Classification (Part 2)

Some slides adapted from Stanford data mining course, "Introduction to Data Mining " by Kumar etc, and UIC data mining course

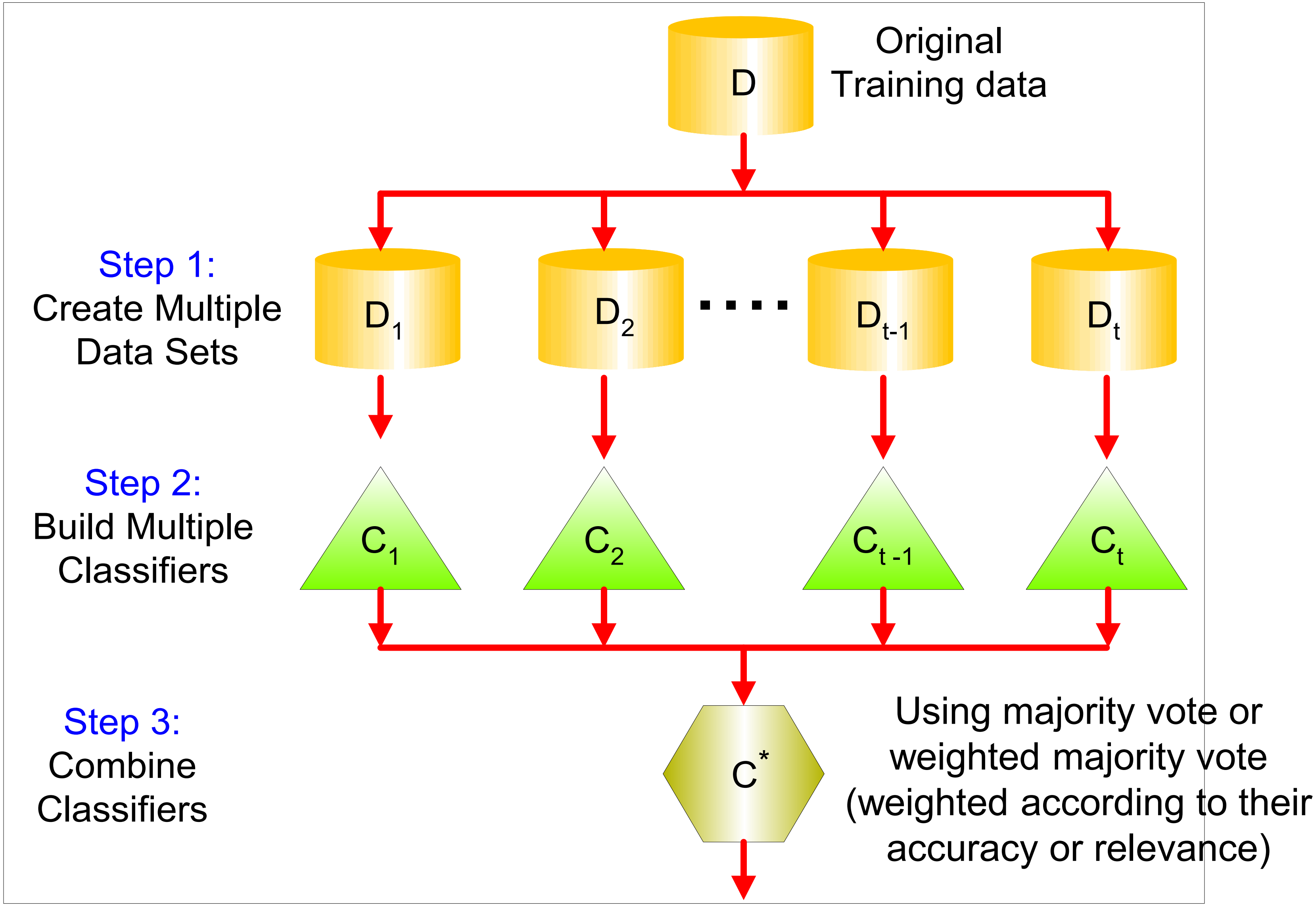
Outline

- Classification Techniques
  - Decision Tree
  - Classification based on association rules
  - Ensemble classifier
  - Overfitting
  - Classification evaluation

Ensemble Methods

- Construct a set of classifiers from the training data
- Predict class label of previously unseen records by aggregating predictions made by multiple classifiers, such as majority of voting
- Assumption:
  - Individual classifiers (voters) could be lousy (stupid), but the aggregate (electorate) can usually classify (decide) correctly.

General Idea



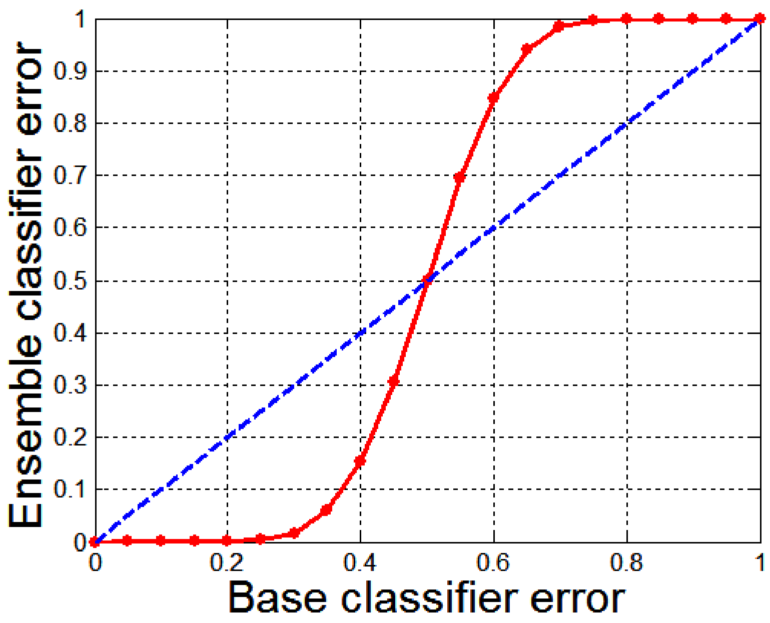
Example: Why Do Ensemble Methods Work?

- 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.

Examples of Ensemble Methods

- How to generate an ensemble of classifiers?
  - Bagging
  - Boosting

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

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.$\}$

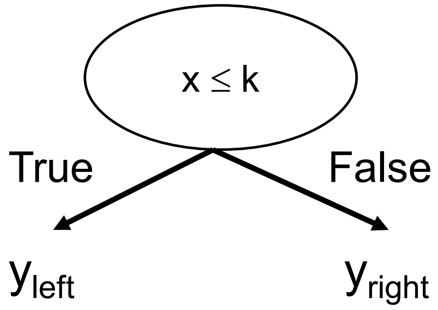
Bagging Example

- 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

Improvement of Bagging: Random Forest

- Train a **Bagged Decision Tree**
- But use a modified tree learning algorithm that selects (at each candidate split) **a random subset of features**
  - If we have d features, consider $\sqrt{d}$ random features

- **This is called: Feature bagging**
  - **Benefit:** Breaks correlation between trees
    - If one feature is very strong predictor, then every tree will select it, causing trees to be correlated.

- **Random Forests achieve state-of-the-art results in many classification problems!**

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, sampling weights may change at the end of boosting round
- Successful algorithms
  - Example 1: adaBoost (some slides for your information or self-study)
  - Example 2: Gradient Boosted Decision Trees

Boosting

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

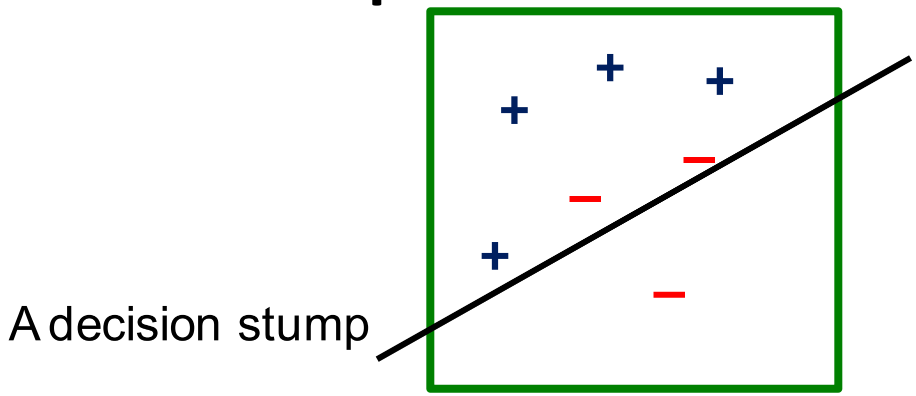
Build Decision Trees with AdaBoost

Suppose we have training data $\{(x_i, y_i)\}_{i=1}^{N}$, $y_i \in \{1, -1\}$

- Initialize equal weights for all observations
- At each iteration t:
  1. **Train a stump G_t** using data weighted by w_i
  2. **Compute the misclassification error** adjusted by w_i
  3. **Compute the weight of the current tree**
  4. **Reweight each observation** based on prediction accuracy

AdaBoost: Weak learner

- **1. build Decision "stumps":**
  - 1-level decision tree
  - A decision boundary based on one feature
    - E.g.: If someone is not a smoker, then predict them to live past 80 years old
  - Building blocks of AdaBoost algorithm
  - **Decision stump** is a **weak learner**



Boosting theory:
if weak learners have >50% accuracy then we can learn a perfect classifier.

Update Step

2. Calculate the weighted misclassification error

$$err_t = \frac{\sum_{i=1}^{N} w_i \, I\left(y_i \neq G_t(x_i)\right)}{\sum_{i=1}^{N} w_i}$$

3. Use the error score to weight the current tree in the final classifier:

$$\alpha_t = log\left(\frac{1 - err_t}{err_t}\right)$$

A classifier with 50% accuracy is given a weight of zero;

4. Use misclassification error and tree weight to reweight the training data:

$$w_i \leftarrow w_i exp\left[\alpha_t I\left(y_i \neq G_t(x_i)\right)\right]$$

Harder to classify training instances get higher weight

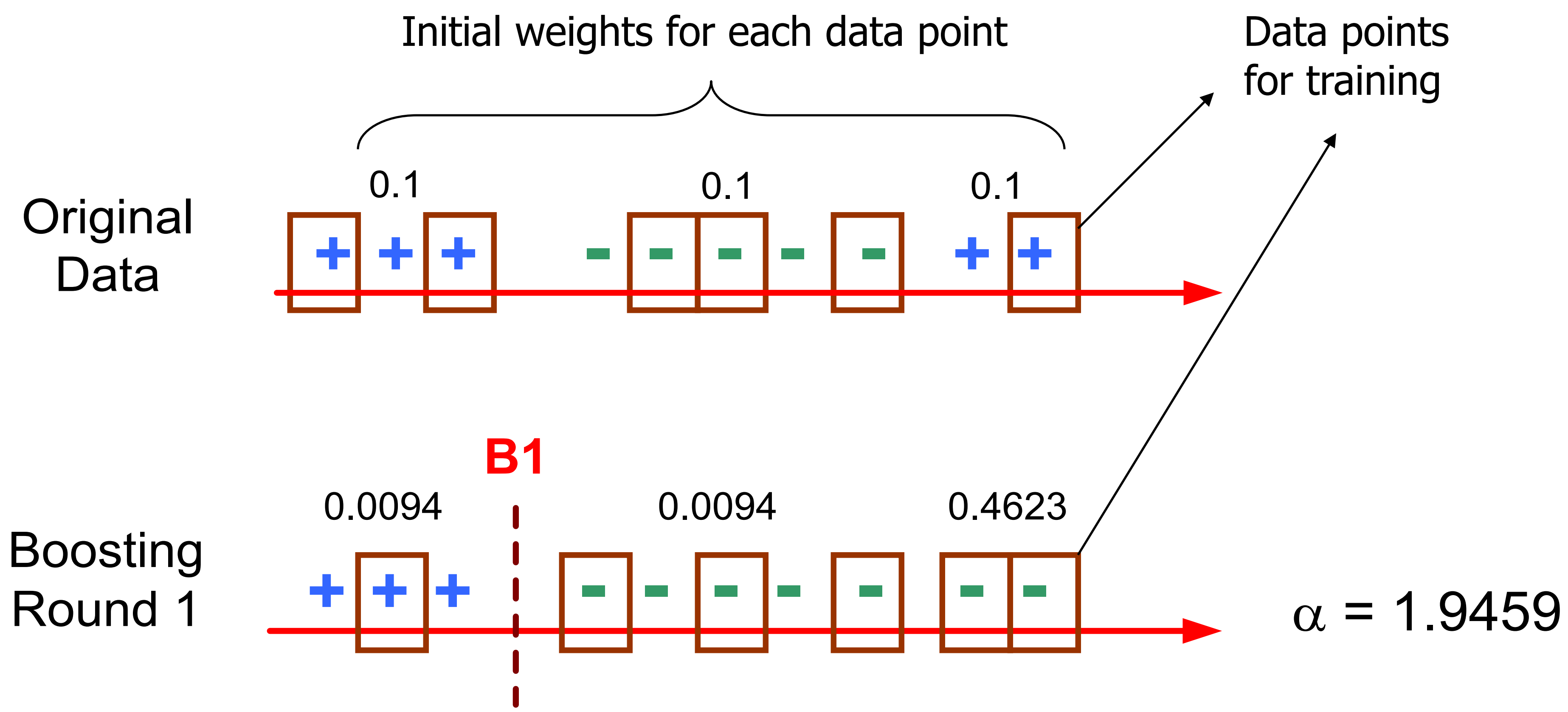
Final Prediction

- **Final prediction is a weighted sum of the predictions from each stump:**

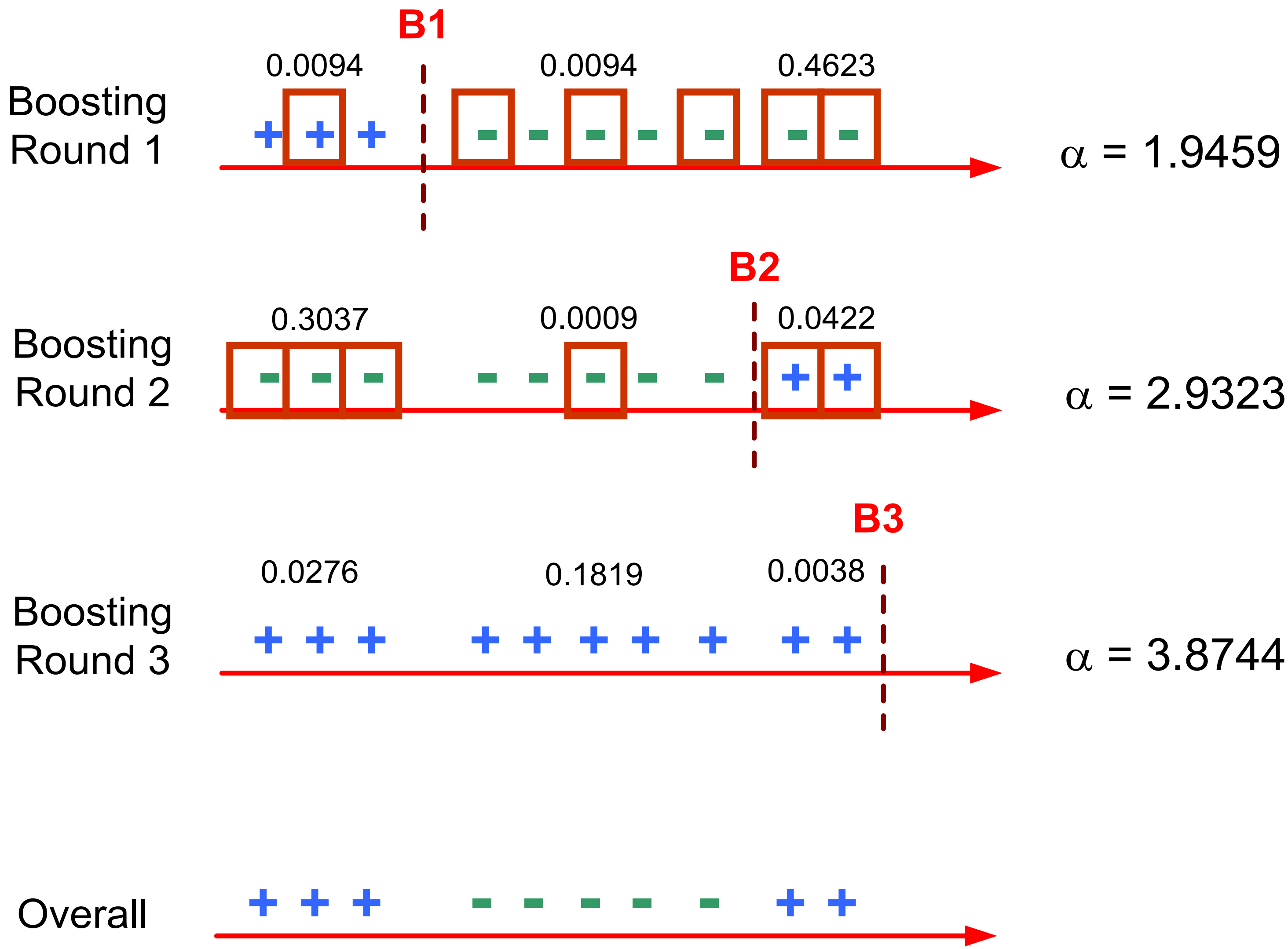
$$G(x) = sign\left[\sum_{t=1}^{T} \alpha_t \, G_t(x)\right]$$

- **More accurate trees are weighted higher in the final model**

Illustrating AdaBoost



Illustrating AdaBoost



Outline

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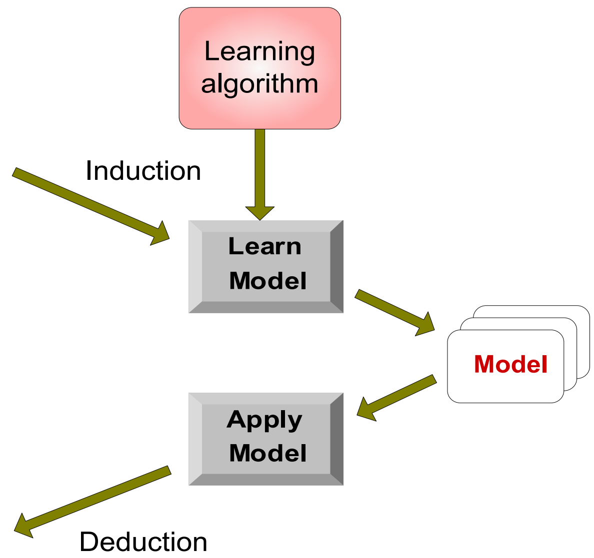
  - Decision Tree
  - Classification based on association rules
  - Ensemble classifier
  - Overfitting
  - Classification evaluation

Classification Errors

- **Training errors**: Errors committed on the training set
- **Test errors**: Errors committed on the test set
- **Generalization errors**: Expected error of a model over random selection of records from same distribution

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

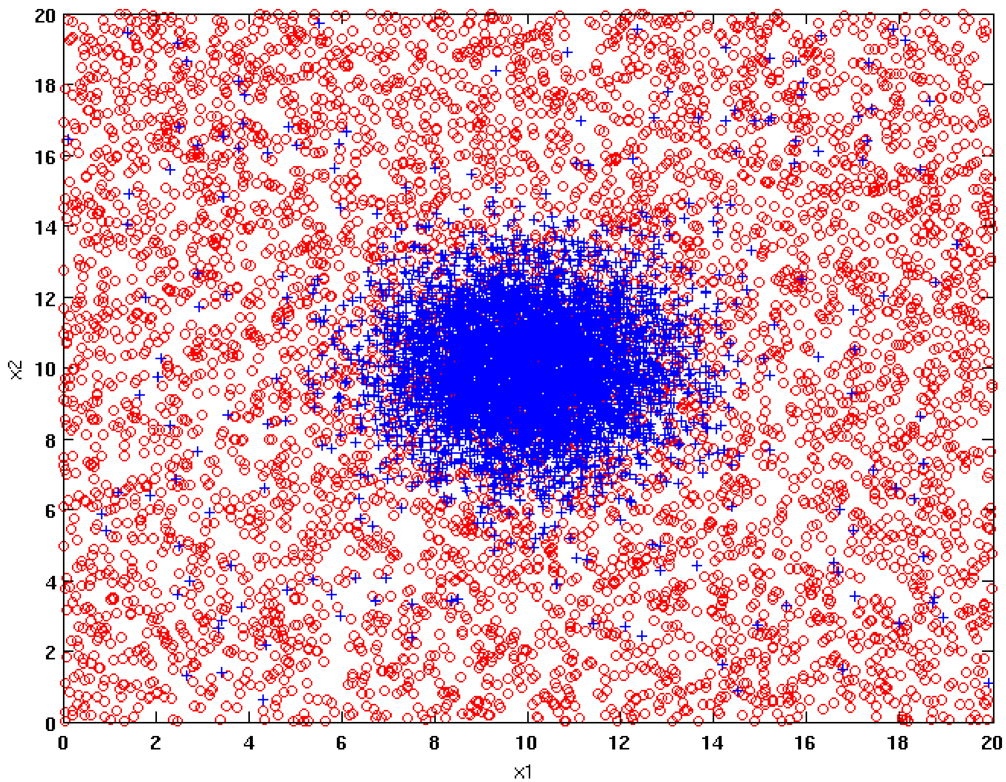
Training Set



Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set

Example Data Set



Two class problem:

+ : 5400 instances

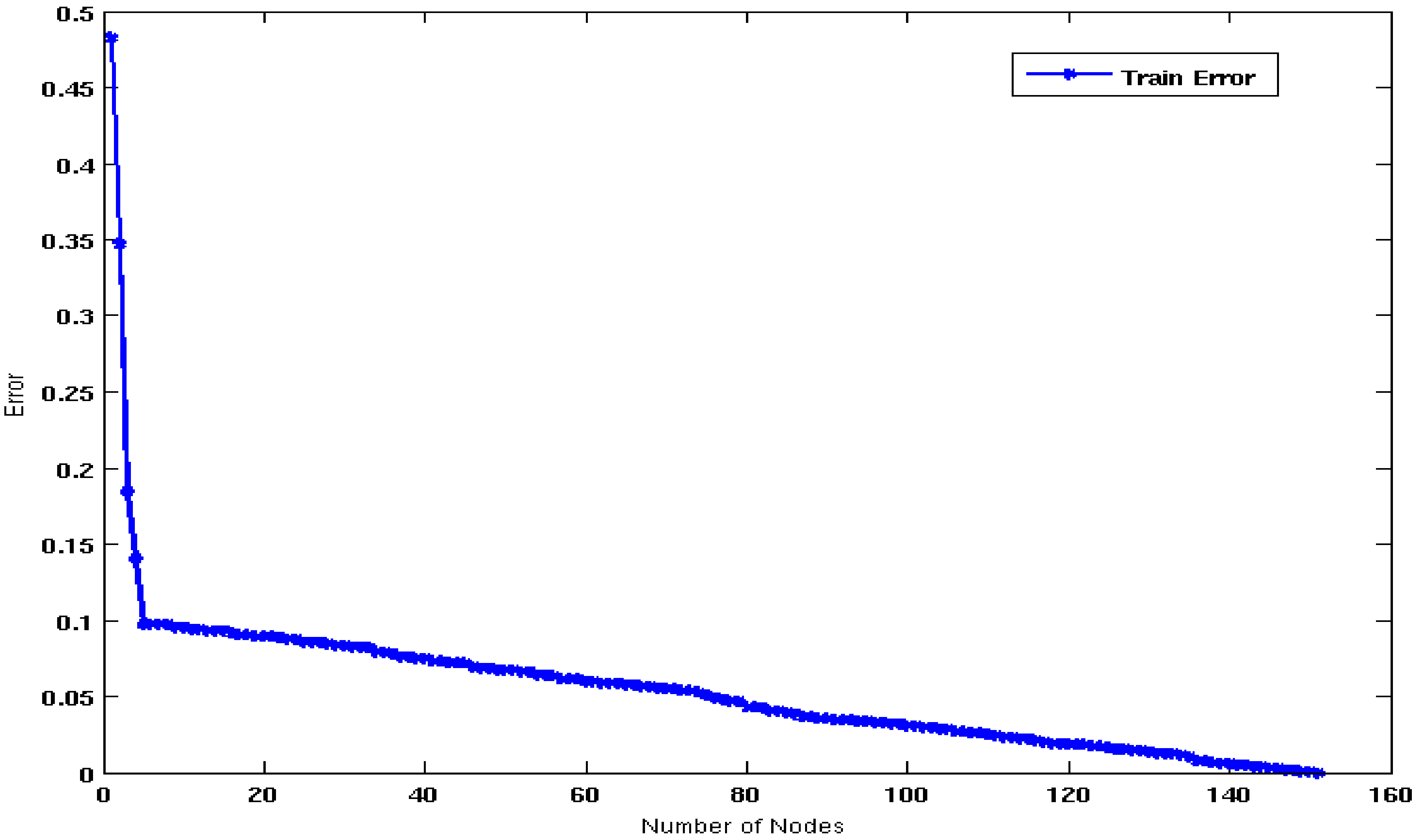
- **5000 instances generated from a Gaussian centered at (10,10)**
- **400 noisy instances added**

o : 5400 instances

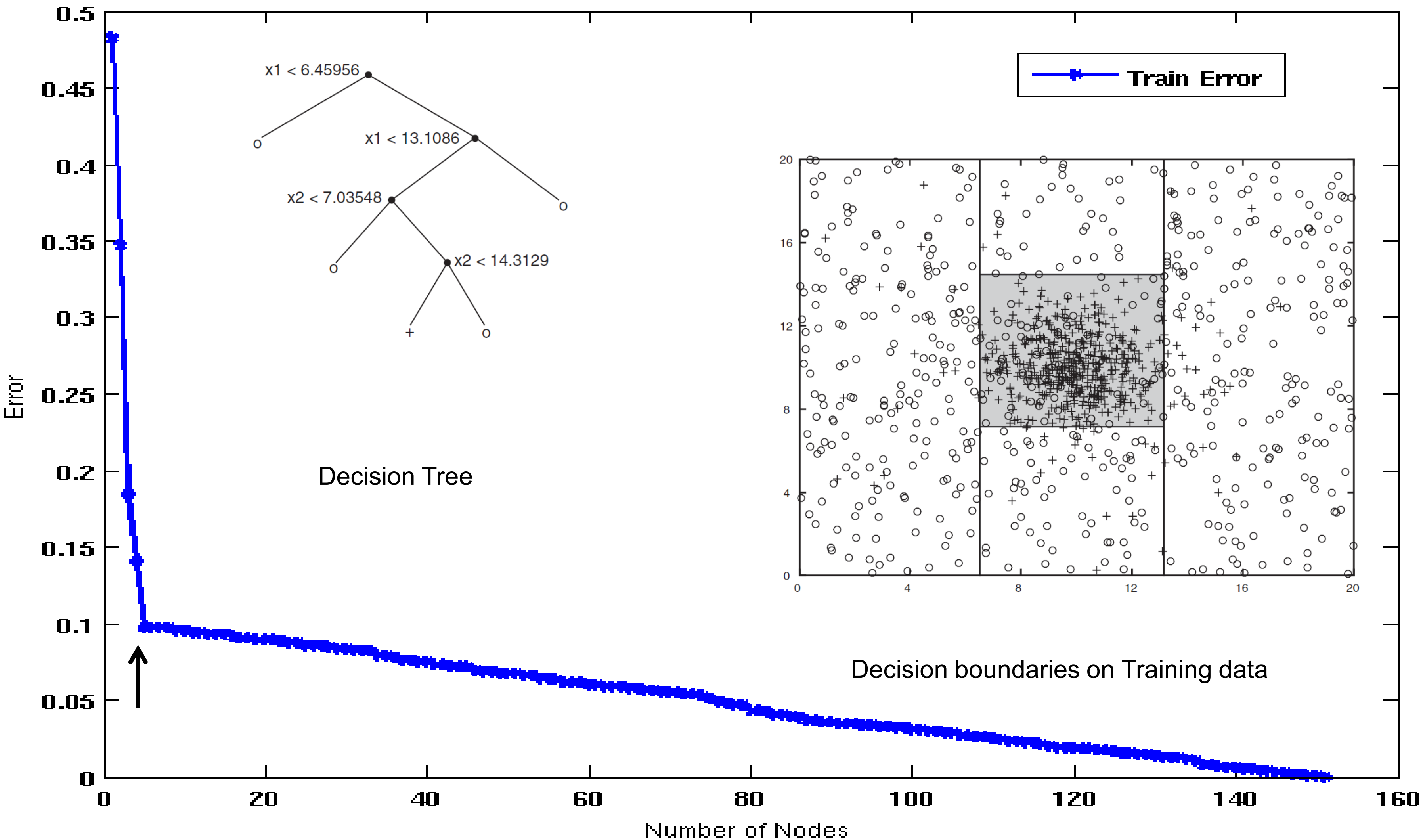
- **Generated from a uniform distribution**

10 % of the data used for training and 90% of the data used for testing

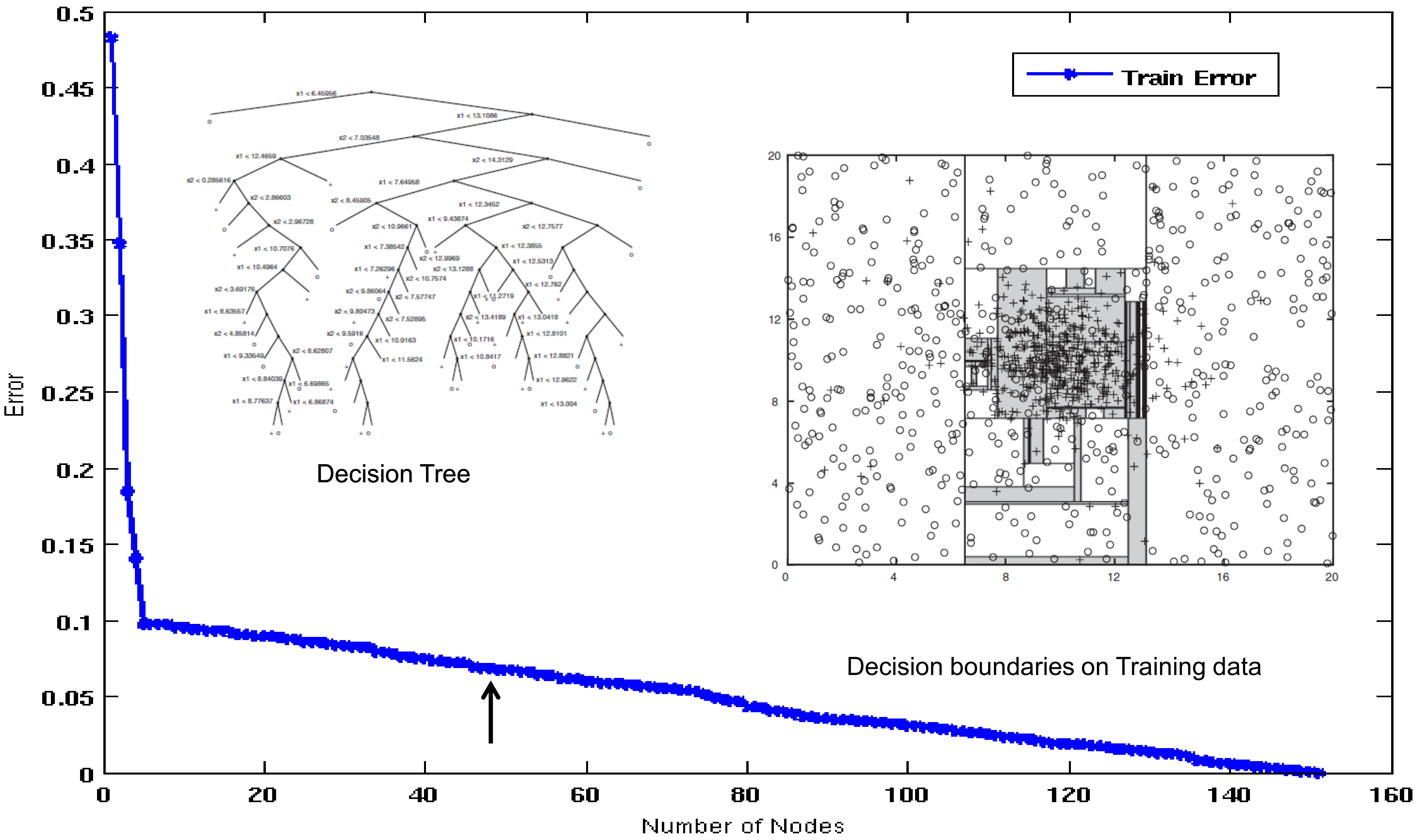
Increasing number of nodes in Decision Trees



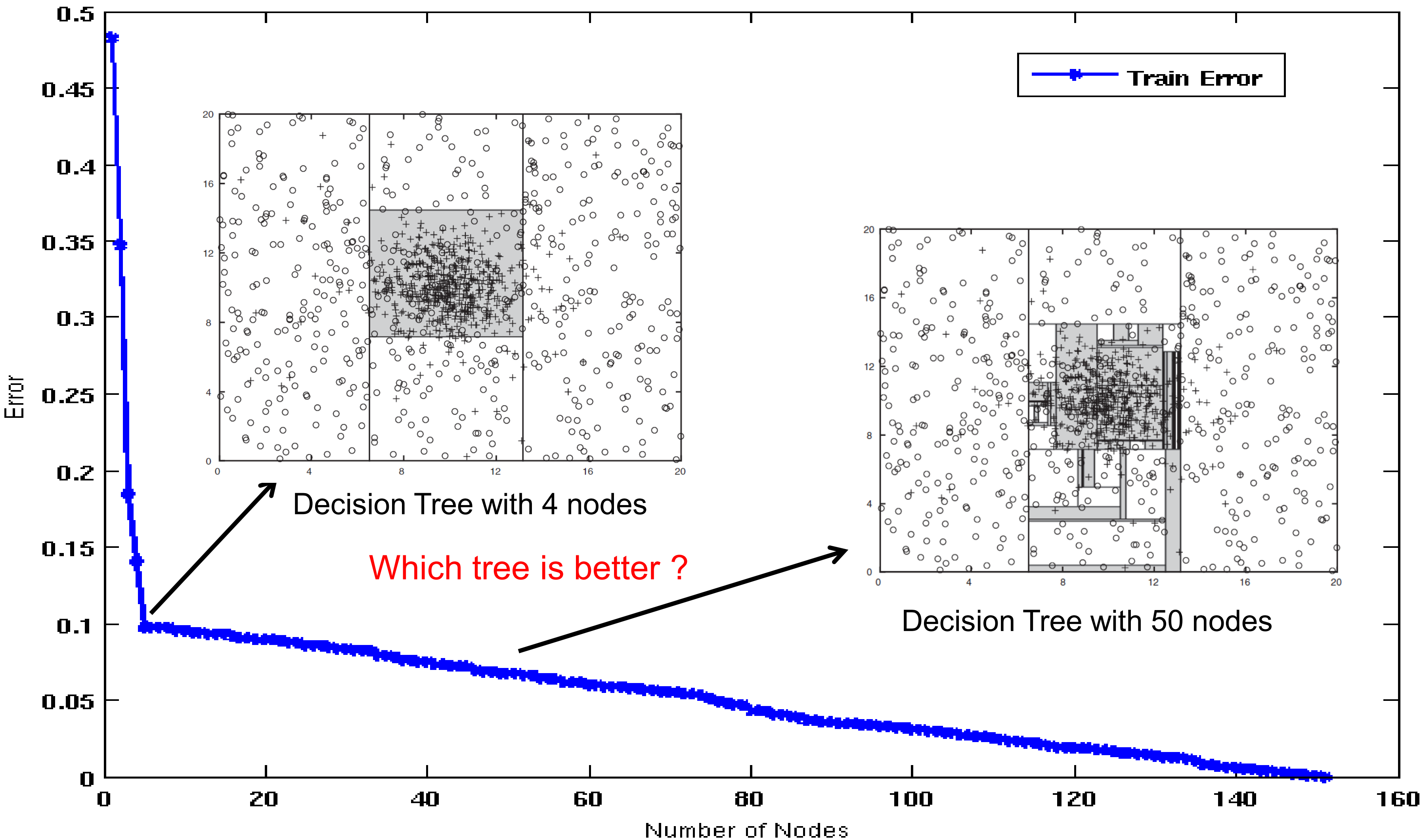
Decision Tree with 4 nodes



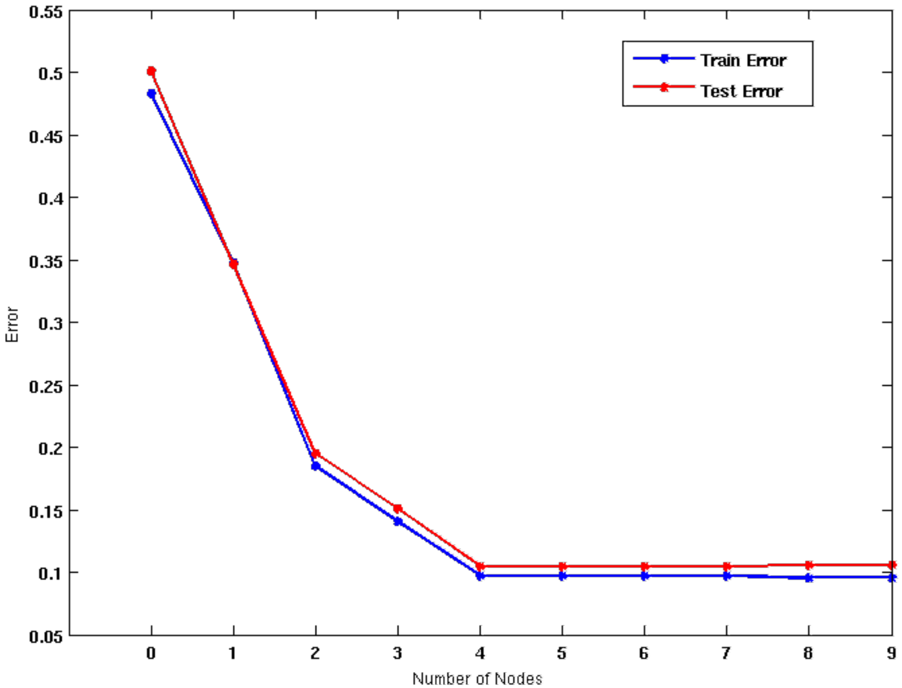
Decision Tree with 50 nodes

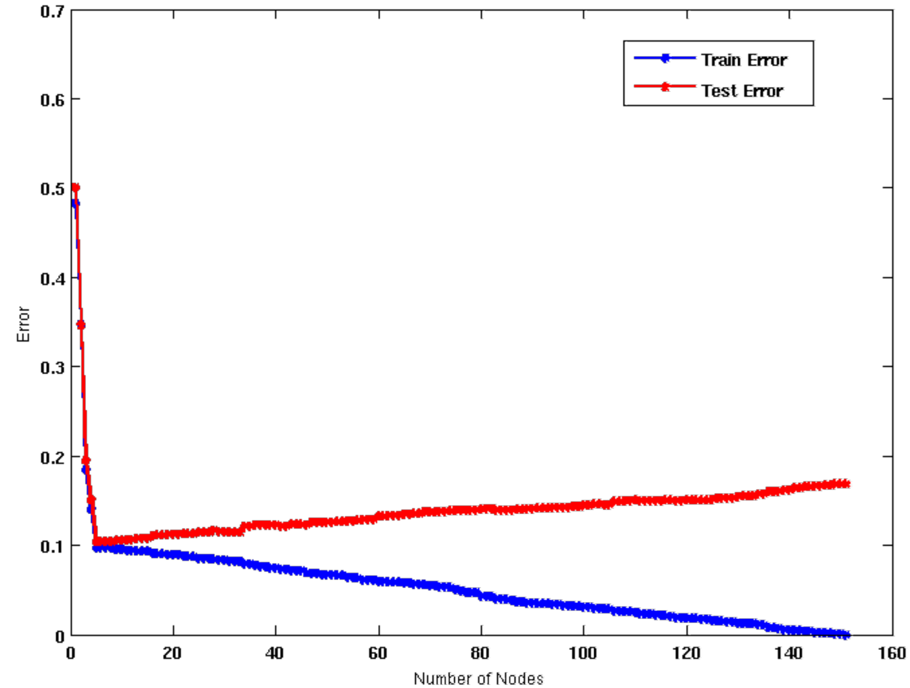


Which tree is better?



Model Underfitting and Overfitting



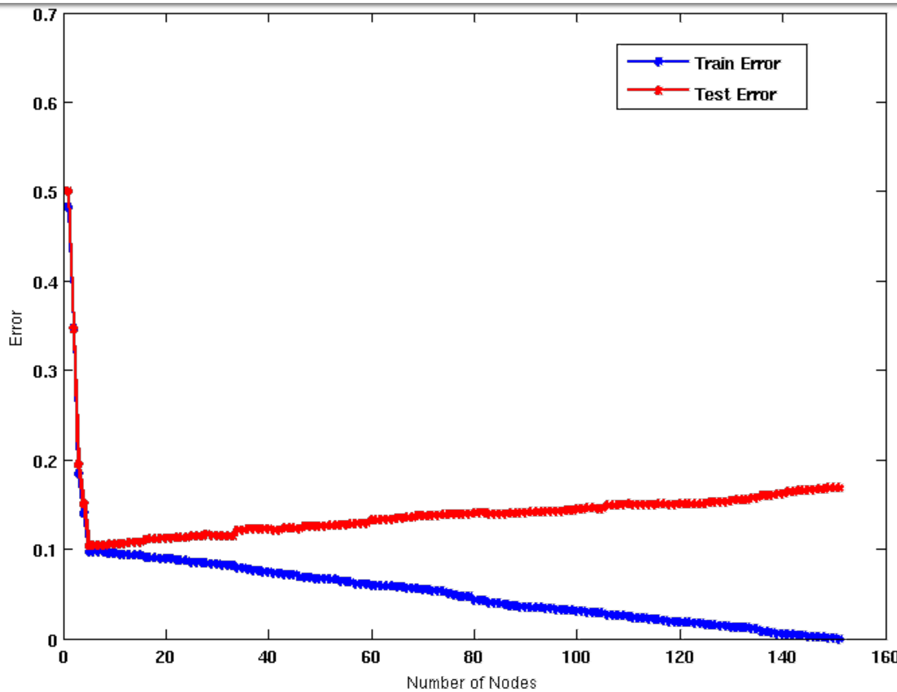


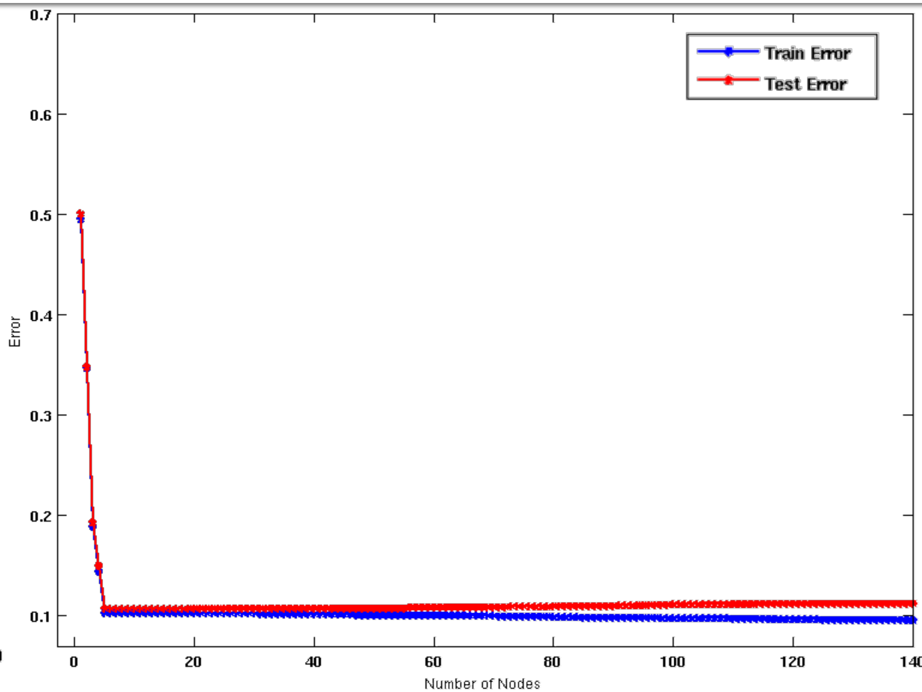
- As the model becomes more and more complex, test errors can start increasing even though training error may be decreasing

Underfitting: when model is too simple, both training and test errors are large

Overfitting: when model is too complex, training error is small but test error is large

Model Overfitting – Impact of Training Data Size

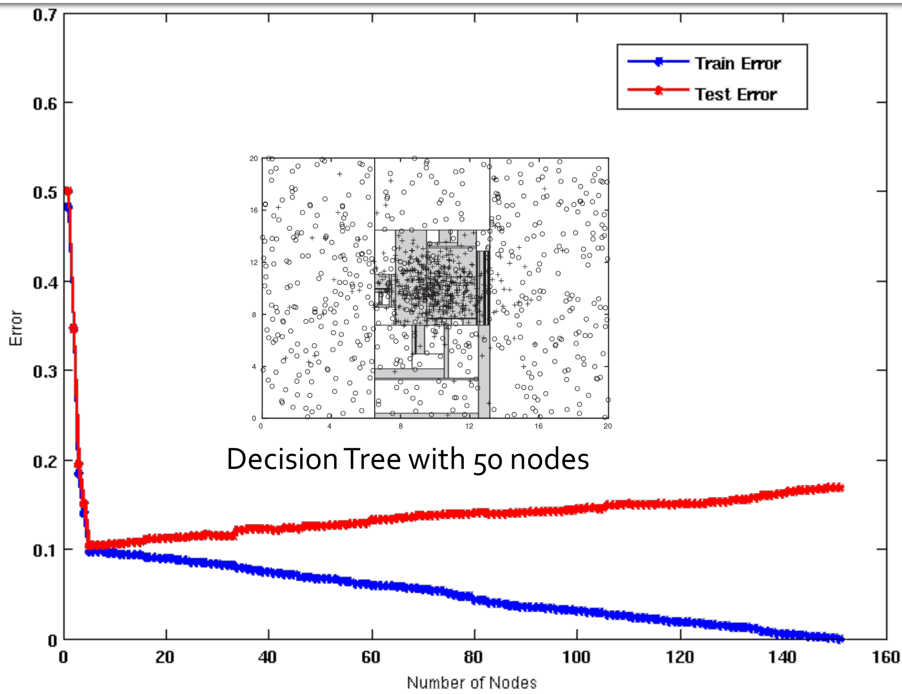




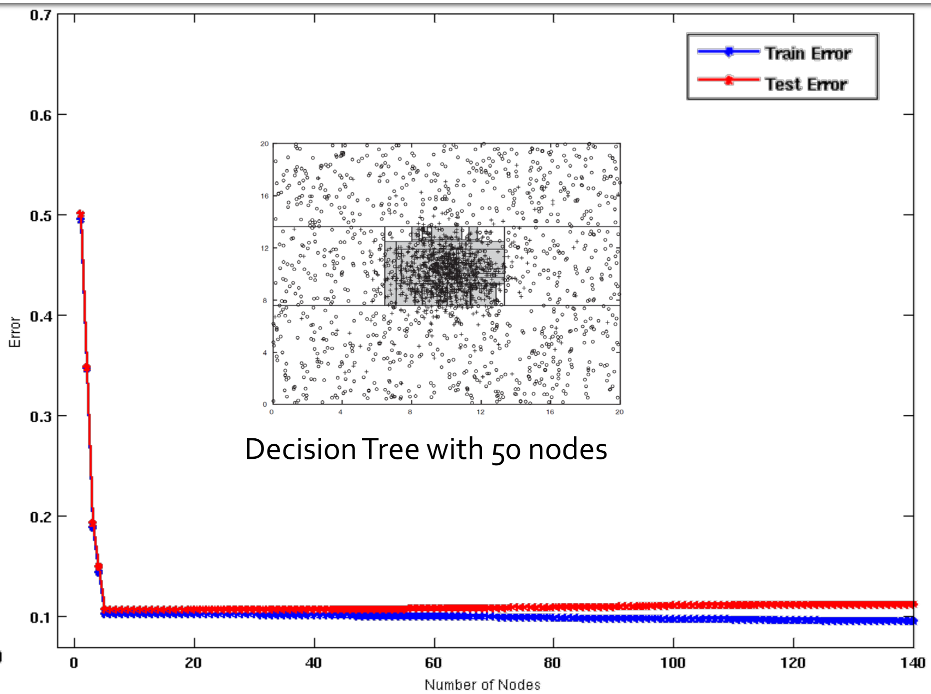
Using twice the number of data instances

- Increasing the size of training data reduces the difference between training and testing errors at a given size of model

Model Overfitting – Impact of Training Data Size



Decision Tree with 50 nodes



Decision Tree with 50 nodes

Using twice the number of data instances

- Increasing the size of training data reduces the difference between training and testing errors at a given size of model

Reasons for Model Overfitting

- Not enough training data

- High model complexity
  - Multiple Comparison Procedure

Notes on Overfitting

Use decision trees as an example:

- Overfitting results in decision trees that are more complex than necessary
- Training error does not provide a good estimate of how well the tree will perform on previously unseen records
- Need ways for estimating generalization errors

Model Selection

- Performed during model building
- Purpose is to ensure that model is not overly complex (to avoid overfitting)
- Need to estimate generalization error
  - Using Validation Set
  - Incorporating Model Complexity (e.g., number of leaf nodes in decision trees) in model training
    - Given two models of similar generalization errors, one should prefer the simpler model over the more complex model

Using Validation Set

- Divide training data into two parts:
  - Training set:
    - use for model building
  - Validation set:
    - use for estimating generalization error
    - Note: validation set is not the same as test set

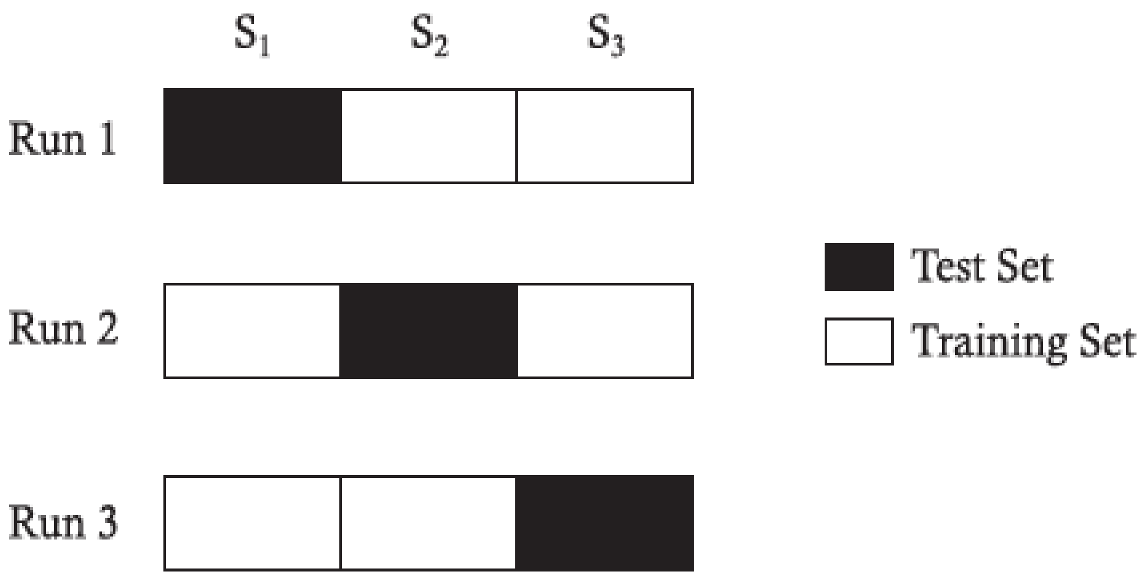
- Drawback:
  - Less data available for training

Classification Model Evaluation

- Purpose:
  - To estimate performance of classifier on previously unseen data (test set)
- Holdout
  - Reserve k% for training and (100-k)% for testing
  - Random subsampling: repeated holdout
- Cross validation
  - Partition data into k disjoint subsets
  - k-fold: train on k-1 partitions, test on the remaining one
  - Leave-one-out: k=n

Cross-validation Example

- 3-fold cross-validation



Summary

- Classification Techniques
  - Decision Tree
  - Classification based on association rules
  - Ensemble classifier
    - Understand the high-level idea
  - Overfitting
    - Understand the high-level idea
  - Classification evaluation
    - Understand the high-level idea