Review from last week

1. Supervised Learning
2. Classification: a two-step process
3. Validation of partition
4. Cross validation: K-fold
5. Overfitting: accuracy vs. generalization, bias vs. variance
6. KNN algorithm
   1. Distance function and different function
   2. Normalization
   3. Weighted voting
   4. Attributed relevance

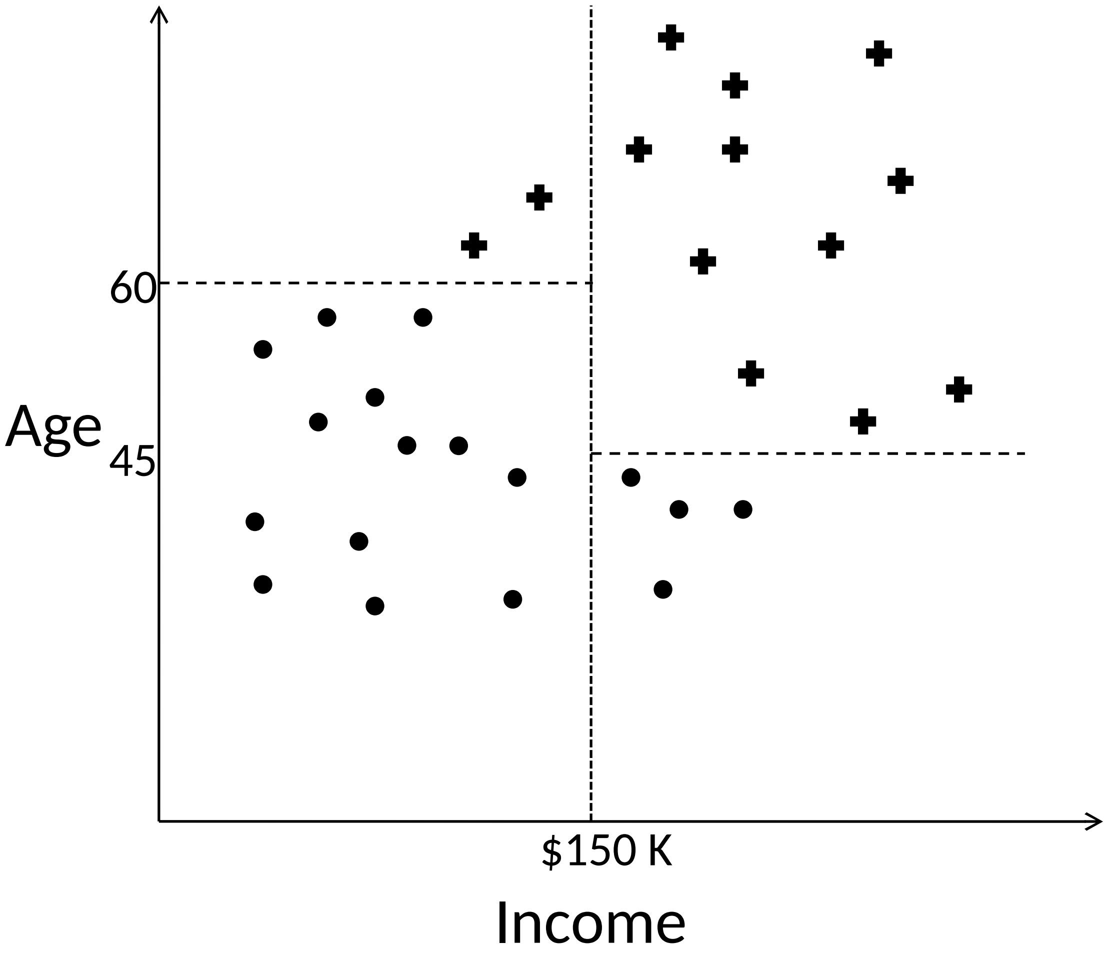
Classification: Decision Trees, Naïve Bayes, and Evaluation Metrics

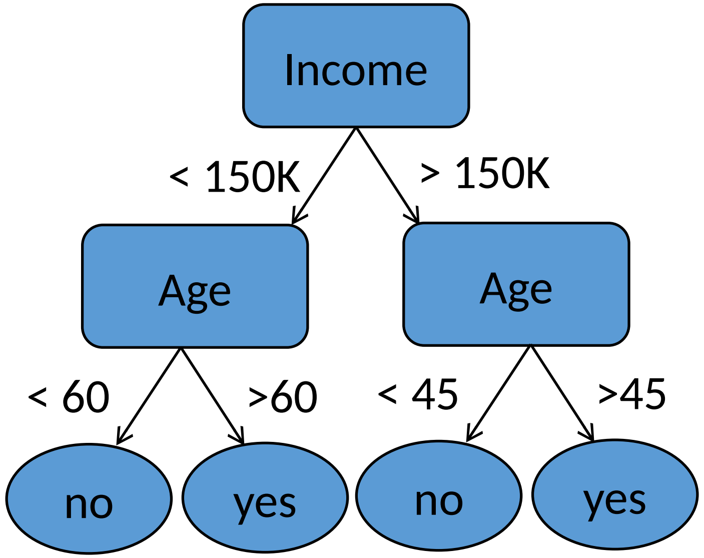
Decision Trees

- Uses a flowchart-like tree structure.
- Collection of <u>decision nodes,</u> connected by <u>branches</u>, extending downward from <u>root node</u> to terminating <u>leaf nodes</u>
  - Each node represents a test on an attribute
  - Each branch represents an outcome
  - Each leaf node holds a class label

- Intuitive and popular classifier
- Very simple but with randomization can be the best!

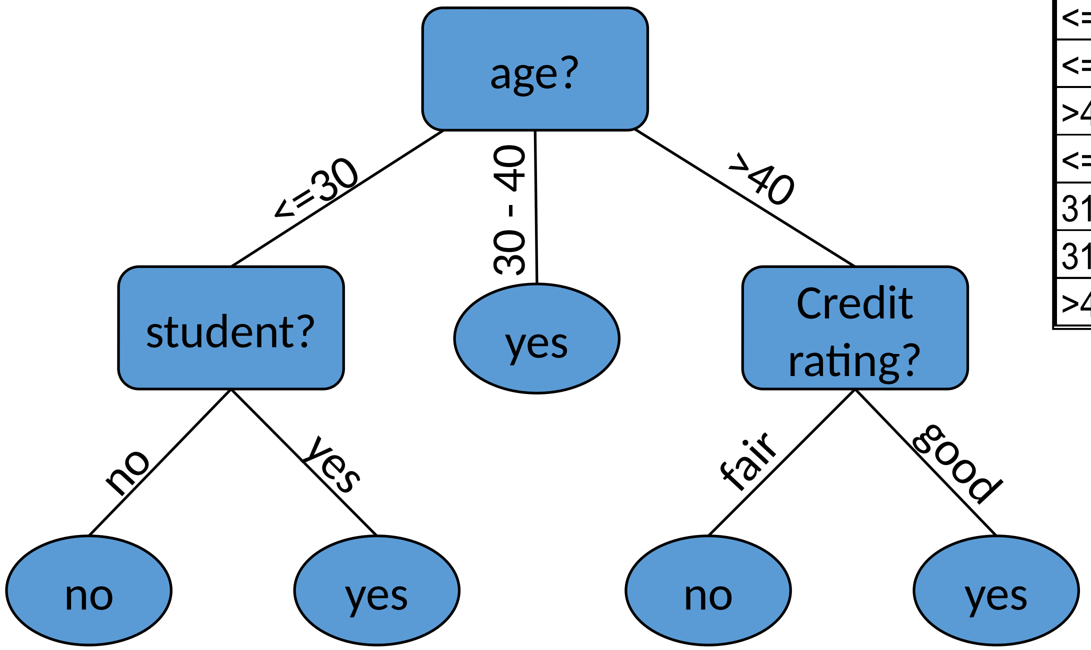
Decision Trees: Basic Concept





Decision Tree: Another Example

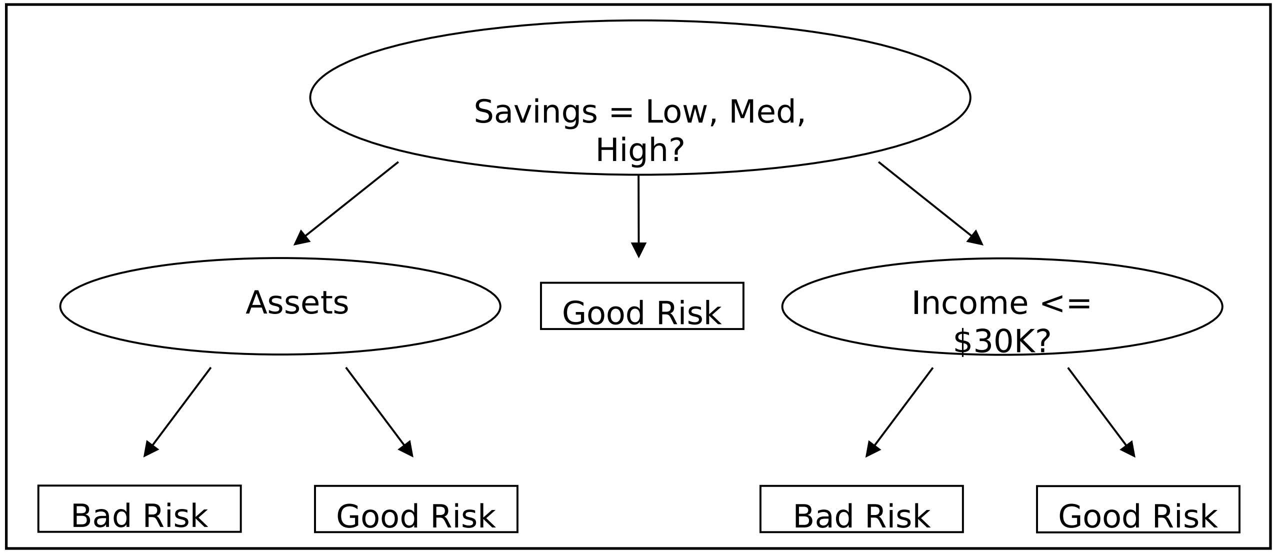
- Target Attribute: Buys_computer
- Resulting tree:



age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

Decision Trees: Another Example (*cont'd*)

- Example
  - *Credit Risk* is the target variable
  - Customers are classified as either "Good Risk" or "Bad Risk"
  - Predictor variables are *Savings* (Low, Med, High), *Assets* (Low, High) and *Income*



Requirements for Using Decision Trees

- Supervised learning
  - requires a pre-classified target variable for training

- The training dataset should be rich and **varied**, providing the algorithm with a representative cross section of the data

- The target attribute class must be **discrete/categorical**

Algorithm for Decision Tree Induction

- Basic algorithm (a greedy (non-backtracking) algorithm)
  - Tree is constructed in a top-down recursive divide-and-conquer manner
  - At start, all the training examples are at the root
  - Attributes are categorical (continuous-values are discretized in advance)
  - Examples are partitioned recursively based on selected attributes
  - Test attributes are selected on the basis of a heuristic or statistical measure (e.g., information gain)

- Conditions for stopping partitioning
  - All samples for a given node belong to the same class
  - Or: No remaining attributes for further partitioning – majority voting is employed for classifying the leaf
  - Or: There are no samples left

Algorithms and Attribute Selection

- Which attribute **best** partitions the data?
- A number of measures are used to determine the best attribute for partitioning

- Algorithms:
  - ID3 (Information Gain)
  - C4.5 (Gain Ratio)
  - CART (Gini Index)

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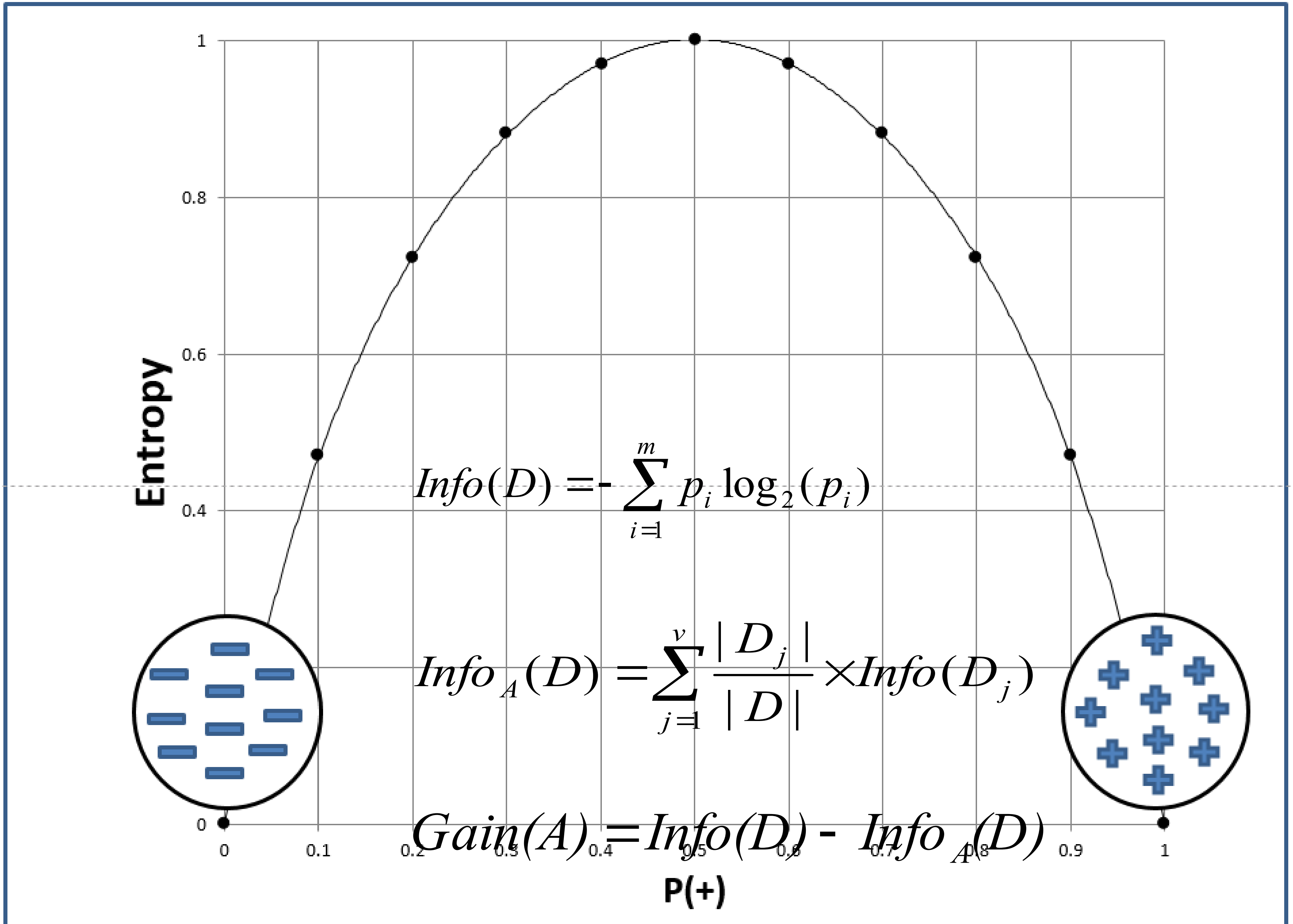


$$Info(D) = -\sum_{i=1}^{m} p_i \log_2(p_i)$$

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times Info(D_j)$$

$$Gain(A) = Info(D) - Info_A(D)$$

Attribute Selection

$$Info(D) = -\left(\frac{9}{14}log_2\frac{9}{14} + \frac{5}{14}log_2\frac{5}{14}\right) = 0.940$$

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

$$Info_{age}(D) = \frac{5}{14} \times \left(-\frac{2}{5}log_2\frac{2}{5} - \frac{3}{5}log_2\frac{3}{5}\right)$$

$$+\frac{4}{14} \times \left(-\frac{4}{4}log_2\frac{4}{4}\right)$$

$$+\frac{5}{14} \times \left(-\frac{3}{5}log_2\frac{3}{5} - \frac{2}{5}log_2\frac{2}{5}\right)$$

= 0.694

$$Gain(age) = 0.940 - 0.694 = 0.246$$

$$Gain(income) = 0.029$$
$$Gain(student) = 0.151$$
$$Gain(credit_{rating}) = 0.048$$

Information Gain Exercise

Color	Size	Shape	Edible?
Yellow	Small	Round	Yes
Yellow	Small	Round	No
Green	Small	Irregular	Yes
Green	Large	Irregular	No
Yellow	Large	Round	Yes
Yellow	Small	Round	Yes
Yellow	Small	Round	Yes
Yellow	Small	Round	Yes
Green	Small	Round	No
Yellow	Large	Round	No
Yellow	Large	Round	Yes
Yellow	Large	Round	No
Yellow	Large	Round	No
Yellow	Large	Round	No
Yellow	Small	Irregular	Yes
Yellow	Large	Irregular	Yes

Summary: ID3

- Calculate the entropy of every attribute using the data set
- Split the original set into subsets using the attribute for which the resulting entropy (after splitting) is minimum (or, equivalently, information gain is maximum)
- Make a decision tree node containing that attribute.

  Recursively on subsets using remaining attributes.

Computing Information-Gain for Continuous Attributes

- Let attribute *A* be a continuous-valued attribute
- Must determine the ***best split point*** for *A*
  - Sort the value *A* in increasing order
  - Typically, the midpoint between each pair of adjacent values is considered as a possible *split point*
    - $(a_i+a_{i+1})/2$ is the midpoint between the values of a_i and a_{i+1}
  - The point with the *minimum expected information requirement* for *A* is selected as the split-point for *A*
- Split:
  - D_1 is the set of tuples in *D* satisfying *A* ≤ split-point, and D_2 is the set of tuples in *D* satisfying *A* > split-point

Gain Ratio for Attribute Selection (C4.5)

- Information gain measure is biased towards attributes with a large number of values
- C4.5 (a successor of ID3) uses **gain ratio** to overcome the problem (normalization of information gain)

$$SplitInfo_A(D) = -\sum_{j=1}^{v} \frac{|D_j|}{|D|} \times \log_2\left(\frac{|D_j|}{|D|}\right)$$

  – *GainRatio(A) = Gain(A)/SplitInfo(A)*

- Ex. $SplitInfo_{income}(D) = -\frac{4}{14} \times \log_2\left(\frac{4}{14}\right) - \frac{6}{14} \times \log_2\left(\frac{6}{14}\right) - \frac{4}{14} \times \log_2\left(\frac{4}{14}\right) = 1.557$

  – *gain_ratio(income) = 0.029/1.557 = 0.019*

- The attribute with the maximum gain ratio is selected as the splitting attribute

Gini Index (CART, IBM Intelligent Miner)

- If a data set D contains examples from n classes, gini index, *gini*(D) is defined as

$$Gini(D) = 1 - \sum_{i=1}^{n} p_i^2$$

  where p_i is the relative frequency of class i in D

- If a data set D is split on A into two subsets D_1 and D_2, the *Gini* index $Gini_A(D)$ is defined as

$$Gini_A(D) = \frac{|D_1|}{|D|} Gini(D_1) + \frac{|D_2|}{|D|} Gini(D_2)$$

- Reduction in Impurity:

$$\Delta Gini(A) = Gini(D) - Gini_A(D)$$

- The attribute that provides the largest reduction in impurity is chosen to split the node (*need to enumerate all the possible splitting points for each attribute*)

Computation of Gini Index

Example *D* has 9 tuples in buys_computer = "yes" and 5 in "no"

$$gini(D) = 1 - \left(\frac{9}{14}\right)^2 - \left(\frac{5}{14}\right)^2 = 0.459$$

- Suppose the attribute income partitions *D* into 10 in D_1: {low,medium} and 4 in D_2 {high}:

$$gini_{income \in \{low,medium\}}(D) = \left(\frac{10}{14}\right) Gini(D_1) + \left(\frac{4}{14}\right) Gini(D_1)$$

$$= \frac{10}{14}\left(1 - \left(\frac{7}{10}\right)^2 - \left(\frac{3}{10}\right)^2\right) + \frac{4}{14}\left(1 - \left(\frac{2}{4}\right)^2 - \left(\frac{2}{4}\right)^2\right)$$
$$= 0.443$$
$$= Gini_{income \in \{high\}}(D).$$

❑ $Gini_{\{low, medium\}}$ is 0.443; $Gini_{\{medium, high\}}$ is 0.450. Thus, split on the {low, medium} (and {high}) since it has the lowest Gini index resulting in the largest reduction in impurity.

Comparing Attribute Selection Measures

- The three measures, in general, return good results but
  - **Information gain**:
    - biased toward multivalued attributes
  - **Gain ratio**:
    - tends to prefer unbalanced splits in which one partition is much smaller than the others
  - **Gini index**:
    - biased toward multivalued attributes
    - provides binary split
    - has difficulty when # of classes is large
    - tends to favor tests that result in equal-sized partitions and purity in both partitions

Comparing Attribute Selection Measures: Example

Customer	Savings	Assets	Income	Credit Risk
1	Medium	High	High	Good
2	Low	Low	Medium	Bad
3	High	Medium	Low	Bad
4	Medium	Medium	Medium	Good
5	Low	Medium	High	Good
6	High	High	Low	Good
7	Low	Low	Low	Bad
8	Medium	Medium	High	Good

Gain (Savings)	0.360073065
Gain (Assets)	**0.548794941**
Gain (Income)	0.468036283
GainRatio (Savings)	0.230627112
GainRatio (Assets)	**0.365863294**
GainRatio (Income)	0.299777647

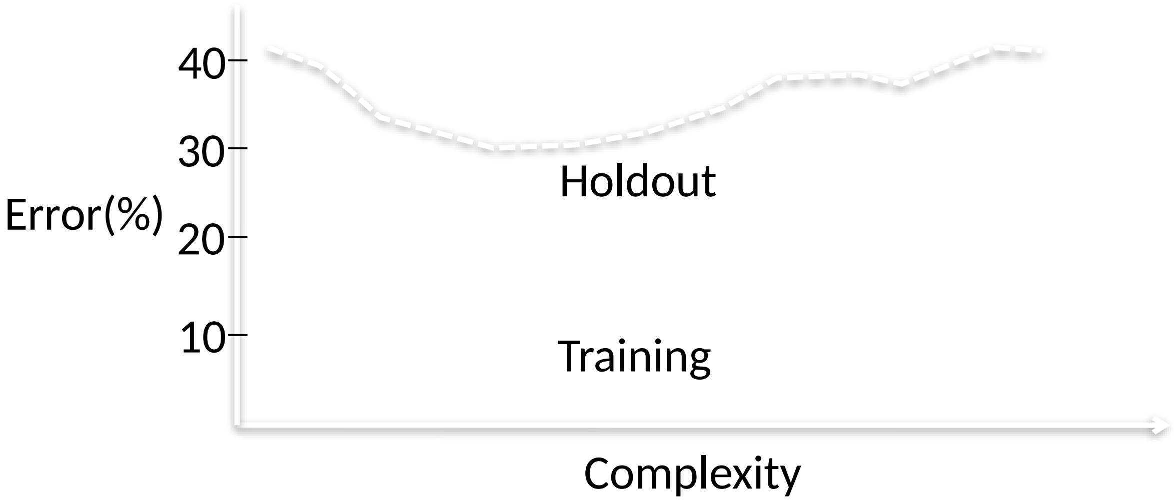
Candidate Split	Left Child Node	Right Child Node	Gini(D)	Gini(A)	Impurity
1	Savings = Low	Savings = {Medium,High}	0.46875	0.666666667	-0.197916667
2	Savings = Medium	Savings = {Low,High}	0.46875	0.5	-0.03125
3	Savings = High	Savings = {Low,Medium}	0.46875	0.75	-0.28125
4	Assets = Low	Assets = {Medium,High}	0.46875	0.625	-0.15625
5	Assets = Medium	Assets = {Low,High}	0.46875	0.5625	-0.09375
6	Assets = High	Assets = {Low,Medium}	0.46875	0.625	-0.15625
7	Income = Low	Income = {Medium, High}	0.46875	0.666666667	-0.197916667
8	Income = Medium	Income = {Low, High}	0.46875	0.75	-0.28125
9	**Income = High**	**Income = {Low, Medium}**	**0.46875**	**0.5**	**-0.03125**

Other Attribute Selection Measures

- CHAID: a popular decision tree algorithm measure based on χ^2 test for independence
- C-SEP: performs better than information gain and gini index in certain cases
- G-statistic: has a close approximation to χ^2 distribution
- MDL (Minimal Description Length) principle (i.e., the simplest solution is preferred):
  - The best tree is the one that requires the fewest # of bits to both (1) encode the tree, and (2) encode the exceptions to the tree
- Multivariate splits (partition based on multiple variable combinations)
  - CART: finds multivariate splits based on a linear combination of attributes
- Which attribute selection measure is the best?
  - Most give good results, none is significantly superior than others

Overfitting

- Overfitting: the tendency of data mining procedures to tailor models to the training data
  - An induced tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Model does not represent general population
  - Poor accuracy for **unseen** samples



Avoiding Overfitting in Decision Trees

- Two approaches to avoid overfitting
  - Prepruning: *Halt tree construction early*- do not split a node if this would result in the goodness measure falling below a threshold
    - Difficult to choose an appropriate threshold
  - Postpruning: *Remove branches* from a “fully grown” tree—get a sequence of progressively pruned trees
    - Use a set of data **different** from the training data to decide which is the “best pruned tree”

Enhancements to Basic Decision Tree Induction

- Allow for **continuous-valued attributes**
  - Dynamically define new discrete-valued attributes that partition the continuous attribute value into a discrete set of intervals
- Handle **missing attribute values**
  - Assign the most common value of the attribute
  - Assign probability to each of the possible values
- **Attribute construction**
  - Create new attributes based on existing ones that are sparsely represented
  - This reduces fragmentation, repetition, and replication

Bayesian Classification

- Simple probabilistic classifier
- Based on **Bayes' theorem**
- Assumes strong (naïve) **independence** between features
  - For example:
    - A fruit can be considered an apple if it is red, round and about 10 cm in diameter
    - Red, round, and diameter are all independent

Bayes' Theorem

- Let ***X*** be a data sample ("*evidence*"): class label is unknown
- Let H be a *hypothesis* that ***X*** belongs to class *C*
- Classification is to determine *P(H|**X**)*, (*posterior probability*), the probability that the hypothesis holds <u>given</u> the observed data sample ***X***
- **Example:** Given the evidence of age and income, predict of someone buys a computer
- *P(H)* (*prior probability*), the initial probability
  - ***X*** will buy computer, regardless of age, income, …
- *P(**X**)*: probability that sample data is observed
  - Probability that ***X*** is 31..40, medium income
- *P(**X**|H)* (likelihood), the probability of observing the sample ***X***, given that the hypothesis holds
  - Given that ***X*** will buy computer, the probability that ***X*** is 31..40, medium income

Bayes' Theorem

- Given training data $\mathbf{X}$, *posterior probability of a hypothesis H, P(H|**X**)*, follows the Bayes theorem

$$P(H|\mathbf{X}) = \frac{P(\mathbf{X}|H)P(H)}{P(\mathbf{X})}$$

- Informally, this can be written as

*posteriori = likelihood * prior/evidence*

- Predicts that $\mathbf{X}$ belongs to C_i **iff** the probability $P(C_i|\mathbf{X})$ is the highest among all the $P(C_k|X)$ for all the *k* classes
- Practical difficulty: <u>requires the initial knowledge of many probabilities, significant computational cost</u>

Towards Naïve Bayesian Classifier

- Let *D* be a training set of tuples and their associated class labels, and each tuple is represented by an n-attribute vector ***X*** = (x_1, x_2, …, x_n)
- Suppose there are *m* classes C_1, C_2, …, C_m.
- Classification is to derive the ***maximum posteriori***, i.e., the maximal $P(C_i|\boldsymbol{X})$
- This can be derived from Bayes' theorem

$$P(C_i|\mathbf{X}) = \frac{P(\mathbf{X}|C_i)P(C_i)}{P(\mathbf{X})}$$

- Since *P(X)* is constant for all classes, only

$$P(C_i|\mathbf{X}) = P(\mathbf{X}|C_i)P(C_i)$$

needs to be maximized

Derivation of Naïve Bayes Classifier

- A simplified assumption: attributes are **conditionally independent** (i.e., no dependence relation between attributes):

$$P(\mathbf{X}|C_i) = \prod_{k=1}^{n} P(x_k|C_i) = P(x_1|C_i) \times P(x_2|C_i) \times \ldots \times P(x_n|C_i)$$

- This greatly reduces the computation cost: Only counts the **class distribution**
- If A_k is categorical, $P(x_k|C_i)$ is the # of tuples in C_i having value x_k for A_k divided by $|C_{i, D}|$ (# of tuples of C_i in D)
- If A_k is continuous-valued, $P(x_k|C_i)$ is usually computed based on a Gaussian distribution with a mean μ and standard deviation σ

$$g(x,\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

and $P(x_k|C_i)$ is

$$P(\mathbf{X}|C_i) = g(x_k, \mu_{C_i}, \sigma_{C_i})$$

Naïve Bayesian Classifier: Training Dataset

Class:

C_1: buys_computer = 'yes'

C_2: buys_computer = 'no'

Data sample

X = (age <=30, Income = medium, Student = yes, Credit_rating = Fair)

age	income	student	credit_rating	_com
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

Naïve Bayesian Classifier: An Example

- ***X*** = (age <= 30 , income = medium, student = yes, credit_rating = fair)
- ***P(C_i)***: P(buys_computer = "yes") = 9/14 = **0.643**
  P(buys_computer = "no") = 5/14= **0.357**
- Compute *P*(*X*|C_i) for each class
  P(age = "<=30" | buys_computer = "yes") = 2/9 = 0.222
  P(age = "<= 30" | buys_computer = "no") = 3/5 = 0.6
  P(income = "medium" | buys_computer = "yes") = 4/9 = 0.444
  P(income = "medium" | buys_computer = "no") = 2/5 = 0.4
  P(student = "yes" | buys_computer = "yes) = 6/9 = 0.667
  P(student = "yes" | buys_computer = "no") = 1/5 = 0.2
  P(credit_rating = "fair" | buys_computer = "yes") = 6/9 = 0.667
  P(credit_rating = "fair" | buys_computer = "no") = 2/5 = 0.4
- ***P(X|C_i)***: P(X|buys_computer = "yes") = 0.222 x 0.444 x 0.667 x 0.667 = **0.044**
  P(X|buys_computer = "no") = 0.6 x 0.4 x 0.2 x 0.4 = **0.019**

P(C_i|X)=P(X|C_i)*P(C_i): P(X|buys_computer = "yes") * P(buys_computer = "yes") = **0.028**
P(X|buys_computer = "no") * P(buys_computer = "no") = **0.007**

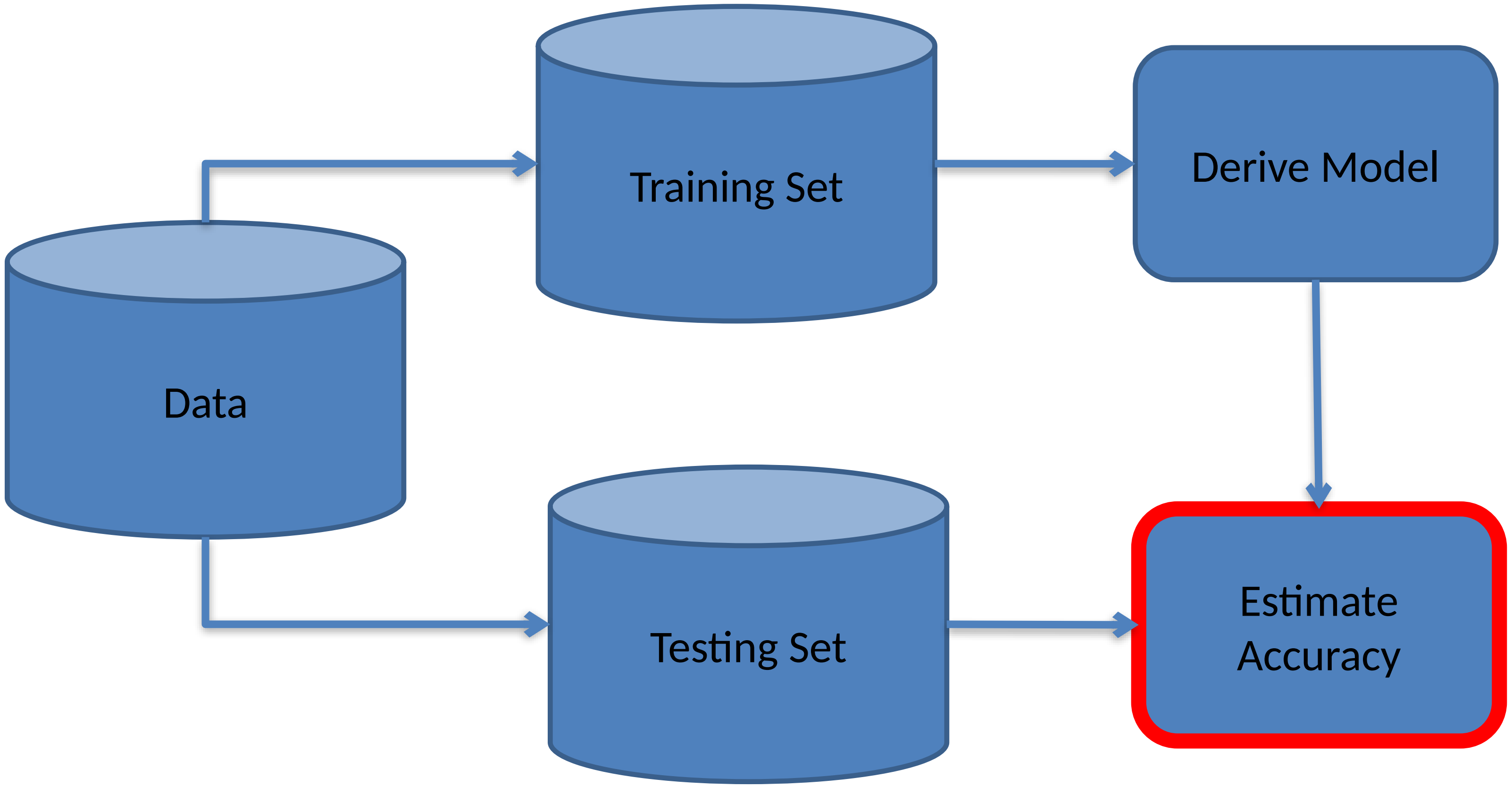
Therefore, *X* belongs to class ("buys_computer = yes")

Evaluating Classifiers

- How well can a classifier be expected to perform on new data?
- Choice of performance measure
- How close is the estimated performance to the true performance?

- Evaluating Classifiers:
  - Performance Metrics
  - Experimental Design

Review: Supervised Learning



Confusion Matrix

Confusion Matrix:

Actual class\Predicted class	C_1	$\neg C_1$
C_1	**True Positives (TP)**	**False Negatives (FN)**
$\neg C_1$	**False Positives (FP)**	**True Negatives (TN)**

Example of Confusion Matrix:

Actual class\Predicted class	buy_computer = yes	buy_computer = no	Total
buy_computer = yes	**6954**	**46**	7000
buy_computer = no	**412**	**2588**	3000
Total	7366	2634	10000

- Given *m* classes, an entry, $\boldsymbol{CM_{i,j}}$ in a **confusion matrix** indicates # of tuples in class *i* that were labeled by the classifier as class *j*
- May have extra rows/columns to provide totals

Accuracy and Error Rate

- Classifier Accuracy, or recognition rate:
  - percentage of test set tuples that are correctly classified
  - Accuracy = *(TP + TN)/All*
- Error rate:
  - *1 – accuracy*, or
  - Error rate = *(FP + FN)/All*

A\P	C	¬C	
C	**TP**	**FN**	**P**
¬C	**FP**	**TN**	**N**
	P’	**N’**	**All**

Sensitivity and Specificity

- Class Imbalance Problem:
  - One class may be *rare*, e.g. fraud, or HIV-positive
  - Significant *majority of the negative class* and minority of the positive class
- Sensitivity: True Positive recognition rate
  - Sensitivity = *TP/P*
- Specificity: True Negative recognition rate
  - Specificity = *TN/N*
  - False Alarm = *FP/(TN+FP)*

A\P	C	¬C	
C	**TP**	**FN**	**P**
¬C	**FP**	**TN**	**N**
	P'	**N'**	**All**

- Accuracy is a function of sensitivity and specificity
  - *accuracy = sensitivity*P/(P+N) + specificity*N/(P+N)*

Precision and Recall

- **Precision**: exactness – what % of tuples that the classifier labeled as positive are actually positive

$$precision = \frac{TP}{TP + FP}$$

- **Recall**: completeness – what % of positive tuples did the classifier label as positive?

$$recall = \frac{TP}{TP + FN}$$

- Perfect score is 1.0
- Inverse relationship between precision & recall

F- Measures

- ***F* measure (*F*$_1$ or *F*-score)**:
- Accuracy measure which considers both precision and recall
- Score between 0 and 1
- Traditional F measure is the harmonic mean of precision and recall

$$F = \frac{2 \times precision \times recall}{precision + recall}$$

- ***F*$_\beta$:** weighted measure of precision and recall
  - assigns ß times as much weight to recall as to precision

$$F_\beta = \frac{(1+\beta^2) \times precision \times recall}{\beta^2 \times precision + recall}$$

Evaluation Metrics: Example 1

Actual\Predicted	Student = Yes	Student = No	Total
Student = Yes	120	10	130
Student = No	5	100	105
Total	125	110	235

- Accuracy = (120 + 100) / 235 = **0.936**
- Error Rate = 1 - 0.936 = **0.064**
- Sensitivity = 120 / 130 = **0.923**
- Specificity = 100 / 105 = **0.952**
- Precision = 120 / 125 = **0.96**
- Recall = 120 / 130 = **0.923**
- F_1 measure = (2 * 0.96 * 0.923) / (0.96 + 0.923) = **0.941**
- F_2 measure = ((1+4) * 0.96 * 0.923) / (4 * 0.96 + 0.923) = **0.93**
- $F_{0.5}$ measure = ((1+0.25) * 0.96 * 0.923) / (0.25 * * 0.96 + 0.923) = 0.952

Evaluation Metrics: Example 2

Actual\Predicted	Cancer = Yes	Cancer = No	Total
Cancer = Yes	90	210	300
Cancer = No	140	9560	9700
Total	230	9770	10000

- Accuracy = (90 + 9560)/10000 = 0.965
- Error Rate = 1 - 0.965 = 0.035
- Sensitivity = 90 / 300 = 0.3
- Specificity = 9560 / 9700 = 0.986
- Precision = 90/230 = 0.3913
- Recall = 90/300 = 0.3
- F measure = (2 * 0.3913 * 0. 3) / (0.3913 + 0.3) = 0.3
- F_2 measure = ((1+4) * 0.3913 * 0.3) / (4 * 0.3913 + 0.3) = 0.3
- $F_{0.5}$ measure = ((1+0.25) * 0.3913 * 0.3) / (0.25 * 0.3913 + 0.3) = 0.368

Measuring Classifier Performance

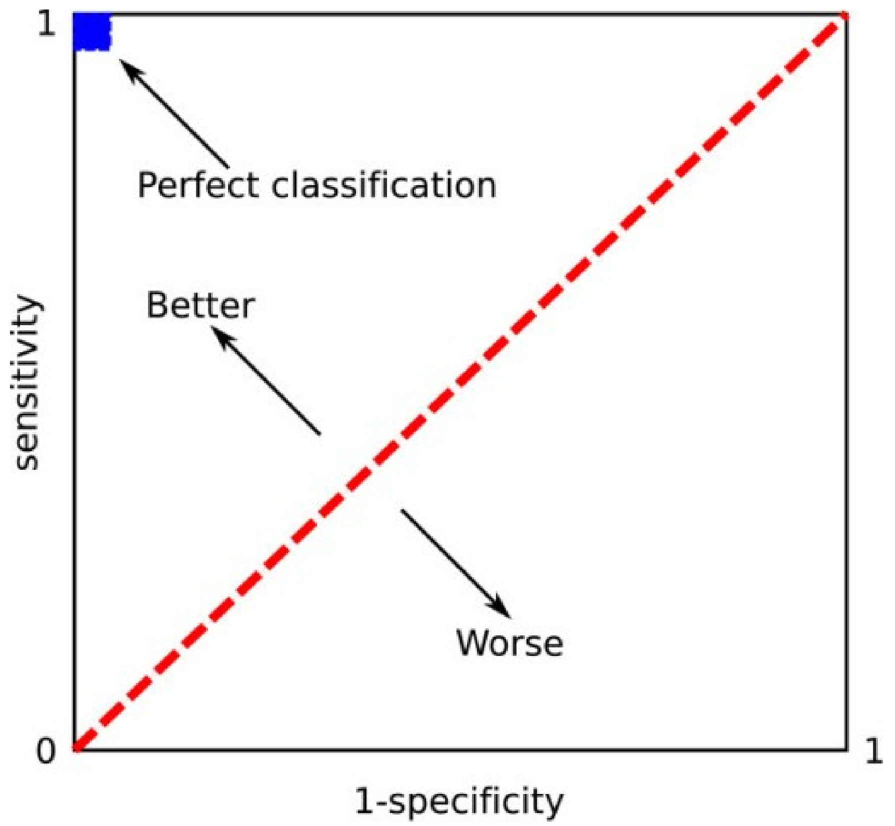
- TP, FP, TN, FN provide the relevant information
- No single measure tells the whole story
- A classifier with 90% accuracy is useless where 90% of the population does not have cancer and the 10% that do are misclassified
- Use of multiple measures recommended
- When you wrap up your results, always include the formula to avoid confusion!

ROC Curves

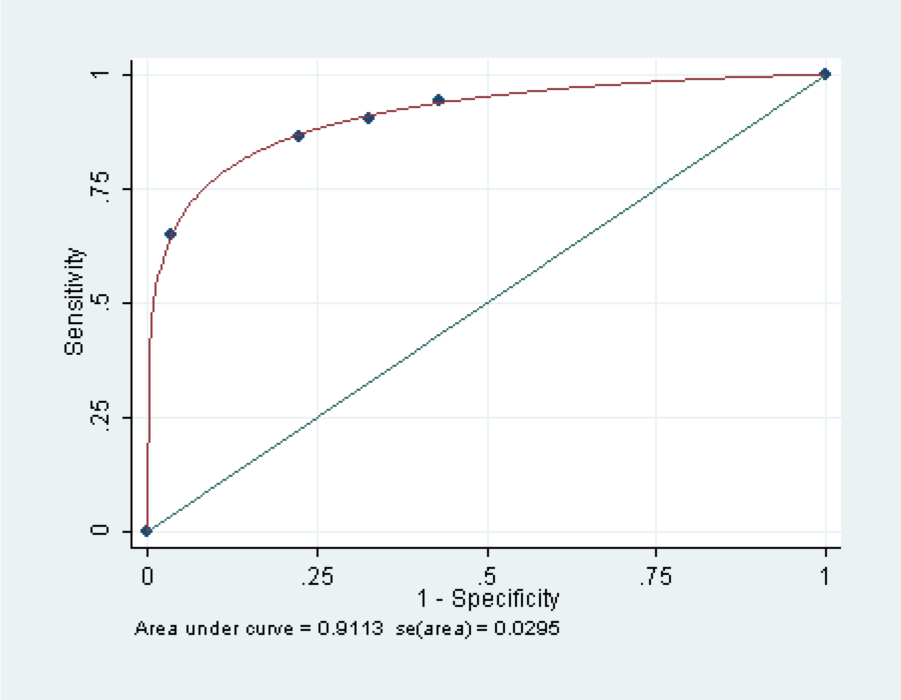
- ROC (Receiver Operating Characteristics) curves: for visual comparison of classification models
- Originated from signal detection theory
- Shows the trade-off between the true positive rate and the false positive rate
- The area under the ROC curve is a measure of the accuracy of the model
- Rank the test tuples in decreasing order: the one that is most likely to belong to the positive class appears at the top of the list
- The closer to the diagonal line (i.e., the closer the area is to 0.5), the less accurate is the model

ROC Space

- ROC curve is a plot of TPR against FPR which depicts relative trade-offs between benefits (true positives) and costs (false positives)



ROC Curves



- Vertical axis: the true positive rate
- Horizontal axis: the false positive rate
- The plot also shows a diagonal line
- The closer an ROC curve is to the diagonal line, the less accurate the model