Data Mining
Classification: Basic Concepts, Decision Trees, and Model Evaluation

Thanks to Tan,Steinbach, Kumar

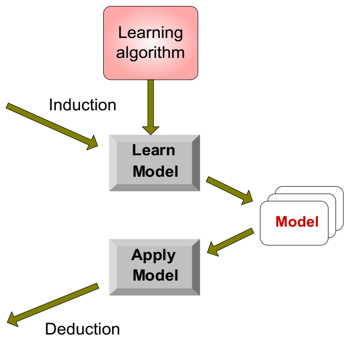
Classification: Definition

- Given a collection of records (*training set*)
  - Each record contains a set of *attributes*, one of the attributes is the *class*.
- Find a *model* for class attribute as a function of the values of other attributes.
- Goal: previously unseen records should be assigned a class as accurately as possible.
  - A *test set* is used to determine the accuracy of the model. Usually, the given data set is divided into training and test sets, with training set used to build the model and test set used to validate it.

Illustrating Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set



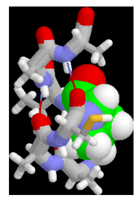
Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set

Examples of Classification Task

- Predicting tumor cells as benign or malignant
- Classifying credit card transactions as legitimate or fraudulent

- Classifying secondary structures of protein as alpha-helix, beta-sheet, or random coil



- Categorizing news stories as finance, weather, entertainment, sports, etc

Classification Techniques

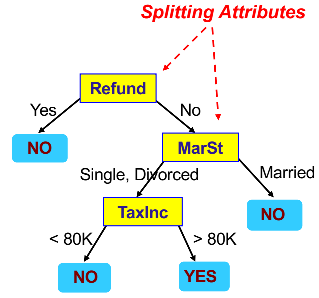
- Decision Tree based Methods
- Rule-based Methods
- Memory based reasoning, Instanse-Based Learning
- Neural Networks, Deep Neural Networks
- Naïve Bayes and Bayesian Belief Networks
- Support Vector Machines
- Ensemble Methods
- Concept Lattice based Methods
- …

Example of a Decision Tree

categorical categorical continuous class

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	90K	Yes

Training Data



Model: Decision Tree

Another Example of Decision Tree

categorical categorical continuous class

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
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3	No	Single	70K	No
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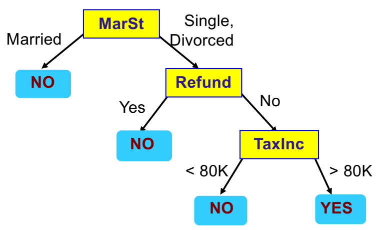
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



There could be more than one tree that fits the same data!

Decision Tree Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
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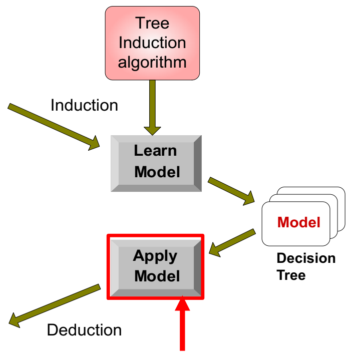
Training Set



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11	No	Small	55K	?
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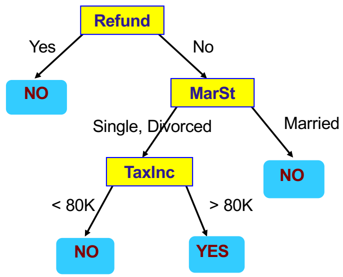
Test Set

Apply Model to Test Data

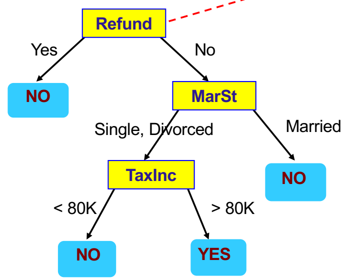
Start from the root of tree.



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data



Test Data

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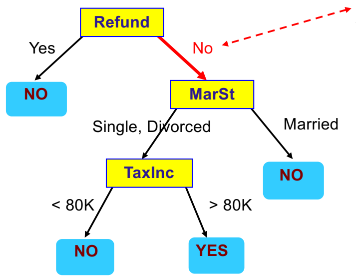

Test Data

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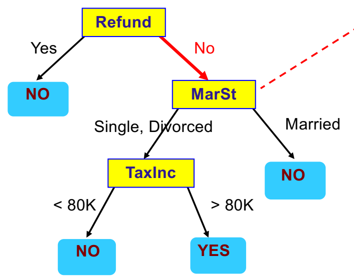
No	Married	80K	?

Apply Model to Test Data



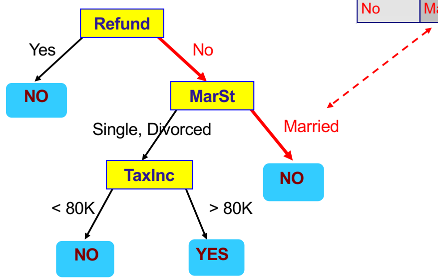
Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Apply Model to Test Data

Test Data

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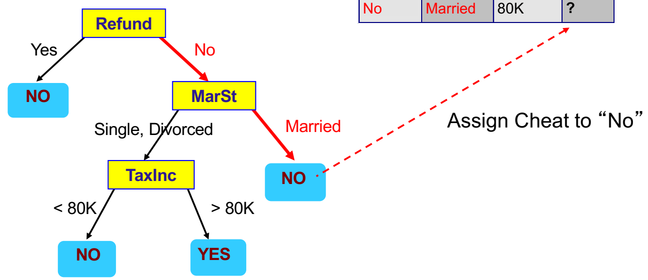

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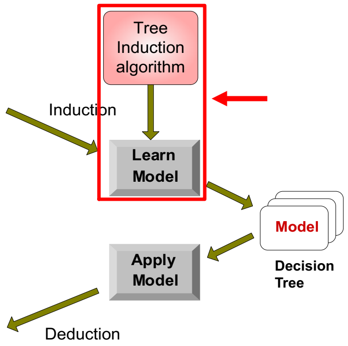
Training Set



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Test Set

Decision Tree Induction

- Many Algorithms:
  - Hunt's Algorithm (one of the earliest)
  - CART
  - ID3, C4.5
  - …

General Structure of Hunt's Algorithm

- Let D_t be the set of training records that reach a node t
- General Procedure:
  - If D_t contains records that belong the same class y_t, then t is a leaf node labeled as y_t
  - If D_t is an empty set, then t is a leaf node labeled by the default class, y_d
  - If D_t contains records that belong to more than one class, use an attribute test to split the data into smaller subsets. Recursively apply the procedure to each subset.

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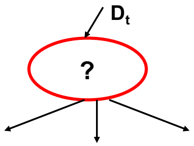

Hunt's Algorithm

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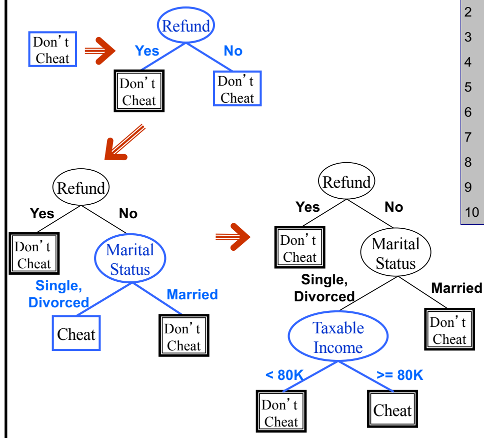

Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting

Tree Induction

- Greedy strategy.
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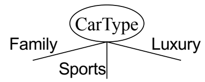
How to Specify Test Condition?

- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

Splitting Based on Nominal Attributes

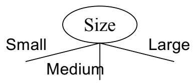
- Multi-way split: Use as many partitions as distinct values.



- Binary split: Divides values into two subsets. Need to find optimal partitioning.

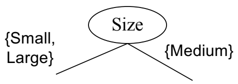
Splitting Based on Ordinal Attributes

- Multi-way split: Use as many partitions as distinct values.



- Binary split: Divides values into two subsets. Need to find optimal partitioning.

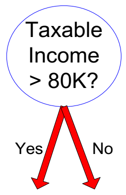
- What about this split?



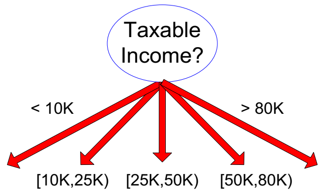
Splitting Based on Continuous Attributes

- Different ways of handling
  - Discretization to form an ordinal categorical attribute
    - Static – discretize once at the beginning
    - Dynamic – ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
  - Binary Decision: $(A < v)$ or $(A \geq v)$
    - consider all possible splits and finds the best cut
    - can be more compute intensive

Splitting Based on Continuous Attributes



(i) Binary split



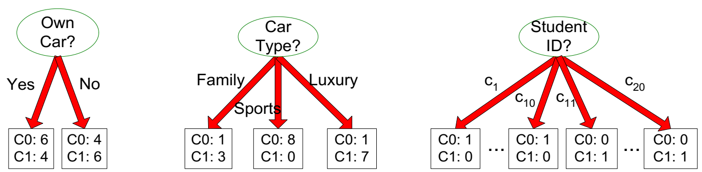
(ii) Multi-way split

Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting

How to determine the Best Split

Before Splitting: 10 records of class 0,
10 records of class 1



Which test condition is the best?

How to determine the Best Split

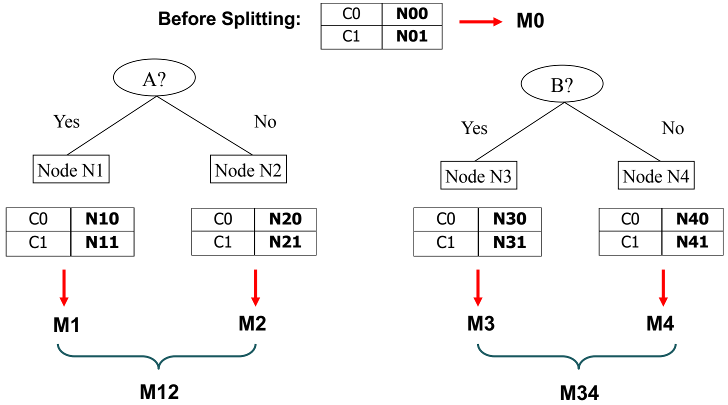
- Greedy approach:
  - Nodes with homogeneous class distribution are preferred
- Need a measure of node impurity:

C0: 5 C1: 5	C0: 9 C1: 1
Non-homogeneous, **High degree of impurity**	**Homogeneous,** **Low degree of impurity**

Measures of Node Impurity

- Gini Index
- Entropy
- Misclassification error

How to Find the Best Split



Gain = M0 – M12 vs M0 – M34

Measure of Impurity: GINI

- Gini Index for a given node t :

$$GINI(t) = 1 - \sum_j [p(j \mid t)]^2$$

(NOTE: $p(j \mid t)$ is the relative frequency of class j at node t).

- Maximum ($1 - 1/n_c$) when records are equally distributed among all classes, implying least interesting information
- Minimum (0.0) when all records belong to one class, implying most interesting information

C1	**0**
C2	**6**
Gini=0.000	

C1	**1**
C2	**5**
Gini=0.278	

C1	**2**
C2	**4**
Gini=0.444	

C1	**3**
C2	**3**
Gini=0.500	

Examples for computing GINI

$$GINI(t) = 1 - \sum_j [p(j \mid t)]^2$$

C1	**0**
C2	**6**

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1

Gini = 1 – P(C1)^2 – P(C2)^2 = 1 – 0 – 1 = 0

C1	**1**
C2	**5**

P(C1) = 1/6 P(C2) = 5/6

Gini = 1 – (1/6)^2 – (5/6)^2 = 0.278

C1	**2**
C2	**4**

P(C1) = 2/6 P(C2) = 4/6

Gini = 1 – (2/6)^2 – (4/6)^2 = 0.444

Splitting Based on GINI

- Used in CART, SLIQ, SPRINT.
- When a node p is split into k partitions (children), the quality of split is computed as,

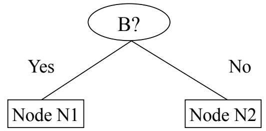
$$GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)$$

where, n_i = number of records at child i,

n = number of records at node p.

Binary Attributes: Computing GINI Index

- Splits into two partitions
- Effect of Weighing partitions:
  – Larger and Purer Partitions are sought for.



	Parent
C1	6
C2	6
Gini = 0.500	

Gini(N1)
= 1 – $(5/7)^2$ – $(2/7)^2$
= 0.41

Gini(N2)
= 1 – $(1/5)^2$ – $(4/5)^2$
= 0.32

	N1	N2
C1	5	1
C2	2	4
Gini=0.369		

Gini(Children)
= 7/12 * 0.41 +
5/12 * 0.32
= 0.369

Categorical Attributes: Computing Gini Index

- For each distinct value, gather counts for each class in the dataset
- Use the count matrix to make decisions

Multi-way split

	CarType		
	Family	Sports	Luxury
C1	1	2	1
C2	4	1	1
Gini	0.393		

Two-way split
(find best partition of values)

	CarType	
	{Sports, Luxury}	{Family}
C1	3	1
C2	2	4
Gini	0.400	

	CarType	
	{Sports}	{Family, Luxury}
C1	2	2
C2	1	5
Gini	0.419	

Continuous Attributes: Computing Gini Index

- Use Binary Decisions based on one value
- Several Choices for the splitting value
  – Number of possible splitting values = Number of distinct values
- Each splitting value has a count matrix associated with it
  – Class counts in each of the partitions, A < v and A ≥ v
- Simple method to choose best v
  – For each v, scan the database to gather count matrix and compute its Gini index
  – Computationally Inefficient! Repetition of work.

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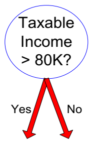


Continuous Attributes: Computing Gini Index...

- For efficient computation: 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 least gini index

Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No
	Taxable Income									
Sorted Values →	60	70	75	85	90	95	100	120	125	220

Split Positions →	55		65		72		80		87		92		97		110		122		172		230	
	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
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	0.420		0.400		0.375		0.343		0.417		0.400		*0.300*		0.343		0.375		0.400		0.420	

Alternative Splitting Criteria based on INFO

- Entropy at a given node t:

$$Entropy(t) = -\sum_j p(j \mid t) \log p(j \mid t)$$

(NOTE: $p(j \mid t)$ is the relative frequency of class j at node t).

- Measures homogeneity of a node.
  - Maximum ($\log n_c$) when records are equally distributed among all classes implying least information
  - Minimum (0.0) when all records belong to one class, implying most information
- Entropy based computations are similar to the GINI index computations

Examples for computing Entropy

$$Entropy(t) = -\sum_j p(j \mid t) \log_2 p(j \mid t)$$

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) = 5/6

Entropy = – (1/6) $\log_2$ (1/6) – (5/6) $\log_2$ (1/6) = 0.65

C1	**2**
C2	**4**

P(C1) = 2/6 P(C2) = 4/6

Entropy = – (2/6) $\log_2$ (2/6) – (4/6) $\log_2$ (4/6) = 0.92

Splitting Based on INFO...

- 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 and C4.5
- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.

Splitting Based on INFO...

- Gain Ratio:

$$GainRATIO_{split} = \frac{GAIN_{Split}}{SplitINFO} \qquad SplitINFO = -\sum_{i=1}^{k} \frac{n_i}{n} \log \frac{n_i}{n}$$

Parent Node, p is split into k partitions
n_i is the 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

Splitting Criteria based on Classification Error

- Classification error at a node t :

$$Error(t) = 1 - \max_i P(i \mid t)$$

- Measures misclassification error made by a node.
  - Maximum (1 - $1/n_c$) when records are equally distributed among all classes, implying least interesting information
  - Minimum (0.0) when all records belong to one class, implying most interesting information

Examples for Computing Error

$$Error(t) = 1 - \max_i P(i \mid t)$$

C1	**0**
C2	**6**

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1

Error = 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

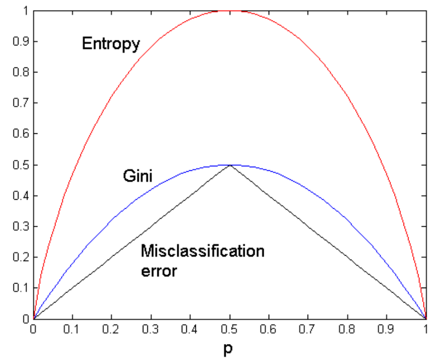
C1	**2**
C2	**4**

P(C1) = 2/6 P(C2) = 4/6

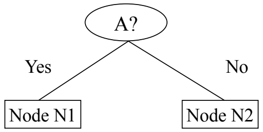
Error = 1 – max (2/6, 4/6) = 1 – 4/6 = 1/3

Comparison among Splitting Criteria

For a 2-class problem:



Misclassification Error vs Gini



	Parent
C1	**7**
C2	**3**
Gini = 0.42	

Gini(N1)
$= 1 - (3/3)^2 - (0/3)^2$
$= 0$

Gini(N2)
$= 1 - (4/7)^2 - (3/7)^2$
$= 0.489$

	N1	N2
C1	**3**	**4**
C2	**0**	**3**
Gini=0.342		

Gini(Children)
$= 3/10 * 0$
$+ 7/10 * 0.489$
$= 0.342$

Gini improves !!

Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - 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
- Stop expanding a node when all the records have similar attribute values
- Early termination

Decision Tree Based Classification

- Advantages:
  - 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
- Sorts Continuous Attributes at each node.
- Needs entire data to fit in memory.
- Unsuitable for Large Datasets.
  - Needs out-of-core sorting.

Model Evaluation

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

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Metrics for Performance Evaluation

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a	b
	Class=No	c	d

a: TP (true positive)
b: FN (false negative)
c: FP (false positive)
d: TN (true negative)

Metrics for Performance Evaluation…

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

- Most widely-used metric:

$$\text{Accuracy} = \frac{a+d}{a+b+c+d} = \frac{TP+TN}{TP+TN+FP+FN}$$

Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10
- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
  - Accuracy is misleading because model does not detect any class 1 example

Cost Matrix

	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|j): Cost of misclassifying class j example as class i

Computing Cost of Classification

Cost Matrix	PREDICTED CLASS		
ACTUAL CLASS	C(i|j)	**+**	**-**
	+	-1	100
	-	1	0

Model M_1	PREDICTED CLASS		
ACTUAL CLASS		**+**	**-**
	+	150	40
	-	60	250

Accuracy = 80%

Cost = 3910

Model M_2	PREDICTED CLASS		
ACTUAL CLASS		**+**	**-**
	+	250	45
	-	5	200

Accuracy = 90%

Cost = 4255

Cost vs Accuracy

Count	PREDICTED CLASS	
	Class=Yes	Class=No
ACTUAL CLASS Class=Yes	a	b
ACTUAL CLASS Class=No	c	d

Accuracy is proportional to cost if
1. C(Yes|No)=C(No|Yes) = q
2. C(Yes|Yes)=C(No|No) = p

N = a + b + c + d

Accuracy = (a + d)/N

Cost	PREDICTED CLASS	
	Class=Yes	Class=No
ACTUAL CLASS Class=Yes	p	q
ACTUAL CLASS Class=No	q	p

Cost = p (a + d) + q (b + c)
= p (a + d) + q (N – a – d)
= q N – (q – p)(a + d)
= N [q – (q-p) × Accuracy]

Cost-Sensitive Measures

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

$$\text{Recall (r)} = \frac{a}{a+b}$$

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

- Precision is biased towards C(Yes|Yes) & C(Yes|No)
- Recall is biased towards C(Yes|Yes) & C(No|Yes)
- F-measure is biased towards all except C(No|No)

$$\text{Weighted Accuracy} = \frac{w_1 a + w_4 d}{w_1 a + w_2 b + w_3 c + w_4 d}$$

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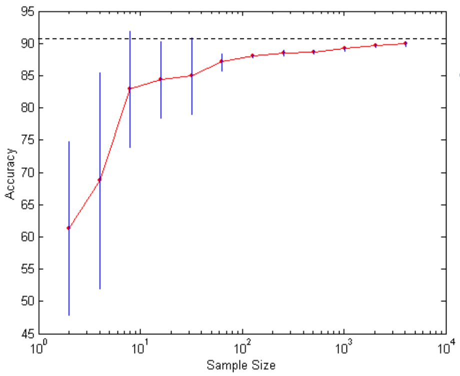
Methods for Performance Evaluation

- How to obtain a reliable estimate of performance?
- Performance of a model may depend on other factors besides the learning algorithm:
  - Class distribution
  - Cost of misclassification
  - Size of training and test sets

Learning Curve



- Learning curve shows how accuracy changes with varying sample size
- Requires a sampling schedule for creating learning curve:
  - Arithmetic sampling (Langley, et al)
  - Geometric sampling (Provost et al)

Effect of small sample size:
- Bias in the estimate
- Variance of estimate

Methods of Estimation

- Holdout
  - Reserve 2/3 for training and 1/3 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
- Stratified sampling
  - oversampling vs undersampling
- Bootstrap
  - Sampling with replacement

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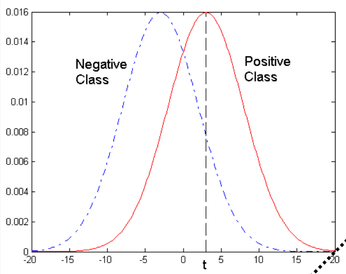
ROC (Receiver Operating Characteristic)

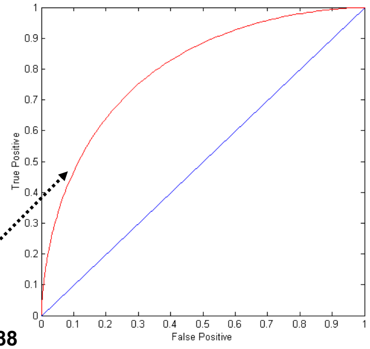
- Developed in 1950s for signal detection theory to analyze noisy signals
  - Characterize the trade-off between positive hits and false alarms
- ROC curve plots TP (on the y-axis) against FP (on the x-axis)
- Performance of each classifier represented as a point on the ROC curve
  - changing the threshold of algorithm, sample distribution or cost matrix changes the location of the point

ROC Curve

- 1-dimensional data set containing 2 classes (positive and negative)

- any points located at x > t is classified as positive





At threshold t:

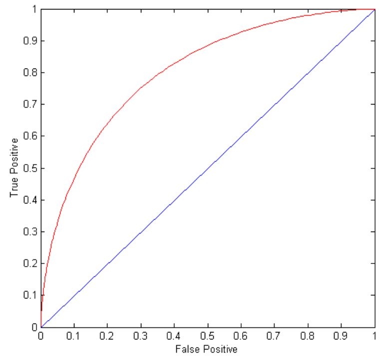
TP=0.5, FN=0.5, FP=0.12, FN=0.88

ROC Curve

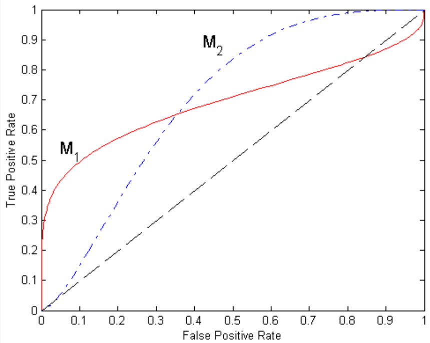
(TP,FP):

- (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



- No model consistently outperform the other
  - M_1 is better for small FPR
  - M_2 is better for large FPR
- Area Under the ROC curve
  - Ideal:
    - Area = 1
  - Random guess:
    - Area = 0.5

How to Construct an ROC curve

Instance	P(+|A)	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

- Use classifier that produces posterior probability for each test instance P(+|A)
- Sort the instances according to P(+|A) in decreasing order
- Apply threshold at each unique value of P(+|A)
- Count the number of TP, FP, TN, FN at each threshold
- TP rate, TPR = TP/(TP+FN)
- FP rate, FPR = FP/(FP + TN)

How to construct an ROC curve

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3	3	2	2	1	0
FP	5	5	4	4	3	2	1	1	0	0	0
TN	0	0	1	1	2	3	4	4	5	5	5
FN	0	1	1	2	2	2	2	3	3	4	5
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4	0.2	0
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0	0	0

ROC Curve: