Machine Learning
10-701/15-781, Spring 2010

Theory of Classification and Nonparametric Classifier

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Reading: Chap. 2, 5 CB and handouts

Classification

- Representing data:

- Hypothesis (classifier)
Outline

- What is theoretically the best classifier
  - Probabilistic theory of classification
  - Discrete 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 machine
Continuous Distributions

- Uniform Probability Density Function
  \[ p(x) = \begin{cases} \frac{1}{b-a} & \text{for } a \leq x \leq b \\ 0 & \text{elsewhere} \end{cases} \]

- 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, \( \mu \) (mean) and \( \sigma \) (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
  \[
p(X; \mu, \Sigma) = \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp \left( -\frac{1}{2} (X - \mu)^T \Sigma^{-1} (X - \mu) \right)
\]

Class-Conditional Probability

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

  \[
p(X | Y = 1) = p_1(X; \mu_1, \Sigma_1)
  \]

  \[
p(X | Y = 2) = p_2(X; \mu_2, \Sigma_2)
  \]

- Class prior (i.e., "weight"): \( P(Y) \)
The Bayes Rule

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

\[ P(Y \mid X) = \frac{p(X \mid Y)p(Y)}{p(X)} \]

This is Bayes Rule


The Bayes Decision Rule for Minimum Error

- The a posteriori probability of a sample

\[ P(Y = i \mid X) = \frac{p(X \mid Y = i)p(Y = i)}{p(X)} = \frac{\pi_i p_i(X)}{\sum \pi_i p_i(X)} = q_i(X) \]

- Bayes Test:

- Likelihood Ratio:

\[ \ell(X) = \]

- Discriminant function:

\[ h(X) = \]
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?

$$\epsilon = \min\{q_1(X), q_2(X)\}$$

- The Bayes error (the expected risk):

$$\epsilon = E[r(X)] = \int r(x)p(x)dx$$

$$= \int \min[p_1(x), p_2(x)]dx$$

$$= \pi_1 \int_{L_1} p_1(x)dx + \pi_2 \int_{L_2} p_2(x)dx$$

$$= \pi_1 \epsilon_1 + \pi_2 \epsilon_2$$
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:
    \[
    c_1 = \int_{\ln(\pi_1/\pi_2)}^{+\infty} p_1(x)dx \\
    c_2 = \int_{-\infty}^{\ln(\pi_2/\pi_1)} p_2(x)dx
    \]

Learning Classifier

- The decision rule:
  \[
  h(X) = -\ln p_1(X) + \ln p_2(X) > \ln \frac{\pi_1}{\pi_2}
  \]

- 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
K-Nearest Neighbor (kNN) classifier

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

Where does kNN come from?

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

- Bayes classifier based on kNN density estimator:
  
  $$\begin{align*}
  h(X) &= -\ln p_1(X) - \ln (k_1 - 1)N_2V_2(X) > \ln \pi_1 \\
  p_2(X) &= -\ln (k_2 - 1)N_1V_1(X) < \ln \pi_2
  \end{align*}$$

- Voting kNN classifier

  Pick $K_1$ and $K_2$ implicitly by picking $K_1 + K_2 = K$, $V_1 = V_2$, $N_1 = N_2$
Voting kNN

- The procedure

Asymptotic Analysis

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

- Assuming \( k = 1 \)

\[
\begin{align*}
    r_1(X, X_{NN}) &= P_r \left\{ \left[ X \rightarrow 1 \right] \cup \left[ X \rightarrow 2 \right] \right\} \cup \left\{ X \rightarrow 1 \right\} \mid X_{NN} \\
    &= P_r \left\{ \left[ X \rightarrow 1 \right] \cup \left[ X \rightarrow 2 \right] \right\} \cdot P_r \left\{ \left[ X \rightarrow 1 \right] \mid X_{NN} \right\} \\
    &= q_1(X)q_2(X_{NN}) + q_2(X)q_1(X_{NN})
\end{align*}
\]

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

\[
r_k^*(X) = 2q_1(X)q_2(X) = 2\zeta(X)
\]
Asymptotic Analysis, cont.

- Recall conditional Bayes risk:
  \[ r^*(X) = \min[q_1(X), q_2(X)] \]
  \[ = \frac{1}{2} - \frac{1}{2} \sqrt{1 - 4\xi(X)} \]
  \[ = \sum_{i=1}^{\infty} \frac{j}{i(i-1)} \epsilon(X) \]

  This is called the MacLaurin series expansion

- 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

\[ \frac{1}{2} \epsilon^* \leq \epsilon^*_{2NN} \leq \epsilon^*_{4NN} \leq \ldots \leq \epsilon^* \leq \ldots \leq \epsilon^*_{3NN} \leq \epsilon^*_{NN} \leq 2\epsilon^* \]

- 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
  - …
1-Nearest Neighbor (kNN) classifier

2-Nearest Neighbor (kNN) classifier
3-Nearest Neighbor (kNN) classifier

5-Nearest Neighbor (kNN) classifier
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

Case Study: kNN for Web Classification

- Dataset
  - 20 News Groups (20 classes)
  - 61,118 words, 18,774 documents
  - Class labels descriptions

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<tr>
<th>comp.graphics</th>
<th>rec.autos</th>
<th>sci.crypt</th>
</tr>
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<tbody>
<tr>
<td>comp.os.ms-windows</td>
<td>rec.motorcycles</td>
<td>sci.electronics</td>
</tr>
<tr>
<td>misc</td>
<td>rec.sport.baseball</td>
<td>sci.med</td>
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<td>comp.sys.mac.hardware</td>
<td>rec.sport.hockey</td>
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<tbody>
<tr>
<td>talk.politics.misc</td>
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<tr>
<td>talk.politics.guns</td>
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<tr>
<td>talk.politics.mideast</td>
</tr>
<tr>
<td>talk.religion.misc</td>
</tr>
<tr>
<td>alt.atheism</td>
</tr>
<tr>
<td>soc.religion.christian</td>
</tr>
</tbody>
</table>
Experimental Setup

- **Training/Test Sets:**
  - 50%-50% randomly split.
  - 10 runs
  - report average results
- **Evaluation Criteria:**
  \[
  \text{Accuracy} = \frac{\sum \mathbb{1}(\text{predict}_i = \text{true label}_i)}{\# \text{ of test samples}}
  \]

Results: Binary Classes

<table>
<thead>
<tr>
<th>Class Pair</th>
<th>Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>alt.atheism vs. comp.graphics</td>
<td></td>
</tr>
<tr>
<td>rec.autos vs. rec.sport.baseball</td>
<td></td>
</tr>
<tr>
<td>comp.windows.x vs. rec.motorcycles</td>
<td></td>
</tr>
</tbody>
</table>
Results: Multiple Classes

Random select 5-out-of-20 classes, repeat 10 runs and average

Accuracy

All 20 classes

Is kNN ideal? … more later
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

Sample size and dimensionality

\[
E[\epsilon_{NN}] \cong \epsilon_{NN} + \beta_1 f(X)
\]

From page 316, Fukumaga
Neighborhood size

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.