Ensemble Methods

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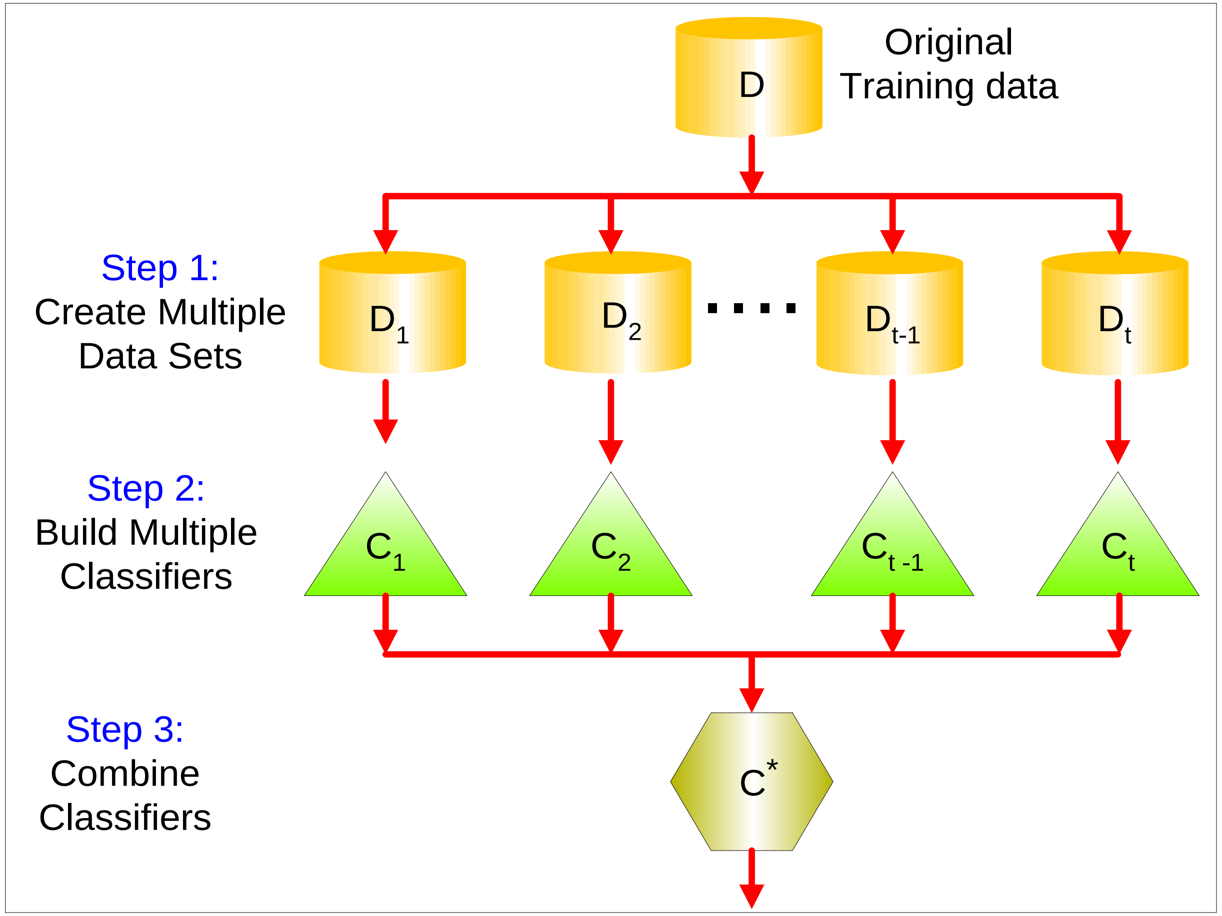
Ensemble Methods

- Improves the accuracy by **aggregating the predictions** of multiple classifiers.
- Construct a set of **base classifiers** from the training data.
- Predict class label of test records by combining the predictions made by multiple classifiers.



Back to Machine Learning

It will exploit *Wisdom of crowd* ideas for specific tasks

- By combining classifier predictions and
- aims to combine independent and diverse classifiers.

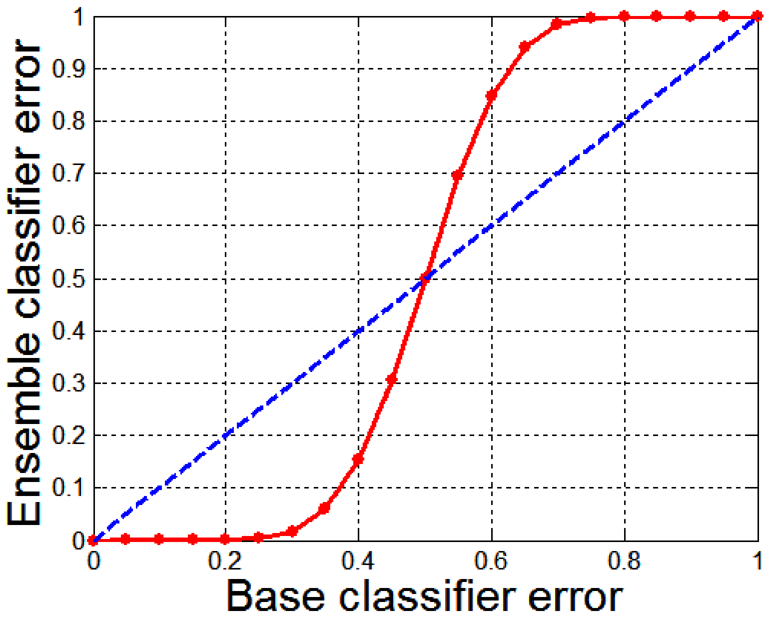
But it will use labelled training data

- to identify the **expert** classifiers in the pool;
- to identify **complementary** classifiers;
- to indicate how to the best **combine** them.

Why Ensemble Methods work?

Suppose there are 25 base classifiers

- Each classifier has error rate, ε = 0.35
- Assume errors made by classifiers are uncorrelated
- Probability that the ensemble classifier makes a wrong prediction:



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

Types of Ensemble Methods

- Manipulate data distribution
  - Example: bagging, boosting
- Manipulate input features
  - Example: random forests
- Manipulate class labels
  - Example: error-correcting output coding

Bagging

Bagging (a.k.a. Bootstrap AGGregatING)

- 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
- Each sample has probability (1 – 1/n)n of being selected

Algorithm 5.6 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) = argmax_y Σ_i δ(C_i(x) = y), {δ(·) = 1 if its argument is true, and 0 otherwise.}
```

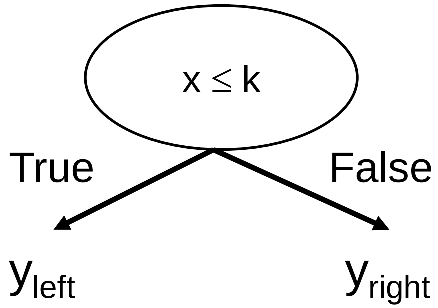
Bagging Example

- 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 rule: x <= 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 Training sets:

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

- Assume test set is the same as the original data
- Use majority vote 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

Boosting

Boosting

- An iterative procedure to adaptively change distribution of training data by focusing more on previously misclassified records.

- Initially, all the records are assigned equal weights.

- Unlike bagging, weights may change at the end of each boosting round.

Boosting

- Records that are wrongly classified will have their weights increased.
- Records that are classified correctly will have their weights decreased.

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

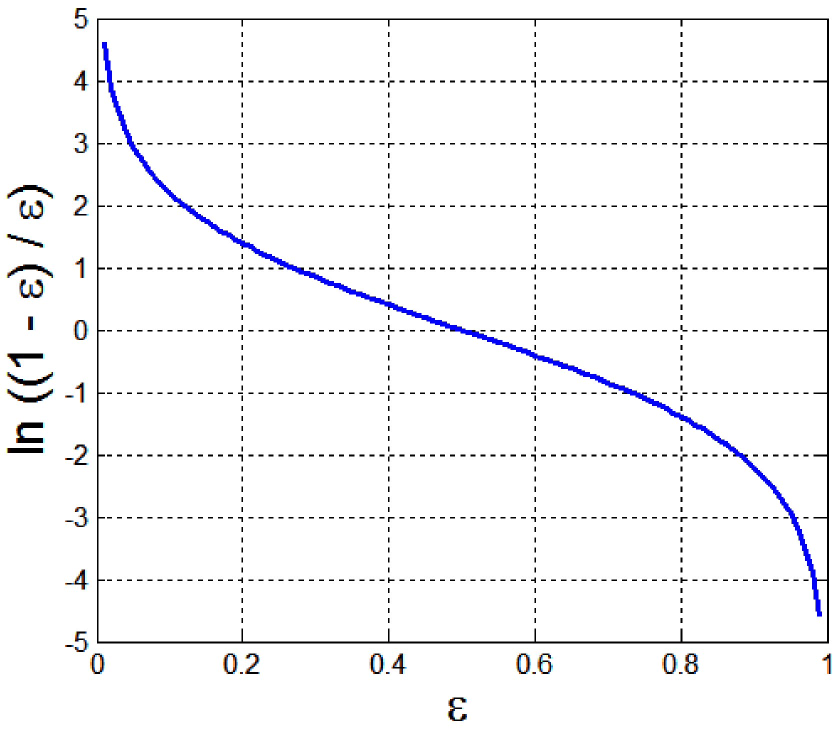
AdaBoost

- Base classifiers: C_1, C_2, …, C_T
- Error rate:

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

- Importance of a classifier depends on its error rate:

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



High positive importance when error is close to 0,
High negative importance when error is close to 1

AdaBoost Algorithm

- Weight update:

Weight associated to x_i during the j boosting round

$$w_i^{(j+1)} = \frac{w_i^{(j)}}{Z_j} \begin{cases} \exp^{-\alpha_j} & \text{if } C_j(x_i) = y_i \\ \exp^{\alpha_j} & \text{if } C_j(x_i) \neq y_i \end{cases}$$

where Z_j 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:

$$C^*(x) = \arg\max_y \sum_{j=1}^{T} \alpha_j \delta\big(C_j(x) = y\big)$$

AdaBoost Algorithm

Algorithm 5.7 AdaBoost Algorithm

1: $\mathbf{w} = \{w_j = 1/n \mid j = 1, 2, \cdots, n\}$. {Initialize the weights for all n instances.}
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 instances 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: $\mathbf{w} = \{w_j = 1/n \mid j = 1, 2, \cdots, n\}$. {Reset the weights for all n instances.}
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 instance according to equation (5.88).
14: **end for**
15: $C^*(\mathbf{x}) = \arg\max_y \sum_{j=1}^{T} \alpha_j \delta(C_j(\mathbf{x}) = y)$.

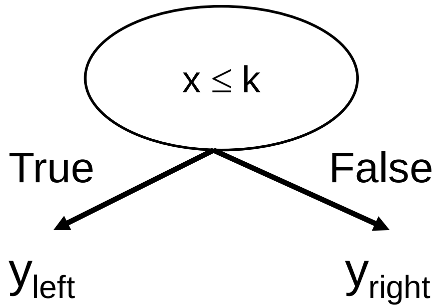
AdaBoost Example

- 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: $x \leq k$ 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

- 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

AdaBoost Example

- 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

- Classification

$$C^*(x) = \arg\max_{y} \sum_{j=1}^{T} \alpha_j \delta\left(C_j(x) = y\right)$$

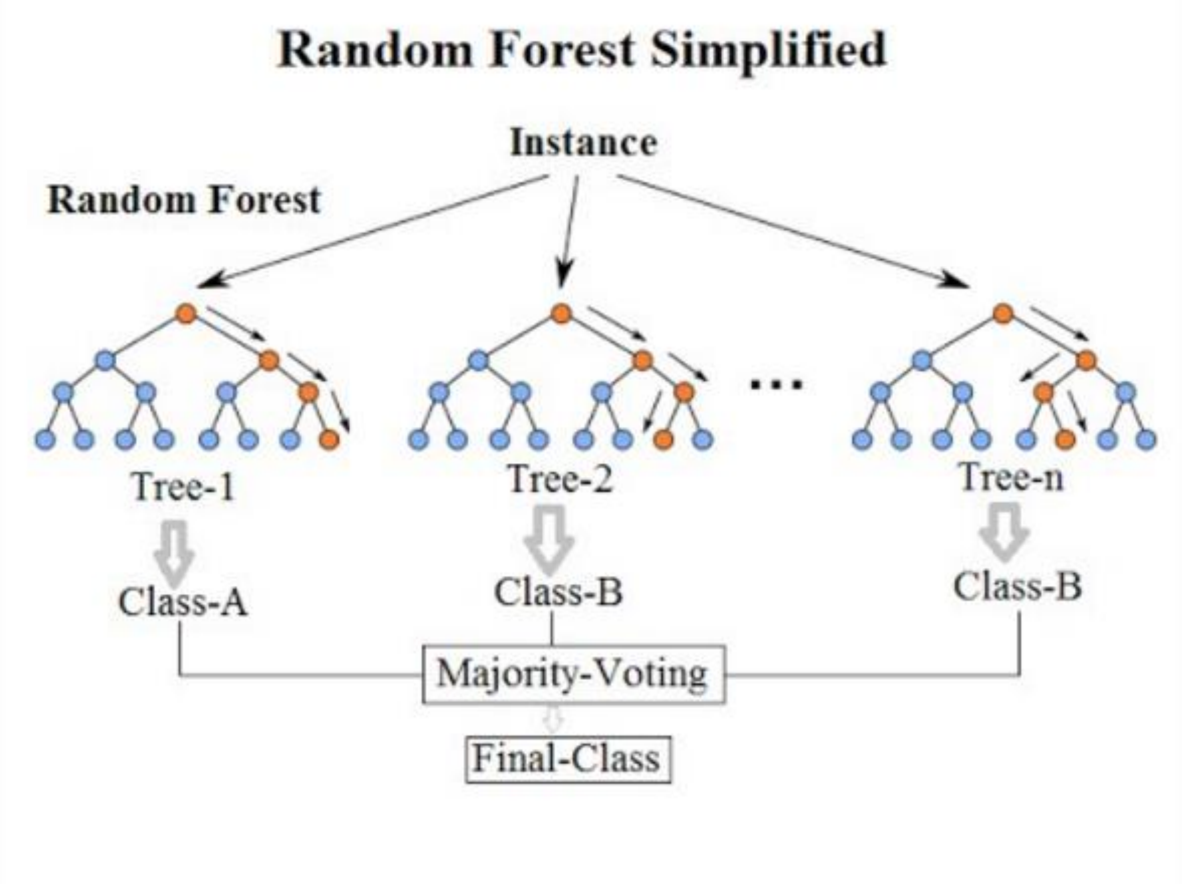
Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	-1	-1	-1	-1	-1	-1	-1	1	1	1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	-1	-1	-1	-1	-1	-1	-1
Sum	5.16	5.16	5.16	-3.08	-3.08	-3.08	-3.08	0.397	0.397	0.397
Sign	1	1	1	-1	-1	-1	-1	1	1	1

Predicted Class

Random Forests

Random Forests

- Is a class of ensemble methods specifically designed for **decision trees**.
- It combines the predictions made by multiple decision trees and outputs the class that **is the mode of the class's output** by individual trees.



Random Forest

- Each decision tree is built on a **bootstrap sample** based on the values of an **independent** set of random vectors.
  - Unlike AdaBost, the random vector are generated from a fixed probability distribution.
  - Bagging using decision trees is a special case of random forests where randomness is injected into the model-building process.
- Each decision tree is evaluated among ***m*** **randomly chosen attributes** from the M available attributes
  - m ~ $\sqrt{M}$ or m ~ $\log M$+1

Random Forest - Advantages

- It is one of the most accurate learning algorithms available. For many data sets, it produces a high accurate classifier.
- It runs efficiently on large databases.
- 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.

References

- Ensemble Methods. Chapter 5.6. Introduction to Data Mining.