Chapter 6. Classification and Prediction

- What is classification? What is prediction?
- Issues regarding classification and prediction
- Classification by decision tree induction
- Classification by back propagation
- Lazy learners (or learning from your neighbors)
- Frequent-pattern-based classification
- Other classification methods
- Prediction
- Accuracy and error measures

Supervised vs. Unsupervised Learning

- Supervised learning (classification)
  - Supervision: The training data (observations, measurements, etc.) are accompanied by labels indicating the class of the observations
  - New data is classified based on the training set
- Unsupervised learning (clustering)
  - The class labels of training data is unknown
  - Given a set of measurements, observations, etc. with the aim of establishing the existence of classes or clusters in the data

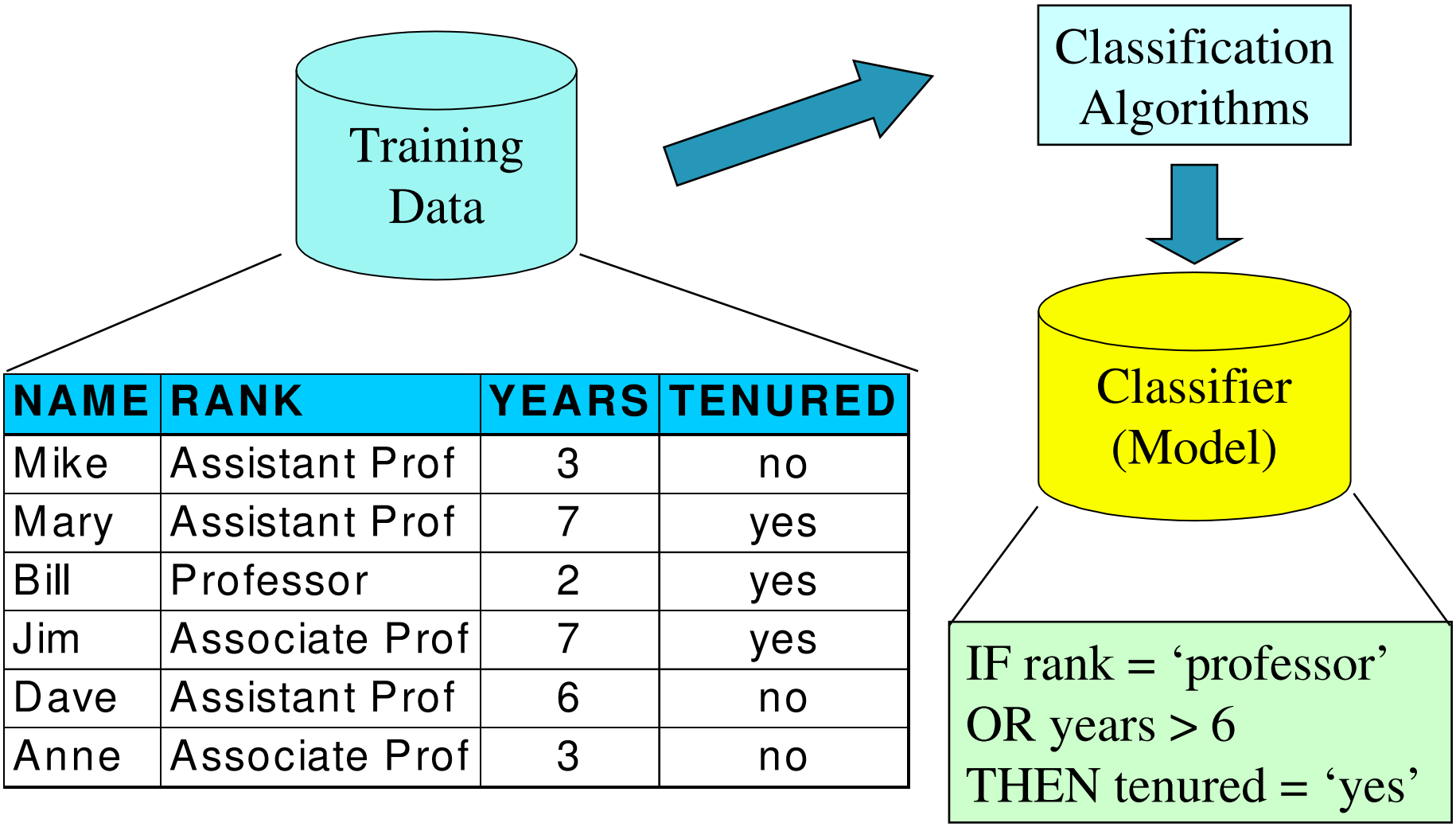
Classification vs. Prediction

- Classification
  - predicts categorical class labels (discrete or nominal)
  - classifies data (constructs a model) based on the training set and the values (class labels) in a classifying attribute and uses it in classifying new data
- Prediction
  - models continuous-valued functions, i.e., predicts unknown or missing values
- Typical applications
  - Credit/loan approval:
  - Medical diagnosis: if a tumor is cancerous or benign
  - Fraud detection: if a transaction is fraudulent
  - Web page categorization: which category it is

Classification—A Two-Step Process

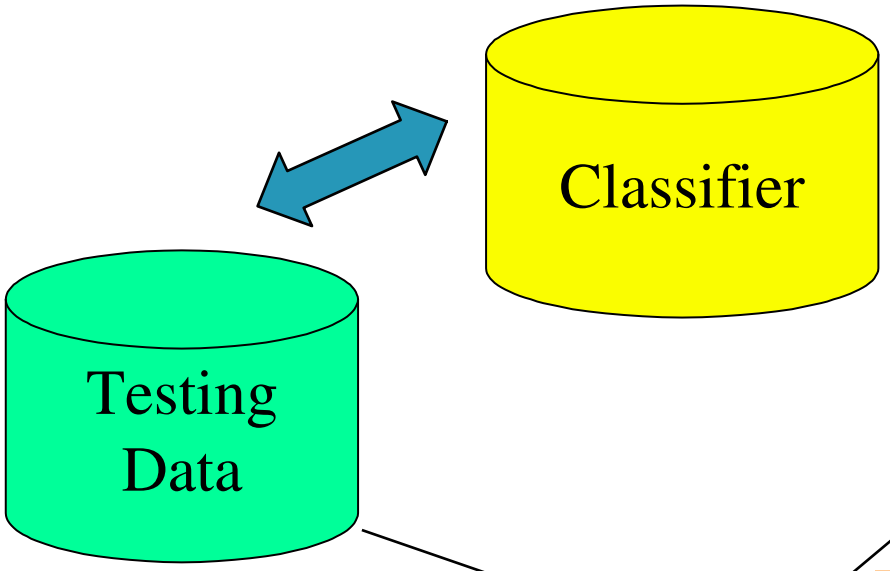
- Model construction: describing a set of predetermined classes
  - Each tuple/sample is assumed to belong to a predefined class, as determined by the class label attribute
  - The set of tuples used for model construction is training set
  - The model is represented as classification rules, decision trees, or mathematical formulae
- Model usage: for classifying future or unknown objects
  - Estimate accuracy of the model
    - The known label of test sample is compared with the classified result from the model
    - Accuracy rate is the percentage of test set samples that are correctly classified by the model
    - Test set is independent of training set, otherwise over-fitting will occur
  - If the accuracy is acceptable, use the model to classify data tuples whose class labels are not known

Process (1): Model Construction



NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no

Process (2): Using the Model in Prediction



NAME	RANK	YEARS	TENURED
Tom	Assistant Prof	2	no
Merlisa	Associate Prof	7	no
George	Professor	5	yes
Joseph	Assistant Prof	7	yes

(Jeff, Professor, 4)

Tenured?

Yes

Issues: Data Preparation

- Data cleaning
  - Preprocess data in order to reduce noise and handle missing values
- Relevance analysis (feature selection)
  - Remove the irrelevant or redundant attributes
- Data transformation
  - Generalize and/or normalize data

Issues: Evaluating Classification Methods

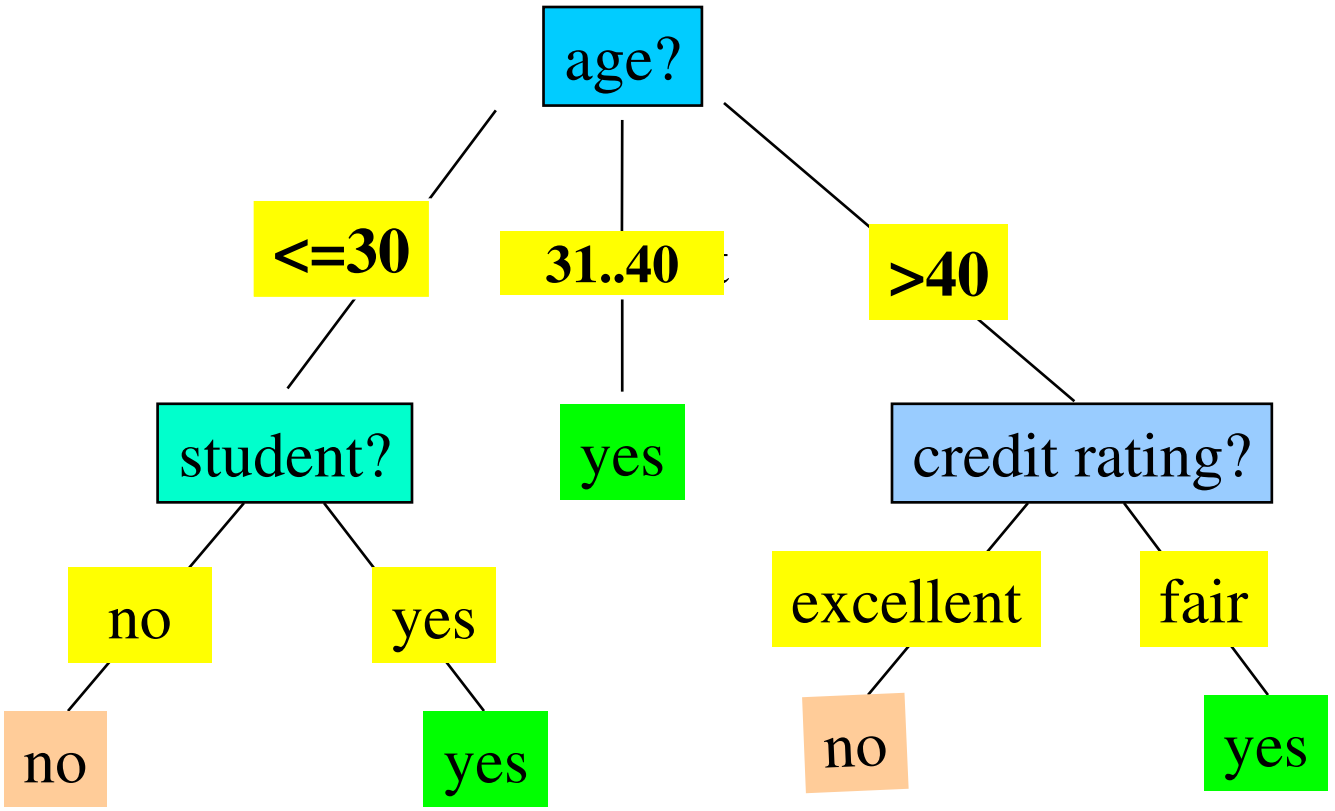
- Accuracy
  - classifier accuracy: predicting class label
  - predictor accuracy: guessing value of predicted attributes
- Speed
  - time to construct the model (training time)
  - time to use the model (classification/prediction time)
- Robustness: handling noise and missing values
- Scalability: efficiency in disk-resident databases
- Interpretability
  - understanding and insight provided by the model
- Other measures, e.g., goodness of rules, such as decision tree size or compactness of classification rules

Decision Tree Induction: Training Dataset

This follows an example of Quinlan's ID3 (Playing Tennis)

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

Output: A Decision Tree for "*buys_computer*"



Algorithm for Decision Tree Induction

- Basic algorithm (a greedy 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 (if continuous-valued, they 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
  - There are no remaining attributes for further partitioning – majority voting is employed for classifying the leaf
  - There are no samples left

Attribute Selection Measure: Information Gain (ID3/C4.5)

- Select the attribute with the highest information gain
- Let p_i be the probability that an arbitrary tuple in D belongs to class C_i, estimated by $|C_{i,D}|/|D|$
- Expected information (entropy) needed to classify a tuple in D:

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

- Information needed (after using A to split D into v partitions) to classify D:

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

- Information gained by branching on attribute A

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

Attribute Selection: Information Gain

- Class P: buys_computer = "yes"
- Class N: buys_computer = "no"

$$Info(D) = I(9,5) = -\frac{9}{14}\log_2(\frac{9}{14}) - \frac{5}{14}\log_2(\frac{5}{14}) = 0.940$$

$$Info_{age}(D) = \frac{5}{14} I(2,3) + \frac{4}{14} I(4,0) + \frac{5}{14} I(3,2) = 0.694$$

age	p_i	n_i	$I(p_i, n_i)$
<=30	2	3	0.971
31…40	4	0	0
>40	3	2	0.971

$\frac{5}{14} I(2,3)$ means "age <=30" has 5 out of 14 samples, with 2 yes'es and 3 no's. Hence

$$Gain(age) = Info(D) - Info_{age}(D) = 0.246$$

Similarly,

$$Gain(income) = 0.029$$
$$Gain(student) = 0.151$$
$$Gain(credit\_rating) = 0.048$$

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

Computing Information-Gain for Continuous-Value 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:
  - D1 is the set of tuples in D satisfying A ≤ split-point, and D2 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 to 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. $SplitInfo_A(D) = -\frac{4}{14} \times \log_2\left(\frac{4}{14}\right) - \frac{6}{14} \times \log_2\left(\frac{6}{14}\right) - \frac{4}{14} \times \log_2\left(\frac{4}{14}\right) = 0.926$
  - gain_ratio(income) = 0.029/0.926 = 0.031
- The attribute with the maximum gain ratio is selected as the splitting attribute

Gini index (CART, IBM IntelligentMiner)

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

$$gini(D) = 1 - \sum_{j=1}^{n} p_j^2$$

  where p_j is the relative frequency of class j in D

- If a data set D is split on A into two subsets D_1 and D_2, the *gini* index $gini(D)$ 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 provides the smallest $gini_{split}(D)$ (or the largest reduction in impurity) is chosen to split the node (*need to enumerate all the possible splitting points for each attribute*)

Gini index (CART, IBM IntelligentMiner)

- Ex. 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

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

$$= \frac{10}{14}(1 - (\frac{6}{10})^2 - (\frac{4}{10})^2) + \frac{4}{14}(1 - (\frac{1}{4})^2 - (\frac{3}{4})^2)$$

$$= 0.450$$

$$= Gini_{income \in \{high\}}(D)$$

but $gini_{\{medium,high\}}$ is 0.30 and thus the best since it is the lowest

- All attributes are assumed continuous-valued
- May need other tools, e.g., clustering, to get the possible split values
- Can be modified for categorical attributes

Comparing Attribute Selection Measures

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

Overfitting and Tree Pruning

- Overfitting: An induced tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Poor accuracy for unseen samples
- 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"

Classification in Large Databases

- Classification—a classical problem extensively studied by statisticians and machine learning researchers
- Scalability: Classifying data sets with millions of examples and hundreds of attributes with reasonable speed
- Why decision tree induction in data mining?
  - relatively faster learning speed (than other classification methods)
  - convertible to simple and easy to understand classification rules
  - can use SQL queries for accessing databases
  - comparable classification accuracy with other methods

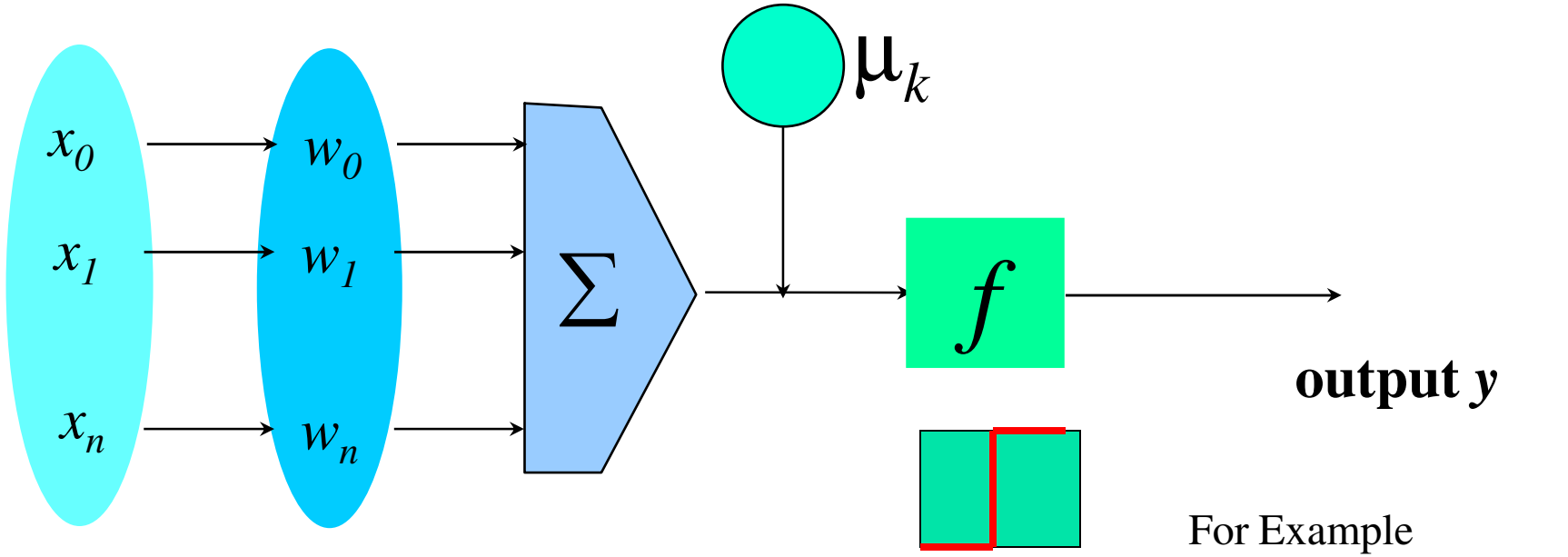
Classification by Backpropagation

- Backpropagation: A **neural network** learning algorithm
- Started by psychologists and neurobiologists to develop and test computational analogues of neurons
- A neural network: A set of connected input/output units where each connection has a **weight** associated with it
- During the learning phase, the **network learns by adjusting the weights** so as to be able to predict the correct class label of the input tuples
- Also referred to as **connectionist learning** due to the connections between units

Neural Network as a Classifier

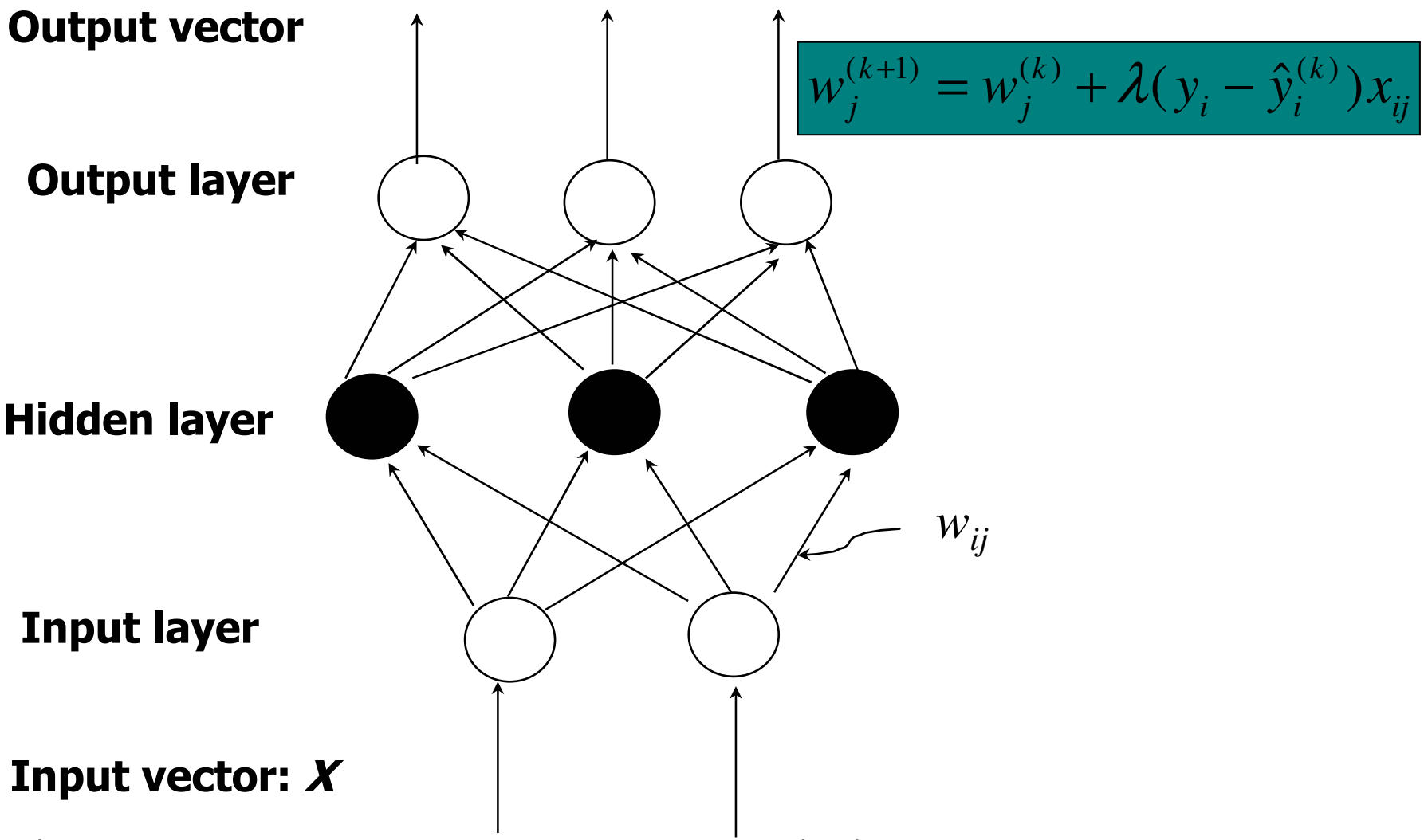
- Weakness
  - Long training time
  - Require a number of parameters typically best determined empirically, e.g., the network topology or "structure."
  - Poor interpretability: Difficult to interpret the symbolic meaning behind the learned weights and of "hidden units" in the network
- Strength
  - High tolerance to noisy data
  - Ability to classify untrained patterns
  - Well-suited for continuous-valued inputs and outputs
  - Successful on a wide array of real-world data
  - Algorithms are inherently parallel
  - Techniques have recently been developed for the extraction of rules from trained neural networks

A Neuron (= a perceptron)



- The *n*-dimensional input vector **x** is mapped into variable y by means of the scalar product and a nonlinear function mapping

A Multi-Layer Feed-Forward Neural Network



How A Multi-Layer Neural Network Works?

- The **inputs** to the network correspond to the attributes measured for each training tuple
- Inputs are fed simultaneously into the units making up the **input layer**
- They are then weighted and fed simultaneously to a **hidden layer**
- The number of hidden layers is arbitrary, although usually only one
- The weighted outputs of the last hidden layer are input to units making up the **output layer**, which emits the network's prediction
- The network is **feed-forward** in that none of the weights cycles back to an input unit or to an output unit of a previous layer
- From a statistical point of view, networks perform **nonlinear regression**: Given enough hidden units and enough training samples, they can closely approximate any function

Defining a Network Topology

- First decide the **network topology:** # of units in the *input layer*, # of *hidden layers* (if > 1), # of units in *each hidden layer*, and # of units in the *output layer*
- Normalizing the input values for each attribute measured in the training tuples to [0.0—1.0]
- One **input** unit per domain value, each initialized to 0
- **Output**, if for classification and more than two classes, one output unit per class is used
- Once a network has been trained and its accuracy is **unacceptable**, repeat the training process with a *different network topology* or a *different set of initial weights*

Backpropagation

- Iteratively process a set of training tuples & compare the network's prediction with the actual known target value
- For each training tuple, the weights are modified to **minimize the mean squared error** between the network's prediction and the actual target value
- Modifications are made in the "**backwards**" direction: from the output layer, through each hidden layer down to the first hidden layer, hence "**backpropagation**"
- Steps
  - Initialize weights (to small random #s) and biases in the network
  - Propagate the inputs forward (by applying activation function)
  - Backpropagate the error (by updating weights and biases)
  - Terminating condition (when error is very small, etc.)

Backpropagation and Interpretability

- Efficiency of backpropagation: Each epoch (one interation through the training set) takes O(|D| * *w*), with |D| tuples and *w* weights, but # of epochs can be exponential to n, the number of inputs, in the worst case
- Rule extraction from networks: network pruning
  - Simplify the network structure by removing weighted links that have the least effect on the trained network
  - Then perform link, unit, or activation value clustering
  - The set of input and activation values are studied to derive rules describing the relationship between the input and hidden unit layers
- Sensitivity analysis: assess the impact that a given input variable has on a network output. The knowledge gained from this analysis can be represented in rules

Lazy vs. Eager Learning

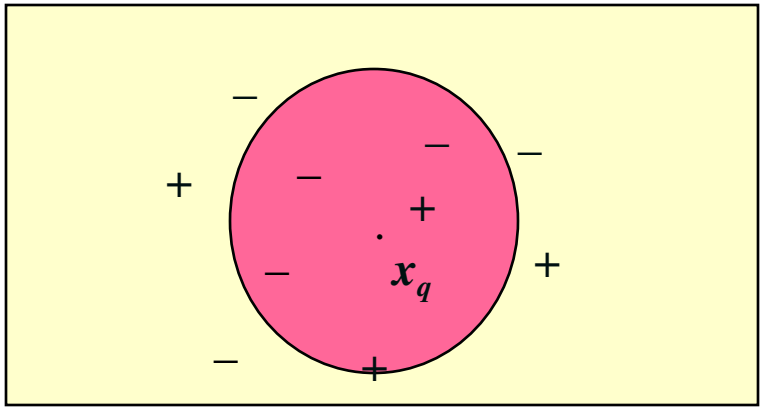
- Lazy vs. eager learning
  - Lazy learning (e.g., instance-based learning): Simply stores training data (or only minor processing) and waits until it is given a test tuple
  - Eager learning (the above discussed methods): Given a set of training set, constructs a classification model before receiving new (e.g., test) data to classify
- Lazy: less time in training but more time in predicting
- Accuracy
  - Lazy method effectively uses a richer hypothesis space since it uses many local linear functions to form its implicit global approximation to the target function
  - Eager: must commit to a single hypothesis that covers the entire instance space

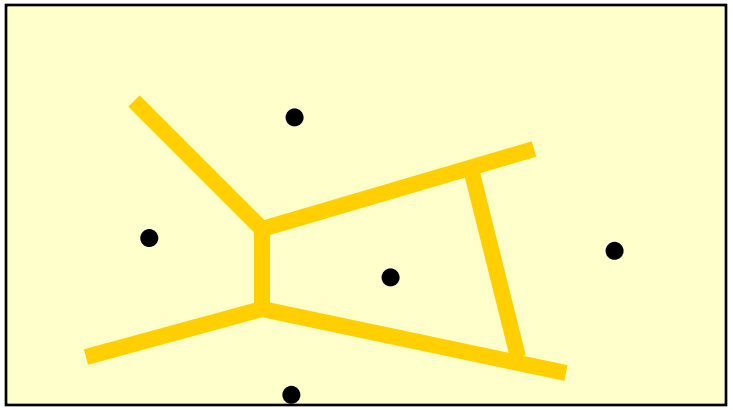
Lazy Learner: Instance-Based Methods

- Instance-based learning:
  - Store training examples and delay the processing ("lazy evaluation") until a new instance must be classified
- Typical approaches
  - *k*-nearest neighbor approach
    - Instances represented as points in a Euclidean space.
  - Locally weighted regression
    - Constructs local approximation
  - Case-based reasoning
    - Uses symbolic representations and knowledge-based inference

The *k*-Nearest Neighbor Algorithm

- All instances correspond to points in the n-D space
- The nearest neighbor are defined in terms of Euclidean distance, dist($\mathbf{X_1}$, $\mathbf{X_2}$)
- Target function could be discrete- or real- valued
- For discrete-valued, *k*-NN returns the most common value among the *k* training examples nearest to x_q
- Vonoroi diagram: the decision surface induced by 1-NN for a typical set of training examples





Discussion on the *k*-NN Algorithm

- k-NN for real-valued prediction for a given unknown tuple
  - Returns the mean values of the *k* nearest neighbors
- Distance-weighted nearest neighbor algorithm
  - Weight the contribution of each of the k neighbors according to their distance to the query x_q
    - Give greater weight to closer neighbors

$$w \equiv \frac{1}{d(x_q, x_i)^2}$$

- Robust to noisy data by averaging k-nearest neighbors
- Curse of dimensionality: distance between neighbors could be dominated by irrelevant attributes
  - To overcome it, axes stretch or elimination of the least relevant attributes

Genetic Algorithms (GA)

- Genetic Algorithm: based on an analogy to biological evolution
- An initial **population** is created consisting of randomly generated rules
  - Each rule is represented by a string of bits
  - E.g., if A_1 and $\neg A_2$ then C_2 can be encoded as 100
  - If an attribute has k > 2 values, k bits can be used
- Based on the notion of survival of the **fittest**, a new population is formed to consist of the fittest rules and their offsprings
- The fitness of a rule is represented by its *classification accuracy* on a set of training examples
- Offsprings are generated by *crossover* and *mutation*
- The process continues until a population P evolves *when each rule in P satisfies a prespecified threshold*
- Slow but easily parallelizable

What Is Prediction?

- (Numerical) prediction is similar to classification
  - construct a model
  - use model to predict continuous or ordered value for a given input
- Prediction is different from classification
  - Classification refers to predict categorical class label
  - Prediction models continuous-valued functions
- Major method for prediction: regression
  - model the relationship between one or more *independent* or **predictor** variables and a *dependent* or **response** variable
- Regression analysis
  - Linear and multiple regression
  - Non-linear regression
  - Other regression methods: generalized linear model, Poisson regression, log-linear models, regression trees

Linear Regression

- Linear regression: involves a response variable y and a single predictor variable x

  $y = w_0 + w_1 x$

  where w_0 (y-intercept) and w_1 (slope) are regression coefficients
- Method of least squares: estimates the best-fitting straight line

$$w_1 = \frac{\sum_{i=1}^{|D|}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{|D|}(x_i - \bar{x})^2} \qquad w_0 = \bar{y} - w_1 \bar{x}$$

- Multiple linear regression: involves more than one predictor variable
  - Training data is of the form $(\mathbf{X_1}, y_1)$, $(\mathbf{X_2}, y_2)$,…, $(\mathbf{X_{|D|}}, y_{|D|})$
  - Ex. For 2-D data, we may have: $y = w_0 + w_1 x_1 + w_2 x_2$
  - Solvable by extension of least square method or using SAS, S-Plus
  - Many nonlinear functions can be transformed into the above

Nonlinear Regression

- Some nonlinear models can be modeled by a polynomial function
- A polynomial regression model can be transformed into linear regression model. For example,

$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$

convertible to linear with new variables: $x_2 = x^2$, $x_3 = x^3$

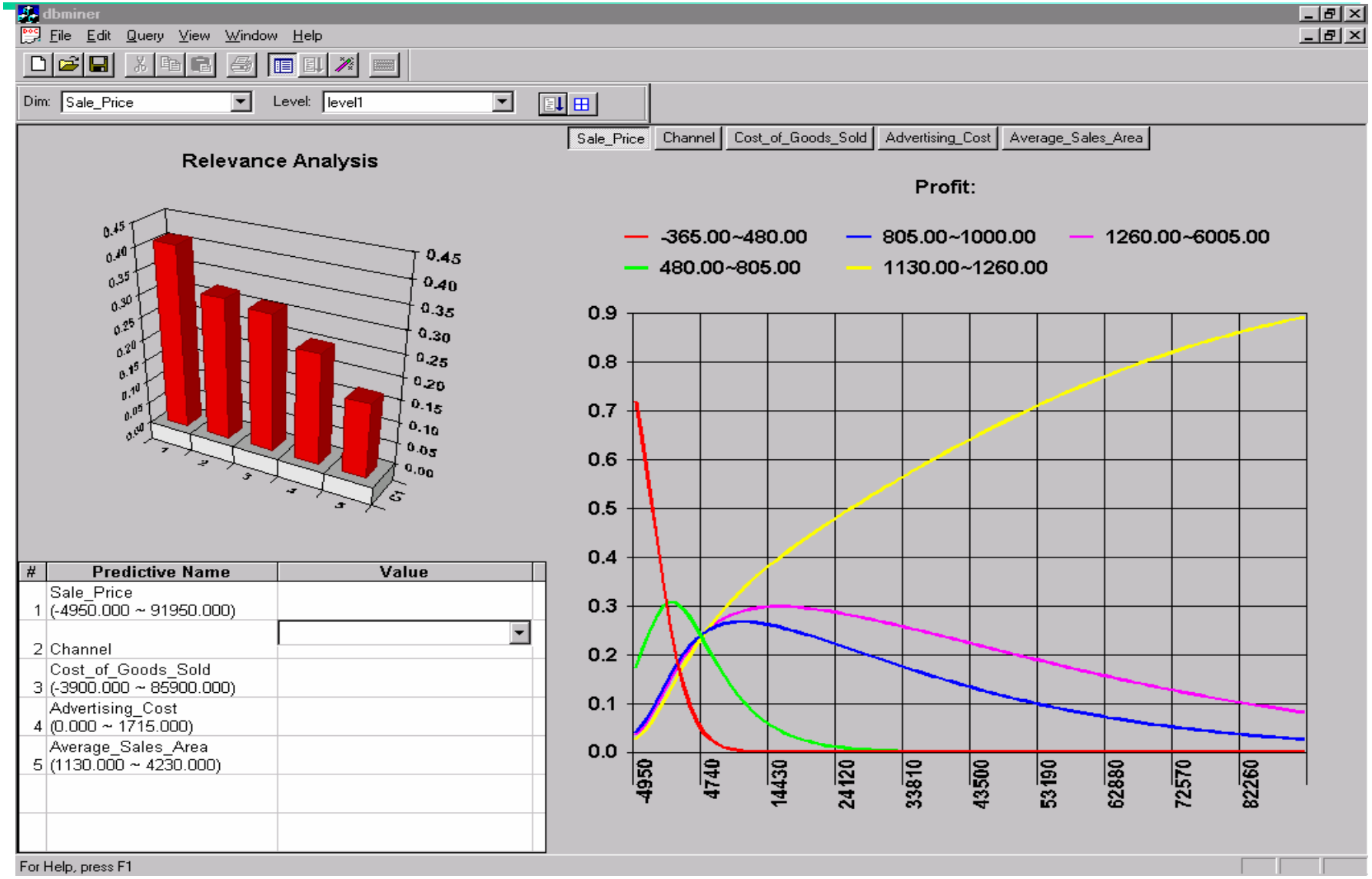
$$y = w_0 + w_1 x + w_2 x_2 + w_3 x_3$$

- Other functions, such as power function, can also be transformed to linear model
- Some models are intractable nonlinear (e.g., sum of exponential terms)
  - possible to obtain least square estimates through extensive calculation on more complex formulae

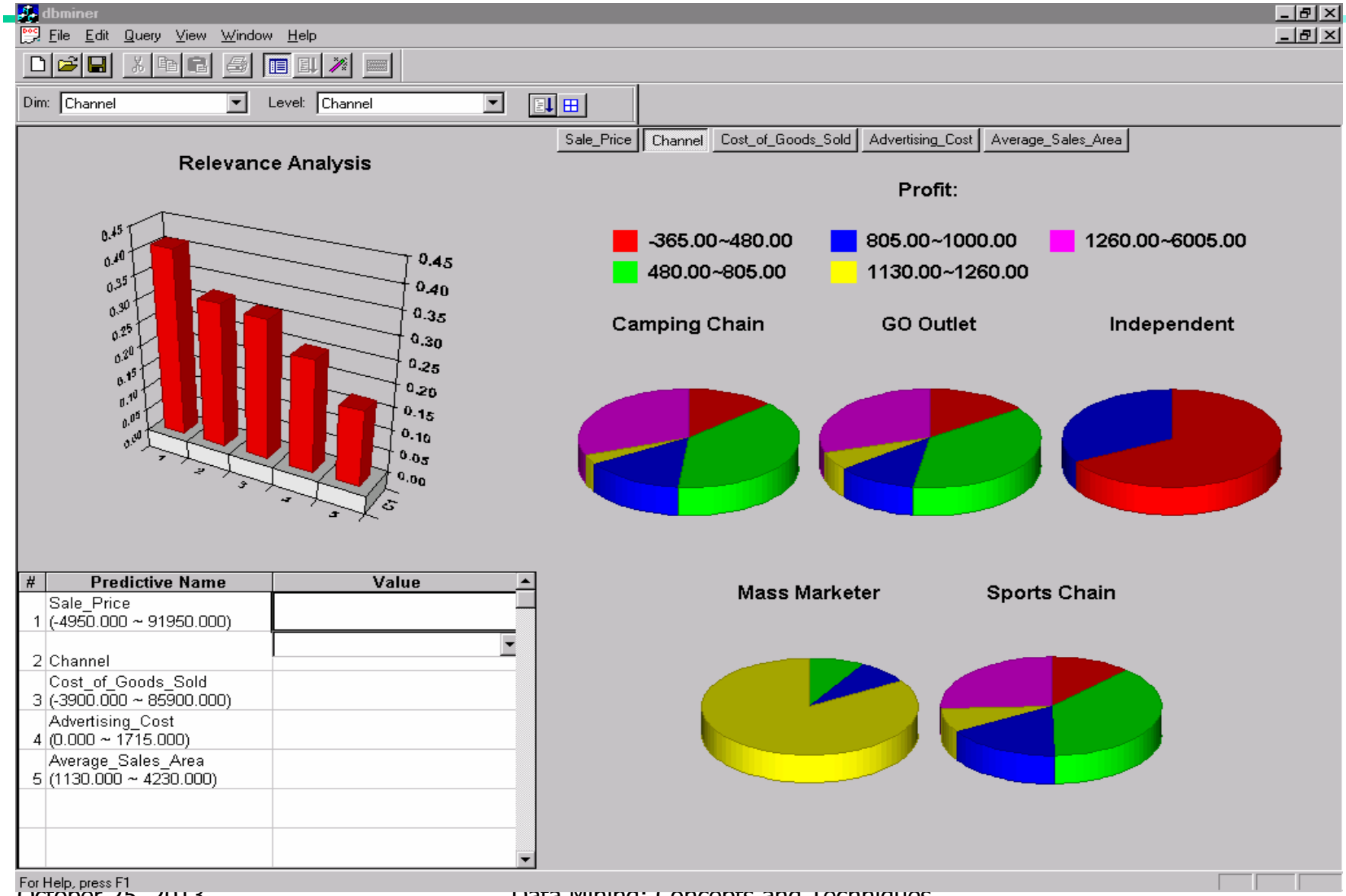
Other Regression-Based Models

- Generalized linear model:
  - Foundation on which linear regression can be applied to modeling categorical response variables
  - Variance of y is a function of the mean value of y, not a constant
  - Logistic regression: models the prob. of some event occurring as a linear function of a set of predictor variables
  - Poisson regression: models the data that exhibit a Poisson distribution
- Log-linear models: (for categorical data)
  - Approximate discrete multidimensional prob. distributions
  - Also useful for data compression and smoothing
- Regression trees and model trees
  - Trees to predict continuous values rather than class labels

Prediction: Numerical Data



Prediction: Categorical Data



Classifier Accuracy Measures

Real class\Predicted class	C_1	$\sim C_1$
C_1	True positive	False negative
$\sim C_1$	False positive	True negative

Real class\Predicted class	buy_computer = yes	buy_computer = no	total	recognition(%)
buy_computer = yes	6954	46	7000	99.34
buy_computer = no	412	2588	3000	86.27
total	7366	2634	10000	95.52

- Accuracy of a classifier M, acc(M): percentage of test set tuples that are correctly classified by the model M
  - Error rate (misclassification rate) of M = 1 – acc(M)
  - Given *m* classes, $CM_{i,j}$, an entry in a **confusion matrix**, indicates # of tuples in class *i* that are labeled by the classifier as class *j*
- Alternative accuracy measures (e.g., for cancer diagnosis)

  sensitivity = t-pos/pos /* true positive recognition rate */

  specificity = t-neg/neg /* true negative recognition rate */

  precision = t-pos/(t-pos + f-pos)

  accuracy = sensitivity * pos/(pos + neg) + specificity * neg/(pos + neg)
  - This model can also be used for cost-benefit analysis

Predictor Error Measures

- Measure predictor accuracy: measure how far off the predicted value is from the actual known value
- **Loss function**: measures the error betw. y_i and the predicted value y_i'
  - Absolute error: $| y_i - y_i' |$
  - Squared error: $(y_i - y_i')^2$
- Test error (generalization error): the average loss over the test set
  - Mean absolute error: $\frac{\sum_{i=1}^{d} | y_i - y_i' |}{d}$ Mean squared error: $\frac{\sum_{i=1}^{d} (y_i - y_i')^2}{d}$
  - Relative absolute error: $\frac{\sum_{i=1}^{d} | y_i - y_i' |}{\sum_{i=1}^{d} | y_i - \bar{y} |}$ Relative squared error: $\frac{\sum_{i=1}^{d} (y_i - y_i')^2}{\sum_{i=1}^{d} (y_i - \bar{y})^2}$

  The mean squared-error exaggerates the presence of outliers

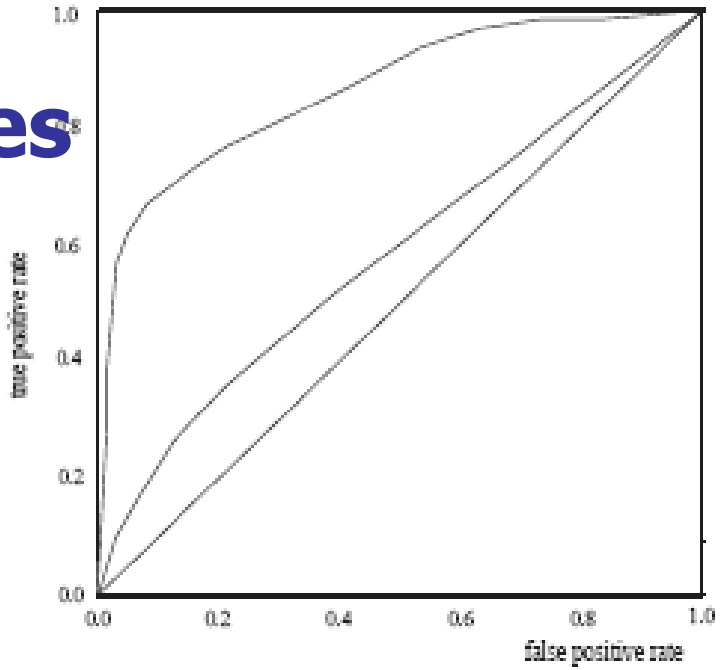
  Popularly use (square) root mean-square error, similarly, root relative squared error

Evaluating the Accuracy of a Classifier or Predictor (I)

- Holdout method
  - Given data is randomly partitioned into two independent sets
    - Training set (e.g., 2/3) for model construction
    - Test set (e.g., 1/3) for accuracy estimation
  - Random sampling: a variation of holdout
    - Repeat holdout k times, accuracy = avg. of the accuracies obtained
- Cross-validation (*k*-fold, where k = 10 is most popular)
  - Randomly partition the data into *k mutually exclusive* subsets, each approximately equal size
  - At *i*-th iteration, use D_i as test set and others as training set
  - Leave-one-out: k folds where k = # of tuples, for small sized data
  - Stratified cross-validation: folds are stratified so that class dist. in each fold is approx. the same as that in the initial data

Model Selection: 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



- Vertical axis represents the true positive rate
- Horizontal axis rep. the false positive rate
- The plot also shows a diagonal line
- A model with perfect accuracy will have an area of 1.0