# Data Mining

Ensemble Techniques

Introduction to Data Mining, 2nd Edition

by

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# Ensemble Methods

- Construct a set of base classifiers learned from the training data

- Predict class label of test records by combining the predictions made by multiple classifiers (e.g., by taking majority vote)

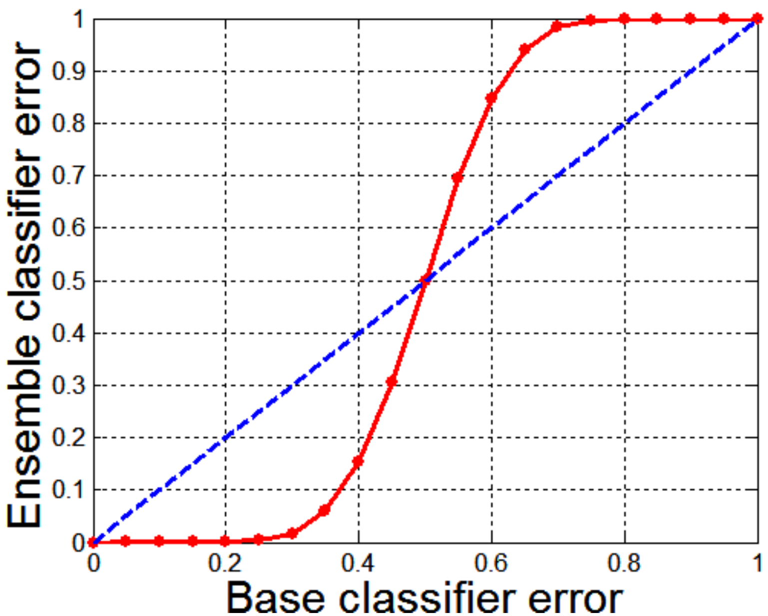
# Example: Why Do Ensemble Methods Work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate, $\epsilon$ = 0.35
  - Majority vote of classifiers used for classification
  - If all classifiers are identical:
    - Error rate of ensemble = $\epsilon$ (0.35)
  - If all classifiers are independent (errors are uncorrelated):
    - Error rate of ensemble = probability of having more than half of base classifiers being wrong

$$e_{\text{ensemble}} = \sum_{i=13}^{25} \binom{25}{i} \epsilon^i (1-\epsilon)^{25-i} = 0.06$$

# Necessary Conditions for Ensemble Methods

- Ensemble Methods work better than a single base classifier if:
  1. All base classifiers are independent of each other
  2. All base classifiers perform better than random guessing (error rate < 0.5 for binary classification)

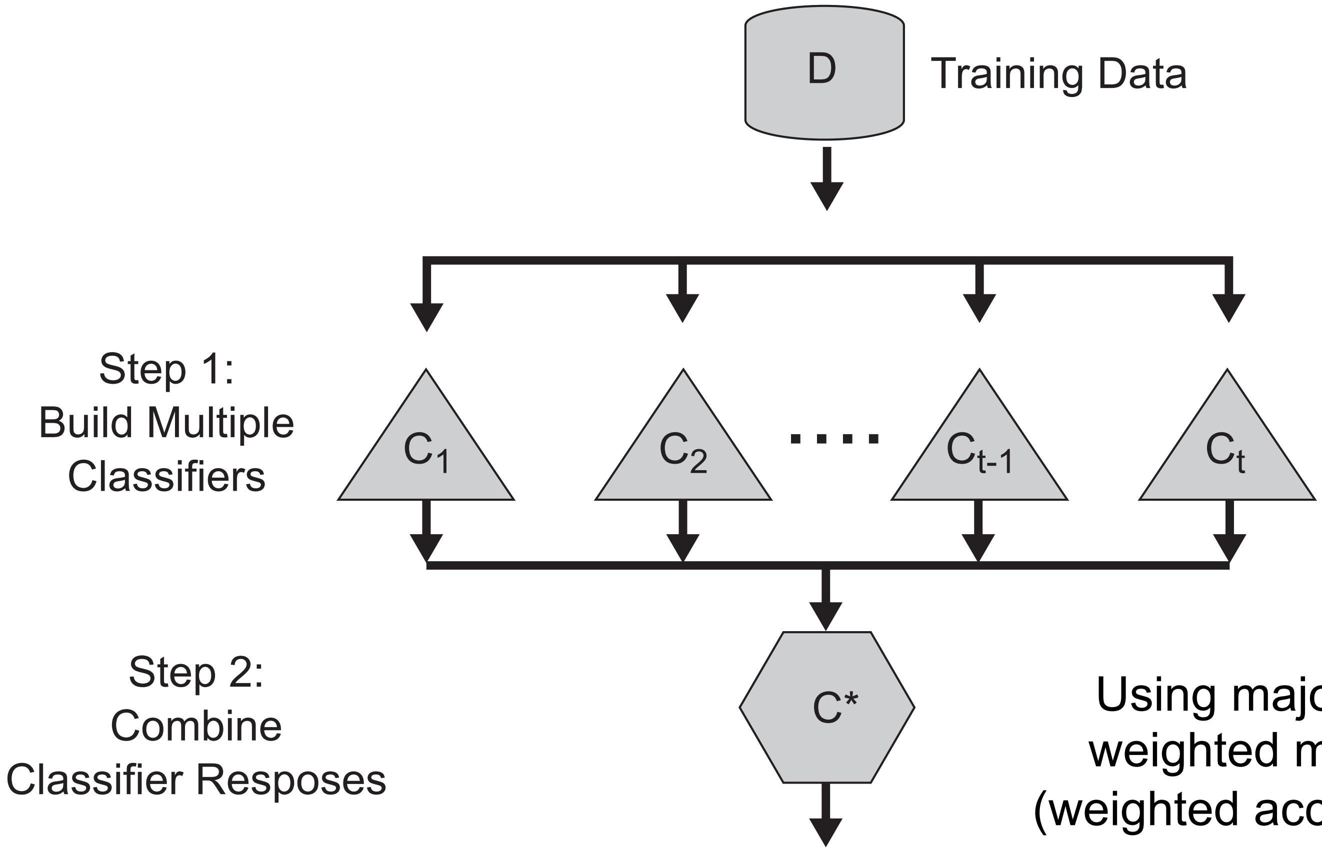



Classification error for an ensemble of 25 base classifiers, assuming their errors are uncorrelated.

# Rationale for Ensemble Learning

- Ensemble Methods work best with **unstable base classifiers**
  - Classifiers that are sensitive to minor perturbations in training set, due to *high model complexity*
  - Examples: Unpruned decision trees, ANNs, …

# General Approach of Ensemble Learning




Using majority vote or weighted majority vote (weighted according to their accuracy or relevance)

# Constructing Ensemble Classifiers

- By manipulating training set
  - Example: bagging, boosting, random forests
- By manipulating input features
  - Example: random forests
- By manipulating class labels
  - Example: error-correcting output coding
- By manipulating learning algorithm
  - Example: injecting randomness in the initial weights of ANN

# Bagging (Bootstrap AGGregatING)

- Bootstrap sampling: sampling with replacement

| **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 |

- Build classifier on each bootstrap sample

- Probability of a training instance being selected in a bootstrap sample is:
  - $1 - (1 - 1/n)^n$ (n: number of training instances)
  - ~0.632 when n is large

# Bagging Algorithm

**Algorithm 4.5** Bagging algorithm.

1: Let $k$ be the number of bootstrap samples.
2: **for** $i = 1$ to $k$ **do**
3: Create a bootstrap sample of size $N$, $D_i$.
4: Train a base classifier $C_i$ on the bootstrap sample $D_i$.
5: **end for**
6: $C^*(x) = \underset{y}{\operatorname{argmax}} \sum_i \delta\big(C_i(x) = y\big)$.
$\{\delta(\cdot) = 1$ if its argument is true and 0 otherwise.$\}$

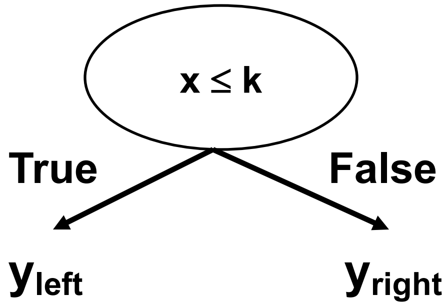
# Bagging Example

- Consider 1-dimensional data set:

**Original Data:**

| x | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1 |
|---|---|---|---|---|---|---|---|---|---|---|
| y | 1 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |

- Classifier is a decision stump (decision tree of size 1)
  - Decision rule: $x \leq k$ versus $x > k$
  - Split point k is chosen based on entropy



# Bagging Example

Bagging Round 1:

| x | 0.1 | 0.2 | 0.2 | 0.3 | 0.4 | 0.4 | 0.5 | 0.6 | 0.9 | 0.9 |
|---|---|---|---|---|---|---|---|---|---|---|
| y | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 |

**x <= 0.35 → y = 1**
**x > 0.35 → y = -1**

# Bagging Example

Bagging Round 1:

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| x | 0.1 | 0.2 | 0.2 | 0.3 | 0.4 | 0.4 | 0.5 | 0.6 | 0.9 | 0.9 |
| y | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 |

x <= 0.35 → y = 1
x > 0.35 → y = -1

Bagging Round 2:

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| x | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.5 | 0.9 | 1 | 1 | 1 |
| y | 1 | 1 | 1 | -1 | -1 | -1 | 1 | 1 | 1 | 1 |

x <= 0.7 → y = 1
x > 0.7 → y = 1

Bagging Round 3:

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| x | 0.1 | 0.2 | 0.3 | 0.4 | 0.4 | 0.5 | 0.7 | 0.7 | 0.8 | 0.9 |
| y | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 |

x <= 0.35 → y = 1
x > 0.35 → y = -1

Bagging Round 4:

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| x | 0.1 | 0.1 | 0.2 | 0.4 | 0.4 | 0.5 | 0.5 | 0.7 | 0.8 | 0.9 |
| y | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 |

x <= 0.3 → y = 1
x > 0.3 → y = -1

Bagging Round 5:

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| x | 0.1 | 0.1 | 0.2 | 0.5 | 0.6 | 0.6 | 0.6 | 1 | 1 | 1 |
| y | 1 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |

x <= 0.35 → y = 1
x > 0.35 → y = -1

# Bagging Example

Bagging Round 6:

| x | 0.2 | 0.4 | 0.5 | 0.6 | 0.7 | 0.7 | 0.7 | 0.8 | 0.9 | 1 |
|---|---|---|---|---|---|---|---|---|---|---|
| y | 1 | -1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |

x <= 0.75 → y = -1
x > 0.75 → y = 1

Bagging Round 7:

| x | 0.1 | 0.4 | 0.4 | 0.6 | 0.7 | 0.8 | 0.9 | 0.9 | 0.9 | 1 |
|---|---|---|---|---|---|---|---|---|---|---|
| y | 1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 | 1 | 1 |

x <= 0.75 → y = -1
x > 0.75 → y = 1

Bagging Round 8:

| x | 0.1 | 0.2 | 0.5 | 0.5 | 0.5 | 0.7 | 0.7 | 0.8 | 0.9 | 1 |
|---|---|---|---|---|---|---|---|---|---|---|
| y | 1 | 1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |

x <= 0.75 → y = -1
x > 0.75 → y = 1

Bagging Round 9:

| x | 0.1 | 0.3 | 0.4 | 0.4 | 0.6 | 0.7 | 0.7 | 0.8 | 1 | 1 |
|---|---|---|---|---|---|---|---|---|---|---|
| y | 1 | 1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |

x <= 0.75 → y = -1
x > 0.75 → y = 1

Bagging Round 10:

| x | 0.1 | 0.1 | 0.1 | 0.1 | 0.3 | 0.3 | 0.8 | 0.8 | 0.9 | 0.9 |
|---|---|---|---|---|---|---|---|---|---|---|
| y | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

x <= 0.05 → y = 1
x > 0.05 → y = 1

# Bagging Example

- Summary of Trained Decision Stumps:

| Round | Split Point | Left Class | Right Class |
|---|---|---|---|
| 1 | 0.35 | 1 | -1 |
| 2 | 0.7 | 1 | 1 |
| 3 | 0.35 | 1 | -1 |
| 4 | 0.3 | 1 | -1 |
| 5 | 0.35 | 1 | -1 |
| 6 | 0.75 | -1 | 1 |
| 7 | 0.75 | -1 | 1 |
| 8 | 0.75 | -1 | 1 |
| 9 | 0.75 | -1 | 1 |
| 10 | 0.05 | 1 | 1 |

# Bagging Example

- Use majority vote (sign of sum of predictions) to determine class of ensemble classifier

| Round | x=0.1 | x=0.2 | x=0.3 | x=0.4 | x=0.5 | x=0.6 | x=0.7 | x=0.8 | x=0.9 | x=1.0 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 3 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| 4 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| 5 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| 6 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |
| 7 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |
| 8 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |
| 9 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |
| 10 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Sum | 2 | 2 | 2 | -6 | -6 | -6 | -6 | 2 | 2 | 2 |
| Sign | 1 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |

**Predicted Class**

- Bagging can also increase the complexity (representation capacity) of simple classifiers such as decision stumps

# Boosting

- An iterative procedure to adaptively change distribution of training data by focusing more on previously misclassified records
  - Initially, all N records are assigned equal weights (for being selected for training)
  - Unlike bagging, weights may change at the end of each boosting round

# Boosting

- Records that are wrongly classified will have their weights increased in the next round
- Records that are classified correctly will have their weights decreased in the next round

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

- Example 4 is hard to classify
- Its weight is increased, therefore it is more likely to be chosen again in subsequent rounds

# AdaBoost

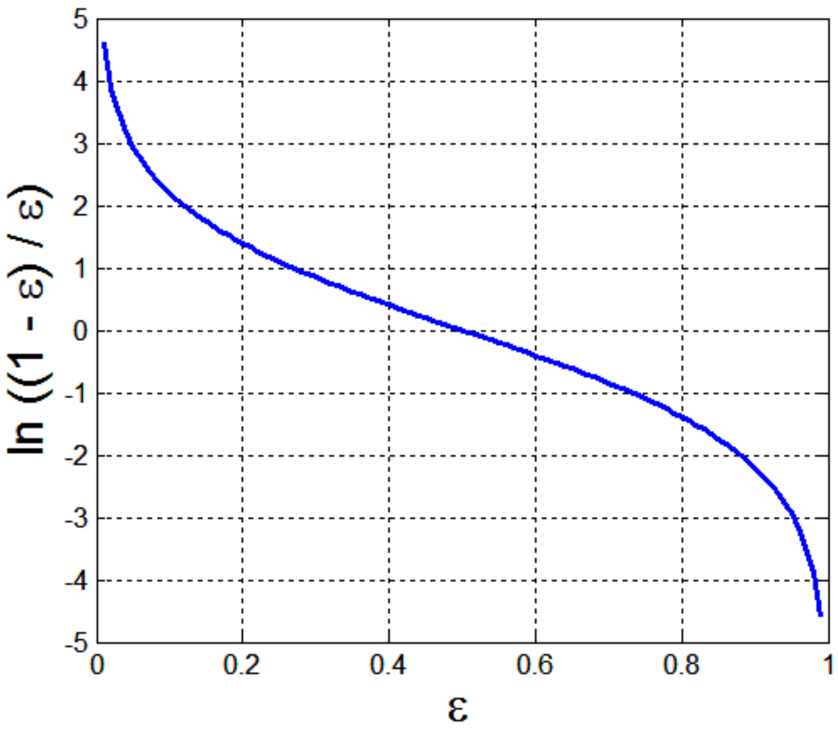
- Base classifiers: $C_1, C_2, \ldots, C_T$

- Error rate of a base classifier:

$$\epsilon_i = \frac{1}{N}\sum_{j=1}^{N} w_j^{(i)}\ \delta\left(C_i(x_j) \neq y_j\right)$$

- Importance of a classifier:

$$\alpha_i = \frac{1}{2}\ln\left(\frac{1-\varepsilon_i}{\varepsilon_i}\right)$$



# AdaBoost Algorithm

- Weight update:

$$w_j^{(i+1)} = \frac{w_j^{(i)}}{Z_i} \times \begin{cases} e^{-\alpha_i} & \text{if } C_i(x_j) = y_j \\ e^{\alpha_i} & \text{if } C_i(x_j) \neq y_j \end{cases}$$

Where $Z_i$ is the normalization factor

- If any intermediate rounds produce error rate higher than 50%, the weights are reverted back to 1/n and the resampling procedure is repeated
- Classification:

$$C^*(x) = \arg\max_y \sum_{i=1}^{T} \alpha_i \delta(C_i(x) = y)$$

# AdaBoost Algorithm

**Algorithm 4.6** AdaBoost algorithm.

1: $\mathbf{w} = \{w_j = 1/N \mid j = 1, 2, \ldots, N\}$. {Initialize the weights for all $N$ examples.}  
2: Let $k$ be the number of boosting rounds.  
3: **for** $i = 1$ to $k$ **do**  
4: Create training set $D_i$ by sampling (with replacement) from $D$ according to $\mathbf{w}$.  
5: Train a base classifier $C_i$ on $D_i$.  
6: Apply $C_i$ to all examples in the original training set, $D$.  
7: $\epsilon_i = \frac{1}{N}\left[\sum_j w_j \, \delta\big(C_i(x_j) \neq y_j\big)\right]$ {Calculate the weighted error.}  
8: **if** $\epsilon_i > 0.5$ **then**  
9: $\mathbf{w} = \{w_j = 1/N \mid j = 1, 2, \ldots, N\}$. {Reset the weights for all $N$ examples.}  
10: Go back to Step 4.  
11: **end if**  
12: $\alpha_i = \frac{1}{2} \ln \frac{1-\epsilon_i}{\epsilon_i}$.  
13: Update the weight of each example according to Equation 4.103.  
14: **end for**  
15: $C^*(\mathbf{x}) = \underset{y}{\operatorname{argmax}} \sum_{j=1}^{T} \alpha_j \delta(C_j(\mathbf{x}) = y)\big)$.

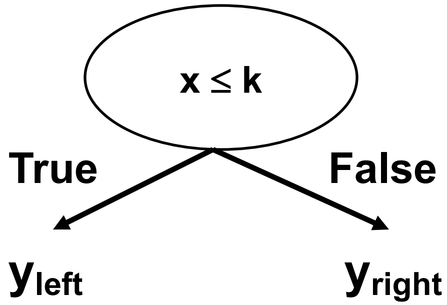
# AdaBoost Example

- Consider 1-dimensional data set:

**Original Data:**

| x | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1 |
|---|---|---|---|---|---|---|---|---|---|---|
| y | 1 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |

- Classifier is a decision stump
  - Decision rule: $x \le k$ versus $x > k$
  - Split point k is chosen based on entropy



# AdaBoost Example

- Training sets for the first 3 boosting rounds:

Boosting Round 1:

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **x** | **0.1** | **0.4** | **0.5** | **0.6** | **0.6** | **0.7** | **0.7** | **0.7** | **0.8** | **1** |
| **y** | **1** | **-1** | **-1** | **-1** | **-1** | **-1** | **-1** | **-1** | **1** | **1** |

Boosting Round 2:

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **x** | **0.1** | **0.1** | **0.2** | **0.2** | **0.2** | **0.2** | **0.3** | **0.3** | **0.3** | **0.3** |
| **y** | **1** | **1** | **1** | **1** | **1** | **1** | **1** | **1** | **1** | **1** |

Boosting Round 3:

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **x** | **0.2** | **0.2** | **0.4** | **0.4** | **0.4** | **0.4** | **0.5** | **0.6** | **0.6** | **0.7** |
| **y** | **1** | **1** | **-1** | **-1** | **-1** | **-1** | **-1** | **-1** | **-1** | **-1** |

- Summary:

| Round | Split Point | Left Class | Right Class | alpha |
|---|---|---|---|---|
| 1 | 0.75 | -1 | 1 | 1.738 |
| 2 | 0.05 | 1 | 1 | 2.7784 |
| 3 | 0.3 | 1 | -1 | 4.1195 |

# AdaBoost Example

- Weights

| Round | x=0.1 | x=0.2 | x=0.3 | x=0.4 | x=0.5 | x=0.6 | x=0.7 | x=0.8 | x=0.9 | x=1.0 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 |
| 2 | 0.311 | 0.311 | 0.311 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 |
| 3 | 0.029 | 0.029 | 0.029 | 0.228 | 0.228 | 0.228 | 0.228 | 0.009 | 0.009 | 0.009 |

- Classification

| Round | x=0.1 | x=0.2 | x=0.3 | x=0.4 | x=0.5 | x=0.6 | x=0.7 | x=0.8 | x=0.9 | x=1.0 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |
| 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 3 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| Sum | 5.16 | 5.16 | 5.16 | -3.08 | -3.08 | -3.08 | -3.08 | 0.397 | 0.397 | 0.397 |
| Sign | 1 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 |

**Predicted Class**

# Random Forest Algorithm

- Construct an ensemble of decision trees by manipulating training set as well as features
  - Use bootstrap sample to train every decision tree (similar to Bagging)
  - Use the following tree induction algorithm:
    - At every internal node of decision tree, randomly sample p attributes for selecting split criterion
    - Repeat this procedure until all leaves are pure (unpruned tree)

# Characteristics of Random Forest

- Base classifiers are unpruned trees and hence are *unstable classifiers*
- Base classifiers are *decorrelated* (due to randomization in training set as well as features)
- Random forests reduce variance of unstable classifiers without negatively impacting the bias
- Selection of hyper-parameter p
  - Small value ensures lack of correlation
  - High value promotes strong base classifiers
  - Common default choices: $\sqrt{d}, \ \log_2(d+1)$

# Gradient Boosting

- Constructs a series of models
  - Models can be any predictive model that has a differentiable loss function
  - Commonly, trees are the chosen model
    - XGboost (extreme gradient boosting) is a popular package because of its impressive performance
- Boosting can be viewed as optimizing the loss function by iterative functional gradient descent.
- Implementations of various boosted algorithms are available in Python, R, Matlab, and more.