# Classification fundamentals

Data Base and Data Mining Group of Politecnico di Torino

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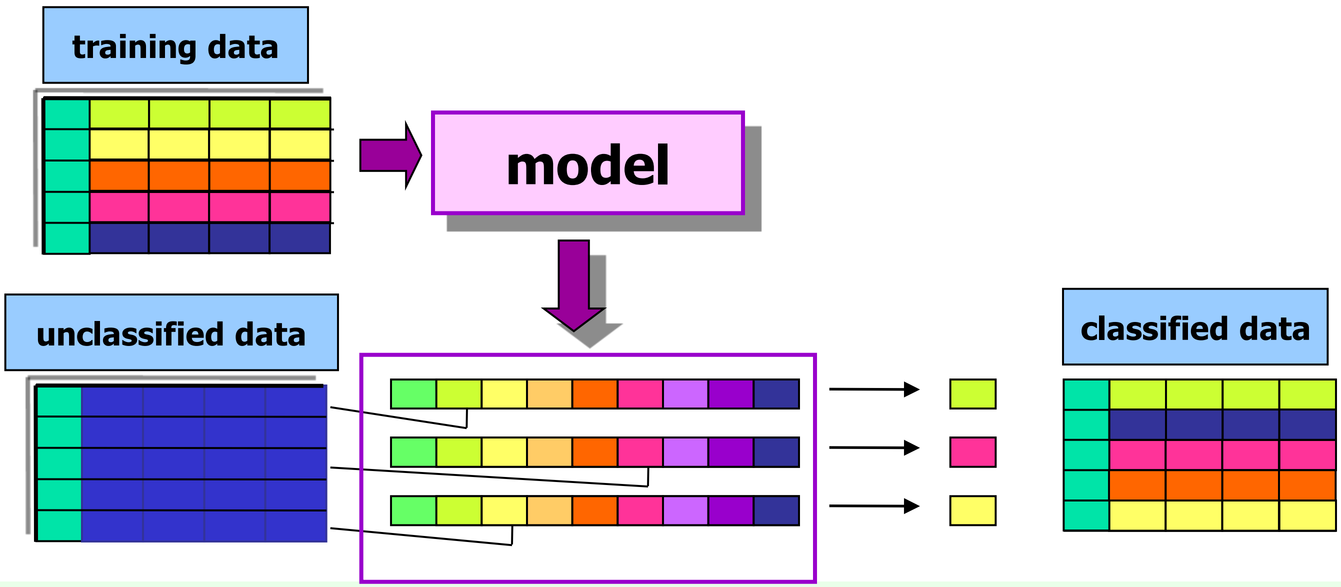
# Classification

- Objectives
  - prediction of a class label
  - definition of an interpretable model of a given phenomenon



# Classification: definition

- Given
  - a collection of class labels
  - a collection of data objects labelled with a class label
- Find a descriptive profile of each class, which will allow the assignment of unlabeled objects to the appropriate class

# Definitions

- Training set
  - Collection of labeled data objects used to learn the classification model
- Test set
  - Collection of labeled data objects used to validate the classification model

# Classification techniques

- Decision trees
- Classification rules
- Association rules
- Neural Networks
- Naïve Bayes and Bayesian Networks
- k-Nearest Neighbours (k-NN)
- Support Vector Machines (SVM)
- ….

# Evaluation of classification techniques

- Accuracy
  - quality of the prediction
- Efficiency
  - model building time
  - classification time
- Scalability
  - training set size
  - attribute number
- Robustness
  - noise, missing data
- Interpretability
  - model interpretability
  - model compactness

# Decision trees

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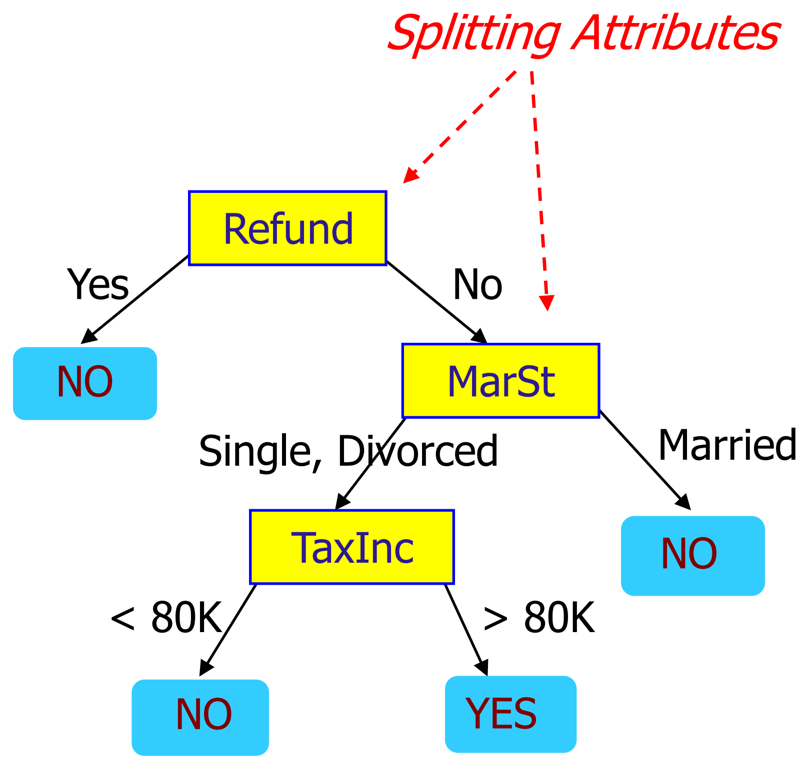
# Example of decision tree

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

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Another example of decision tree

categorical categorical continuous class

| Tid | Refund | Marital Status | Taxable Income | Cheat |
|---|---|---|---|---|
| 1 | Yes | Single | 125K | No |
| 2 | No | Married | 100K | No |
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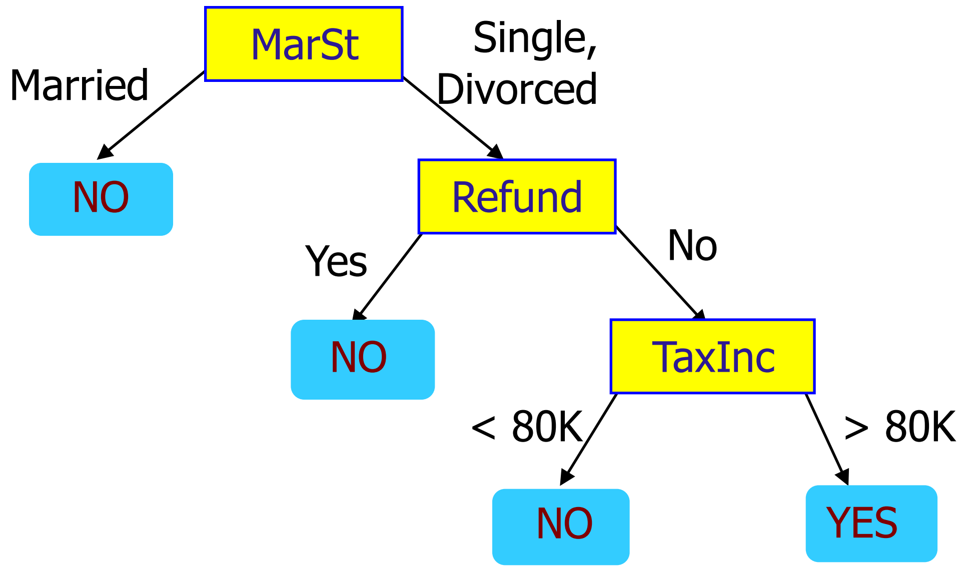
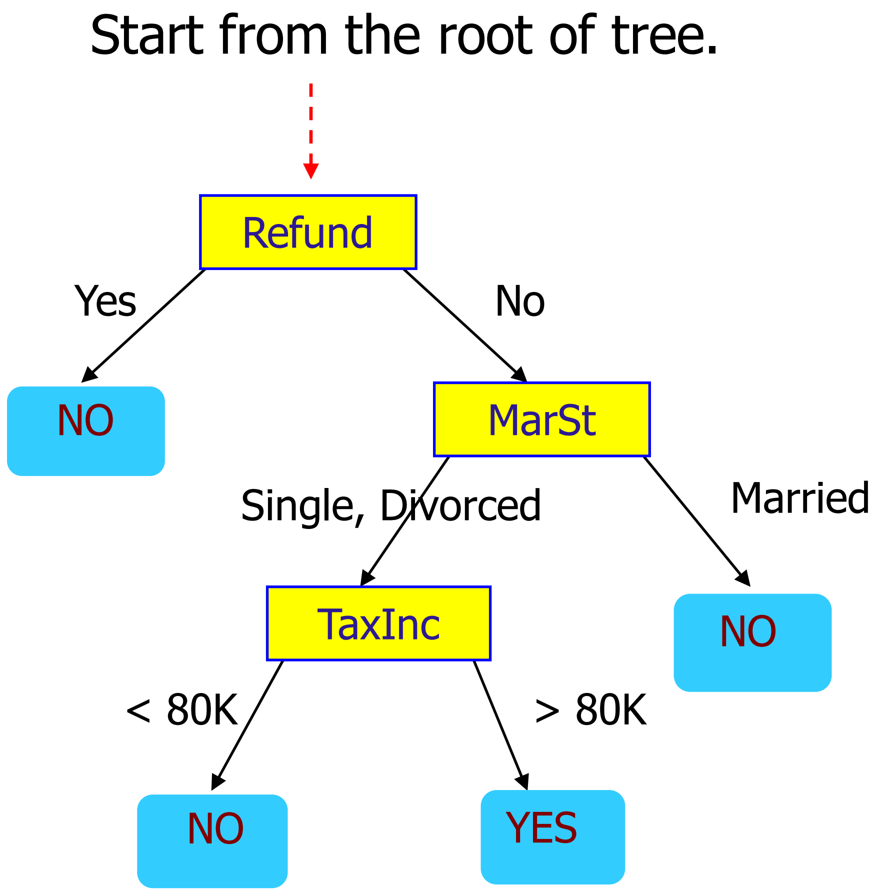



There could be more than one tree that fits the same data!

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

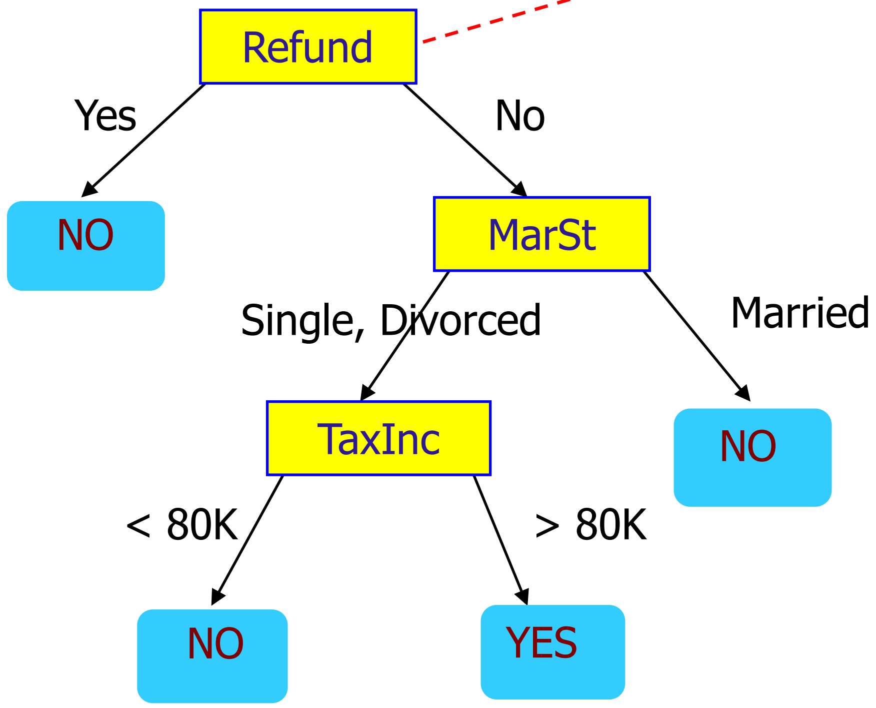
# Apply Model to Test Data




## Test Data

| Refund | Marital Status | Taxable Income | Cheat |
|---|---|---|---|
| No | Married | 80K | ? |

# Apply Model to Test Data




Test Data

| Refund | Marital Status | Taxable Income | Cheat |
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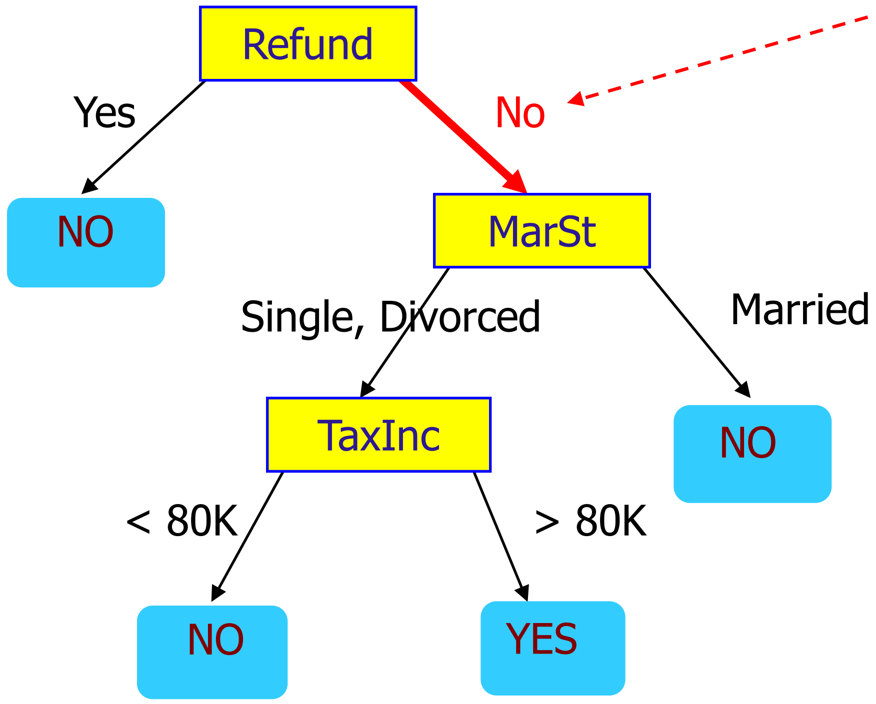
| No | Married | 80K | ? |

# Apply Model to Test Data



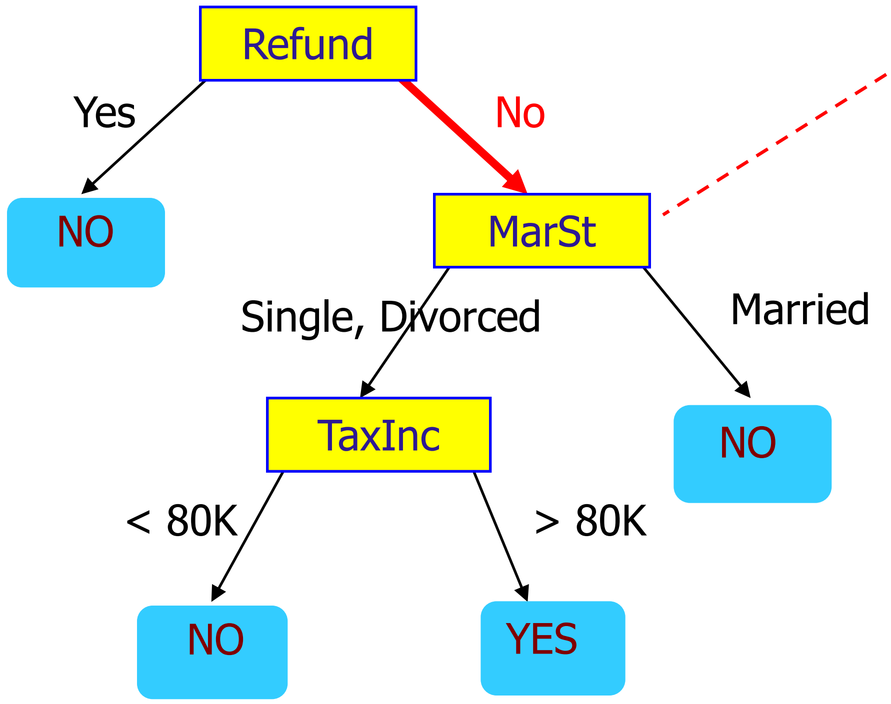

### Test Data

| 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

| Refund | Marital Status | Taxable Income | Cheat |
|---|---|---|---|
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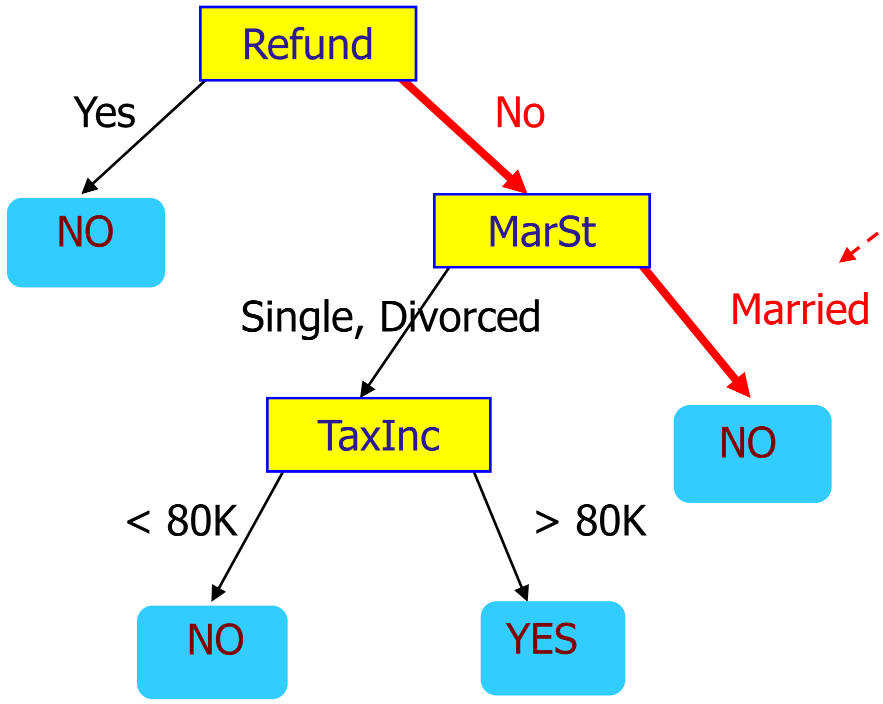

# Apply Model to Test Data

Test Data

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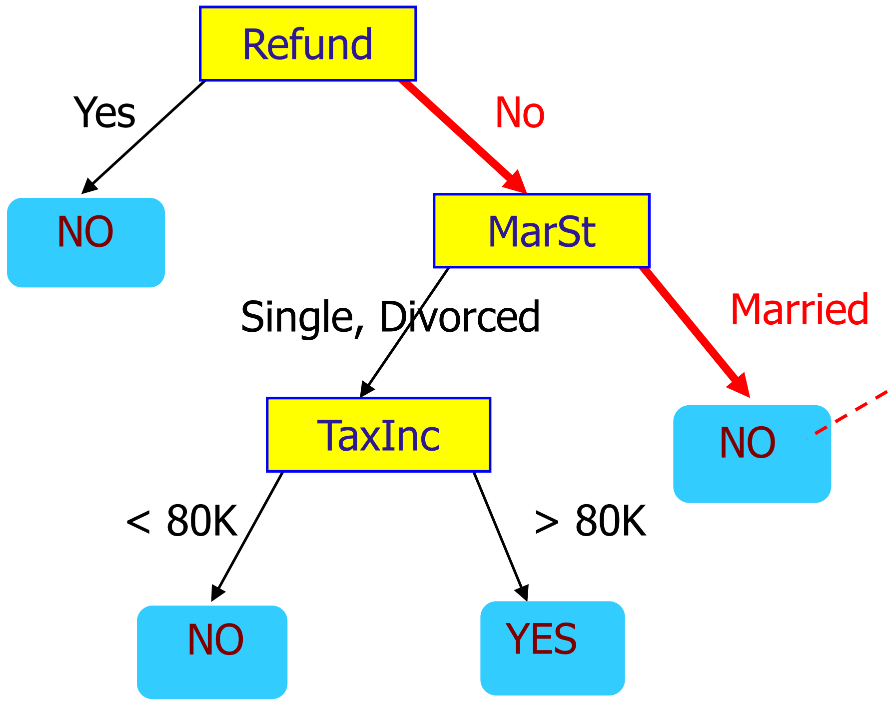


Assign Cheat to "No"

# Decision tree induction

- Many algorithms to build a decision tree
  - Hunt's Algorithm (one of the earliest)
  - CART
  - ID3, C4.5, C5.0
  - SLIQ, SPRINT

# General structure of Hunt's algorithm

| Tid | Refund | Marital Status | Taxable Income | Cheat |
|---|---|---|---|---|
| 1 | Yes | Single | 125K | No |
| 2 | No | Married | 100K | No |
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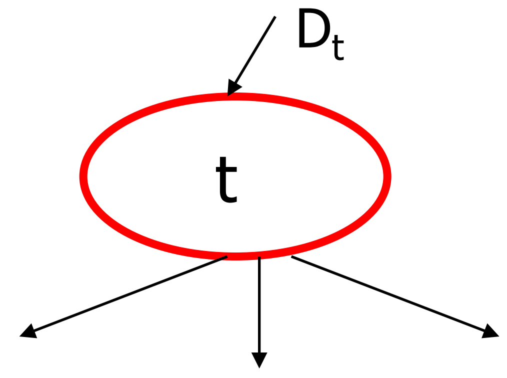
Basic steps

- If $D_t$ contains records that belong to the same class $y_t$
  - then t is a leaf node labeled as $y_t$
- If $D_t$ contains records that belong to more than one class
  - select the "best" attribute A on which to split $D_t$ and label node t as A
  - split $D_t$ into smaller subsets and recursively apply the procedure to each subset
- If $D_t$ is an empty set
  - then t is a leaf node labeled as the default (majority) class, $y_d$

$D_{t,}$, set of training records that reach a node t




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Decision tree induction

- Adopts a greedy strategy
  - "Best" attribute for the split is selected locally at each step
    - not a global optimum
- Issues
  - Structure of test condition
    - Binary split versus multiway split
  - Selection of the best attribute for the split
  - Stopping condition for the algorithm

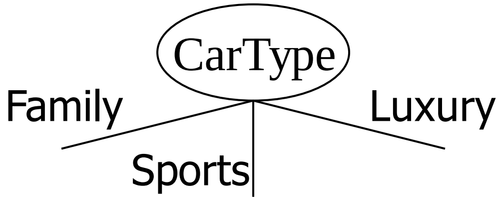
# Structure of test condition

- Depends on attribute type
  - nominal
  - ordinal
  - continuous
- Depends on number of outgoing edges
  - 2-way split
  - multi-way split

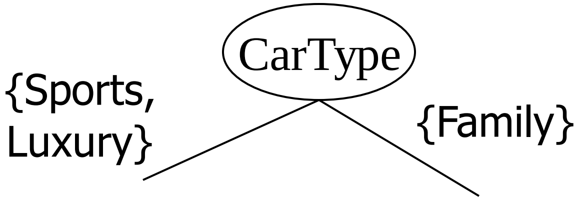
From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Splitting on nominal attributes

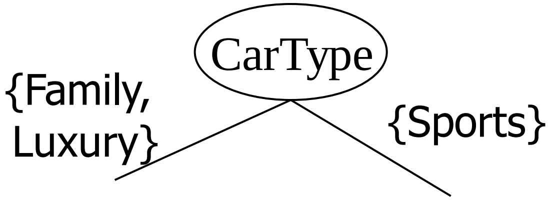
- Multi-way split
  - use as many partitions as distinct values




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



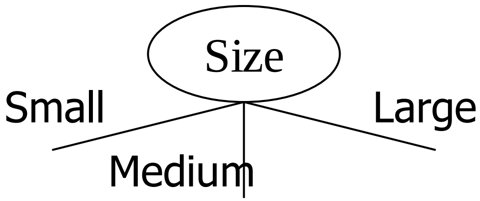

OR



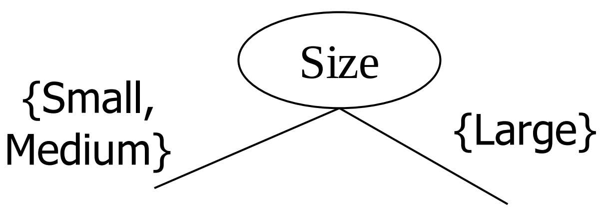

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Splitting on ordinal attributes

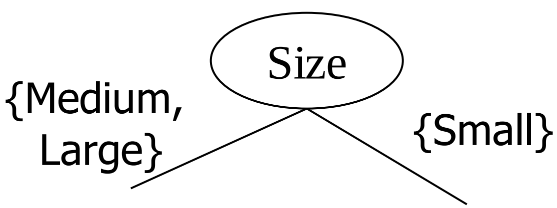
- Multi-way split
  - use as many partitions as distinct values



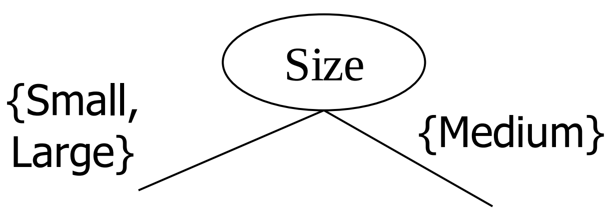

- Binary split
  - Divides values into two subsets
  - Need to find optimal partitioning




OR




What about this split?




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Splitting on continuous attributes

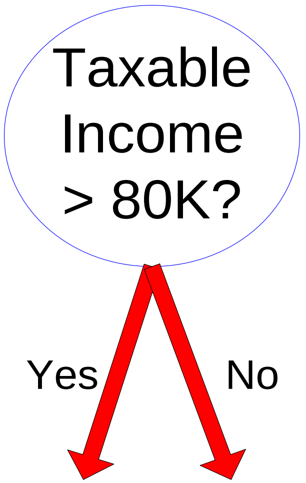
- Different techniques
  - Discretization to form an ordinal categorical attribute
    - Static – discretize once at the beginning
    - Dynamic – discretize during tree induction

    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 find the best cut
    - more computationally intensive

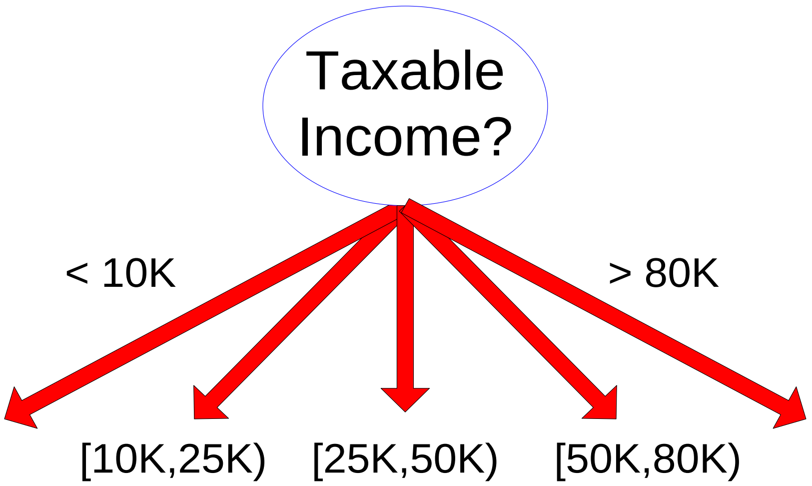


From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Splitting on continuous attributes




(i) Binary split

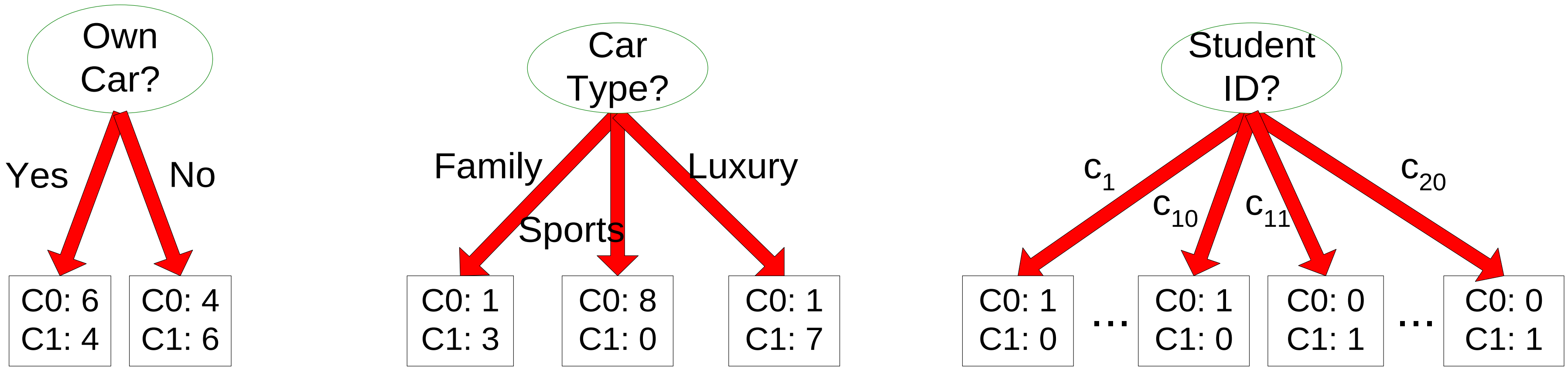



(ii) Multi-way split

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Selection of the best attribute

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




Which attribute (test condition) is the best?

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Selection of the best attribute

- Attributes with *homogeneous* class distribution are preferred
- Need a measure of node impurity

| C0: 5 |
|---|
| C1: 5 |

Non-homogeneous, high degree of impurity

| C0: 9 |
|---|
| C1: 1 |

Homogeneous, low degree of impurity

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Measures of node impurity

- Many different measures available
  - Gini index
  - Entropy
  - Misclassification error
- Different algorithms rely on different measures



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# 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
- Disadvantages
  - accuracy may be affected by missing data

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Associative classification

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# Associative classification

- The classification model is defined by means of association rules

$$(\textit{Condition}) \rightarrow y$$

  - rule body is an itemset
- Model generation
  - Rule selection & sorting
    - based on support, confidence and correlation thresholds
  - Rule pruning
    - Database coverage: the training set is covered by selecting topmost rules according to previous sort

# Associative classification

- Strong points
  - interpretable model
  - higher accuracy than decision trees
    - correlation among attributes is considered
  - efficient classification
  - unaffected by missing data
  - good scalability in the training set size
- Weak points
  - rule generation may be slow
    - it depends on support threshold
  - reduced scalability in the number of attributes
    - rule generation may become unfeasible

# Neural networks

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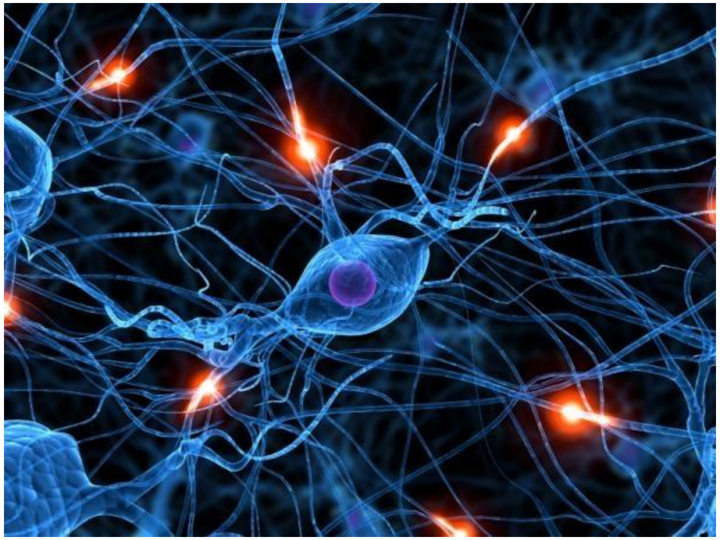
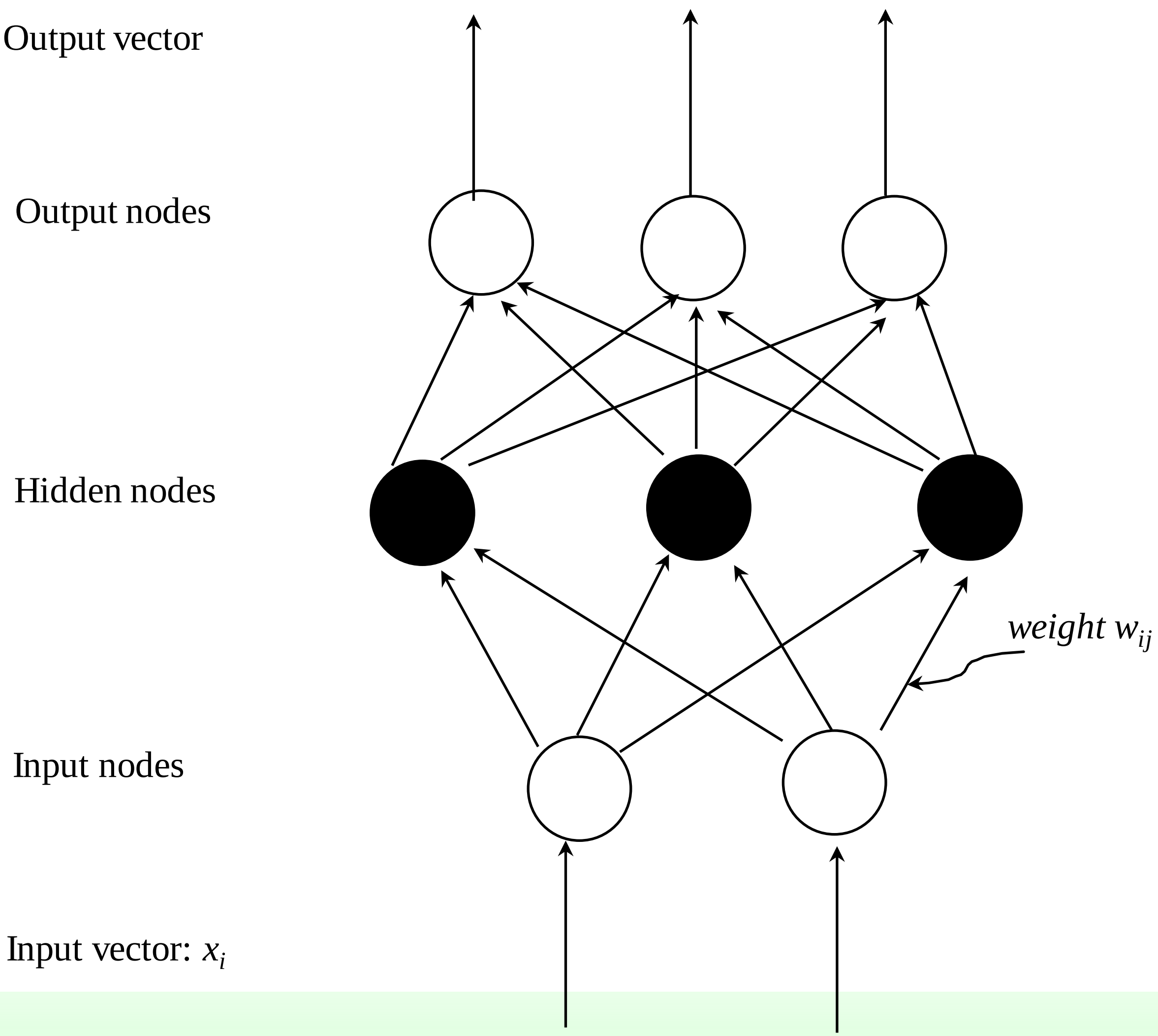
# Neural networks

- Inspired to the structure of the human brain
  - Neurons as elaboration units
  - Synapses as connection network

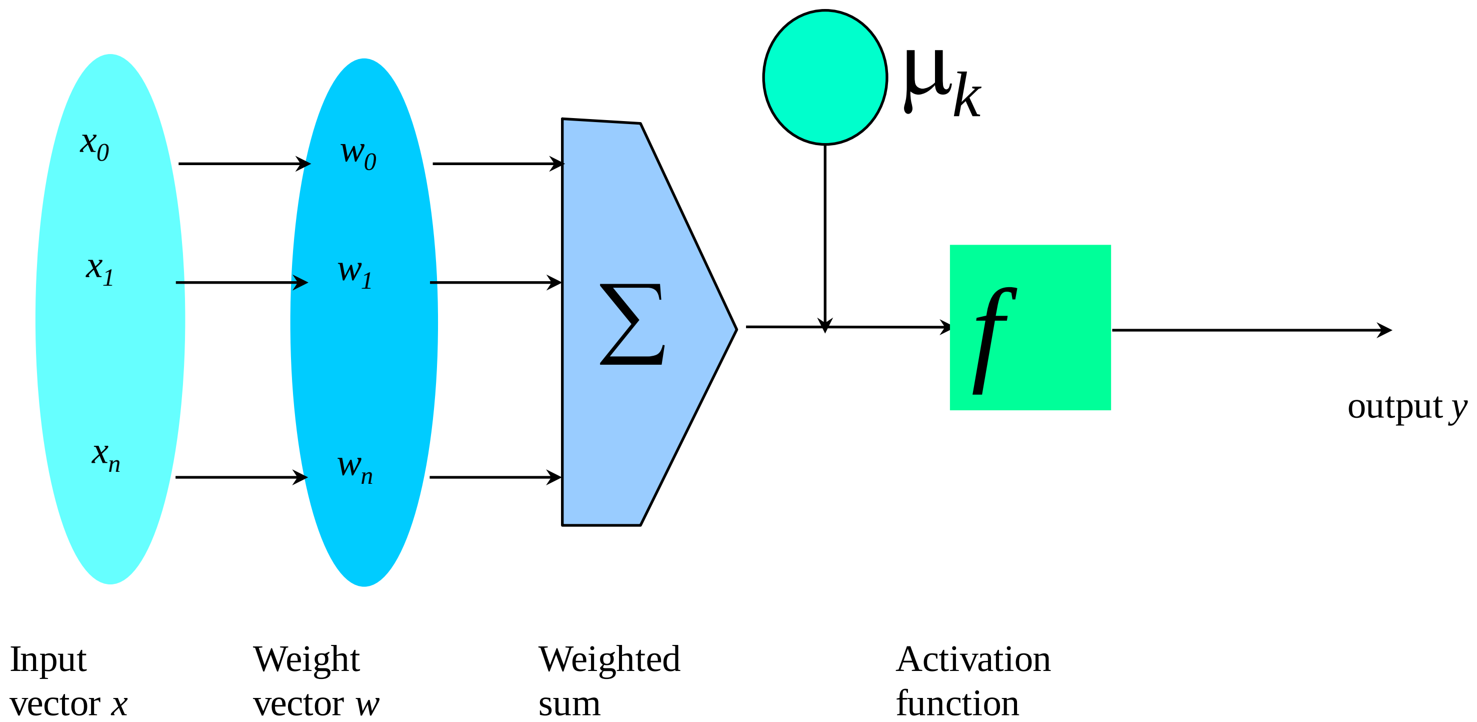


# Structure of a neural network




From: Han, Kamber,"Data mining; Concepts and Techniques", Morgan Kaufmann 2006

# Structure of a neuron

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# Construction of the neural network

- For each node, definition of
  - set of weights
  - offset value

  providing the highest accuracy on the training data
- Iterative approach on training data instances

# Neural networks

- Strong points
  - High accuracy
  - Robust to noise and outliers
  - Supports both discrete and continuous output
  - Efficient during classification
- Weak points
  - Long training time
    - weakly scalable in training data size
    - complex configuration
  - Not interpretable model
    - application domain knowledge cannot be exploited in the model

# Bayesian Classification

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# Bayes theorem

- Let C and X be random variables

$$P(C,X) = P(C|X)\,P(X)$$

$$P(C,X) = P(X|C)\,P(C)$$

- Hence

$$P(C|X)\,P(X) = P(X|C)\,P(C)$$

- and also

$$P(C|X) = P(X|C)\,P(C) \,/\, P(X)$$

# Bayesian classification

- Let the class attribute and all data attributes be random variables
  - C = any class label
  - X = <$x_1$,…,$x_k$> record to be classified
- Bayesian classification
  - compute P(C|X) for all classes
    - probability that record X belongs to C
  - assign X to the class with *maximal* P(C|X)
- Applying Bayes theorem

$$P(C|X) = P(X|C) \cdot P(C) / P(X)$$

  - P(X) constant for all C, disregarded for maximum computation
  - P(C) a priori probability of C

$$P(C) = N_c/N$$

# Bayesian classification

- How to estimate $P(X|C)$, i.e. $P(x_1,\ldots,x_k|C)$?
- Naïve hypothesis

$$P(x_1,\ldots,x_k|C) = P(x_1|C)\ P(x_2|C)\ \ldots\ P(x_k|C)$$

  - *statistical independence* of attributes $x_1,\ldots,x_k$
  - not always true
    - model quality may be affected
- Computing $P(x_k|C)$
  - for discrete attributes

$$P(x_k|C) = |x_{kC}| / N_c$$

    - where $|x_{kC}|$ is number of instances having value $x_k$ for attribute k and belonging to class C
  - for continuous attributes, use probability distribution
- Bayesian networks
  - allow specifying a subset of dependencies among attributes

# Bayesian classification: Example

| Outlook | Temperature | Humidity | Windy | Class |
|---|---|---|---|---|
| sunny | hot | high | false | N |
| sunny | hot | high | true | N |
| overcast | hot | high | false | P |
| rain | mild | high | false | P |
| rain | cool | normal | false | P |
| rain | cool | normal | true | N |
| overcast | cool | normal | true | P |
| sunny | mild | high | false | N |
| sunny | cool | normal | false | P |
| rain | mild | normal | false | P |
| sunny | mild | normal | true | P |
| overcast | mild | high | true | P |
| overcast | hot | normal | false | P |
| rain | mild | high | true | N |

From: Han, Kamber,"Data mining; Concepts and Techniques", Morgan Kaufmann 2006

# Bayesian classification: Example

| | |
|---|---|
| **outlook** | |
| P(sunny\|p) = 2/9 | P(sunny\|n) = 3/5 |
| P(overcast\|p) = 4/9 | P(overcast\|n) = 0 |
| P(rain\|p) = 3/9 | P(rain\|n) = 2/5 |
| **temperature** | |
| P(hot\|p) = 2/9 | P(hot\|n) = 2/5 |
| P(mild\|p) = 4/9 | P(mild\|n) = 2/5 |
| P(cool\|p) = 3/9 | P(cool\|n) = 1/5 |
| **humidity** | |
| P(high\|p) = 3/9 | P(high\|n) = 4/5 |
| P(normal\|p) = 6/9 | P(normal\|n) = 2/5 |
| **windy** | |
| P(true\|p) = 3/9 | P(true\|n) = 3/5 |
| P(false\|p) = 6/9 | P(false\|n) = 2/5 |

| |
|---|
| P(p) = 9/14 |
| P(n) = 5/14 |

From: Han, Kamber,"Data mining; Concepts and Techniques", Morgan Kaufmann 2006

# Bayesian classification: Example

- Data to be labeled

  X = <rain, hot, high, false>

- For class p

  $P(X|p) \cdot P(p) =$
  $= P(rain|p) \cdot P(hot|p) \cdot P(high|p) \cdot P(false|p) \cdot P(p)$
  $= 3/9 \cdot 2/9 \cdot 3/9 \cdot 6/9 \cdot 9/14 = 0.010582$

- For class n

  $P(X|n) \cdot P(n) =$
  $= P(rain|n) \cdot P(hot|n) \cdot P(high|n) \cdot P(false|n) \cdot P(n)$
  $= 2/5 \cdot 2/5 \cdot 4/5 \cdot 2/5 \cdot 5/14 =$ 0.018286



From: Han, Kamber,"Data mining; Concepts and Techniques", Morgan Kaufmann 2006

# Model evaluation

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# Model evaluation

- Methods for performance evaluation
  - Partitioning techniques for training and test sets
- Metrics for performance evaluation
  - Accuracy, other measures
- Techniques for model comparison
  - ROC curve

# Methods of estimation

- Partitioning labeled data in
  - training set for model building
  - test set for model evaluation
- Several partitioning techniques
  - holdout
  - cross validation
- Stratified sampling to generate partitions
  - without replacement
- Bootstrap
  - Sampling with replacement

# Holdout

- Fixed partitioning
  - reserve 2/3 for training and 1/3 for testing
- Appropriate for large datasets
  - may be repeated several times
    - repeated holdout

# Cross validation

- Cross validation
  - partition data into k disjoint subsets (i.e., folds)
  - k-fold: train on k-1 partitions, test on the remaining one
    - repeat for all folds
  - reliable accuracy estimation, not appropriate for very large datasets
- Leave-one-out
  - cross validation for k=n
  - only appropriate for very small datasets

# Metrics for model evaluation

- Evaluate the predictive accuracy of a model
- Confusion matrix
  - binary classifier

| | | 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)



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Accuracy

- Most widely-used metric for model evaluation

$$\text{Accuracy} = \frac{\text{Number of correctly classified objects}}{\text{Number of classified objects}}$$

- Not always a reliable metric

# Accuracy

- For a binary classifier

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

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



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Limitations of accuracy

- Consider a binary problem
  - Cardinality of Class 0 = 9900
  - Cardinality of Class 1 = 100
- Model

$$() \rightarrow \textit{class 0}$$

  - Model predicts everything to be class 0
    - accuracy is 9900/10000 = 99.0 %
- Accuracy is misleading because the model does not detect any class 1 object

# Limitations of accuracy

- Classes may have different importance
  - Misclassification of objects of a given class is more important
  - e.g., ill patients erroneously assigned to the healthy patients class
- Accuracy is not appropriate for
  - unbalanced class label distribution
  - different class relevance

# Class specific measures

- Evaluate separately for each class

$$\text{Recall (r)} = \frac{\text{Number of objects correctly assigned to C}}{\text{Number of objects belonging to C}}$$

$$\text{Precision (p)} = \frac{\text{Number of objects correctly assigned to C}}{\text{Number of objects assigned to C}}$$

- Maximize

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

# Class specific measures

- For a binary classification problem
  - on the confusion matrix, for the positive class

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

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

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



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006