Classification error

- The errors committed by a classification model are generally divided into two types
  - Training errors
  - Generalization errors
- Training error is the number of misclassification errors committed on training records.
- Training error is also known as resubstitution error or apparent error.
- Generalization error is the expected error of the model on previously unseen records.

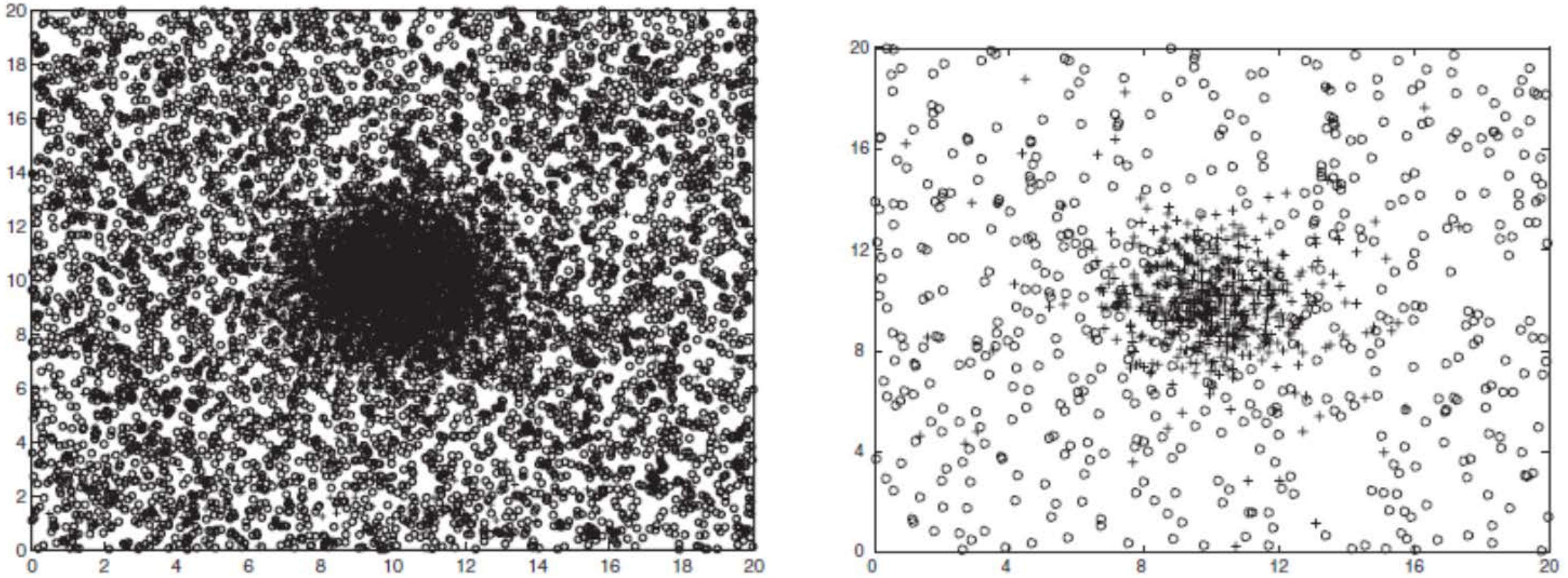
Classification error

- A good classification model should
  - Fit the training data well. (low training error)
  - Accurately classify records it has never seen before. (low generalization error)
- A model that fits the training data too well can have a poor generalization error.
- This is known as model overfitting.

Classification error

- We consider the 2-D data set in the following figure.
- The data set contains data points that belong to two different classes.
- 10% of the points are chosen for training, while the remaining 90% are used for testing.
- Decision tree classifiers with different numbers of leaf nodes are built using the training set.

Classification error

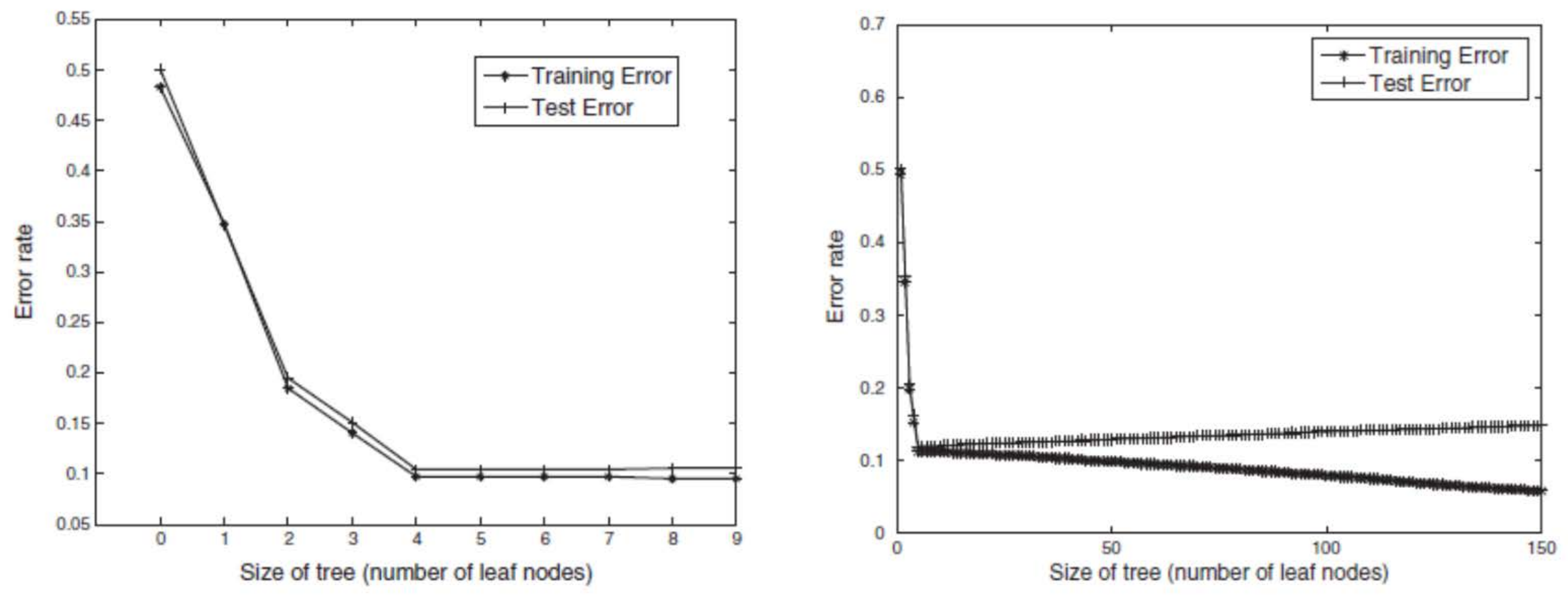


(a) Example of a 2-D data. (b) Training set using 10% data.

Classification error

- The following figure shows the training and test error rates of the decision tree.
- Both error rates are large when the size of the tree is very small.
- This situation is known as model underfitting.
- Underfitting occurs because the model cannot learn the true structure of the data.
- It performs poorly on both the training and test sets.

Classification error



(a) Varying tree size from 1 to 8. (b) Varying tree size from 1 to 150.

Classification error

- When the tree becomes too large
  - The training error rate continues to decrease.
  - However, the test error rate begins to increase.
- This phenomenon is known as model overfitting.

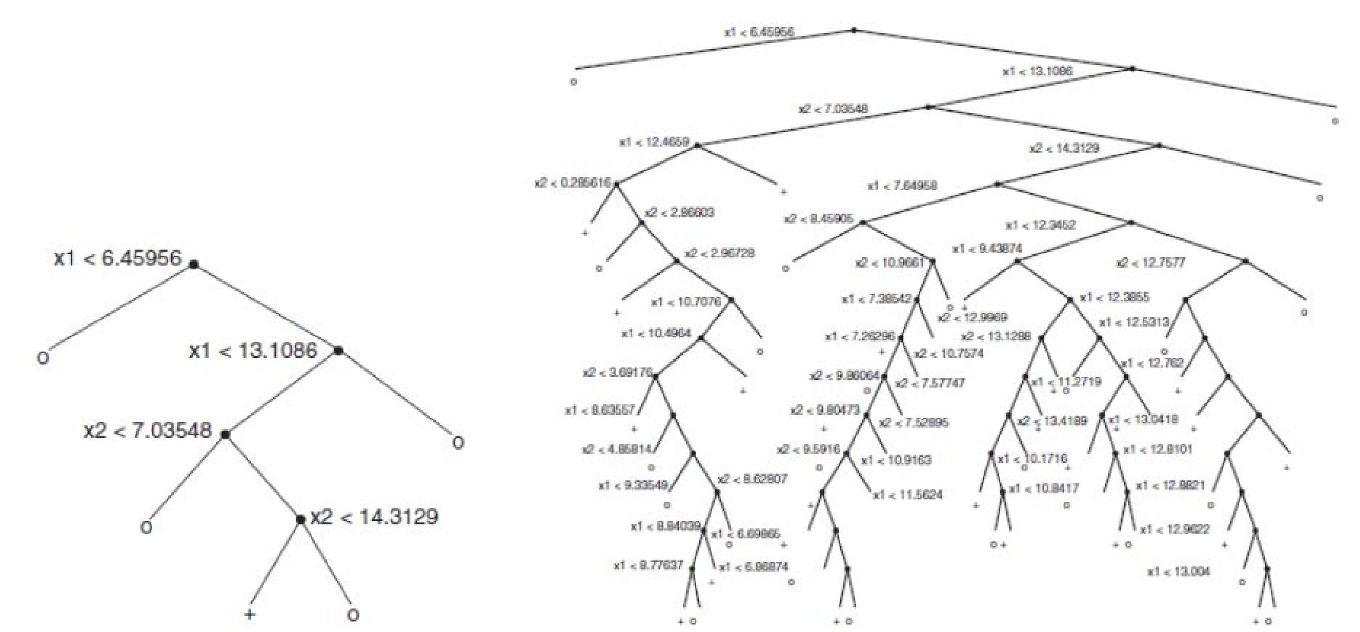
Overfitting

- The training error can be reduced by increasing the model complexity.
- However, the test error can be large because the model may accidentally fit some of the noise points in the training data.
- In other words, the performance of the model on the training set does not generalize well to the test examples.

Overfitting

- We consider two decision trees, one with 5 leaf nodes and one with 50 leaf nodes.
- The two decision trees and their corresponding decision boundaries are shown in the following figures.

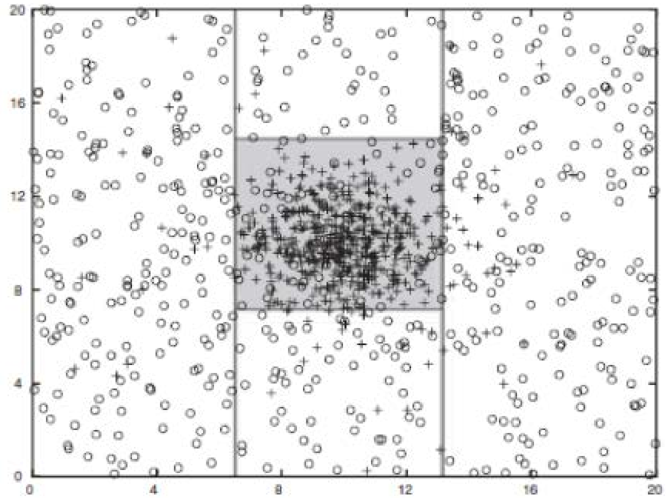
Overfitting



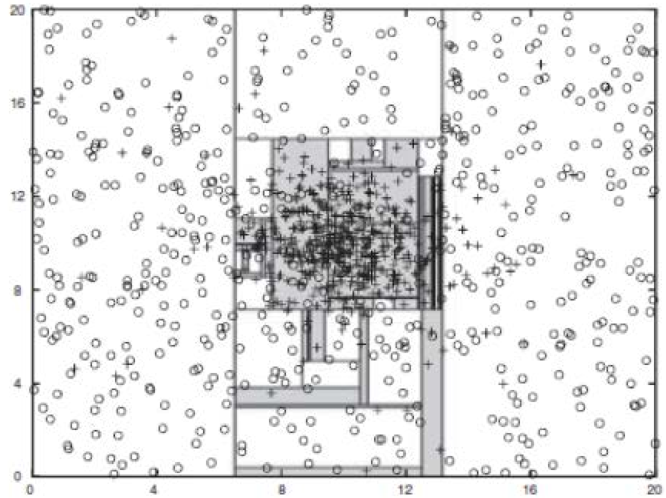
(a) Decision tree with 5 leaf nodes.

(b) Decision tree with 50 leaf nodes.

Overfitting



(c) Decision boundary for tree with 5 leaf nodes.



(d) Decision boundary for tree with 50 leaf nodes.

Overfitting

- The decision boundaries constructed by the tree with 5 leaf nodes represent a reasonable approximation of the optimal solution.
- It is expected that this set of decision boundaries will result in a good classification performance on the test set.

Overfitting

- On the other hand, the tree with 50 leaf nodes generates a set of complicated decision boundaries.
- Some of the shaded regions corresponding to the ‘+’ class only contain a few ‘+’ training instances, among a large number of surrounding ‘○’ instances.
- This excessive fine-tuning to specific patterns in the data will lead to unsatisfactory classification performance on the test set.

Generalization error estimation

- The ideal classification model is the one that produces the lowest generalization error.
- The problem is that the model has no knowledge of the test set.
- It has access only to the training set.
- We consider the following approaches to estimate the generalization error
  - Resubstitution estimate
  - Estimates incorporating model complexity
  - Using a validation set

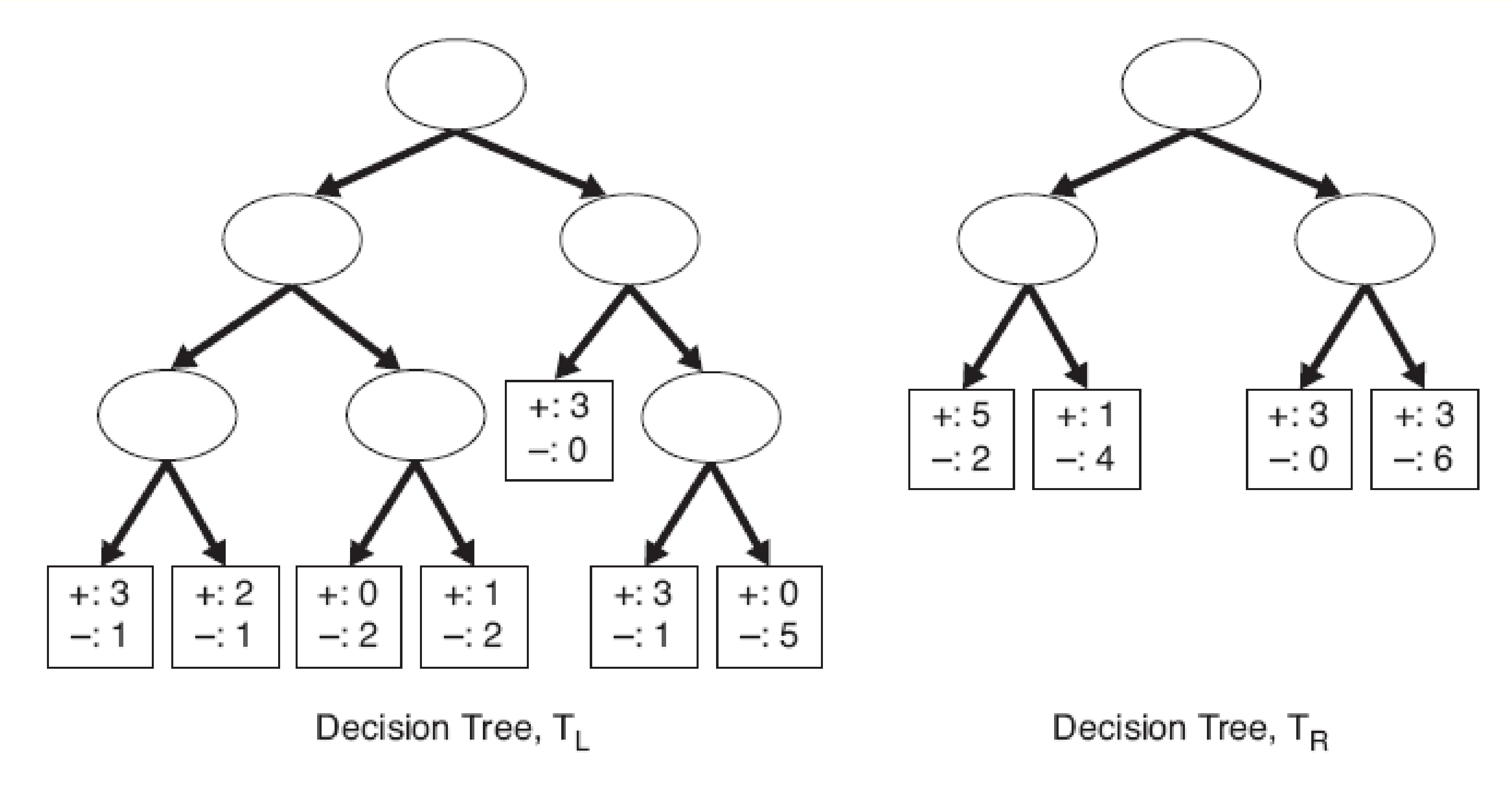
Resubstitution estimate

- The resubstitution estimate approach assumes that the training set is a good representation of the overall data.
- However, the training error is usually an optimistic estimate of the generalization error.

Resubstitution estimate

- We consider the two decision trees shown in the following figure.
- The left tree T_L is more complex than the right tree T_R.
- The training error rate for T_L is $e(T_L)=4/24=0.167$.
- The training error rate for T_R is $e(T_R)=6/24=0.25$.
- Based on the resubstitution estimate, T_L is considered better than T_R.

Resubstitution estimate



Estimates incorporating model complexity

- The chance for model overfitting increases as the model becomes more complex.
- As a result, we should prefer simpler models.
- Based on this principle, we can estimate the generalization error as the sum of
  - Training error and
  - A penalty term for model complexity.

Estimates incorporating model complexity

- We consider the previous two decision trees T_L and T_R.
- We assume that the penalty term is equal to 0.5 for each leaf node.
- The error rate estimate for T_L is

$$e_c(T_L) = \frac{4 + 7 \times 0.5}{24} = \frac{7.5}{24} = 0.3125$$

- The error rate estimate for T_R is

$$e_c(T_R) = \frac{6 + 4 \times 0.5}{24} = \frac{8}{24} = 0.3333$$

Estimates incorporating model complexity

- Based on this penalty term, T_L is better than T_R.
- For a binary tree, a penalty term of 0.5 means that a node should always be expanded into its two child nodes if it improves the classification of at least one training record.
- This is because expanding a node, which is the same as adding 0.5 to the overall error, is less costly than committing one training error.

Estimates incorporating model complexity

- Suppose the penalty term is equal to 1 for all the leaf nodes.
- The error rate estimate for T_L becomes 0.458.
- The error rate estimate for T_R becomes 0.417.
- Based on this penalty term, T_R is better than T_L.
- A penalty term of 1 means that, for a binary tree, a node should not be expanded unless it reduces the classification error by more than one training record.

Using a validation set

- In this approach, the original training data is divided into two smaller subsets.
- One of the subsets is used for training.
- The other, known as the validation set, is used for estimating the generalization error.

Using a validation set

- This approach can be used in the case where the complexity of the model is determined by a parameter.
- We can adjust the parameter until the resulting model attains the lowest error on the validation set.
- This approach provides a better way for estimating how well the model performs on previously unseen records.
- However, less data are available for training.

Handling overfitting in decision tree

- There are two approaches for avoiding model overfitting in decision tree
  - Pre-pruning
  - Post-pruning

Pre-pruning

- In this approach, the tree growing algorithm is halted before generating a fully grown tree that perfectly fits the training data.
- To do this, an alternative stopping condition could be used.
- For example, we can stop expanding a node when the observed change in impurity measure falls below a certain threshold.

Pre-pruning

- The advantage of this approach is that it avoids generating overly complex sub-trees that overfit the training data.
- However, it is difficult to choose the right threshold for the change in impurity measure.
- A threshold which is too high will result in underfitted models.
- A threshold which is too low may not be sufficient to overcome the model overfitting problem.

Post-pruning

- In this approach, the decision tree is initially grown to its maximum size.
- This is followed by a tree pruning step, which trims the fully grown tree.

Post-pruning

- Trimming can be done by replacing a sub-tree with a new leaf node whose class label is determined from the majority class of records associated with the node.
- The tree pruning step terminates when no further improvement is observed.

Post-pruning

- Post-pruning tends to give better results than pre-pruning because it makes pruning decisions based on a fully grown tree.
- On the other hand, pre-pruning can suffer from premature termination of the tree growing process.
- However, for post-pruning, the additional computations for growing the full tree may be wasted when some of the sub-trees are pruned.

Classifier evaluation

- There are a number of methods to evaluate the performance of a classifier
  - Hold-out method
  - Cross validation

Hold-out method

- In this method, the original data set is partitioned into two disjoint sets.
- These are called the training set and test set respectively.
- The classification model is constructed from the training set.
- The performance of the model is evaluated using the test set.

Hold-out method

- The hold-out method has a number of well known limitations.
- First, fewer examples are available for training.
- Second, the model may be highly dependent on the composition of the training and test sets.

Cross validation

- In this approach, each record is used the same number of times for training, and exactly once for testing.
- To illustrate this method, suppose we partition the data into two equal-sized subsets.
- First, we choose one of the subsets for training and the other for testing.
- We then swap the roles of the subsets so that the previous training set becomes the test set, and vice versa.

Cross validation

- The estimated error is obtained by averaging the errors on the test sets for both runs.
- In this example, each record is used exactly once for training and once for testing.
- This approach is called two-fold cross-validation.

Cross validation

- The k-fold cross validation method generalizes this approach by segmenting the data into k equal-sized partitions.
- During each run
  - One of the partitions is chosen for testing.
  - The rest of them are used for training.
- This procedure is repeated k times so that each partition is used for testing exactly once.
- The estimated error is obtained by averaging the errors on the test sets for all k runs.