Pattern Recognition

K-Nearest Neighbor Linear Discriminant Functions

k-Nearest Neighbors Classifier

• The k_n nearest neighbor (KNN) density estimate is given by:

$$p_n(\mathbf{x}) = \frac{k_n}{nV_n},$$

• V_n is the volume of the smallest possible x centered cell that contains k_n training samples, and n is the total number of training samples

K-Nearest Neighbor Example



Disadvantages

- The distance to all sample points should be computed at each classification. This computation can be very time consuming
- The accuracy of the *k*-NN algorithm can be severely degraded by the presence of noisy or irrelevant features.

Optimizing K Parameter

• 1-NNR versus k-NNR

- The use of large values of k has two main advantages
 - Yields smoother decision regions
 - Provides probabilistic information; The ratio of examples for each class gives information about the ambiguity of the decision
- However, too large values of k are harmful; They destroy the locality of the estimation since farther examples are taken into account
- In addition, it increases the computational burden

Example

1-NNR

5-NNR

п

05

0.5

.0.5

-0.5

20-NNR





0 ×,

Distance Metrics

Requirements for a distance metric:

- 1. $L(a, b) \ge 0$
- 2. L(a, b) = 0 if and only if a = b.
- 3. L(a, b) = L(b, a)
- 4. $L(a, b) + L(b, c) \ge L(a, c)$.

Sample Distance Metrics

- Euclidean metric
- Minkowski metrics

$$L(\mathbf{a}, \mathbf{b}) = ||\mathbf{a} - \mathbf{b}|| = \sqrt{\sum_{i=1}^{d} (a_i - b_i)^2}.$$
$$L_m(\mathbf{a}, \mathbf{b}) = (\sum_{i=1}^{d} (|a_i - b_i|^m)^{1/m}.$$

• L-infinity metric

$$L_{\infty}(\mathbf{a},\mathbf{b}) = \max_{i} |a_i - b_i|.$$

• Mahalanobis-distance

$$L_{Mahalanobis,C}(\mathbf{a},\mathbf{b}) = \sqrt{(\mathbf{a}-\mathbf{b})^T C^{-1}(\mathbf{a}-\mathbf{b})}$$

Improving KNN Classifier

- Classify all the examples in the training set and remove those examples that are misclassified, in an attempt to separate classification regions by removing ambiguous points
- The opposite alternative is to remove training examples that are classified correctly, in an attempt to define the boundaries between classes by eliminating points in the interior of the regions
- A different alternative is to reduce the training examples to a set of prototypes that are representative of the underlying data.
- [The issue of selecting prototypes will be the subject of the lectures on clustering]

Example



Improving KNN Search Algorithm

Bucketing

- In the Bucketing algorithm, the space is divided into identical cells and for each cell the data points inside it are stored in a list.
- The cells are examined in order of increasing distance from the query point and for each cell the distance is computed between its internal data points and the query point
- The search terminates when the distance from the query point to the cell exceeds the distance to the closest point already visited

Improving KNN Search Algorithm

k-d trees

- A k-d tree is a generalization of a binary search tree in high dimensions. Each internal node in a k-d tree is associated with a hyper-rectangle and a hyper-plane orthogonal to one of the coordinate axis
- The hyper-plane splits the hyper-rectangle into two parts, which are associated with the child nodes
- The partitioning process goes on until the number of data points in the hyperrectangle falls below some given threshold
- The effect of a k-d tree is to partition the (multi-dimensional) sample space according to the underlying distribution of the data, the partitioning being finer in regions where the density of pints is higher
- For a given query point, the algorithm works by first descending the tree to find the data points lying in the cell that contains the query point
- Then it examines surrounding cells if they overlap the ball centered at the query point and the closest data point so far

K-d Tree Example









Discriminant Function

• For each class, there exists a discriminant function g_i , i = 1, ..., cwhose input is a feature vector x. The sample identified by the feature vector x is assigned to ω_i if

 $g_i(\mathbf{x}) > g_j(\mathbf{x})$ for all j = 1, . . . , c and i \neq j

Linear Classifiers

• A discriminant function is said to be linear if it can written as:

$$g_i(\mathbf{x}) = \mathbf{w}_i^T \mathbf{x} + w_{i0} = \sum_{j=1}^d w_{ij} x_j + w_{i0},$$

where $w_i = [w_{i1}, \ldots, w_{id}]^T$ is the weight vector and the scalar w_{i0} is threshold weight

The classifier relying only on the linear discriminant functions is called linear classifier

Example: Linear Classifier



Linearly Separable Training Samples If there exists a linear classifier that classifies all the training samples correctly, i.e.

$$\begin{split} g(\mathbf{x}_{1j}) &> 0, \quad \text{ for all } j = 1, \dots, n_1 \text{ and} \\ g(\mathbf{x}_{2j}) &< 0 \quad \text{ for all } j = 1, \dots, n_2 \end{split}$$

Then we say that the training sets/samples D_1 and D_2 are linearly separable.

Linearly Inseparable Sets (Example)



Non-Linear Classification (Example 2)





Non-Linear Classification (Example 1)





- Problem definition: Classification based on thresholding in feature space cannot separate classes in many cases.
- Instead on mapping feature values on the feature vector axes, a different line can be used (Linear classification is assumed)









• Fisher Linear Classifier tries to maximize between class scatter, and minimize within class scatter.

• where
$$J(\mathbf{w}) = \frac{\mathbf{w}^T S_B \mathbf{w}}{\mathbf{w}^T S_W \mathbf{w}}$$

$$S_B = \sum_{c} (\boldsymbol{\mu}_c - \bar{\mathbf{x}}) (\boldsymbol{\mu}_c - \bar{\mathbf{x}})^T$$
$$S_W = \sum_{c} \sum_{i \in c} (\mathbf{x}_i - \boldsymbol{\mu}_c) (\mathbf{x}_i - \boldsymbol{\mu}_c)^T$$

• W is obtained from

$$w^* = \arg \max \left[\frac{w^T S_B w}{w^T S_W w} \right] = S_W^{-1} (\mu_1 - \mu_2)$$

Example $X1 = \{(4,1), (2,4), (2,3), (3,6), (4,4)\}$ $X2 = \{(9,10), (6,8), (9,5), (8,7), (10,8)\}$ $S_1 = \begin{bmatrix} .8 & -.4 \\ & 2.64 \end{bmatrix}$ $S_2 = \begin{bmatrix} 1.84 & -.04 \\ & 2.64 \end{bmatrix}$ $\mu_1 = [3.0 \ 3.6]^T; \ \mu_2 = [8.4 \ 7.6]^T$ $S_B = \begin{bmatrix} 29.16 & 21.6 \\ 16.0 \end{bmatrix} \quad S_W = \begin{bmatrix} 2.64 & -.44 \\ 5.28 \end{bmatrix}$

$$w^* = S_W^{-1}(\mu_1 - \mu_2) = [-.91 - .39]^T$$

Reducing Feature Space Dimension

- Feature selection methods find a subset of the original features or attributes.
- In some cases, data analysis can be done in the reduced space more accurately than in the original space.
- Curse of dimensionality reduces the accuracy of the classifier
- Dimension reduction can be done once.
- Adaptive dimension reduction combines unsupervised learning with dimension reduction adaptively.

Questions?