

Nonparametric Density Estimation
Intro
Parzen Windows

Non-Parametric Methods

- Neither probability distribution nor discriminant function is known
 - Happens quite often
- All we have is labeled data



- Estimate the probability distribution from the labeled data

*a lot is
known
"easier"*

*little is
known
"harder"*

NonParametric Techniques: Introduction

- In previous lectures we assumed that either
 1. someone gives us the density $p(\mathbf{x}/\mathbf{c}_j)$
 - In pattern recognition applications this never happens
 2. someone gives us $p(\mathbf{x}/\theta_{c_j})$
 - Does happen sometimes, **but**
 - we are likely to suspect whether the given $p(\mathbf{x}/\theta)$ models the data well
 - Most parametric densities are unimodal (have a single local maximum), whereas many practical problems involve multi-modal densities

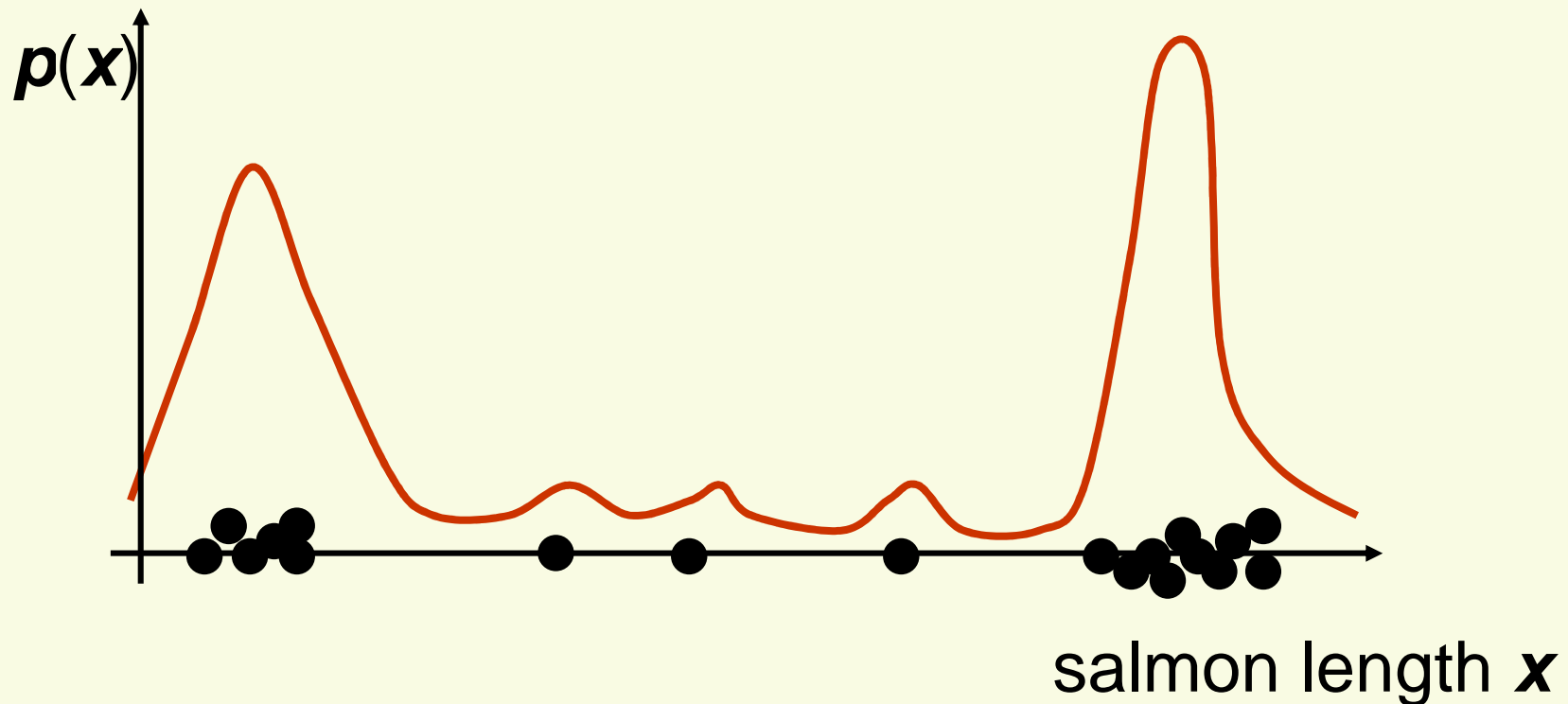
NonParametric Techniques: Introduction

- Nonparametric procedures can be used with arbitrary distributions and without any assumption about the forms of the underlying densities
- There are two types of nonparametric methods:
 - Parzen windows
 - Estimate likelihood $p(\mathbf{x} | \mathbf{c}_j)$
 - Nearest Neighbors
 - Bypass likelihood and go directly to posterior estimation $P(\mathbf{c}_j | \mathbf{x})$

NonParametric Techniques: Introduction

- Nonparametric techniques attempt to estimate the underlying density functions from the training data
 - Idea: the more data in a region, the larger is the density function

$$Pr[X \in \mathcal{R}] = \int_{\mathcal{R}} f(\mathbf{x}) d\mathbf{x}$$



NonParametric Techniques: Introduction

$$Pr[X \in \mathcal{R}] = \int_{\mathcal{R}} f(x) dx$$

- How can we approximate $Pr[X \in \mathcal{R}_1]$ and $Pr[X \in \mathcal{R}_2]$?

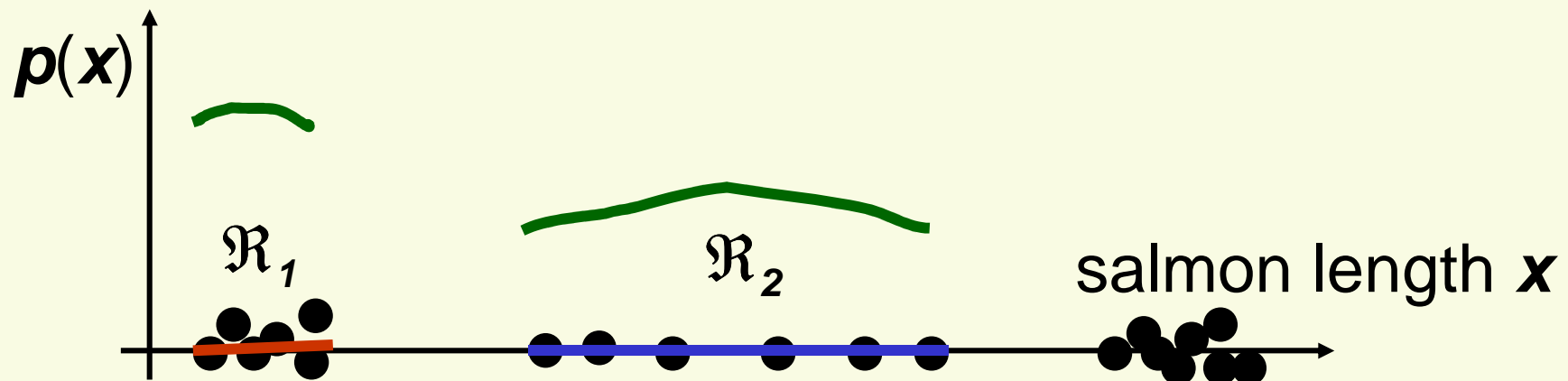
- $Pr[X \in \mathcal{R}_1] \approx \frac{6}{20}$ and $Pr[X \in \mathcal{R}_2] \approx \frac{6}{20}$

- Should the density curves above \mathcal{R}_1 and \mathcal{R}_2 be equally high?

- No, since \mathcal{R}_1 is smaller than \mathcal{R}_2

$$Pr[X \in \mathcal{R}_1] = \int_{\mathcal{R}_1} f(x) dx \approx \int_{\mathcal{R}_2} f(x) dx = Pr[X \in \mathcal{R}_2]$$

- To get density, normalize by region size



NonParametric Techniques: Introduction

- Assuming $f(\mathbf{x})$ is basically flat inside \mathcal{R} ,

$$\frac{\text{\# of samples in } \mathcal{R}}{\text{total \# of samples}} \approx \text{Pr}[X \in \mathcal{R}] = \int_{\mathcal{R}} f(\mathbf{y}) d\mathbf{y} \approx f(\mathbf{x}) * \text{Volume}(\mathcal{R})$$

- Thus, density at a point \mathbf{x} inside \mathcal{R} , can be approximated

$$f(\mathbf{x}) \approx \frac{\text{\# of samples in } \mathcal{R}}{\text{total \# of samples}} \frac{1}{\text{Volume}(\mathcal{R})}$$

- Now let's derive this formula more formally

Binomial Random Variable

- Let us flip a coin n times (each one is called “trial”)
 - Probability of head ρ , probability of tail is $1-\rho$
- Binomial random variable K counts the number of heads in n trials

$$P(K = k) = \binom{n}{k} \rho^k (1 - \rho)^{n-k}$$

where $\binom{n}{k} = \frac{n!}{k!(n-k)!}$

- Mean is $E(K) = n\rho$
- Variance is $\text{var}(K) = n\rho(1 - \rho)$

Density Estimation: Basic Issues

- From the definition of a density function, probability ρ that a vector \mathbf{x} will fall in region \mathcal{R} is:

$$\rho = \Pr[\mathbf{x} \in \mathcal{R}] = \int_{\mathcal{R}} p(\mathbf{x}') d\mathbf{x}'$$

- Suppose we have samples $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ drawn from the distribution $p(\mathbf{x})$. The probability that k points fall in \mathcal{R} is then given by binomial distribution:

$$\Pr[K = k] = \binom{n}{k} \rho^k (1 - \rho)^{n-k}$$

- Suppose that k points fall in \mathcal{R} , we can use MLE to estimate the value of ρ . The likelihood function is

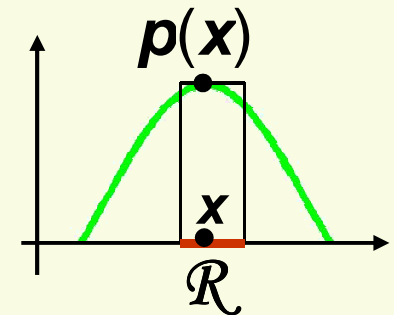
$$p(\mathbf{x}_1, \dots, \mathbf{x}_n | \rho) = \binom{n}{k} \rho^k (1 - \rho)^{n-k}$$

Density Estimation: Basic Issues

$$p(\mathbf{x}_1, \dots, \mathbf{x}_n | \rho) = \binom{n}{k} \rho^k (1 - \rho)^{n-k}$$

- This likelihood function is maximized at $\rho = \frac{k}{n}$
- Thus the MLE is $\hat{\rho} = \frac{k}{n}$
- Assume that $p(\mathbf{x})$ is continuous and that the region \mathcal{R} is so small that $p(\mathbf{x})$ is approximately constant in \mathcal{R}

$$\int_{\mathcal{R}} p(\mathbf{x}') d\mathbf{x}' \cong p(\mathbf{x})V$$

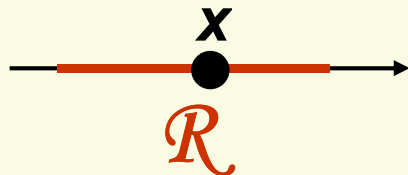


- \mathbf{x} is in \mathcal{R} and V is the volume of \mathcal{R}
- Recall from the previous slide: $\rho = \int_{\mathcal{R}} p(\mathbf{x}') d\mathbf{x}'$
- Thus $p(\mathbf{x})$ can be approximated: $p(\mathbf{x}) \approx \frac{k/n}{V}$

Density Estimation: Basic Issues

- This is exactly what we had before:

$$p(\mathbf{x}) \approx \frac{k/n}{V}$$



x is inside some region \mathcal{R}
k = number of samples inside \mathcal{R}
n = total number of samples
V = volume of \mathcal{R}

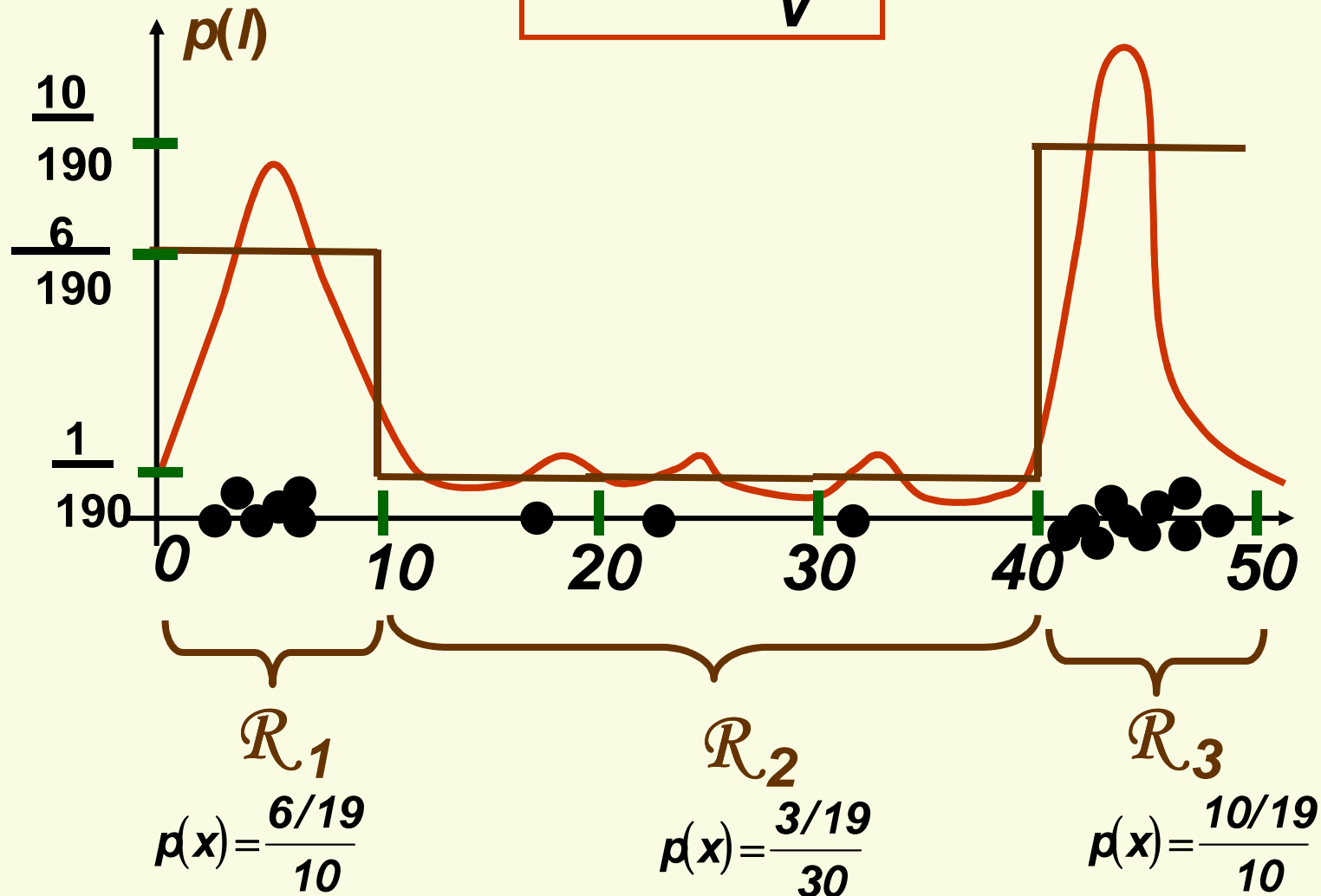
- Our estimate will always be the average of true density over \mathcal{R}

$$p(\mathbf{x}) \approx \frac{k/n}{V} = \frac{\hat{\rho}}{V} \approx \frac{\int_{\mathcal{R}} p(\mathbf{x}') d\mathbf{x}'}{V}$$

- Ideally, $p(\mathbf{x})$ should be constant inside \mathcal{R}

Density Estimation: Histogram

$$p(x) \approx \frac{k/n}{v}$$



- If regions \mathcal{R}_i 's do not overlap, we have a histogram

Density Estimation: Accuracy

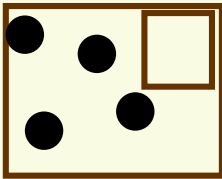
- How accurate is density approximation $p(\mathbf{x}) \approx \frac{k/n}{V}$?
- We have made two approximations

1. $\hat{\rho} = \frac{k}{n}$

- as n increases, this estimate becomes more accurate

2. $\int_{\mathcal{R}} p(\mathbf{x}') d\mathbf{x}' \cong p(\mathbf{x})V$

- as \mathcal{R} grows smaller, the estimate becomes more accurate



- As we shrink \mathcal{R} we have to make sure it contains samples, otherwise our estimated $p(\mathbf{x}) = 0$ for all \mathbf{x} in \mathcal{R}

- Thus in theory, if we have an unlimited number of samples, we get convergence as we simultaneously increase the number of samples n , and shrink region \mathcal{R} , but not too much so that \mathcal{R} still contains a lot of samples

Density Estimation: Accuracy

$$p(\mathbf{x}) \approx \frac{k/n}{V}$$

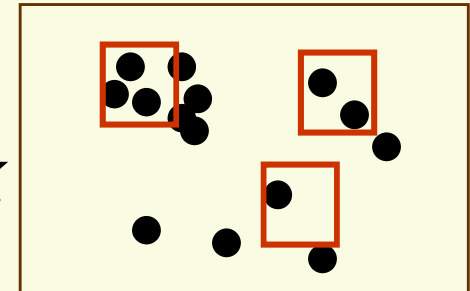
- In practice, the number of samples is always fixed
- Thus the only available option to increase the accuracy is by decreasing the size of \mathcal{R} (V gets smaller)
 - If V is too small, $p(\mathbf{x})=0$ for most \mathbf{x} , because most regions will have no samples
 - Thus have to find a compromise for V
 - not too small so that it has enough samples
 - but also not too large so that $p(\mathbf{x})$ is approximately constant inside V

Density Estimation: Two Approaches

$$p(\mathbf{x}) \approx \frac{k/n}{V}$$

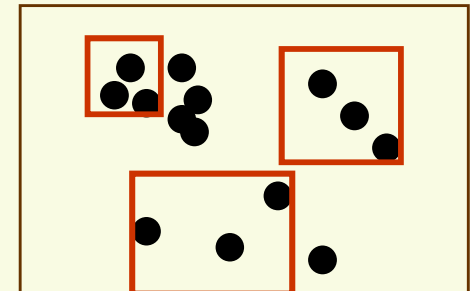
1. Parzen Windows:

- Choose a fixed value for volume V and determine the corresponding k from the data



2. k-Nearest Neighbors

- Choose a fixed value for k and determine the corresponding volume V from the data



- Under appropriate conditions and as number of samples goes to infinity, both methods can be shown to converge to the true $p(\mathbf{x})$

Parzen Windows

$$p(\mathbf{x}) \approx \frac{k/n}{V}$$

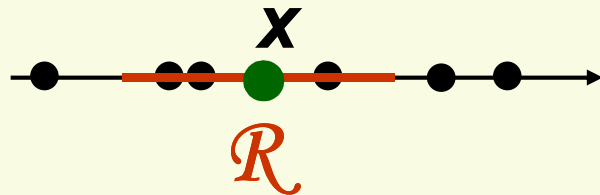
\mathbf{x} is inside some region \mathcal{R}

k = number of samples inside \mathcal{R}

n = total number of samples

V = volume of \mathcal{R}

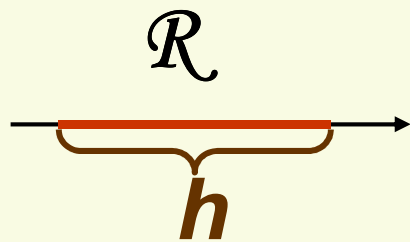
- To estimate the density at point \mathbf{x} , simply center the region \mathcal{R} at \mathbf{x} , count the number of samples in \mathcal{R} , and substitute everything in our formula



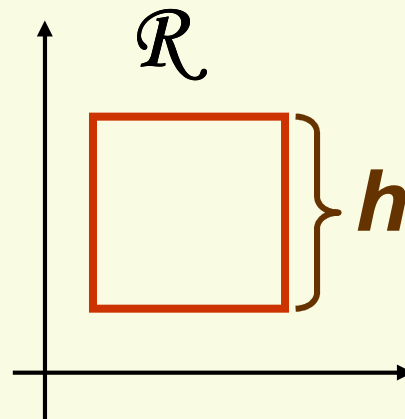
$$p(\mathbf{x}) \approx \frac{3/6}{10}$$

Parzen Windows

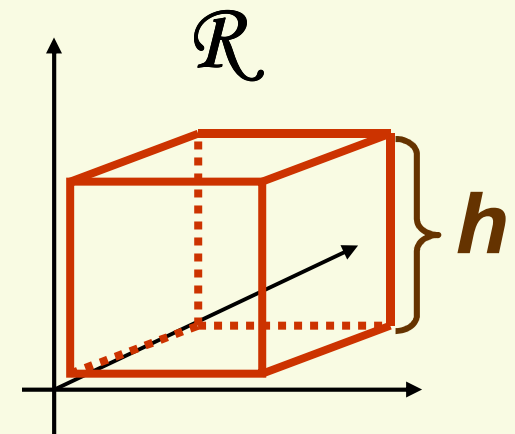
- In Parzen-window approach to estimate densities we fix the size and shape of region \mathcal{R}
- Let us assume that the region \mathcal{R} is a d -dimensional hypercube with side length h thus it's volume is h^d



1 dimension



2 dimensions

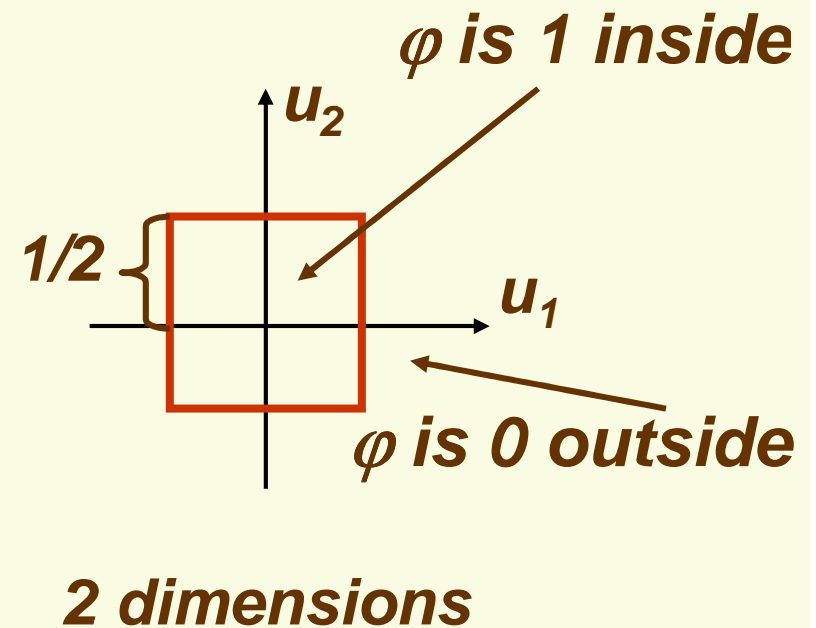
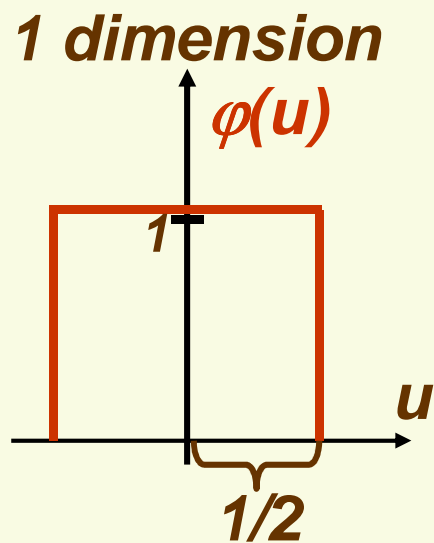


3 dimensions

Parzen Windows

- Let $u = [u_1, u_2, \dots, u_d]$ and define a **window function**

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

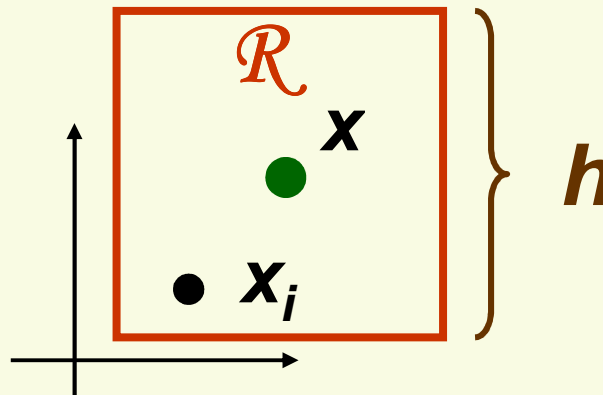


Parzen Windows

- Recall we have d -dimensional samples $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$. Let x_{ij} be the j th coordinate of sample \mathbf{x}_i . Then

$$\varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right) = \begin{cases} 1 & |x_j - x_{ij}| \leq \frac{h}{2} \quad j = 1, \dots, d \\ 0 & \text{otherwise} \end{cases}$$

$|u_j| \leq \frac{1}{2}$



$$\varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right) = \begin{cases} 1 & \text{if } \mathbf{x}_i \text{ is inside the hypercube with} \\ & \text{width } h \text{ and centered at } \mathbf{x} \\ 0 & \text{otherwise} \end{cases}$$

Parzen Windows

- How do we count the total number of sample points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ which are inside the hypercube with side h and centered at \mathbf{x} ?

$$\mathbf{k} = \sum_{i=1}^{i=n} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)$$

- Recall $p(\mathbf{x}) \approx \frac{\mathbf{k}/n}{V}$, $V=h^d$
- Thus we get the desired analytical expression for the estimate of density $p_\varphi(\mathbf{x})$

$$p_\varphi(\mathbf{x}) = \frac{\sum_{i=1}^{i=n} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right) / n}{h^d} = \frac{1}{n} \sum_{i=1}^{i=n} \frac{1}{h^d} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)$$

Parzen Windows

$$p_{\varphi}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{i=n} \frac{1}{h^d} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)$$

- Let's make sure $p_{\varphi}(\mathbf{x})$ is in fact a density

- $p_{\varphi}(\mathbf{x}) \geq 0 \quad \forall \mathbf{x}$

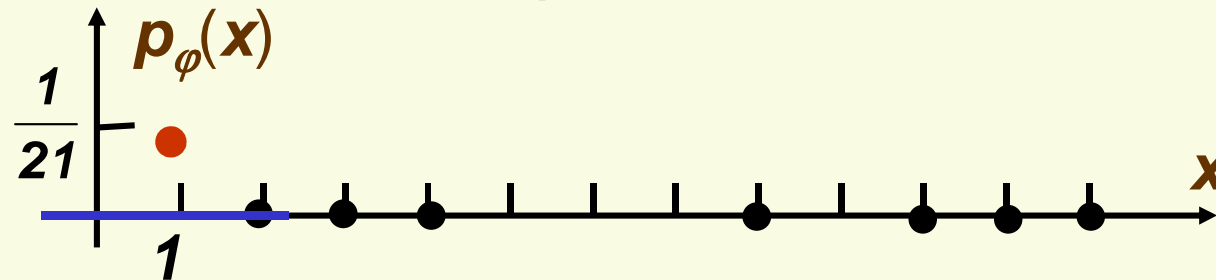
volume of hypercube

- $$\int p_{\varphi}(\mathbf{x}) d\mathbf{x} = \int \frac{1}{n} \sum_{i=1}^{i=n} \frac{1}{h^d} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right) d\mathbf{x} = \frac{1}{h^d n} \sum_{i=1}^{i=n} \int \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right) d\mathbf{x}$$
$$= \frac{1}{n} \frac{1}{h^d} \sum_{i=1}^{i=n} h^d = 1$$

Parzen Windows: Example in 1D

$$p_\varphi(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \frac{1}{h^d} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)$$

- Suppose we have 7 samples $\mathbf{D}=\{2,3,4,8,10,11,12\}$



- Let window width $h=3$, estimate density at $x=1$

$$p_\varphi(1) = \frac{1}{7} \sum_{i=1}^7 \frac{1}{3} \varphi\left(\frac{1-x_i}{3}\right) = \frac{1}{21} \left[\varphi\left(\frac{1-2}{3}\right) + \varphi\left(\frac{1-3}{3}\right) + \varphi\left(\frac{1-4}{3}\right) + \dots + \varphi\left(\frac{1-12}{3}\right) \right]$$

$$\left|-\frac{1}{3}\right| \leq 1/2 \quad \left|-\frac{2}{3}\right| > 1/2 \quad |-1| > 1/2 \quad \left|-\frac{11}{3}\right| > 1/2$$

$$p_\varphi(1) = \frac{1}{7} \sum_{i=1}^7 \frac{1}{3} \varphi\left(\frac{1-x_i}{3}\right) = \frac{1}{21} [1 + 0 + 0 + \dots + 0] = \frac{1}{21}$$

Parzen Windows: Sum of Functions

- Now let's look at our density estimate $\mathbf{p}_\varphi(\mathbf{x})$ again:

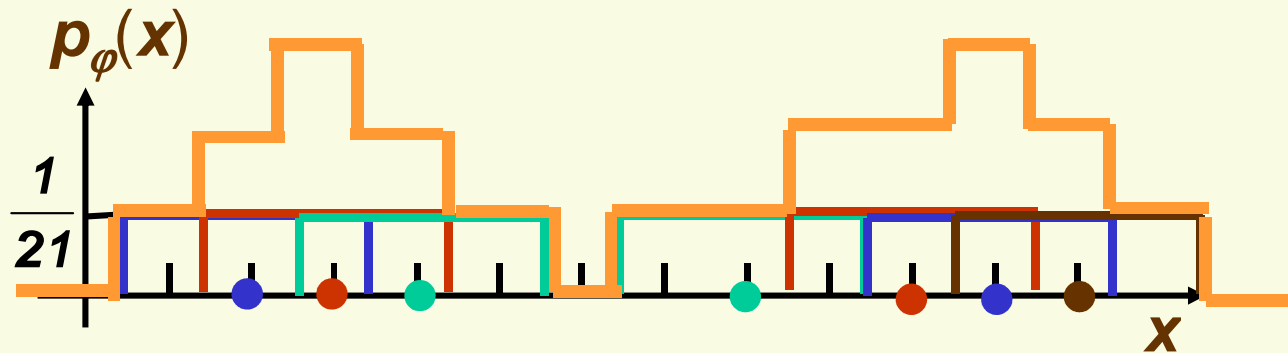
$$\mathbf{p}_\varphi(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{i=n} \frac{1}{h^d} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right) = \sum_{i=1}^{i=n} \underbrace{\frac{1}{nh^d} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)}$$

1 inside square centered at \mathbf{x}_i
0 otherwise

- Thus $\mathbf{p}_\varphi(\mathbf{x})$ is just a sum of n “box like” functions each of height $\frac{1}{nh^d}$

Parzen Windows: Example in 1D

- Let's come back to our example
 - 7 samples $D=\{2,3,4,8,10,11,12\}$, $h=3$

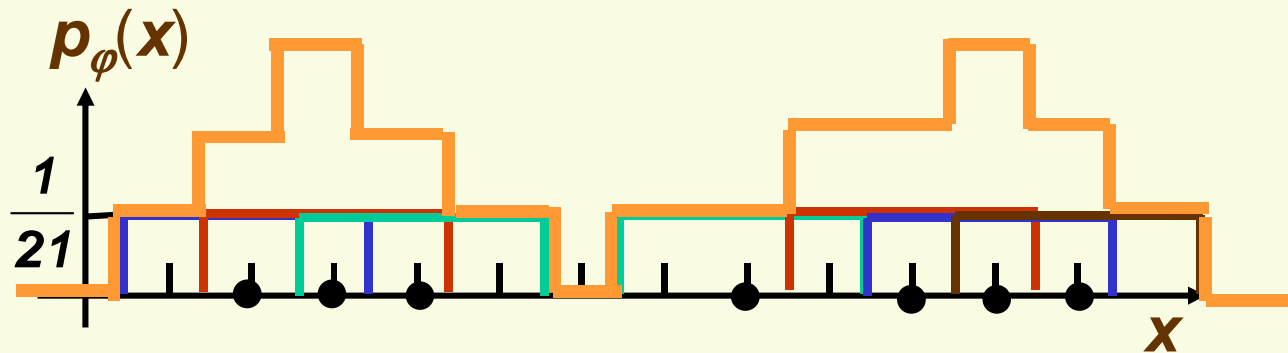


- To see what the function looks like, we need to generate 7 boxes and add them up
- The width is $h=3$ and the height is

$$\frac{1}{nh^d} = \frac{1}{21}$$

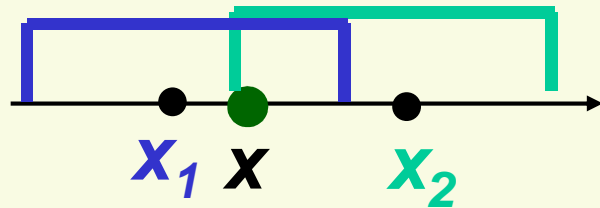
Parzen Windows: Interpolation

- In essence, window function φ is used for interpolation: each sample \mathbf{x}_i contributes to the resulting density at \mathbf{x} if \mathbf{x} is close enough to \mathbf{x}_i



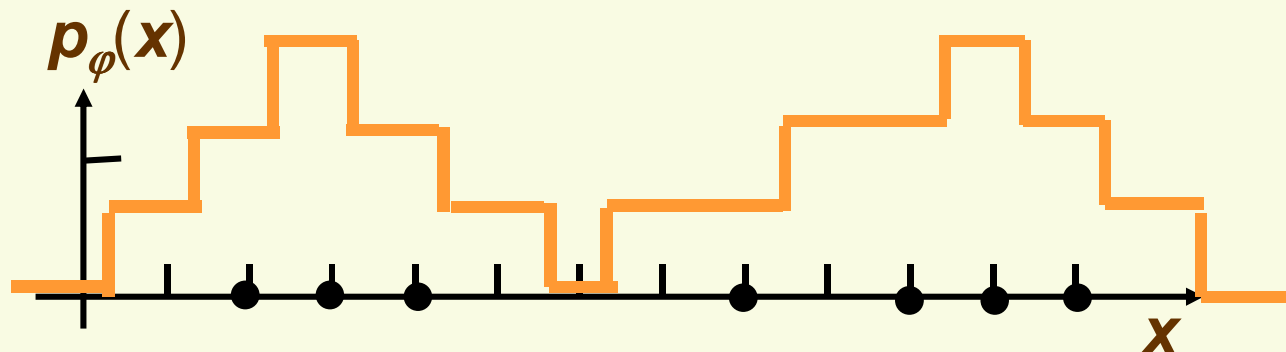
Parzen Windows: Drawbacks of Hypercube φ

- As long as sample point \mathbf{x}_i and \mathbf{x} are in the same hypercube, the contribution of \mathbf{x}_i to the density at \mathbf{x} is constant, regardless of how close \mathbf{x}_i is to \mathbf{x}



$$\varphi\left(\frac{\mathbf{x} - \mathbf{x}_1}{h}\right) = \varphi\left(\frac{\mathbf{x} - \mathbf{x}_2}{h}\right) = 1$$

- The resulting density $p_\varphi(\mathbf{x})$ is not smooth, it has discontinuities



Parzen Windows: general φ

$$p_{\varphi}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \frac{1}{h^d} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)$$

- We can use a general window φ as long as the resulting $p_{\varphi}(\mathbf{x})$ is a legitimate density, i.e.

1. $p_{\varphi}(\mathbf{u}) \geq 0$

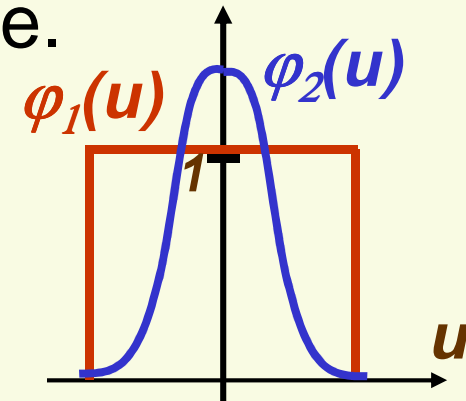
- satisfied if $\varphi(\mathbf{u}) \geq 0$

2. $\int p_{\varphi}(\mathbf{x}) d\mathbf{x} = 1$

- satisfied if $\int \varphi(\mathbf{u}) d\mathbf{u} = 1$

$$\int p_{\varphi}(\mathbf{x}) d\mathbf{x} = \frac{1}{nh^d} \sum_{i=1}^n \int \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right) d\mathbf{x} = \frac{1}{nh^d} \sum_{i=1}^n \int h^d \varphi(\mathbf{u}) d\mathbf{u} = 1$$

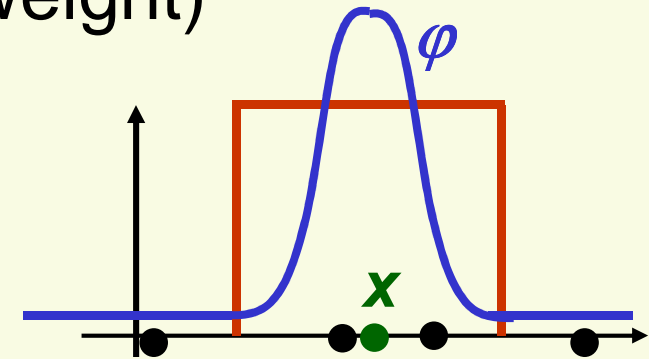
change coordinates to $u = \frac{\mathbf{x} - \mathbf{x}_i}{h}$, thus $du = \frac{d\mathbf{x}}{h}$



Parzen Windows: general φ

$$p_{\varphi}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \frac{1}{h^d} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)$$

- Notice that with the general window φ we are no longer counting the number of samples inside \mathcal{R} .
- We are counting the weighted average of potentially every single sample point (although only those within distance h have any significant weight)



- With infinite number of samples, and appropriate conditions, it can still be shown that

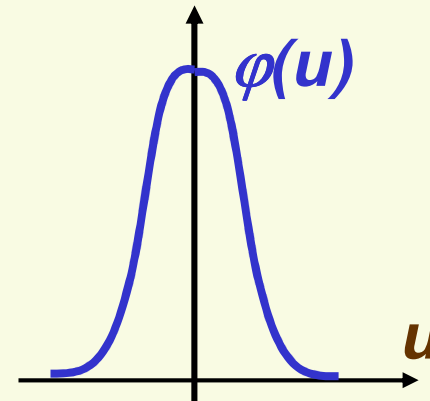
$$p_{\varphi}^n(\mathbf{x}) \rightarrow p(\mathbf{x})$$

Parzen Windows: Gaussian φ

$$p_{\varphi}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{i=n} \frac{1}{h^d} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)$$

- A popular choice for φ is $\mathbf{N}(\mathbf{0}, \mathbf{1})$ density

$$\varphi(\mathbf{u}) = \frac{1}{\sqrt{2\pi}} e^{-u^2/2}$$

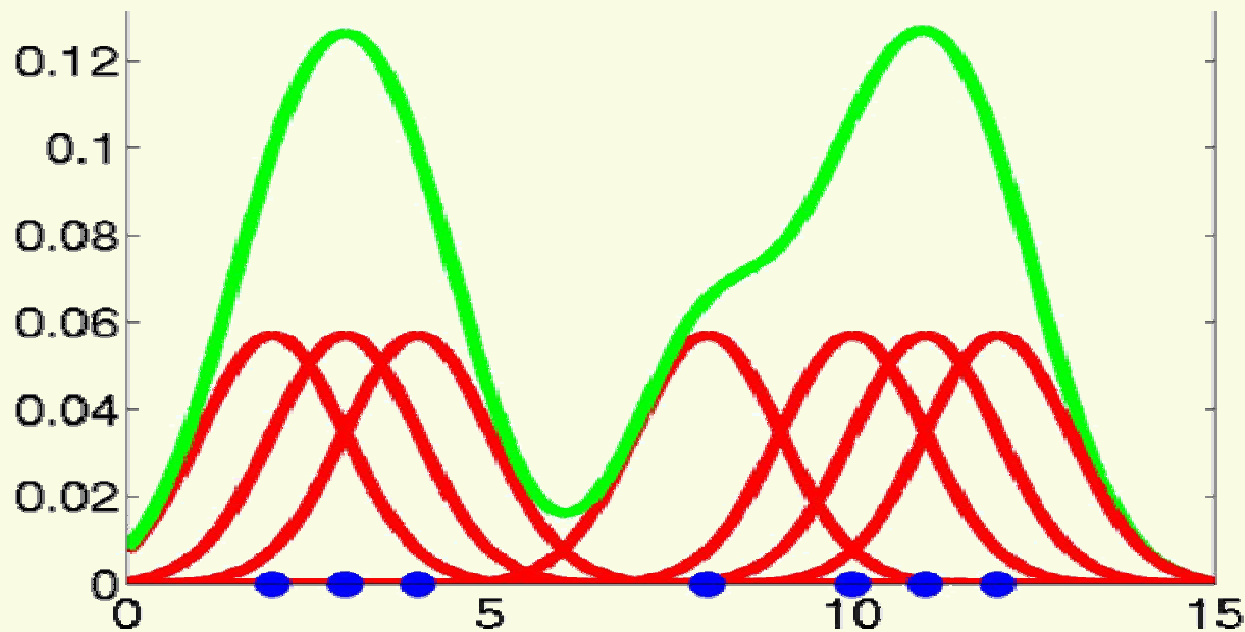


- Solves both drawbacks of the “box” window
 - Points \mathbf{x} which are close to the sample point \mathbf{x}_i receive higher weight
 - Resulting density $p_{\varphi}(\mathbf{x})$ is smooth

Parzen Windows: Example with General φ

- Let's come back to our example
 - 7 samples $D=\{2,3,4,8,10,11,12\}$, $h=1$

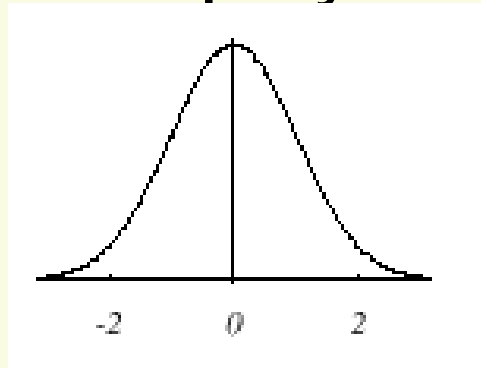
$$p_{\varphi}(\mathbf{x}) = \frac{1}{7} \sum_{i=1}^{i=7} \varphi(\mathbf{x} - \mathbf{x}_i)$$



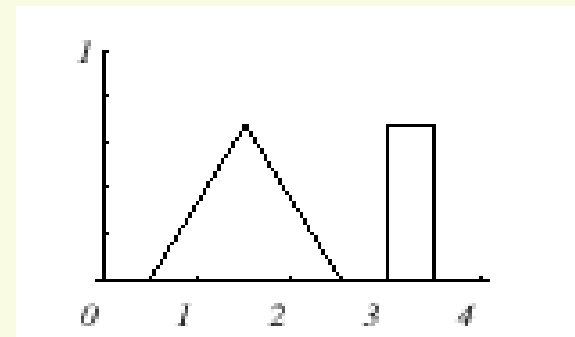
- $p_{\varphi}(\mathbf{x})$ is the sum of 7 Gaussians, each centered at one of the sample points, and each scaled by $1/7$

Parzen Windows: Did We Solve the Problem?

- Let's test if we solved the problem
 1. Draw samples from a known distribution
 2. Use our density approximation method and compare with the true density
- We will vary the number of samples n and the window size h
- We will play with 2 distributions

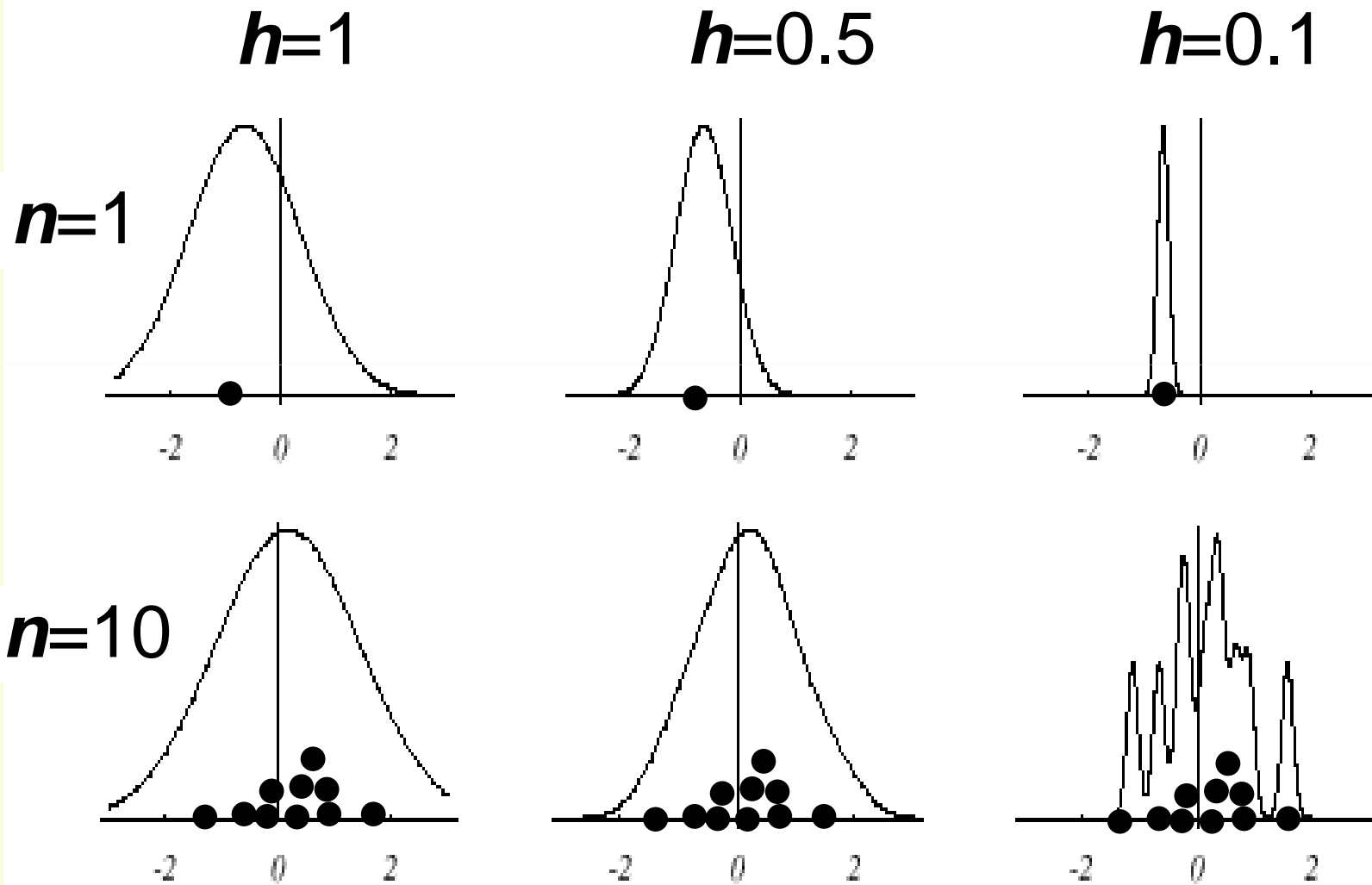
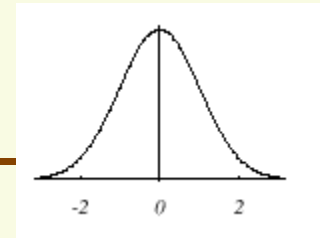


$N(0, 1)$



***triangle and
uniform mixture***

Parzen Windows: True Density $N(0,1)$



Parzen Windows: True Density $N(0,1)$

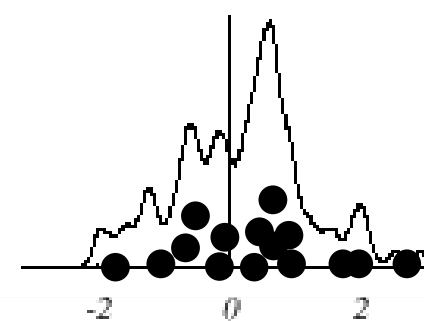
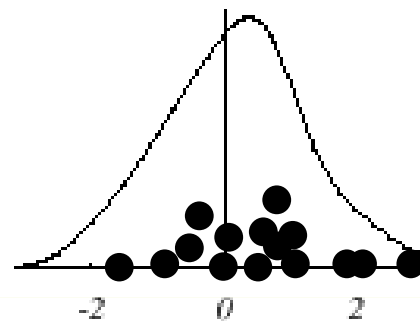
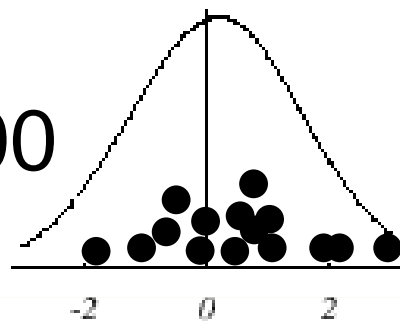


$h=1$

$h=0.5$

$h=0.1$

$n=100$



$n=\infty$

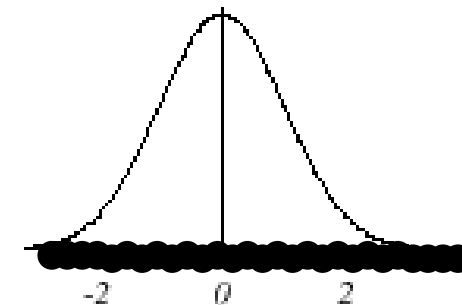
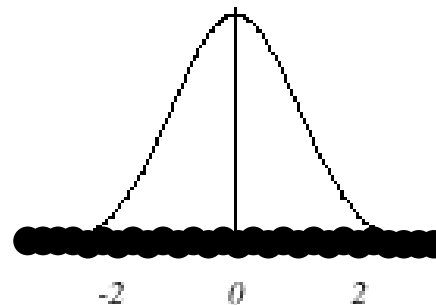
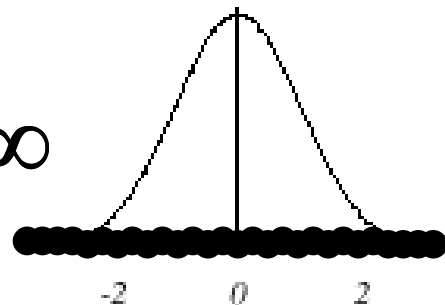
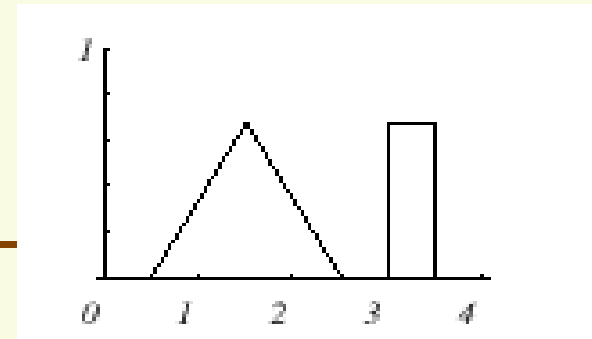


FIGURE 4.5. Parzen-window estimates of a univariate normal density using different window widths and numbers of samples. The vertical axes have been scaled to best show the structure in each graph. Note particularly that the $n = \infty$ estimates are the same (and match the true density function), regardless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

Parzen Windows: True density is Mixture of Uniform and Triangle

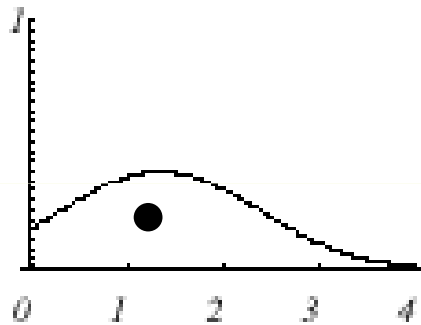


$h=1$

$h_j=1$

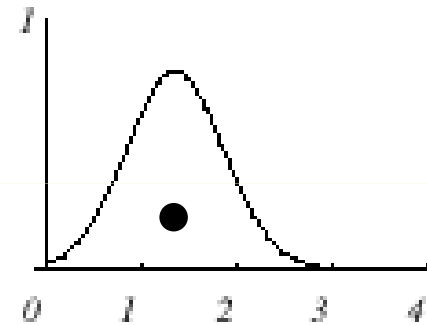
$n=1$

$r=1$



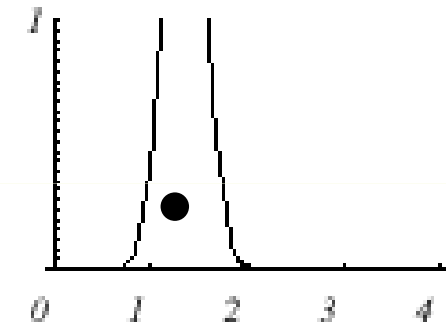
$h=0.5$

$h_j=0.5$

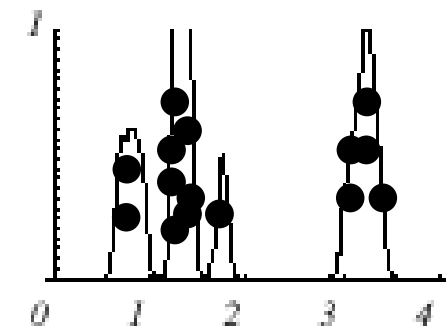
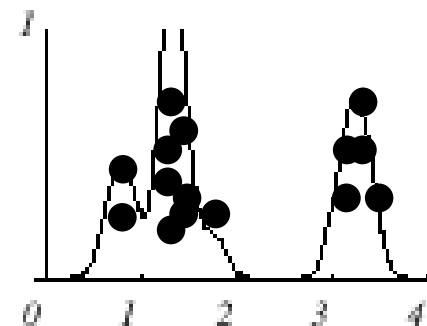
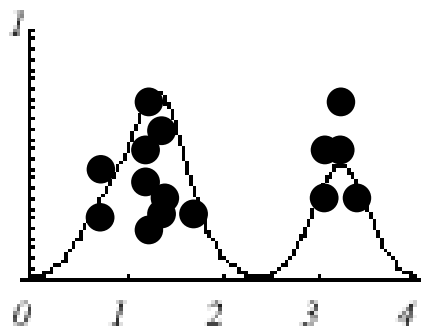


$h=0.2$

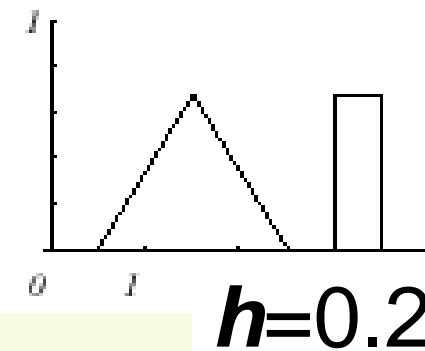
$h_j=0.2$



$n=16$



Parzen Windows: True density is Mixture of Uniform and Triangle



$h=1$

$h=0.5$

$h=0.2$

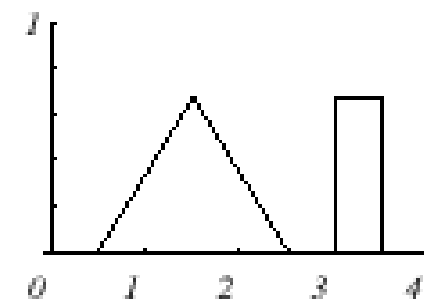
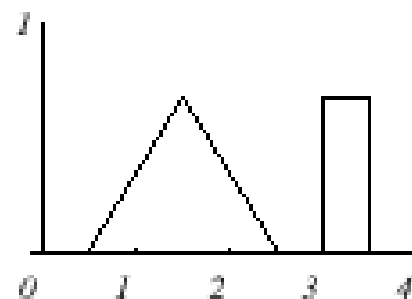
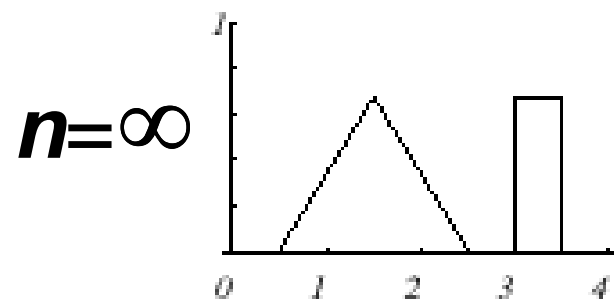
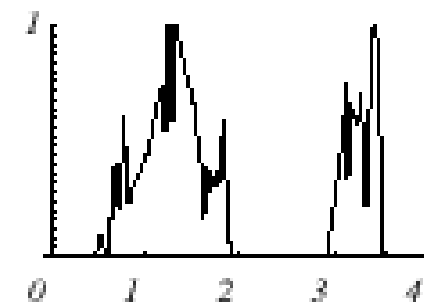
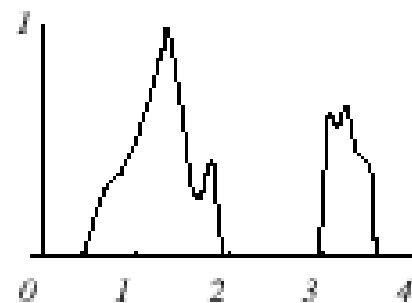
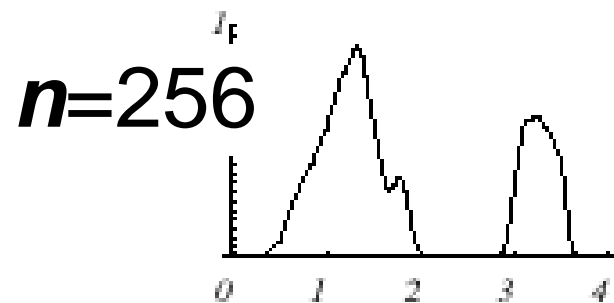
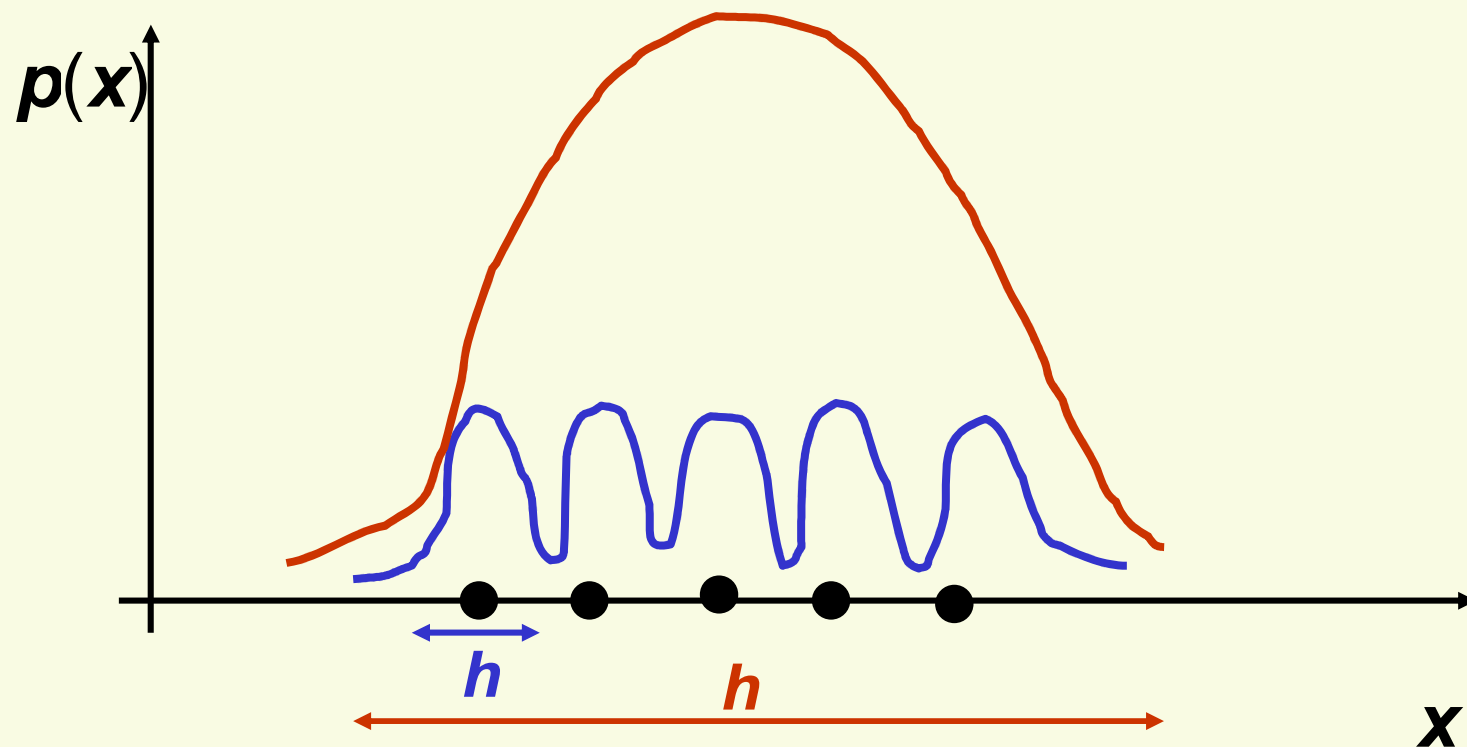


FIGURE 4.7. Parzen-window estimates of a bimodal distribution using different window widths and numbers of samples. Note particularly that the $n = \infty$ estimates are the same (and match the true distribution), regardless of window width. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern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

Parzen Windows: Effect of Window Width h

- By choosing h we are guessing the region where density is approximately constant
- Without knowing anything about the distribution, it is really hard to guess where the density is approximately constant



Parzen Windows: Effect of Window Width h

- If h is small, we superimpose n sharp pulses centered at the data
 - Each sample point x_i influences too small range of x
 - **Smoothed too little**: the result will look noisy and not smooth enough
- If h is large, we superimpose broad slowly changing functions,
 - Each sample point x_i influences too large range of x
 - **Smoothed too much**: the result looks oversmoothed or “out-of-focus”
- Finding the best h is challenging, and indeed no single h may work well
 - May need to adapt h for different sample points
- **However we can try to learn the best h to use from our labeled data**

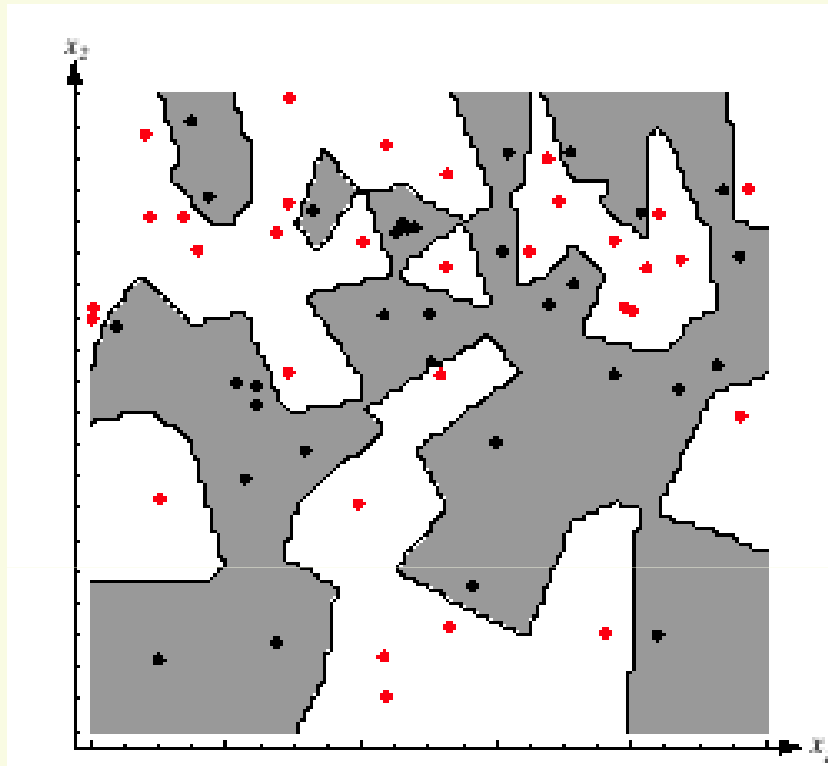
Learning window width h From Labeled Data

- Divide labeled data into *training* set, *validation* set, *test* set
- For a range of different values of h (possibly using binary search), construct density estimate $p(x)$ using Parzen windows
- Test the classification performance on the ***validation*** set for each value of h you tried
- For the final density estimate, choose h giving the smallest error on the ***validation*** set
- Now you can test the performance of the classifier on the test set
 - Notice we need validation set to find best parameter h , we can't use test set for this because test set cannot be used for training
 - In general, need validation set if our classifier has some tunable parameters

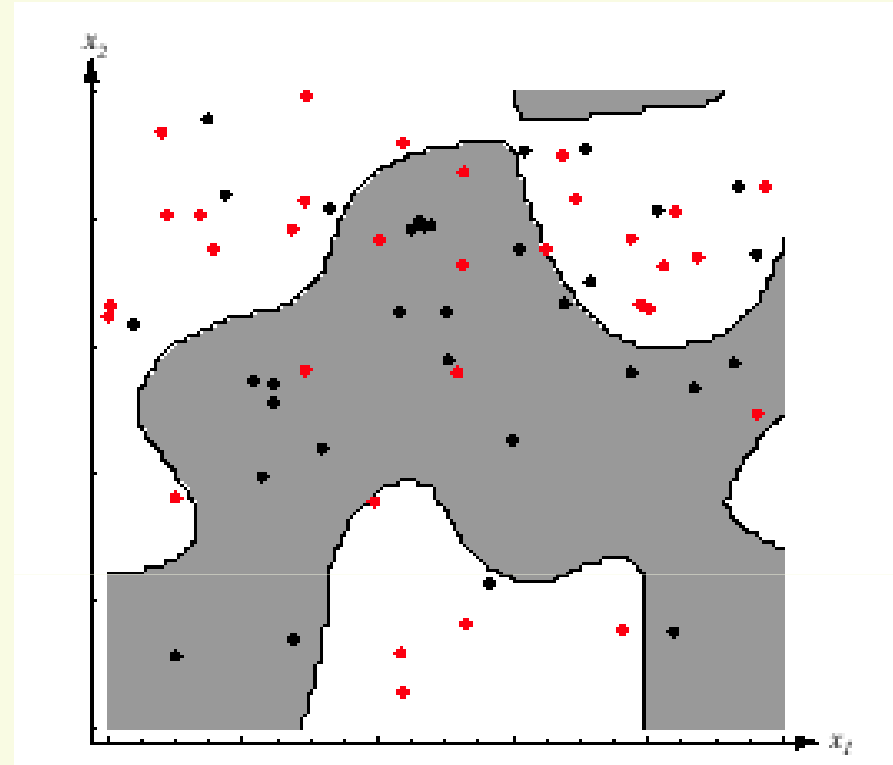
Parzen Windows: Classification Example

- 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

Parzen Windows: Classification Example



- For **small** enough window size h the classification on training data is perfect
- However decision boundaries are complex and this solution is not likely to generalize well to novel data



- For **larger** window size h , classification on training data is not perfect
- However decision boundaries are simpler and this solution is more likely to generalize well to novel data

Parzen Windows: Summary

- Advantages

- Can be applied to the data from any distribution
- In theory can be shown to converge as the number of samples goes to infinity

- Disadvantages

- Number of training data is limited in practice, and so choosing the appropriate window size h is difficult
- May need large number of samples for accurate estimates
- Computationally heavy, to classify one point we have to compute a function which potentially depends on all samples

$$p_{\varphi}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{i=n} \frac{1}{h^d} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)$$

- **But we need a lot of samples for accurate density estimation!**