

Data Mining

Model Overfitting

Introduction to Data Mining, 2nd Edition
by
Tan, Steinbach, Karpatne, Kumar

02/03/2021

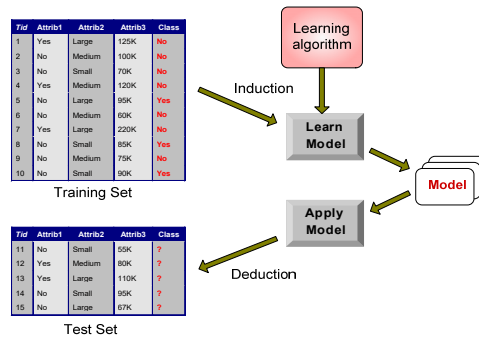
Introduction to Data Mining, 2nd Edition

1

1

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



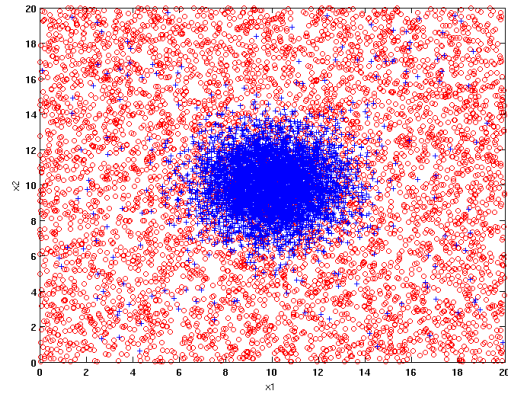
02/03/2021

Introduction to Data Mining, 2nd Edition

2

2

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

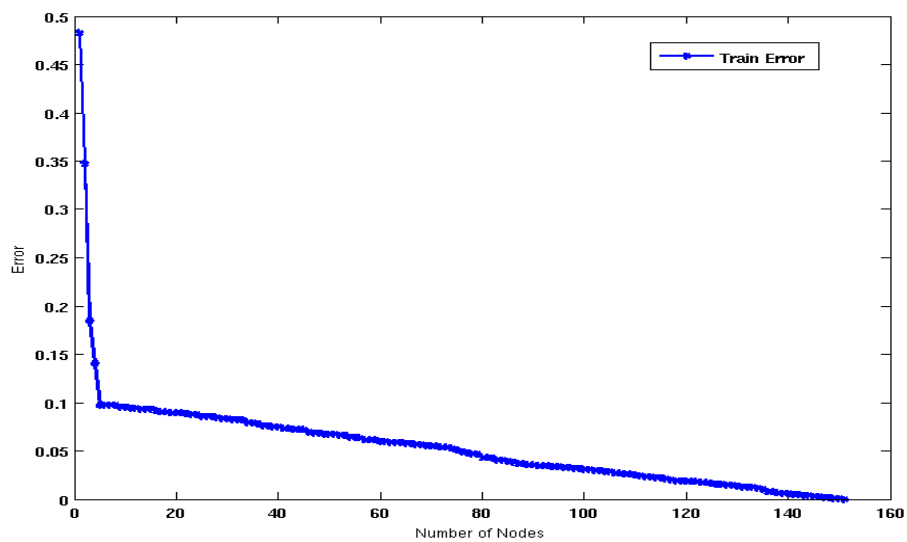
02/03/2021

Introduction to Data Mining, 2nd Edition

3

3

Increasing number of nodes in Decision Trees



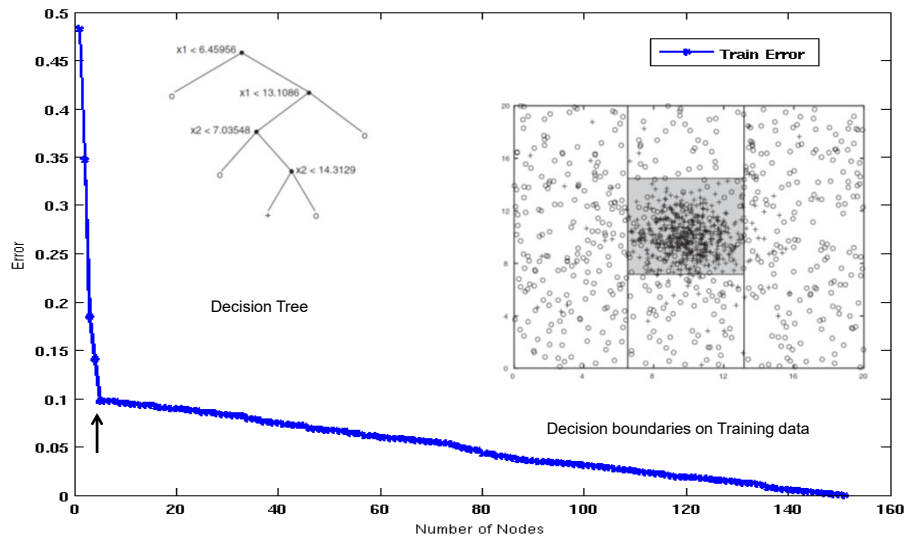
02/03/2021

Introduction to Data Mining, 2nd Edition

4

4

Decision Tree with 4 nodes



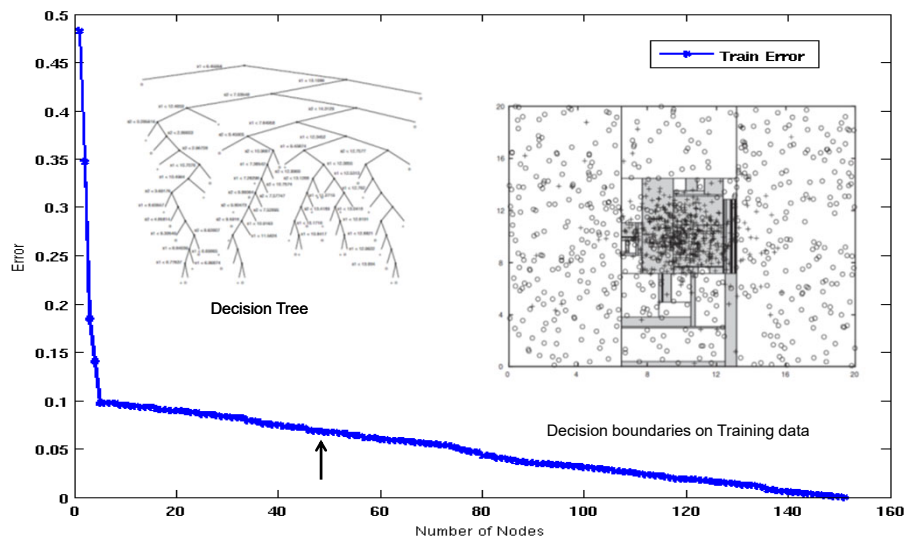
02/03/2021

Introduction to Data Mining, 2nd Edition

5

5

Decision Tree with 50 nodes



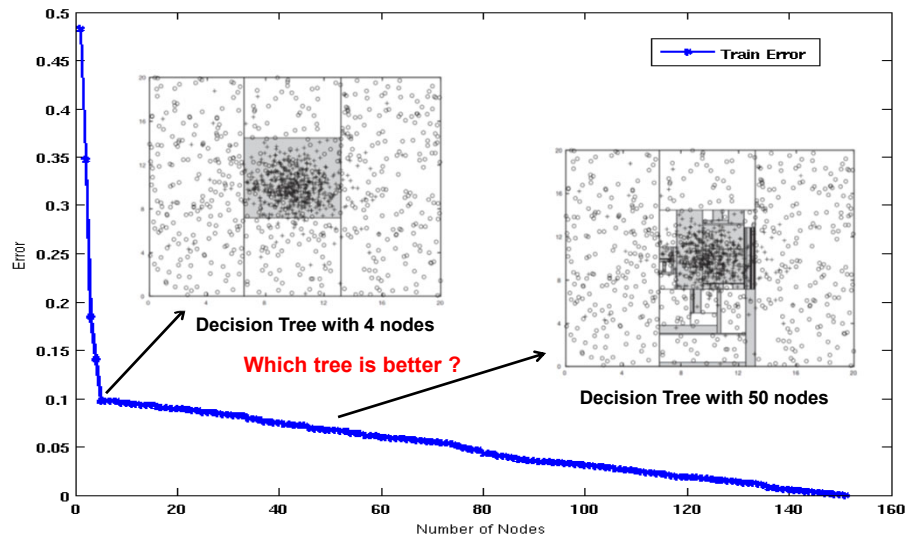
02/03/2021

Introduction to Data Mining, 2nd Edition

6

6

Which tree is better?



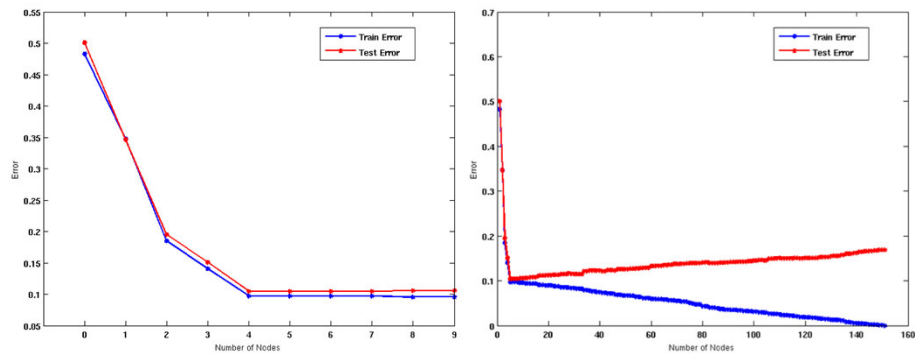
02/03/2021

Introduction to Data Mining, 2nd Edition

7

7

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

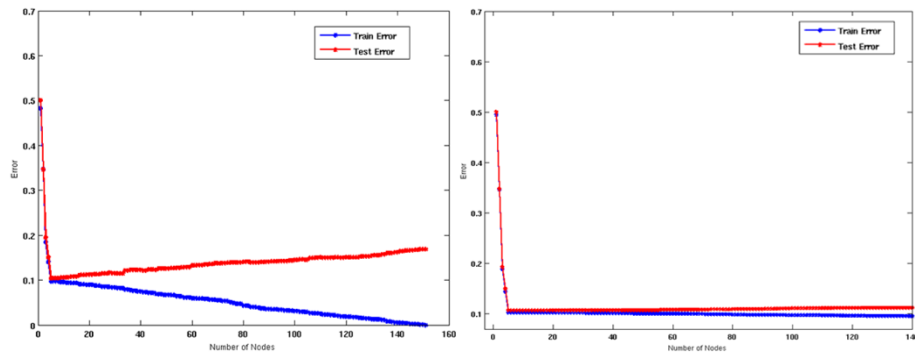
02/03/2021

Introduction to Data Mining, 2nd Edition

8

8

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

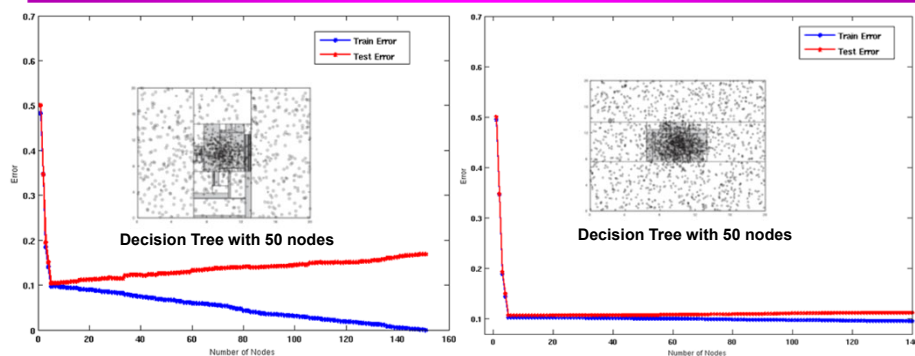
02/03/2021

Introduction to Data Mining, 2nd Edition

9

9

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

02/03/2021

Introduction to Data Mining, 2nd Edition

10

10

Reasons for Model Overfitting

- Not enough training data
- High model complexity
 - Multiple Comparison Procedure

02/03/2021

Introduction to Data Mining, 2nd Edition

11

11

Effect of Multiple Comparison Procedure

- Consider the task of predicting whether stock market will rise/fall in the next 10 trading days
- Random guessing:
 $P(\text{correct}) = 0.5$
- Make 10 random guesses in a row:

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

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

02/03/2021

Introduction to Data Mining, 2nd Edition

12

12

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

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

Effect of Multiple Comparison Procedure

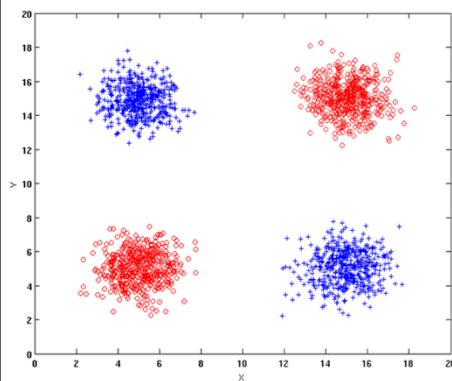
□ Many algorithms employ the following greedy strategy:

- Initial model: M
- Alternative model: $M' = M \cup \gamma$,
where 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, $\Gamma = \{\gamma_1, \gamma_2, \dots, \gamma_k\}$

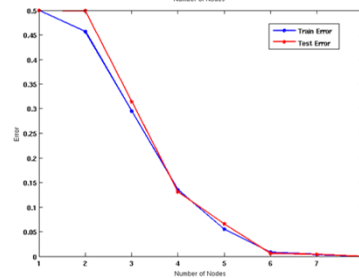
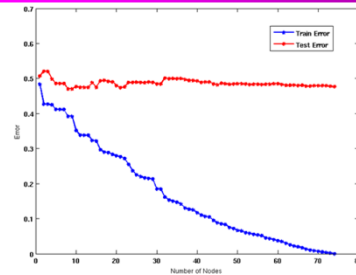
□ If many alternatives are available, one may inadvertently add irrelevant components to the model, resulting in model overfitting

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

02/03/2021

Introduction to Data Mining, 2nd Edition

15

15

Notes on Overfitting

- 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

02/03/2021

Introduction to Data Mining, 2nd Edition

16

16

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

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

02/03/2021

Introduction to Data Mining, 2nd Edition

19

19

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
- 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

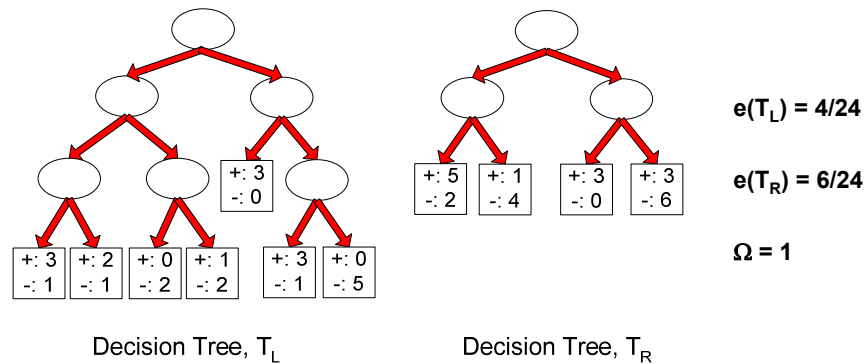
02/03/2021

Introduction to Data Mining, 2nd Edition

20

20

Estimating the Complexity of Decision Trees: Example



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

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

02/03/2021

Introduction to Data Mining, 2nd Edition

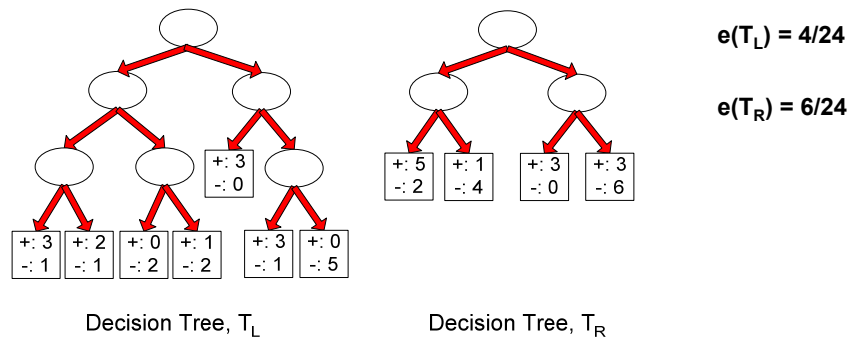
21

21

Estimating the Complexity of Decision Trees

□ Resubstitution Estimate:

- Using training error as an **optimistic** estimate of generalization error
- Referred to as **optimistic error** estimate



02/03/2021

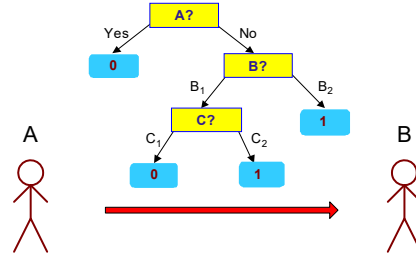
Introduction to Data Mining, 2nd Edition

22

22

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	?

- $\text{Cost}(\text{Model}, \text{Data}) = \text{Cost}(\text{Data}|\text{Model}) + \alpha \times \text{Cost}(\text{Model})$
 - Cost is the number of bits needed for encoding.
 - Search for the least costly model.
- $\text{Cost}(\text{Data}|\text{Model})$ encodes the misclassification errors.
- $\text{Cost}(\text{Model})$ uses node encoding (number of children) plus splitting condition encoding.

02/03/2021

Introduction to Data Mining, 2nd Edition

23

23

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 χ^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

02/03/2021

Introduction to Data Mining, 2nd Edition

24

24

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

02/03/2021

Introduction to Data Mining, 2nd Edition

25

25

Example of Post-Pruning

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

Training Error (Before splitting) = 10/30

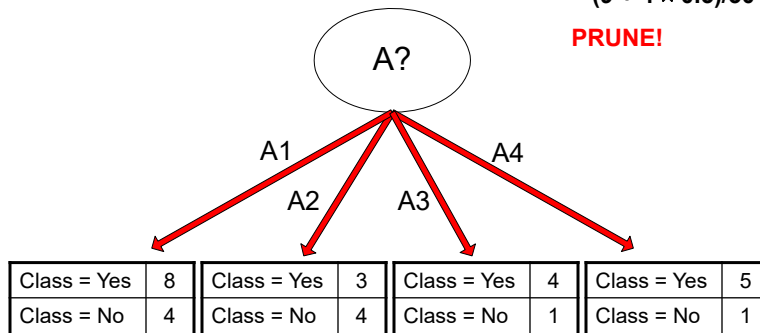
Pessimistic error = $(10 + 0.5)/30 = 10.5/30$

Training Error (After splitting) = 9/30

Pessimistic error (After splitting)

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

PRUNE!



02/03/2021

Introduction to Data Mining, 2nd Edition

26

26

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

```

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

```

Subtree
Raising

Subtree
Replacement

02/03/2021

Introduction to Data Mining, 2nd Edition

27

27

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

02/03/2021

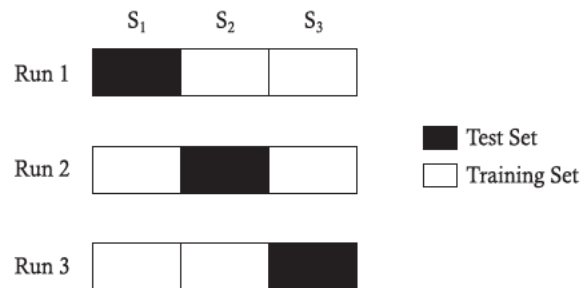
Introduction to Data Mining, 2nd Edition

28

28

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