

Machine Learning

10-701/15-781, Spring2010

Theory of Classification and Nonparametric Classifier



Eric Xing

Lecture 3, January 18, 2010

Reading: Chap. 2, 5 CB and handouts

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Miscellaneous

- Homework 1 due this Wed
- My office hour moved to this Wed 12:30-1:30. (only this week)

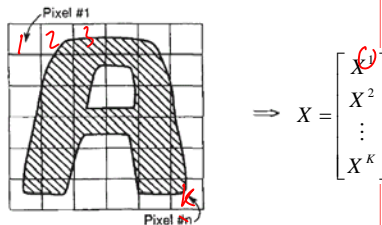
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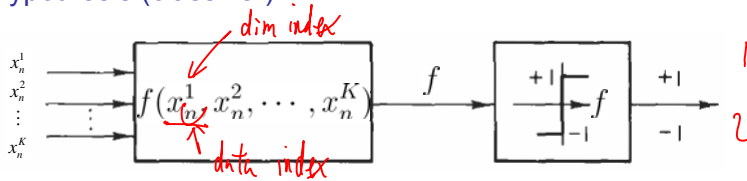
Classification



- Representing data:



- Hypothesis (classifier)



Outline

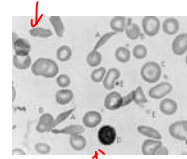
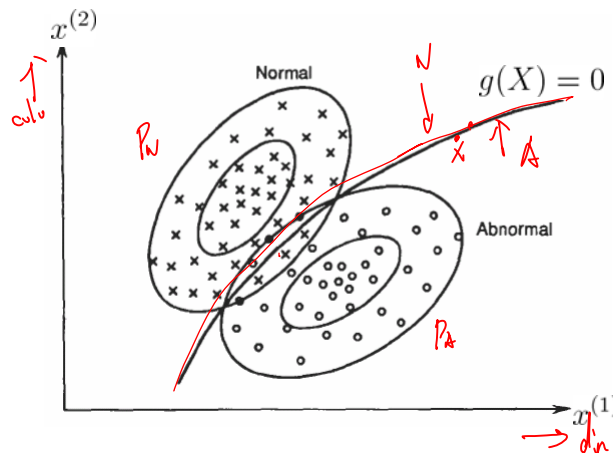


- What is theoretically the best classifier
 - Probabilistic theory of classification
 - Density estimation and Bayesian theorem
 - Bayesian decision rule for Minimum Error
- Nonparametric Classifier (Instance-based learning)
 - Nonparametric density estimation
 - K-nearest-neighbor classifier
 - Optimality of kNN
 - Problem of kNN

Decision-making as dividing a high-dimensional space



- Distributions of samples from normal and abnormal cells



$P_A, P_B \rightarrow g(x)$

Continuous Distributions



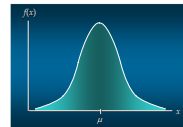
- Uniform Probability Density Function

$$p(x) = \begin{cases} 1/(b-a) & \text{for } a \leq x \leq b \\ 0 & \text{elsewhere} \end{cases}$$



- Normal (Gaussian) Probability Density Function

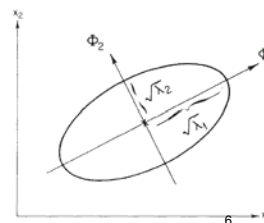
$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$



- The distribution is symmetric, and is often illustrated as a bell-shaped curve.
- Two parameters, μ (mean) and σ (standard deviation), determine the location and shape of the distribution.
- The highest point on the normal curve is at the mean, which is also the median and mode.
- The mean can be any numerical value: negative, zero, or positive.

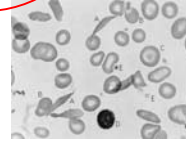
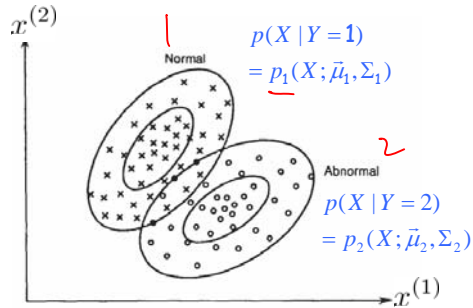
- Multivariate Gaussian

$$p(X; \bar{\mu}, \Sigma) = \frac{1}{(\sqrt{2\pi})^n |\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(X - \bar{\mu})^T \Sigma^{-1} (X - \bar{\mu})\right\}$$



Class-Conditional Probability

- Classification-specific Dist.: $P(X|Y)$



$$P(Y|X) \neq P(Y=2|X)$$

$$\begin{matrix} > & 1 \\ < & 2 \end{matrix}$$

- Class prior (i.e., "weight"): $P(Y)$

$$P(Y=1) = \pi_1 = 0.5$$

The Bayes Rule

- What we have just did leads to the following general expression:

$$P(Y|X) = \frac{P(X|Y)p(Y)}{P(X) = \sum_y P(X|Y)p(Y)}$$

This is Bayes Rule

Bayes, Thomas (1763) An essay towards solving a problem in the doctrine of chances. *Philosophical Transactions of the Royal Society of London*, 53:370-418



The Bayes Decision Rule for Minimum Error



- The *a posteriori* probability of a sample

$$P(Y=i|X) = \frac{p(X|Y=i)P(Y=i)}{p(X)} = \frac{\pi_i p_i(X)}{\sum_i \pi_i p_i(X)} \equiv q_i(X)$$

- Bayes Test:

$$q_1(x) \geq q_2(x) \Rightarrow \pi_1 p_1(x) \geq \pi_2 p_2(x) \quad \frac{p_1(x)}{p_2(x)} \geq \frac{\pi_2}{\pi_1}$$

- Likelihood Ratio:

$$l(X) = \frac{p_1(x)}{p_2(x)}$$

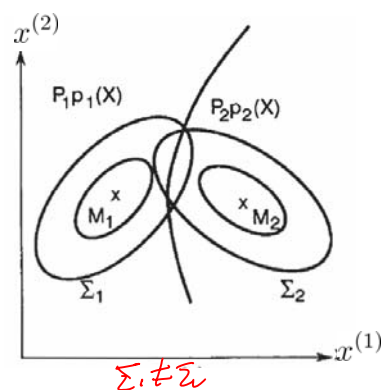
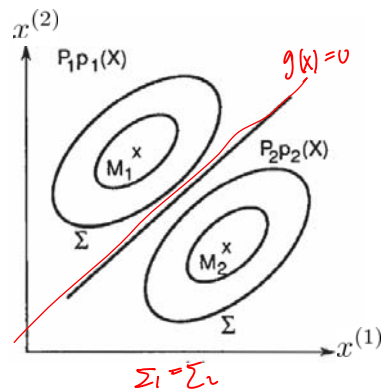
- Discriminant function:

$$h(x) = \ln l(x) = \ln p_1(x) - \ln p_2(x) \geq \ln \frac{\pi_2}{\pi_1} = 0$$

Example of Decision Rules



- When each class is a normal ...



- We can write the decision boundary analytically in some cases ... homework!!

Bayes Error



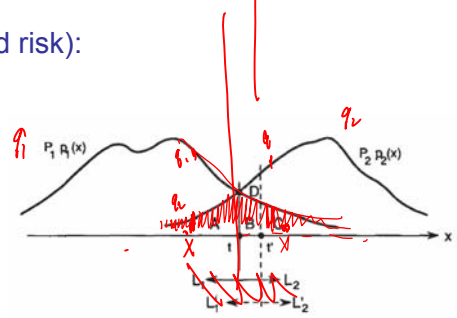
- We must calculate the **probability of error**
 - the probability that a sample is assigned to the wrong class
- Given a datum X , what is the **risk**?

q_1
 q_2
 $P(\xi) = P(\xi | X, E_w)$
 $+P(\xi \neq X, E_w)$
 $E_1: q_1 > q_2$
 $E_2: q_2 > q_1$

$$r(X) = \min[q_1(X), q_2(X)]$$

- The Bayes error (the expected risk):

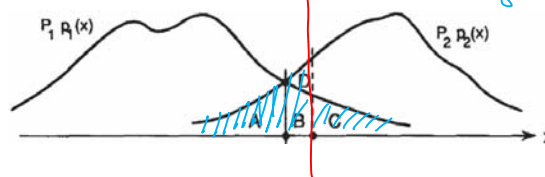
$$\begin{aligned} \epsilon &= E[r(X)] = \int r(x)p(x)dx \\ &= \int \min[\pi_1 p_1(x), \pi_2 p_2(x)]dx \\ &= \pi_1 \int_{L_1} p_1(x)dx + \pi_2 \int_{L_2} p_2(x)dx \\ &= \pi_1 \epsilon_1 + \pi_2 \epsilon_2 \end{aligned}$$



More on Bayes Error



- Bayes error is the lower bound of probability of classification error



- Bayes classifier is the theoretically best classifier that minimizes probability of classification error
- Computing Bayes error is in general a very complex problem. Why?
 - Density estimation:
 - Integrating density function:

$$\epsilon_1 = \int_{\ln(\pi_1/\pi_2)}^{+\infty} p_1(x)dx \quad \epsilon_2 = \int_{-\infty}^{\ln(\pi_1/\pi_2)} p_2(x)dx$$

Learning Classifier



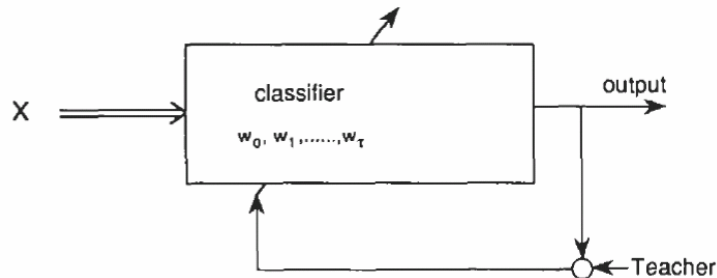
- The decision rule:

$$h(X) = -\ln p_1(X) + \ln p_2(X) \begin{matrix} > \ln \frac{\pi_1}{\pi_2} \\ < \ln \frac{\pi_1}{\pi_2} \end{matrix}$$

- Learning strategies

- Generative Learning
 - Parametric
 - Nonparametric
- Discriminative Learning
 - Parametric
 - Nonparametric
- Instance-based Learning (Store all past experience in memory)
 - A special case of nonparametric classifier

Supervised Learning



- K-Nearest-Neighbor Classifier:
where the $h(X)$ is represented by all the data, and by an algorithm

Recall: Vector Space Representation



- Each document is a vector, one component for each term (= word).

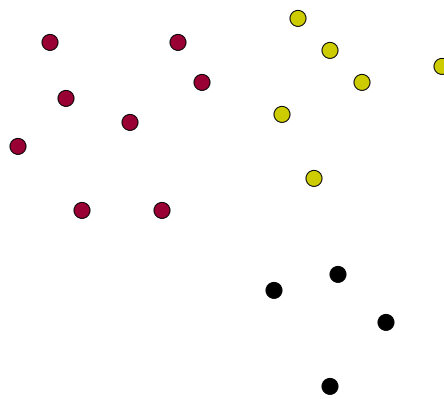
	Doc 1	Doc 2	Doc 3	...
Word 1	3	0	0	...
Word 2	0	8	1	...
Word 3	12	1	10	...
...	0	1	3	...
...	0	0	0	...

- Normalize to unit length.
- High-dimensional vector space:
 - Terms are axes, 10,000+ dimensions, or even 100,000+
 - Docs are vectors in this space

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Classes in a Vector Space

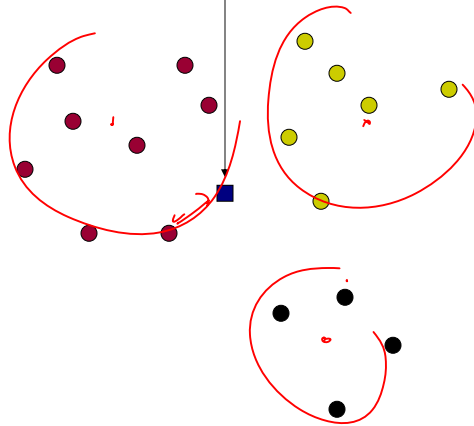


- Sports
- Science
- Arts

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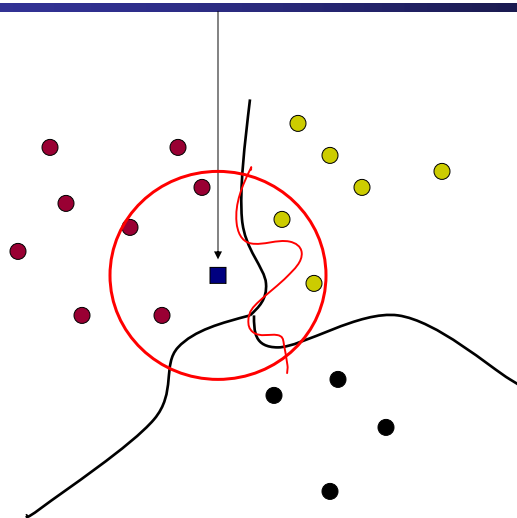
16

Test Document = ?



- Sports
- Science
- Arts
-

K-Nearest Neighbor (kNN) classifier

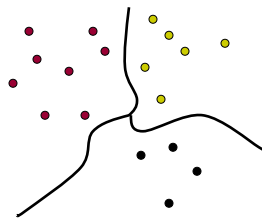


- Sports
- Science
- Arts

kNN Is Close to Optimal



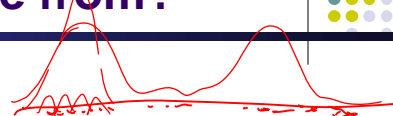
- Cover and Hart 1967
- Asymptotically, the error rate of 1-nearest-neighbor classification is less than twice the Bayes rate [error rate of classifier knowing model that generated data]
- In particular, asymptotic error rate is 0 if Bayes rate is 0.
- Decision boundary:



Where does kNN come from?



- How to estimation $p(X)$?
- Nonparametric density estimation



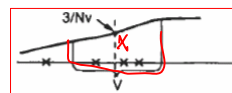
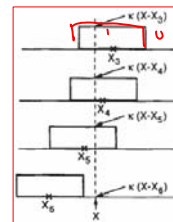
- Parzen density estimate

E.g. (Kernel density est.):

$$\hat{p}(X) = \frac{1}{N} \sum_{i=1}^N \kappa(X - x_i)$$

More generally: $\hat{p}(X) = \frac{1}{N} \frac{k(X)}{V}$

Handwritten red notes:
 + long
 # of part in V.
 fix volume.



Where does kNN come from?



- Nonparametric density estimation

- Parzen density estimate $\hat{p}(X) = \frac{1}{N} \frac{k(X)}{V}$

- kNN density estimate $\hat{p}(X) = \frac{1}{N} \frac{(k-1)}{V(X)}$

Handwritten notes: "k-1" with arrow pointing to the numerator, "size of volume" with arrow pointing to the denominator, and a circled "k" to the right.

- Bayes classifier based on kNN density estimator:

$$h(X) = -\ln \frac{p_1(X)}{p_2(X)} = -\ln \frac{(k_1 - 1)N_2 V_2(X)}{(k_2 - 1)N_1 V_1(X)} > \ln \frac{\pi_1}{\pi_2}$$

Handwritten notes: A red circle around the right side of the equation, and a red arrow pointing from the circle to the text below.

- Voting kNN classifier

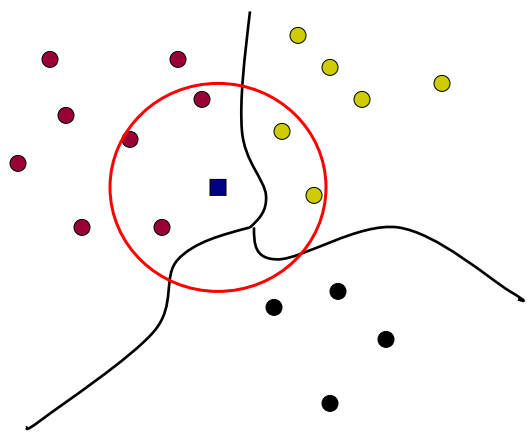
Pick K_1 and K_2 implicitly by picking $K_1 + K_2 = K$, $V_1 = V_2$, $N_1/p_1 = N_2/p_2$

Handwritten note: $\ln \frac{k_1}{k_2}$

Voting kNN



- The procedure



- Sports
- Science
- Arts

Asymptotic Analysis



- Condition risk: $r_k(X, X_{NN})$
 - Test sample X
 - NN sample X_{NN}
 - Denote the event X is class l as $X \leftrightarrow l$

- Assuming $k=1$

$$\begin{aligned} r_1(X, X_{NN}) &= Pr\left\{ \{X \leftrightarrow 1 \ \& \ X_{NN} \leftrightarrow 2\} \text{ or } \{X \leftrightarrow 2 \ \& \ X_{NN} \leftrightarrow 1\} \mid X, X_{NN} \right\} \\ &= Pr\left\{ \{X \leftrightarrow 1 \ \& \ X_{NN} \leftrightarrow 2\} \mid X, X_{NN} \right\} + Pr\left\{ \{X \leftrightarrow 2 \ \& \ X_{NN} \leftrightarrow 1\} \mid X, X_{NN} \right\} \\ &= q_1(X)q_2(X_{NN}) + q_2(X)q_1(X_{NN}) \end{aligned}$$

- When an infinite number of samples is available, X_{NN} will be so close to X

$$r_1^*(X) = 2q_1(X)q_2(X) = 2\xi(X)$$

Asymptotic Analysis, cont.



- Recall conditional Bayes risk:

$$\begin{aligned} r^*(X) &= \min[q_1(X), q_2(X)] \\ &= \frac{1}{2} - \frac{1}{2}\sqrt{1 - 4\xi(X)} \\ &= \sum_{i=1}^{\infty} \frac{1}{i} \binom{2i-2}{i-1} \xi^i(X) \quad \text{This is called the MacLaurin series expansion} \end{aligned}$$

- Thus the asymptotic condition risk

$$r_1^*(X) = 2\xi(X) \leq 2r^*(X)$$

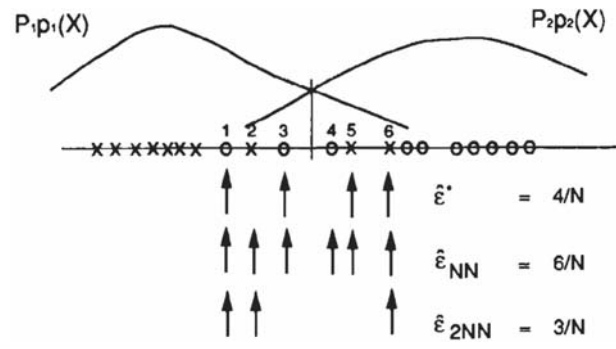
- It can be shown that $\epsilon_1^* \leq 2\epsilon^*$
 - This is remarkable, considering that the procedure does not use any information about the underlying distributions and only the class of the single nearest neighbor determines the outcome of the decision.

In fact



$$\frac{1}{2}\epsilon^* \leq \epsilon_{2NN}^* \leq \epsilon_{4NN}^* \leq \dots \leq \epsilon^* \leq \dots \leq \epsilon_{3NN}^* \leq \epsilon_{NN}^* \leq 2\epsilon^*$$

- Example:



kNN is an instance of Instance-Based Learning



- What makes an Instance-Based Learner?
 - A distance metric
 - How many nearby neighbors to look at?
 - A weighting function (optional)
 - How to relate to the local points?

Euclidean Distance Metric

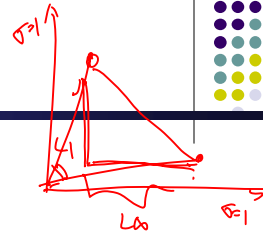
$$D(x, x') = \sqrt{\sum_i \sigma_i^2 (x_i - x'_i)^2}$$

- Or equivalently,

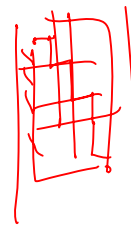
$$D(x, x') = \sqrt{(x - x')^T \Sigma (x - x')}$$

- Other metrics:

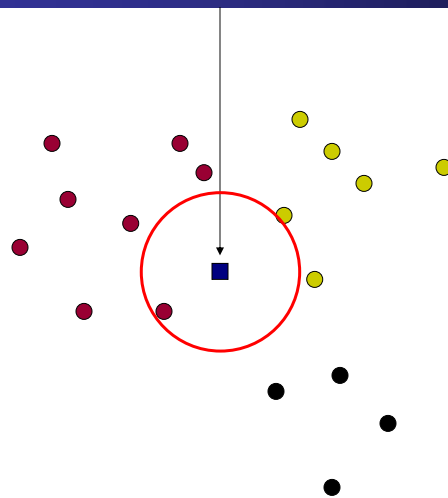
- L_1 norm: $|x - x'|$
- L_∞ norm: $\max |x - x'|$ (elementwise ...)
- Mahalanobis: where Σ is full, and symmetric
- Correlation
- Angle
- Hamming distance, Manhattan distance
- ...



$$\Sigma = \begin{bmatrix} \sigma_1^2 & & \\ & \sigma_2^2 & \\ & & \ddots \end{bmatrix}$$

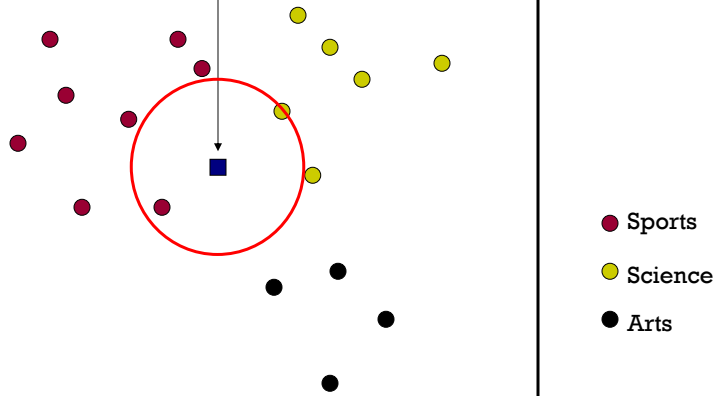


1-Nearest Neighbor (kNN) classifier

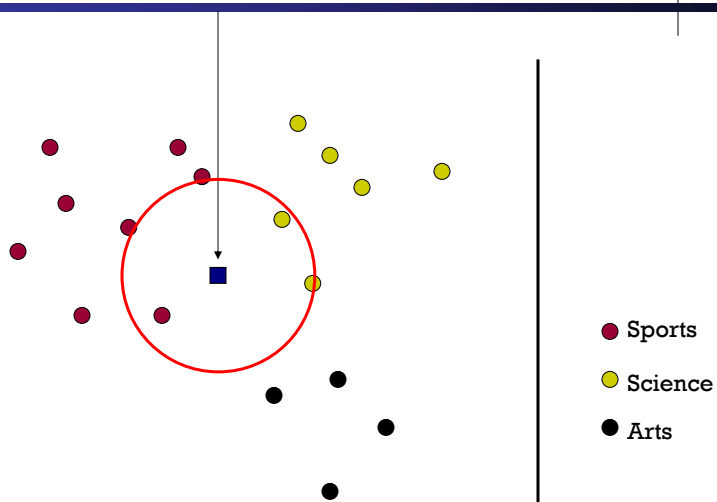


- Sports
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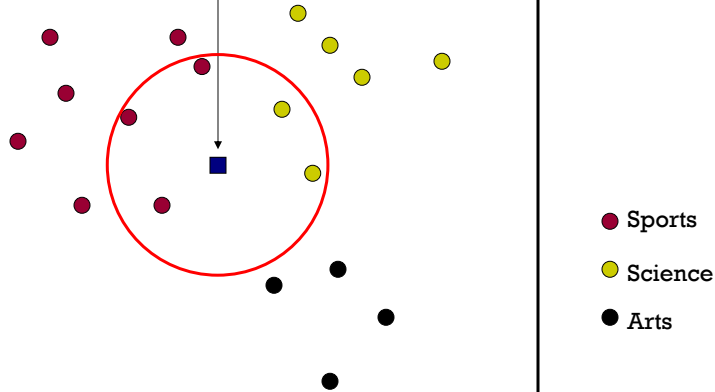
2-Nearest Neighbor (kNN) classifier



3-Nearest Neighbor (kNN) classifier



5-Nearest Neighbor (kNN) classifier



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Nearest-Neighbor Learning Algorithm



- Learning is just storing the representations of the training examples in D .
- Testing instance x :
 - Compute similarity between x and all examples in D .
 - Assign x the category of the most similar example in D .
- Does not explicitly compute a generalization or category prototypes.
- Also called:
 - Case-based learning
 - Memory-based learning
 - Lazy learning

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Case Study: kNN for Web Classification



- Dataset
 - 20 News Groups (20 classes)
 - Download : (<http://people.csail.mit.edu/jrennie/20Newsgroups/>)
 - 61,118 words, 18,774 documents
 - Class labels descriptions

comp.graphics comp.os.ms-windows.misc comp.sys.ibm.pc.hardware comp.sys.mac.hardware comp.windows.x	rec.autos rec.motorcycles rec.sport.baseball rec.sport.hockey	sci.crypt sci.electronics sci.med sci.space
misc.forsale	talk.politics.misc talk.politics.guns talk.politics.mideast	talk.religion.misc alt.atheism soc.religion.christian

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Experimental Setup



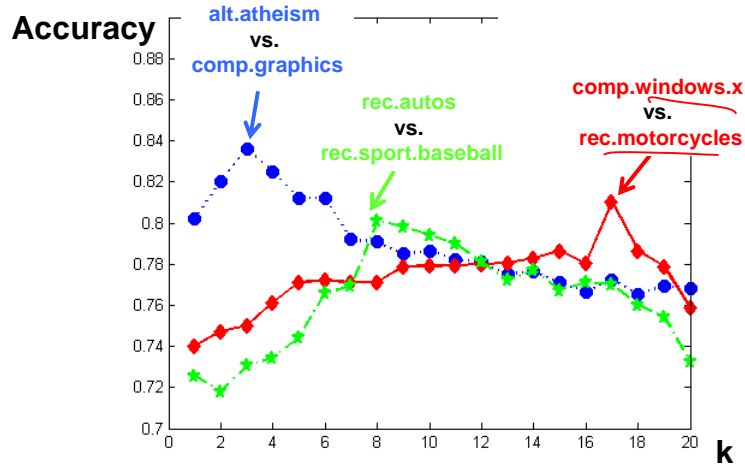
- Training/Test Sets:
 - 50%-50% randomly split.
 - 10 runs
 - report average results
- Evaluation Criteria:

$$Accuracy = \frac{\sum_{i \in \text{test set}} I(\text{predict}_i = \text{true label}_i)}{\# \text{ of test samples}}$$

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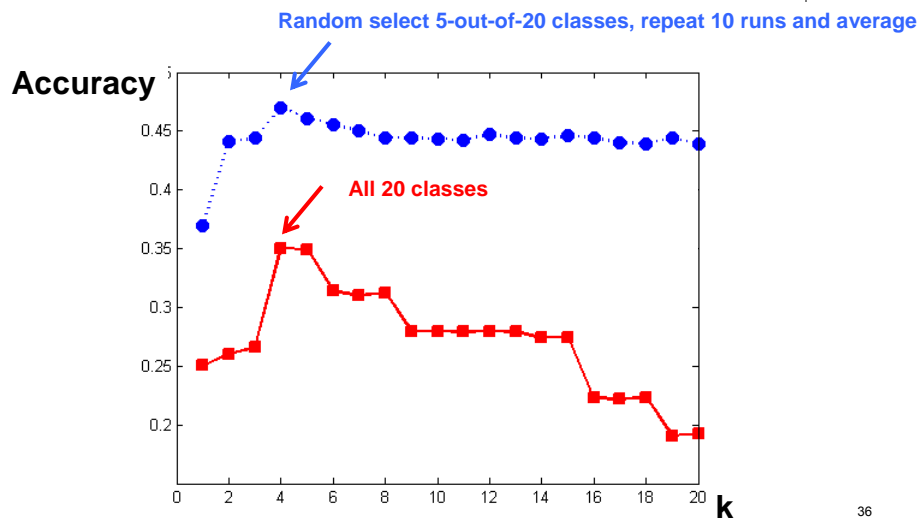
Results: Binary Classes



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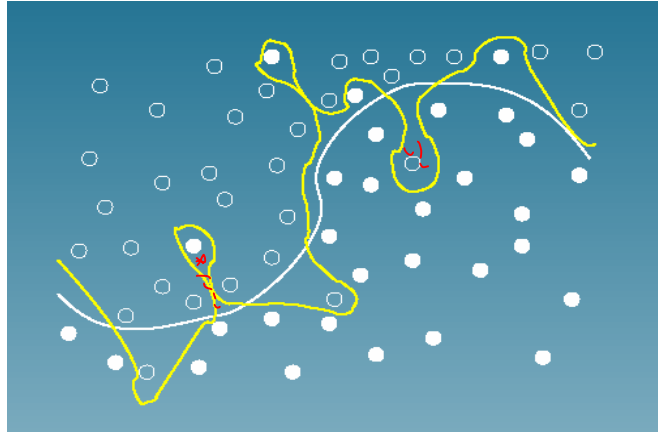
Results: Multiple Classes



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Is kNN ideal? ... more later



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Effect of Parameters

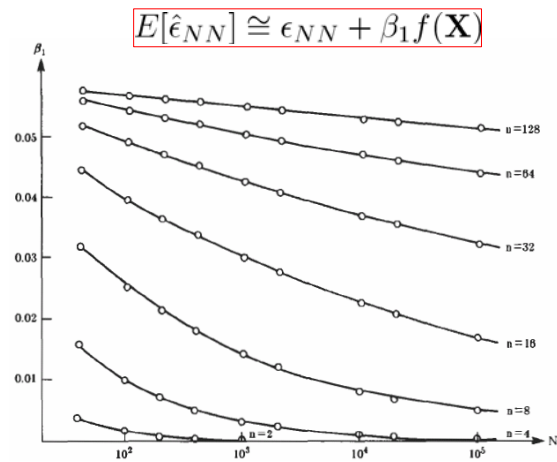


- Sample size
 - The more the better
 - Need efficient search algorithm for NN
- Dimensionality
 - Curse of dimensionality
- Density
 - How smooth?
- Metric
 - The relative scalings in the distance metric affect region shapes.
- Weight
 - Spurious or less relevant points need to be downweighted
- K

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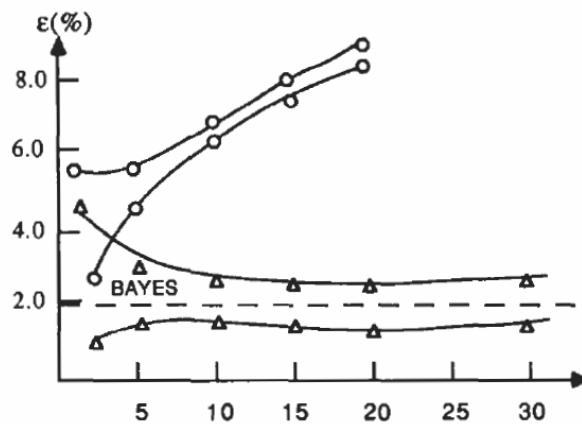
Sample size and dimensionality



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From page 316, Fukumaga

Neighborhood size



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From page 350, Fukumaga

Summary



- **Bayes classifier** is the best classifier which minimizes the probability of classification error.
- Nonparametric and parametric classifier
- A nonparametric classifier does not rely on any assumption concerning the structure of the underlying density function.
- A classifier becomes the **Bayes classifier** if the density estimates converge to the true densities
 - when an infinite number of samples are used
 - The resulting error is the **Bayes error**, the smallest achievable error given the underlying distributions.