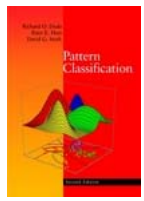
Chapter 4 (Part 1): Non-Parametric Classification

- Introduction
- Density Estimation
- Parzen Windows



Introduction

- All Parametric densities are unimodal (have a single local maximum), whereas many practical problems involve multi-modal densities
- Nonparametric procedures can be used with arbitrary distributions and without the assumption that the forms of the underlying densities are known
- There are two types of nonparametric methods:
  - Estimating $P(x \mid \omega_j)$
  - Bypass probability and go directly to a-posteriori probability estimation

Density Estimation

- **Basic idea:**

  Probability that a vector x will fall in region R is:

$$P = \int_{\Re} p(x')dx' \qquad (1)$$

  P is a smoothed (or averaged) version of the density function p(x) if we have a sample of size n; therefore, the probability that k points fall in R is then:

$$P_k = \binom{n}{k} P^k (1-P)^{n-k} \qquad (2)$$

  and the expected value for k is:

$$E(k) = nP \qquad (3)$$

ML estimation of $P = \theta$

$\mathbf{Max}_{\theta}(P_k \mid \theta)$ is reached for $\hat{\theta} = \frac{k}{n} \cong P$

Therefore, the ratio k/n is a good estimate for the probability P and hence for the density function p.

p(x) is continuous and that the region R is so small that p does not vary significantly within it, we can write:

$$\int_{\Re} p(x')dx' \cong p(x)V \qquad (4)$$

where is a point within R and V the volume enclosed by R.

Combining equation (1) , (3) and (4) yields: $p(x) \cong \frac{k/n}{V}$

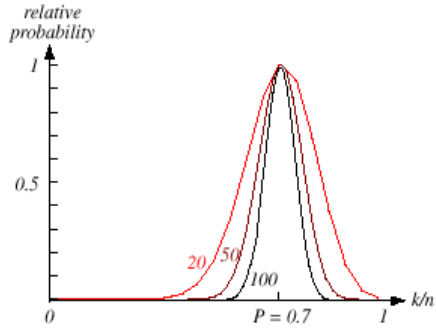


FIGURE 4.1. The relative probability an estimate given by Eq. 4 will yield a particular value for the probability density, here where the true probability was chosen to be 0.7. Each curve is labeled by the total number of patterns n sampled, and is scaled to give the same maximum (at the true probability). The form of each curve is binomial, as given by Eq. 2. For large n, such binomials peak strongly at the true probability. In the limit $n \to \infty$, the curve approaches a delta function, and we are guaranteed that our estimate will give the true probability. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

- Density Estimation (cont'd)
  - Justification of equation (4)

$$\int_{\Re} p(x')dx' \cong p(x)V \qquad (4)$$

We assume that p(x) is continuous and that region R is so small that p does not vary significantly within R. Since p(x) = constant, it is not a part of the sum.

$$\int_{\Re} p(x')dx' = p(x')\int_{\Re} dx' = p(x')\int_{\Re} 1 I_{\Re}(x)dx' = p(x')\mu(\Re)$$

Where: $\mu(R)$ is: a surface in IR^2
a volume in IR^3
a hypervolume in IR^n

Since $p(x) \cong p(x') = \text{constant}$, therefore in IR^3:

$$\int_{\Re} p(x')dx' \cong p(x).V$$

$$\text{and } p(x) \cong \frac{k}{nV}$$

- Condition for convergence

The fraction k/(nV) is a space averaged value of p(x). p(x) is obtained only if V approaches zero.

$$\lim_{V \to 0, k=0} p(x) = 0 \quad (\text{if } n = \text{fixed})$$

This is the case where no samples are included in R: it is an uninteresting case!

$$\lim_{V \to 0, k \neq 0} p(x) = \infty$$

In this case, the estimate diverges: it is an uninteresting case!

The volume V needs to approach 0 anyway if we want to use this estimation

- Practically, V cannot be allowed to become small since the number of samples is always limited
- One will have to accept a certain amount of variance in the ratio k/n
- Theoretically, if an unlimited number of samples is available, we can circumvent this difficulty

  To estimate the density of x, we form a sequence of regions R_1, R_2,…containing x: the first region contains one sample, the second two samples and so on.

  Let V_n be the volume of R_n, k_n the number of samples falling in R_n and $p_n(x)$ be the n^{th} estimate for p(x):

$$p_n(x) = (k_n/n)/V_n \qquad (7)$$

Three necessary conditions should apply if we want $p_n(x)$ to converge to p(x)

$$\textbf{1)} \lim_{n\to\infty} V_n = 0$$

$$\textbf{2)} \lim_{n\to\infty} k_n = \infty$$

$$\textbf{3)} \lim_{n\to\infty} k_n / n = 0$$

There are two different ways of obtaining sequences of regions that satisfy these conditions:

(a) Shrink an initial region where $V_n = 1/\sqrt{n}$ and show that

$$p_n(x) \underset{n\to\infty}{\rightarrow} p(x)$$

This is called "the Parzen-window estimation method"

(b) Specify k_n as some function of n, such as $k_n = \sqrt{n}$; the volume V_n is grown until it encloses k_n neighbors of x. This is called "the k_n-nearest neighbor estimation method"

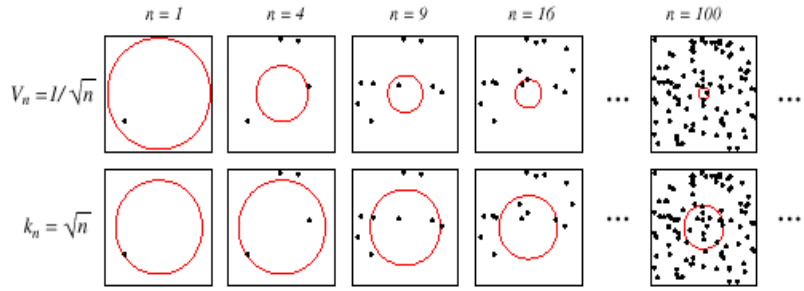


FIGURE 4.2. There are two leading methods for estimating the density at a point, here at the center of each square. The one shown in the top row is to start with a large volume centered on the test point and shrink it according to a function such as $V_n = 1/\sqrt{n}$. The other method, shown in the bottom row, is to decrease the volume in a data-dependent way, for instance letting the volume enclose some number $k_n = \sqrt{n}$ of sample points. The sequences in both cases represent random variables that generally converge and allow the true density at the test point to be calculated. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

Parzen Windows

- Parzen-window approach to estimate densities assume that the region R_n is a d-dimensional hypercube

$$V_n = h_n^d \quad (h_n : \text{length of the edge of } \Re_n)$$

Let $\varphi(u)$ be the following window function :

$$\varphi(u) = \begin{cases} 1 & |u_j| \le \frac{1}{2} \quad j = 1,\ldots,d \\ 0 & \text{otherwise} \end{cases}$$

- $\varphi((x-x_i)/h_n)$ is equal to unity if x_i falls within the hypercube of volume V_n centered at x and equal to zero otherwise.

- The number of samples in this hypercube is:

$$k_n = \sum_{i=1}^{i=n} \varphi\left(\frac{x - x_i}{h_n}\right)$$

By substituting k_n in equation (7), we obtain the following estimate:

$$p_n(x) = \frac{1}{n}\sum_{i=1}^{i=n} \frac{1}{V_n} \varphi\left(\frac{x - x_i}{h_n}\right)$$

$P_n(x)$ estimates $p(x)$ as an average of functions of x and the samples (x_i) $(i = 1,\ldots,n)$. These functions φ can be general!

- Illustration
  - The behavior of the Parzen-window method
    - Case where $p(x) \rightarrow N(0,1)$

      Let $\varphi(u) = (1/\sqrt{(2\pi)}) \exp(-u^2/2)$ and $h_n = h_1/\sqrt{n}$ $(n>1)$

      (h_1: known parameter)

      Thus:

$$p_n(x) = \frac{1}{n}\sum_{i=1}^{i=n} \frac{1}{h_n} \varphi\left(\frac{x - x_i}{h_n}\right)$$

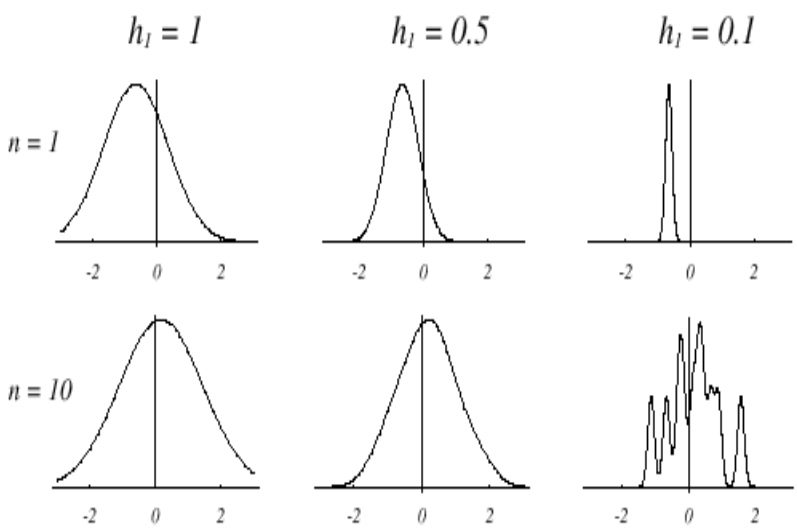
      is an average of normal densities centered at the samples x_i.

– **Numerical results:**

For n = 1 and h_1=1

$$p_1(x) = \varphi(x - x_1) = \frac{1}{\sqrt{2\pi}} e^{-1/2 (x - x_1)^2} \rightarrow N(x_1,1)$$

For n = 10 and h = 0.1, the contributions of the individual samples are clearly observable !



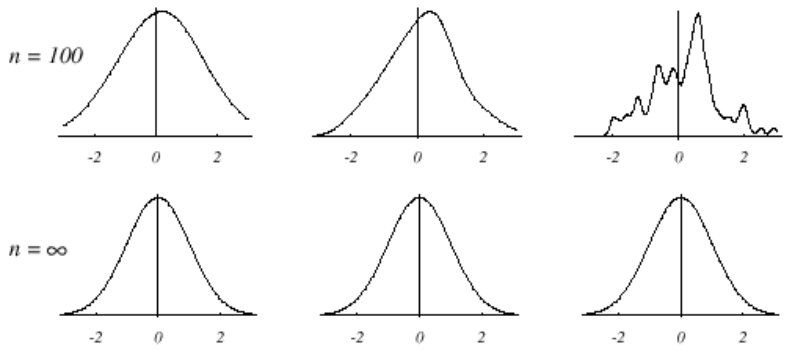
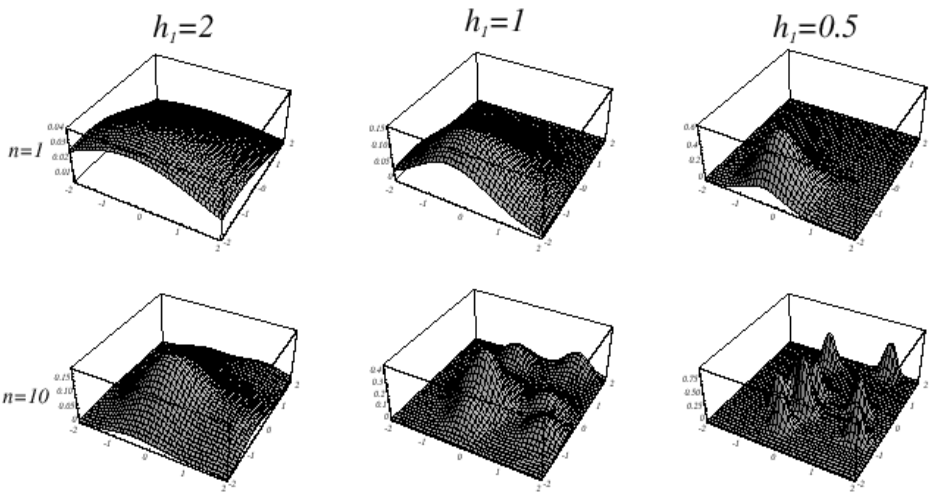


FIGURE 4.5. Parzen-window estimates of a univariate normal density using different window widths and numbers of samples. The vertical axes have been scaled to best show the structure in each graph. Note particularly that the $n = \infty$ estimates are the same (and match the true density function), regardless of window width. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

Analogous results are also obtained in two dimensions as illustrated:



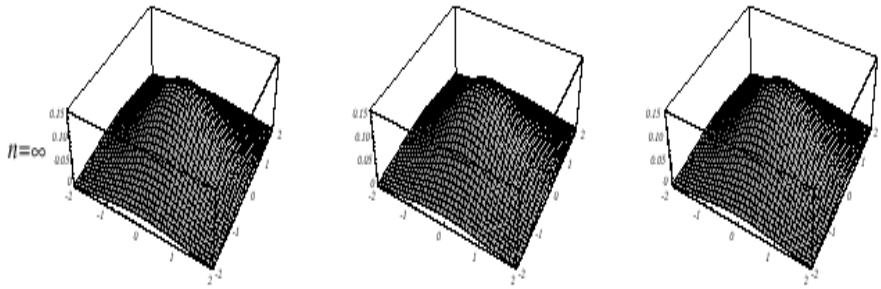
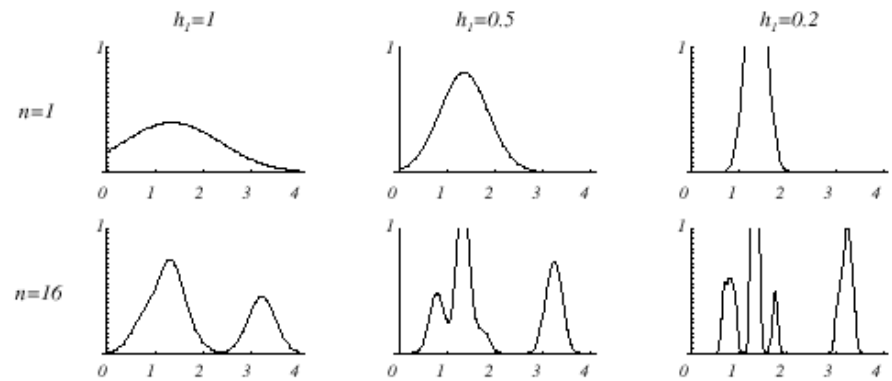


FIGURE 4.6. Parzen-window estimates of a bivariate normal density using different window widths and numbers of samples. The vertical axes have been scaled to best show the structure in each graph. Note particularly that the $n = \infty$ estimates are the same (and match the true distribution), regardless of window width. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

– Case where $p(x) = \lambda_1.U(a,b) + \lambda_2.T(c,d)$ (unknown density) (mixture of a uniform and a triangle density)



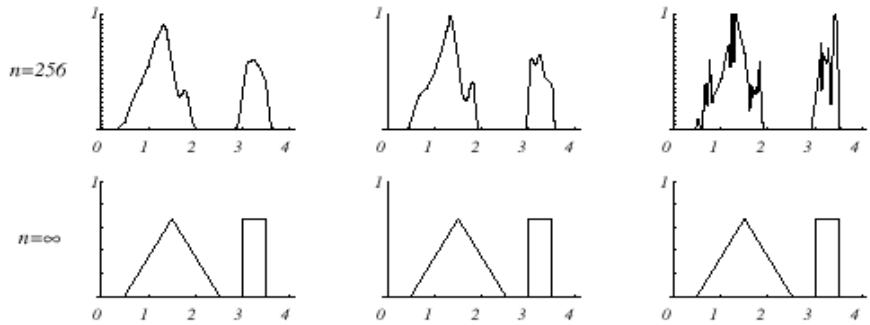


FIGURE 4.7. Parzen-window estimates of a bimodal distribution using different window widths and numbers of samples. Note particularly that the $n = \infty$ estimates are the same (and match the true distribution), regardless of window width. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

- Classification example

  In classifiers based on Parzen-window estimation:

  - We estimate the densities for each category and classify a test point by the label corresponding to the maximum posterior
  - The decision region for a Parzen-window classifier depends upon the choice of window function as illustrated in the following figure.

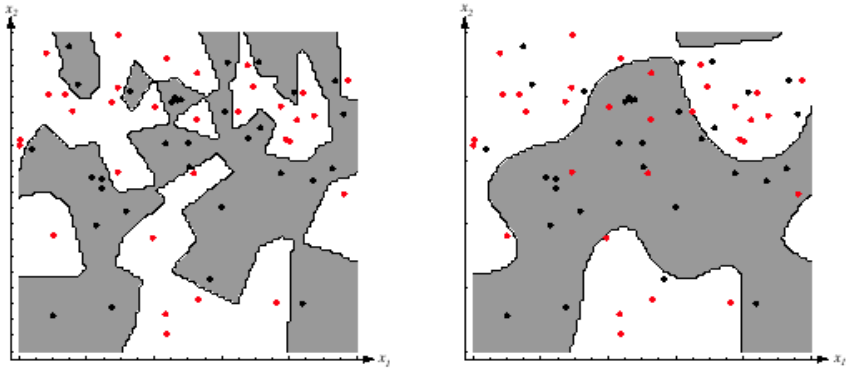


FIGURE 4.8. The decision boundaries in a two-dimensional Parzen-window dichotomizer depend on the window width h. At the left a small h leads to boundaries that are more complicated than for large h on same data set, shown at the right. Apparently, for these data a small h would be appropriate for the upper region, while a large h would be appropriate for the lower region; no single window width is ideal overall. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.