Artificial Intelligence for Medicine II

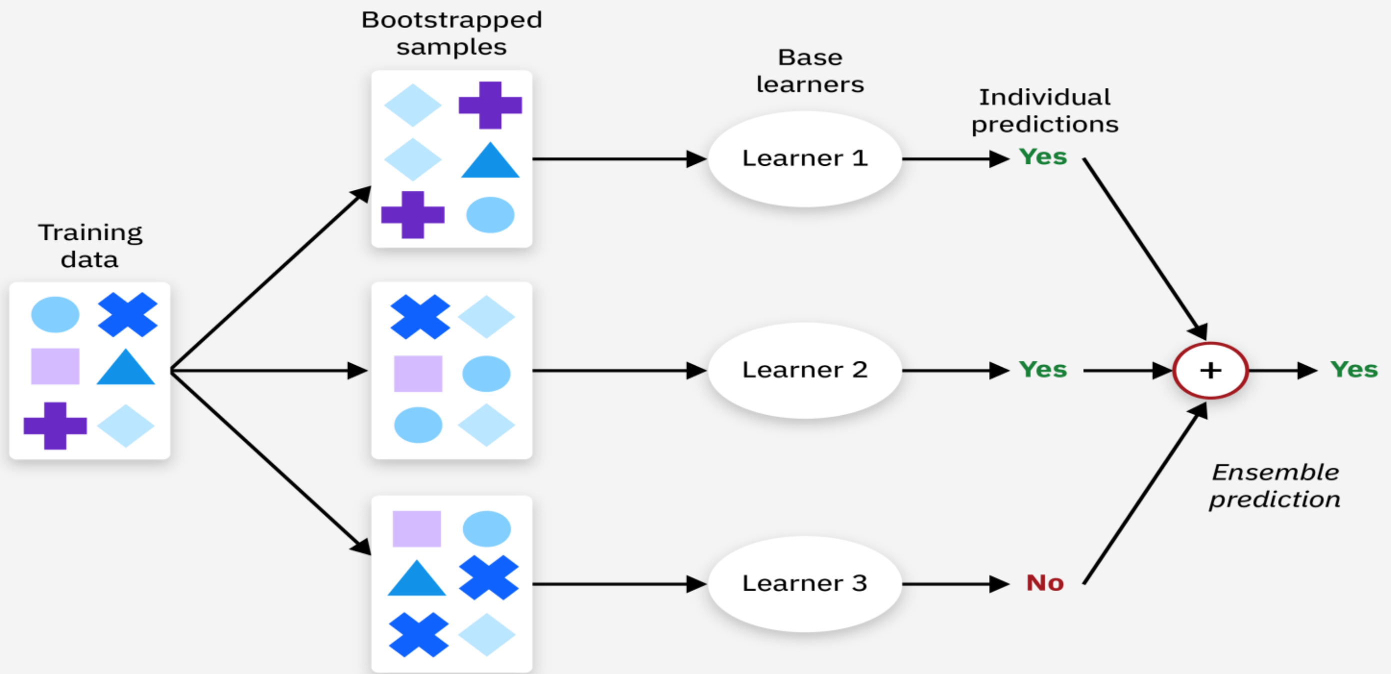
Spring 2025

Lecture 62: Supervised Learning
ENSEMBLE LEARNING

(Many slides adapted from Bing Liu, Han, Kamber & Pei; Tan, Steinbach, Kumar and the web)

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)



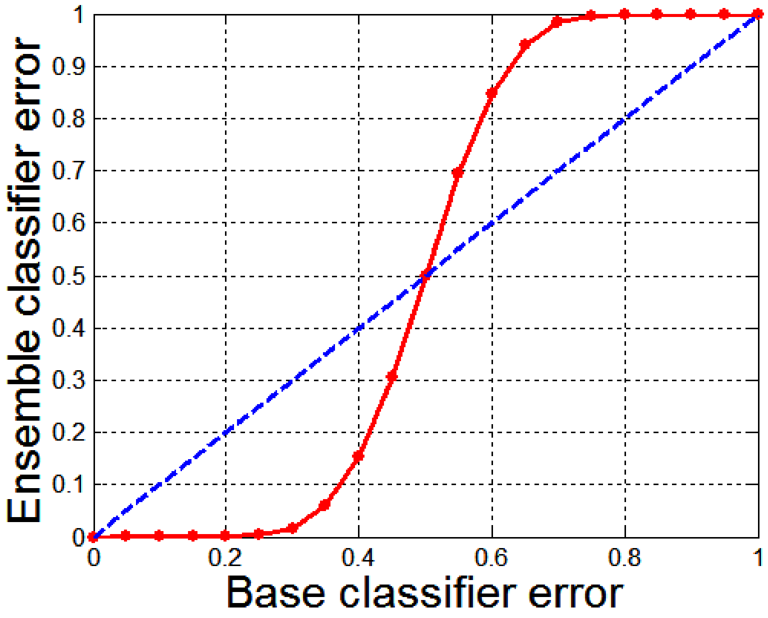
Example: Why Do Ensemble Methods Work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate, ϵ = 0.35
  - Majority vote of classifiers used for classification
  - If all classifiers are identical:
    - Error rate of ensemble = ϵ (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, …

The bias-variance problem

- The bias-variance problem is a fundamental issue in machine learning and statistics, particularly in the context of supervised learning. It involves finding the right balance between two types of errors that can affect the performance of a model:

- **Bias:** This error occurs when a model makes overly simplistic assumptions about the data, leading to underfitting. High bias means the model is not flexible enough to capture the underlying patterns in the data.

- **Variance**: This error happens when a model is too sensitive to small fluctuations in the training data, leading to overfitting. High variance means the model captures noise in the training data rather than the actual patterns.

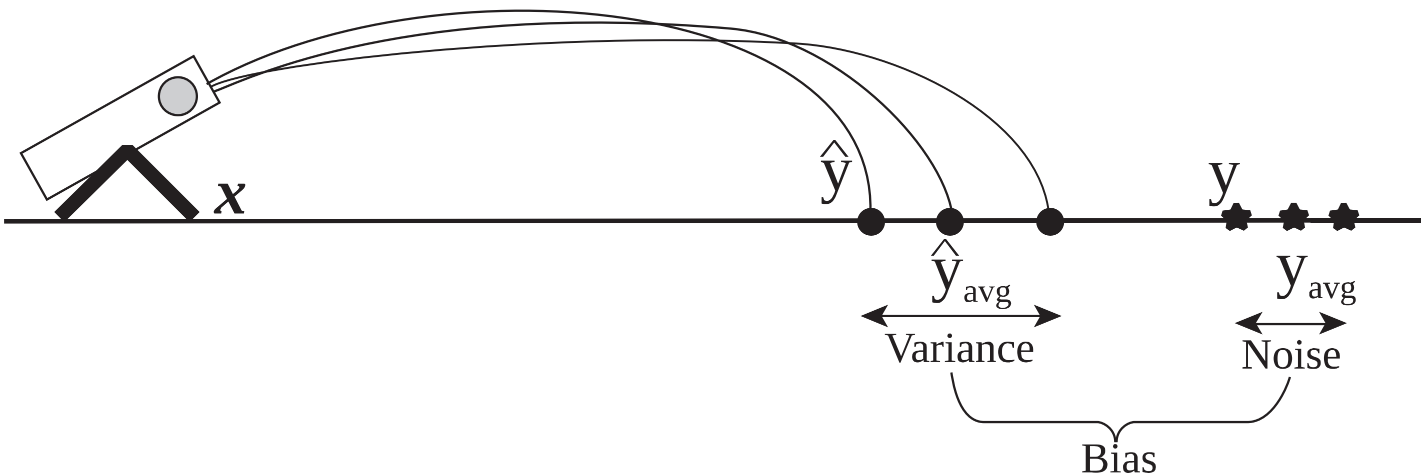
- The goal is to find a balance between bias and variance to achieve optimal model performance. This is known as the bias-variance tradeoff. A model with low bias and low variance is ideal, but in practice, achieving this balance can be challenging.

Bias and Variance Error

- **Error due to Bias**: The error due to bias is taken as the difference between the expected (or average) prediction of our model and the correct value which we are trying to predict.
  - Of course, you only have one model so talking about expected or average prediction values might seem a little strange. However, imagine you could repeat the whole model building process more than once: each time you gather new data and run a new analysis creating a new model. Due to randomness in the underlying data sets, the resulting models will have a range of predictions. Bias measures how far off in general these models' predictions are from the correct value.
- **Error due to Variance**: The error due to variance is taken as the variability of a model prediction for a given data point.
  - Again, imagine you can repeat the entire model building process multiple times. The variance is how much the predictions for a given point vary between different realizations of the model.

Bias-Variance Decomposition

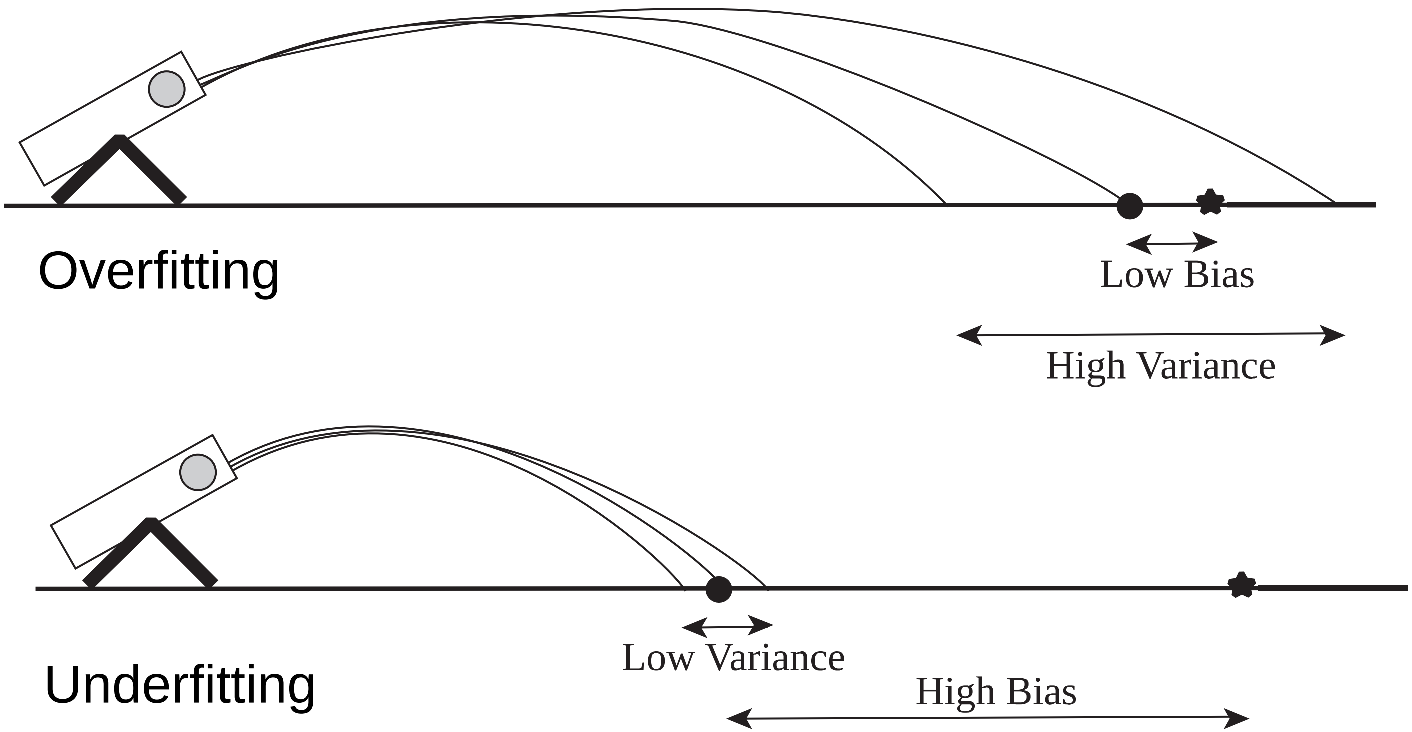
- Analogous problem of reaching a target y by firing projectiles from x (regression problem)



- For classification, the generalization error of model m can be given by:

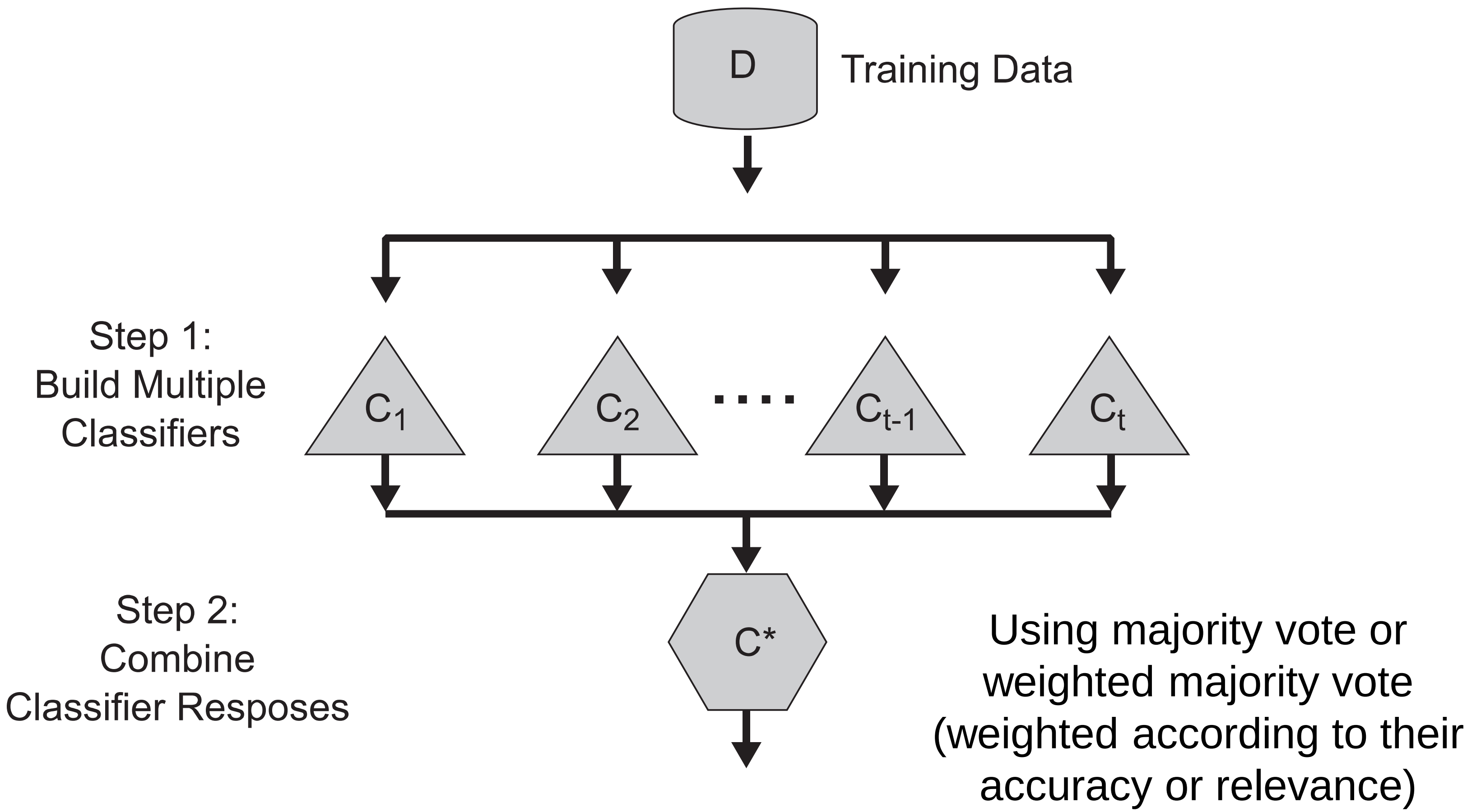
$$gen.error(m) = c_1 + bias(m) + c_2 \times variance(m)$$

Bias-Variance Trade-off and Overfitting



- Ensemble methods try to reduce the variance of complex models (with low bias) by *aggregating* responses of multiple base classifiers

General Approach of Ensemble Learning



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.

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

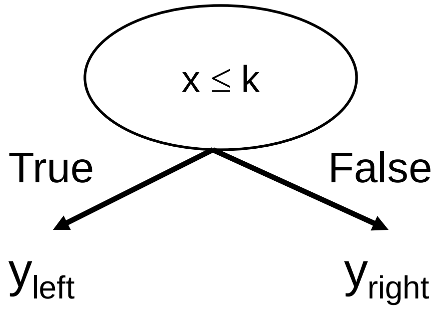
Bagging Example

- 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

AdaBoost (short for Adaptive Boosting) is a machine learning meta-algorithm developed by Yoav Freund and Robert Schapire in 1995. It isused to improve the performance of other learning algorithms by combining multiple weak learners into a strong classifier.

Here's how AdaBoost works:

1. **Initialization**: Start with equal weights for all training samples.
2. **Training**: Train a weak learner (e.g., a decision stump) on the weighted training data.
3. **Weight Update**: Increase the weights of misclassified samples so that the next weak learner focuses more on these difficult cases.
4. **Combination**: Combine the outputs of all weak learners into a final strong classifier, typically using a weighted sum.

AdaBoost is adaptive because it adjusts the weights of the training samples based on the errors of previous learners. This process helps the algorithm to focus on harder-to-classify examples.

AdaBoost

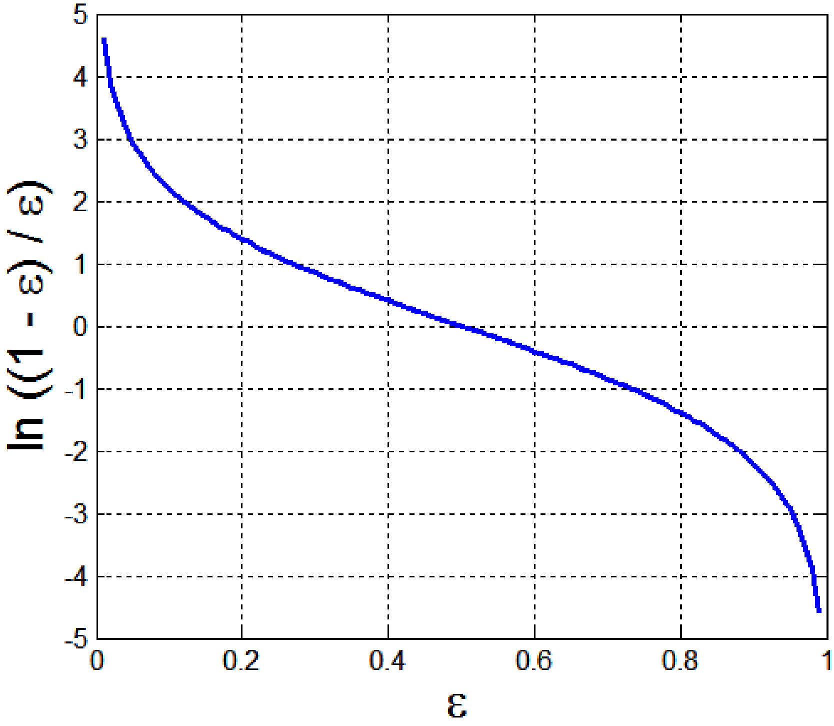
- Base classifiers: $C_1, C_2, \ldots, C_T$

- Error rate of a base classifier:

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

- 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: $C^*(\mathbf{x}) = \underset{y}{\operatorname{argmax}} \sum_{j=1}^{T} \alpha_j \delta\big(C_j(\mathbf{x}) = y\big)$.

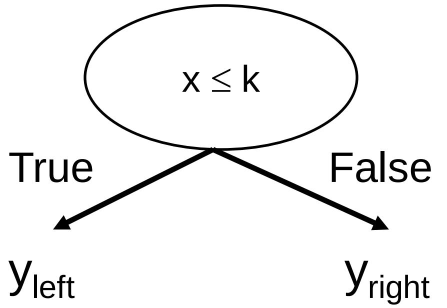
AdaBoost Example

- 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

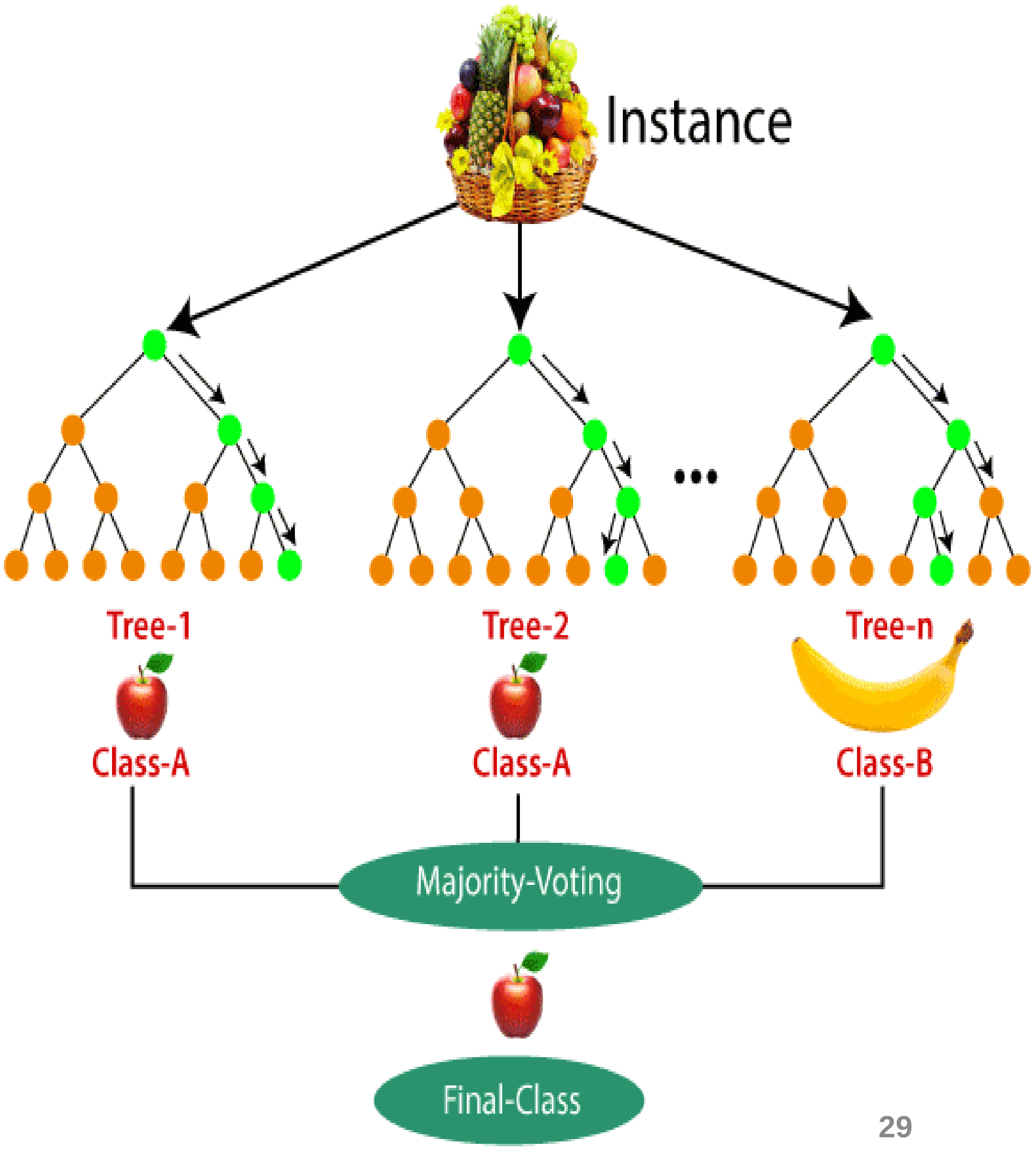
- Classification

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)

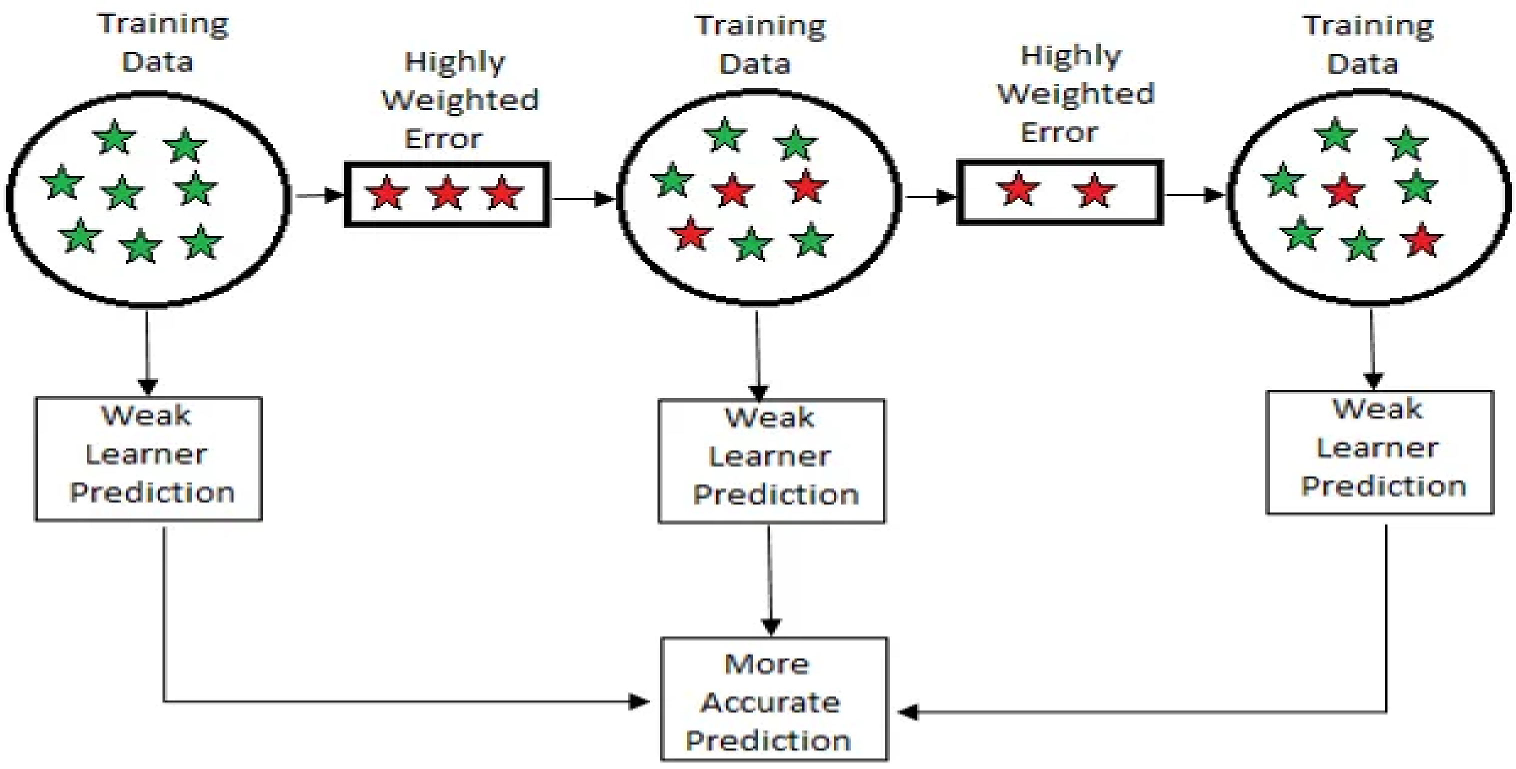


Characteristics of Random Forest

- 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



Gradient Boosting

Gradient boosting is a powerful machine learning technique used to create predictive models. It works by combining multiple weak learners, typically decision trees, into a single strong learner. Here are some key points about gradient boosting:

1. **Boosting Method**: Gradient boosting is a type of boosting method that iteratively improves the model by minimizing a loss function.
2. **Weak Learners**: It uses weak learners, which are models that perform slightly better than random guessing. Decision trees are commonly used as weak learners.
3. **Applications**: Gradient boosting can be applied to various tasks such as regression, classification, ranking, and survival analysis.
4. **Libraries**: Popular libraries for implementing gradient boosting include XGBoost and LightGBM.

Implementations of various boosted algorithms are available in Python, R, Matlab, and more.