Introduction to Data Mining

Chapter 3 Classification – Basic Concepts

by Michael Hahsler

Based in Slides by Tan, Steinbach, Karpatne, Kumar

R Code Examples

 Available R Code examples are indicated on slides by the R logo



The Examples are available at <u>https://mhahsler.github.io/Introduction_to_Data_Mining_R_Examples/</u>





Topics

- Introduction
- Decision Trees
 - -Overview
 - -Tree Induction
- Overfitting and other Practical Issues
- Model Selection and Evaluation
 - -Metrics for Performance Evaluation
 - -Methods to Obtain Reliable Estimates
 - -Model Comparison (Relative Performance)
- Feature Selection

Supervised Learning – Learning from Examples

Examples

- -Input-output pairs: $E = (x_1, y_1), ..., (x_i, y_i), ..., (x_N, y_N).$
- —We assume that the examples are produced iid (with noise and errors) from a target function y = f(x).
- Learning problem
 - -Given a hypothesis space H
 - -Find a hypothesis $h \in H$ such that $\hat{y}_i = h(x_i) \approx y_i$
 - —That is, we want to approximate f by h using E.



Includes

- -**Regression** (outputs = real numbers). Goal: Predict the number accurately. E.g., x is a house and f(x) is its selling price.
- -**Classification** (outputs = class labels). Goal: Assign new records to a class. E.g., x is an email and f(x) is spam / ham

You already know linear regression. We focus on Classification.

Illustrating Classification Task



Figure 4.3. General approach for building a classification model.

Examples of Classification Task

- Predicting tumor cells as benign or malignant.
- Classifying credit card transactions as legitimate or fraudulent.
- Categorizing news stories as finance, weather, entertainment, sports, etc.







Topics

- Introduction
- Decision Trees
 - -Overview
 - -Tree Induction
- Overfitting and other Practical Issues
- Model Selection and Evaluation
 - -Metrics for Performance Evaluation
 - —Methods to Obtain Reliable Estimates
 - -Model Comparison (Relative Performance)
- Feature Selection

Example of a Decision Tree





Training Data

Model: Decision Tree

Another Example of Decision Tree





fits the same data!

Decision Tree: Deduction



Figure 4.3. General approach for building a classification model.



Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?





YES

NO

Refund Marital Taxable Cheat **Status** Income 80K ? Married No Refund Yés No NO **MarSt** Married Single, Divorced **TaxInc** NO < 8⁄0K > 80K



Refund Marital Taxable Cheat Income **Status** 80K ? Married No Refund Yés No NO **MarSt** Married Single, Divorced **TaxInc** NO < 8⁄0K > 80K **YES** NO

Cheat **Status** Income 80K ? Married No Refund Yés No **MarSt** NO Assign Cheat to "No" Married Single, Divorced **TaxInc** NO < 8⁄0K > 80K **YES** NO

Test Data

Marital

Taxable

Refund



Topics

- Introduction
- Decision Trees
 - -Overview
 - -Tree Induction
- Overfitting and other Practical Issues
- Model Selection and Evaluation
 - -Metrics for Performance Evaluation
 - —Methods to Obtain Reliable Estimates
 - -Model Comparison (Relative Performance)
- Feature Selection

Decision Tree: Induction



Figure 4.3. General approach for building a classification model.

Decision Tree Induction

Many Algorithms:

- —Hunt's Algorithm (one of the earliest)
- -CART (Classification And Regression Tree)
- -ID3, C4.5, C5.0 (by Ross Quinlan, introduced information gain)
- -CHAID (CHi-squared Automatic Interaction Detection)
- -MARS (Improvement for numerical features)
- -SLIQ, SPRINT
- -Conditional Inference Trees (recursive partitioning using statistical tests)

All algorithms use a simple, greedy top-down splitting strategy!

The Effect of a Split



Every split partitions the data set into two subsets.



Example: Creating a Decision Tree



Decision trees can only cut parallel to an axis!

Example: Creating a Decision Tree



Tree Induction

Greedy strategy

-Split the records based on an attribute test that optimizes a certain criterion.



Tree Induction

- Greedy strategy
 - —Split the records based on an attribute test that optimizes a certain criterion.

Issues

- -Determine how to split the records using different attribute types.
- -How to determine the best split variable?
- -Determine when to stop splitting.

How to Specify Test Condition?

- Depends on attribute types
 - -Nominal
 - -Ordinal
 - -Continuous (interval/ratio)

Splitting Based on Nominal Attributes

- Divide the unordered values into two subsets.
- We need to find optimal partitioning.



Best decision depends on what we want to predict!

Splitting Based on Ordinal Attributes

Divide the ordered values into two subsets.



Splitting Based on Continuous AttributesBinary splitMulti-way split



Discretization to form an ordinal categorical attribute:

- **Static** discretize the data set once at the beginning (equal interval, equal frequency, etc.).
- **Dynamic** discretize during the tree construction.
 - Example: For a binary decision (A < v) or $(A \ge v)$ consider all possible splits and finds the best cut. This can be done efficiently.

Tree Induction

- Greedy strategy
 - -Split the records based on an attribute test that optimizes a certain criterion.

Issues

- -Determine how to split the records using different attribute types.
- -How to determine the best split variable?
- -Determine when to stop splitting

How to determine the Best Split



Which splitting variable is the best?

Determine the Quality of a Node: Node Impurity

- Nodes represent a subset of data that satisfy the splitting condition.
- We want to create nodes with homogeneous class distributions.
- Need a measure of node impurity:



Non-homogeneous, High degree of impurity This is preferredC0:9C1:1

Homogeneous, Low degree of impurity

- General rule for measures of impurity:
 - -Smaller is better.
 - -0 represents the complete purity.

Find the Best Split: General Framework

Assume we have a measure **M** that tells us how "pure" a node is.



We look at the improvement called the gain: Gain = M0 – MA vs. M0 – MB → Choose best split

Measures of Node Impurity







Gini Index

Entropy

Classification error

Measure of Impurity: Gini Index of a Node

Gini Index for a given node t :

$$GINI(t) = \sum_{j} p(j | t)(1 - p(j | t)) = 1 - \sum_{j} p(j | t)^{2}$$

p(j | t) is estimated as the relative frequency of class j at node t

- Origin: The Gini index is a measure of statistical dispersion intended to represent the income inequality within nations. Here it is used as a statistical measure that quantifies how mixed or impure the class distribution in a node is.
- Maximum Impurity: $1 1/n_c$ (number of classes) when records are equally distributed among all classes. For a binary decision it is 0.5.
- Minimum Impurity: 0 when all records belong to one class.

Examples

Gini=	0.000	Gini=	0.278	Gini=	0.444	Gini=	0.500
C2	6	C2	5	C2	4	C2	3
C1	0	C1	1	C1	2	C1	3

Examples: Gini Index of a Node

$$GINI(t) = 1 - \sum_{j} p(j \mid t)^2$$

C1	0
C2	6

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1Gini = 1 - $P(C1)^2 - P(C2)^2 = 1 - 0 - 1 = 0$

C1	1
C2	5

P(C1) = 1/6 P(C2) = 5/6Gini = 1 - (1/6)² - (5/6)² = **0.278**

C1	2
C2	4

P(C1) = 2/6 P(C2) = 4/6Gini = 1 - (2/6)² - (4/6)² = **0.444**

Maximal impurity here is $\frac{1}{2} = .5$
Splitting Based on the Gini Index

When a node *p* is split into *k* partitions (children), the quality of the split is computed as a weighted:



where n_i is the number of records at child i, and n is the number of records at node p.

Used in the algorithms CART, SLIQ, SPRINT.

Example: Splitting based on the Gini Index

 Effect of weighing partitions: Larger and purer partitions are preferred.



$$Gini(N1) = 1 - (5/8)^2 - (3/8)^2 = 0.469$$

 $Gini(N2) = 1 - (1/4)^2 - (3/4)^2 = 0.375$

Gain = 0.5 – 0.438 = 0.062

GINI improves!

Continuous Attributes: Computing Gini Index

- How does the algorithm choose the splitting value v? (= dynamic discretization)
 - Number of possible splitting values
 Number of distinct values
- Efficient Method: for each attribute,
 - -Sort the attribute on values
 - -Linearly scan these values, each time updating the count matrix and computing Gini index
 - -Choose the split position that has the smallest Gini index

	Cheat		No		No)	N	0	Ye	S	Ye	S	Ye	es	N	0	N	0	N	0		No	
			Taxable Income																				
Sorted Values	s>		60		70)	7	5	85	;	9()	9	5	10	0	12	20	12	25		220	
Split Position	s 🔶	5	5	6	5	7	2	8	0	8	7	9	2	9	7	11	10	12	22	17	2	23	0
		;	>	<=	>		>	;	>	۲	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
	Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	3	0
	No	0	7	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	7	0
	Gini	0.4	20	0.4	00	0.3	75	0.3	43	0.4	17	0.4	100	<u>0.3</u>	<u>800</u>	0.3	43	0.3	375	0.4	00	0.4	20

Tid	Refund	Marital Status	Taxable Income	Cheat	
1	Yes	Single	125K	No	
2	No	Married	100K	No	
3	No	Single	70K	No	
4	Yes	Married	120K	No	
5	No	Divorced	95K	Yes	
6	No	Married	60K	No	
7	Yes	Divorced	220K	No	
8	No	Single	85K	Yes	
9	No	Married	75K	No	
10	No	Single	90	Yes	
		Yes	Taxabl e ncome > 97K) ı No	v = 97

Measures of Node Impurity







Gini Index

Entropy

Classification error

Measure of Impurity: Entropy

Entropy at a given node t:

Entropy(t) =
$$-\sum_{j} p(j \mid t) \log(p(j \mid t))$$

 $p(j \mid t)$ is the relative frequency of class j at node t; $0 \log(0) \stackrel{\text{def}}{=} 0$ is used!

- Origin: In information theory, entropy quantifies the amount of uncertainty involved in the value of a random. Here the random variable is the class label of a randomly chosen observation in a node.
- Maximum Impurity: $log(n_c)$ when records are equally distributed among all classes.
- Minimum Impurity: 0 when all records belong to one class. We can perfectly predict the class label of each observation in the node.

Examples: Entropy

Entropy(t) =
$$-\sum_{j} p(j \mid t) \log(p(j \mid t))$$

C1	0
C2	6

$$P(C1) = 0/6 = 0$$
 $P(C2) = 6/6 = 1$
Entropy = $-0 \log 0 - 1 \log 1 = -0 - 0 = 0$

C1	1
C2	5

P(C1) = 1/6 P(C2) = 5/6Entropy = - (1/6) $\log_2 (1/6) - (5/6) \log_2 (1/6) = 0.65$

C1	3
C2	3

P(C1) = 3/6 P(C2) = 3/6Entropy = - (3/6) $\log_2 (3/6) - (3/6) \log_2 (3/6) = 1$

Splitting based on Information Gain

$$GAIN_{split} = Entropy(p) - \left(\sum_{i=1}^{k} \frac{n_i}{n} Entropy(i)\right)$$

Parent Node, p is split into k partitions; n_i is number of records in partition i

- Measures reduction in Entropy achieved because of the split. Choose the split that achieves most reduction (maximizes GAIN)
- Used in ID3, C4.5 and C5.0
- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.

Splitting based on the Gain Ratio

$$GainRato_{split} = \frac{GAIN_{split}}{SplitInfo}$$
$$SplitInfo = -\sum_{i=1}^{k} \frac{n_i}{n} \log\left(\frac{n_i}{n}\right)$$

Parent Node, p is split into k partitions; n_i is number of records in partition i

- Adjusts Information Gain by the entropy of the partitioning (SplitInfo). Higher entropy partitioning (large number of small partitions) is penalized!
- Used in C4.5
- Designed to overcome the disadvantage of Information Gain.

Measures of Node Impurity







G	i	r	١	i	r	٦	d	ex	

Entropy

Classification error

Splitting Criteria based on Classification Error

Classification error at a node t :

$$Error(t) = 1 - \max_{i} p(i | t)$$

p(j | t) is the relative frequency of class j at node t

- Measures the classification error made in a node by a simple classifier that always predict the majority class (given by the $max(\cdot)$ in the equation).
- Maximum Impurity: $1 \frac{1}{n_c}$ when records are equally distributed among all classes (maximal error).
- Minimum Impurity: 0 when all records belong to one class = maximal purity (no error)
- Splitting decision: Use weighted averages or gain as for the other indices to make the splitting decision.

Examples: Classification Error

$$Error(t) = 1 - \max_{i} p(i | t)$$

C1	0
C2	6

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1Error = 1 - max (0, 1) = 1 - 1 = 0

C1	1
C2	5

$$P(C1) = 1/6$$
 $P(C2) = 5/6$
Error = 1 - max (1/6, 5/6) = 1 - 5/6 = 1/6

C1	3
C2	3

P(C1) = 3/6 P(C2) = 3/6Error = 1 - max (3/6, 3/6) = 1 - 3/6 = .5

Comparison among Splitting Criteria

For a 2-class problem: Probability of the majority class p is always > .5



Note: The order is the same no matter what splitting criterion is used, however, the gain (differences) are not since they depend on the slope.

Tree Induction

Greedy strategy

—Split the records based on an attribute test that optimizes a certain criterion.

Issues

-Determine how to split the record using different attribute types.

- -How to determine the best split?
- -Determine when to stop splitting

Stopping Criteria for Tree Induction

Stop expanding a node when all the records belong to the same class (used Hunt's algorithm).

Stop expanding a node when all the records in the node have the same attribute values. Splitting becomes impossible.

 Early termination criterion. Stop when more splits will lead to overfitting the training data. We will discuss this later with tree pruning.

Standard method

Advantages of Decision Trees









INEXPENSIVE TO CONSTRUCT EXTREMELY FAST AT CLASSIFYING UNKNOWN RECORDS

EASY TO INTERPRET FOR SMALL-SIZED TREES ACCURACY IS COMPARABLE TO OTHER CLASSIFICATION TECHNIQUES FOR MANY SIMPLE DATA SETS

Example: C4.5

- Simple depth-first construction.
- Uses Information Gain (improvement of the entropy measure).
- Handling both continuous and discrete attributes (continuous attributes are split at threshold).
- Needs entire data to fit in memory (unsuitable for large datasets).
- Final trees are pruned to remove branches that hurt performance.
- Code available at
 - -http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.gz
 - -Open-Source implementation as J48 in Weka/rWeka





Topics

- Introduction
- Decision Trees
 - -Overview
 - -Tree Induction
- Overfitting and other Practical Issues
- Model Selection and Evaluation
 - -Metrics for Performance Evaluation
 - -Methods to Obtain Reliable Estimates
 - —Model Comparison (Relative Performance)
- Feature Selection

Model Selection: Bias vs. Variance



Note: This trade-off applies to any model.

Example: Underfitting and Overfitting



How is the data generated?

500 circular and 500 triangular data points.

Circular points: $0.5 \ge sqrt(x_1^2 + x_2^2) \le 1$

Triangular points:

 $sqrt(x_1^2 + x_2^2) < 0.5 \text{ or}$ $sqrt(x_1^2 + x_2^2) > 1$

Example: Underfitting and Overfitting



Underfitting: The model is too simple, both training and test errors are large.Overfitting: The model is too complicated and starts memorizing the training data.Generalization error goes up again.

Example: Underfitting due to Insufficient Examples



Lack of training data points in the lower half of the diagram makes it difficult to predict correctly the class labels of that region

Example: Overfitting due to Noise



Decision boundary is distorted to accommodate a noise point

Training Error vs. Generalization Error

- Training error is reduced by overfitting and 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 new example (e.g., test data).
- We need to estimate the Generalization Error expected for new data.

Estimating the Generalization Error

- Resubstitution error e: error on training set
- Generalization error e': error on testing set

Methods for estimating generalization errors:

- **1. Optimistic approach**: assume e' = e
- **2.** Pessimistic approach:
 - Estimate as $e' = e + N \times 0.5$ (N: number of leaf nodes)
 - For a tree with 30 leaf nodes and 10 errors on training out of 1000 training instances:

Training error e = 10/1000 = 1%Estimated generalization error $e' = (10 + 30 \times 0.5)/1000 = 2.5\%$

3. Validation approach:

 uses a validation (test) data set (or cross-validation) to estimate the generalization error.

Penalty for model complexity! 0.5 per leave node is often used for binary splits.



"Simpler is better"

Occam's Razor

The Principle of Parsimony

- Given two models of similar generalization errors, one should prefer the simpler model over the more complex model.
- Reason: Complex models have a greater chance of overfitting.
 I.e., it fitted accidentally errors in the training data.

Therefore, one should consider also model complexity when evaluating a model.

How to Address Overfitting in Decision Trees

Full tree (will overfit)

- Stop if all instances belong to the **same class.**
- Stop if all the **attribute values are the same.**

Reduce overfitting with pre-pruning / early stopping

- Stop if **number of instances** is less than some user-specified threshold (estimates become bad for small sets of instances).
- Stop if class distribution of instances are **independent** of the available features (e.g., using a χ^2 test).
- Stop if expanding the current node **does not improve impurity** measures more than a user-specified threshold (e.g., Gini or information gain).

How to Address Overfitting in Decision Trees

Reduce overfitting with post-pruning

- 1. Grow complete decision tree.
- 2. Try to prune sub-trees of the decision tree in a bottom-up fashion.

Options:

- -Generalization error: If generalization error improves after pruning a sub-tree, replace the sub-tree by a leaf node with the majority class of the training instances as the predicted label.
- —Penalty for complexity: You can use Maximum Description Length (MDL).

Refresher: Minimum Description Length (MDL)



- Cost(Model) encodes each node (splitting condition and children).
- Cost(Data|Model) encodes information to correct misclassification errors.
- $Cost(Model, Data) = Cost(Data|Model) + Cost(Model) \rightarrow min$ -Cost is the number of bits needed for encoding.

Penalty for model complexity! This is equivalent to the pessimistic generalization error.

Example: Post-Pruning



Other issues:

Data Fragmentation and Search Strategy

Data Fragmentation

- Number of instances gets smaller as you traverse down the tree and can become too small to make a statistically significant decision (splitting or determining the class in a leaf node)
- → Many algorithms stop when a node has not enough instances.

Search Strategy

- Finding an optimal decision tree is NP-hard
- → Most algorithm use a greedy, top-down, recursive partitioning strategy to induce a reasonable solution.

Other issues: Tree Replication



- Same subtree appears in multiple branches.
- Makes the model more complicated and harder to interpret.

Decision Boundary of a Classifier



- The border line between two neighboring regions of different classes is known as the decision boundary.
- The decision boundary of decision trees is parallel to the axes because each test condition represents a threshold on a single attribute.
- Not expressive enough for modeling continuous variables directly. Discretization is performed for the splits.



- The test condition may involve multiple attributes.
- More expressive representation.
- Finding the optimal test condition is computationally expensive!

Not used in practice for decision trees but Linear Discriminant Analysis (LDA) can learn a single oblique decision boundary.

EVALUATION

Relevance Efficiency Effectiveness Sustainability Impact ★ ○ ○ ○ ○
◇ ○ ▲ ○ ○ ○
◇ ○ ○ ○ ▲ ○
○ ○ ○ ○ ▲ ○

Topics

- Introduction
- Decision Trees
 - -Overview
 - -Tree Induction
- Overfitting and other Practical Issues
- Model Selection and Evaluation
 - —Metrics for Performance Evaluation
 - -Methods to Obtain Reliable Estimates
 - —Model Comparison (Relative Performance)
- Feature Selection

Metrics for Performance Evaluation: Confusion Matrix

- Focuses on the predictive capability of a model (not speed, scalability, etc.)
- For simplicity, we will present a binary classification problem here, but most measures generalize to multi-class problems.

Confusion Matrix

	PRE			
		Class=Yes	Class=No	a: TP (true positive)
	Class=Yes	а	b	b: FN (false negative)
ACIUAL		(TP)	(FN)	d: TN (true negative)
ULASS	Class=No	С	d	
		(FP)	(TN)	

Metrics for Performance Evaluation: Statistical Test

From Statistics: Null Hypotheses H0 is that the actual class is Yes.

	PRE			
		Class=Yes	Class=No	•
ACTUAL	Class=Yes		Type I error (FN)	← <i>H</i> 0
CLASS	Class=No	Type II error (FP)		

Type I error: $P(NO \mid HO \text{ is true})$ Type II error: $P(\text{Yes} \mid H0 \text{ is false})$

 \rightarrow Significance level α \rightarrow Power $1 - \beta$
Metrics for Performance Evaluation: Accuracy

Most widely-used metric:

How many do we predict correct (in percent)?

	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a (TP)	b (FN)
	Class=No	с (FP)	d (TN)

$$Accuracy = \frac{a+d}{a+b+c+d} = \frac{TP+TN}{N}$$

Limitation of Accuracy

It is best to always say Class 0

Consider a 2-class problem with a total population of

-Number of Class 0 examples = 9990

-Number of Class 1 examples = 10

A model that predicts everything to be class 0, has an accuracy of 9990/10000 = 99.9%

Accuracy is misleading because the model does not detect any class 1 example!

→ This is a very common problem called the class imbalance problem

Cost Matrix

Different types of error can have different cost!

	PREDICTED CLASS		
ACTUAL CLASS	C(i j)	Class=Yes	Class=No
	Class=Yes	C(Yes Yes)	C(No Yes)
	Class=No	C(Yes No)	C(No No)

 $C(i \mid j)$: Cost of misclassifying class j example as class i

Computing the Cost of Classification

Cost Matrix	PREDICTED CLASS		CLASS	
	C(i j)	+	-	Missing a '+' case is really expensive!
ACTUAL CLASS	+	-1	100 _	
	-	1	0	

Model M ₁	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	150	40
	-	60	250

Accuracy = 80%

Cost = -1*150+100*40+ 1*60+0*250 = **3910** Model M2PREDICTED CLASSACTUAL
CLASS+-+25045-5200

Accuracy = 90%

Cost = **4255**

Cost-Biased Measures (from Information Retrieval)

Precision
$$(p) = \frac{a}{a+c}$$

Recall $(r) = \frac{a}{a+b}$
F - measure $(F) = \frac{2rp}{r+p} = \frac{2a}{2a+b+c}$

	PREDICTED CLASS		
ACTUAL CLASS		Class Yes	Class No
	Class Yes	a (TP)	b (FN)
	Class No	c (FP)	d (TN)

- Precision only considers cost for examples predicted as Yes.
- Recall only considers cost for examples that are truly Yes.
- F-measure combines precision and recall and ignores d.

Kappa Statistic

Idea: Compare the accuracy of the classifier with a **random classifier**. The classifier should be better than random!

	PREDICTED CLASS		
ACTUAL CLASS		Class Yes	Class No
	Class Yes	a (TP)	b (FN)
	Class No	с (FP)	d (TN)

$$\kappa = \frac{\text{total accuracy} - \text{random accuracy}}{1 - \text{random accuracy}}$$

total accuracy =
$$\frac{TP + TN}{\frac{N}{P + FP \times TN + FN + FN + TN \times FP + TP}}{\frac{N^2}{N^2}}$$



Receiver Operating Characteristic (ROC)

- Developed in 1950s for signal detection theory to analyze noisy signals to characterize the trade-off between positive hits and false alarms.
- Works only for binary classification (twoclass problems).
- ROC curve plots TPR (true positive rate) on the y-axis against FPR (false positive rate) on the x-axis.
- Performance of each classifier represented as a point. Changing the threshold of the algorithm, sample distribution or cost matrix changes the location of the point and forms a curve.

ROC Curve

- Example with 1-dimensional data set containing 2 classes (positive and negative)
- Any points located at x > t is classified as positive



Move t to get the other points on the ROC curve.

ROC Curve

(TPR,FPR):

- (0,0): declare everything to be negative class
- (1,1): declare everything to be positive class
- (1,0): ideal

Diagonal line:

- -Random guessing
- Below diagonal line: prediction is opposite of the true class



Using ROC for Model Comparison



EVALUATION

Relevance Efficiency Effectiveness Sustainability Impact

Topics

- Introduction
- Decision Trees
 - -Overview
 - -Tree Induction
- Overfitting and other Practical Issues
- Model Selection and Evaluation
 - -Metrics for Performance Evaluation
 - -Methods to Obtain Reliable Estimates
 - —Model Comparison (Relative Performance)
- Feature Selection

Learning Curve

Accuracy and variance between runs depend on the size of the training data.



Estimating the Generalization Error Using Test Data

- To estimate generalization error we need to separate the data into a set to train and a set to test.
- Holdout testing/Random splits: Split the data randomly into, e.g., 80% training and 20% testing.

Very important: the algorithm can never look at the test set during learning!



k-fold Cross Validation

k-fold cross validation: Use data better to estimate the generalization error:

- Split the data randomly into k folds.
- For k rounds hold 1 fold back for testing and use the remaining k 1 folds for training.
- Use the average of the error/accuracy as a better estimate.
- Some algorithms/tools do that internally.



Training and Testing with Hyperparameters

Hyperparameters: Many algorithms allow choices for learning. E.g.,

- -maximal decision tree depth
- -selected features

We do not want to overfit the hyperparameters!!!

Use a generalization error estimate twice:

- 1. Train: Learn models on the training data (without the validation data) using different hyperparameters.
 - Å grid of possible hyperparameter combinations
 greedy search
- 2. Model Selection: Evaluate the models using the validation data and choose the hyperparameters with the best accuracy. Rebuild the model using all the training data.
- 3. Test the final model using the test data.



Typical Data Use with Model Selection



Confidence Interval for Accuracy

- The observed accuracy is an **estimate** of the true accuracy of the model. How good is the estimate?
- Each prediction can be regarded as a Bernoulli trial: A Bernoulli trial (a biased coin toss) has 2 possible outcomes: heads (correct) or tails (wrong)



We use *p* for the true chance that a prediction is correct (= true accuracy).

- Predictions for a test set of size N are a collection of N Bernoulli trials. The number of correct predictions x has a Binomial distribution:
 X ~ Binomial(N, p)
- Example: Toss a fair coin 50 times, how many heads would turn up? Expected number of heads $E[X] = Np = 50 \times 0.5 = 25$
- Application for Accuracy: If we observe x correct predictions then the observed accuracy is

$$\hat{p} = x/N$$

Can we give bounds for the true accuracy of model p?

Confidence Interval for Accuracy

For large test sets (N > 30) we can approximate the Binomial distribution $X \sim Binomial(N, p)$

by a Normal distribution:

$$X \sim Normal(Np, Np(1-p))$$

Confidence Interval for $p = \frac{X}{N}$ (Wald Method):

$$\hat{p} \pm z_{\alpha/2} \sqrt{\frac{\hat{p}(1-\hat{p})}{N}}$$



Confidence Interval for Accuracy

Consider a model that produces an accuracy of 80% when evaluated on 100 test instances:

1.
$$N = 100, \ acc = 0.8$$

2. Let $1 - \alpha = 0.95$ (95% confidence)
3. Find the critical value for the normal distribution.
 $z_{\alpha/2} = 1.96$
4. Calculate the interval around the accuracy.
 $\hat{p} \pm z_{\alpha/2} \sqrt{\frac{\hat{p}(1-\hat{p})}{N}} = \begin{cases} 0.722\\ 0.878 \end{cases}$
 $\frac{0.90}{N} = \begin{cases} 0.722}{Table \text{ or } R \ qnorm(1-\alpha/2) \end{cases}$

Data mining tools typically calculate this for us.



EVALUATION

Relevance Efficiency Effectiveness Sustainability Impact

Topics

- Introduction
- Decision Trees
 - -Overview
 - -Tree Induction
- Overfitting and other Practical Issues
- Model Selection and Evaluation
 - -Metrics for Performance Evaluation
 - -Methods to Obtain Reliable Estimates
 - -Model Comparison (Relative Performance)
- Feature Selection

Comparing Performance between 2 Models

Given two models, say M_1 and M_2 , which is better? This is a statistical **model selection** problem.

For large test sets (N > 30) we can approximate the observed accuracies (sampled from a Binomial distribution) using the true but unknown model accuracies p_1 and p_2 :

 $acc_1 \sim Normal(Np_1, Np_1(1-p_1))$ $acc_2 \sim Normal(Np_2, Np_2(1-p_2))$

Perform a paired t-test with:

H0: There is no difference between the observed accuracies of the models.

H1: There is a difference.

Notes

- Hyperparameter tuning is also a model selection problem.
- Comparing more than two models: You need to correct for multiple comparisons! For example, using Bonferroni correction or False Discovery Rate (FDR).





Topics

- Introduction
- Decision Trees
 - -Overview
 - -Tree Induction
- Overfitting and other Practical Issues
- Model Selection and Evaluation
 - -Metrics for Performance Evaluation
 - -Methods to Obtain Reliable Estimates
 - —Model Comparison (Relative Performance)
- Feature Selection

Feature Selection

What features should be used in the model?

Univariate feature importance score

- Measures how related each feature is to the class variable.
- E.g., chi-squared statistic, information gain.

Feature subset selection

- Tries to find the best set of features.
- Often uses a black box approach where different subsets are evaluated using a greedy search strategy.
- E.g.: Stepwise backward selection tries to remove one feature at a time.





Conclusion

- Classification is supervised learning with the goal to find a model that predicts well (i.e., has a low generalization error).
- Generalization error can be estimated using test sets/cross-validation and should be used for model selection.
- Model evaluation and comparison needs to take model complexity into account.