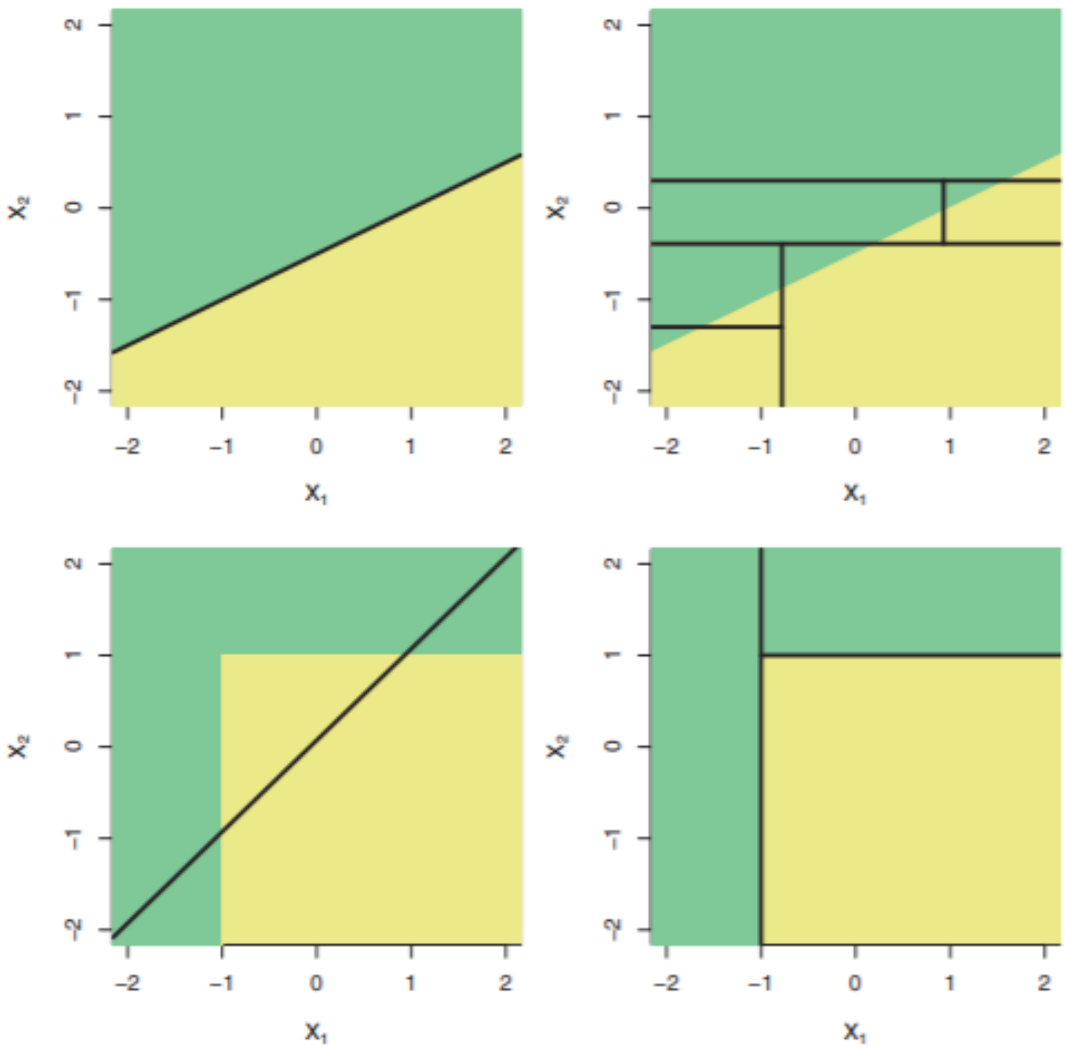
# Decision Boundary

- Decision trees divide the feature space into axis-parallel (hyper-)rectangles
- Each rectangular region is labeled with one label



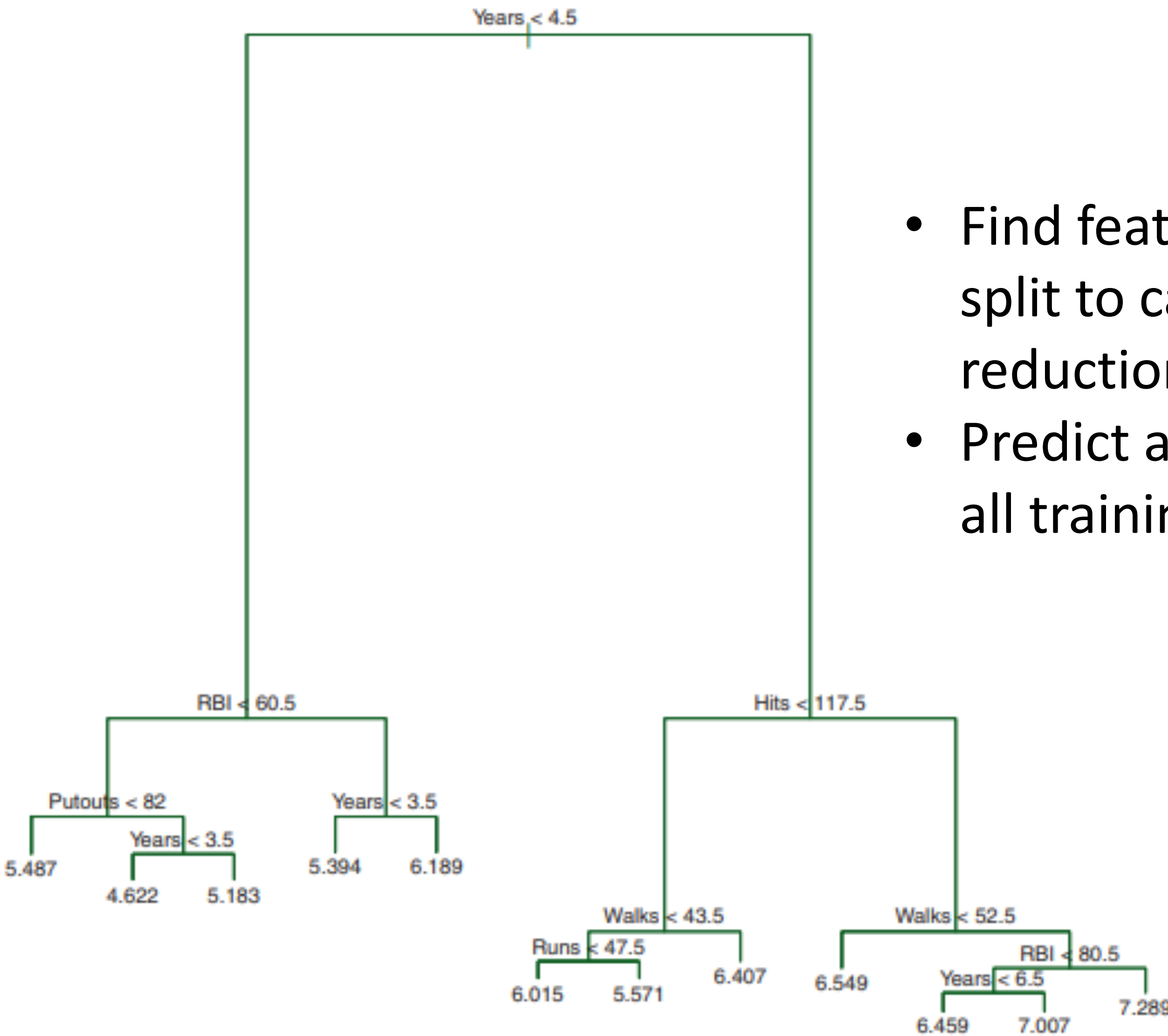
# Decision Trees vs Linear Models




Linear model

Decision tree

# Regression Trees




- Find feature and value to split to cause the maximum reduction in MSE
- Predict average response of all training data at each leaf

# Summary Decision Trees

- Representation: decision trees
- Bias: prefer small decision trees
- Search algorithm: greedy
- Heuristic function: information gain or information content or others
- Overfitting / pruning

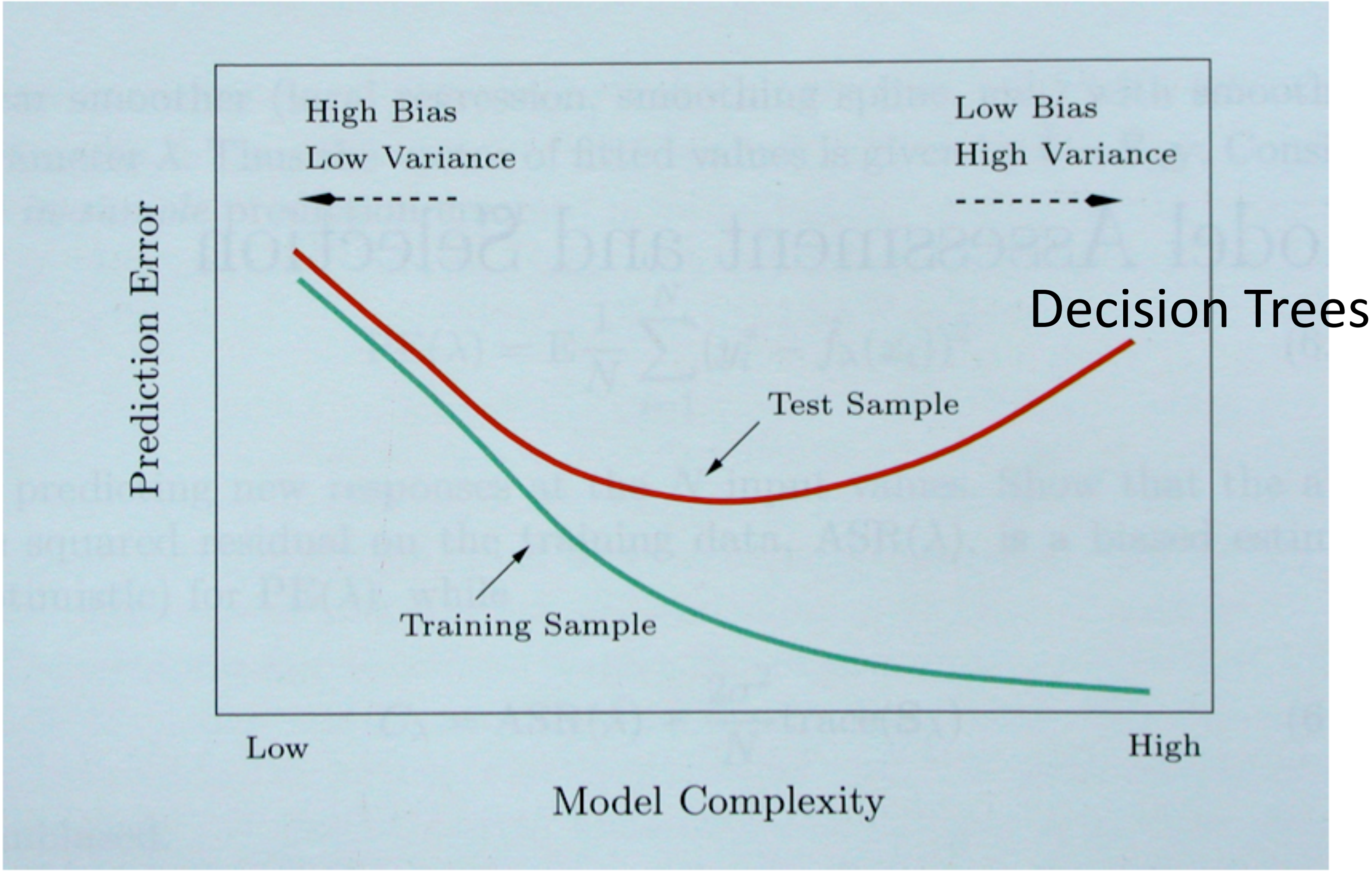
Strengths

- Fast to evaluate
- Interpretable
- Generate rules
- Supports categorical and numerical data

Weaknesses

- Overfitting
- Splitting method might not be optimal
- Accuracy is not always high
- Batch learning

# Bias/Variance Tradeoff




Hastie, Tibshirani, Friedman "Elements of Statistical Learning" 2001

How to reduce variance of single decision tree?

# Ensemble Learning

Consider a set of classifiers $h_1, \ldots, \mathrm{h}_\mathrm{L}$

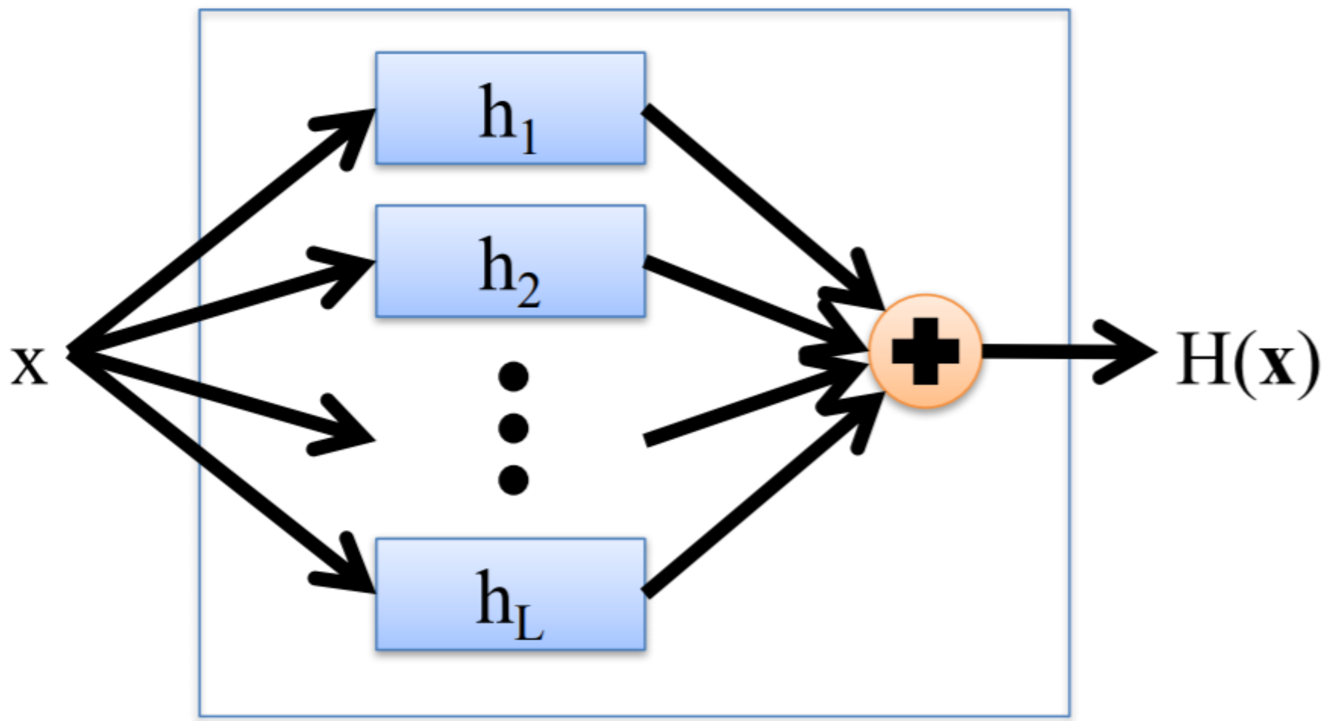
**Idea:** construct a classifier $H(\mathbf{x})$ that combines the individual decisions of $h_1, \ldots, \mathrm{h}_\mathrm{L}$

- e.g., could have the member classifiers vote, or
- e.g., could use different members for different regions of the instance space

Successful ensembles require **diversity**

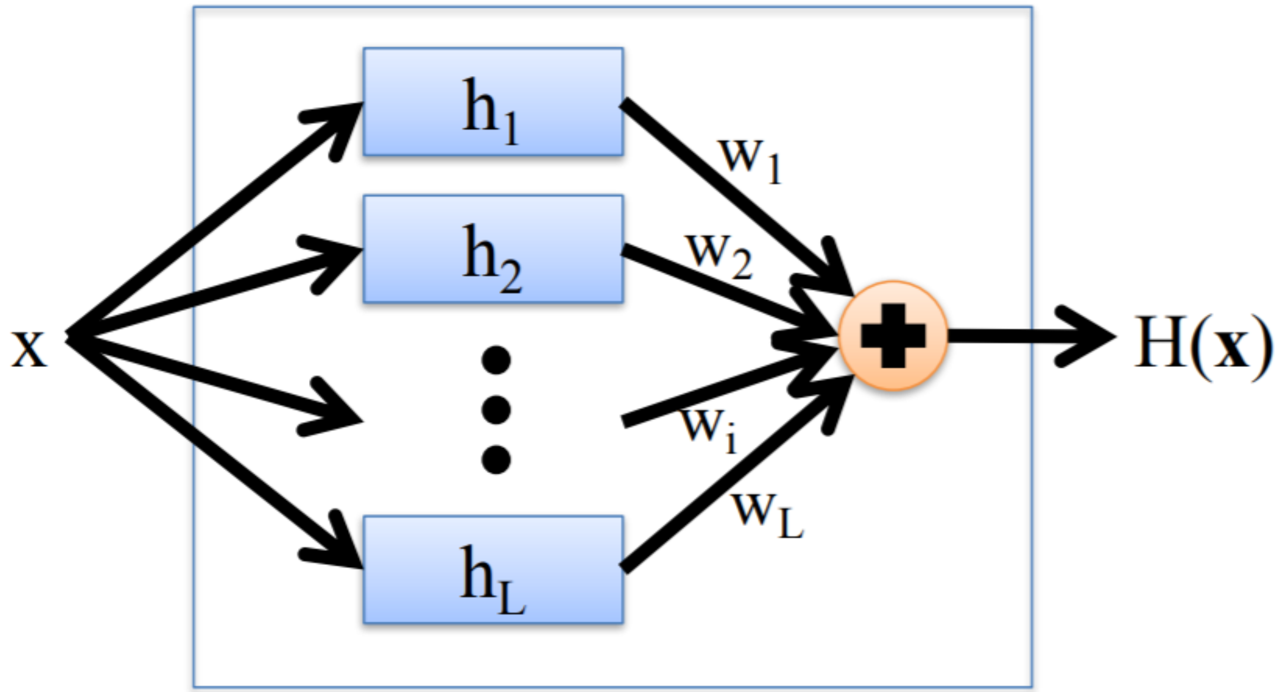
- Classifiers should make different mistakes
- Can have different types of base learners

# Combining Classifiers: Averaging




- Final hypothesis is a simple vote of the members

# Combining Classifiers: Weighted Averaging




- Coefficients of individual members are trained using a validation set

# Practical Applications

**Goal:** predict how a user will rate a movie

- Based on the user's ratings for other movies
- and other peoples' ratings
- with no other information about the movies

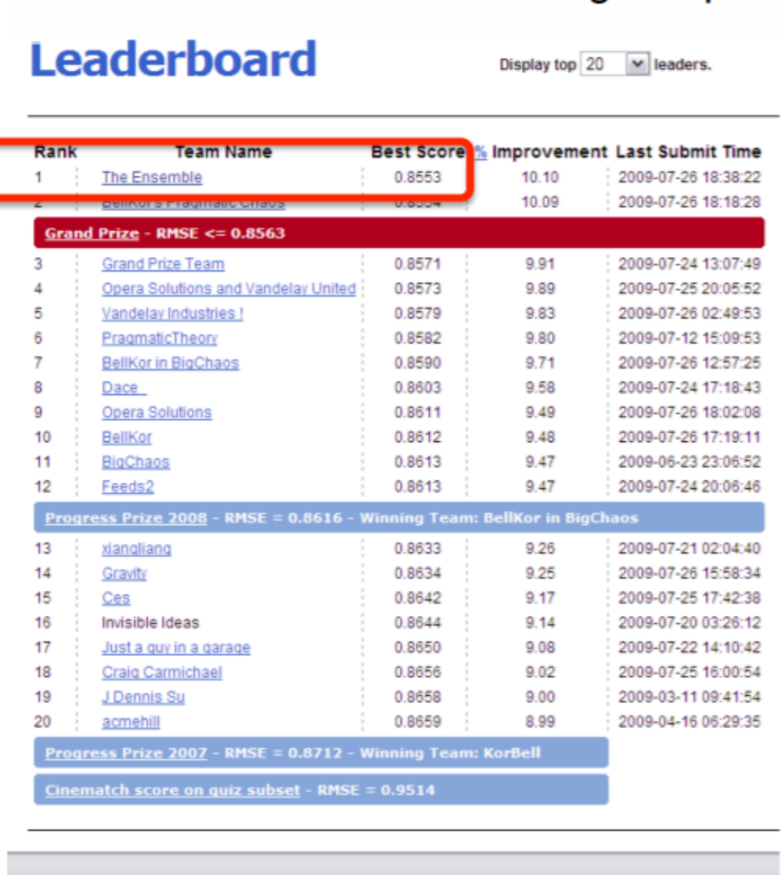
This application is called "collaborative filtering"

**Netflix Prize:** \$1M to the first team to do 10% better then Netflix' system (2007-2009)

**Winner:** BellKor's Pragmatic Chaos – an ensemble of more than 800 rating systems

# Netflix Prize

Machine learning competition with a $1 million prize



## Leaderboard

Display top 20 leaders.

| Rank | Team Name | Best Score | % Improvement | Last Submit Time |
|---|---|---|---|---|
| 1 | The Ensemble | 0.8553 | 10.10 | 2009-07-26 18:38:22 |
| 2 | BellKor's Pragmatic Chaos | [illegible] | 10.09 | 2009-07-26 18:18:28 |
| Grand Prize - RMSE <= 0.8563 | | | | |
| 3 | Grand Prize Team | 0.8571 | 9.91 | 2009-07-24 13:07:49 |
| 4 | Opera Solutions and Vandelay United | 0.8573 | 9.89 | 2009-07-25 20:05:52 |
| 5 | Vandelay Industries ! | 0.8579 | 9.83 | 2009-07-26 02:49:53 |
| 6 | PragmaticTheory | 0.8582 | 9.80 | 2009-07-12 15:09:53 |
| 7 | BellKor in BigChaos | 0.8590 | 9.71 | 2009-07-26 12:57:25 |
| 8 | Dace_ | 0.8603 | 9.58 | 2009-07-24 17:18:43 |
| 9 | Opera Solutions | 0.8611 | 9.49 | 2009-07-26 18:02:08 |
| 10 | BellKor | 0.8612 | 9.48 | 2009-07-26 17:19:11 |
| 11 | BigChaos | 0.8613 | 9.47 | 2009-06-23 23:06:52 |
| 12 | Feeds2 | 0.8613 | 9.47 | 2009-07-24 20:06:46 |
| Progress Prize 2008 - RMSE = 0.8616 - Winning Team: BellKor in BigChaos | | | | |
| 13 | xiangliang | 0.8633 | 9.26 | 2009-07-21 02:04:40 |
| 14 | Gravity | 0.8634 | 9.25 | 2009-07-26 15:58:34 |
| 15 | Ces | 0.8642 | 9.17 | 2009-07-25 17:42:38 |
| 16 | Invisible Ideas | 0.8644 | 9.14 | 2009-07-20 03:26:12 |
| 17 | Just a guy in a garage | 0.8650 | 9.08 | 2009-07-22 14:10:42 |
| 18 | Craig Carmichael | 0.8656 | 9.02 | 2009-07-25 16:00:54 |
| 19 | J Dennis Su | 0.8658 | 9.00 | 2009-03-11 09:41:54 |
| 20 | acmehill | 0.8659 | 8.99 | 2009-04-16 06:29:35 |
| Progress Prize 2007 - RMSE = 0.8712 - Winning Team: KorBell | | | | |
| Cinematch score on quiz subset - RMSE = 0.9514 | | | | |


users

| movies | | | | | | |
|---|---|---|---|---|---|---|
| | 1 | | ? | 3 | 5 | ? |
| | ? | 1 | | | | 2 |
| | | 4 | | 4 | 5 | ? |

# Reduce error

- 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:

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

# Reduce Variance

- Averaging reduces variance:

$$Var(\overline{X}) = \frac{Var(X)}{N}$$

(when predictions are **independent**)

Average models to reduce model variance

One problem:

only one training set

where do multiple models come from?

# How to Achieve Diversity

- Avoid overfitting
  - Vary the training data
- Features are noisy
  - Vary the set of features

Two main ensemble learning methods

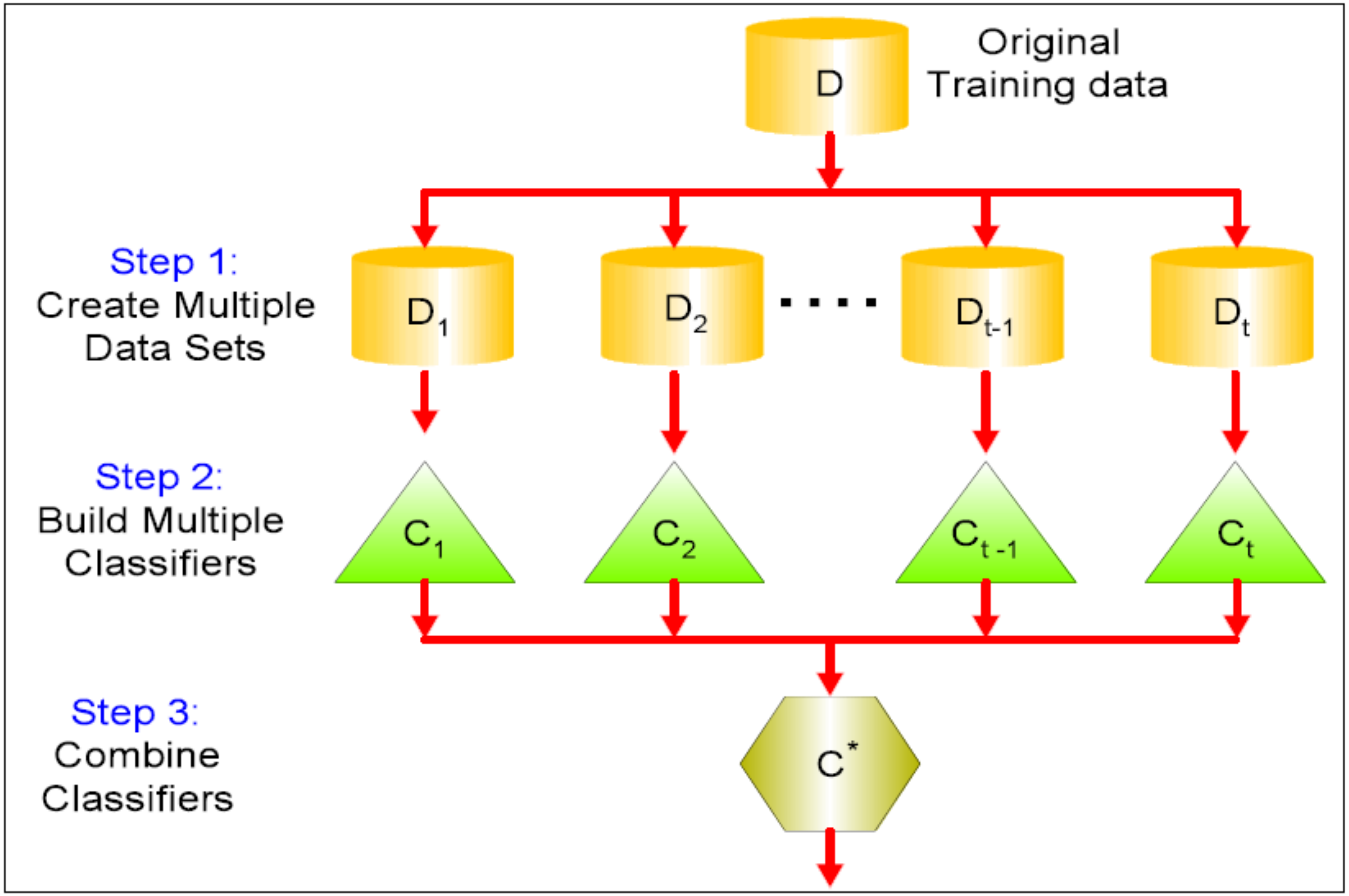
- Bagging (e.g., Random Forests)
- Boosting (e.g., AdaBoost)

# Bagging

- Leo Breiman (1994)
- Take repeated bootstrap samples from training set $D$
- *Bootstrap sampling*: Given set $D$ containing $N$ training examples, create $D'$ by drawing $N$ examples at random with replacement from $D$.

- Bagging:
  - Create $k$ bootstrap samples $D_1 \ldots D_k$.
  - Train distinct classifier on each $D_i$.
  - Classify new instance by majority vote / average.

# General Idea




Majority Votes

# Example of Bagging

- Sampling with replacement

Training Data

Data ID

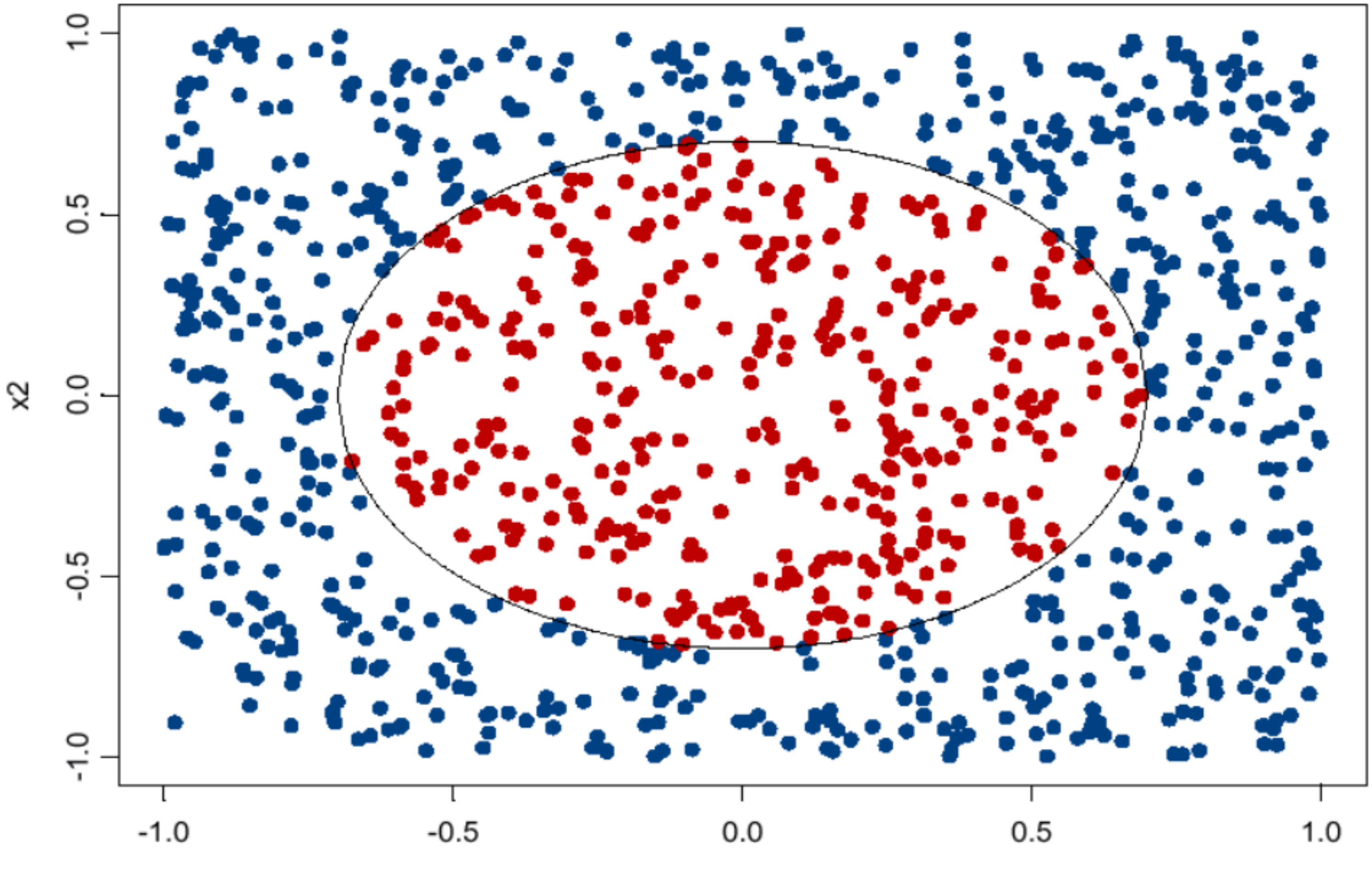
| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Original Data** | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| **Bagging (Round 1)** | 7 | 8 | 10 | 8 | 2 | 5 | 10 | 10 | 5 | 9 |
| **Bagging (Round 2)** | 1 | 4 | 9 | 1 | 2 | 3 | 2 | 7 | 3 | 2 |
| **Bagging (Round 3)** | 1 | 8 | 5 | 10 | 5 | 5 | 9 | 6 | 3 | 7 |

- Sample each training point with probability 1/n
- Out-Of-Bag (OOB) observation: point not in sample
  - For each point: prob $(1-1/n)^n$
  - About 1/3 of data
  - OOB error: error on OOB samples
- OOB average error
  - Compute across all models in Ensemble
  - Use instead of Cross-Validation error

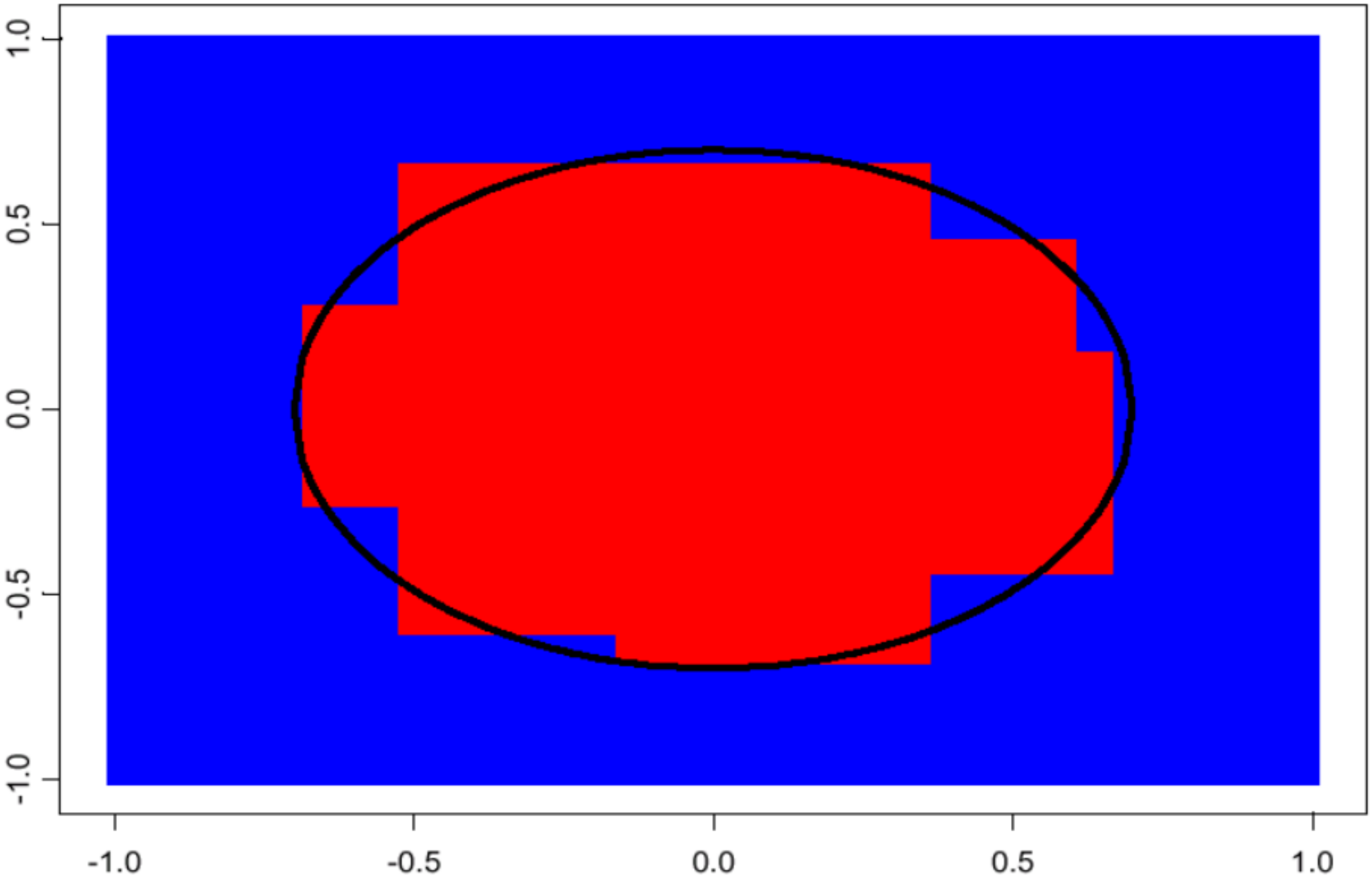
# Bagging

- Can be applied to multiple classification models
- Very successful for decision trees
  - Decision trees have high variance
  - Don’t prune the individual trees, but grow trees to full extent
  - Precision accuracy of decision trees improved substantially
- OOB average error used instead of Cross Validation

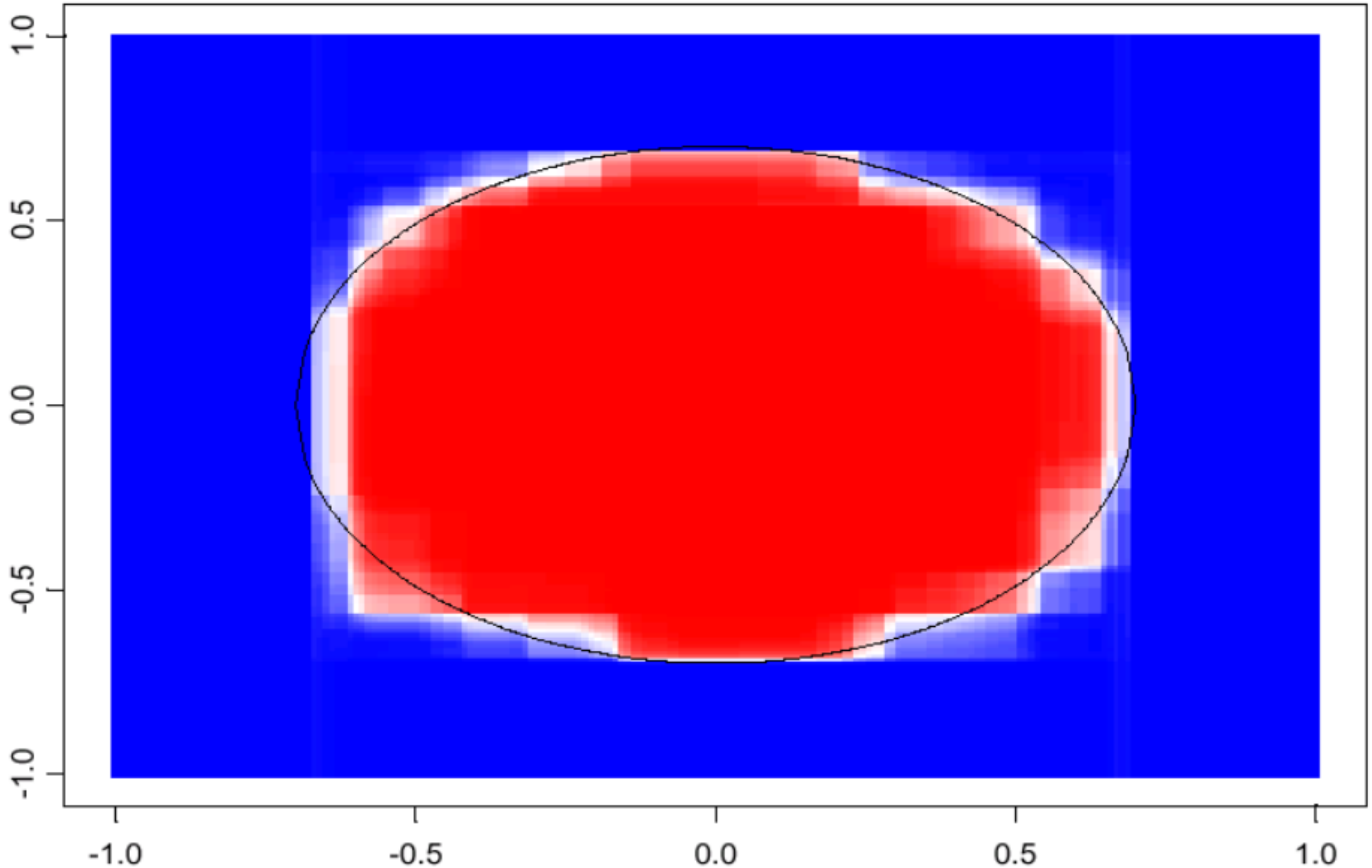
# Example Distribution



# Decision Tree Decision Boundary



# 100 Bagged Trees




shades of blue/red indicate strength of vote for particular classification

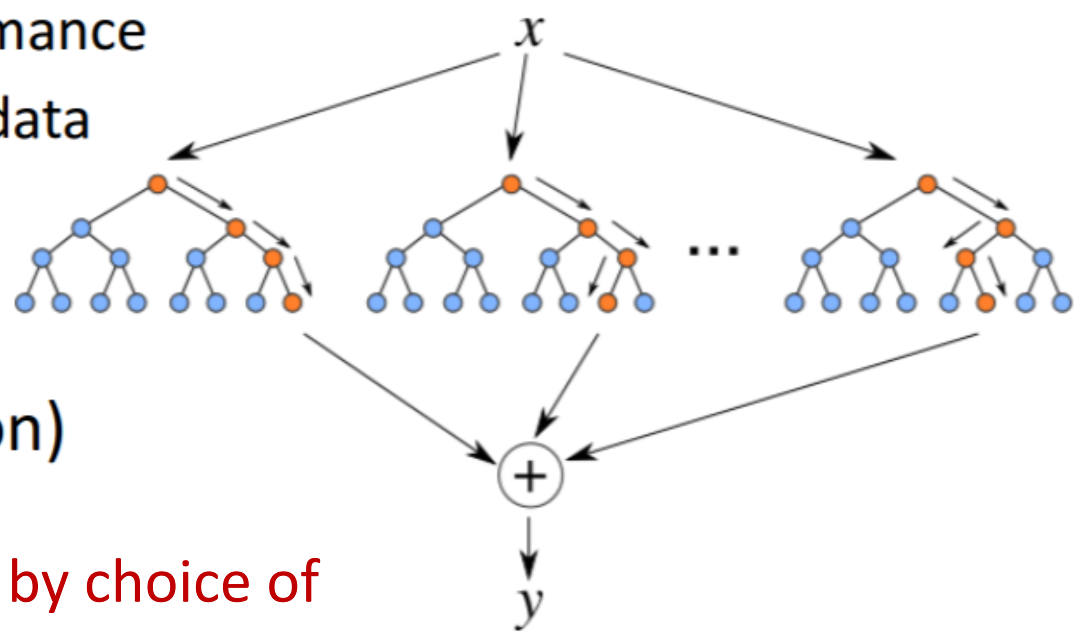
# Random Forests

- Ensemble method specifically designed for decision tree classifiers

- Introduce two sources of randomness: "Bagging" and "Random input vectors"
  - Bagging method: each tree is grown using a bootstrap sample of training data
  - Random vector method: At each node, best split is chosen from a random sample of *m* attributes instead of all attributes

# Random Forests

- Construct decision trees on bootstrap replicas
  - Restrict the node decisions to a small subset of features picked randomly for each node
- Do not prune the trees
  - Estimate tree performance on out-of-bootstrap data
- Average the output of all trees (or choose mode decision)




Trees are de-correlated by choice of random subset of features

# Random Forest Algorithm

1. For $b = 1$ to $B$:

   (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size $N$ from the training data.

   (b) Grow a random-forest tree $T_b$ to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size $n_{min}$ is reached.

      i. Select $m$ variables at random from the $p$ variables.

      ii. Pick the best variable/split-point among the $m$.

      iii. Split the node into two daughter nodes.

2. Output the ensemble of trees $\{T_b\}_1^B$.

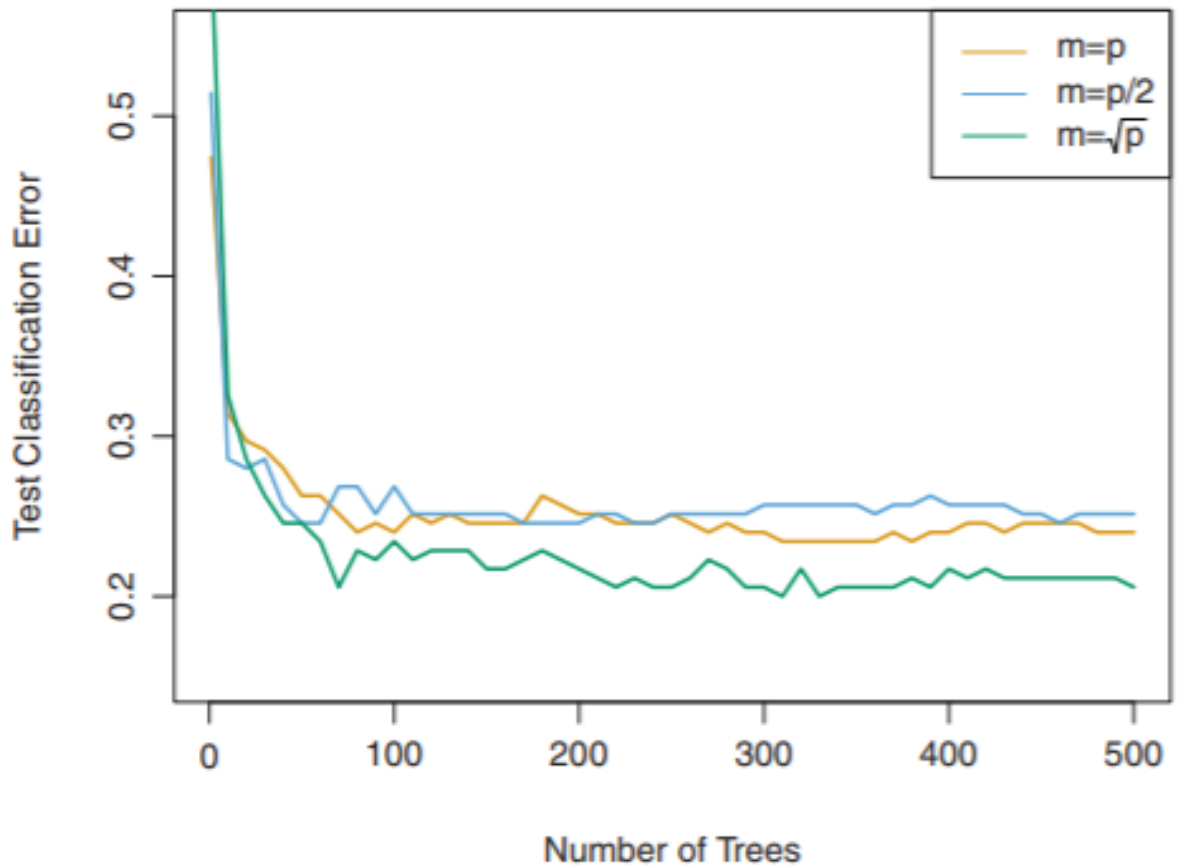
To make a prediction at a new point $x$:

*Regression:* $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.

*Classification:* Let $\hat{C}_b(x)$ be the class prediction of the $b$th random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \textit{majority vote}\ \{\hat{C}_b(x)\}_1^B$.

If m=p, this is equivalent to Bagging with Decision Trees as base learner

# Effect of Number of Predictors




- $p$ = total number of predictors; $m$ = predictors chosen in each split
- Random Forests uses $m = \sqrt{p}$

# Variable Importance

- Ensemble of trees looses somewhat interpretability of decision trees
- Which variables contribute mostly to prediction?
- Random Forests computes a Variable Importance metric per feature
  - For each tree in the ensemble, consider the split by the particular feature
  - How much information gain / Gini index decreases after the split
  - Average over all trees

# Variable Importance Plots

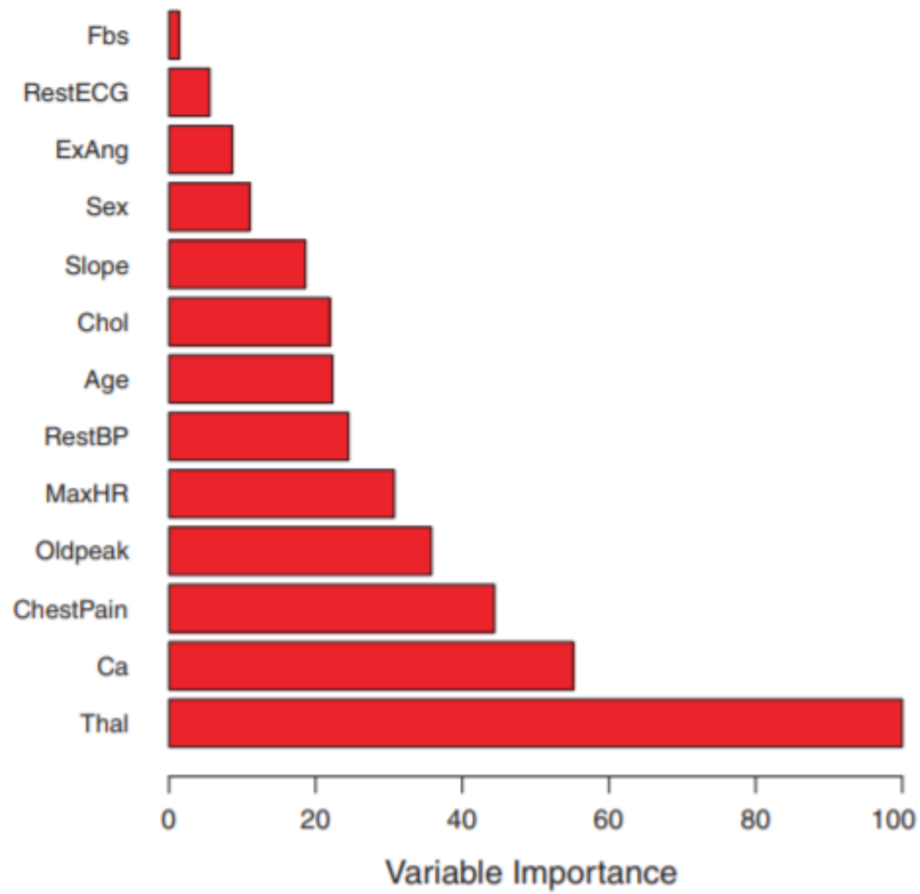



**FIGURE 8.9.** *A variable importance plot for the* `Heart` *data. Variable importance is computed using the mean decrease in Gini index, and expressed relative to the maximum.*

# Variable Importance

- Ensembles of trees loose in interpretability
  - Variable importance helps with determining important features
- Can be used as a filter method for feature selection
  - Train Random Forest model
  - Compute variable importance
  - Select top k features by highest important
  - Train other models with the k features

# How to Achieve Diversity

- Avoid overfitting
  - Vary the training data
- Features are noisy
  - Vary the set of features

Two main ensemble learning methods

- Bagging (e.g., Random Forests)
- $\boxed{\text{Boosting (e.g., AdaBoost)}}$

# AdaBoost

- A meta-learning algorithm with great theoretical and empirical performance
- Turns a base learner (i.e., a “weak hypothesis”) into a high performance classifier
- Creates an ensemble of weak hypotheses by repeatedly emphasizing mispredicted instances

Adaptive Boosting
Freund and Schapire 1997

# Overview of AdaBoost

- Mis-classified examples get higher weights
- Correct examples get lower weights

Better classifiers will get higher weights

Uniform weights

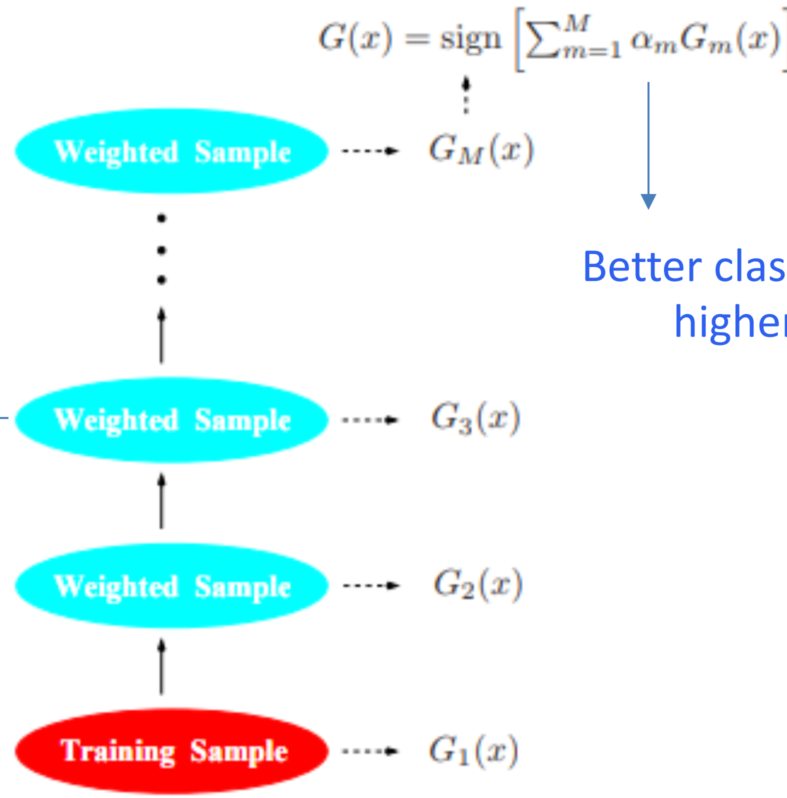



**FIGURE 10.1.** *Schematic of AdaBoost. Classifiers are trained on weighted versions of the dataset, and then combined to produce a final prediction.*

# Boosting [Shapire '89]

- **Idea:** given a weak learner, run it multiple times on (reweighted) training data, then let learned classifiers vote
- On each iteration $t$:
  - weight each training example by how incorrectly it was classified
  - Learn a weak hypothesis – $h_t$
  - A strength for this hypothesis – ( $\beta_t$
- Final classifier: $\boxed{H(x) = sign(\sum \beta_t h_t(x))}$

Convergence bounds with minimal assumptions on weak learner

If each weak learner $h_t$ is slightly better than random guessing ($\varepsilon_t < 0.5$), then training error of AdaBoost decays exponentially fast in number of rounds T.

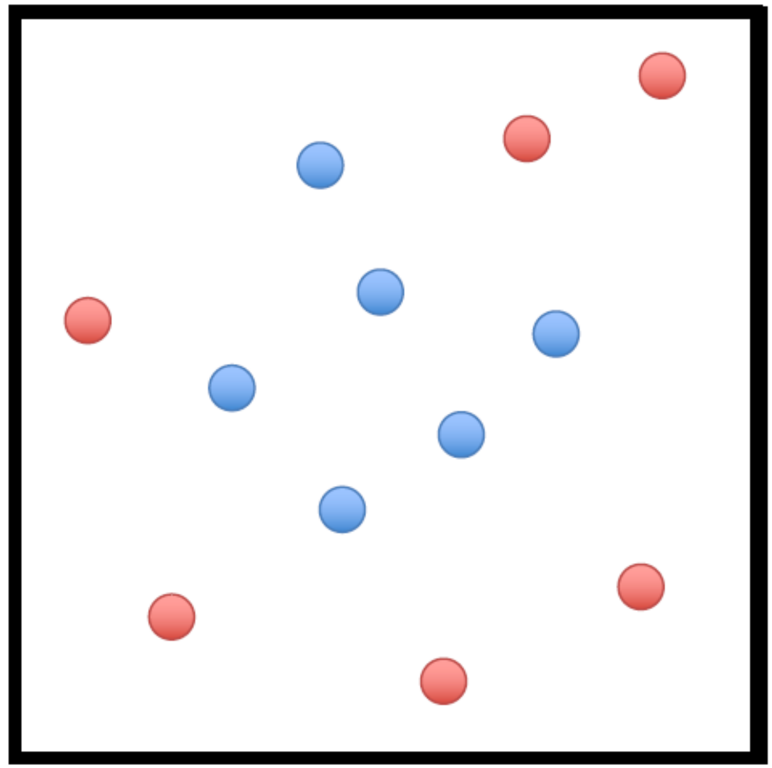
# AdaBoost

Initialize a vector of $n$ uniform weights $\mathbf{w}_1$
**for** $t = 1, \ldots, T$
  Train model $h_t$ on $X, y$ with weights $\mathbf{w}_t$
  Compute the weighted training error of $h_t$
  Choose $\beta_t = \frac{1}{2} \ln \left( \frac{1-\epsilon_t}{\epsilon_t} \right)$
  Update all instance weights:

$$w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\mathbf{x}_i)\right)$$

  Normalize $\mathbf{w}_{t+1}$ to be a distribution
**end for**
**Return** the hypothesis

$$H(\mathbf{x}) = \operatorname{sign}\left( \sum_{t=1}^{T} \beta_t h_t(\mathbf{x}) \right)$$



- Size of point represents the instance's weight

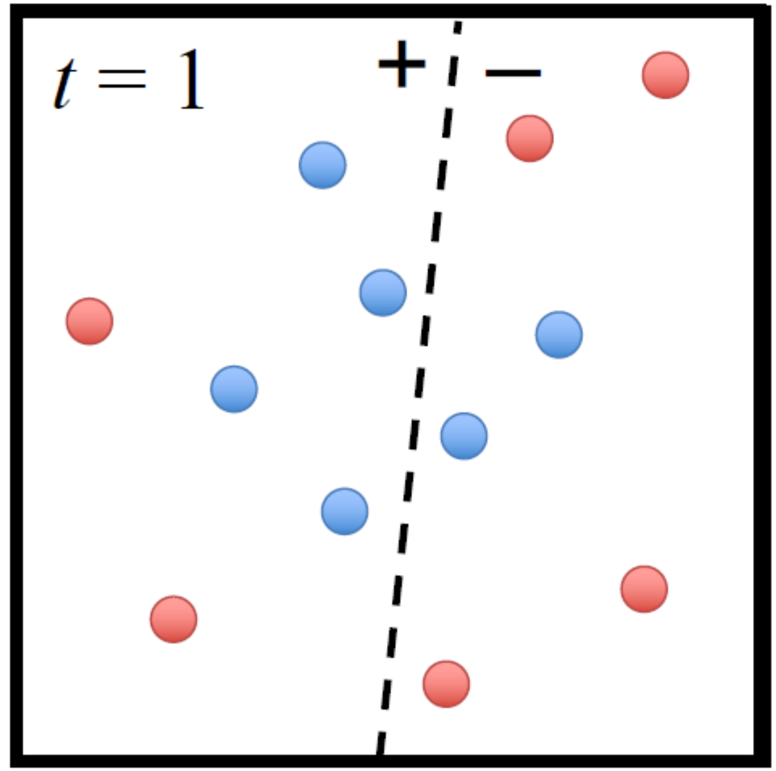
# AdaBoost

Initialize a vector of $n$ uniform weights $\mathbf{w}_1$
**for** $t = 1, \ldots, T$
  Train model $h_t$ on $X, y$ with weights $\mathbf{w}_t$
  Compute the weighted training error of $h_t$
  Choose $\beta_t = \frac{1}{2} \ln \left( \frac{1-\epsilon_t}{\epsilon_t} \right)$
  Update all instance weights:

$$w_{t+1,i} = w_{t,i} \exp \left( -\beta_t y_i h_t(\mathbf{x}_i) \right)$$

  Normalize $\mathbf{w}_{t+1}$ to be a distribution
**end for**
**Return** the hypothesis

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



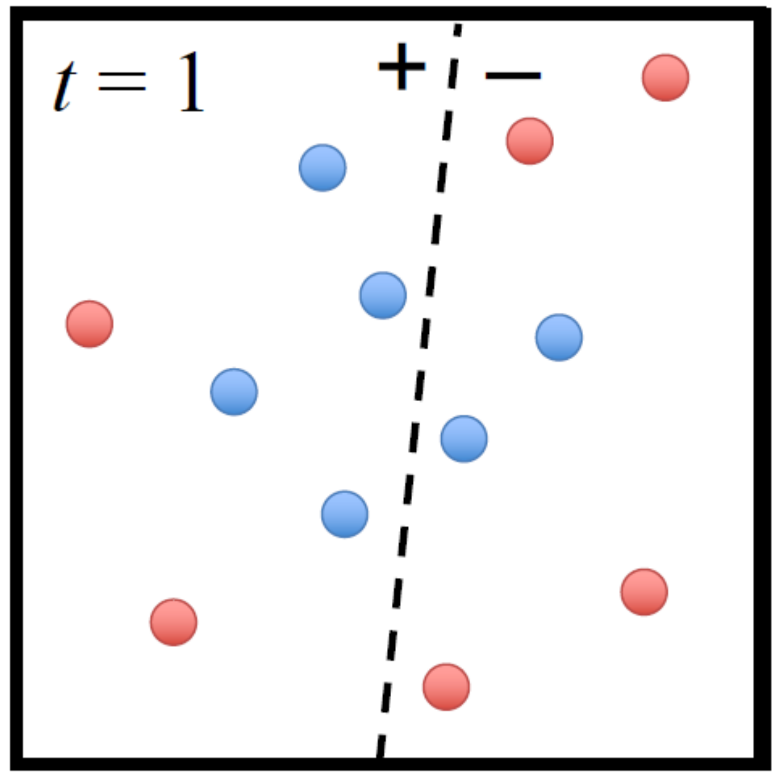
# AdaBoost

Initialize a vector of $n$ uniform weights $\mathbf{w}_1$
**for** $t = 1, \ldots, T$
    Train model $h_t$ on $X, y$ with weights $\mathbf{w}_t$
    Compute the weighted training error of $h_t$
    Choose $\beta_t = \frac{1}{2} \ln \left( \frac{1-\epsilon_t}{\epsilon_t} \right)$
    Update all instance weights:

$$w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\mathbf{x}_i)\right)$$

    Normalize $\mathbf{w}_{t+1}$ to be a distribution
**end for**
**Return** the hypothesis

$$H(\mathbf{x}) = \operatorname{sign}\left( \sum_{t=1}^{T} \beta_t h_t(\mathbf{x}) \right)$$



# Acknowledgements

- Slides made using resources from:
  - Andrew Ng
  - Eric Eaton
  - David Sontag
  - Andrew Moore
- Thanks!