# Non-parametric Density Estimation: Introduction

- Useful parametric densities are limited in the shape they take on-- they may not fit your data well.
- 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 via Binning

– Basic idea:
Probability that a vector x will fall in region $\Re$ is:

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

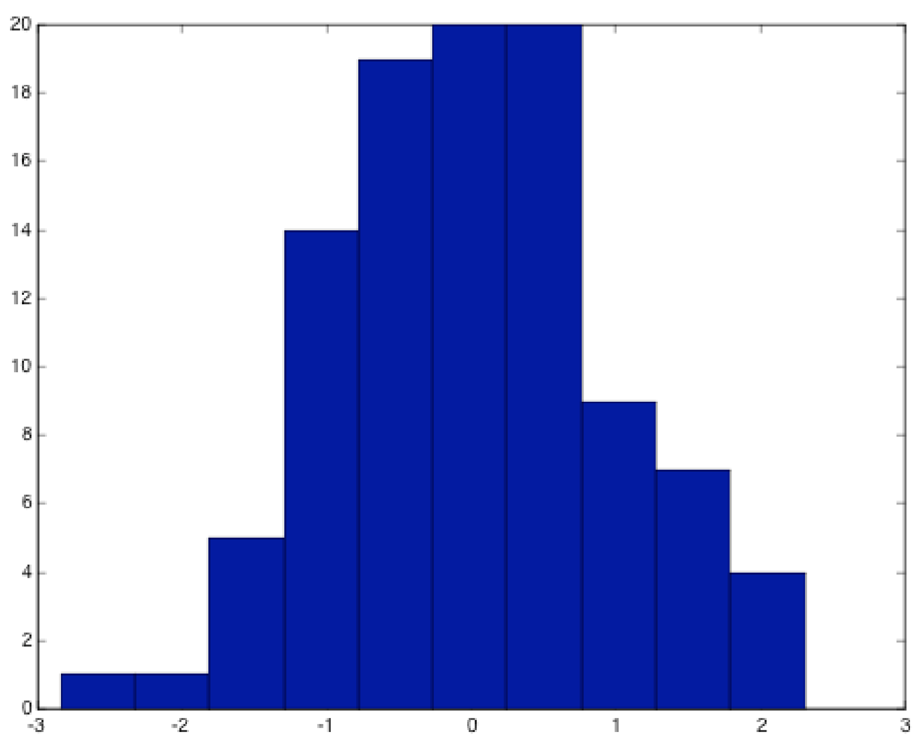
– P is a smoothed (or averaged) version of the density function *p(x)* if we have a sample of size *n*; therefore, the probability that *k* points fall in $\Re$ is then:

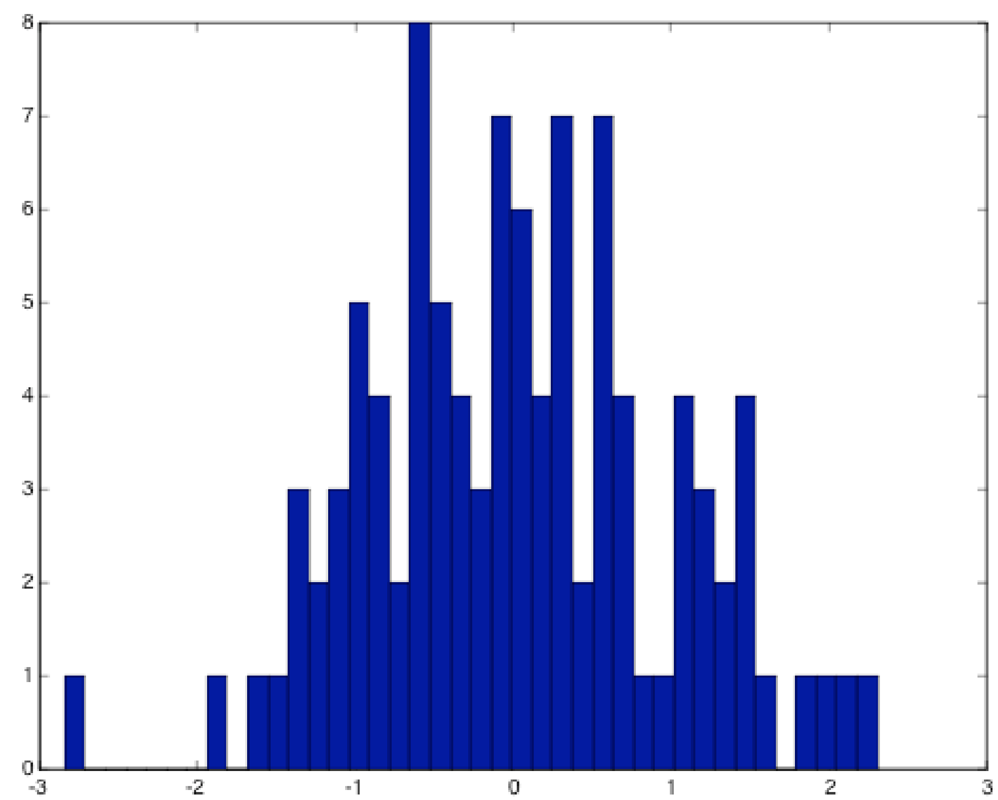
$$P_k = \binom{n}{k} P^k (1-P)^{n-k} \qquad (2)$$

and the expected value for *k* is:

$$\mathbf{E}(k) = nP \qquad (3)$$

# Histogram



ML estimation of $\theta = P$

$\arg\max_{\theta} P_k(\theta)$ is reached for $\hat{\boldsymbol{\theta}} = \dfrac{\boldsymbol{k}}{\boldsymbol{n}} \cong \boldsymbol{P}$

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 $\mathcal{R}$ is so small that p does not vary significantly within it, we can write:

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

Where *x'* is a point within $\mathcal{R}$ and *V* the volume enclosed by $\mathcal{R}$.

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

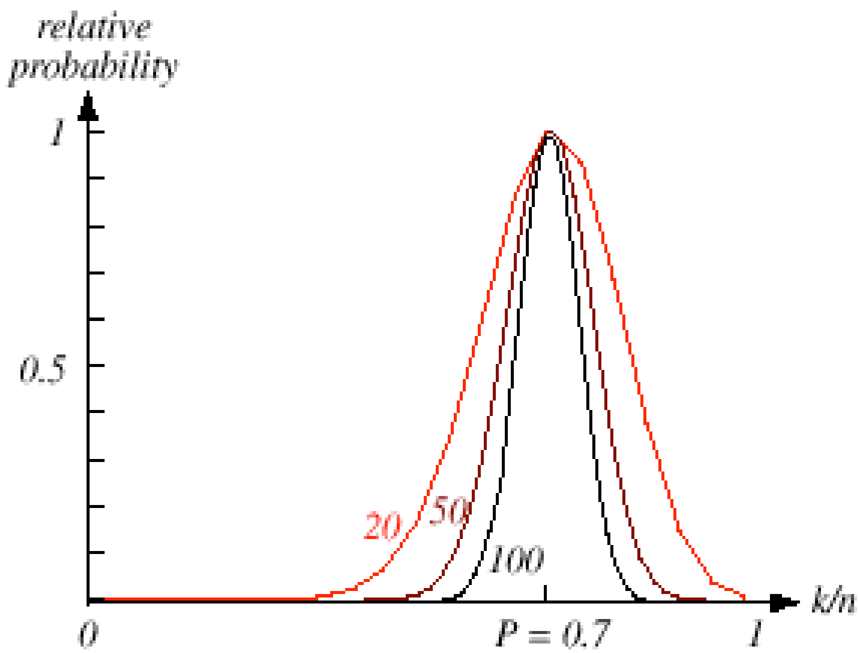



**FIGURE 4.1.** The relative probability an estimate given by Eq. 4 will yield a particular value for the probability density, here where the true probability was chosen to be 0.7. Each curve is labeled by the total number of patterns $n$ sampled, and is scaled to give the same maximum (at the true probability). 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.

$$\int_{\Re} p(x)dx = p(x')\int_{\Re} dx = p(x')\int_{-\infty}^{\infty} 1_{\Re}(x)dx = p(x')\mu(\Re)$$

Where: $\mu(R)$ is: an area in the Euclidean space $R^2$

a volume in the Euclidean space $R^3$

a hypervolume in the Euclidean space $R^n$

Since $p(x) \cong p(x') =$ constant, therefore in the Euclidean space $R^3$:

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

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

– Condition for convergence

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

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

This is the case where no samples are included in $\mathcal{R}$: 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

    $\mathcal{R}_1, \mathcal{R}_2, \ldots$ containing x: the first region contains one sample, the second two samples and so on.

    Let $V_n$ be the volume of $\mathcal{R}_n$, $k_n$ the number of samples falling in $\mathcal{R}_n$ 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 $p(x)$:

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

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

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

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"

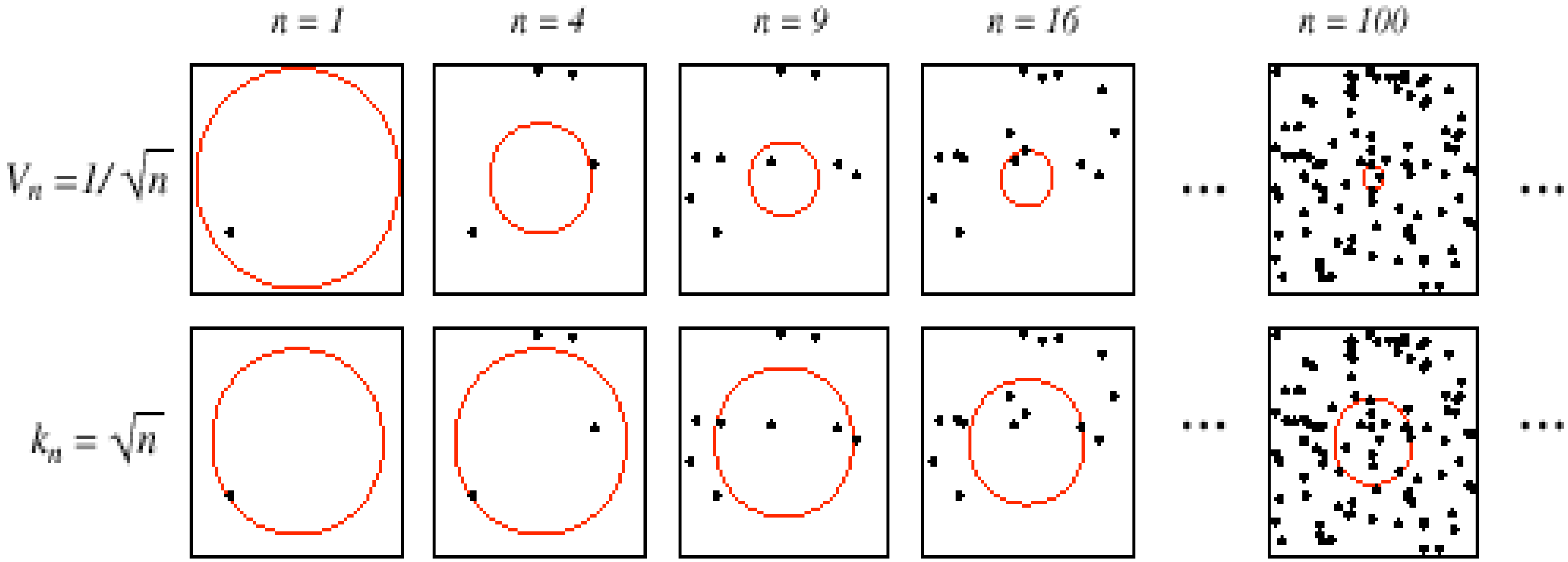



**FIGURE 4.2.** There are two leading methods for estimating the density at a point, here at the center of each square. The one shown in the top row is to start with a large volume centered on the test point and shrink it according to a function such as $V_n = 1/\sqrt{n}$. The other method, shown in 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 $\mathcal{R}_n$ is a d-dimensional hypercube

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

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

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

– $\varphi((x-x_i)/h_n)$ 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:

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

Which yields the probability estimate:

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

$P_n(x)$ estimates $p(x)$ as an average of functions of $x$ and the samples $(x_i)$ $(i = 1, \ldots, n)$. These functions $\varphi$ 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:

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

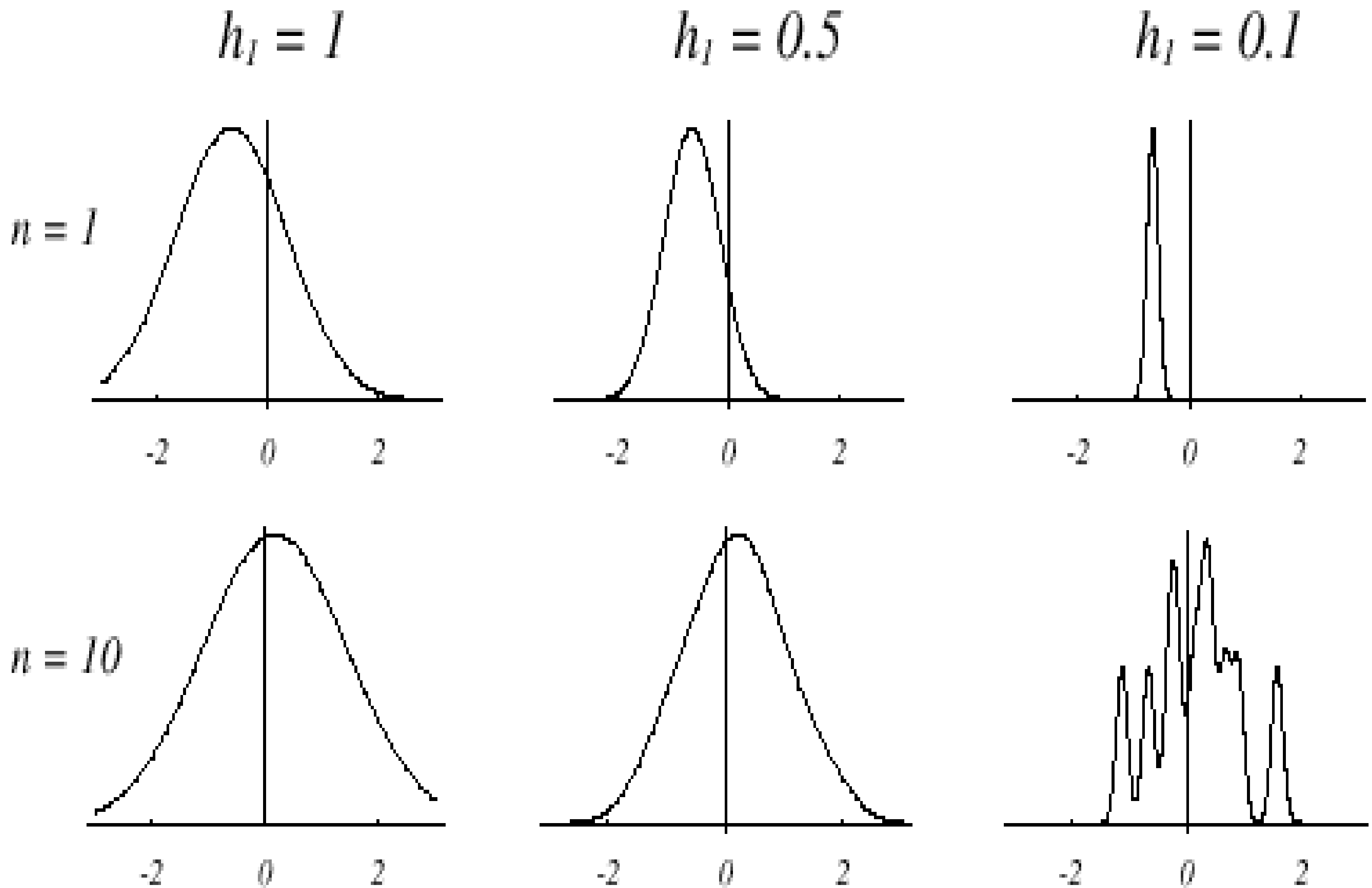
  is an average of normal densities centered at the samples $x_i$.

– 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 !



h1 = 1
h1 = 0.5
h1 = 0.1
n = 1
n = 10
-2
0
2

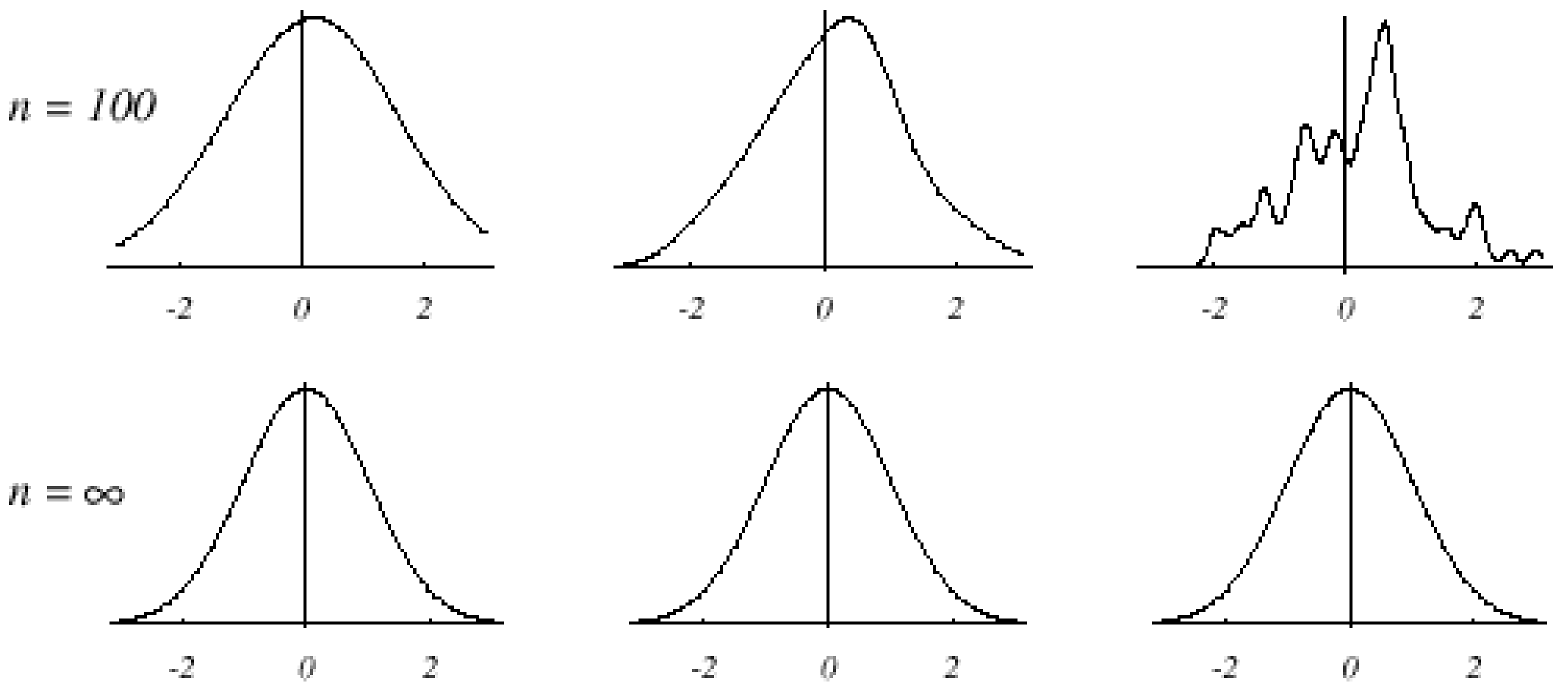
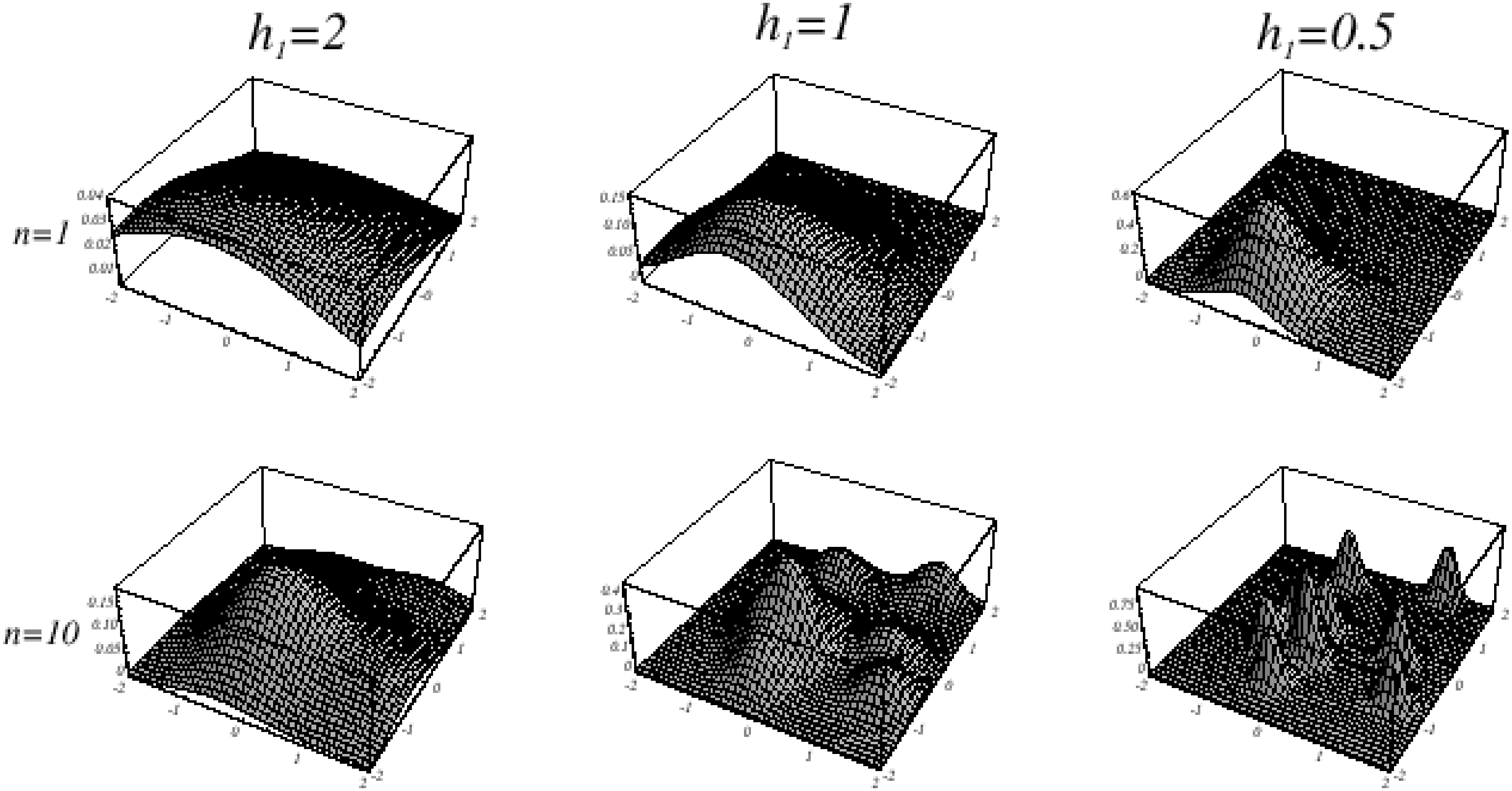



**FIGURE 4.5.** Parzen-window estimates of a univariate normal density using different window widths and numbers of samples. The vertical axes have been scaled to best show the structure in each graph. Note particularly that the $n = \infty$ estimates are the same (and match the true density function), 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:



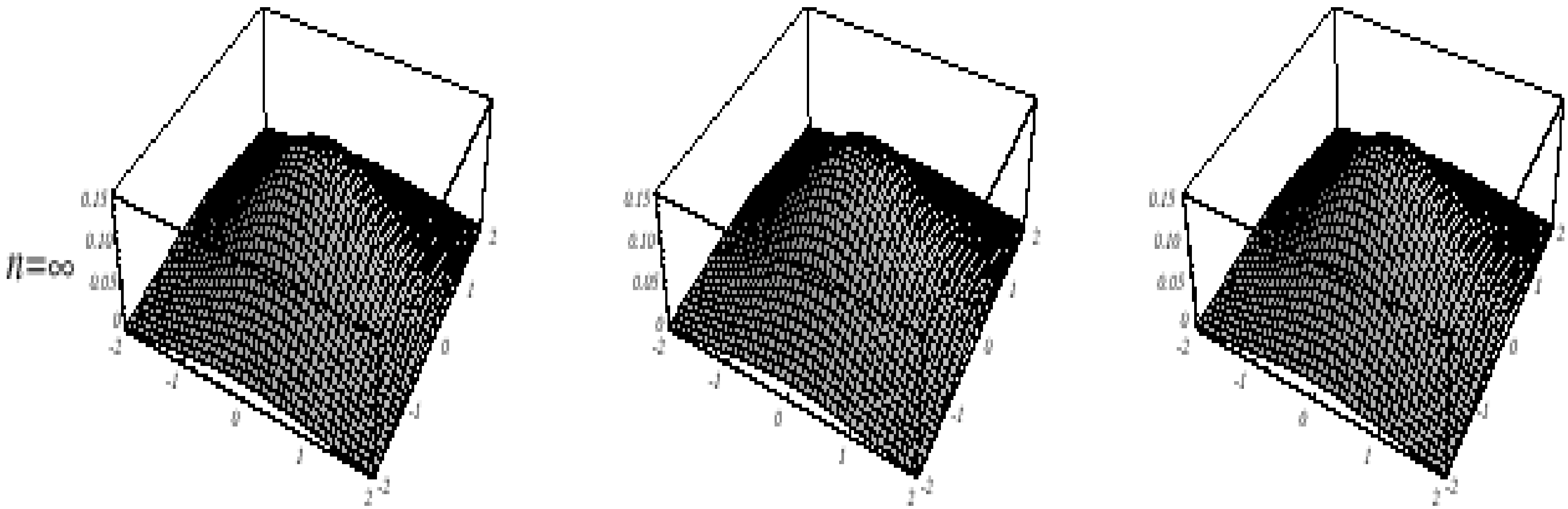
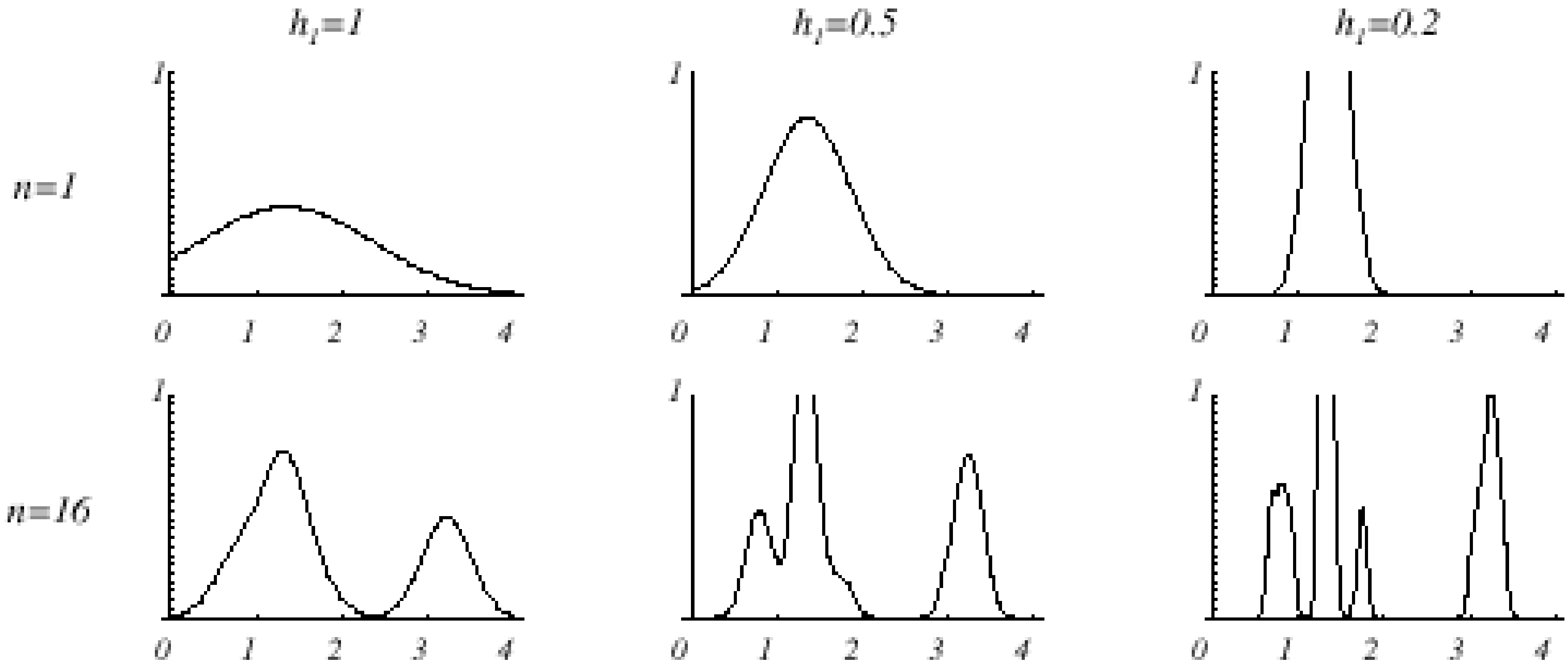



**FIGURE 4.6.** Parzen-window estimates of a bivariate normal density using different window widths and numbers of samples. The vertical axes have been scaled to best show the structure in each graph. Note particularly that the $n = \infty$ estimates are the same (and match the true distribution), regardless 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)



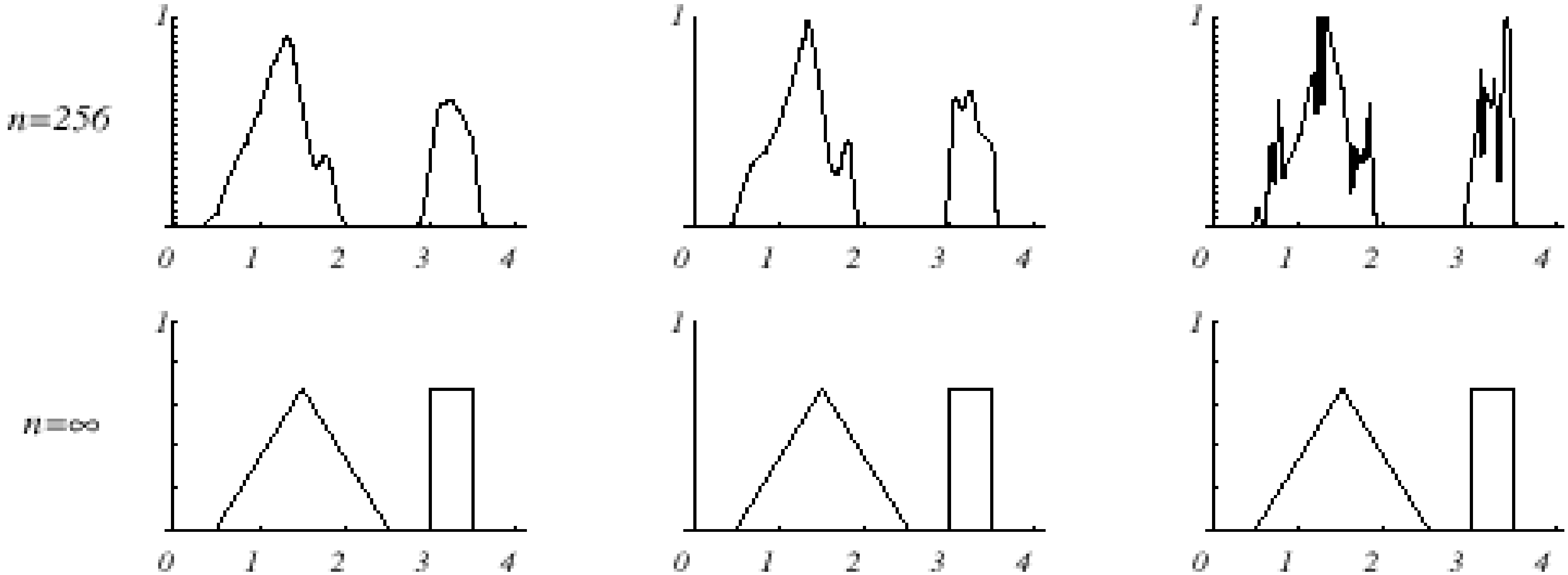



**FIGURE 4.7.** Parzen-window estimates of a bimodal distribution using different window widths and numbers of samples. Note particularly that the $n = \infty$ estimates are the same (and match the true distribution), regardless of window width. From: Richard O. Duda, Peter E. Hart, and David G. Stork,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

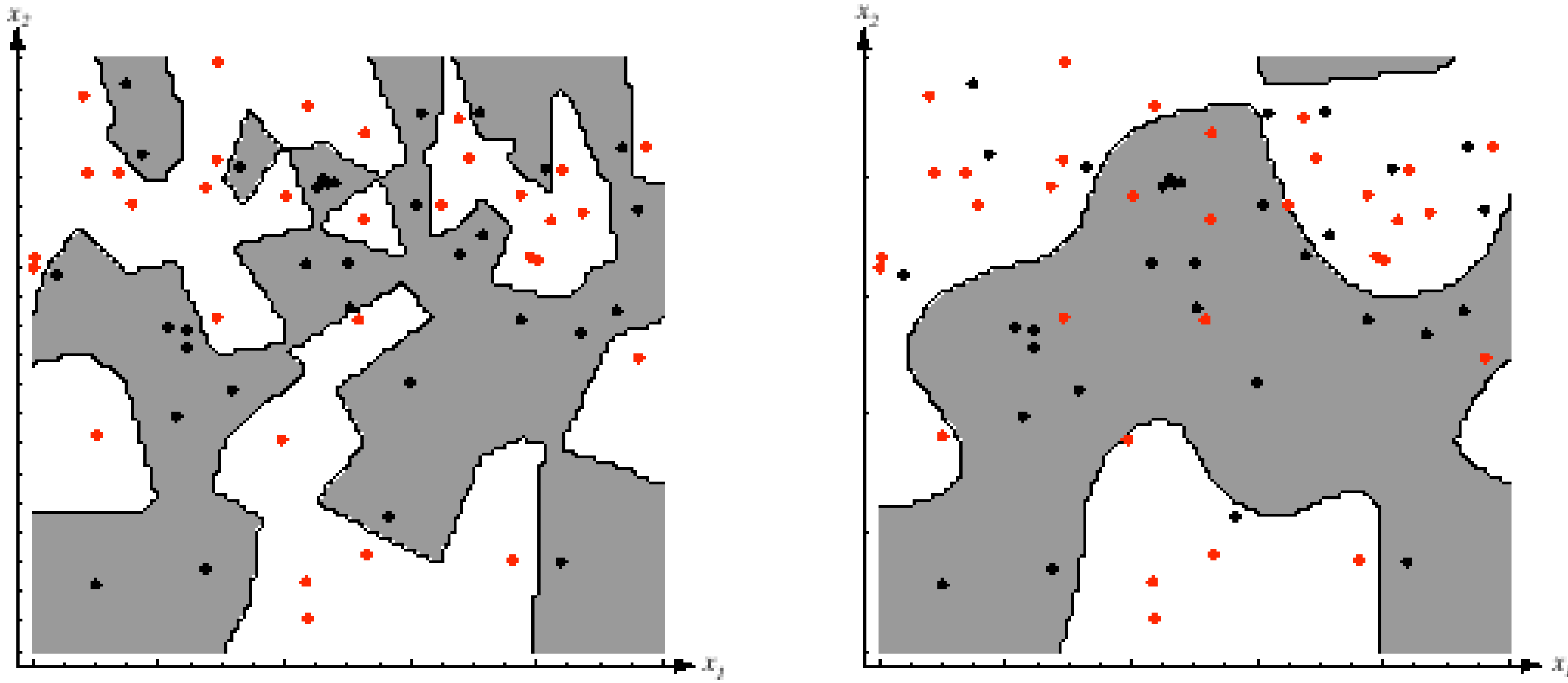


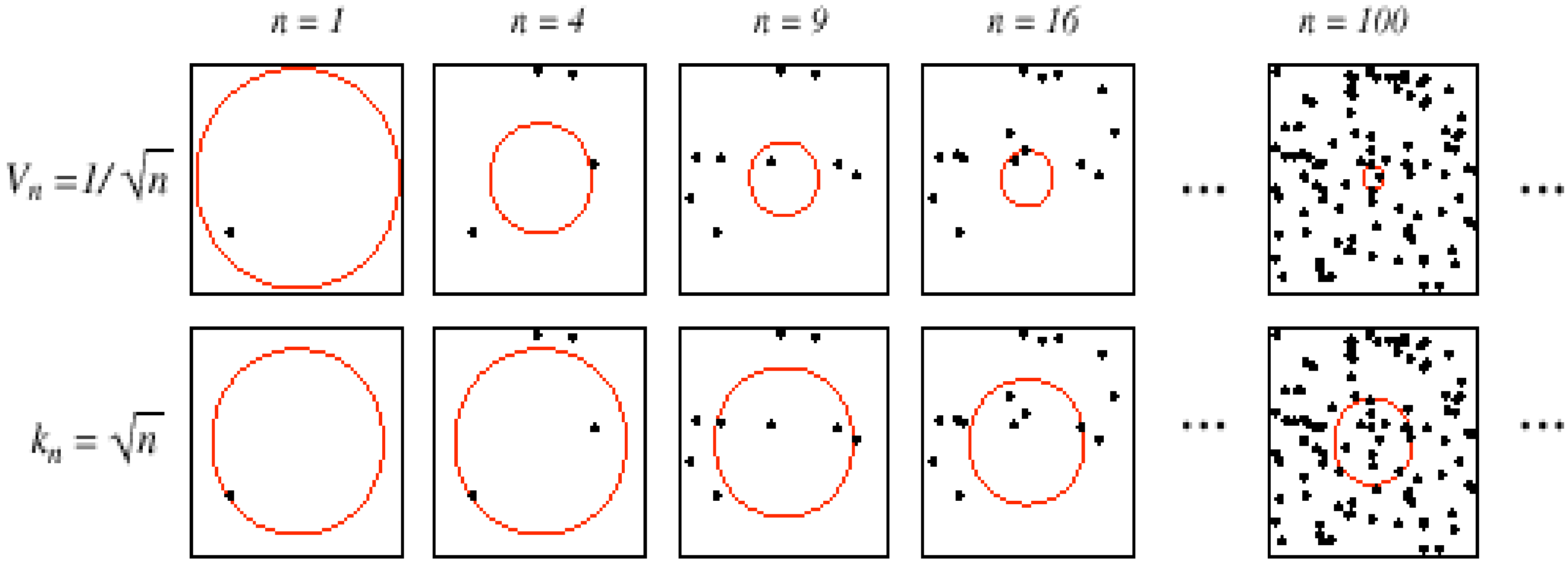

**FIGURE 4.8.** The decision boundaries in a two-dimensional Parzen-window dichotomizer depend on the window width *h*. At the left a small *h* leads to boundaries that are more complicated than for large *h* on same data set, shown at the right. Apparently, for these data a small *h* would be appropriate 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*. 

# Nearest Neighbor Approach

- Problem with Parzen (kernel):
  - Unknown "best" window function

- Nearest Neighbor Approach:
  - let the cell volume be a function of the training data, by centering a cell about each point $x$ and increasing the volume until $k_n$ samples are contained, where $k_n$ depends on $n$.
  - *These samples are the $k_n$ nearest-neighbors of $x$.*

$$p_n(\mathbf{x}) = \frac{k_n/n}{V_n}$$

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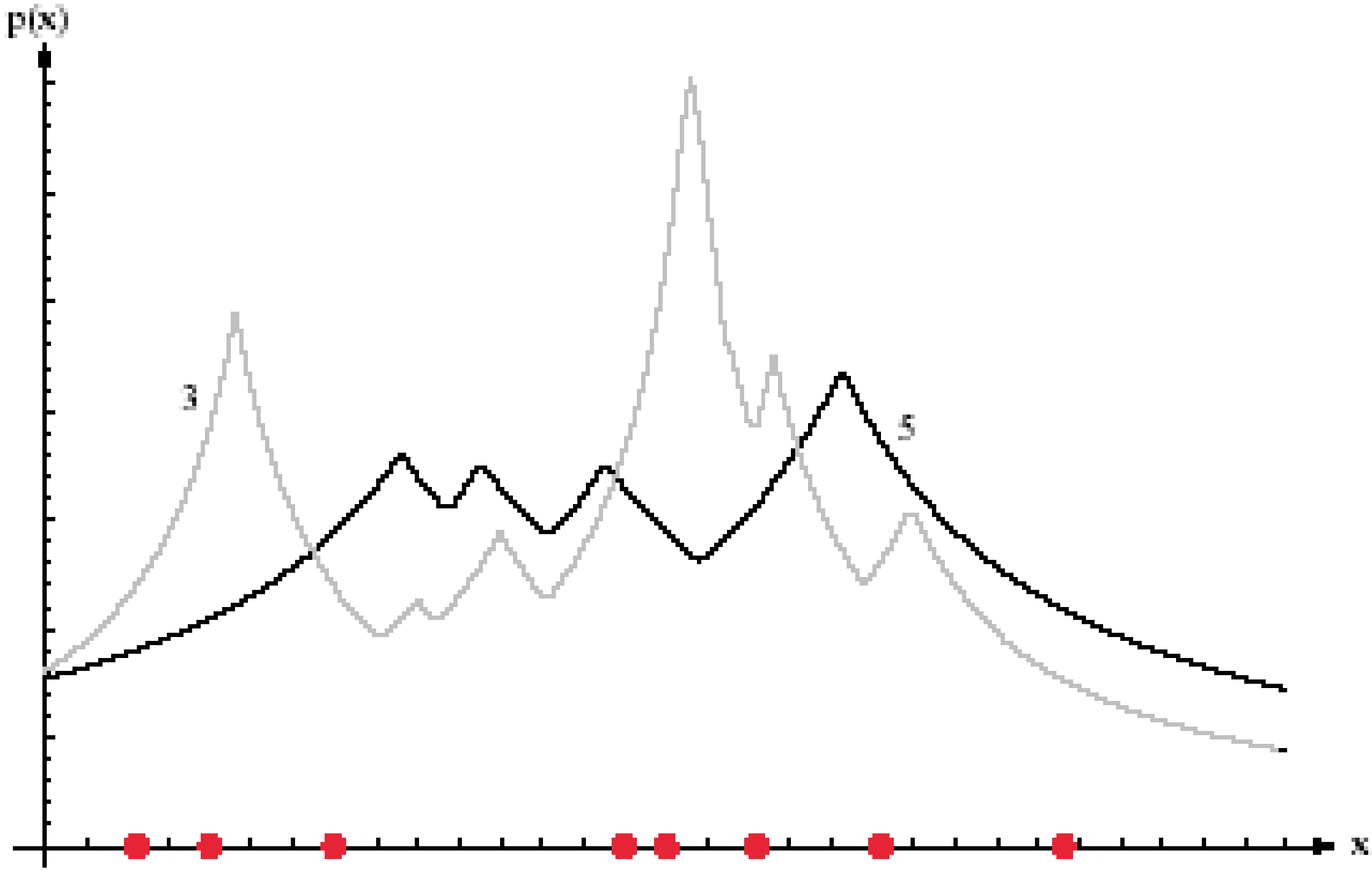
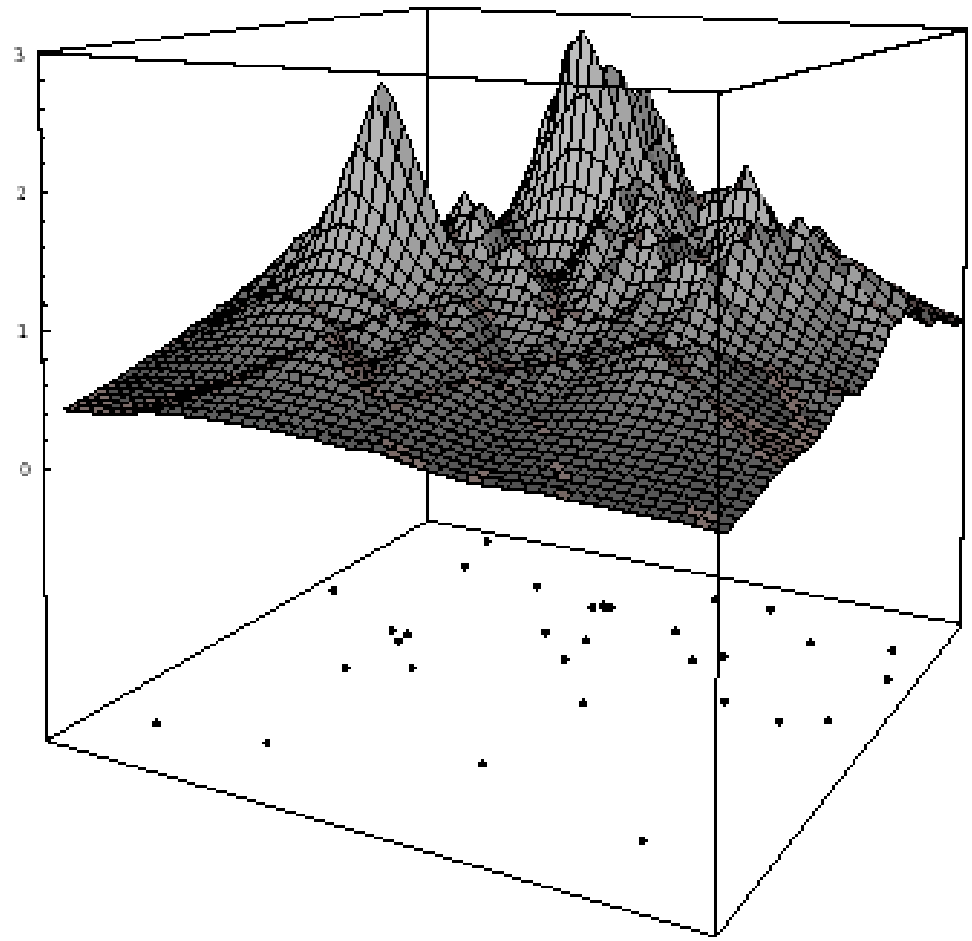
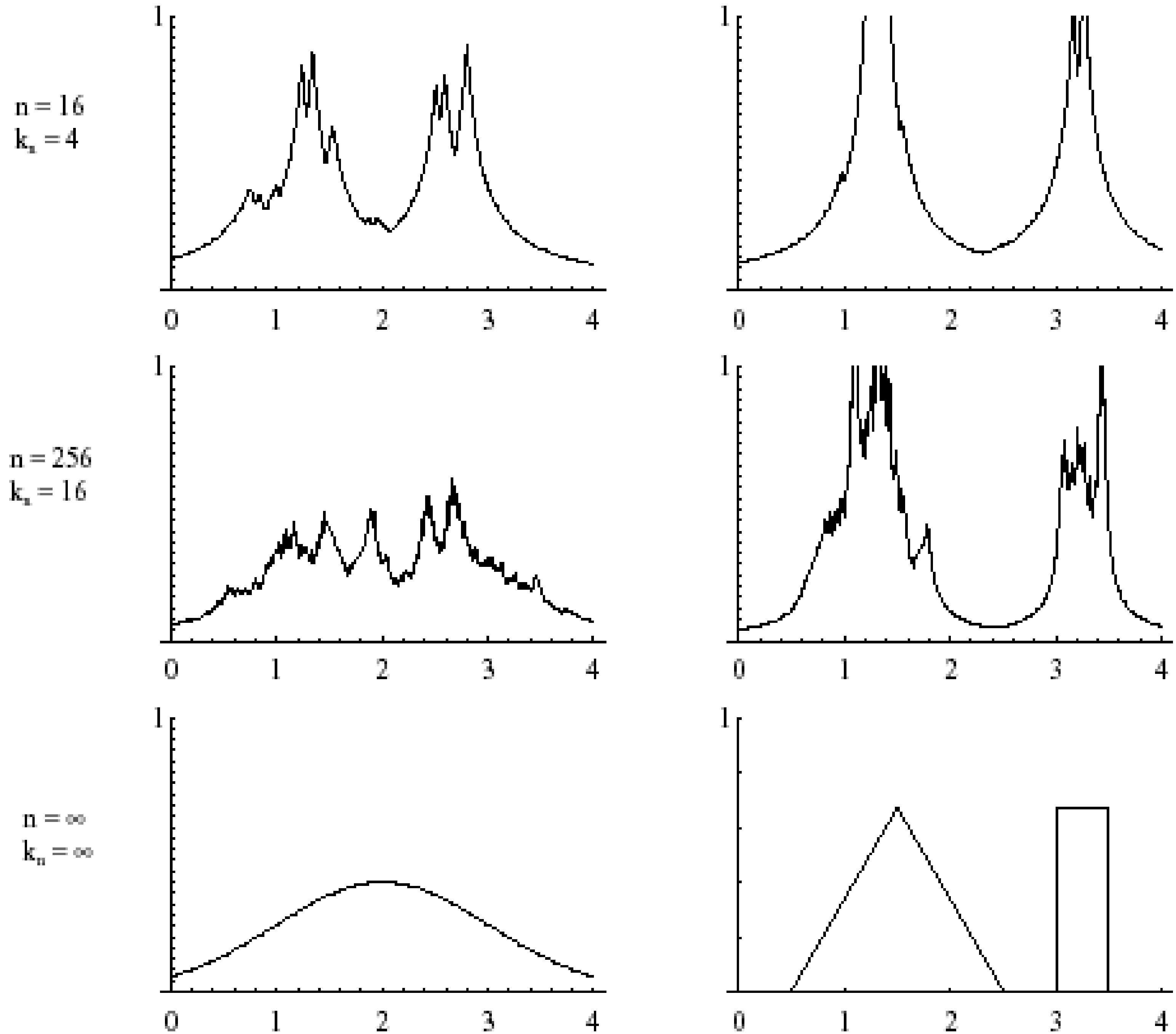



Figure 4.10: Eight points in one dimension and the $k$-nearest-neighbor density estimates, for $k = 3$ and 5. Note especially that the discontinuities in the slopes in the estimates generally occur *away* fom the positions of the points themselves.




- The $k$-nearest-neighbor estimate of a two-dimensional density for $k = 5$.



n = 16
$k_n$ = 4
n = 256
$k_n$ = 16
n = ∞
$k_n$ = ∞
1
0
1
2
3
4

# Estimation of aposteriori Prob

$$p_n(\mathbf{x}, \omega_i) = \frac{k_i/n}{V},$$

$$P_n(\omega_i|\mathbf{x}) = \frac{p_n(\mathbf{x}, \omega_i)}{\sum_{j=1}^{c} p_n(\mathbf{x}, \omega_j)} = \frac{k_i}{k}.$$

Thus, the estimate is just the fraction of the samples in a cell from the $i^{th}$ class

$$P(\omega_m|\mathbf{x}) = \max_i P(\omega_i|\mathbf{x}),$$

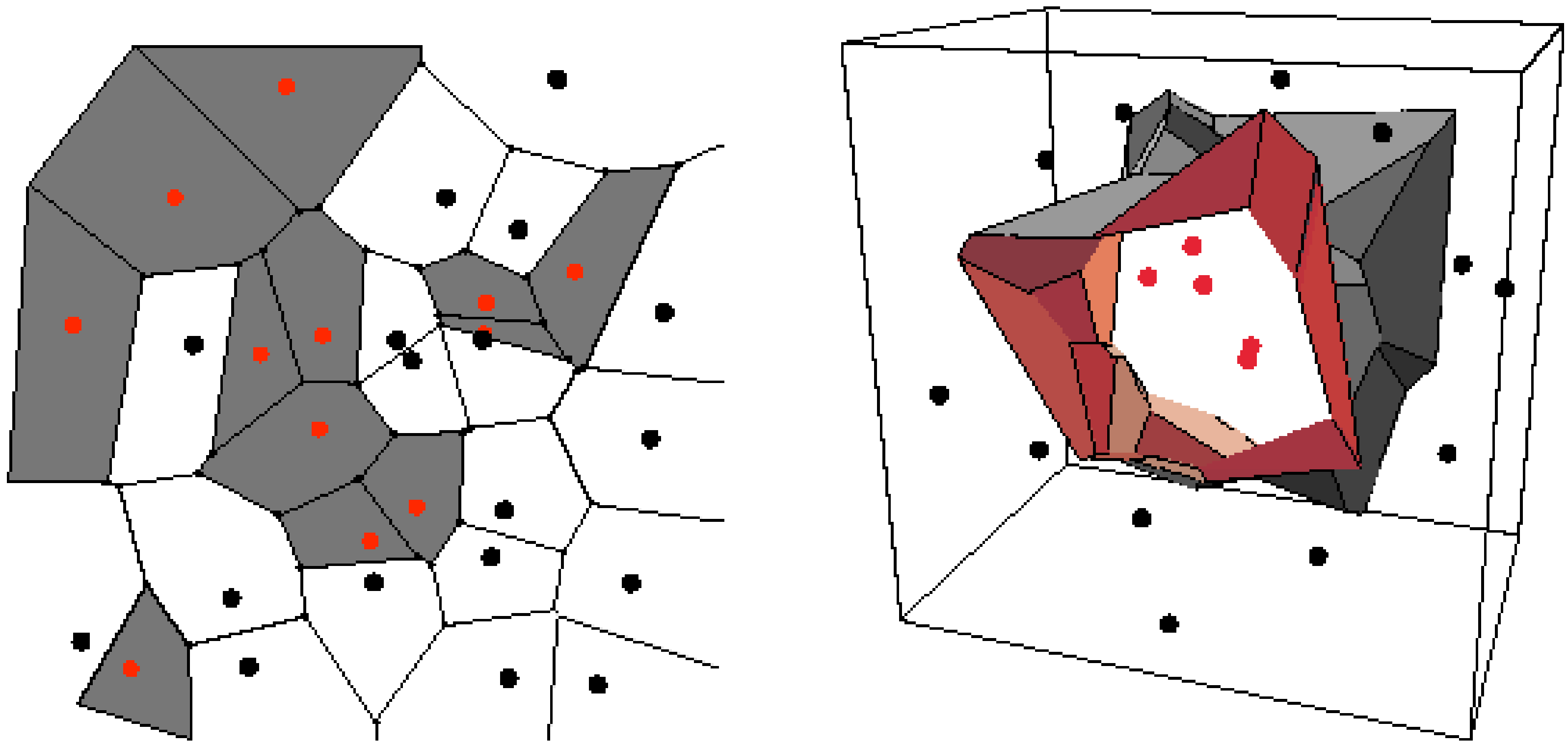


Figure 4.13: In two dimensions, the nearest-neighbor algorithm leads to a partitioning of the input space into Voronoi cells, each labelled by the category of the training point it contains. In three dimensions, the cells are three-dimensional, and the decision boundary resembles the surface of a crystal.