6. Nonparametric techniques
Motivation

Problem: how to decide on a suitable model (e.g. which type of Gaussian)

Idea: just use the original data (lazy learning)
Idea 1: Each data point represents a piece of probability

\[ P(x) \]

\[ x_2 \quad x_1 \quad x_3 \]

A Parzen Window Method
Idea 2:
ignore probabilities
just measure distance to training data

- Consider two class problem

k-nearest neighbor classifier
Idea 2:
ignoring probabilities
just measure distance to training data

- Consider two class problem

k-nearest neighbor classifier
6.1. Density Estimation
Goal

- Determine probability density $P(\bar{x})$
- Given: training data $\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n$
- Consider region $\mathbb{R}$
Estimate probability $P$ inside a region

- Probability of $x$ being in $R$

$$P = \int_{R} P(\vec{x})d\vec{x}$$

- Suppose $k$ training vectors are inside $R$ from a total of $n$ training vectors

$$P \approx \frac{k}{n}$$

What’s an estimate for $P$?
Limit of infinite number of training samples

Consider \( n \to \infty \)

Sequences \( V_n \) (volume of region) and \( k_n \)

Resulting sequence of probabilities:

\[
P_n(x) = \frac{k_n}{nV_n}
\]
Expanding Number of Samples/Shrinking Volume in $k$-Nearest-Neighbour Estimation

$$k_n = \sqrt{n}$$

From: Duda+Hart: Pattern Classification
Necessary conditions for convergence

Convergence means $P_n(x) \to P(x)$ for $n \to \infty$

$P(x)$ is local property: $V_n \to 0$ for $n \to \infty$

Reliability of estimate: $k_n \to \infty$ for $n \to \infty$

$\frac{k_n}{n} \to 0$ for $n \to \infty$: otherwise volume cannot shrink to zero
Possible choice for $k_n$

$$k_n = \sqrt{n}$$

and pick $V_n$ such that is include exactly $k_n$ samples
Expanding Number of Samples/Shrinking Volume in k-Nearest-Neighbour Estimation

\[ k_n = \sqrt{n} \]

From: Duda+Hart: Pattern Classification
6.2. Parzen Windows
Introduction

• Each piece of training contributes it’s own bit of probability distribution

• Possible choice:
  • Cubes
  • Sphere
  • Normal distribution

For the beginning start with cubes
Volume of d-dimensional cubes

- Length of edge $h_n$
- Volume of cube

$$V_n = h_n^d$$

$d$: dimension of features space

"Home work": volume of a d-dimensional sphere?
Introduce Window Function

- Goal: generalize and formalize method

\[ \varphi(\bar{x}) = \begin{cases} 
1 & \text{if } |x^j| \leq \frac{1}{2} \text{ for all } j = 1...d \\
0 & \text{else}
\end{cases} \]

\( x^j \) : j-th component of \( \bar{x} \)

Unit cube centered at origin

Draw a unit cube for \( d=1 \) and \( d=2 \)
Shift and scale the unit cube

What is the window function for a cube centered at \( \vec{x}_i \) with length of edge \( h_n \) ???

\[ \varphi(\frac{\vec{x} - \vec{x}_i}{h_n}) \]
Number of Samples at a point inside the volume $V_n$

Express number of data points $\tilde{x}_i$ that contribute in terms of window functions

$$\varphi\left(\frac{\tilde{x} - \tilde{x}_i}{h_n}\right)$$

If $\varphi\left(\frac{\tilde{x} - \tilde{x}_i}{h_n}\right) = 1$ then $\tilde{x}_i$ is in the volume $V_n$ and hence contributes to $k_n$

$$k_n = \sum_{i=1}^{n} \varphi\left(\frac{\tilde{x} - \tilde{x}_i}{h_n}\right)$$
Estimate of probability using section 6.1

\[ P_n(x) = \frac{k_n}{nV_n} \]

\[ \sum_{i=1}^{n} \phi\left(\frac{x - x_i}{h_n}\right) = \frac{1}{nV_n} \sum_{i=1}^{n} \phi\left(\frac{x - x_i}{h_n}\right) \]

This formula also works for other window functions
Other Window Functions

- Normal (Gaussian) distribution (covariance matrix is unit matrix)

\[ \phi(\bar{x}) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2} \bar{x}' \cdot \bar{x}} \]

- Sphere

\[ \phi(\bar{x}) = \begin{cases} 
1 & \text{if } |\bar{x}| \leq 1 \\
0 & \text{else}
\end{cases} \]
Gaussian Parzen Window 1 d

\[ h_n = \frac{h_1}{\sqrt{n}} \]
Gaussian Parzen Window 2 d
Gaussian Parzen Window 2 d

Converges for all $h_n$
Gaussian Parzen Window 1 d

- $h_i = 1$
- $n = 1$
- $h_i = 0.5$
- $n = 16$
- $h_i = 0.2$
- $n = 256$
- $n = \infty$
In classifiers based on Parzen-window estimation:

- Estimate probability density using a given window
- Pick suitable $h_n$
- Classify using Bayes decision rule
Classification example

Small $h_n$

Large $h_n$
6.3. $k_n$-nearest Neighbor Estimation
Basic idea

Find k most similar cases to test sample x and claim that x is like majority of these cases.
Other names for similar/related methods

- Instance-Based Methods (IBM), or Instance Based Learning (IBL)
- Memory-Based Methods (MBM),
- Case-Based Methods (CBM),
- Case-Based Reasoning (CBR),
- Memory-Based Reasoning (MBR),
- Similarity-Based Reasoning (SBR),
- Similarity-Based Methods (SBM)
Estimate probability in nearest neighbor case

$x_1, x_2, x_3$: training data
$x$: point where we want probability $P(x)$

$V = 2|x - x_2|$

$P(x) = \frac{1}{2 |x - x_2|}$
kNN-Estimation in 1 Dimension

From: Duda+Hart: Pattern Classification
Estimating the Posterior $P(\omega_i|x)$

$V$ : volume under consideration

$k$ : total number of samples in $V$

$k_i$ : number of samples of class $\omega_i$ in $V$

$$k = \sum_{i=1}^{c} k_i$$

$$P_n(x, \omega_i) = \frac{k_i}{nV}$$

$$P_n(x) = \sum_{i=1}^{c} P_n(x, \omega_i) = \sum_{i=1}^{c} \frac{k_i}{nV} = \frac{k}{nV}$$

$$P_n(\omega_i | x) = \frac{P_n(x, \omega_i)}{P_n(x)} = \frac{\frac{k_i}{nV}}{\frac{k}{nV}} = \frac{k_i}{k}$$

$$P_n(\omega_i | x) = \frac{k_i}{k}$$
6.4. Nearest-Neighbor Rule
Voroni-Tessellation

- See white board
Voronoi Cells in 2 Dimensions

From: Duda+Hart: Pattern Classification
Decision Boundary for a nearest-neighbour classifier in a Simulation (Probability Distribution given)

From: Hastie et al.: Statistical Learning
Voronoi Cells in 3 Dimensions

From: Duda+Hart: Pattern Classification
6.5. Error of Nearest Neighbor Rule
Error of Nearest-Neighbour-Classifier (NN)

NN-Classifier:
- Can be as good as Bayes
- In worst case twice as bad

From: Duda+Hart: Pattern Classification
k-Nearest-Neighbour-Classifier

From: Duda+Hart: Pattern Classification
Error of k-Nearest-Neighbour-Classifier

From: Duda+Hart: Pattern Classification
Missclassification vs. Number of Neighbours

From: Hastie et al.: Statistical Learning
Decision Boundary for a nearest-neighbour classifier in a Simulation (Probability Distribution given)

From: Hastie et al.: Statistical Learning
Decision Boundary for a $k$-nearest-neighbour classifier in a Simulation (Probability Distribution given)

From: Hastie et al.: Statistical Learning

$k=15$
Decision Boundaries of Bayes Classifier for the known Probabilities

From: Hastie et al.: Statistical Learning
Other Popular distance functions

$L_\alpha$ distance from 0:

$$D(X, 0)^\alpha = \sum_{i=1}^{d} |X_i|^\alpha$$

Manhattan distance or $L_1$ norm:

$$D(X, Y) = \sum_{i=1}^{d} |X_i - Y_i|$$

Euclidean distance or $L_2$ norm:

$$D(X, Y)^2 = \sum_{i=1}^{d} |X_i - Y_i|^2$$
Summary

• k-Nearest Neighbour classifier
• Voronoi tessellation