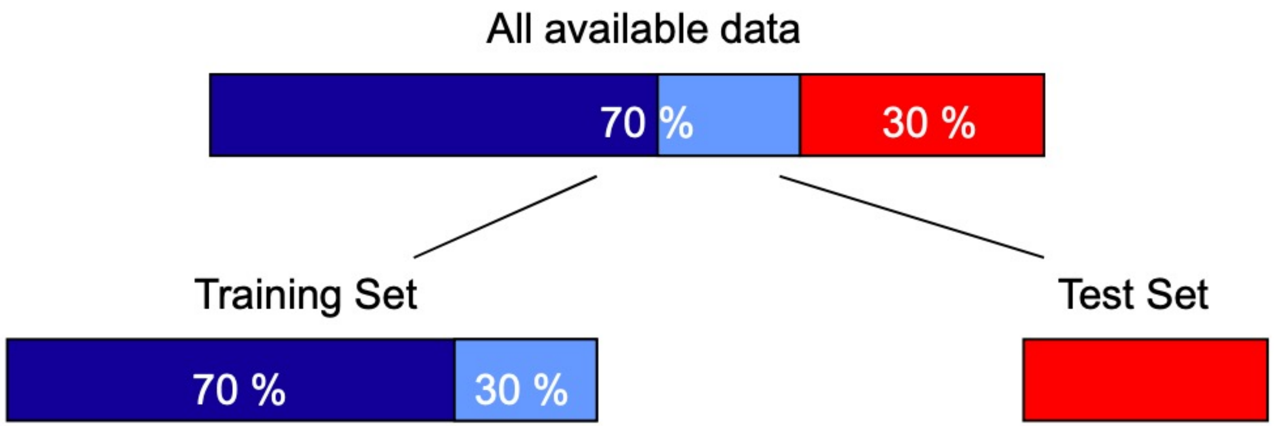
# CLASSIFICATION

# MODEL SELECTION

- Performed during model building
- Select a model that is not overly complex
  - (potential concerns for overly complex model: overfitting)
- Estimate generalization error
  - validation set
  - model complexity

# MODEL SELECTION: USING VALIDATION SET

- Divide training data into two parts:
  - Training set:
  - Validation set:
    - use for estimating generalization error




- 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
  - A complex model has a greater chance of overfitting
  - Include model complexity when evaluating a model

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

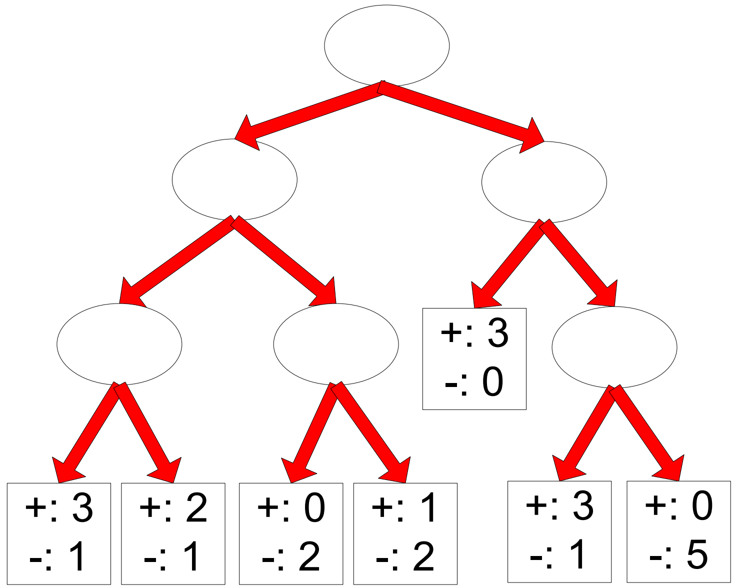
# ESTIMATING THE COMPLEXITY OF DECISION TREES

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

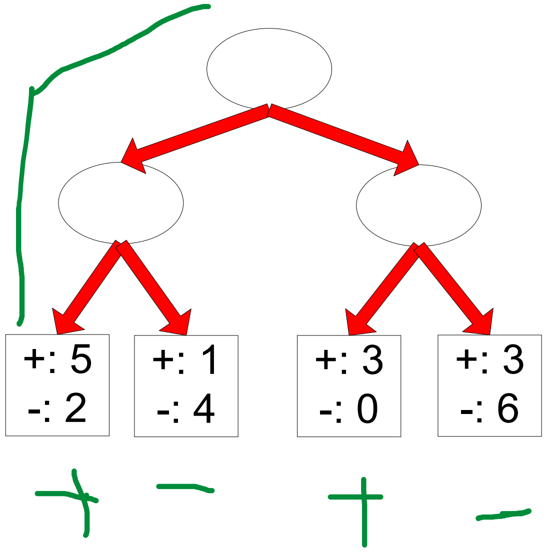
$$err_{gen}(T) = err(T) + \Omega \times \frac{k}{N_{train}}$$

  - 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

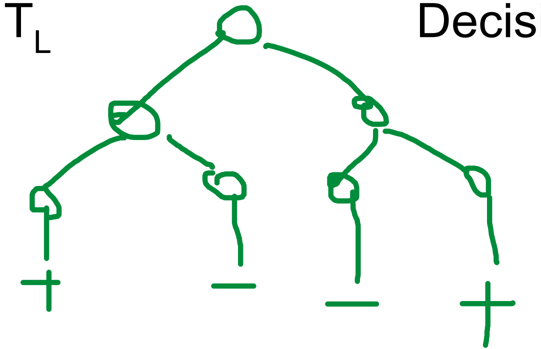
# ESTIMATING THE COMPLEXITY OF DECISION TREES: EXAMPLE




Decision Tree, $T_L$




Decision Tree, $T_R$




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

$e(T_L) = 4/24$

$e(T_R) = 6/24$

$\Omega = 1$

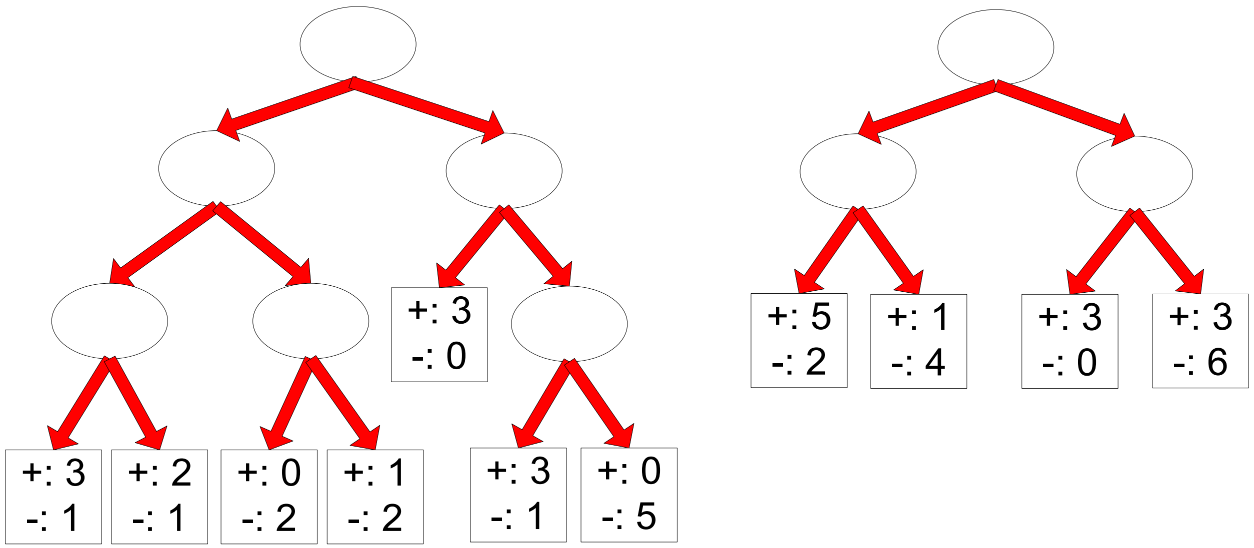
Pessimistic errors for both trees

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

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

# ESTIMATING THE COMPLEXITY OF DECISION TREES

- Resubstitution Estimate:
  - optimistic error estimate: using training error as an estimate of generalization error




Decision Tree, $T_L$

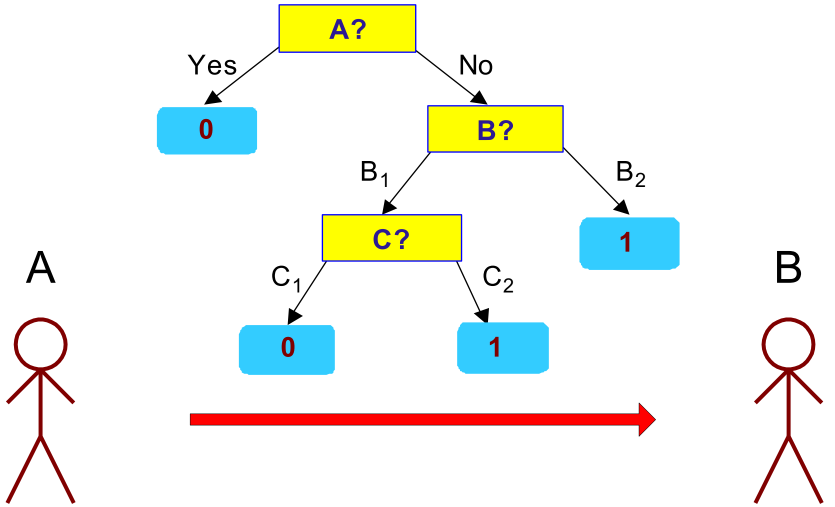
Decision Tree, $T_R$

$e(T_L) = 4/24$

$e(T_R) = 6/24$

# 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) + $\alpha$ 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.

# 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

    or Stop if all the attribute values are the same

  - More restrictive conditions:

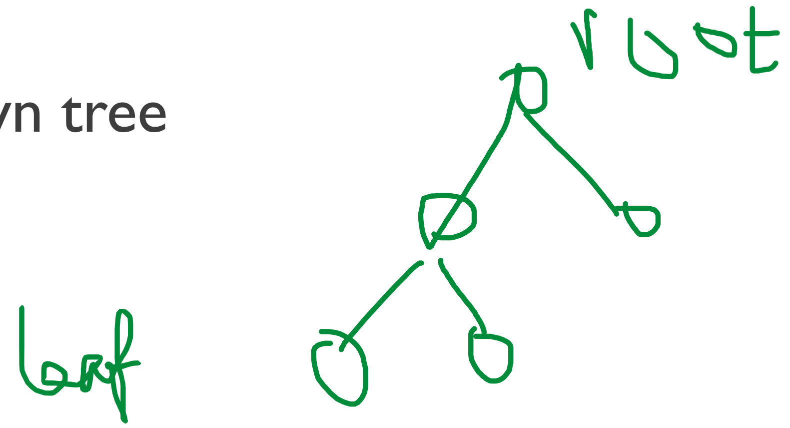
    Stop if the number of instances is < some user-specified threshold

    or Stop if class distribution of instances are independent of the available features (e.g., using $\chi^2$ test)

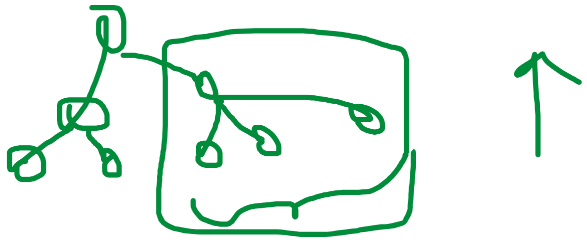
    or Stop if expanding the current node does not improve impurity measures

    (e.g., Gini or information gain).

    or 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

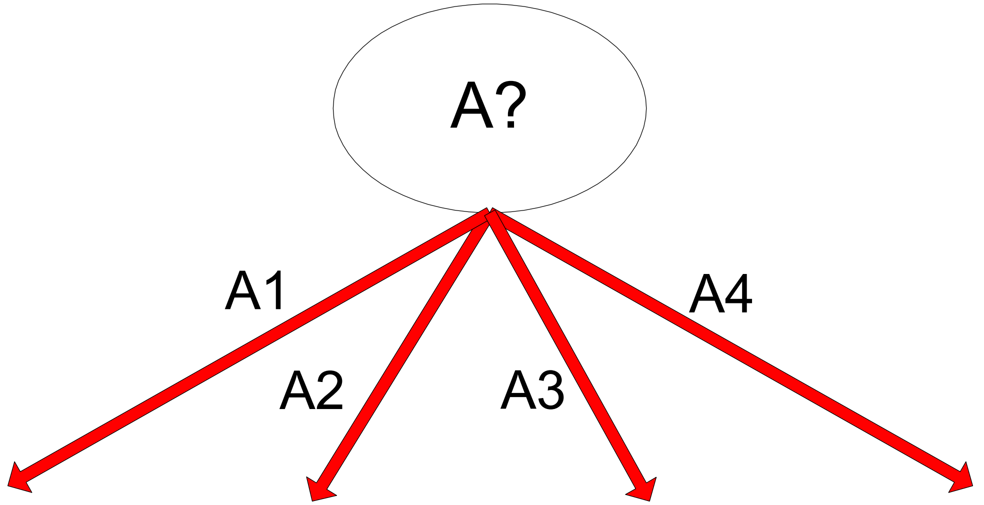
# EXAMPLE OF POST-PRUNING

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

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

Training Error (Before splitting) = 10/30

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




| | |
|---|---|
| Class = Yes | 8 |
| Class = No | 4 |

| | |
|---|---|
| Class = Yes | 3 |
| Class = No | 4 |

| | |
|---|---|
| Class = Yes | 4 |
| Class = No | 1 |

| | |
|---|---|
| Class = Yes | 5 |
| Class = No | 1 |

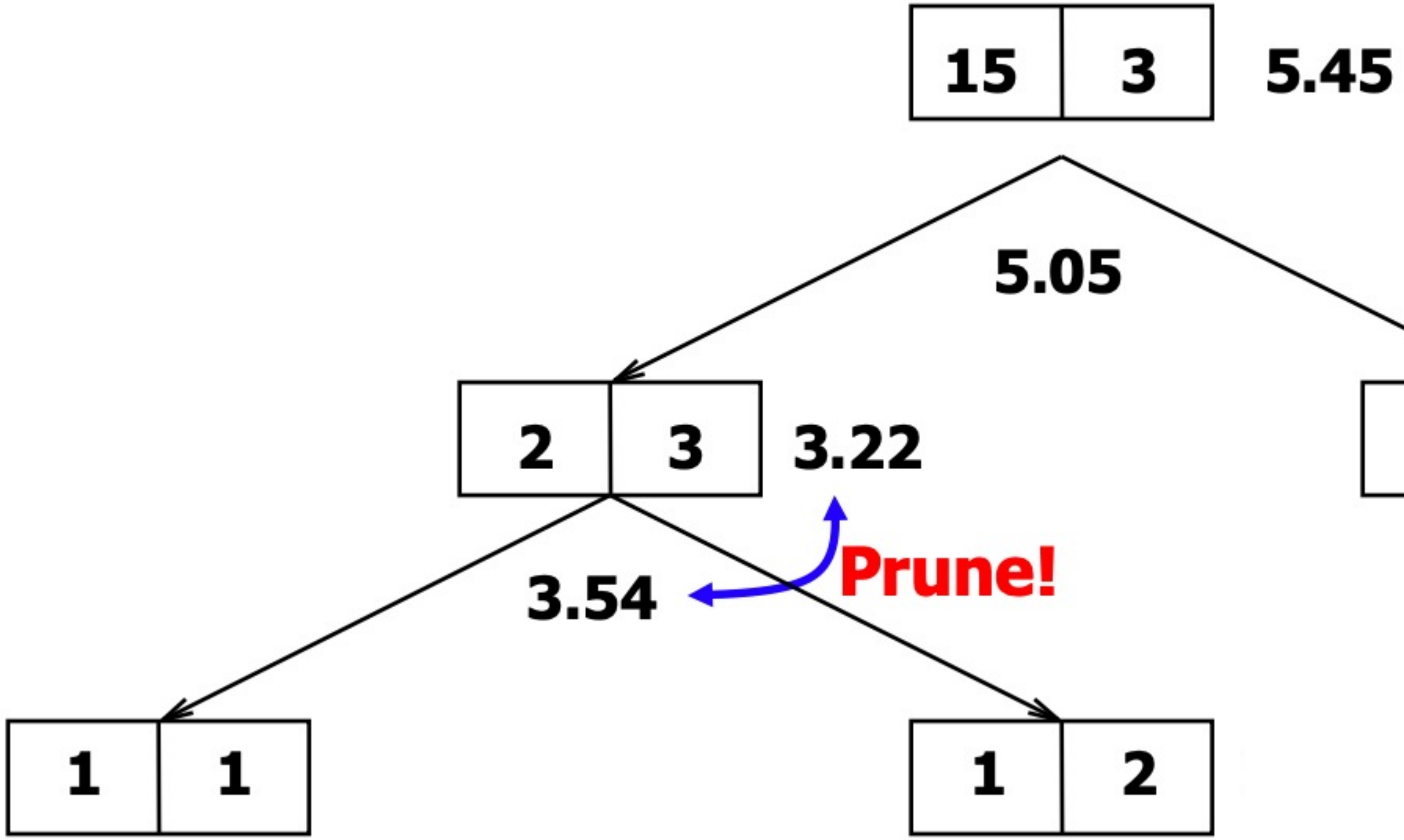
Training Error (After splitting) = 9/30

Pessimistic error (After splitting)

= (9 + 4 $\times$ 0.5)/30 = $\underline{11/30}$ $>$ $\frac{10.5}{30}$

PRUNE!

# EXAMPLE OF POST-PRUNING



# 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:
```

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:
  - Estimate performance of classifier on 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

K fold : 5 groups : { 4b in T
1b in Test

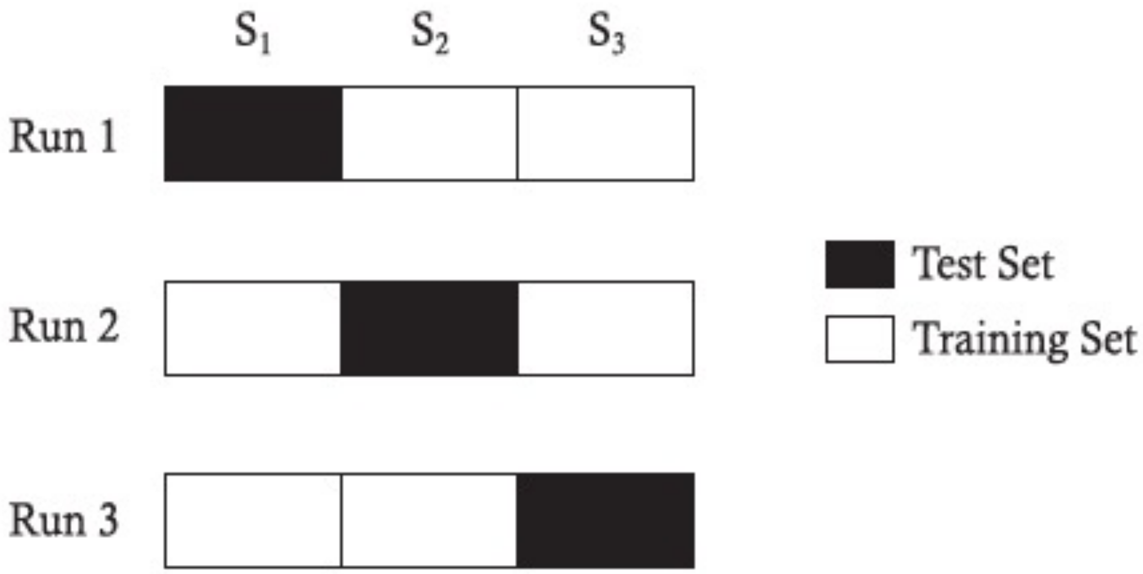
| id | data |
| --- | --- |
| 1 | + |
| 2 | + |
| | |
| | |
| 7 | + |
| | + |
| 10 | - |

$b_1$ $b_2$ $b_5$

$(b_1, b_2, b_3, b_4, \; b_5)$ $(b_1, b_2, b_3, b_4, \; b_5)$

# CROSS-VALIDATION EXAMPLE

- 3-fold cross-validation



# VARIATIONS ON CROSS-VALIDATION

- Repeated cross-validation

  Perform cross-validation for multiple times

  Give an estimate of the variance of the generalization error

- Stratified cross-validation

  Guarantee the same percentage of class labels in training and test

  Good for imbalanced datasets and small samples

- Use nested cross-validation approach for model selection and evaluation