Data Mining

Ensemble Techniques

Introduction to Data Mining, 2nd Edition

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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?

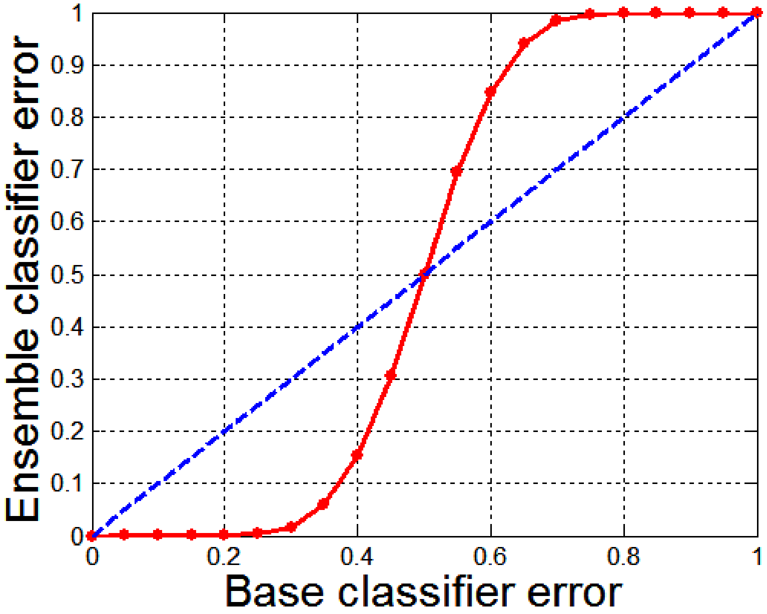
- Suppose there are 25 base classifiers
  - Each classifier has error rate, $\epsilon = 0.35$
  - Majority vote of classifiers used for classification
  - If all classifiers are identical:
    - Error rate of ensemble = ϵ (0.35)
  - If all classifiers are independent (errors are uncorrelated):
    - 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.

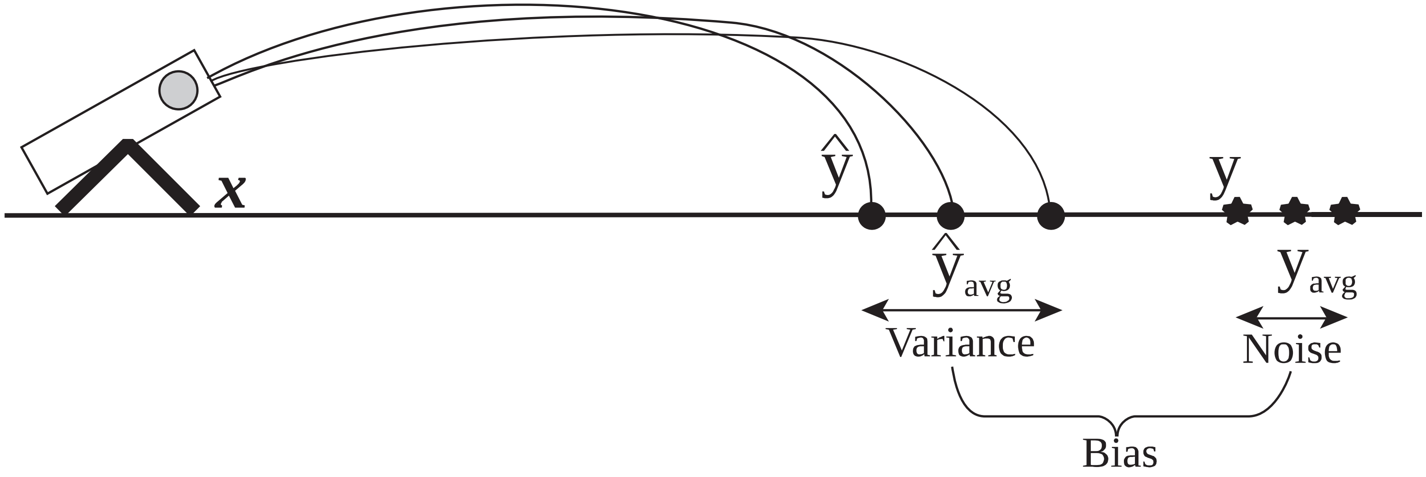
Rationale for Ensemble Learning

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, …

Bias-Variance Decomposition

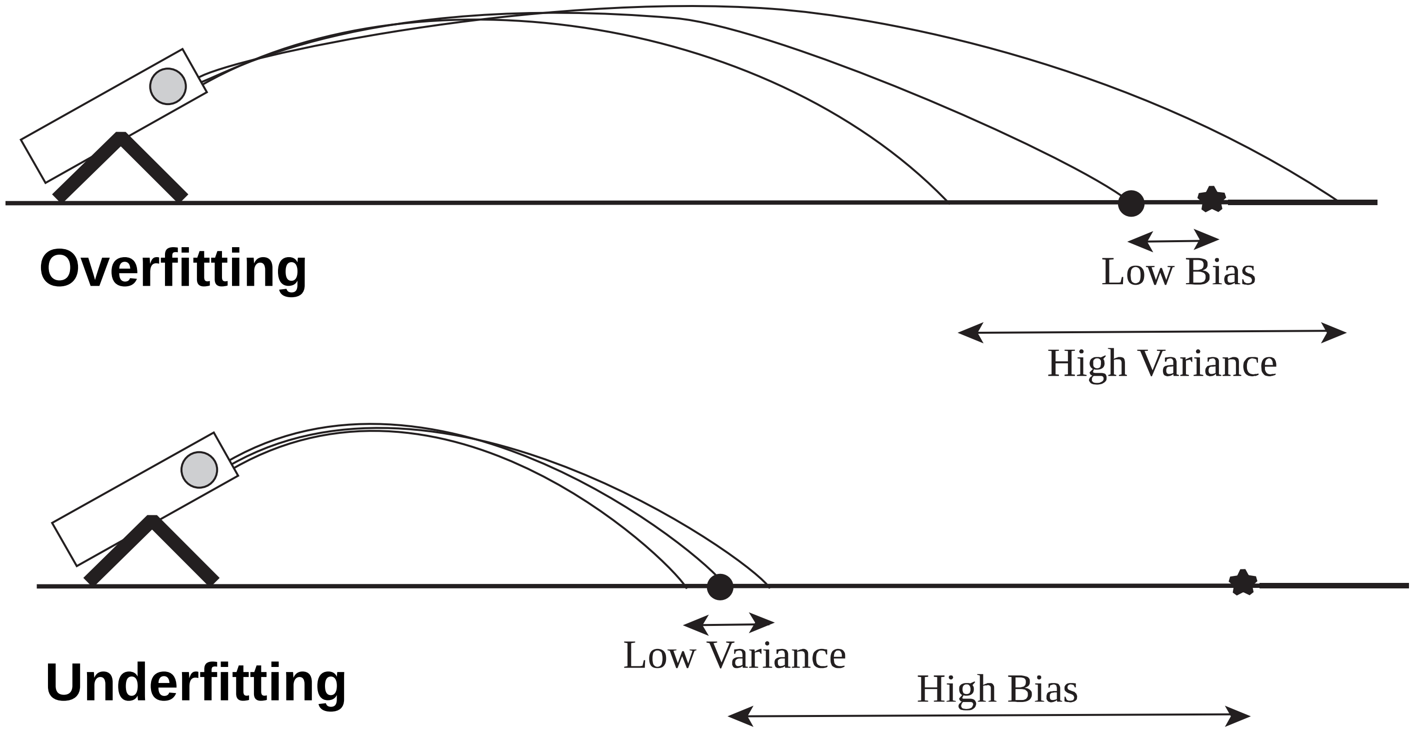
Analogous problem of reaching a target y by firing projectiles from x (regression problem)



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

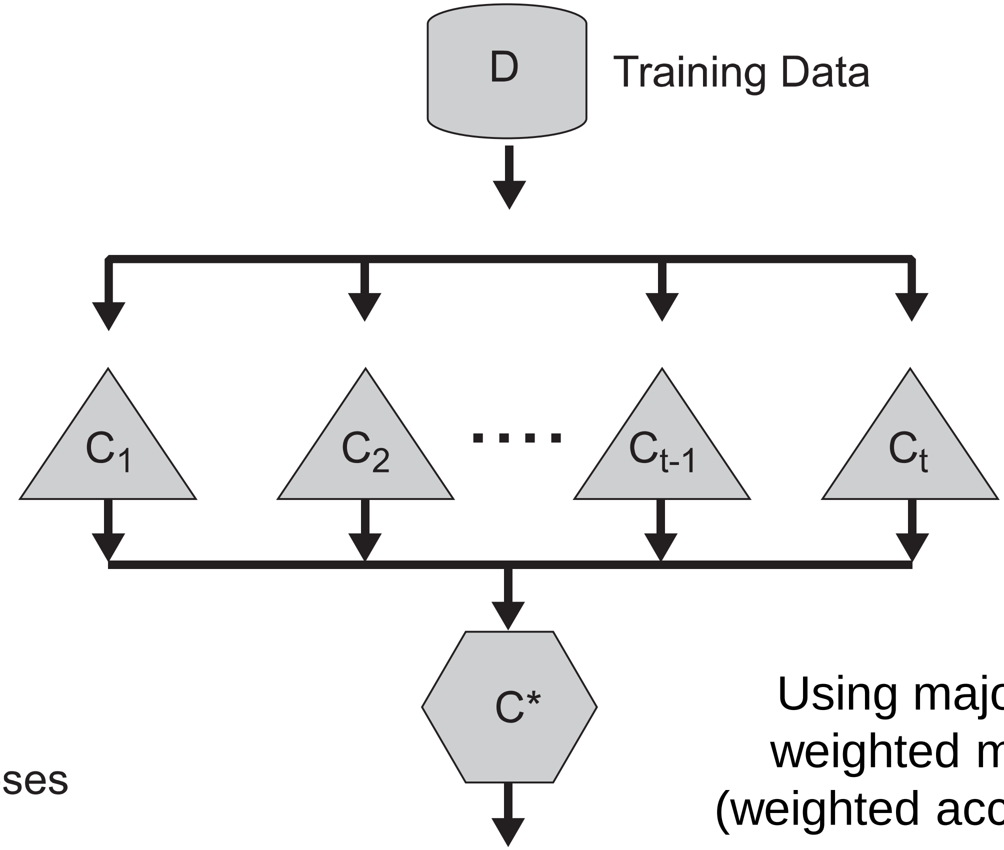
$$gen.error(m) = c_1 + bias(m) + c_2 \times variance(m)$$

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



D

Training Data

Step 1:
Build Multiple
Classifiers

C_1 C_2 .... C_{t-1} C_t

Step 2:
Combine
Classifier Resposes

C*

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

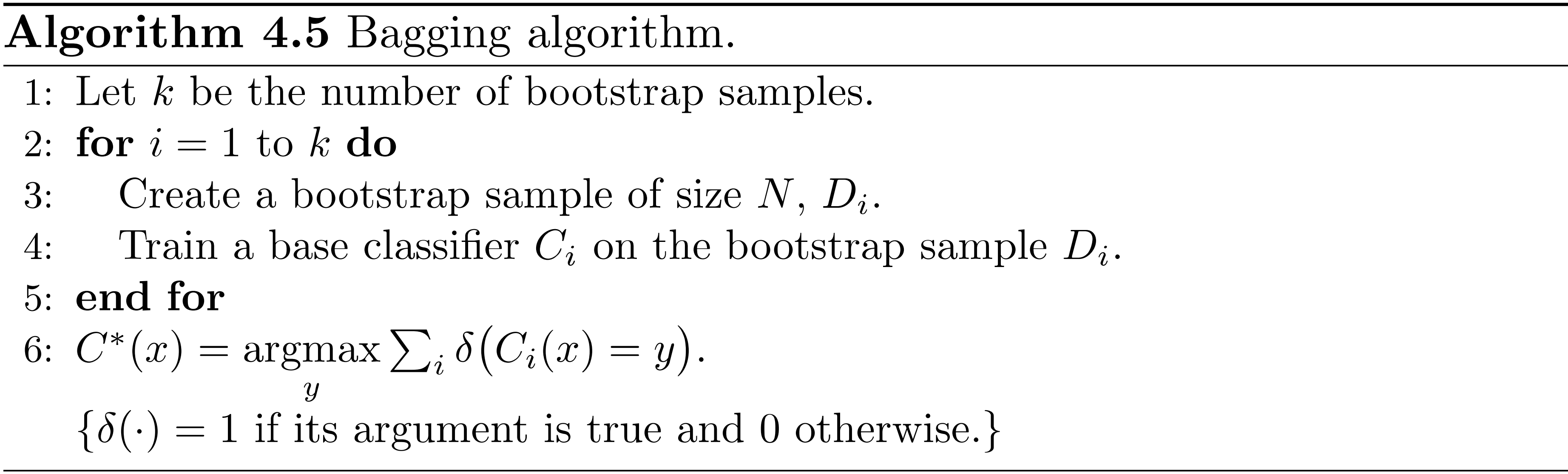
Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

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.

```
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

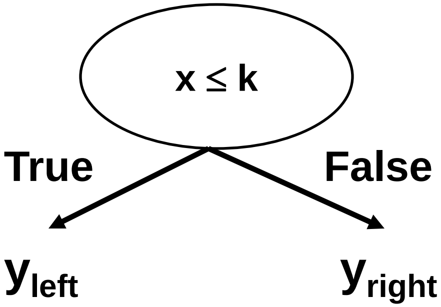
Consider 1-dimensional data set:

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: $x \le k$ 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

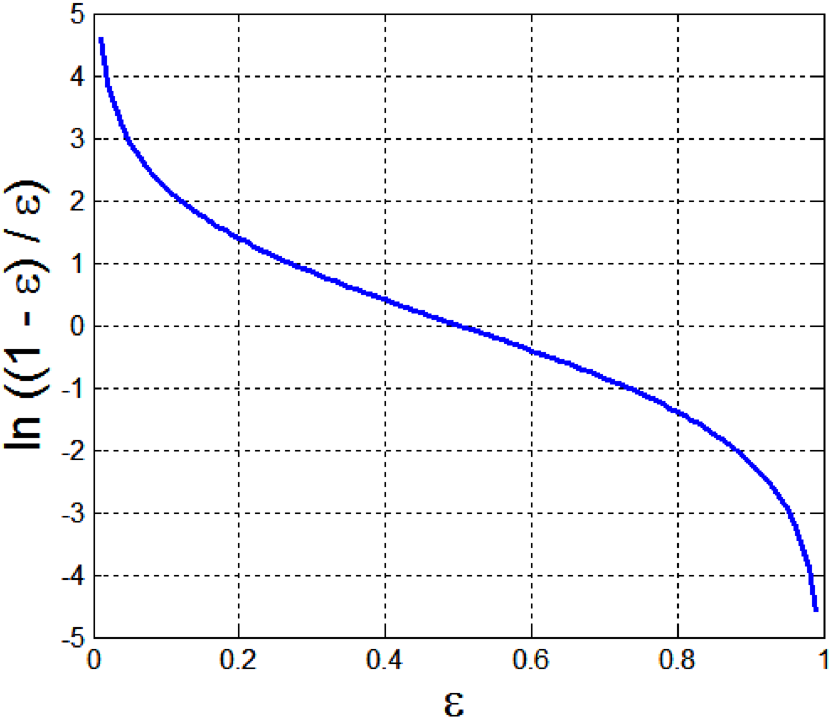
Base classifiers: $C_1, C_2, \ldots, C_T$

Error rate of a base classifier:

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

Importance of a classifier:

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



AdaBoost Algorithm

Weight update:

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

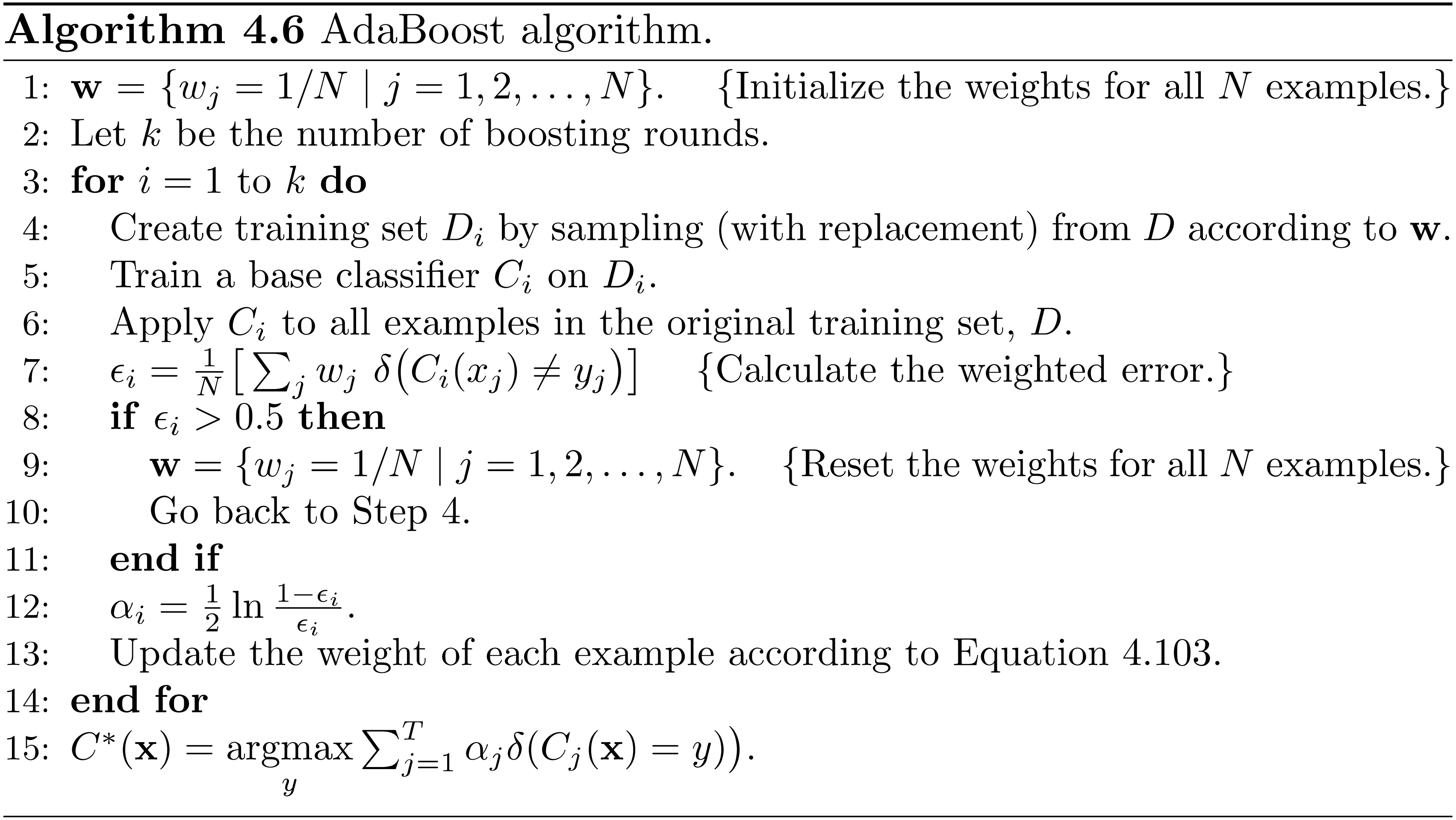
Where Z_i is the normalization factor

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

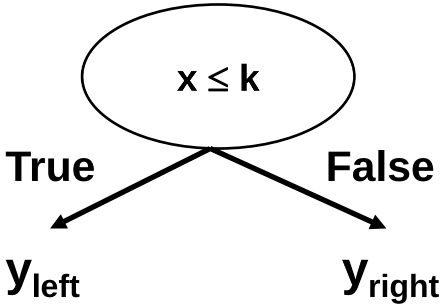
Consider 1-dimensional data set:

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: $x \leq k$ 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

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.