Roadmap

- What is classification? What is prediction?
- Issues regarding classification and prediction
- Classification by decision tree induction
- Bayesian classification ←
- Rule-based classification
- Classification by back propagation
- Support Vector Machines (SVM)
- Associative classification
- Lazy learners (or learning from your neighbors)
- Other classification methods
- Prediction
- Accuracy and error measures
- Ensemble methods
- Model selection
- Summary

Bayesian Classification: Why?

- A statistical classifier: performs *probabilistic prediction, i.e.,* predicts class membership probabilities
- Foundation: Based on Bayes' Theorem.
- Performance: A simple Bayesian classifier, *naïve Bayesian classifier*, has comparable performance with decision tree and selected neural network classifiers
- Incremental: Each training example can incrementally increase/decrease the probability that a hypothesis is correct — prior knowledge can be combined with observed data
- Standard: Even when Bayesian methods are computationally intractable, they can provide a standard of optimal decision making against which other methods can be measured

Bayes Theorem

- Given a hypothesis *H* and data ***X*** which bears on the hypothesis:

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

- *P(H)*: independent probability of *H*: *prior probability*
- *P(**X**)*: independent probability of ***X***
- *P(**X**/H)*: conditional probability of ***X*** given *H*: *likelihood*
- *P(H/**X**)*: conditional probability of *H* given ***X***: *posterior probability*

Bayes Theorem: Basics

- Let **X** be a data sample ("*evidence*"): class label is unknown
- Let H be a *hypothesis* that X belongs to class C
- P(H) (*prior probability*), the initial probability
  - E.g., **X** will buy computer, regardless of age, income, …
- P(**X**): probability that sample data is observed
- P(**X**|H) (*likelihood*), the probability of observing the sample **X**, given that the hypothesis holds
  - E.g., Given that **X** will buy computer, the prob. that **X** is 31..40, medium income
- Classification is to determine the max P(H|**X**) (*posteriori probability*), the probability that the hypothesis holds given the observed data sample **X,** over all the possible H (over all class labels)

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-d attribute vector **X** = (x_1, x_2, …, x_n)
  - x_k is the value of the k-th attribute (A_k) of data tuple **X**
- 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|**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

  needs to be maximized $P(C_i|\mathbf{X}) = P(\mathbf{X}|C_i)P(C_i)$

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 Gaussian distribution with a mean μ and standard deviation σ
$$g(x,\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

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

Naïve Bayesian Classifier: Training Dataset

Class:
C1:buys_computer = 'yes'
C2:buys_computer = 'no'

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

age	income	student	credit_rating	comp
<=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

- 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

- **X = (age <= 30 , income = medium, student = yes, credit_rating = fair)**

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(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")

Implementation Details

- We want to find the class, *i*, that maximizes the following probability: $P(C_i|\mathbf{X}) = P(\mathbf{X}|C_i)P(C_i)$, where

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

- what happens when we multiply all those probabilities?

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- what happens when we multiply all those probabilities?
  - each one of these numbers is between 0 and 1
  - possible underflow!

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- what happens when we multiply all those probabilities?
  - each one of these numbers is between 0 and 1
  - possible underflow!
- solution
  - first compute the log of each probability
  - then convert product to sumation (log(xy) = logx + logy)

Avoiding the 0-Probability Problem

- Naïve Bayesian prediction requires each conditional prob. be non-zero. Otherwise, the predicted prob. will be zero

$$P(X|C_i) = \prod_{k=1}^{n} P(x_k|C_i)$$

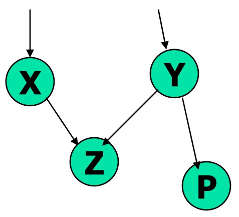
- Ex. Suppose a dataset with 1000 tuples, income=low (0), income= medium (990), and income = high (10),
- Use Laplacian correction (or Laplacian estimator)
  - Adding 1 to each case
    Prob(income = low) = 1/1003
    Prob(income = medium) = 991/1003
    Prob(income = high) = 11/1003
  - The "corrected" prob. estimates are close to their "uncorrected" counterparts

Naïve Bayesian Classifier: Comments

- Advantages
  - Easy to implement
  - Good results obtained in most of the cases
- Disadvantages
  - Assumption: class conditional independence, therefore loss of accuracy
  - Practically, dependencies exist among variables
    - E.g., hospitals: patients: Profile: age, family history, etc.
    Symptoms: fever, cough etc., Disease: lung cancer, diabetes, etc.
    - Dependencies among these cannot be modeled by Naïve Bayesian Classifier
- How to deal with these dependencies?
  - Bayesian Belief Networks

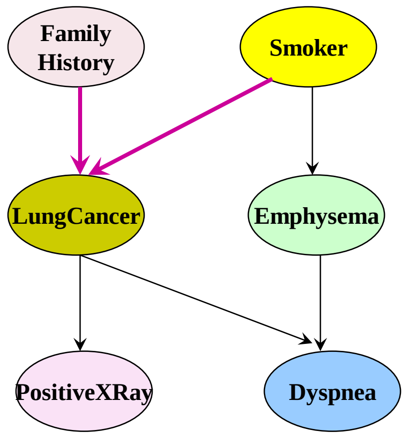
Bayesian Belief Networks

- Bayesian belief network allows a *subset* of the variables be conditionally independent
- A graphical model of causal relationships
  - Represents dependency among the variables
  - Gives a specification of joint probability distribution



❑ Nodes: random variables
❑ Links: dependency
❑ X and Y are the parents of Z, and Y is the parent of P
❑ No dependency between Z and P
❑ Has no loops or cycles

Bayesian Belief Network: An Example



Bayesian Belief Networks

The **conditional probability table** (**CPT**) for variable LungCancer:

	(FH, S)	(FH, ~S)	(~FH, S)	(~FH, ~S)
LC	0.8	0.5	0.7	0.1
~LC	0.2	0.5	0.3	0.9

CPT shows the conditional probability for each possible combination of its parents

Derivation of the probability of a particular combination of values of **X**, from CPT:

$$P(x_1,\ldots,x_n) = \prod_{i=1}^{n} P(x_i \mid Parents(Y_i))$$

Training Bayesian Networks

- Several scenarios:
  - Given both the network structure and all variables observable: *learn only the CPTs*
  - Network structure known, some hidden variables: *gradient descent* (greedy hill-climbing) method, analogous to neural network learning
  - Network structure unknown, all variables observable: search through the model space to *reconstruct network topology*
  - Unknown structure, all hidden variables: No good algorithms known for this purpose
- Ref. D. Heckerman: Bayesian networks for data mining

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Using IF-THEN Rules for Classification

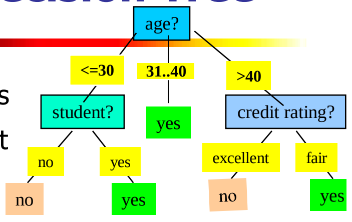
- Represent the knowledge in the form of IF-THEN rules

  R: IF *age* = youth AND *student* = yes THEN *buys_computer* = yes
  - Rule antecedent/precondition vs. rule consequent
- Assessment of a rule: *coverage* and *accuracy*
  - n_{covers} = # of tuples covered by R
  - $n_{correct}$ = # of tuples correctly classified by R

  coverage(R) = n_{covers} /|D| /* D: training data set */

  accuracy(R) = $n_{correct}$ / n_{covers}
- If more than one rule is triggered, need **conflict resolution**
  - Size ordering: assign the highest priority to the triggering rules that has the "toughest" requirement (i.e., with the *most attribute test*)
  - Class-based ordering: decreasing order of *prevalence or misclassification cost per class*
  - Rule-based ordering (**decision list**): rules are organized into one long priority list, according to some measure of rule quality or by experts

Rule Extraction from a Decision Tree



- Rules are easier to understand than large trees
- One rule is created for each path from the root to a leaf
- Each attribute-value pair along a path forms a conjunction: the leaf holds the class prediction
- Rules are mutually exclusive and exhaustive
- Example: Rule extraction from our *buys_computer* decision-tree

  IF *age* = young AND *student* = *no* THEN *buys_computer* = *no*

  IF *age* = young AND *student* = *yes* THEN *buys_computer* = *yes*

  IF *age* = mid-age THEN *buys_computer* = *yes*

  IF *age* = old AND *credit_rating* = *excellent* THEN *buys_computer* = *yes*

  IF *age* = young AND *credit_rating* = *fair* THEN *buys_computer* = *no*

Rule Extraction from the Training Data

- Sequential covering algorithm: Extracts rules directly from training data
- Typical sequential covering algorithms: FOIL, AQ, CN2, RIPPER
- Rules are learned *sequentially*, each for a given class C_i will cover many tuples of C_i but none (or few) of the tuples of other classes
- Steps:
  - Rules are learned one at a time
  - Each time a rule is learned, the tuples covered by the rules are removed
  - The process repeats on the remaining tuples unless *termination condition*, e.g., when no more training examples or when the quality of a rule returned is below a user-specified threshold
- Comp. w. decision-tree induction: learning a set of rules *simultaneously*

How to Learn-One-Rule?

- Star with the most general rule possible: condition = empty
- Adding new attributes by adopting a greedy depth-first strategy
  - Picks the one that most improves the rule quality
- Rule-Quality measures: consider both coverage and accuracy
  - Foil-gain (in FOIL & RIPPER): assesses info_gain by extending condition

$$FOIL\_Gain = pos' \times (\log_2 \frac{pos'}{pos'+neg'} - \log_2 \frac{pos}{pos+neg})$$

It favors rules that have high accuracy and cover many positive tuples

- Rule pruning based on an independent set of test tuples

$$FOIL\_Prune(R) = \frac{pos - neg}{pos + neg}$$

Pos/neg are # of positive/negative tuples covered by R.

If *FOIL_Prune* is higher for the pruned version of R, prune R

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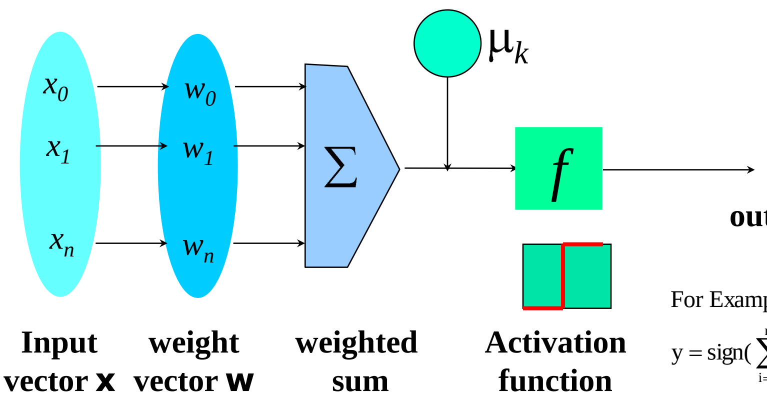
Classification by Backpropagation

- 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)

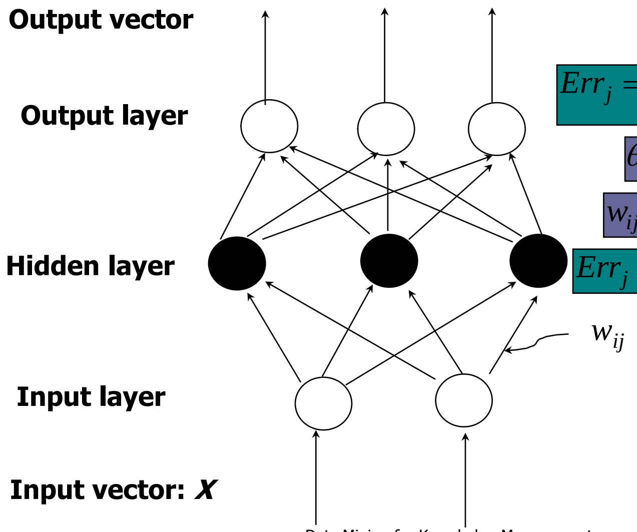


For Example

$$y = \text{sign}\left(\sum_{i=0}^{n} w_i x_i + \mu_k\right)$$

- 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



$$Err_j = O_j(1-O_j)\sum_k Err_k w_{jk}$$

$$\theta_j = \theta_j + (l)Err_j$$

$$w_{ij} = w_{ij} + (l)Err_j O_i$$

$$Err_j = O_j(1-O_j)(T_j - O_j)$$

$$O_j = \frac{1}{1+e^{-I_j}}$$

$$I_j = \sum_i w_{ij} O_i + \theta_j$$

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

Roadmap

SVM—Support Vector Machines

- A new classification method for both linear and nonlinear data
- It uses a nonlinear mapping to transform the original training data into a higher dimension
- With the new dimension, it searches for the linear optimal separating hyperplane (i.e., "decision boundary")
- With an appropriate nonlinear mapping to a sufficiently high dimension, data from two classes can always be separated by a hyperplane
- SVM finds this hyperplane using support vectors ("essential" training tuples) and margins (defined by the support vectors)

SVM—History and Applications

- Vapnik and colleagues (1992)—groundwork from Vapnik & Chervonenkis' statistical learning theory in 1960s
- Features: training can be slow but accuracy is high owing to their ability to model complex nonlinear decision boundaries (margin maximization)
- Used both for classification and prediction
- Applications:
  - handwritten digit recognition, object recognition, speaker identification, benchmarking time-series prediction tests

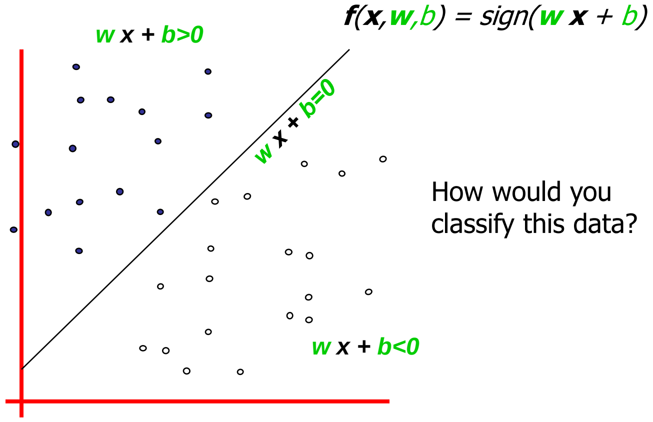
Linear Classifiers

$$\mathbf{x} \xrightarrow{} \boxed{f} \xrightarrow{} y^{est}$$

α (input to f)

● denotes +1

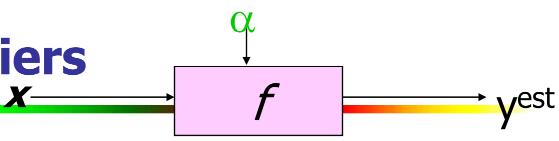
○ denotes -1



$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}\ \mathbf{x} + b)$

How would you classify this data?

Linear Classifiers



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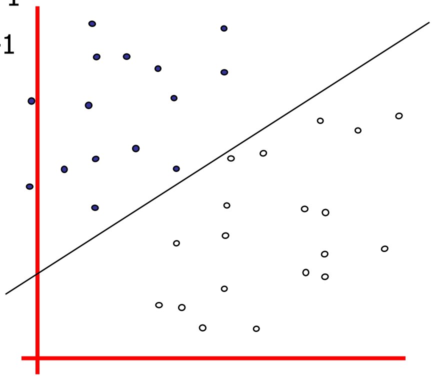

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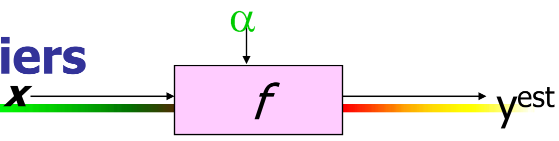

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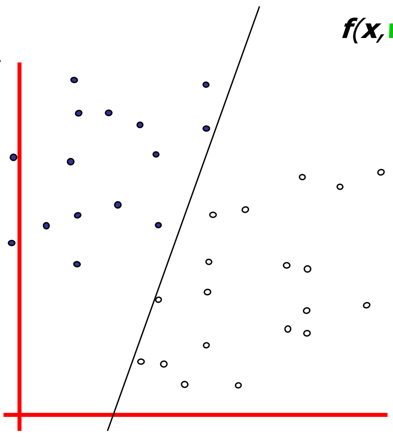

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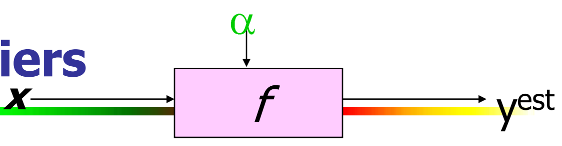
Linear Classifiers



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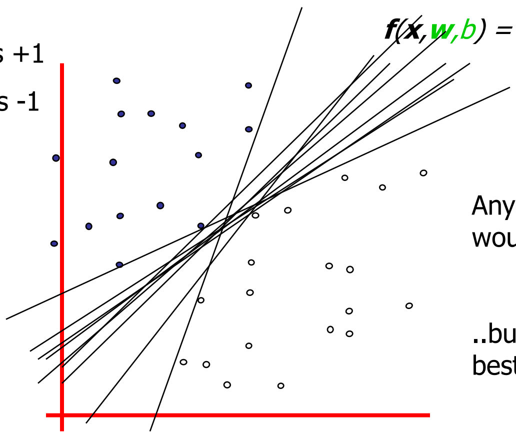
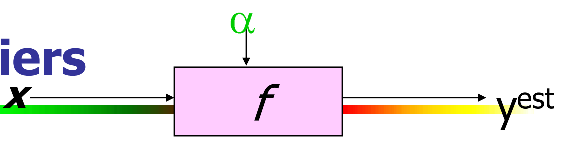


Any of these would be fine..

..but which is best?

Linear Classifiers



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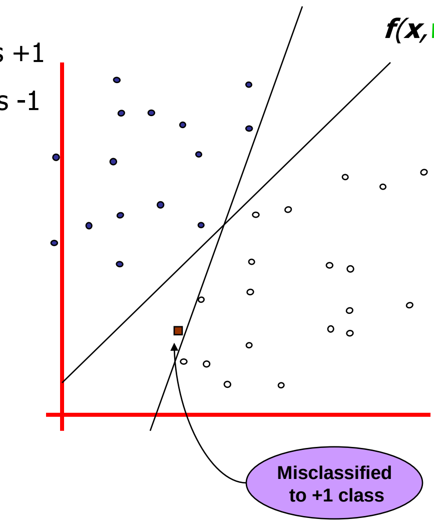
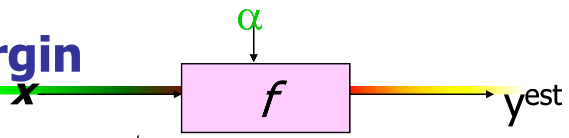
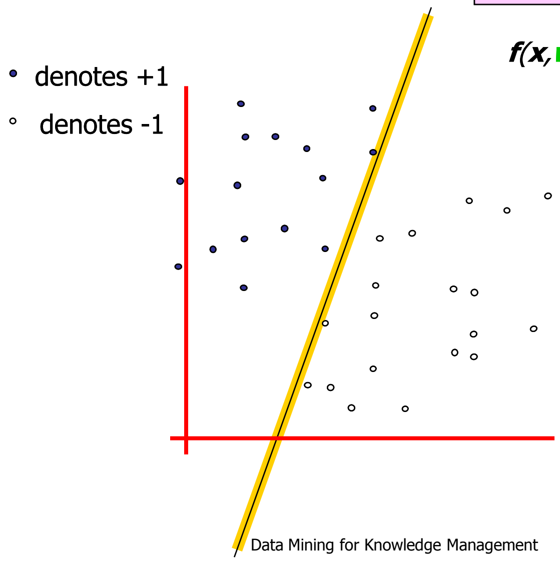


How would you classify this data?

Classifier Margin

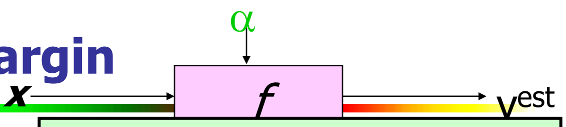


$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}\,\mathbf{x} + b)$

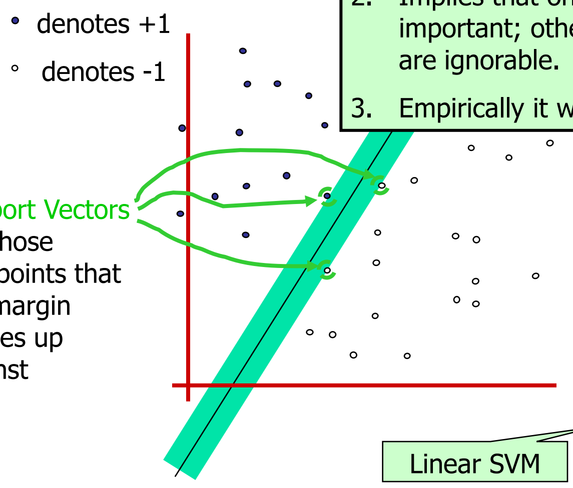


Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a datapoint.

Maximum Margin



1. Maximizing the margin is good
2. Implies that only support vectors are important; other training examples are ignorable.
3. Empirically it works very very well.



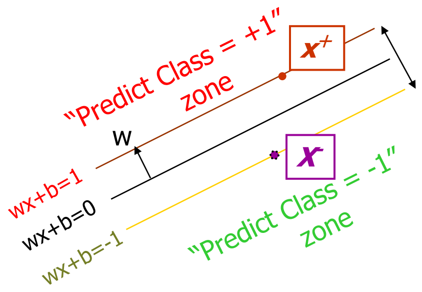
Support Vectors are those datapoints that the margin pushes up against

classifier is the linear classifier with the, um, maximum margin.

This is the simplest kind of SVM (Called an LSVM)

Linear SVM

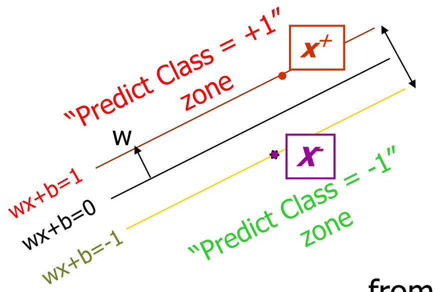
Linear SVM Mathematically



M=Margin Width

- What we know:
- $\mathbf{w} \,.\, \mathbf{x}^+ + b = +1$ (1)
- $\mathbf{w} \,.\, \mathbf{x}^- + b = -1$ (2)
- $\mathbf{x}^+ = \mathbf{x}^- + k\mathbf{w}$ (3)
- $M = |\mathbf{x}^+ - \mathbf{x}^-|$ (4)

Linear SVM Mathematically

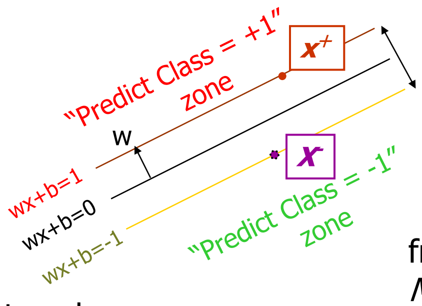


M=Margin Width

- What we know:
- $\mathbf{w} \,.\, \mathbf{x}^+ + b = +1$ (1)
- $\mathbf{w} \,.\, \mathbf{x}^- + b = -1$ (2)
- $\mathbf{x}^+ = \mathbf{x}^- + k\mathbf{w}$ (3)
- $M = |\mathbf{x}^+ - \mathbf{x}^-|$ (4)

from (1) and (3):
$\mathbf{w}\,(\mathbf{x}^- + k\mathbf{w}) + b = +1 \rightarrow$
$\mathbf{w}.\mathbf{x}^- + b + k\mathbf{ww} = +1 \rightarrow$
using (2):
$-1 + k\mathbf{ww} = +1 \rightarrow$
$k = 2/\mathbf{ww}$

Linear SVM Mathematically



M=Margin Width

- What we know:
- $\mathbf{w} \cdot \mathbf{x}^{+} + b = +1$ (1)
- $\mathbf{w} \cdot \mathbf{x}^{-} + b = -1$ (2)
- $\mathbf{x}^{+} = \mathbf{x}^{-} + k\mathbf{w}$ (3)
- $M = |\mathbf{x}^{+} - \mathbf{x}^{-}|$ (4)
- $k = 2/\mathbf{ww}$ (5)

from (4), and (3):

$M = |\mathbf{x}+ - \mathbf{x}-|$
$= |k\mathbf{w}|$
$= k|\mathbf{w}|$
$= k\sqrt{\mathbf{ww}}$, using (5)
$= 2\sqrt{\mathbf{ww}} / \mathbf{ww}$
$= 2 / \sqrt{\mathbf{ww}}$
$= 2 / |\mathbf{w}|$

Linear SVM Mathematically

- Goal: **1) Correctly classify all training data**

$wx_i + b \geq 1$ *if y_i = +1*
$wx_i + b \leq 1$ *if y_i = -1*

$y_i(wx_i + b) \geq 1$ for all i

2) Maximize the Margin $M = \frac{2}{|w|}$

same as minimize $\frac{1}{2} w^t w$

- **We can formulate a Quadratic Optimization Problem and solve for w and b**
- Minimize $\Phi(w) = \frac{1}{2} w^t w$

  subject to $y_i(wx_i + b) \geq 1 \quad \forall i$

Solving the Optimization Problem

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi}(\mathbf{w}) = ½\, \mathbf{w}^T\mathbf{w}$ is minimized;
and for all $\{(\mathbf{x_i}, y_i)\}$: $y_i(\mathbf{w^T x_i} + b) \geq 1$

- **Need to optimize a *quadratic* function subject to *linear* constraints.**
- **Quadratic optimization problems are a well-known class of mathematical programming problems, and many (rather intricate) algorithms exist for solving them.**
- **The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_i is associated with every constraint in the primary problem:**

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - ½\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i^T x_j}$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

The Optimization Problem Solution

- The solution has the form:

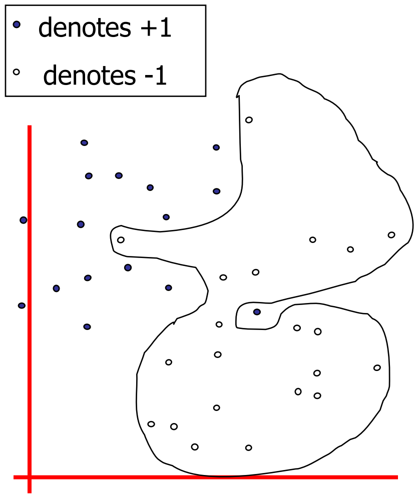
$\mathbf{w} = \Sigma\alpha_i y_i \mathbf{x_i}$ $\quad b = y_k - \mathbf{w^T x_k}$ for any $\mathbf{x_k}$ such that $\alpha_k \neq 0$

- Each non-zero α_i indicates that corresponding $\mathbf{x_i}$ is a support vector.
- Then the classifying function will have the form:

$f(\mathbf{x}) = \Sigma\alpha_i y_i \mathbf{x_i^T x} + b$

- Notice that it relies on an *inner product* between the test point **x** and the support vectors $\mathbf{x_i}$ – we will return to this later.
- Also keep in mind that solving the optimization problem involved computing the inner products $\mathbf{x_i^T x_j}$ between all pairs of training points.

Dataset with noise

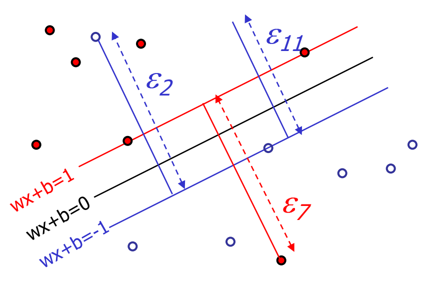


- **Hard Margin:** So far we require all data points be classified correctly
  - No training error
- **What if the training set is noisy?**
  - **Solution 1:** use very powerful kernels

OVERFITTING!

Soft Margin Classification

Slack variables ξi **can be added to allow misclassification of difficult or noisy examples.**



What should our quadratic optimization criterion be?
Minimize

$$\frac{1}{2}\mathbf{w}.\mathbf{w} + C\sum_{k=1}^{R}\varepsilon_k$$

Hard Margin v.s. Soft Margin

- **The old formulation:**

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi}(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{w}$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$
$y_i(\mathbf{w^T x_i} + \mathrm{b}) \geq 1$

- **The new formulation incorporating slack variables:**

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi}(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\Sigma\xi_i$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$
$y_i(\mathbf{w^T x_i} + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$ for all i

- **Parameter *C* can be viewed as a way to control overfitting.**

Linear SVMs: Overview

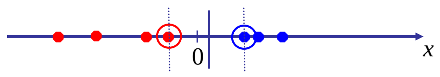
- **The classifier is a *separating hyperplane.***
- **Most "important" training points are support vectors; they define the hyperplane.**
- **Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are support vectors with non-zero Lagrangian multipliers α_i.**
- **Both in the dual formulation of the problem and in the solution training points appear only inside dot products:**

Find $\alpha_1 \ldots \alpha_N$ such that
$Q(\alpha) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \leq \alpha_i \leq C$ for all α_i

$f(\mathbf{x}) = \Sigma\alpha_i y_i \mathbf{x}_i^T\mathbf{x} + b$

Non-linear SVMs

- Datasets that are linearly separable with some noise work out great:



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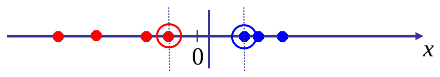
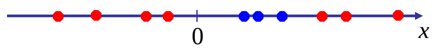


- But what are we going to do if the dataset is just too hard?



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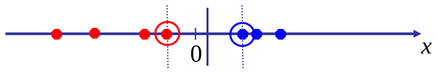

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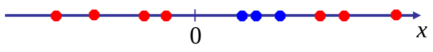
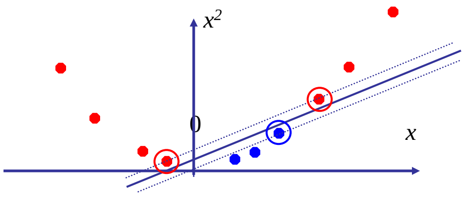
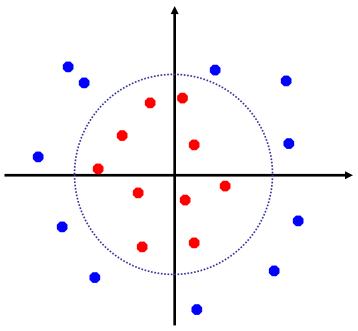


- How about… mapping data to a higher-dimensional space?



Non-linear SVMs: Feature spaces

- General idea: the original input space can always be mapped to some higher-dimensional feature space where the training set is separable:



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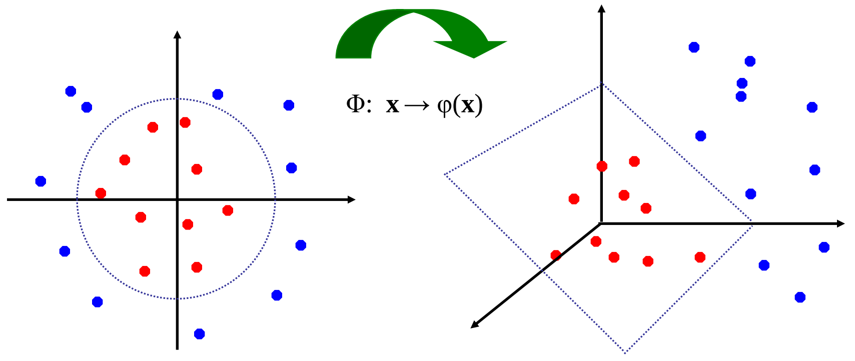


Examples of Kernel Functions

- Linear: $K(\mathbf{x_i},\mathbf{x_j}) = \mathbf{x_i}^T\mathbf{x_j}$
- Polynomial of power p: $K(\mathbf{x_i},\mathbf{x_j}) = (1 + \mathbf{x_i}^T\mathbf{x_j})^p$
- Gaussian (radial-basis function network):

$$K(\mathbf{x_i},\mathbf{x_j}) = \exp\left(-\frac{\|\mathbf{x_i} - \mathbf{x_j}\|^2}{2\sigma^2}\right)$$

- Sigmoid: $K(\mathbf{x_i},\mathbf{x_j}) = \tanh(\beta_0 \mathbf{x_i}^T\mathbf{x_j} + \beta_1)$

Non-linear SVMs Mathematically

- Dual problem formulation:

$$\boxed{\begin{array}{l}\text{Find } \alpha_1 \ldots \alpha_N \text{ such that} \\ Q(\alpha) = \Sigma\alpha_i - ½\Sigma\Sigma\alpha_i\alpha_j y_i y_j K(x_i, x_j) \text{ is maximized and} \\ (1)\ \Sigma\alpha_i y_i = 0 \\ (2)\ \alpha_i \geq 0 \text{ for all } \alpha_i\end{array}}$$

- The solution is:

$$\boxed{f(x) = \Sigma\alpha_i y_i K(x_i, x_j) + b}$$

- Optimization techniques for finding α_i's remain the same!

Nonlinear SVM - Overview

- SVM locates a separating hyperplane in the feature space and classify points in that space
- It does not need to represent the space explicitly, simply by defining a kernel function
- The kernel function plays the role of the dot product in the feature space.

Properties of SVM

- Flexibility in choosing a similarity function
- Sparseness of solution when dealing with large data sets
  - only support vectors are used to specify the separating hyperplane
- Ability to handle large feature spaces
  - complexity does not depend on the dimensionality of the feature space
- Overfitting can be controlled by soft margin approach
- Nice math property: a simple convex optimization problem which is guaranteed to converge to a single global solution
- Feature Selection

Weakness of SVM

- It is sensitive to noise
  - A relatively small number of mislabeled examples can dramatically decrease the performance
- It only considers two classes
  - how to do multi-class classification with SVM?
  - Answer:
  1) with output arity m, learn m SVM's
     - SVM 1 learns "Output==1" vs "Output != 1"
     - SVM 2 learns "Output==2" vs "Output != 2"
     - :
     - SVM m learns "Output==m" vs "Output != m"
  2)To predict the output for a new input, just predict with each SVM and find out which one puts the prediction the furthest into the positive region.

Why Is SVM Effective on High Dimensional Data?

- The complexity of trained classifier is characterized by the # of support vectors rather than the dimensionality of the data
- The support vectors are the essential or critical training examples — they lie closest to the decision boundary (MMH)
- If all other training examples are removed and the training is repeated, the same separating hyperplane would be found
- The number of support vectors found can be used to compute an (upper) bound on the expected error rate of the SVM classifier, which is independent of the data dimensionality
- Thus, an SVM with a small number of support vectors can have good generalization, even when the dimensionality of the data is high

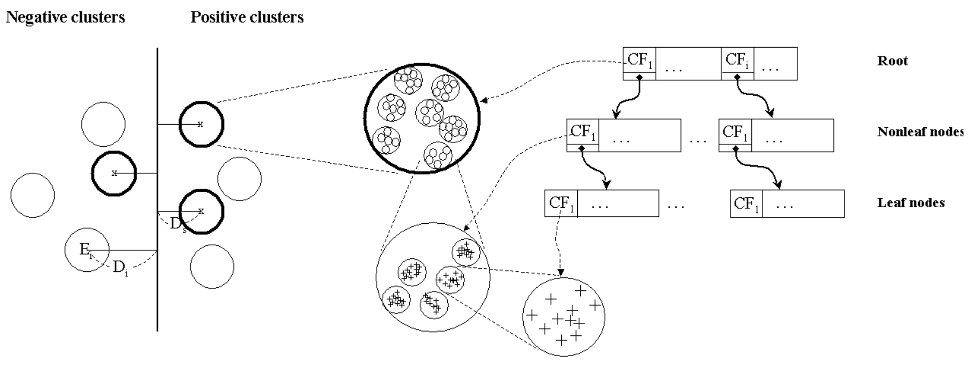
Scaling SVM by Hierarchical Micro-Clustering

- SVM is not scalable to the number of data objects in terms of training time and memory usage
- "Classifying Large Datasets Using SVMs with Hierarchical Clusters Problem" by Hwanjo Yu, Jiong Yang, Jiawei Han, KDD'03
- CB-SVM (Clustering-Based SVM)
  - Given limited amount of system resources (e.g., memory), maximize the SVM performance in terms of accuracy and the training speed
  - Use micro-clustering to effectively reduce the number of points to be considered
  - At deriving support vectors, de-cluster micro-clusters near "candidate vector" to ensure high classification accuracy

CB-SVM: Clustering-Based SVM

- Training data sets may not even fit in memory
- Read the data set once (minimizing disk access)
  - Construct a statistical summary of the data (i.e., hierarchical clusters) given a limited amount of memory
  - The statistical summary maximizes the benefit of learning SVM
- The summary plays a role in indexing SVMs
- Essence of Micro-clustering (Hierarchical indexing structure)
  - Use micro-cluster hierarchical indexing structure
    - provide finer samples closer to the boundary and coarser samples farther from the boundary
  - Selective de-clustering to ensure high accuracy

CF-Tree: Hierarchical Micro-cluster

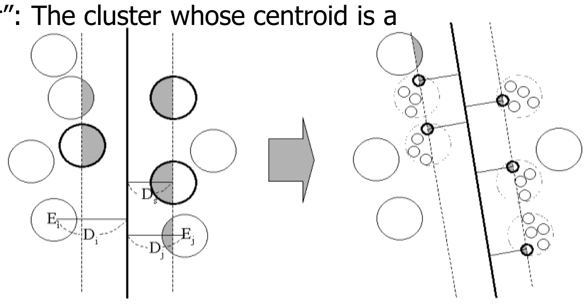


CB-SVM Algorithm: Outline

- Construct two CF-trees from positive and negative data sets independently
  - Need one scan of the data set
- Train an SVM from the centroids of the root entries
- De-cluster the entries near the boundary into the next level
  - The children entries de-clustered from the parent entries are accumulated into the training set with the non-declustered parent entries
- Train an SVM again from the centroids of the entries in the training set
- Repeat until nothing is accumulated

Selective Declustering

- CF tree is a suitable base structure for selective declustering
- De-cluster only the cluster E_i such that
  - $D_i - R_i < D_s$, where D_i is the distance from the boundary to the center point of E_i and R_i is the radius of E_i
  - Decluster only the cluster whose subclusters have possibilities to be the support cluster of the boundary
    - "Support cluster": The cluster whose centroid is a support vector



SVM—Introduction Literature

- "Statistical Learning Theory" by Vapnik: extremely hard to understand, containing many errors too.
- C. J. C. Burges. A Tutorial on Support Vector Machines for Pattern Recognition. *Knowledge Discovery and Data Mining*, 2(2), 1998.
  - Better than the Vapnik's book, but still written too hard for introduction, and the examples are so not-intuitive
- The book "An Introduction to Support Vector Machines" by N. Cristianini and J. Shawe-Taylor
  - Also written hard for introduction, but the explanation about the mercer's theorem is better than above literatures
- The neural network book by Haykins
  - Contains one nice chapter of SVM introduction

Additional Resources

- An excellent tutorial on VC-dimension and Support Vector Machines:

  C.J.C. Burges. A tutorial on support vector machines for pattern recognition. Data Mining and Knowledge Discovery, 2(2):955-974, 1998.

- The VC/SRM/SVM Bible:

  Statistical Learning Theory by Vladimir Vapnik, Wiley-Interscience; 1998

http://www.kernel-machines.org/

Roadmap

Classifier Accuracy Measures

- 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*

predicted class

actual class

classes	buy_computer = yes	buy_computer = no	total	acc(%)
buy_computer = yes	6954	46	7000	99.34
buy_computer = no	412	2588	3000	86.27
total	7366	2634	10000	95.52

Classifier Accuracy Measures

- 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

predicted class

actual class

	C_1	C_2
C_1	True positive	False negative
C_2	False positive	True negative

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

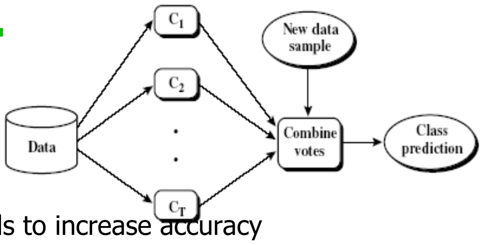
Evaluating the Accuracy of a Classifier or Predictor (II)

- Bootstrap
  - Works well with small data sets
  - Samples the given training tuples uniformly *with replacement*
    - i.e., each time a tuple is selected, it is equally likely to be selected again and re-added to the training set
- Several boostrap methods, and a common one is **.632 boostrap**
  - Suppose we are given a data set of d tuples. The data set is sampled d times, with replacement, resulting in a training set of d samples. The data tuples that did not make it into the training set end up forming the test set. About 63.2% of the original data will end up in the bootstrap, and the remaining 36.8% will form the test set (Prob(not select tuple t)=1-1/d, for a sample of size d: $(1 - 1/d)^d \approx e^{-1} = 0.368$)
  - Repeat the sampling procedue k times, overall accuracy of the model:

$$acc(M) = \sum_{i=1}^{k} (0.632 \times acc(M_i)_{test\_set} + 0.368 \times acc(M_i)_{train\_set})$$

Roadmap

Ensemble Methods: Increasing the Accuracy



- Ensemble methods
  - Use a combination of models to increase accuracy
  - Combine a series of k learned models, M_1, M_2, …, M_k, with the aim of creating an improved model M*
- Popular ensemble methods
  - Bagging: averaging the prediction over a collection of classifiers
  - Boosting: weighted vote with a collection of classifiers
  - Ensemble: combining a set of heterogeneous classifiers

Bagging: Boostrap Aggregation

- Analogy: Diagnosis based on multiple doctors' majority vote
- Training
  - Given a set D of *d* tuples, at each iteration *i*, a training set D_i of *d* tuples is sampled with replacement from D (i.e., boostrap)
  - A classifier model M_i is learned for each training set D_i
- Classification: classify an unknown sample **X**
  - Each classifier M_i returns its class prediction
  - The bagged classifier M* counts the votes and assigns the class with the most votes to **X**
- Prediction: can be applied to the prediction of continuous values by taking the average value of each prediction for a given test tuple
- Accuracy
  - Often significant better than a single classifier derived from D
  - For noise data: not considerably worse, more robust
  - Proved improved accuracy in prediction

Boosting

- Analogy: Consult several doctors, based on a combination of weighted diagnoses—weight assigned based on the previous diagnosis accuracy
- How boosting works?
  - Weights are assigned to each training tuple
  - A series of k classifiers is iteratively learned
  - After a classifier M_i is learned, the weights are updated to allow the subsequent classifier, M_{i+1}, to pay more attention to the training tuples that were misclassified by M_i
  - The final M* combines the votes of each individual classifier, where the weight of each classifier's vote is a function of its accuracy
- The boosting algorithm can be extended for the prediction of continuous values
- Comparing with bagging: boosting tends to achieve greater accuracy, but it also risks overfitting the model to misclassified data

Adaboost (Freund and Schapire, 1997)

- Given a set of *d* class-labeled tuples, ($\mathbf{X_1}$, y_1), …, ($\mathbf{X_d}$, y_d)
- Initially, all the weights of tuples are set the same (1/d)
- Generate k classifiers in k rounds. At round i,
  - Tuples from D are sampled (with replacement) to form a training set D_i of the same size
  - Each tuple's chance of being selected is based on its weight
  - A classification model M_i is derived from D_i
  - Its error rate is calculated using D_i as a test set
  - If a tuple is misclssified, its weight is increased, o.w. it is decreased
- Error rate: err($\mathbf{X_j}$) is the misclassification error of tuple $\mathbf{X_j}$. Classifier M_i error rate is the sum of the weights of the misclassified tuples:

$$error(M_i) = \sum_j^d w_j \times err(\mathbf{X_j})$$

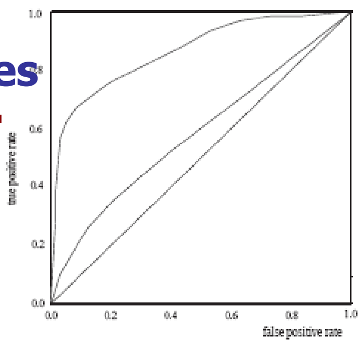
- The weight of classifier M_i's vote is

$$\log \frac{1 - error(M_i)}{error(M_i)}$$

Roadmap

- What is classification? What is prediction?
- Issues regarding classification and prediction
- Classification by decision tree induction
- Bayesian classification
- Rule-based classification
- Classification by back propagation
- Support Vector Machines (SVM)
- Associative classification
- Lazy learners (or learning from your neighbors)
- Other classification methods
- Prediction
- Accuracy and error measures
- Ensemble methods
- Model selection ←
- Summary

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

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Summary (I)

- Classification and prediction are two forms of data analysis that can be used to extract models describing important data classes or to predict future data trends.
- Effective and scalable methods have been developed for decision trees induction, Naive Bayesian classification, Bayesian belief network, rule-based classifier, Backpropagation, Support Vector Machine (SVM), associative classification, nearest neighbor classifiers, and case-based reasoning, and other classification methods such as genetic algorithms, rough set and fuzzy set approaches.
- Linear, nonlinear, and generalized linear models of regression can be used for prediction. Many nonlinear problems can be converted to linear problems by performing transformations on the predictor variables. Regression trees and model trees are also used for prediction.

Summary (II)

- Stratified k-fold cross-validation is a recommended method for accuracy estimation. Bagging and boosting can be used to increase overall accuracy by learning and combining a series of individual models.
- Significance tests and ROC curves are useful for model selection
- There have been numerous comparisons of the different classification and prediction methods, and the matter remains a research topic
- No single method has been found to be superior over all others for all data sets
- Issues such as accuracy, training time, robustness, interpretability, and scalability must be considered and can involve trade-offs, further complicating the quest for an overall superior method

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