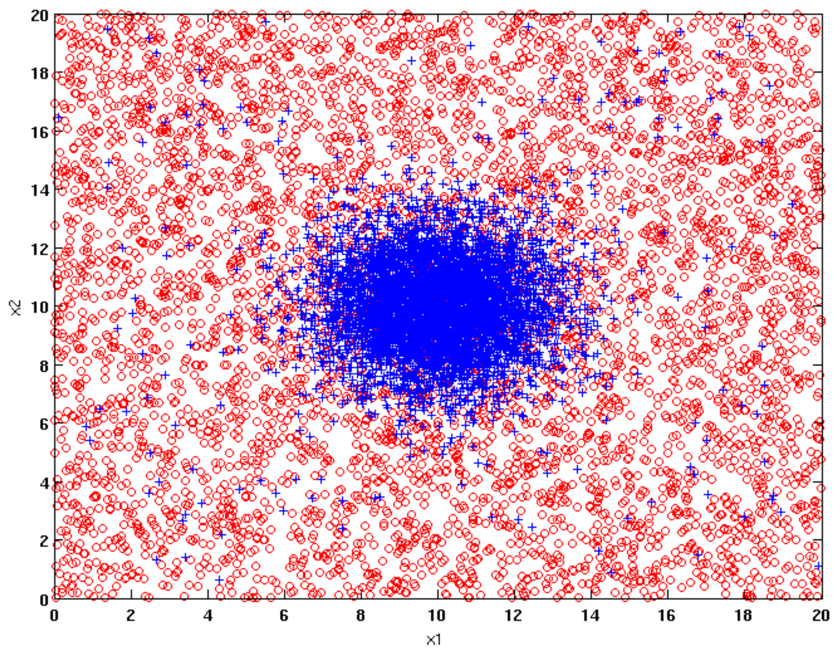
Classification Errors

- Training errors (apparent errors)
  - Errors committed on the training set

- Test errors
  - Errors committed on the test set

- Generalization error
  - Expected error of a model over random selection of records from same distribution

Example Data Set



Two class problem:

+ : 5400 instances

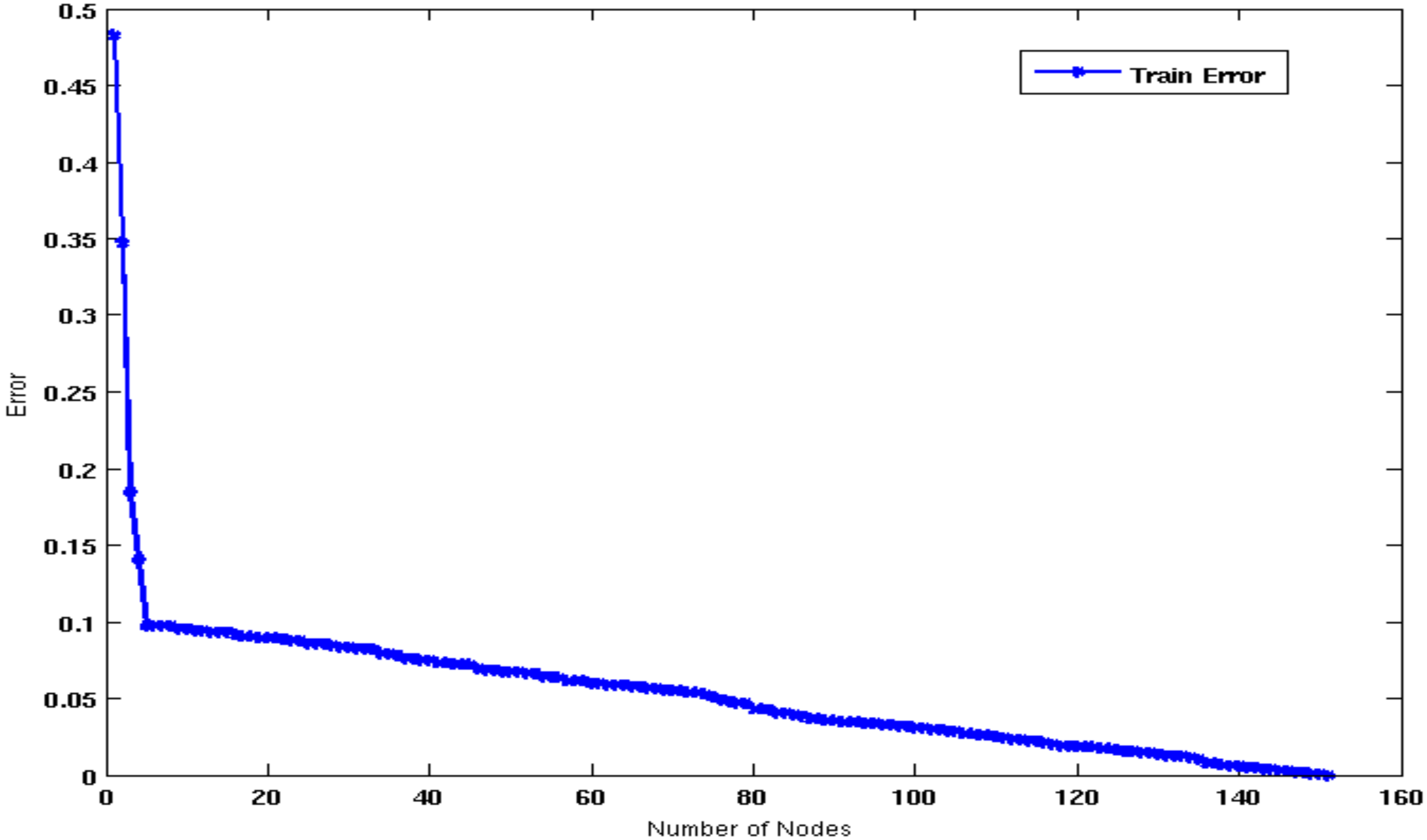
- **5000 instances generated from a Gaussian centered at (10,10)**
- **400 noisy instances added**

o : 5400 instances

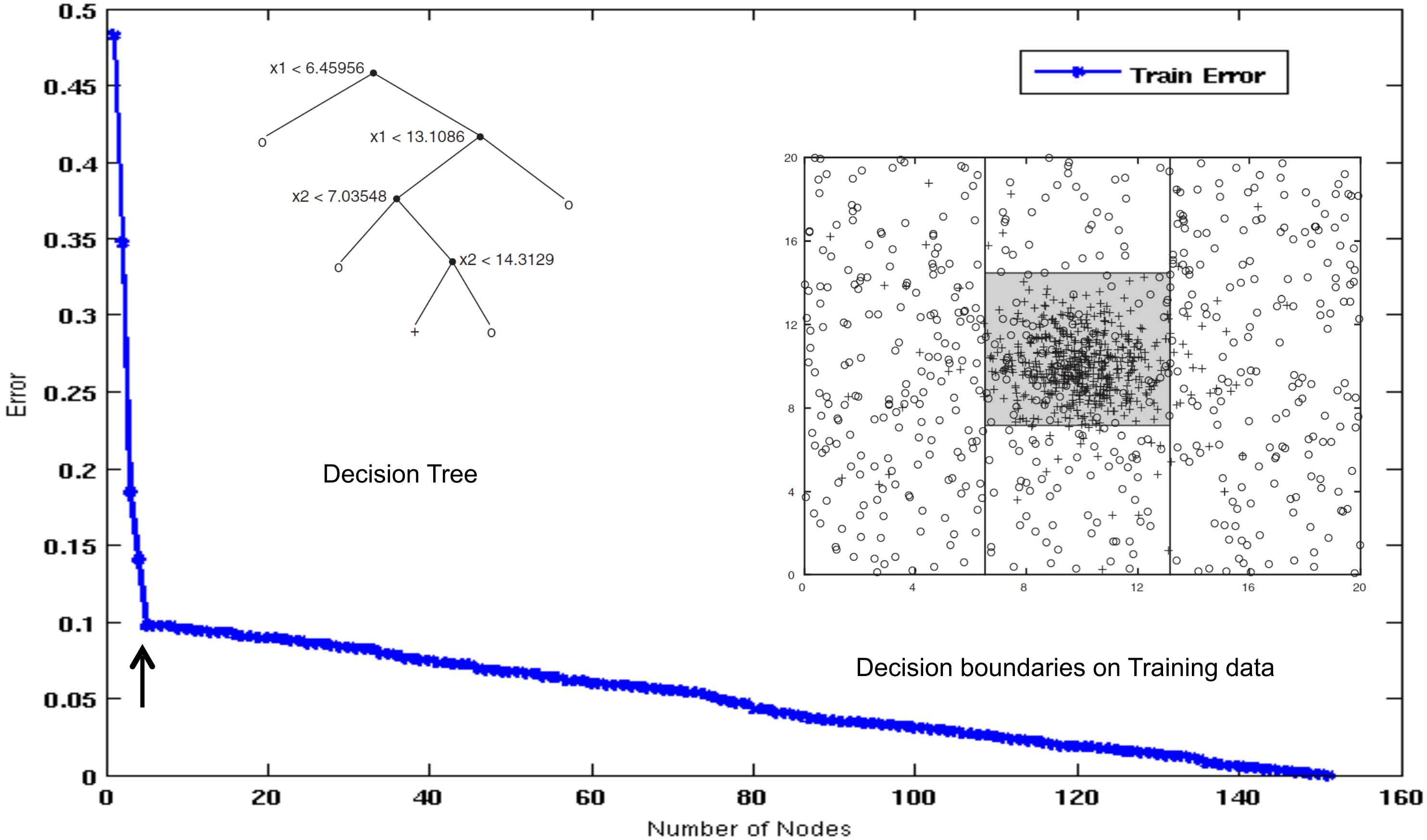
- **Generated from a uniform distribution**

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

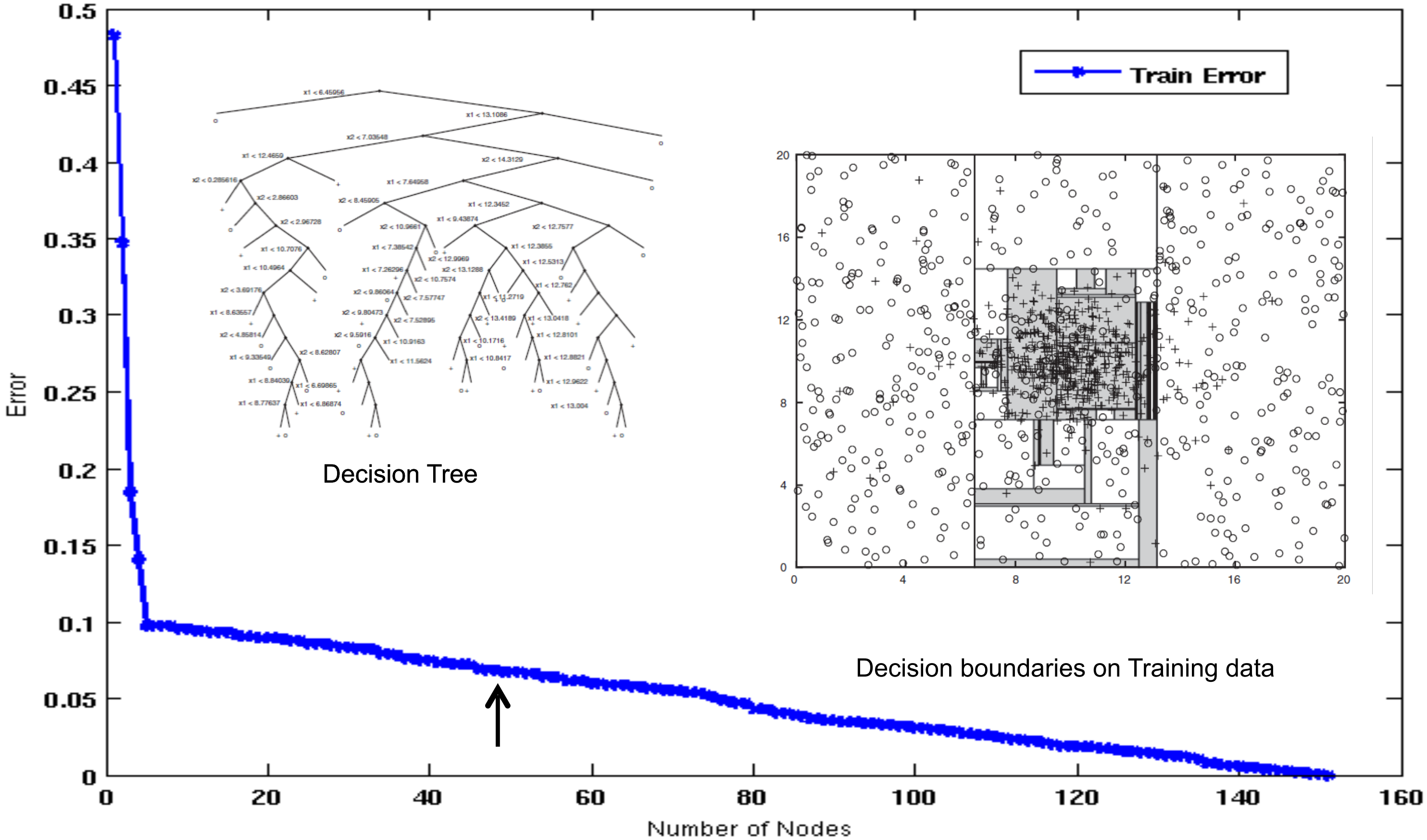
Increasing number of nodes in Decision Trees



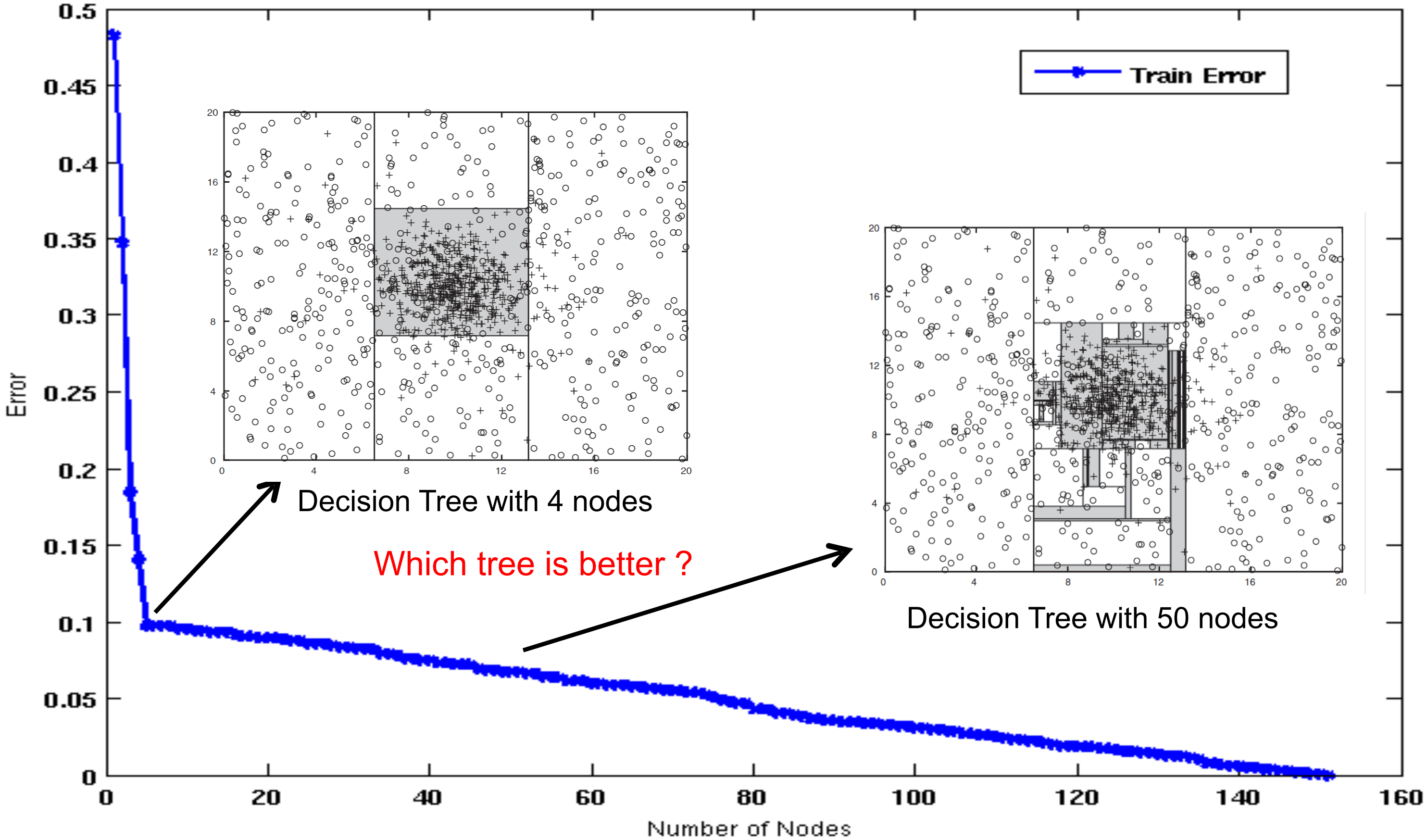
Decision Tree with 4 nodes



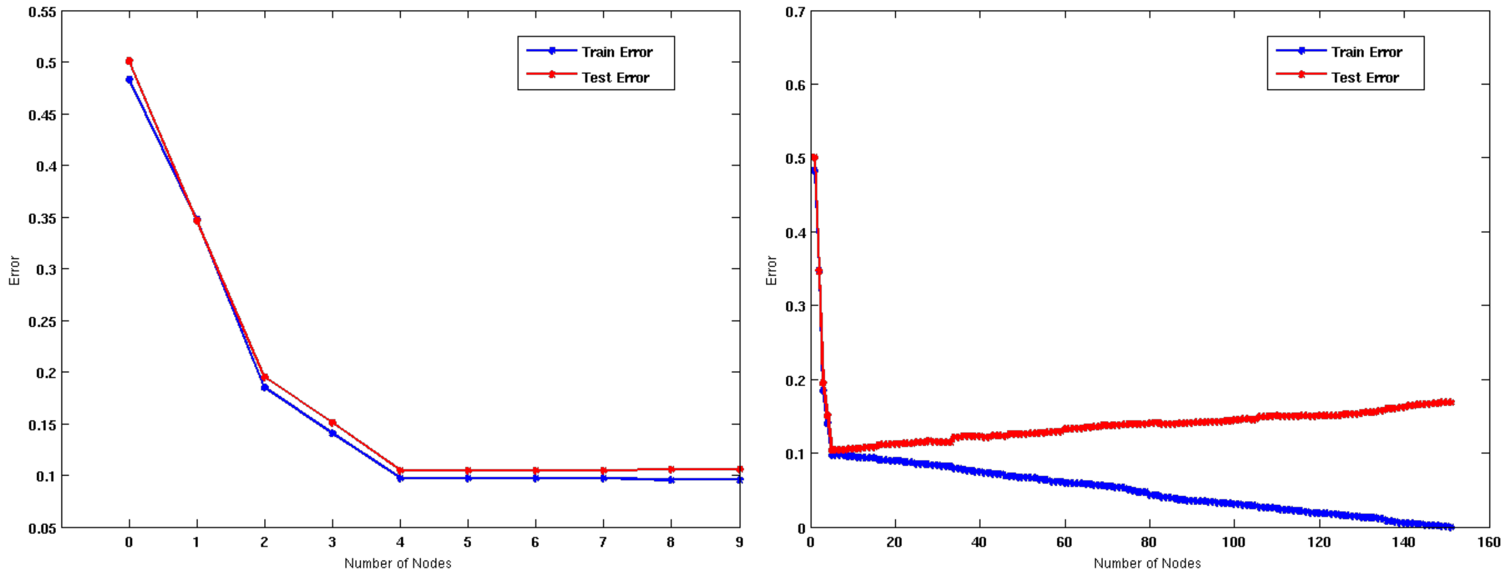
Decision Tree with 50 nodes



Which tree is better?



Model Overfitting

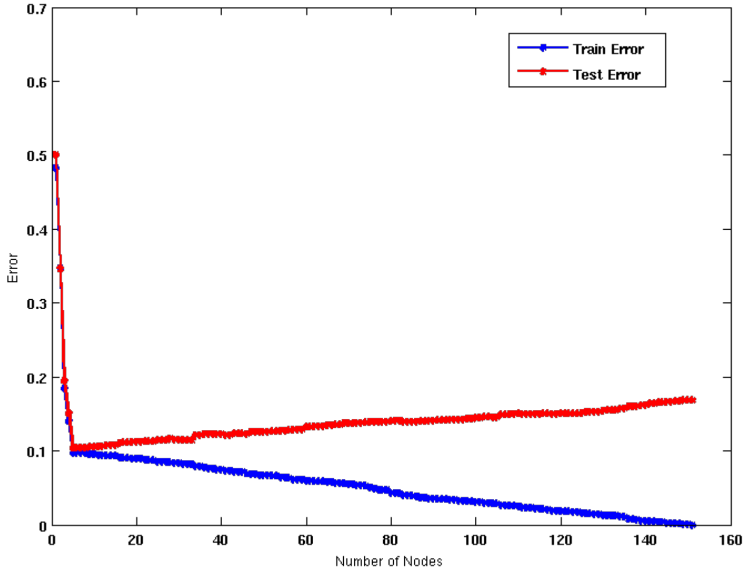


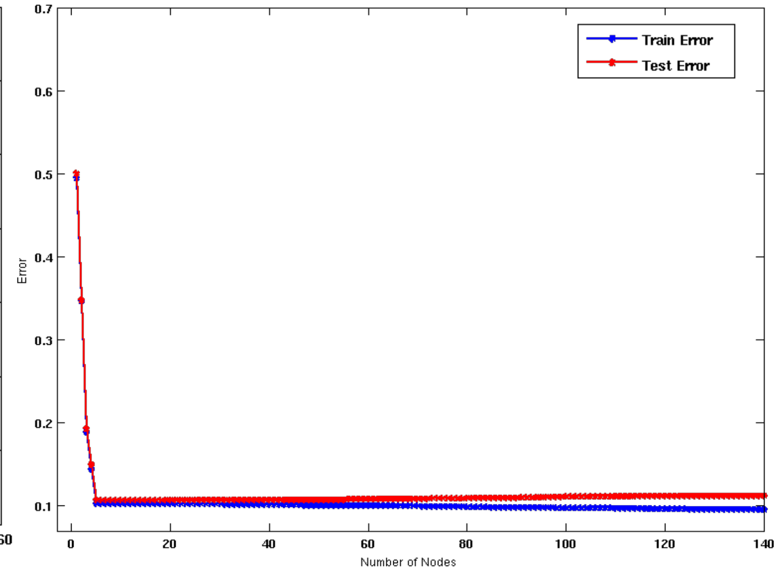
- As the model becomes more and more complex, test error can start increasing even though training error may be decreasing

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

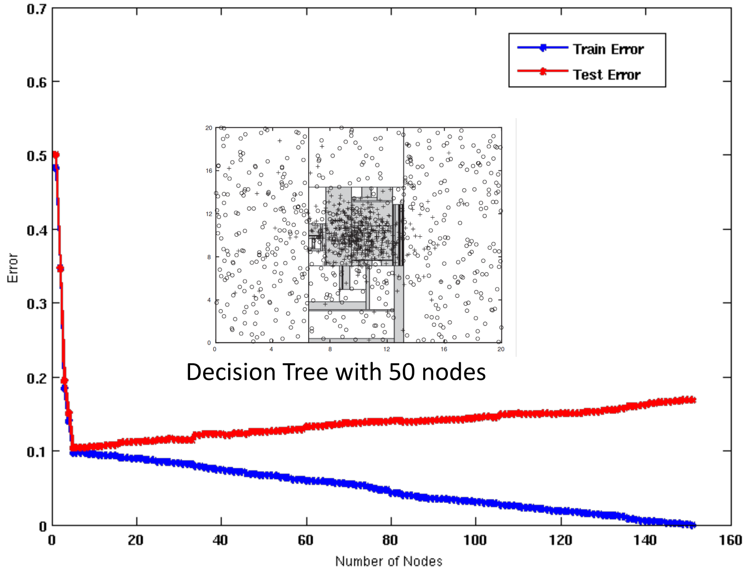


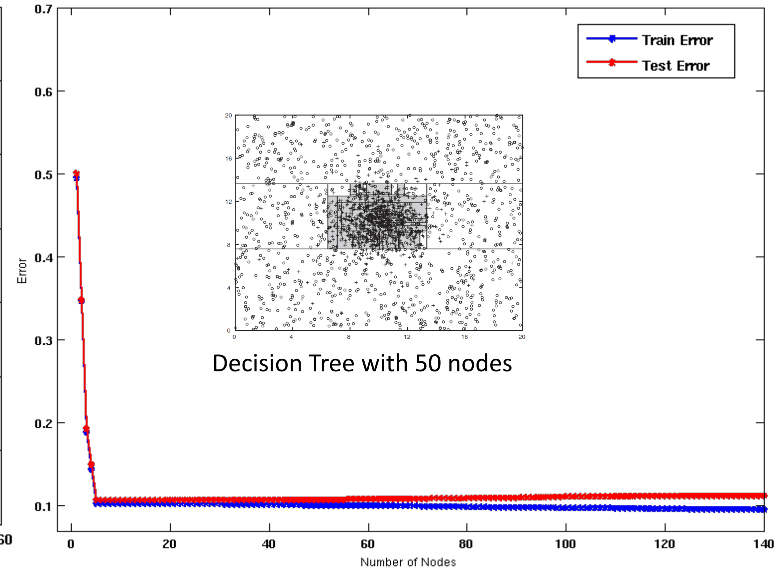


Using twice the number of data instances

- Increasing the size of training data reduces the difference between training and test error for a fixed model size.

Model Overfitting





Using twice the number of data instances

- Increasing the size of training data reduces the difference between training and test error for a fixed model size.

Reasons for Model Overfitting

- Limited Training Size

- High Model Complexity
  - Multiple Comparison Procedure

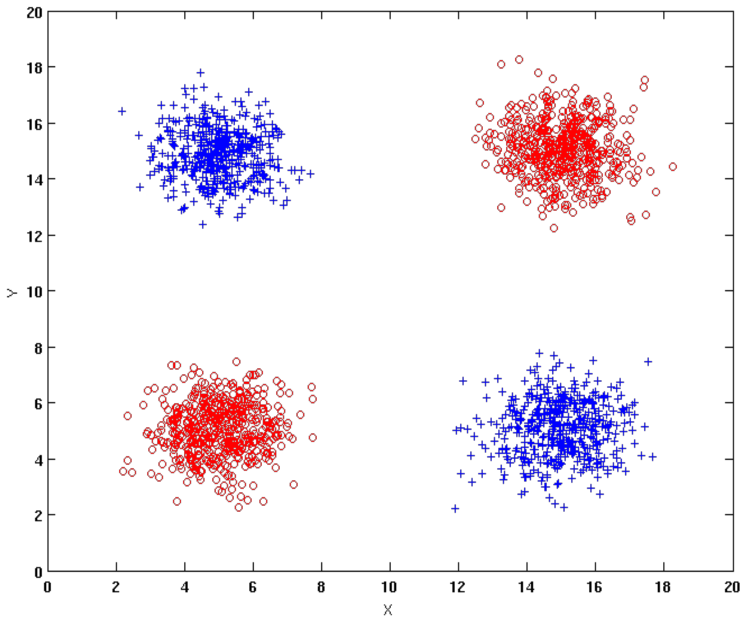
Effect of Multiple Comparison Procedure

- Many algorithms employ the following greedy strategy:
  - Initial model: M
  - Alternative model: $M' = M \cup \gamma$,
    where γ 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, γ is chosen from a set of alternative components, $\Gamma = \{\gamma_1, \gamma_2, \ldots, \gamma_k\}$

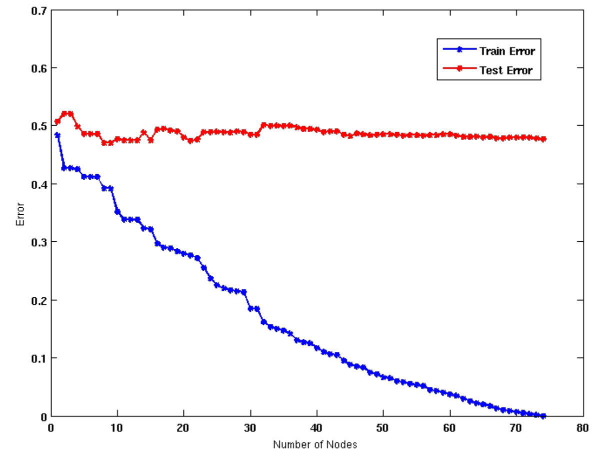
- If many alternatives are available, one may inadvertently add irrelevant components to the model, resulting in model overfitting

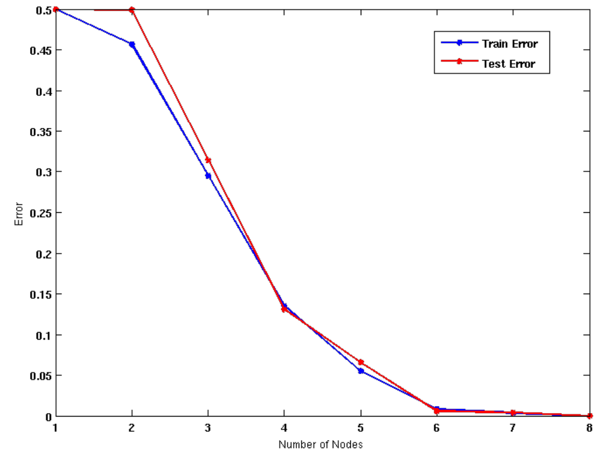
Effect of Multiple Comparison - Example



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 error

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/Cross-Validation
  - Incorporating Model Complexity
  - Estimating Statistical Bounds

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

Incorporating Model Complexity

- Rationale: Occam's Razor
  - Given two models with similar training error, 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

$$\text{Gen. Error(Model)} = \text{Train. Error(Model, Train. Data)} + \alpha \times \text{Complexity(Model)}$$

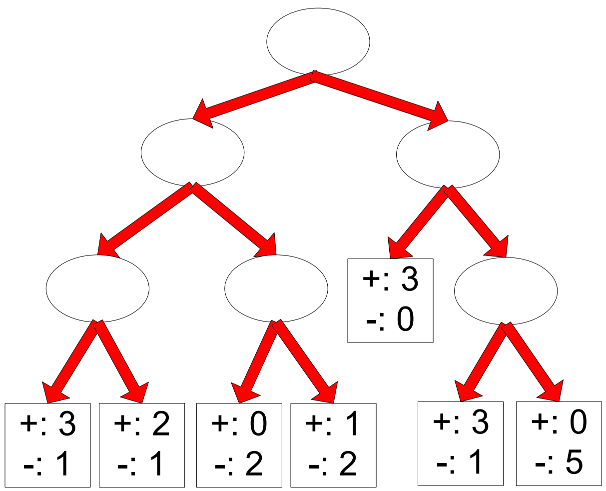
Estimating the Complexity of Decision Trees

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

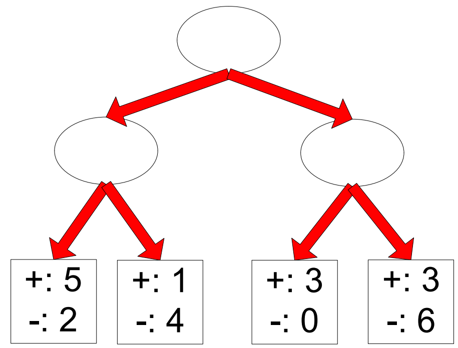
$$err_{gen}(T) = err(T) + \Omega \times \frac{k}{N_{train}}$$

  - err(T): error rate on all training records
  - Ω: trade-off hyper-parameter (similar to α)
    - 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

$e(T_L) = 4/24$

$e(T_R) = 6/24$

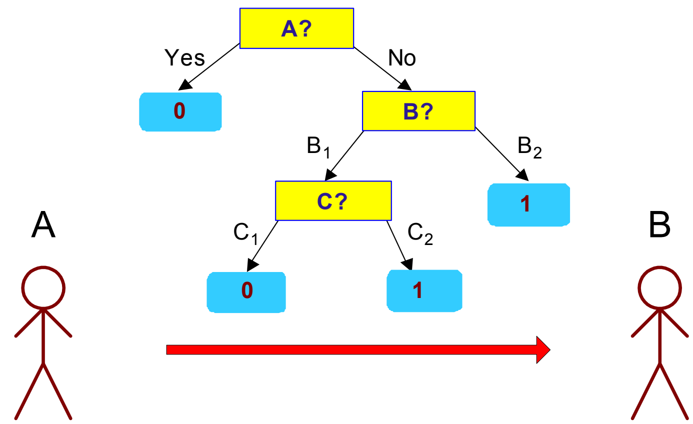
$\Omega = 1$

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

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

Minimum Description Length (MDL)

X	y
X_1	1
X_2	0
X_3	0
X_4	1
…	…
X_n	1



X	y
X_1	?
X_2	?
X_3	?
X_4	?
…	…
X_n	?

- Cost(Model,Data) = Cost(Data|Model) + α x Cost(Model)
  - Cost is the number of bits needed for encoding.
  - Search for the least costly model.
- Cost(Data|Model) encodes the misclassification errors.
- Cost(Model) uses node encoding (number of children) plus splitting condition encoding.