# Model Overfitting

Introduction to Data Mining, 2$^{nd}$ Edition

by

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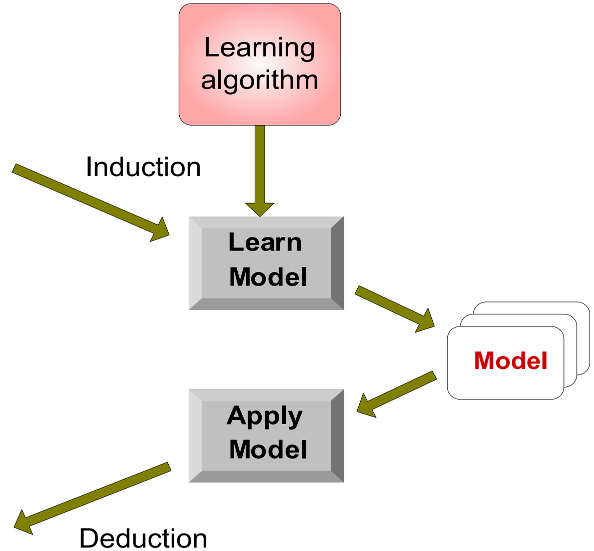
# Classification Errors

- **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 |

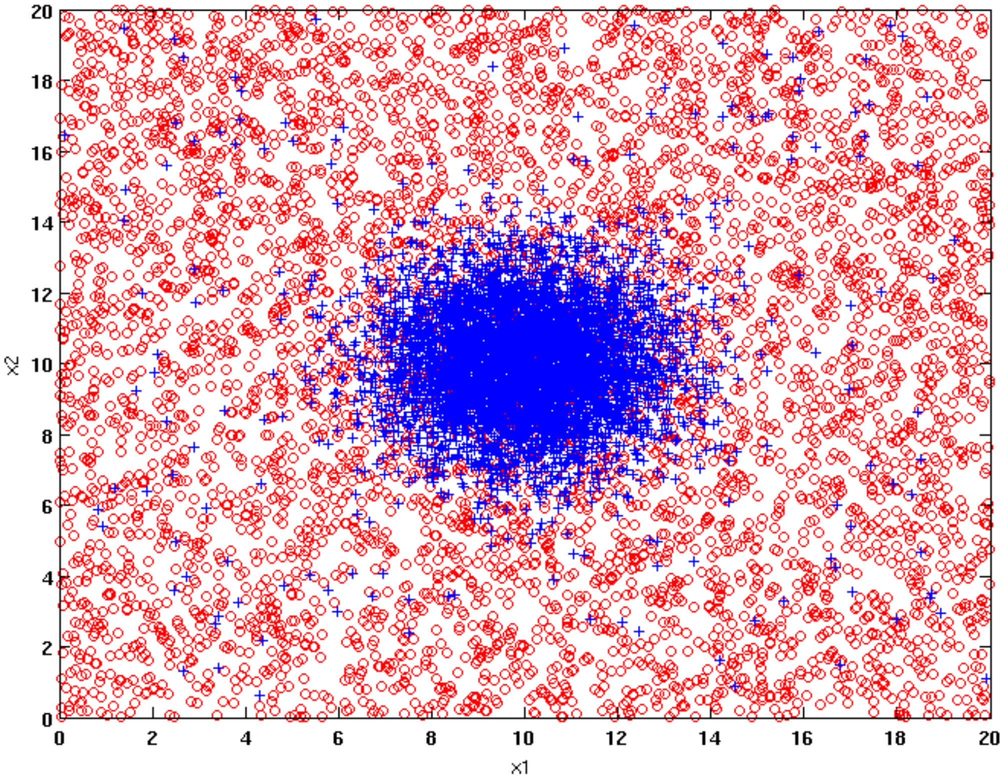
Training Set




| *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**

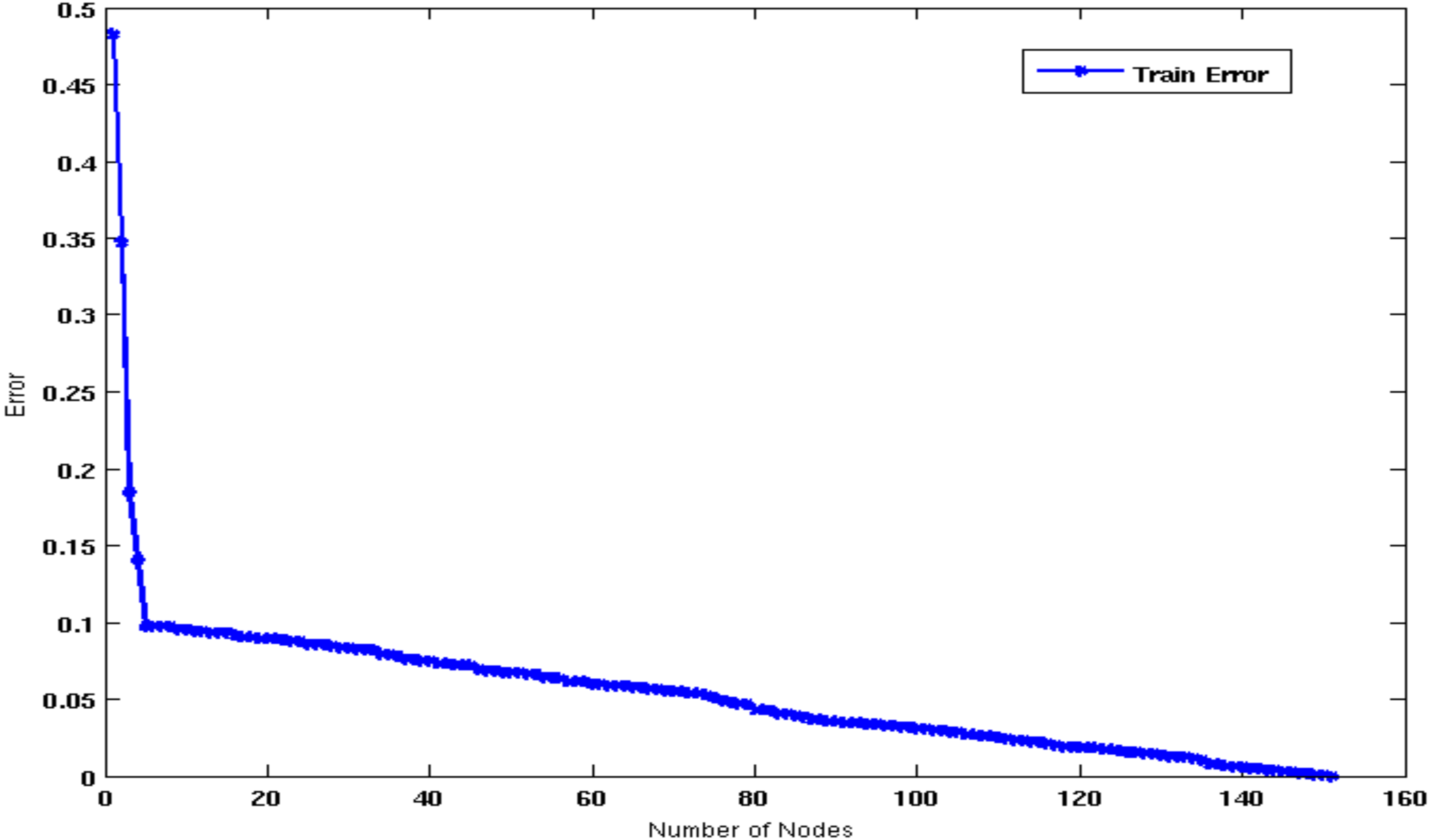
- **5000 instances generated from a Gaussian centered at (10,10)**
- **400 noisy instances added**

**o : 5400 instances**

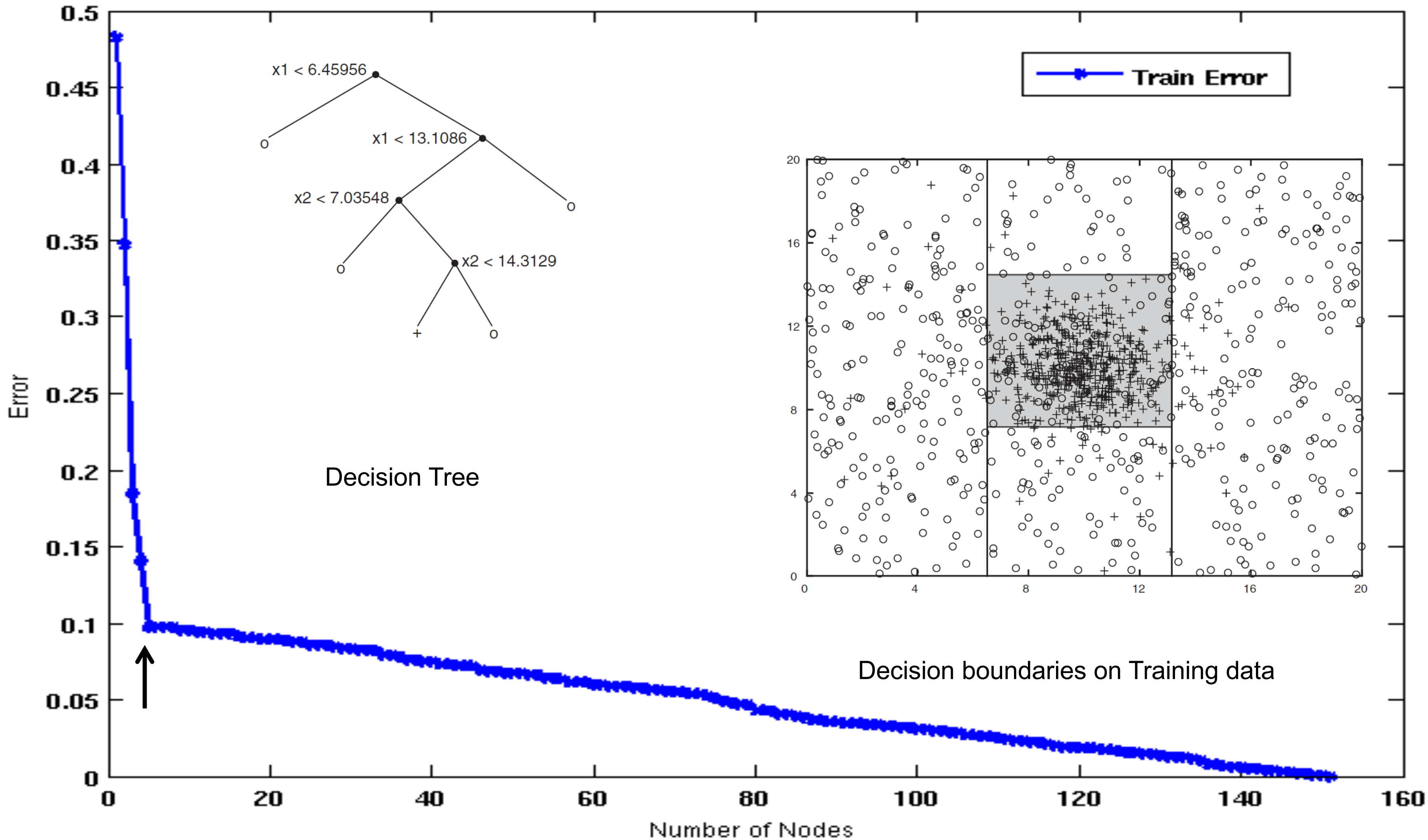
- **Generated from a uniform distribution**

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

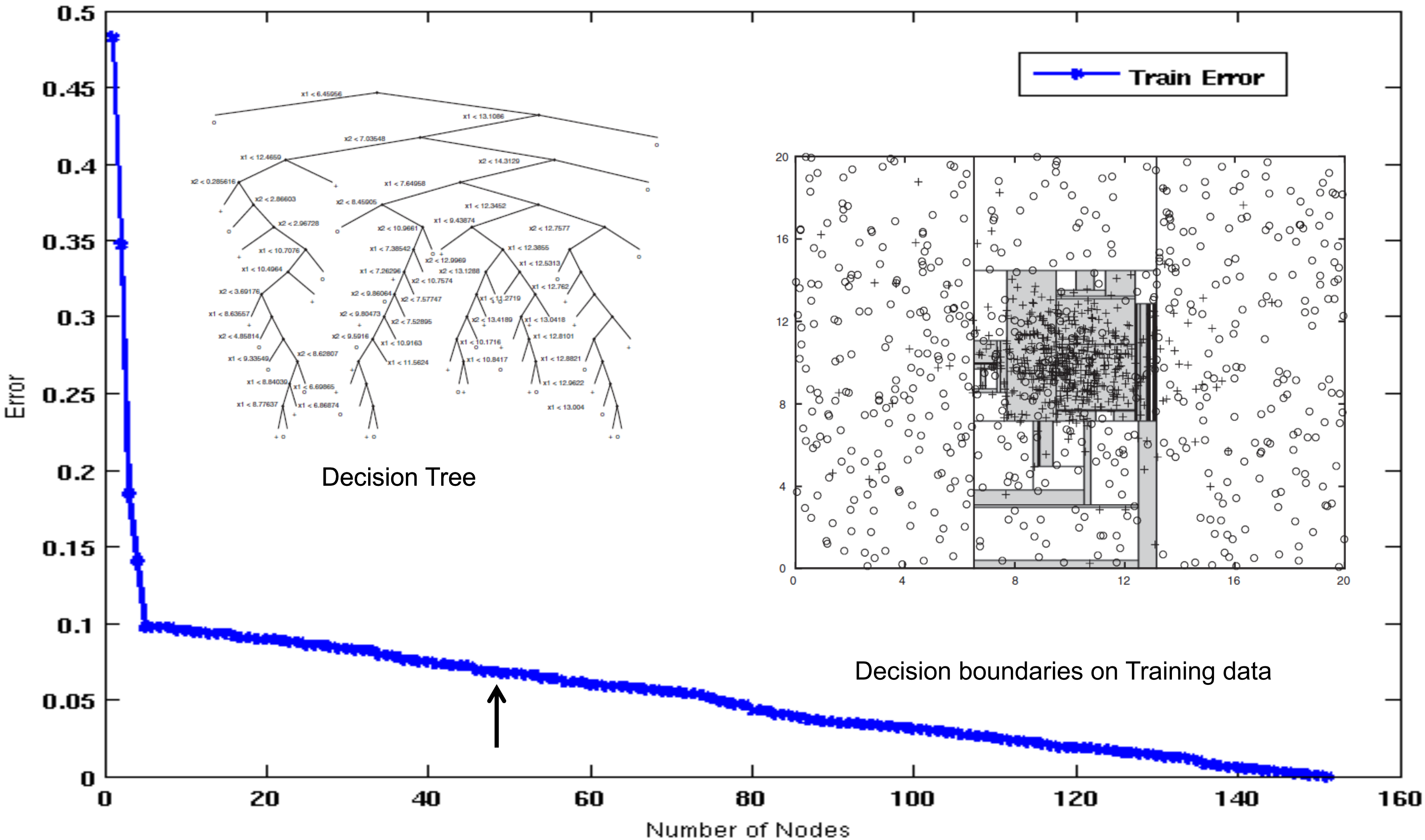
# Increasing number of nodes in Decision Trees



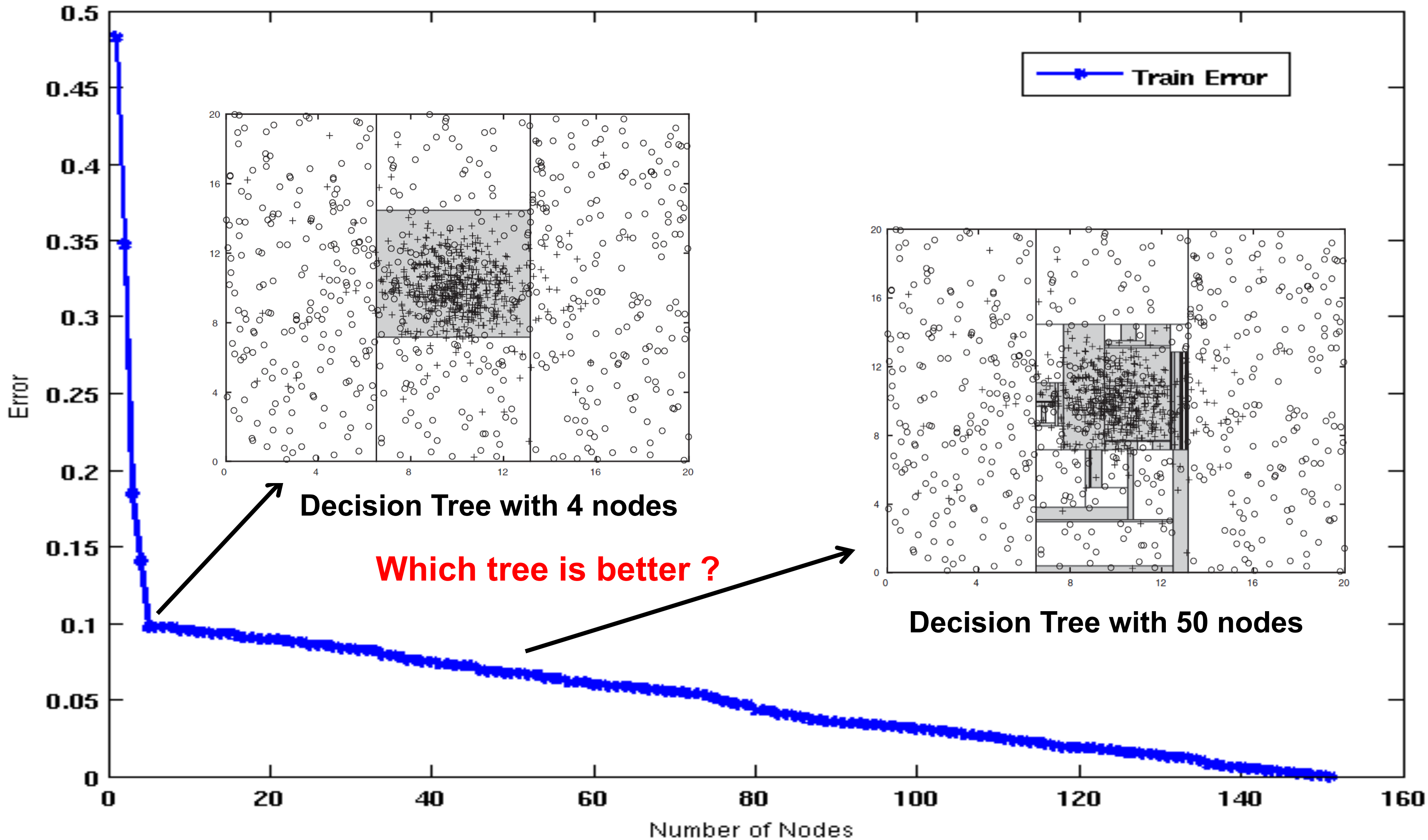
# Decision Tree with 4 nodes



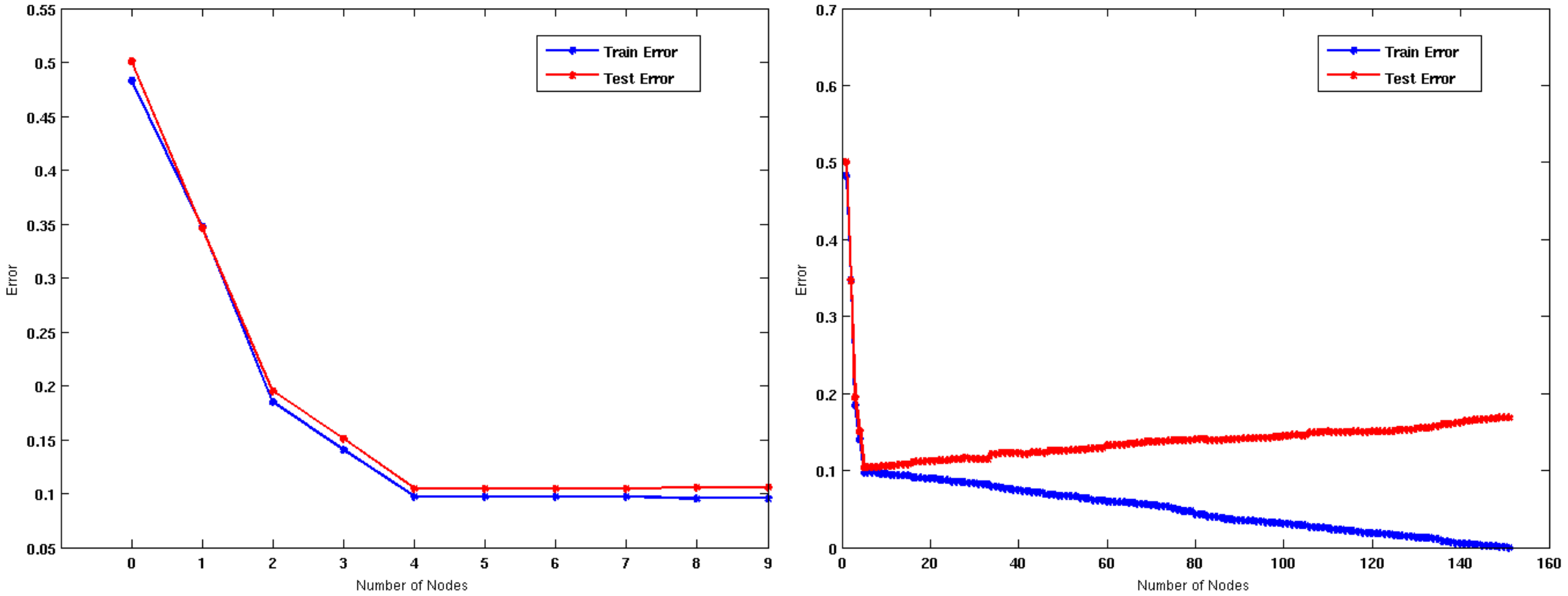
# Decision Tree with 50 nodes



# Which tree is better?



# Model Underfitting and Overfitting

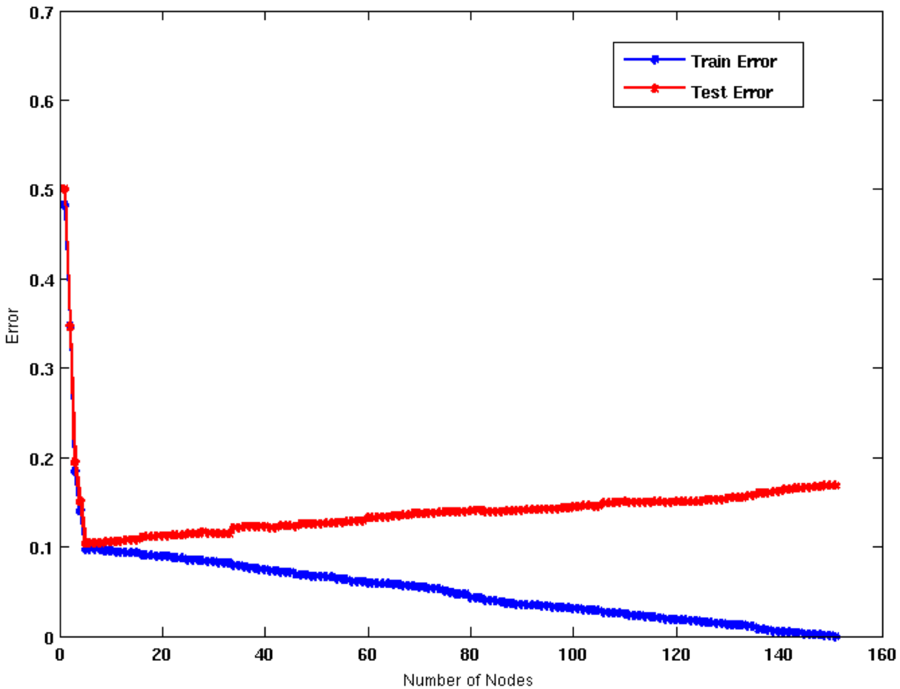


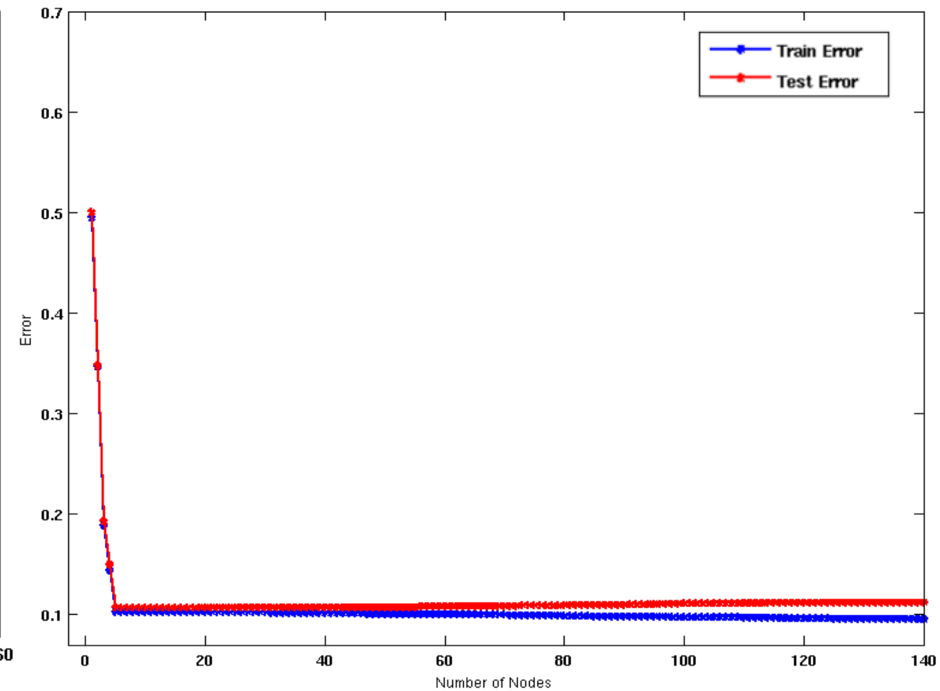

- As the model becomes more and more complex, test errors can start increasing even though training error may be decreasing

**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

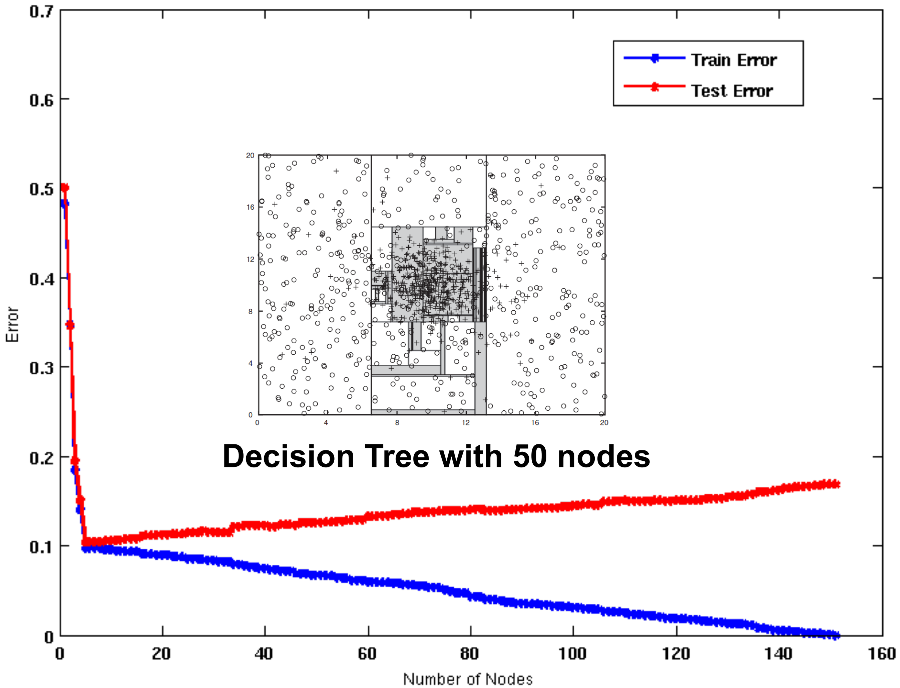


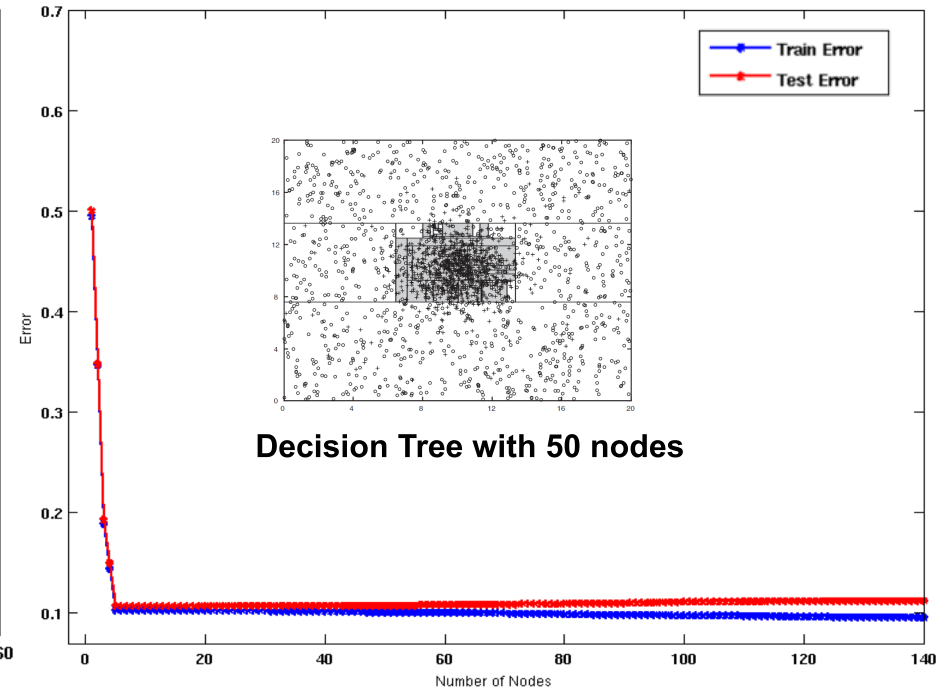




**Using twice the number of data instances**

- 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




**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

# Effect of Multiple Comparison Procedure

- Consider the task of predicting whether stock market will rise/fall in the next 10 trading days

- Random guessing:

  $P(correct) = 0.5$

- Make 10 random guesses in a row:

$$P(\#correct \geq 8) = \frac{\binom{10}{8} + \binom{10}{9} + \binom{10}{10}}{2^{10}} = 0.0547$$

| | |
|---|---|
| Day 1 | Up |
| Day 2 | Down |
| Day 3 | Down |
| Day 4 | Up |
| Day 5 | Down |
| Day 6 | Down |
| Day 7 | Up |
| Day 8 | Up |
| Day 9 | Up |
| Day 10 | Down |

# Effect of Multiple Comparison Procedure

- Approach:
  - Get 50 analysts
  - Each analyst makes 10 random guesses
  - Choose the analyst that makes the most number of correct predictions

- Probability that at least one analyst makes at least 8 correct predictions

$$P(\#correct \geq 8) = 1 - (1 - 0.0547)^{50} = 0.9399$$

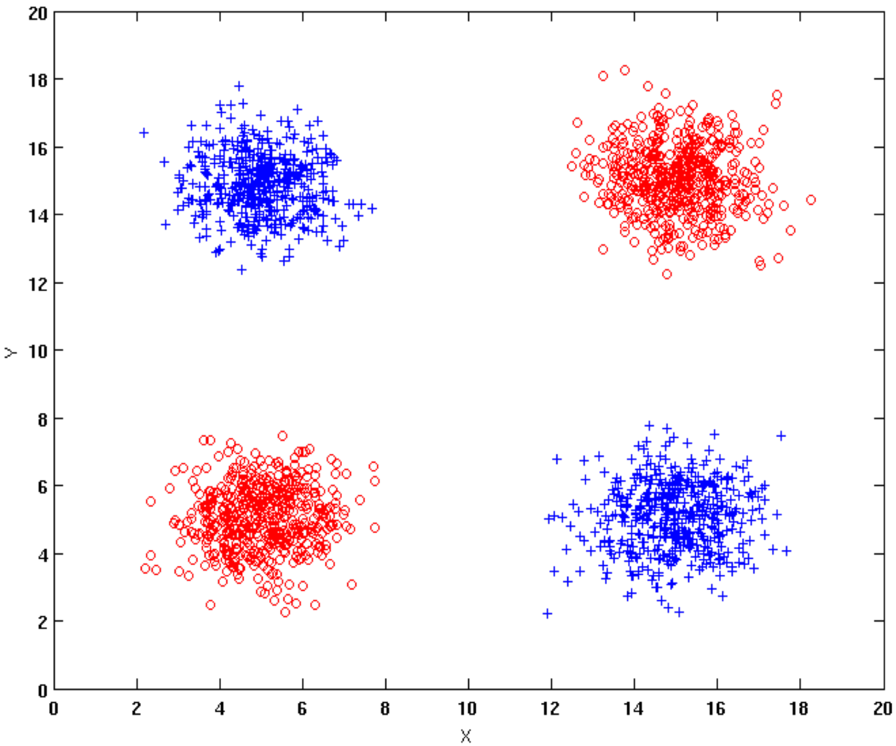
# Effect of Multiple Comparison Procedure

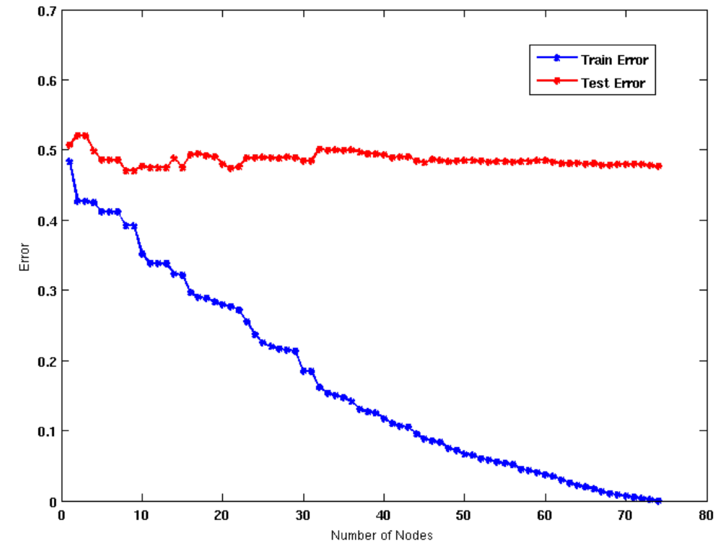
- Many algorithms employ the following greedy strategy:
  - Initial model: M
  - Alternative model: M' = M $\cup$ $\gamma$,
    where $\gamma$ is a component to be added to the model (e.g., a test condition of a decision tree)
  - Keep M' if improvement, $\Delta$(M,M') > $\alpha$

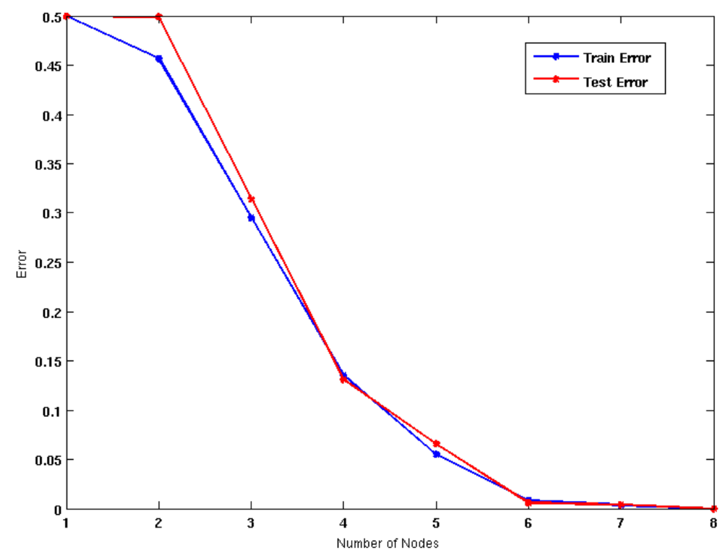
- Often times, $\gamma$ is chosen from a set of alternative components, $\Gamma = \{\gamma_1, \gamma_2, \ldots, \gamma_k\}$

- If many alternatives are available, one may inadvertently add irrelevant components to the model, resulting in model overfitting

# Effect of Multiple Comparison - Example




Use additional 100 noisy variables generated from a uniform distribution along with X and Y as attributes.

Use 30% of the data for training and 70% of the data for testing

**Using only X and Y as attributes**

# Notes on Overfitting

- Overfitting results in decision trees that are <u>more complex</u> 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

## Model Selection:
# 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

Model Selection:

# Incorporating Model Complexity

- Rationale: Occam's Razor
  - Given two models of similar generalization errors, one should prefer the simpler model over the more complex model
  - A complex model has a greater chance of being fitted accidentally
  - Therefore, one should include model complexity when evaluating a model

Gen. Error(Model) = Train. Error(Model, Train. Data) + $\alpha$ x Complexity(Model)

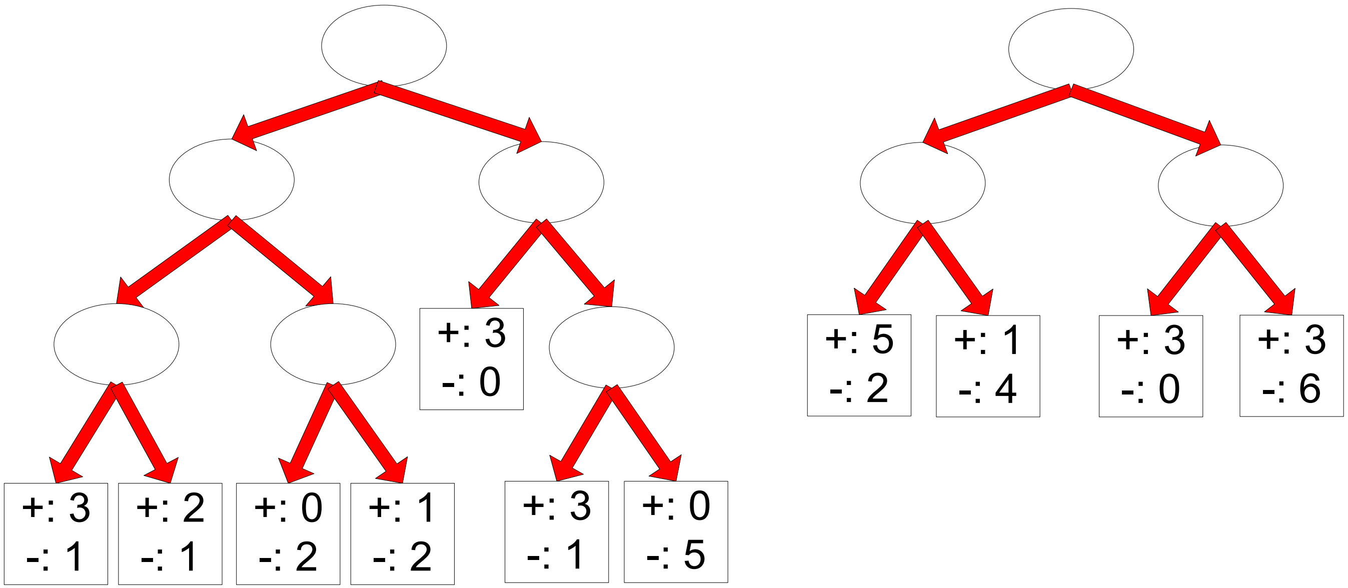
# Estimating the Complexity of Decision Trees

- **Pessimistic Error Estimate** of decision tree $T$ with k leaf nodes:

$$err_{gen}(T) = err(T) + \Omega \times \frac{k}{N_{train}}$$

  - err(T): error rate on all training records
  - $\Omega$: trade-off hyper-parameter (similar to $\alpha$)
    - Relative cost of adding a leaf node
  - k: number of leaf nodes
  - $N_{train}$: total number of training records

# Estimating the Complexity of Decision Trees: Example




Decision Tree, $T_L$ Decision Tree, $T_R$

**$e(T_L) = 4/24$**

**$e(T_R) = 6/24$**

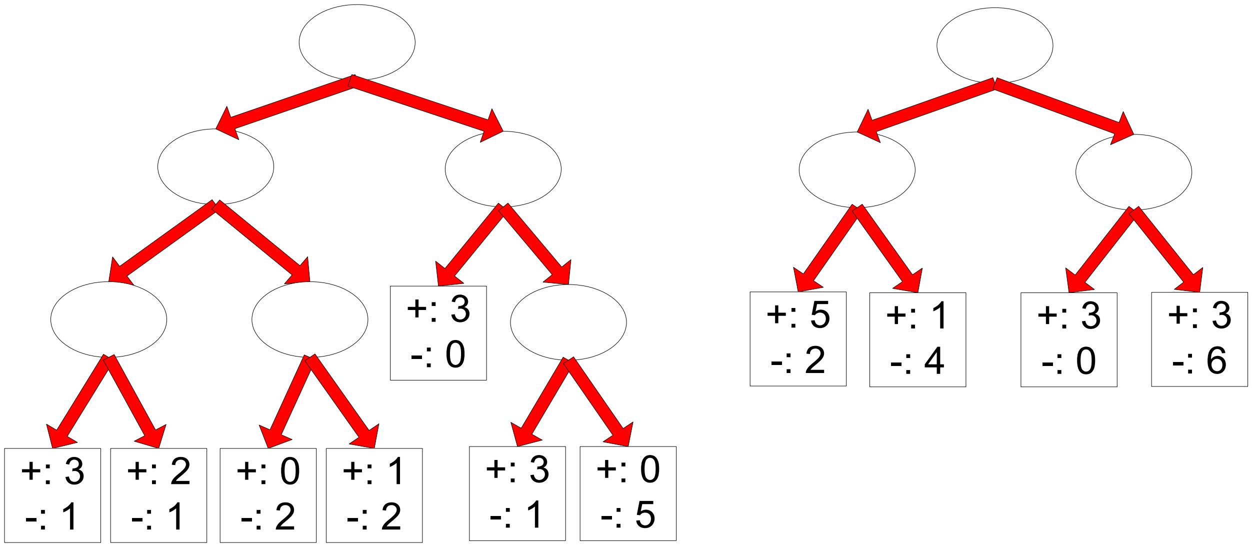
**$\Omega = 1$**

**$e_{gen}(T_L) = 4/24 + 1*7/24 = 11/24 = 0.458$**

**$e_{gen}(T_R) = 6/24 + 1*4/24 = 10/24 = 0.417$**

# Estimating the Complexity of Decision Trees

- Resubstitution Estimate:
  - Using training error as an optimistic estimate of generalization error
  - Referred to as optimistic error estimate




Decision Tree, $T_L$

Decision Tree, $T_R$

$e(T_L) = 4/24$

$e(T_R) = 6/24$

# Model Selection for Decision Trees

- Pre-Pruning (Early Stopping Rule)
  - Stop the algorithm before it becomes a fully-grown tree
  - Typical stopping conditions for a node:
    - Stop if all instances belong to the same class
    - Stop if all the attribute values are the same
  - More restrictive conditions:
    - Stop if number of instances is less than some user-specified threshold
    - Stop if class distribution of instances are independent of the available features (e.g., using $\chi^2$ test)
    - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain).
    - Stop if estimated generalization error falls below certain threshold

# Model Selection for Decision Trees

- Post-pruning
  - Grow decision tree to its entirety
  - Subtree replacement
    - Trim the nodes of the decision tree in a bottom-up fashion
    - If generalization error improves after trimming, replace sub-tree by a leaf node
    - Class label of leaf node is determined from majority class of instances in the sub-tree

# Example of Post-Pruning

| | |
|---|---|
| Class = Yes | 20 |
| Class = No | 10 |
| Error = 10/30 | |

**Training Error (Before splitting) = 10/30**

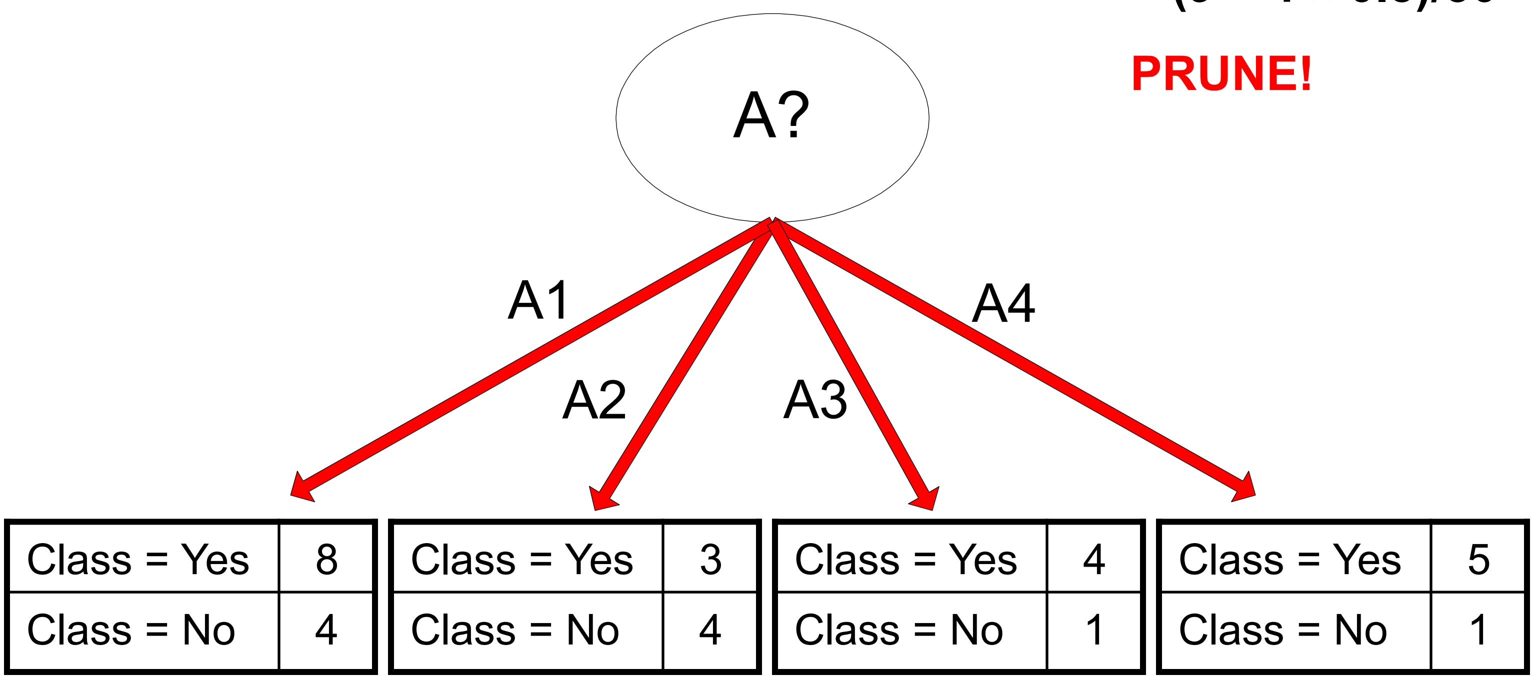
**Pessimistic error = (10 + 0.5)/30 = 10.5/30**

**Training Error (After splitting) = 9/30**

**Pessimistic error (After splitting)**

**$= (9 + 4 \times 0.5)/30 = 11/30$**

**PRUNE!**



# Examples of Post-pruning

**Decision Tree:**

```
depth = 1 :
|   breadth > 7 : class 1
|   breadth <= 7 :
|   |   breadth <= 3 :
|   |   |   ImagePages > 0.375 : class 0
|   |   |   ImagePages <= 0.375 :
|   |   |   |   totalPages <= 6 : class 1
|   |   |   |   totalPages > 6 :
|   |   |   |   |   breadth <= 1 : class 1
|   |   |   |   |   breadth > 1 : class 0
|   |   width > 3 :
|   |   |   MultiIP = 0:
|   |   |   |   ImagePages <= 0.1333 : class 1
|   |   |   |   ImagePages > 0.1333 :
|   |   |   |   |   breadth <= 6 : class 0
|   |   |   |   |   breadth > 6 : class 1
|   |   |   MultiIP = 1:
|   |   |   |   TotalTime <= 361 : class 0
|   |   |   |   TotalTime > 361 : class 1
depth > 1 :
|   MultiAgent = 0:
|   |   depth > 2 : class 0
|   |   depth <= 2 :
|   |   |   MultiIP = 1: class 0
|   |   |   MultiIP = 0:
|   |   |   |   breadth <= 6 : class 0
|   |   |   |   breadth > 6 :
|   |   |   |   |   RepeatedAccess <= 0.0322 : class 0
|   |   |   |   |   RepeatedAccess > 0.0322 : class 1
|   MultiAgent = 1:
|   |   totalPages <= 81 : class 0
|   |   totalPages > 81 : class 1
```

Subtree Raising

Subtree Replacement

**Simplified Decision Tree:**

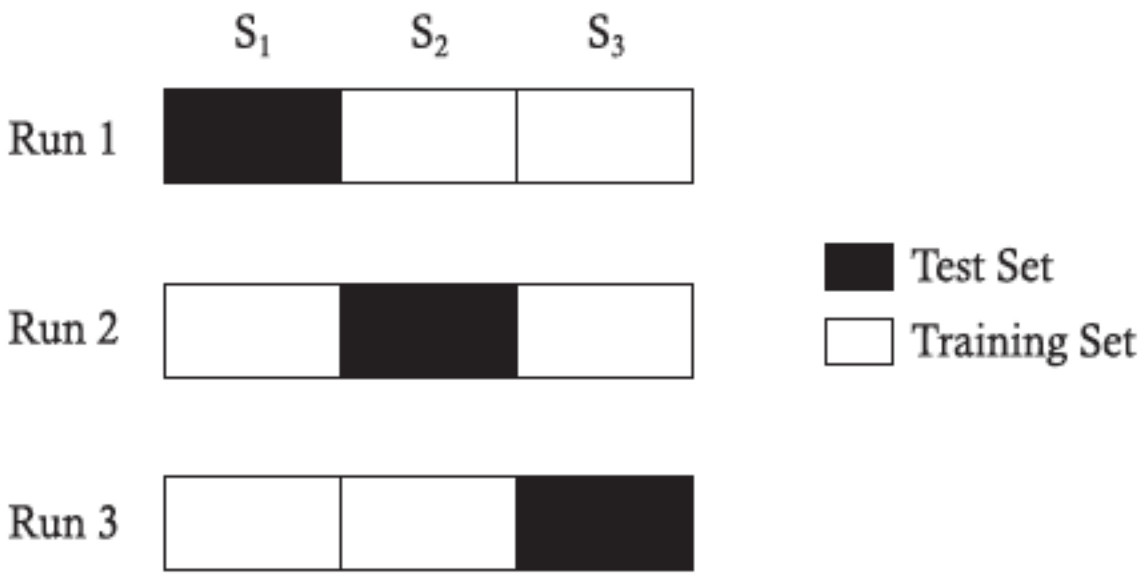
```
depth = 1 :
|   ImagePages <= 0.1333 : class 1
|   ImagePages > 0.1333 :
|   |   breadth <= 6 : class 0
|   |   breadth > 6 : class 1
depth > 1 :
|   MultiAgent = 0: class 0
|   MultiAgent = 1:
|   |   totalPages <= 81 : class 0
|   |   totalPages > 81 : class 1
```

# 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



# Variations on Cross-validation

- Repeated cross-validation
  - Perform cross-validation a number of times
  - Gives an estimate of the variance of the generalization error
- Stratified cross-validation
  - Guarantee the same percentage of class labels in training and test
  - Important when classes are imbalanced and the sample is small
- Use nested cross-validation approach for model selection and evaluation