Nonparametric Density Estimation Intro Parzen Windows

C9

Today

- Introduction to nonparametric techniques
- Basic Issues in Density Estimation
- Two Density Estimation Methods
 - 1. Parzen Windows (today)
 - 2. Nearest Neighbors (next time)

Non-Parametric Methods

 Neither probability distribution nor discriminant function is known

a lot is known "easier"

- Happens quite often
- All we have is labeled data



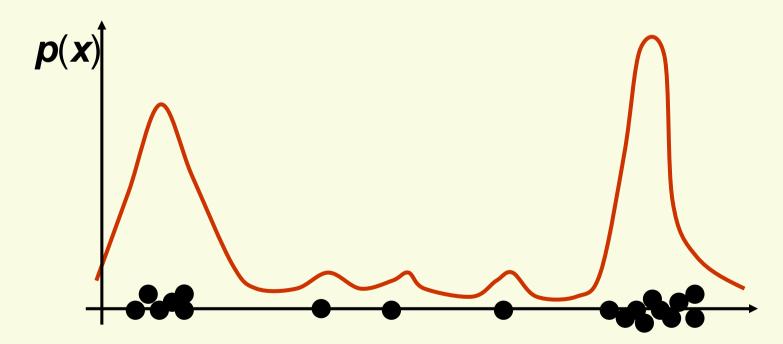
 Estimate the probability distribution from the labeled data

> little is known "harder"

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

- Nonparametric 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 $p(x \mid c_i)$
 - Nearest Neighbors
 - Bypass likelihood and go directly to posterior estimation
 $P(c_i \mid x)$

- 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 $Pr[X \in \Re] = \int f(x) dx$

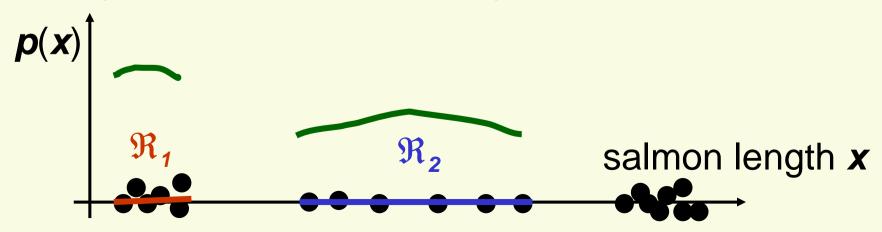


$$Pr[X \in \mathfrak{R}] = \int_{\mathfrak{R}} f(x) dx$$

- How can we approximate $P_r^{\Re}[X \in \Re_1]$ and $P_r[X \in \Re_2]$?
 - $Pr[X \in \mathfrak{R}_1] \approx \frac{6}{20}$ and $Pr[X \in \mathfrak{R}_2] \approx \frac{6}{20}$
- Should the density curves above R₁ and R₂ be equally high?
 - No, since \mathcal{R}_1 is smaller than \mathcal{R}_2

$$Pr[X \in \Re_1] = \int_{\Re_1} f(x) dx \approx \int_{\Re_2} f(x) dx = Pr[X \in \Re_2]$$

To get density, normalize by region size



• Assuming f(x) is basically flat inside R,

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

Thus, density at a point x inside R can be approximated

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

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- ρ
- 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 $var(K) = n\rho(1-\rho)$

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:

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

• Suppose we have samples $x_1, x_2, ..., x_n$ drawn from the distribution p(x). The probability that k points fall in 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 R, we can use MLE to estimate the value of ρ . The likelihood function is

$$p(x_1,...,x_n \mid \rho) = {n \choose k} \rho^k (1-\rho)^{n-k}$$

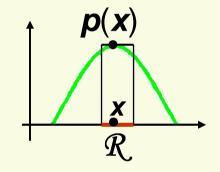
Density Estimation: Basic Issues

$$p(x_1,...,x_n \mid \rho) = {n \choose k} \rho^k (1-\rho)^{n-k}$$

- This likelihood function is maximized at $\rho = \frac{\kappa}{2}$
- Thus the MLE is $\hat{\rho} = \frac{k}{n}$
- Assume that p(x) is continuous and that the region Ris so small that p(x) is approximately constant in R.

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





- Recall from the previous slide: $\rho = \int p(x')dx'$
- Thus p(x) can be approximated: $p(x) \approx \frac{k/n}{1/2}$

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

Density Estimation: Basic Issues

This is exactly what we had before:

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



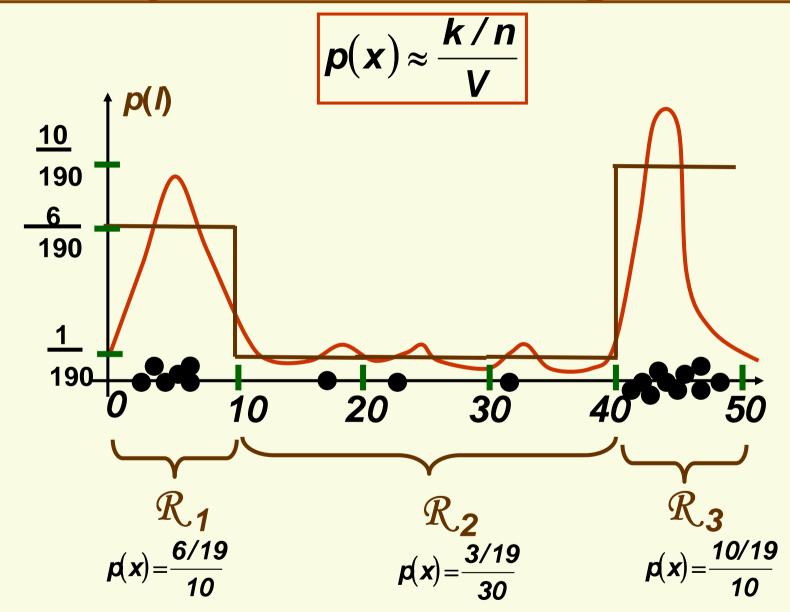
 $k = number of samples inside the following of <math>\mathcal{R}$ $N = number of samples inside the following of <math>\mathcal{R}$ N = number of samples $p(x) \approx \frac{k/n}{V}$ x is inside some region \Re $k = number of samples inside <math>\Re$

 Our estimate will always be the average of true density over R.

$$p(x) \approx \frac{k/n}{V} = \frac{\hat{\rho}}{V} \approx \frac{\int p(x')dx'}{V}$$

• Ideally, p(x) should be constant inside R.

Density Estimation: Histogram



• If regions \mathcal{R}_{i} 's do not overlap, we have a histogram

Density Estimation: Accuracy

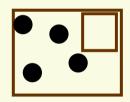
- How accurate is density approximation $p(x) \approx \frac{k/n}{V}$?
- We have made two approximations

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

as n increases, this estimate becomes more accurate

$$2. \int p(x')dx' \cong p(x)V$$

as R grows smaller, the estimate becomes more accurate



- As we shrink \mathcal{R} we have to make sure it contains samples, otherwise our estimated $\mathbf{p}(\mathbf{x}) = 0$ 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 ℝ, but not too much so that ℝ still contains a lot of samples

Density Estimation: Accuracy

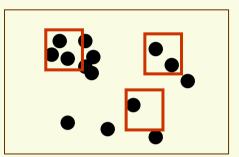
$$p(x) \approx \frac{k/n}{V}$$

- In practice, the number of samples is always fixed
- Thus the only available option to increase the accuracy is by decreasing the size of R (V gets smaller)
 - If V is too small, p(x)=0 for most 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(x) is approximately constant inside V

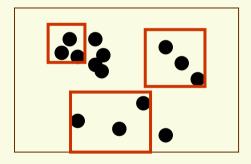
Density Estimation: Two Approaches

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

- 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

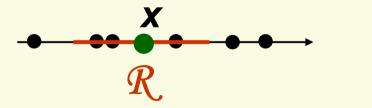


 Under appropriate conditions and as number of samples goes to infinity, both methods can be shown to converge to the true p(x)

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

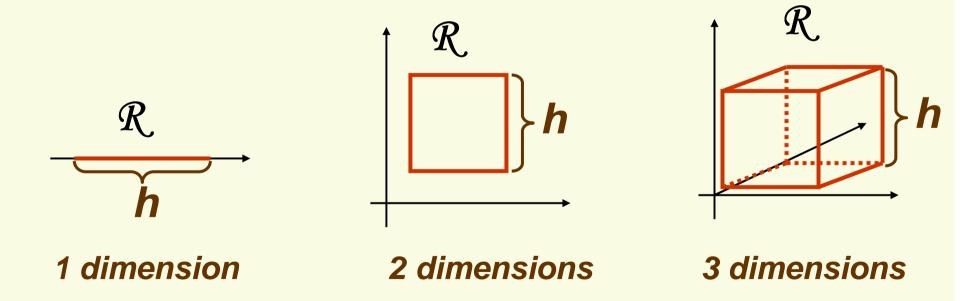
x is inside some region \mathcal{R} k = number of samples inside \mathcal{R} n=total number of samples V = volume of \mathcal{R}

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



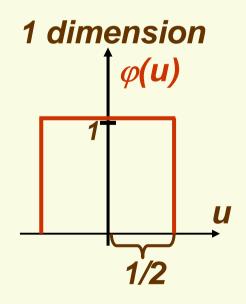
$$p(x) \approx \frac{3/6}{10}$$

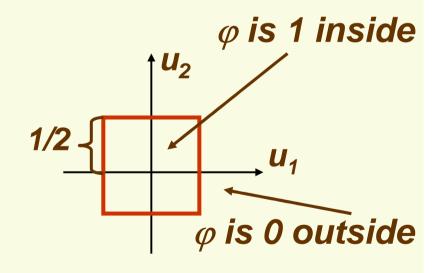
- In Parzen-window approach to estimate densities we fix the size and shape of region R
- Let us assume that the region \mathcal{R} is a d-dimensional hypercube with side length h thus it's volume is h^d



Let u=[u₁, u₂,..., u_d] and define a window function

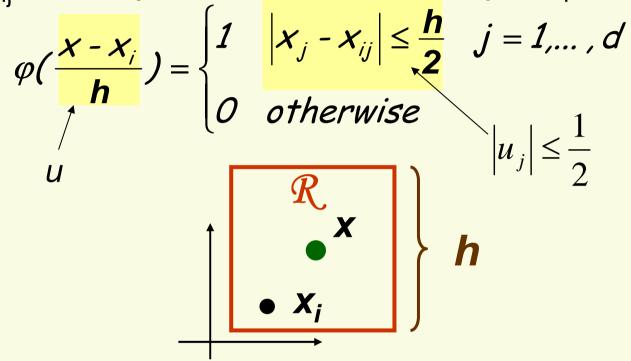
$$\varphi(u) = \begin{cases} 1 & |u_j| \le \frac{1}{2} & j = 1, \dots, d \\ 0 & \text{otherwise} \end{cases}$$





2 dimensions

• Recall we have d-dimensional samples $x_1, x_2, ..., x_n$. Let x_{ij} be the jth coordinate of sample x_i . Then



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

$$0 & \text{otherwise}$$

• How do we count the total number of sample points $x_1, x_2, ..., x_n$ which are inside the hypercube with side h and centered at x?

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

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

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

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

- Let's make sure $p_{\varphi}(x)$ is in fact a density
- $p_{\varphi}(x) \geq 0 \forall x$

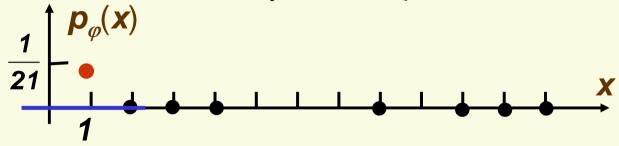
volume of hypercube

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

Parzen Windows: Example in 1D

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

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



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

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

$$\left| -\frac{1}{3} \right| \le 1/2 \qquad \left| -\frac{2}{3} \right| > 1/2 \qquad \left| -1 \right| > 1/2 \qquad \left| -\frac{11}{3} \right| > 1/2$$

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

Parzen Windows: Sum of Functions

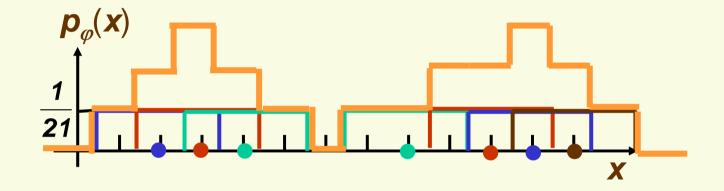
• Now let's look at our density estimate $p_{\omega}(x)$ again:

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

- 1 inside square centered at x_i0 otherwise
- Thus $p_{\varphi}(x)$ 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

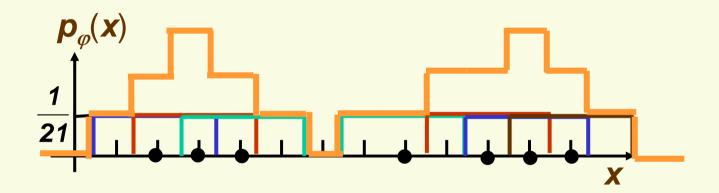


- To see what the function looks like, we need to generate 7 boxes and add them up
- The width is h=3 and the height is

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

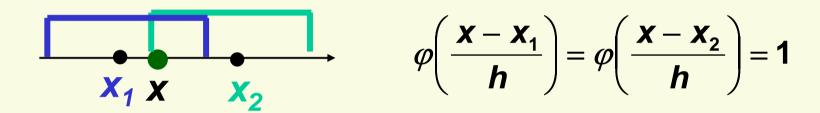
Parzen Windows: Interpolation

• In essence, window function φ is used for interpolation: each sample x_i contributes to the resulting density at x if x is close enough to x_i

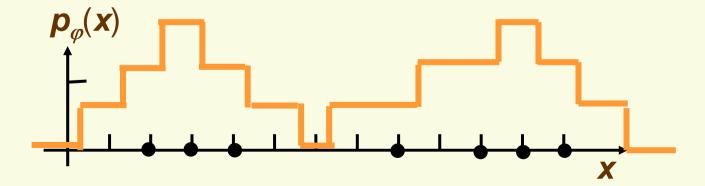


Parzen Windows: Drawbacks of Hypercube φ

 As long as sample point x_i and x are in the same hypercube, the contribution of x_i to the density at x is constant, regardless of how close x_i is to x



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



Parzen Windows: general ϕ

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

- We can use a general window φ as long as the resulting $\mathbf{p}_{\varphi}(\mathbf{x})$ is a legitimate density, i.e.
 - 1. $p_{\varphi}(u) \geq 0$
 - satisfied if $\varphi(u) \ge 0$
 - $2. \int p_{\varphi}(x)dx = 1$
 - satisfied if $\int \varphi(u) du = 1$

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

change coordinates to
$$u = \frac{X - X_i}{h}$$
, thus $du = \frac{dX}{h}$

Parzen Windows: general ϕ

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

- Notice that with the general window φ we are no longer counting the number of samples inside 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

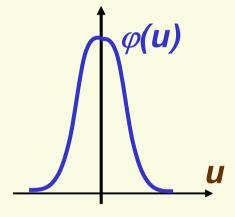
$$p_{\varphi}^{n}(x) \rightarrow p(x)$$

Parzen Windows: Gaussian ϕ

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

• A popular choice for φ is N(0,1) density

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

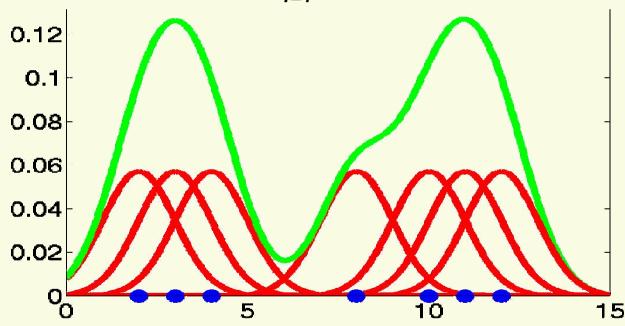


- Solves both drawbacks of the "box" window
 - Points x which are close to the sample point x_i receive higher weight
 - Resulting density $p_{\omega}(x)$ is smooth

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

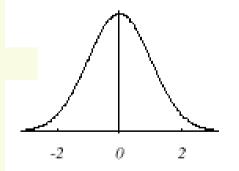
$$p_{\varphi}(x) = \frac{1}{7} \sum_{i=1}^{i=7} \varphi(x - x_i)$$



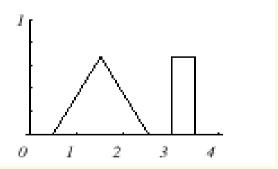
• $p_{\varphi}(x)$ is the sum of of 7 Gaussians, each centered at one of the sample points, and each scaled by 1/7

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

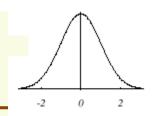


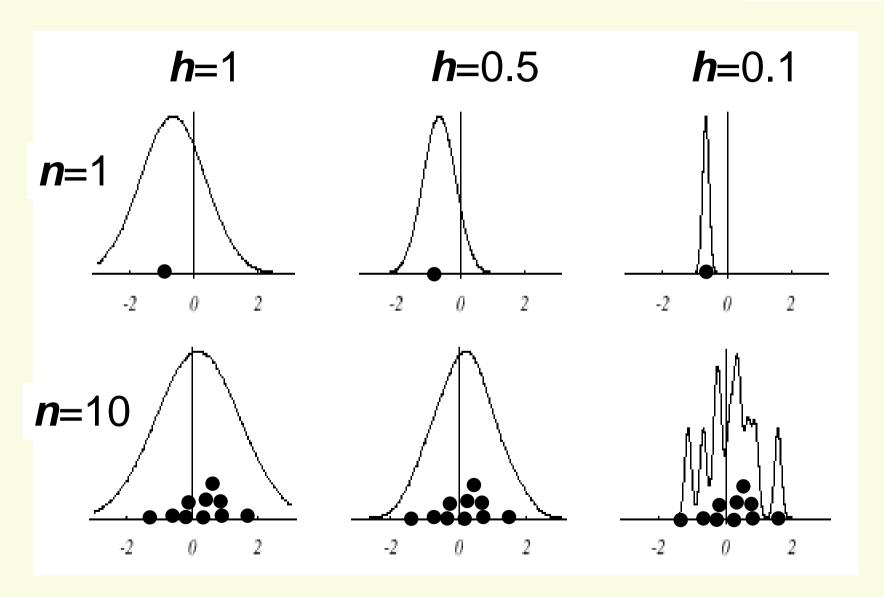
N(0, 1)



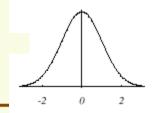
triangle and uniform mixture

Parzen Windows: True Density N(0,1)





Parzen Windows: True Density N(0,1)



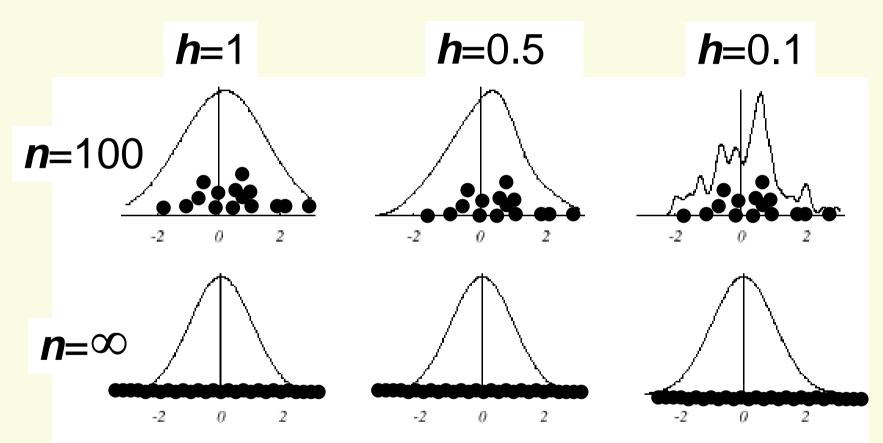
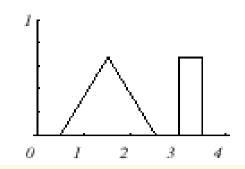
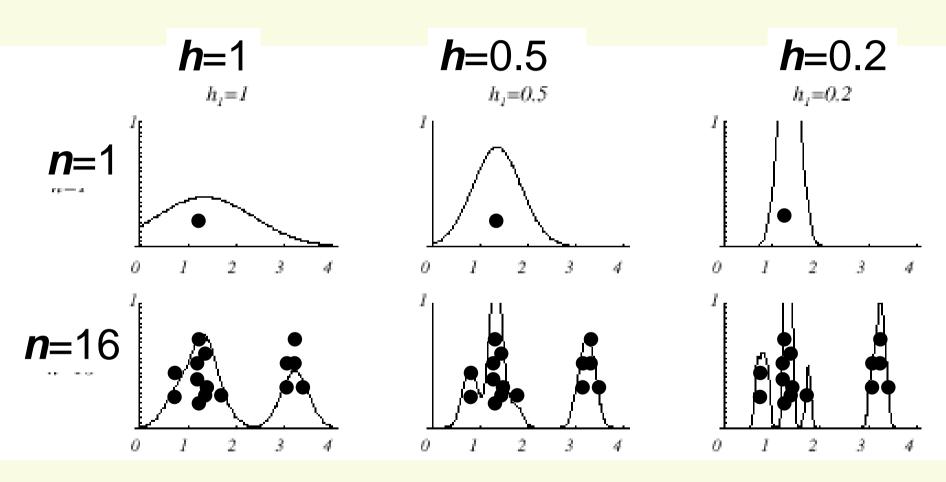


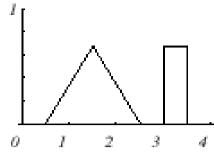
FIGURE 4.5. Parzen-window estimates of a univariate normal density using different window widths and numbers of samples. The vertical axes have been scaled to best show the structure in each graph. Note particularly that the $n = \infty$ estimates are the same (and match the true density function), regardless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

Parzen Windows: True density is Mixture of Uniform and Triangle





Parzen Windows: True density is Mixture of Uniform and Triangle



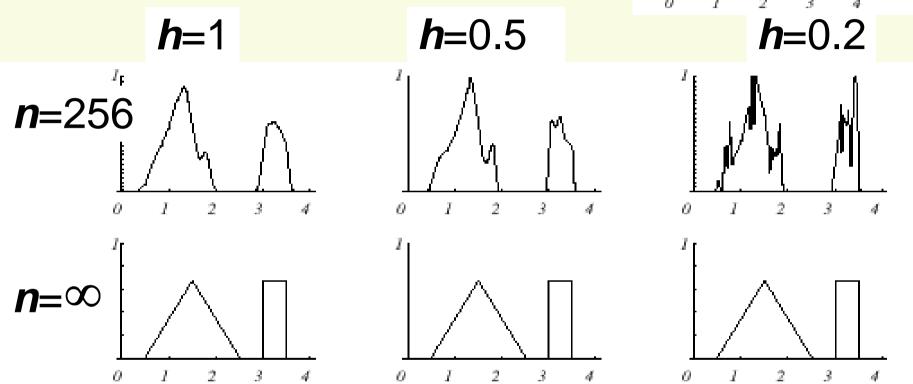
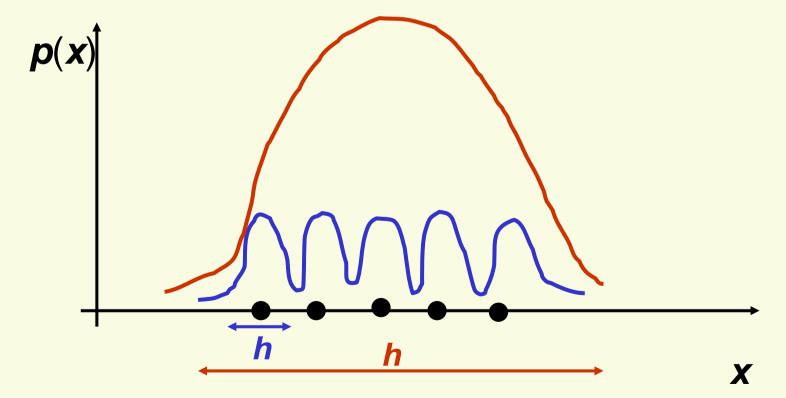


FIGURE 4.7. Parzen-window estimates of a bimodal distribution using different window widths and numbers of samples. Note particularly that the $n=\infty$ estimates are the same (and match the true distribution), regardless of window width. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern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

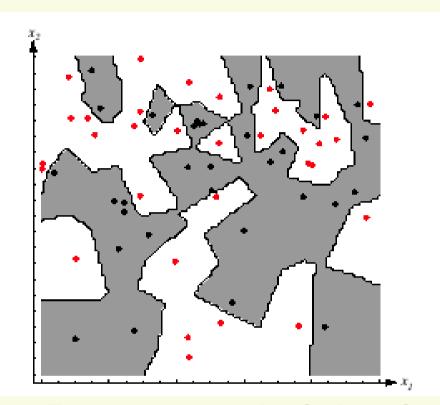
Learning window width h From Labeled Data

- 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

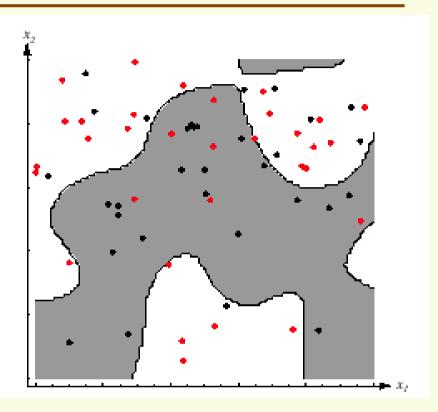
Parzen Windows: Classification Example

- 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

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

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