IIT KHARAGPUR

NPTEL ONLINE CERTIFICATION COURSES

Data Mining

Week 4: K-Nearest Neighbor, Classifier Evaluation

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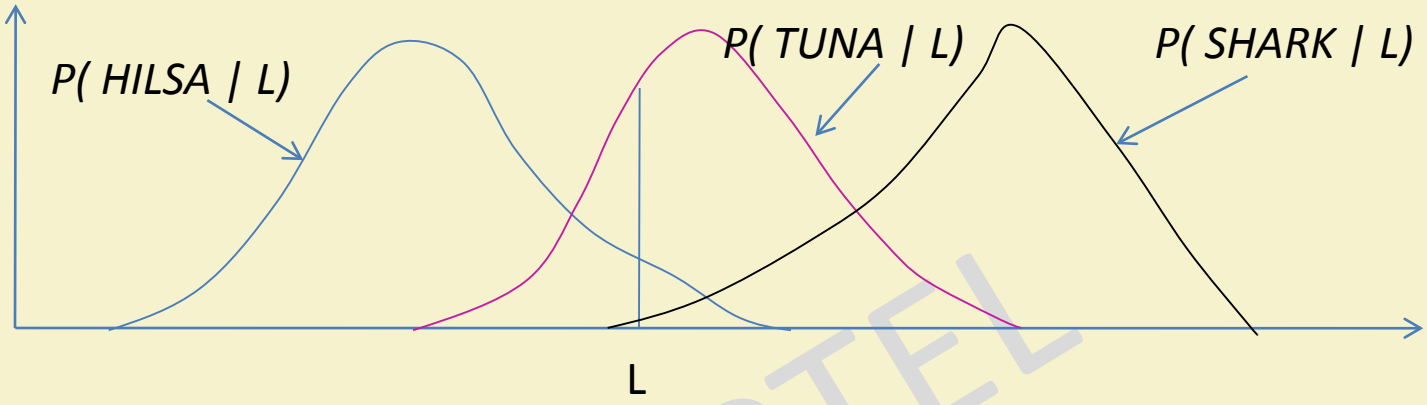
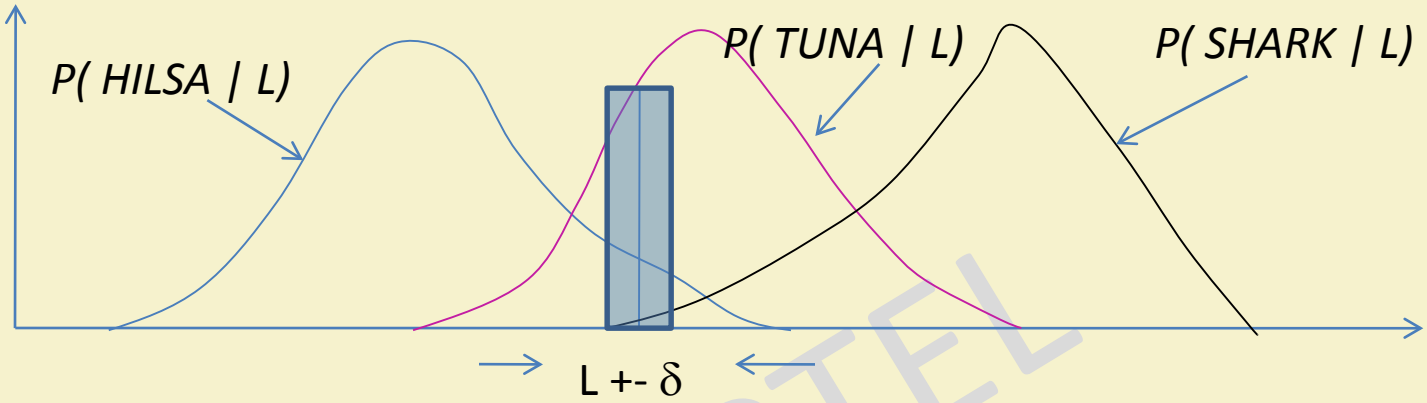
Bayes Classifier: Recap



Maximum Aposteriori (MAP) Rule

Distributions assumed to be of particular family (e.g., Gaussian), and parameters estimated from training data.

Bayes Classifier: Recap

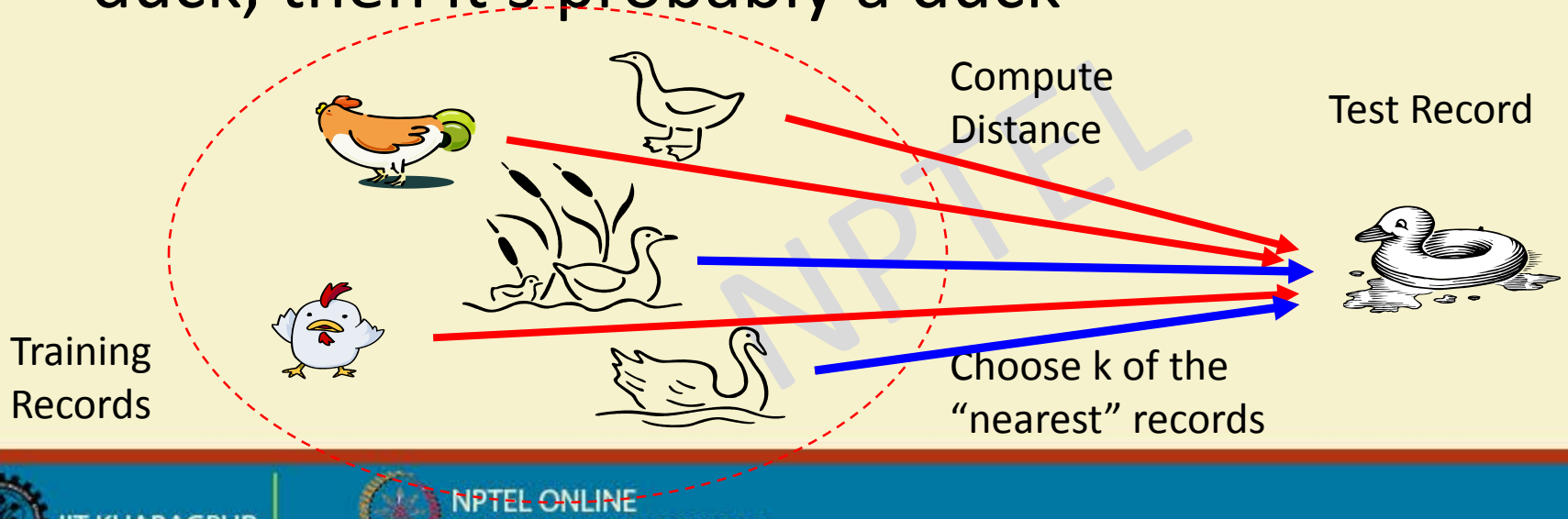


Approximate Maximum Aposteriori (MAP) Rule

Non-parametric (data driven) approach: consider a small window around L, Find which class is most populous in that window.

Nearest Neighbor Classifiers

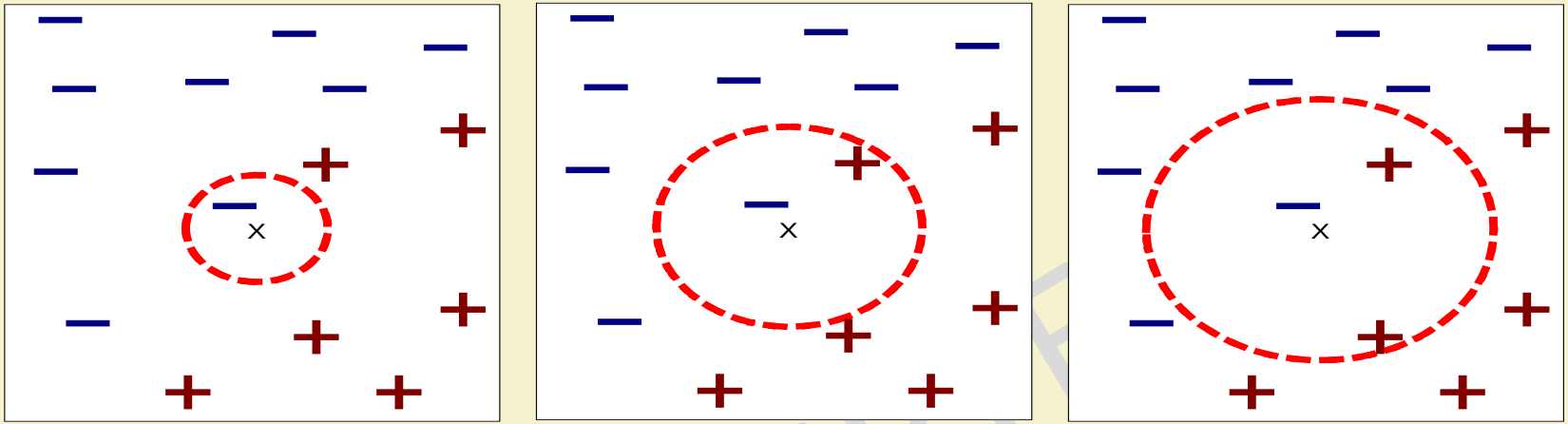
- Basic idea: If it walks like a duck, quacks like a duck, then it's probably a duck



Basic Idea

- *k*-NN classification rule is to assign to a test sample the majority category label of its *k* nearest training samples
- In practice, *k* is usually chosen to be odd, so as to avoid ties
- The *k* = 1 rule is generally called the nearest-neighbor classification rule

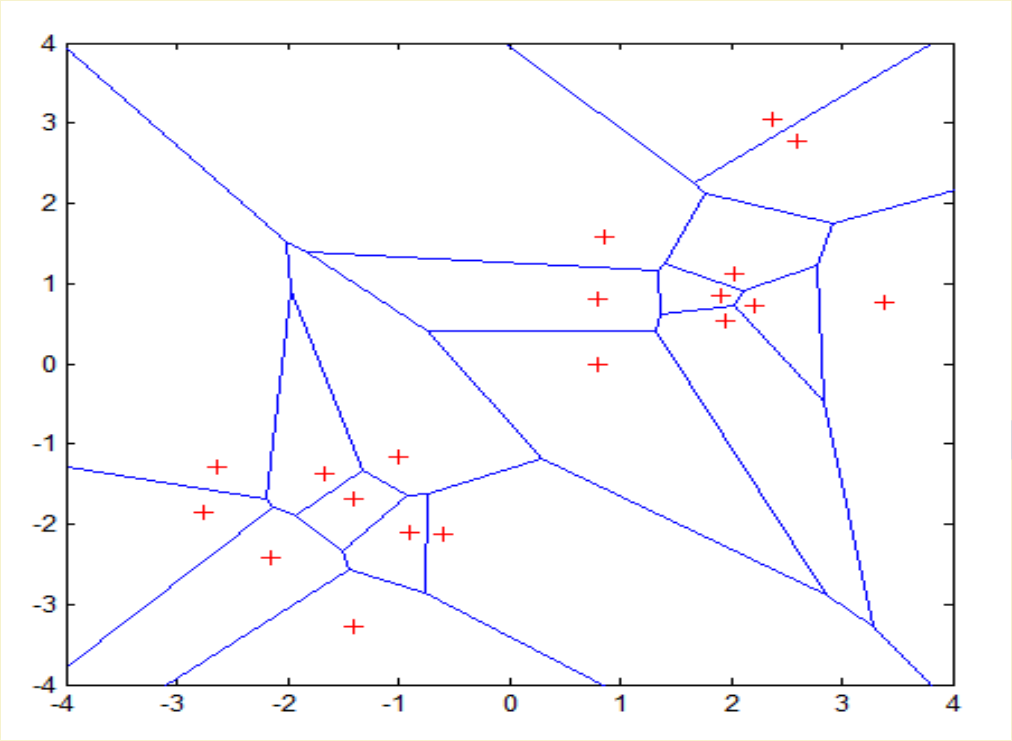
Definition of Nearest Neighbor



(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

K-nearest neighbors of a record x - data points that have the k smallest distance to x

Nearest Neighbor: Voronoi Diagram



Properties:

1) All possible points within a sample's Voronoi cell are the nearest neighboring points for that sample
2) For any sample, the nearest sample is determined by the closest Voronoi cell edge

Distance-weighted *k*-NN

- Replace $\hat{f}(q) = \arg\max_{v \in V} \sum_{i=1}^{k} \delta(v, f(x_i))$ by:

$$\hat{f}(q) = \arg\max_{v \in V} \sum_{i=1}^{k} \frac{1}{d(x_i, x_q)^2} \delta(v, f(x_i))$$

General Kernel functions like Parzen Windows may be considered Instead of inverse distance.

Predicting Continuous Values

- Replace $$\hat{f}(q) = \arg\max_{v \in V} \sum_{i=1}^{k} w_i \delta(v, f(x_i))$$ by:

- Note: unweighted corresponds to w_i=1 for all i

$$\hat{f}(q) = \frac{\sum_{i=1}^{k} w_i f(x_i)}{\sum_{i=1}^{k} w_i}$$

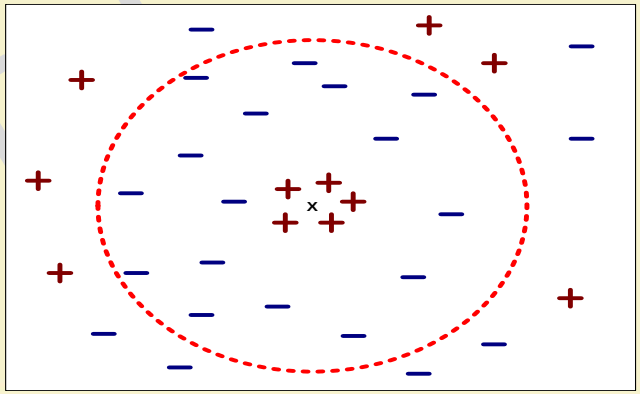
Nearest-Neighbor Classifiers: Issues

- The value of *k*, the number of nearest neighbors to retrieve
- Choice of Distance Metric to compute distance between records
- Computational complexity
  - Size of training set
  - Dimension of data

Value of K

- Choosing the value of k:
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from other classes

Rule of thumb:
K = sqrt(N)
N: number of training points



Distance Metrics

Minkowsky:

$$D(\boldsymbol{x},\boldsymbol{y}) = \left(\sum_{i=1}^{m} |x_i - y_i|^r\right)^{1/r}$$

Euclidean:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sqrt{\sum_{i=1}^{m} (x_i - y_i)^2}$$

Manhattan / city-block:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} |x_i - y_i|$$

Camberra:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} \frac{|x_i - y_i|}{|x_i + y_i|}$$

Chebychev:

$$D(\boldsymbol{x},\boldsymbol{y}) = \max_{i=1}^{m} |x_i - y_i|$$

Quadratic:

$$D(\boldsymbol{x},\boldsymbol{y}) = (\boldsymbol{x} - \boldsymbol{y})^T Q(\boldsymbol{x} - \boldsymbol{y}) = \sum_{j=1}^{m}\left(\sum_{i=1}^{m}(x_i - y_i)q_{ji}\right)(x_j - y_j)$$

Q is a problem-specific positive definite $m \times m$ weight matrix

Mahalanobis:

$$D(\boldsymbol{x},\boldsymbol{y}) = [\det V]^{1/m}(\boldsymbol{x} - \boldsymbol{y})^{\mathrm{T}} V^{-1}(\boldsymbol{x} - \boldsymbol{y})$$

V is the covariance matrix of $A_1..A_m$, and A_j is the vector of values for attribute j occuring in the training set instances $1..n$.

Correlation:

$$D(\boldsymbol{x},\boldsymbol{y}) = \frac{\sum_{i=1}^{m}(x_i - \overline{x_i})(y_i - \overline{y_i})}{\sqrt{\sum_{i=1}^{m}(x_i - \overline{x_i})^2 \sum_{i=1}^{m}(y_i - \overline{y_i})^2}}$$

$\overline{x_i} = \overline{y_i}$ and is the average value for attribute i occuring in the training set.

Chi-square:

$$D(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} \frac{1}{sum_i}\left(\frac{x_i}{size_{\boldsymbol{x}}} - \frac{y_i}{size_{\boldsymbol{y}}}\right)^2$$

sum_i is the sum of all values for attribute i occuring in the training set, and $size_{\boldsymbol{x}}$ is the sum of all values in the vector $\boldsymbol{x}$.

Kendall's Rank Correlation:

$$D(\boldsymbol{x},\boldsymbol{y}) = 1 - \frac{2}{n(n-1)}\sum_{i=1}^{m}\sum_{j=1}^{i-1}\mathrm{sign}(x_i - x_j)\mathrm{sign}(y_i - y_j)$$

sign(x)=-1, 0 or 1 if $x < 0$, $x = 0$, or $x > 0$, respectively.

Figure 1. Equations of selected distance functions. ($\boldsymbol{x}$ and $\boldsymbol{y}$ are vectors of m attribute values).

Distance Measure: Scale Effects

- Different features may have different measurement scales
  - E.g., patient weight in kg (range [50,200]) vs. blood protein values in ng/dL (range [-3,3])
- Consequences
  - Patient weight will have a much greater influence on the distance between samples
  - May bias the performance of the classifier

Standardization

- Transform raw feature values into z-scores

$$z_{ij} = \frac{x_{ij} - \mu_j}{\sigma_j}$$

x_{ij} is the value for the i^{th} sample and j^{th} feature

μ_j is the average of all x_{ij} for feature j

σ_j is the standard deviation of all x_{ij} over all input samples

- Range and scale of z-scores should be similar (providing distributions of raw feature values are alike)

Nearest Neighbor : Dimensionality

- Problem with Euclidean measure:
  - High dimensional data
    - curse of dimensionality
  - Can produce counter-intuitive results
  - Shrinking density – sparsification effect

1 1 1 1 1 1 1 1 1 1 1 0
0 1 1 1 1 1 1 1 1 1 1 1

d = 1.4142

vs

1 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 1

d = 1.4142

Distance for Nominal Attributes

Value Difference Metric (VDM)

[Stanfill & Waltz, 1986]

Providing appropriate distance measurements for nominal attributes.

$$vdm_a(x,y) = \sum_{c=1}^{C} \left(\frac{N_{a,x,c}}{N_{a,x}} - \frac{N_{a,y,c}}{N_{a,y}} \right)^2$$

$N_{a,x}$ = # times attribute a had value x

$N_{a,x,c}$ = # times attribute a had value x and class was c

C = # output classes

Two values are considered closer if they have more similar classifications, i.e., if they have more similar correlations with the output classes.

Distance for Heterogeneous Data

In this section, we define a heterogeneous distance function *HVDM* that returns the distance between two input vectors $\boldsymbol{x}$ and $\boldsymbol{y}$. It is defined as follows:

$$HVDM(\boldsymbol{x},\boldsymbol{y}) = \sqrt{\sum_{a=1}^{m} d_a{}^2(x_a, y_a)} \tag{11}$$

where m is the number of attributes. The function $d_a(x,y)$ returns a distance between the two values x and y for attribute a and is defined as:

$$d_a(x,y) = \begin{cases} 1, & \text{if } x \text{ or } y \text{ is unknown; otherwise...} \\ normalized\_vdm_a(x,y), & \text{if } a \text{ is nominal} \\ normalized\_diff_a(x,y), & \text{if } a \text{ is linear} \end{cases} \tag{12}$$

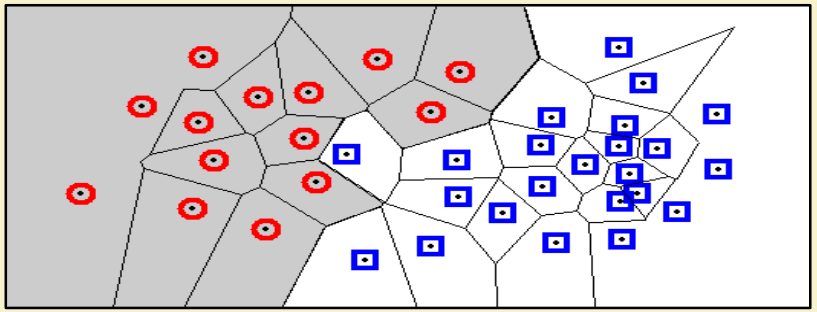
Nearest Neighbour : Computational Complexity

- Expensive
  - To determine the nearest neighbour of a query point *q*, must compute the distance to all *N* training examples
    - \+ Pre-sort training examples into fast data structures (kd-trees)
    - \+ Compute only an approximate distance (LSH)
    - \+ Remove redundant data (condensing)
- Storage Requirements
  - Must store all training data **P**
    - \+ Remove redundant data (condensing)
    - \- Pre-sorting often increases the storage requirements
- High Dimensional Data
  - "Curse of Dimensionality"
    - Required amount of training data increases exponentially with dimension
    - Computational cost also increases dramatically
    - Partitioning techniques degrade to linear search in high dimension

Reduction in Computational Complexity

- Reduce size of training set
  - Condensation, editing
- Use geometric data structure for high dimensional search

Condensation: Decision Regions



Each cell contains one sample, and every location within the cell is closer to that sample than to any other sample.

A Voronoi diagram divides the space into such cells.

Every query point will be assigned the classification of the sample within that cell. The *decision boundary* separates the class regions based on the 1-NN decision rule.

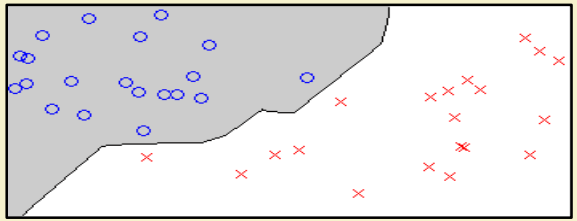
Knowledge of this boundary is sufficient to classify new points.

The boundary itself is rarely computed; many algorithms seek to retain only those points necessary to generate an identical boundary.

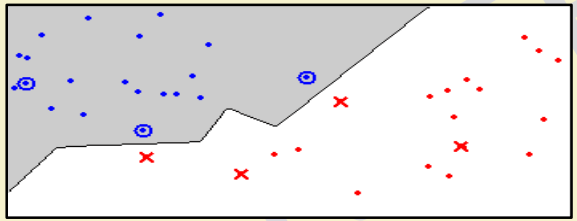
Condensing

- Aim is to reduce the number of training samples
- Retain only the samples that are needed to define the decision boundary

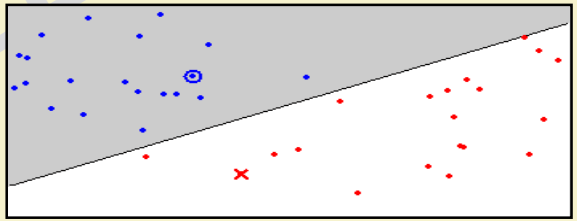
- Decision Boundary Consistent – a subset whose nearest neighbour decision boundary is identical to the boundary of the entire training set
- Minimum Consistent Set – the smallest subset of the training data that correctly classifies all of the original training data



Original data



Condensed data



Minimum Consistent Set

Condensed Nearest Neighbor

- Condensed Nearest Neighbour (CNN)

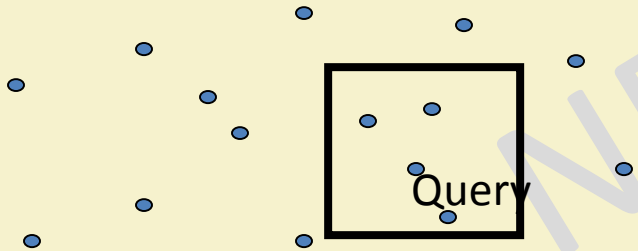
1. Initialize subset with a single (or K) training example
2. Classify all remaining samples using the subset, and transfer any incorrectly classified samples to the subset
3. Return to 2 until no transfers occurred or the subset is full

- Incremental
- Order dependent
- Neither minimal nor decision boundary consistent
- $O(n^3)$ for brute-force method

High dimensional search

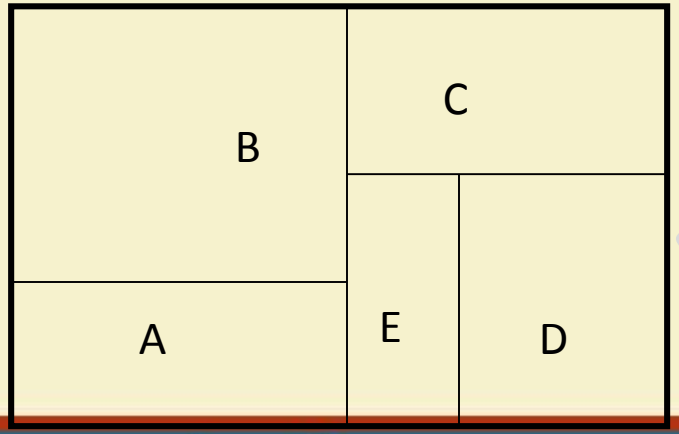
- Given a point set and a nearest neighbor query point

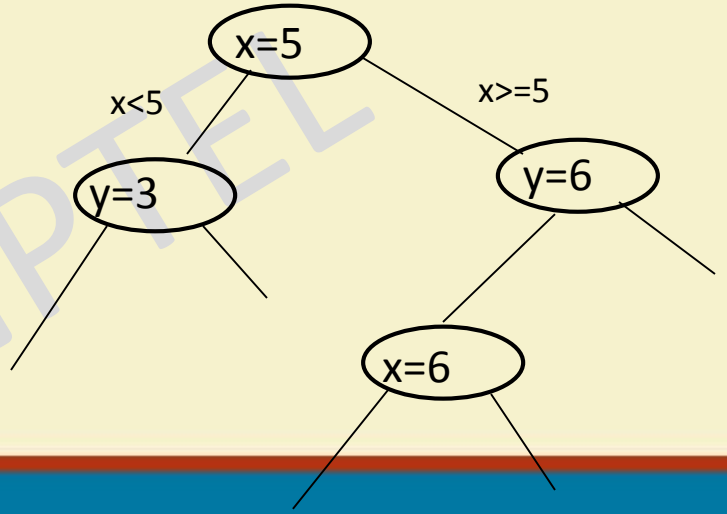
- Find the points enclosed in a rectangle (range) around the query
- Perform linear search for nearest neighbor only in the rectangle



kd-tree: data structure for range search

- Index data into a tree
- Search on the tree
- Tree construction: At each level we use a different dimension to split





KNN: Alternate Terminologies

- Instance Based Learning
- Lazy Learning
- Case Based Reasoning
- Exemplar Based Learning

Text Search: Documents as vectors

- We have a |V|-dimensional vector space
- Terms are axes of the space
- Documents are points or vectors in this space
- Very high-dimensional: tens of millions of dimensions when you apply this to a web search engine
- These are very sparse vectors - most entries are zero.

Queries as vectors

- Key idea 1: Do the same for queries: represent them as vectors in the space
- Key idea 2: Rank documents according to their proximity to the query in this space
- proximity = similarity of vectors
- proximity ≈ inverse of distance
- Recall: We do this because we want to get away from the you're-either-in-or-out Boolean model.
- Instead: rank more relevant documents higher than less relevant documents

Formalizing vector space proximity

- First cut: distance between two points
  - (= distance between the end points of the two vectors)
- Euclidean distance?
- Euclidean distance is a bad idea . . .
- . . . because Euclidean distance is large for vectors of different lengths.

Use angle instead of distance

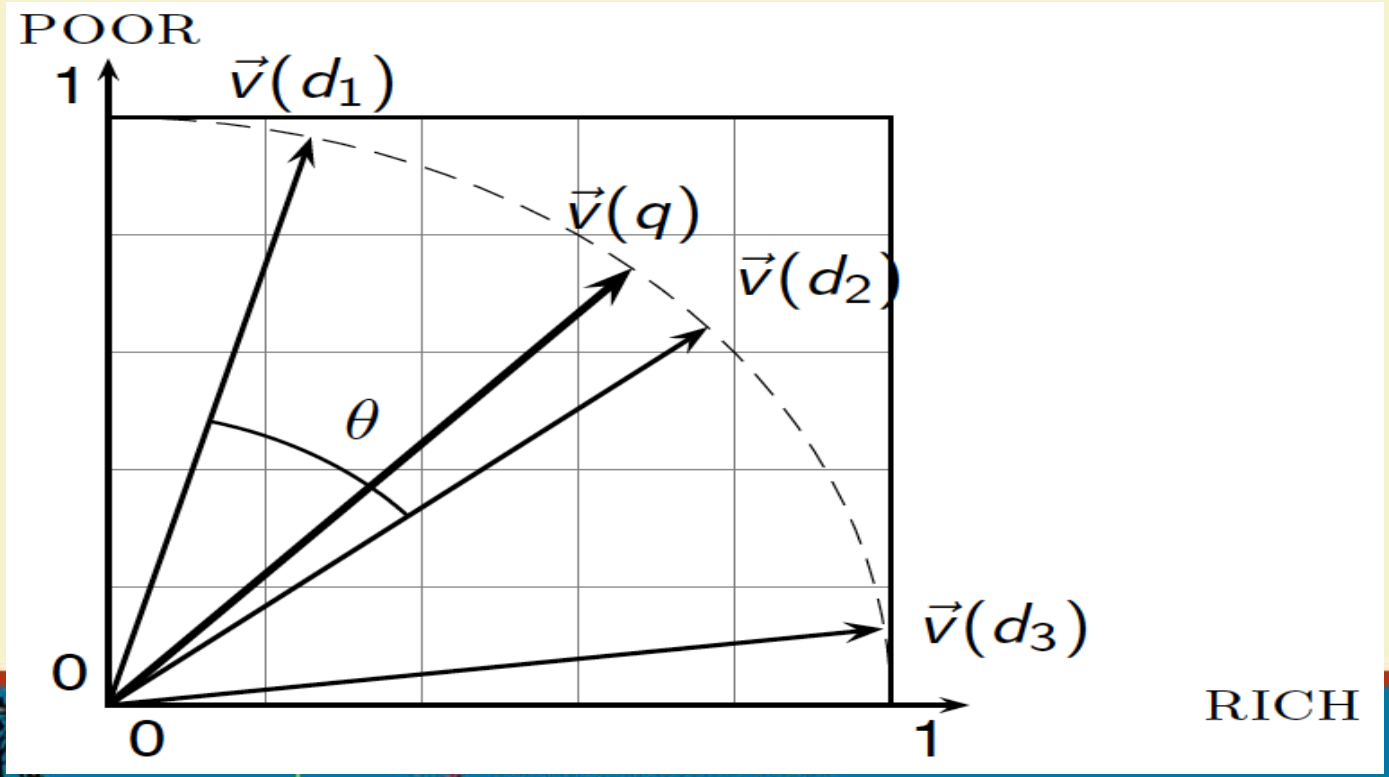
- Thought experiment: take a document *d* and append it to itself. Call this document *d′*.
- "Semantically" d and d′ have the same content
- The Euclidean distance between the two documents can be quite large
- The angle between the two documents is 0, corresponding to maximal similarity.

- Key idea: Rank documents according to angle with query.

From angles to cosines

- The following two notions are equivalent.
  - Rank documents in decreasing order of the angle between query and document
  - Rank documents in increasing order of cosine(query,document)
- Cosine is a monotonically decreasing function for the interval [0^o, 180^o]

Cosine similarity illustrated



End of K-Nearest Neighbor

Classifier Evaluation

Classifier Evaluation

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

Metrics for Performance Evaluation

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

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

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Accuracy

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

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

Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10

- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
  - Accuracy is misleading because model does not detect any class 1 example

Cost Matrix

	PREDICTED CLASS		
ACTUAL CLASS	C(i|j)	**Class=Yes**	**Class=No**
	Class=Yes	C(Yes|Yes)	C(No|Yes)
	Class=No	C(Yes|No)	C(No|No)

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

Cost-Sensitive Measures

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

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

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

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

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

Model Evaluation

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model
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  - How to obtain reliable estimates?
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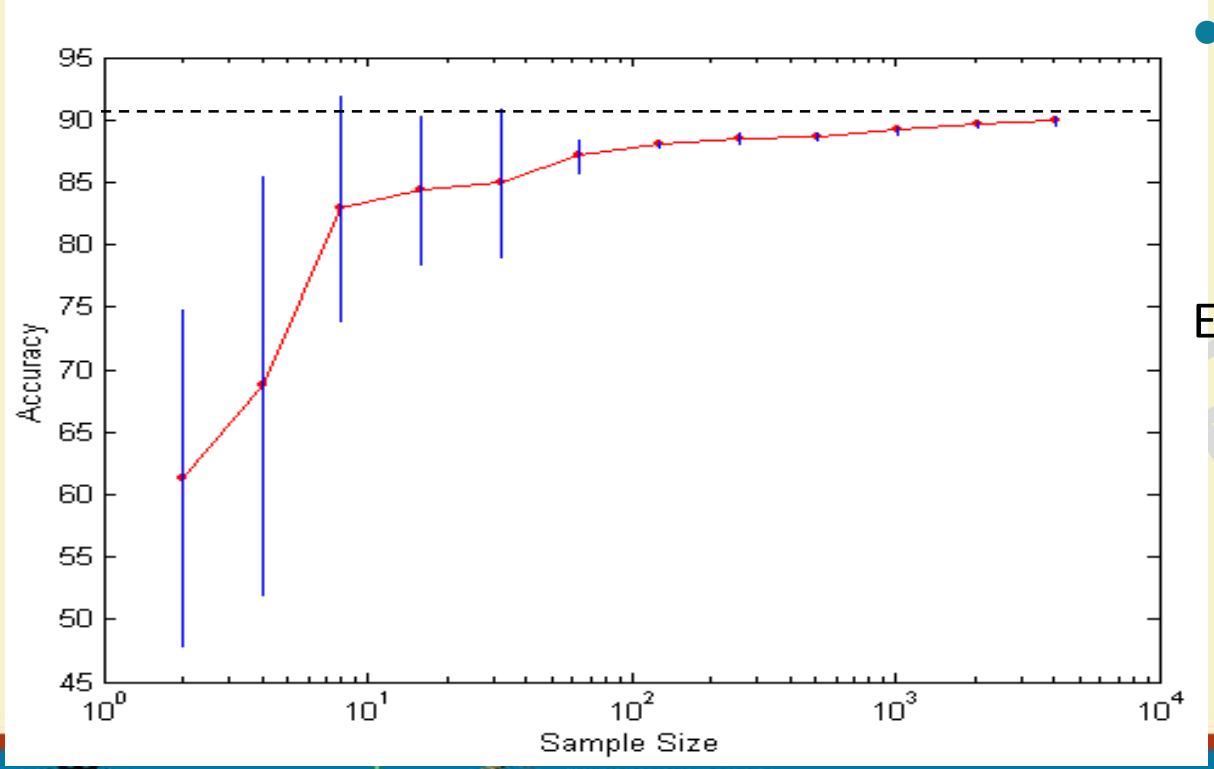
Methods for Performance Evaluation

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

Learning Curve



- Learning curve shows how accuracy changes with varying sample size

Effect of small sample size:

- Bias in the estimate
- Variance of estimate

Methods of Estimation

- Holdout
  - Reserve 2/3 for training and 1/3 for testing
- Random subsampling
  - Repeated holdout
- Cross validation
  - Partition data into k disjoint subsets
  - k-fold: train on k-1 partitions, test on the remaining one
  - Leave-one-out: k=n
- Stratified sampling
  - oversampling vs undersampling
- Bootstrap
  - Sampling with replacement

Model Evaluation

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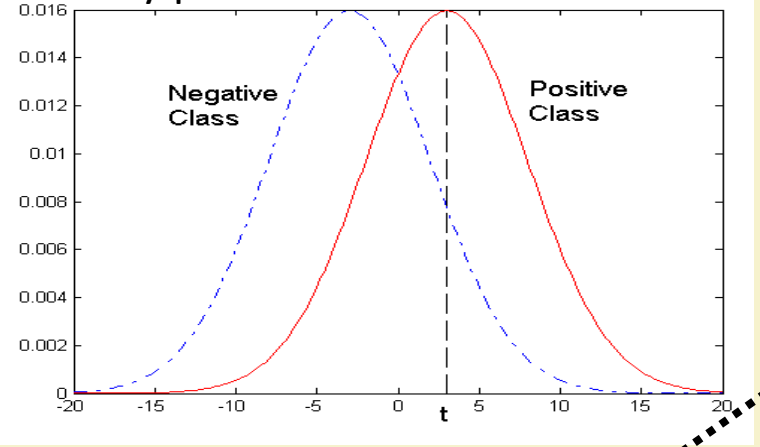
ROC (Receiver Operating Characteristic)

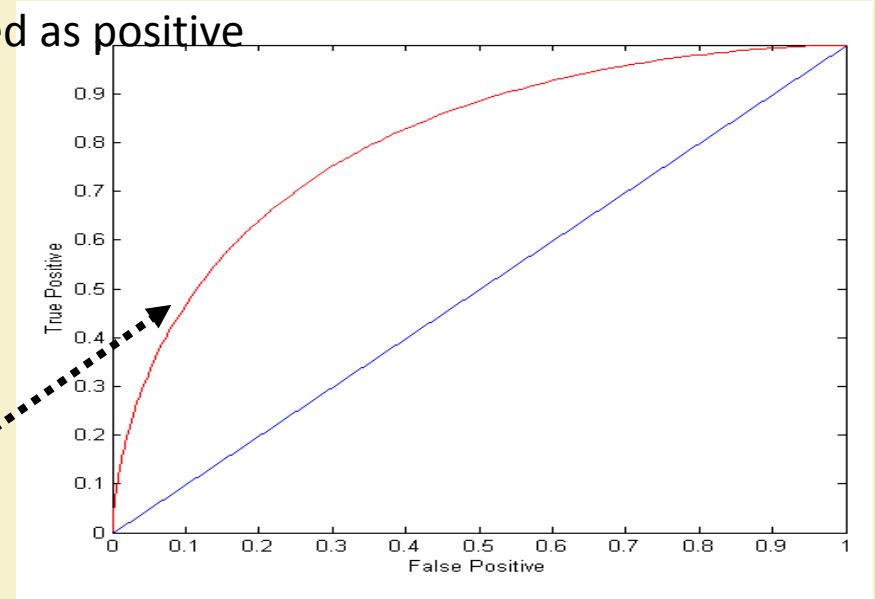
- Developed in 1950s for signal detection theory to analyze noisy signals
  - Characterize the trade-off between positive hits and false alarms
- ROC curve plots TP (on the y-axis) against FP (on the x-axis)
- Performance of each classifier represented as a point on the ROC curve
  - changing the threshold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

ROC Curve

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

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





At threshold t:

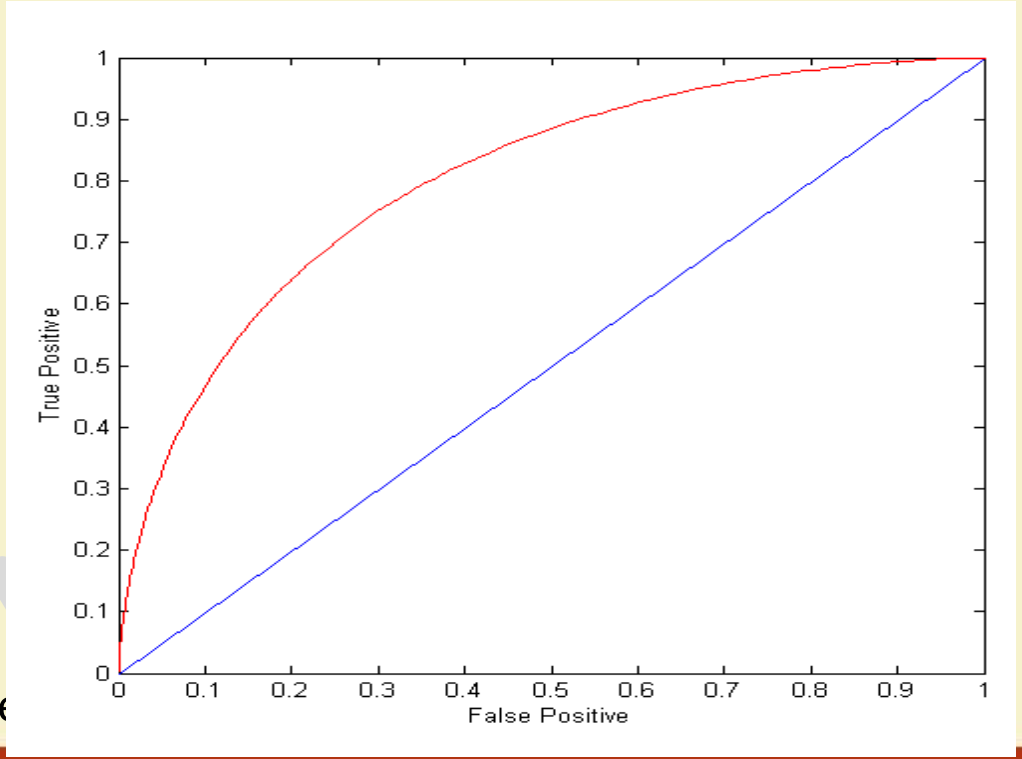
TP=0.5, FN=0.5, FP=0.12, FN=0.88

ROC Curve

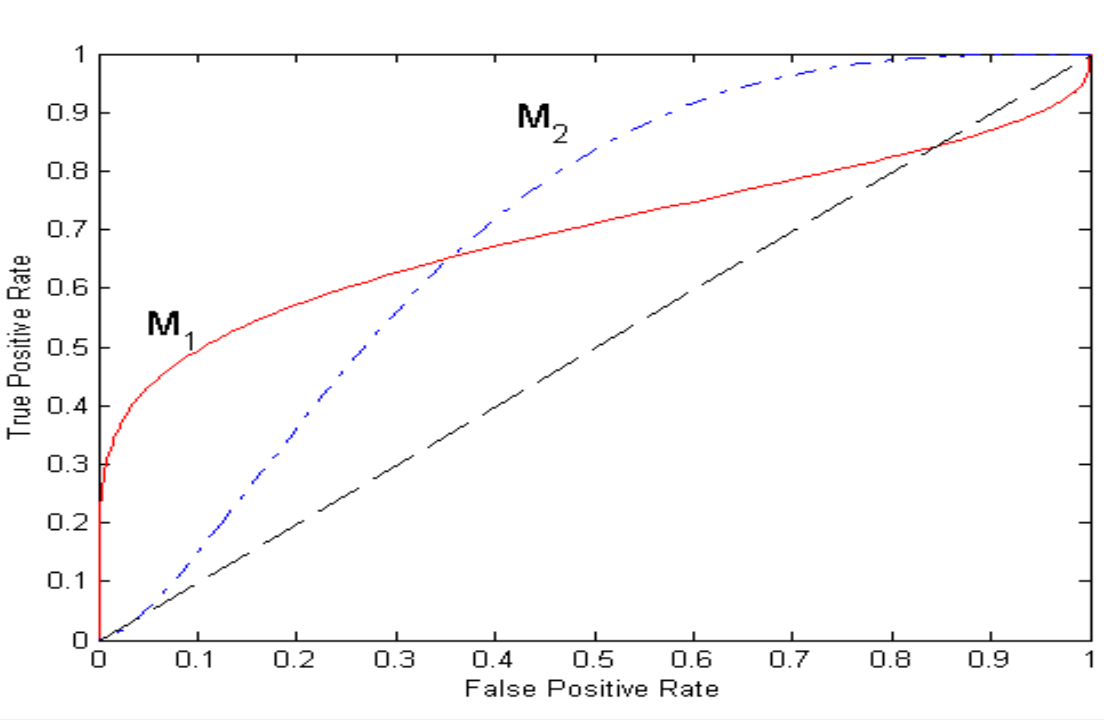
(TP,FP):

- (0,0): declare everything to be negative class
- (1,1): declare everything to be positive class
- (1,0): ideal

- Diagonal line:
  - Random guessing
  - Below diagonal line:
    - prediction is opposite of the true class



Using ROC for Model Comparison



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

Test of Significance

- Given two models:
  - Model M1: accuracy = 85%, tested on 30 instances
  - Model M2: accuracy = 75%, tested on 5000 instances
- Can we say M1 is better than M2?
  - How much confidence can we place on accuracy of M1 and M2?
  - Can the difference in performance measure be explained as a result of random fluctuations in the test set?

Comparing Performance of 2 Models

- Given two models, say M1 and M2, which is better?
  - M1 is tested on D1 (size=n1), found error rate = e_1
  - M2 is tested on D2 (size=n2), found error rate = e_2
  - Assume D1 and D2 are independent
  - If n1 and n2 are sufficiently large, then

$$e_1 \sim N(\mu_1, \sigma_1)$$
$$e_2 \sim N(\mu_2, \sigma_2)$$

  - Approximate: $\hat{\sigma}_i = \frac{e_i(1-e_i)}{n_i}$

Comparing Performance of 2 Models

- To test if performance difference is statistically significant: d = e1 – e2
  - d ~ $N(d_t, \sigma_t)$ where d_t is the true difference
  - Since D1 and D2 are independent, their variance adds up:

$$\sigma_t^2 = \sigma_1^2 + \sigma_2^2 \cong \hat{\sigma}_1^2 + \hat{\sigma}_2^2$$

$$= \frac{e1(1-e1)}{n1} + \frac{e2(1-e2)}{n2}$$

  - At (1-α) confidence level, $d_t = d \pm Z_{\alpha/2}\hat{\sigma}_t$

End of Classifier Evaluation