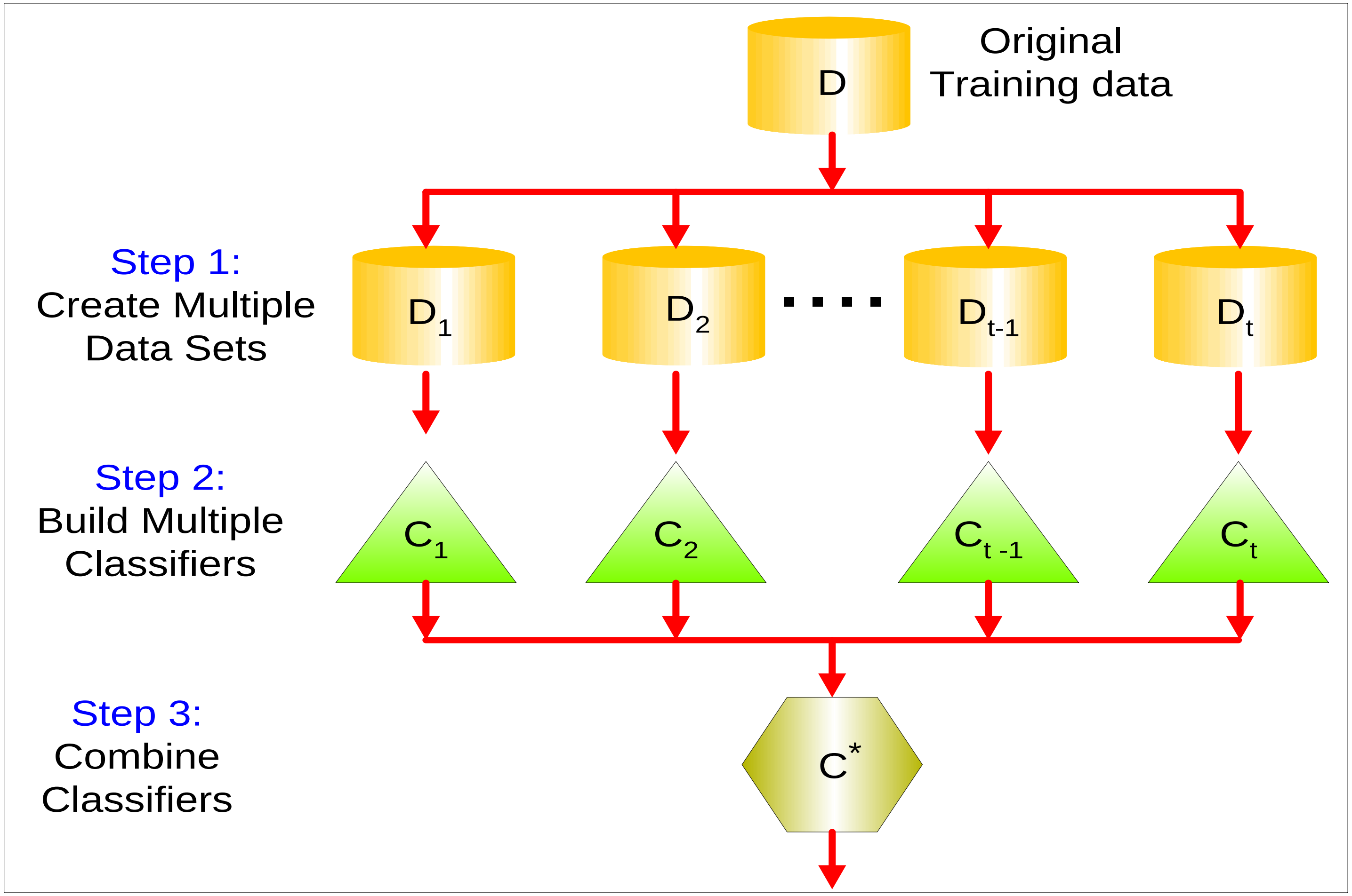
Ensemble Learning: An Introduction

Adapted from Slides by Tan, Steinbach, Kumar

General Idea



Why does it work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate, $\varepsilon = 0.35$
  - Assume classifiers are independent
  - Probability that the ensemble classifier makes a wrong prediction:

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

Examples of Ensemble Methods

- How to generate an ensemble of classifiers?
  - Bagging

  - Boosting

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

- Build classifier on each bootstrap sample
- Each sample has probability $(1 – 1/n)^n$ of being selected as test data
- Training data = 1- $(1 – 1/n)^n$ of the original data

The 0.632 bootstrap

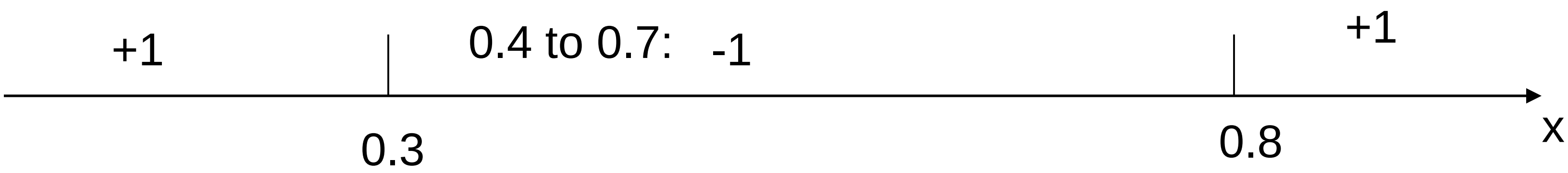
- This method is also called the *0.632 bootstrap*
  - A particular training data has a probability of 1-1/*n* of *not* being picked
  - Thus its probability of ending up in the test data (not selected) is:

$$\left(1-\frac{1}{n}\right)^{n} \approx e^{-1} = 0.368$$

  - This means the training data will contain approximately 63.2% of the instances

Example of Bagging

Assume that the training data is:



Goal: find a collection of 10 simple thresholding classifiers that collectively can classify correctly.
-Each simple (or weak) classifier is:
(x<=K → class = +1 or -1 depending on which value yields the lowest error; where K is determined by entropy minimization)

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	0.8	0.9	1	1	1
y	1	1	1	-1	-1	1	1	1	1	1

x <= 0.65 ==> y = 1
x > 0.65 ==> 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 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

Figure 5.35. Example of bagging.

Bagging (applied to training data)

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
True Class	1	1	1	-1	-1	-1	-1	1	1	1

Figure 5.36. Example of combining classifiers constructed using the bagging approach.

Accuracy of ensemble classifier: 100% ☺

Bagging- Summary

- Works well if the base classifiers are unstable (complement each other)
- Increased accuracy because it ***reduces the variance*** of the individual classifier
- Does not focus on any particular instance of the training data
  - Therefore, less susceptible to model over-fitting when applied to noisy data
- What if we want to focus on a particular instances of training data?

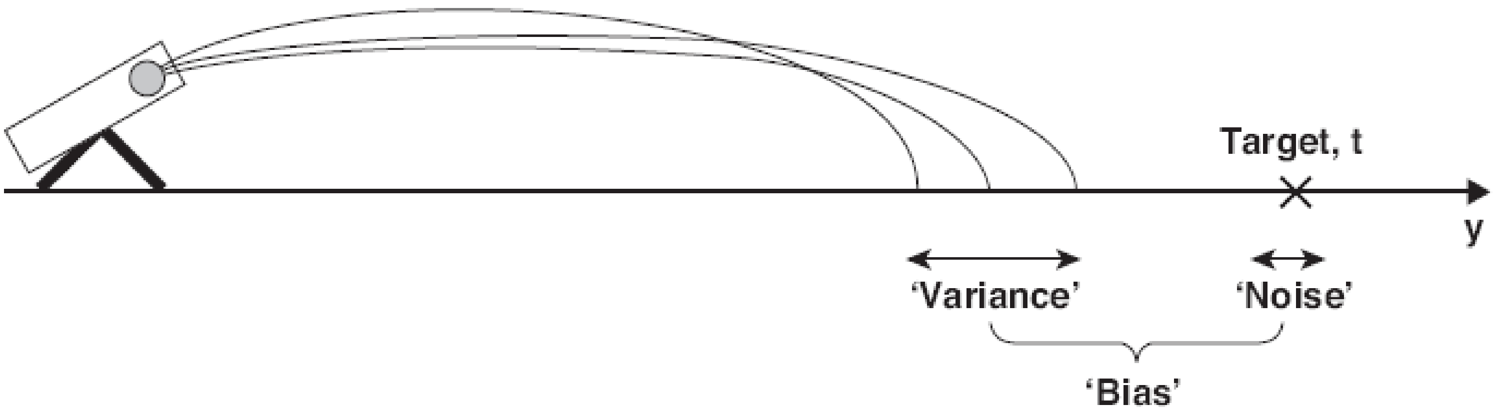
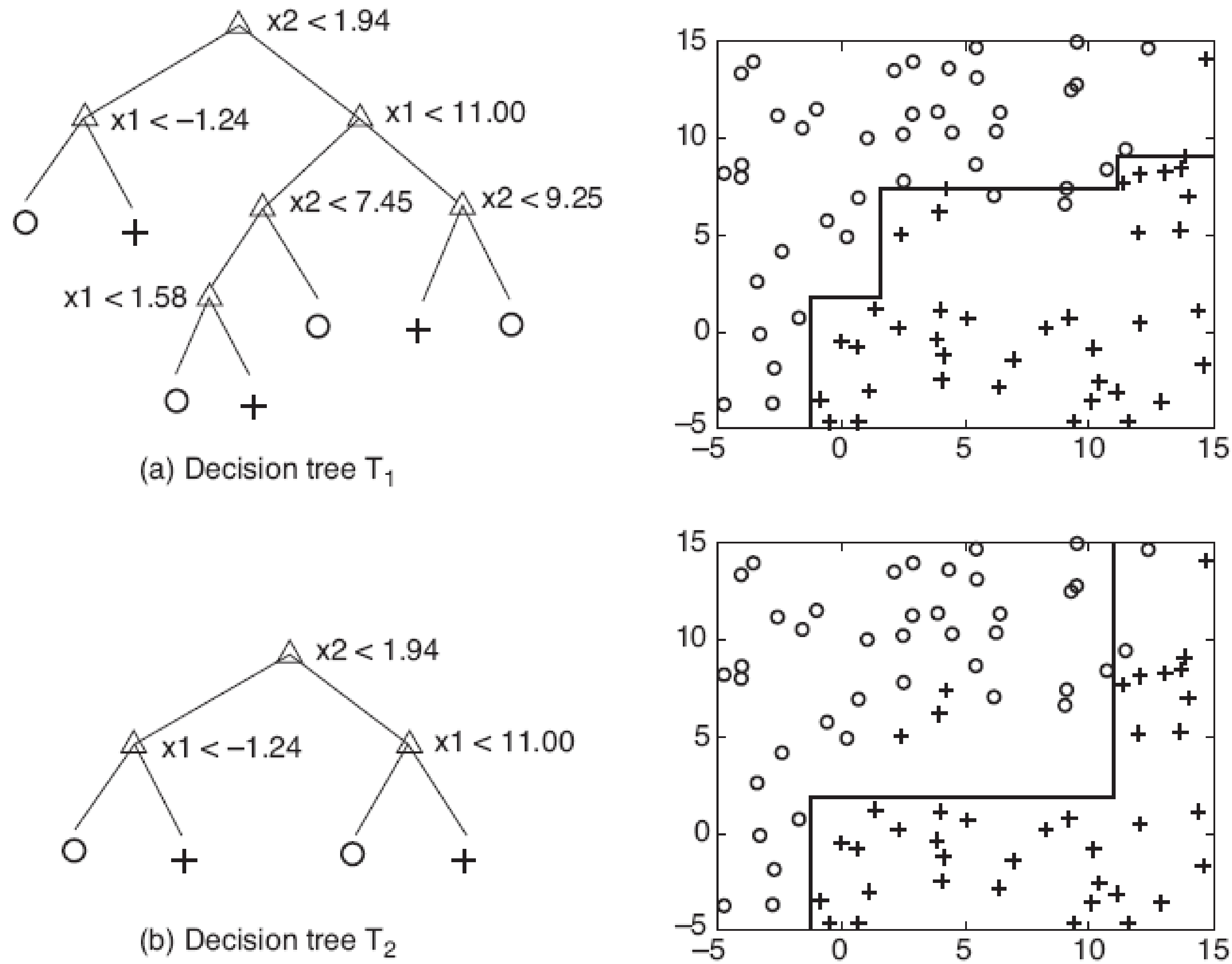


Figure 5.32. Bias-variance decomposition.

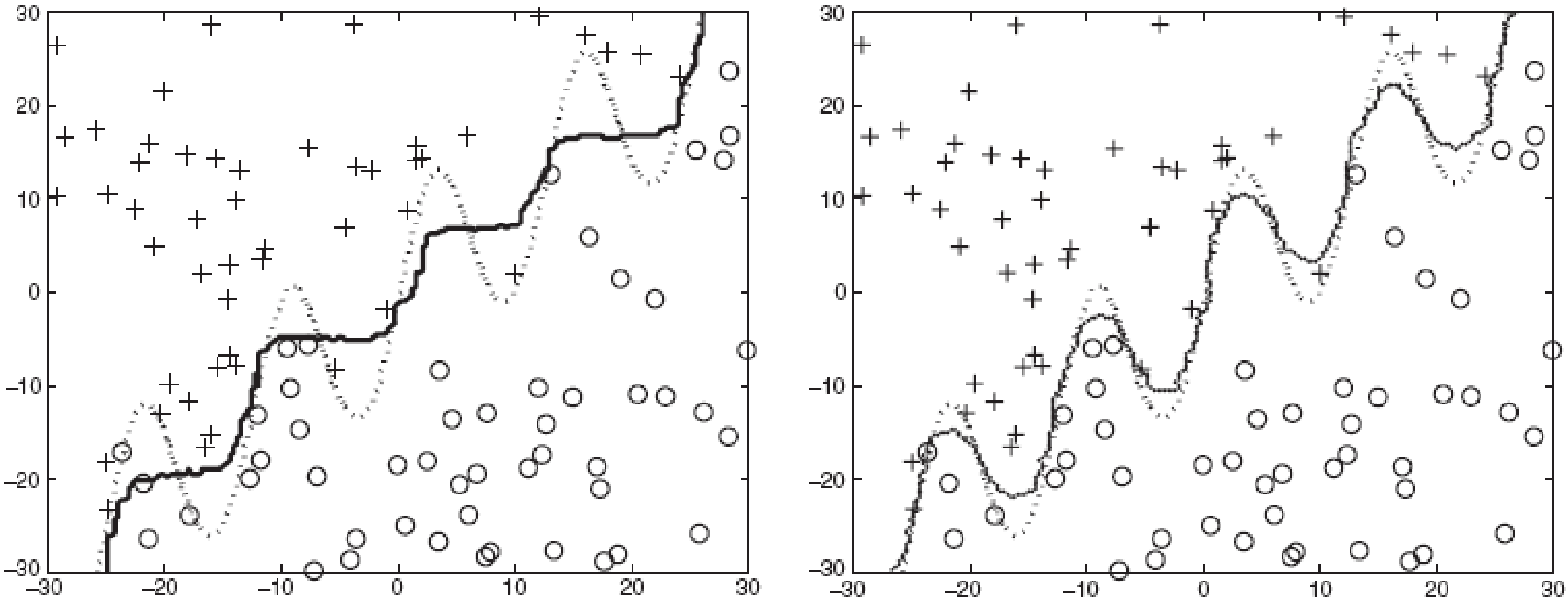
In general,
- Bias is contributed to by the training error; a complex model has low bias.
-Variance is caused by future error; a complex model has High variance.
- Bagging reduces the variance in the base classifiers.



(a) Decision tree T_1

(b) Decision tree T_2

Figure 5.33. Two decision trees with different complexities induced from the same training data.



(a) Decision boundary for decision tree.

(b) Decision boundary for 1-nearest neighbor.

Figure 5.34. Bias of decision tree and 1-nearest neighbor classifiers.

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
  - Unlike bagging, weights may change at the end of a 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

Boosting

- Equal weights are assigned to each training instance (1/d for round 1) at first
- After a classifier C_i is learned, the weights are adjusted to allow the subsequent classifier C_{i+1} to "pay more attention" to data that were misclassified by C_i.
- Final boosted classifier C^* combines the votes of each individual classifier
  - Weight of each classifier's vote is a function of its accuracy
- Adaboost – popular boosting algorithm

Adaboost (Adaptive Boost)

- Input:
  - Training set D containing N instances
  - T rounds
  - A classification learning scheme
- Output:
  - A composite model

Adaboost: Training Phase

- Training data D contain N labeled data (X_1,y_1), (X_2,y_2), (X_3,y_3),….(X_N,y_N)
- Initially assign equal weight 1/d to each data
- To generate *T* base classifiers, we need *T* rounds or iterations
- Round i, data from D are sampled with replacement , to form Di (size *N*)
- Each data's chance of being selected in the next rounds depends on its weight
  - Each time the new sample is generated directly from the training data D with different sampling probability according to the weights; these weights are not zero

Adaboost: Training Phase

- Base classifier C_i, is derived from training data of Di
- Error of C_i is tested using Di
- Weights of training data are adjusted depending on how they were classified
  - Correctly classified: Decrease weight
  - Incorrectly classified: Increase weight
- Weight of a data indicates how hard it is to classify it (directly proportional)

Adaboost: Testing Phase

- The lower a classifier error rate, the more accurate it is, and therefore, the higher its weight for voting should be
- Weight of a classifier C_i's vote is

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

- Testing:
  - For each class c, sum the weights of each classifier that assigned class c to X (unseen data)
  - The class with the highest sum is the WINNER!

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

Example: AdaBoost

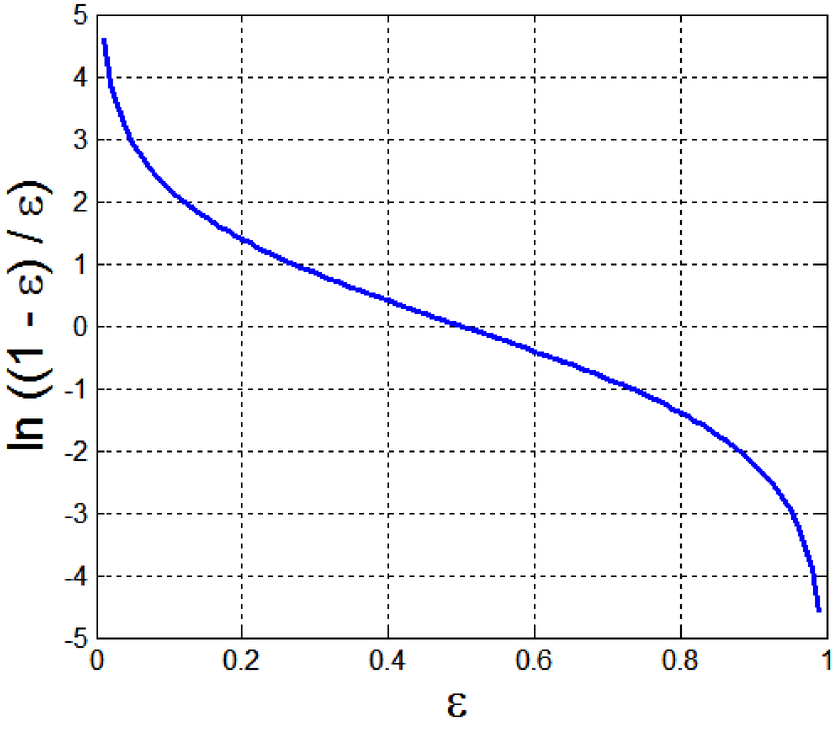
- Base classifiers: $C_1, C_2, \ldots, C_T$

- Error rate: (i = index of classifier, j=index of instance)

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

- Importance of a classifier:

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



Example: AdaBoost

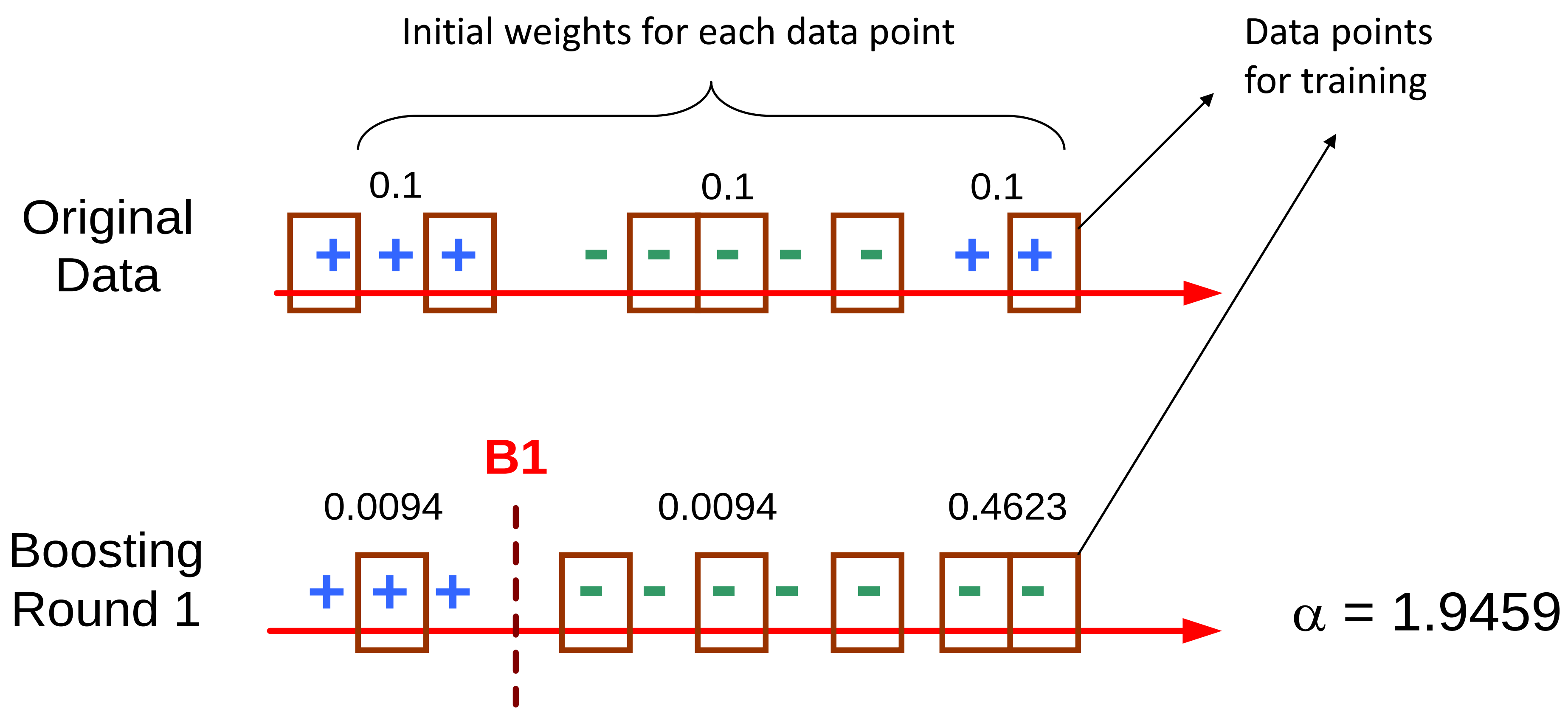
- Assume: *N* training data in D, *T* rounds, (x_j,y_j) are the training data, C_i, a_i are the classifier and weight of the i^{th} round, respectively.
- Weight update on all training data in *D*:

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

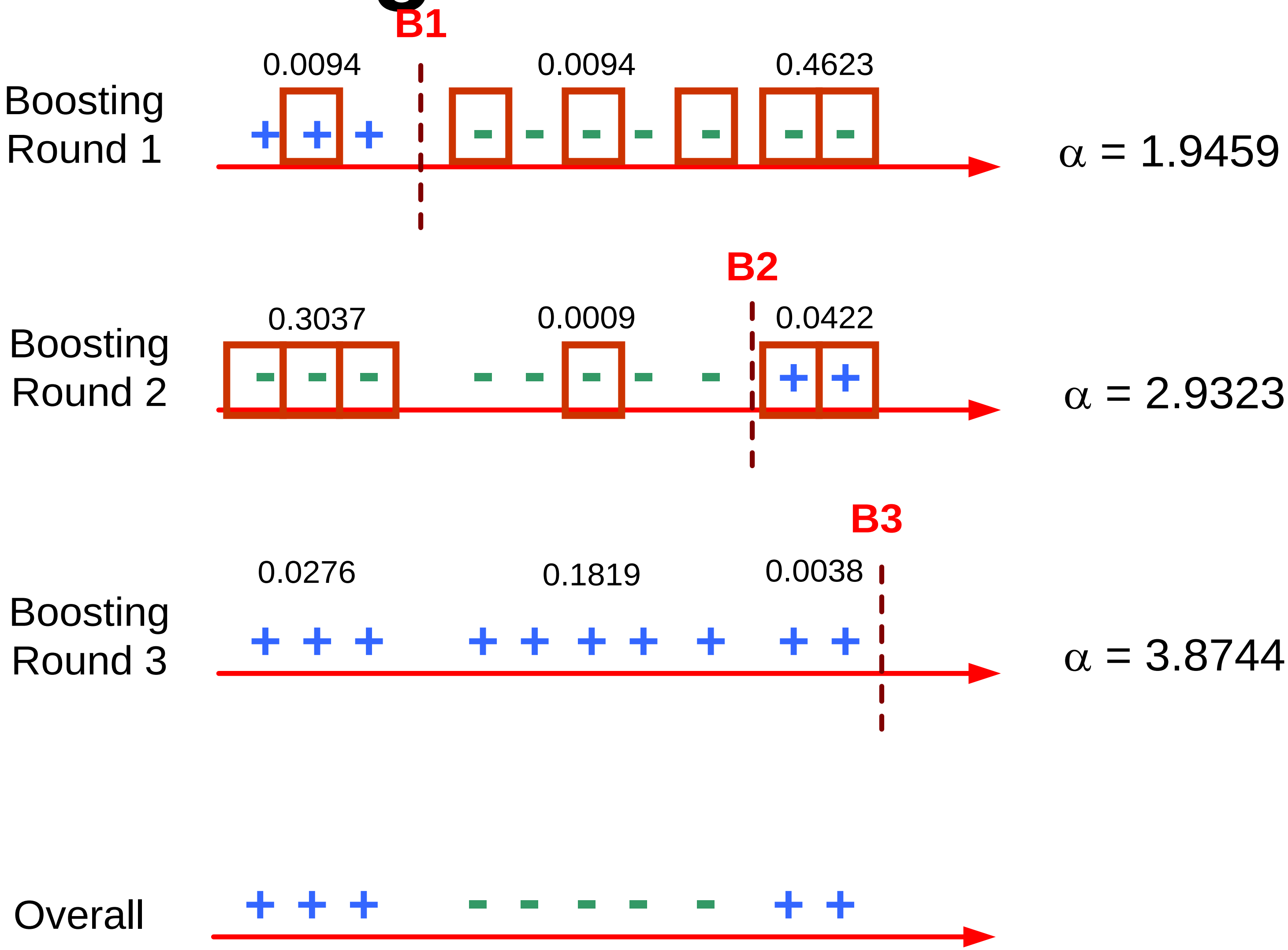
$$\text{where } Z_i \text{ is the normalization factor}$$

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

Illustrating AdaBoost



Illustrating AdaBoost



Random Forests

- Ensemble method specifically designed for decision tree classifiers
- Random Forests grows many trees
  - Ensemble of unpruned decision trees
  - Each base classifier classifies a “new” vector of attributes from the original data
  - Final result on classifying a new instance: voting. Forest chooses the classification result having the most votes (over all the trees in the forest)

Random Forests

- 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

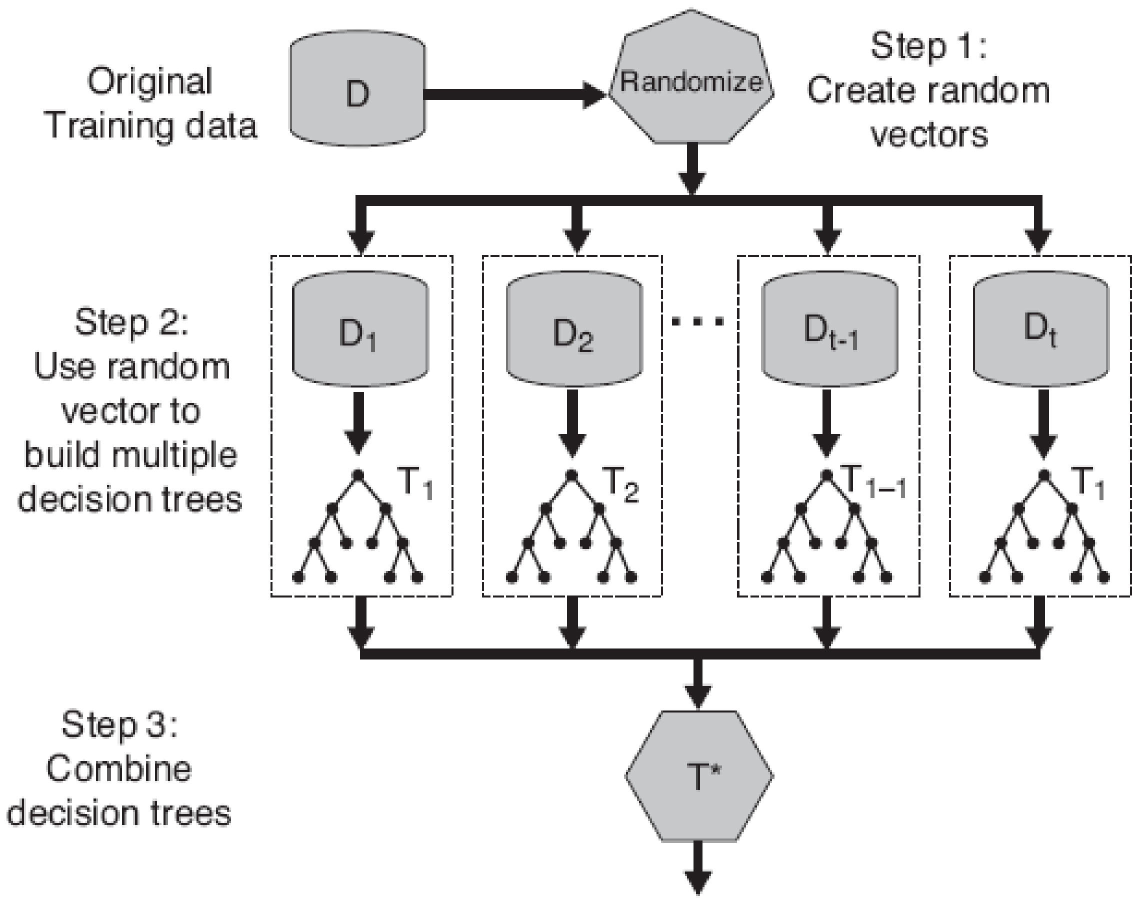


Figure 5.40. Random forests.

Methods for Growing the Trees

- Fix a $m <= M$. At each node
  - Method 1:
    - Choose m attributes randomly, compute their information gains, and choose the attribute with the largest gain to split
  - Method 2:
    - (When M is not very large): select L of the attributes randomly. Compute a linear combination of the L attributes using weights generated from [-1,+1] randomly. That is, new A = Sum(Wi*Ai), i=1..L.
  - Method 3:
    - Compute the information gain of all M attributes. Select the top m attributes by information gain. Randomly select one of the m attributes as the splitting node.

Random Forest Algorithm: method 1 in previous slide

- M input features in training data, a number m<<M is specified such that at each node, m features are selected at random out of the M and the best split on these m features is used to split the node. (In weather data, M=4, and m is between 1 and 4)
- m is held constant during the forest growing
- Each tree is grown to the largest extent possible (deep tree, overfit easily), and there is no pruning

Generalization Error of Random Forests (page 291 of Tan book)

- It can be proven that the generalization Error <= $\rho(1-s^2)/s^2$,
  - ρ is the average correlation among the trees
  - *s* is the strength of the tree classifiers
    - Strength is defined as *how certain* the classification results are on the training data on average
    - How certain is measured Pr(C1|X)-Pr(C2-X), where C1, C2 are class values of two highest probability in decreasing order for input instance X.
- Thus, higher diversity and accuracy is good for performance