CS434b/654b : Pattern Recognition
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Lecture 6

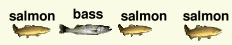
Nonparametric Density Estimation

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
  - 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 $p(\mathbf{x})$
     - In pattern recognition applications this never happens
  2. someone gives us $p(\mathbf{x}/\theta)$
     - 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

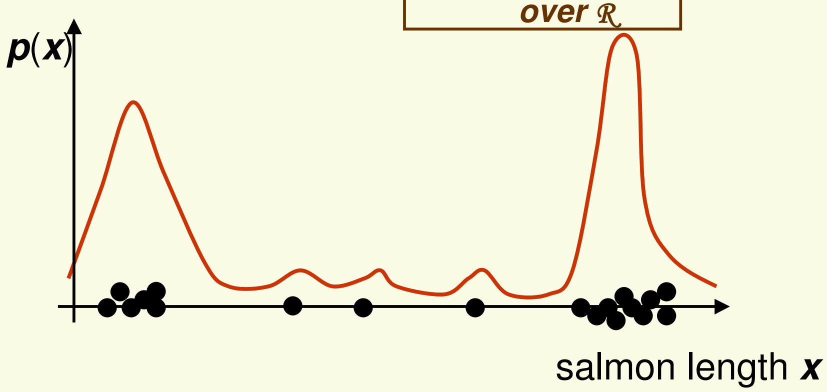
- Nonparametric procedures can be used with arbitrary distributions and without any assumption about the forms of the underlying densities
- There are two types of nonparametric methods:
  - Parzen windows
    - Estimate likelihood $p(x \mid c_j)$
  - Nearest Neighbors
    - Bypass likelihood and go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

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

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

average of f(x) over $\mathcal{R}$



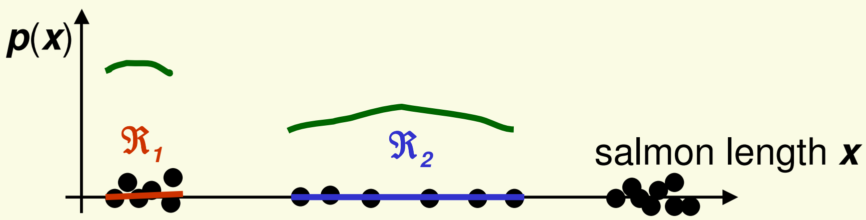
NonParametric Techniques: Introduction

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

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



NonParametric Techniques: Introduction

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

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

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

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

- 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 $\text{var}(K) = n\rho(1-\rho)$

Density Estimation: Basic Issues

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

$$\rho = Pr[x \in \Re] = \int_{\Re} p(x')dx'$$

- Suppose we have samples x_1, x_2,…, x_n drawn from the distribution $p(x)$. 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

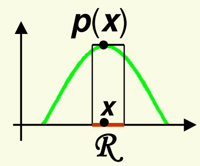
$$p(x_1,\ldots,x_n \mid \rho) = \binom{n}{k}\rho^k(1-\rho)^{n-k}$$

Density Estimation: Basic Issues

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

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

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

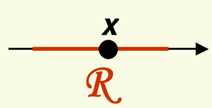


  - ***x*** is in $\mathcal{R}$ and ***V*** is the volume of $\mathcal{R}$
- Recall from the previous slide: $\rho = \int_{\Re} p(x')dx'$
- Thus ***p(x)*** can be approximated: $\boxed{p(x) \approx \dfrac{k/n}{V}}$

Density Estimation: Basic Issues

- This is exactly what we had before:

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



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

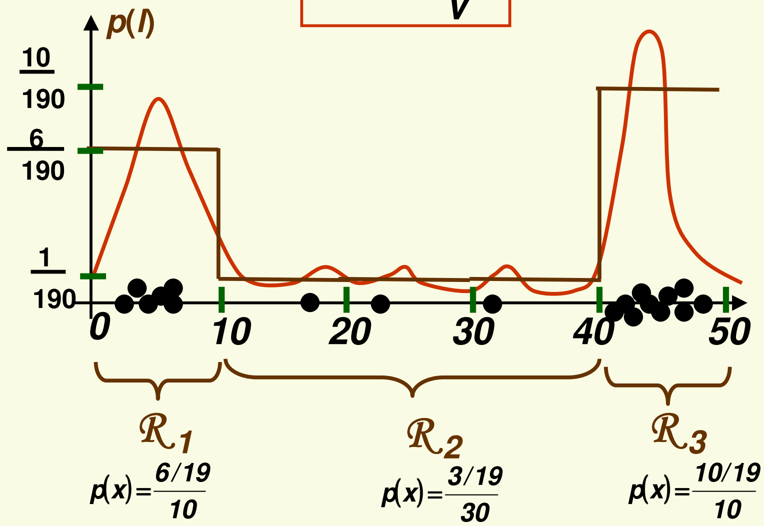
- Our estimate will always be the average of true density over $\mathcal{R}$

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

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

Density Estimation: Histogram

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

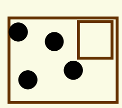


- If regions $\mathcal{R}_i$'s do not overlap, we have a histogram

Density Estimation: Accuracy

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

1. $\hat{\rho} = \frac{k}{n}$
   - as n increases, this estimate becomes more accurate
2. $\int_{\Re} p(x')dx' \cong p(x)V$
   - 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 **$p(x)$** = 0 for all **x** in $\mathcal{R}$

- Thus in theory, if we have an unlimited number of samples, to 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

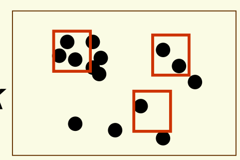
$$p(x) \approx \frac{k/n}{V}$$

- 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***(***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***

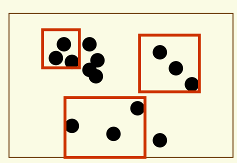
Density Estimation: Two Approaches

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

1. Parzen Windows:
   - Choose a fixed value for volume ***V*** and determine the corresponding ***k*** from the data



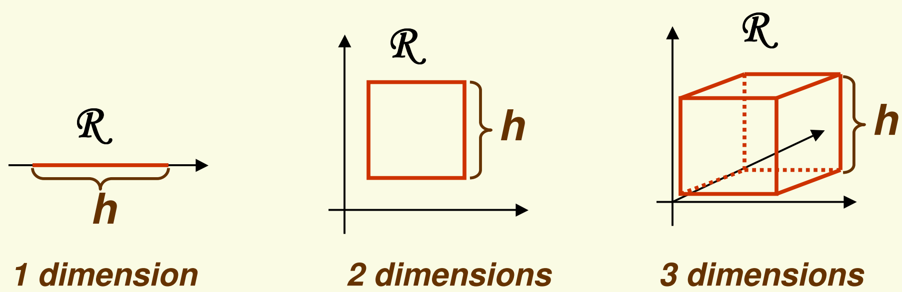
2. k-Nearest Neighbors
   - Choose a fixed value for ***k*** and determine the corresponding volume ***V*** from the data



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

Parzen Windows

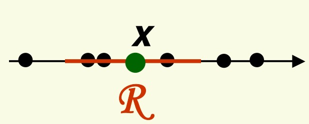
- In Parzen-window approach to estimate densities we fix the size and shape of region $\mathcal{R}$
- Let us assume that the region $\mathcal{R}$ is a ***d***-dimensional hypercube with side length ***h*** thus it's volume is h^d



Parzen Windows

- 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

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



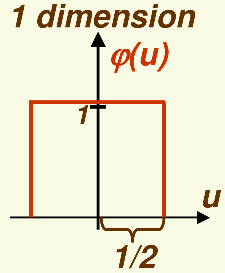
$$p(x) \approx \frac{3/6}{10}$$

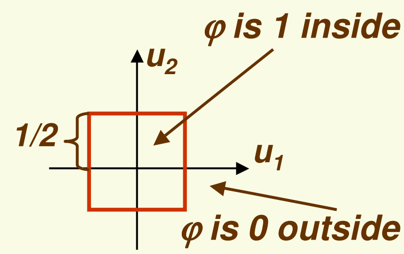
Parzen Windows

- We wish to have an analytic expression for our approximate density $\mathcal{R}$
- Let u=[u_1, u_2,…, u_d] and define a window function

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

1 dimension



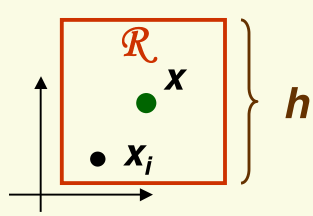


2 dimensions

Parzen Windows

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

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



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

Parzen Windows

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

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

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

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

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
- $p_\varphi(\mathbf{x}) \geq 0 \quad \forall \mathbf{x}$
- $\int p_\varphi(\mathbf{x})d\mathbf{x} = \int \frac{1}{n}\sum_{i=1}^{i=n} \frac{1}{h^d}\varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)d\mathbf{x} = \frac{1}{h^d n}\sum_{i=1}^{i=n} \overbrace{\int \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)d\mathbf{x}}^{\text{volume of hypercube}}$

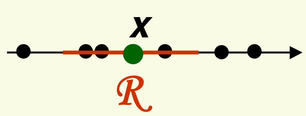
$$= \frac{1}{n}\frac{1}{h^d}\sum_{i=1}^{i=n} h^d = 1$$

Parzen Windows

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

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



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

Parzen Windows

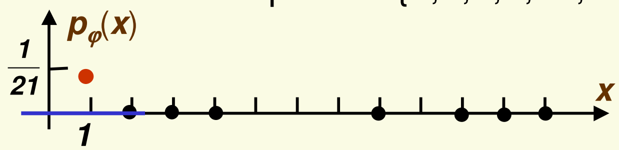
- Formula for Parzen window estimation

$$p_\varphi(x) = \frac{\overbrace{\sum_{i=1}^{i=n} \varphi\left(\frac{x - x_i}{h}\right)}^{=k} \Big/ n}{\underbrace{h^d}_{=V}} = \frac{1}{n} \sum_{i=1}^{i=n} \frac{1}{h^d} \varphi\left(\frac{x - x_i}{h}\right)$$

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

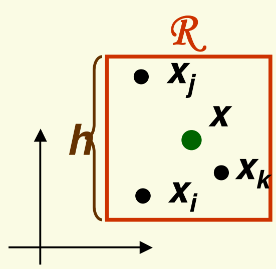
$$p_\varphi(1) = \frac{1}{7}\sum_{i=1}^{i=7}\frac{1}{3}\varphi\left(\frac{1-x_i}{3}\right) = \frac{1}{21}\left[\varphi\left(\frac{1-2}{3}\right)+\varphi\left(\frac{1-3}{3}\right)+\varphi\left(\frac{1-4}{3}\right)+\dots+\varphi\left(\frac{1-12}{3}\right)\right]$$

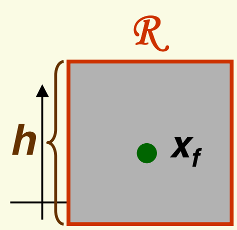
$$\left|-\frac{1}{3}\right| \le 1/2 \qquad \left|-\frac{2}{3}\right| > 1/2 \qquad \left|-1\right| > 1/2 \qquad \left|-\frac{11}{3}\right| > 1/2$$

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

Parzen Windows: Sum of Functions

- Fix x, let i vary and ask
  - For which samples x_i is $\varphi\left(\frac{x-x_i}{h}\right) = 1$?





- Now fix f and let x vary and ask
  - For which x is $\varphi\left(\frac{x-x_f}{h}\right) = 1$? For all x in gray box
- Thus $\varphi\left(\frac{x-x_f}{h}\right) = 1$ is simply a function which is 1 inside square of width h centered at x_f and 0 otherwise!

Parzen Windows: Sum of Functions

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

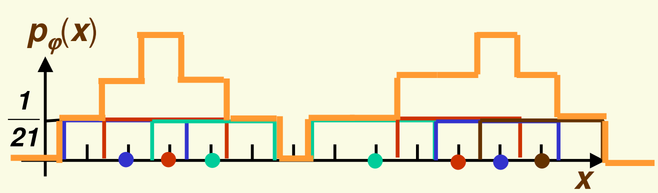
$$p_\varphi(x) = \frac{1}{n}\sum_{i=1}^{i=n}\frac{1}{h^d}\,\varphi\left(\frac{x-x_i}{h}\right) = \sum_{i=1}^{i=n}\frac{1}{nh^d}\,\underbrace{\varphi\left(\frac{x-x_i}{h}\right)}_{}$$

1 inside square centered at x_i
0 otherwise

- Thus $\boldsymbol{p_\varphi}$($\boldsymbol{x}$) is just a sum of ***n*** "box like" functions each of height $\dfrac{1}{nh^d}$

Parzen Windows: Example in 1D

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

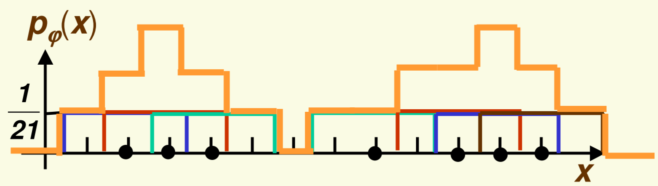


- To see what the function looks like, we need to generate 7 boxes and add them up
- The width is ***h***=3 and the height, according to previous slide is

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

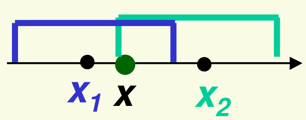
Parzen Windows: Interpolation

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



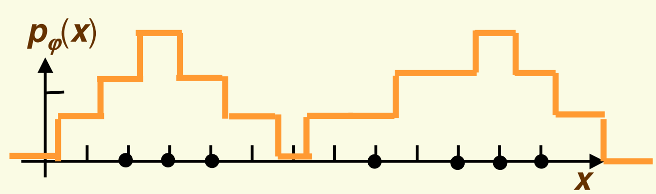
Parzen Windows: Drawbacks of Hypercube φ

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



$$\varphi\left(\frac{x - x_1}{h}\right) = \varphi\left(\frac{x - x_2}{h}\right) = 1$$

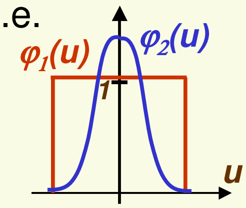
- The resulting density $\boldsymbol{p_\varphi(x)}$ is not smooth, it has discontinuities



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 $p_\varphi(x)$ is a legitimate density, i.e.



1. $p_\varphi(u) \geq 0$
   - satisfied if $\varphi(u) \geq 0$
2. $\int p_\varphi(x)dx = 1$
   - satisfied if $\int \varphi(u)du = 1$

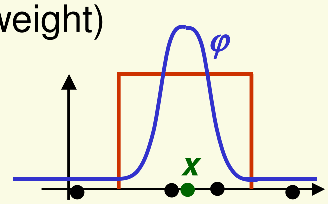
$$\int p_\varphi(x)dx = \frac{1}{nh^d}\sum_{i=1}^{i=n}\int \varphi\left(\frac{x-x_i}{h}\right)dx = \frac{1}{nh^d}\sum_{i=1}^{n}\int h^d\varphi(u)du = 1$$

change coordinates to $u = \frac{x-x_i}{h}$, thus $du = \frac{dx}{h}$

Parzen Windows: general φ

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

- 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

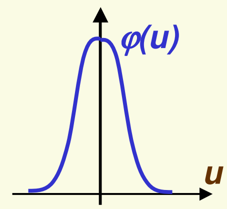
$$p_\varphi^n(x) \to p(x)$$

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

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

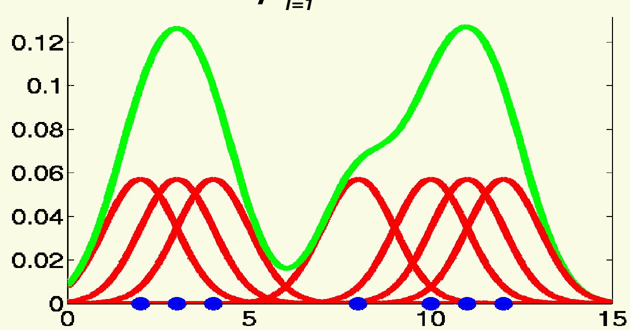


- Solves both drawbacks of the "box" window
  - Points x which are close to the sample point x_i receive higher weight
  - Resulting density $p_\varphi(x)$ is smooth

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

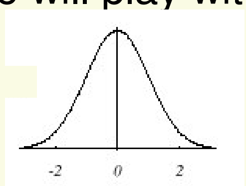
$$p_\varphi(x) = \frac{1}{7}\sum_{i=1}^{i=7}\varphi(x - x_i)$$



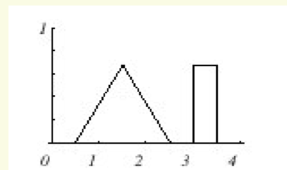
- $p_\varphi(x)$ is the sum of of 7 Gaussians, each centered at one of the sample points, and each scaled by 1/7

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

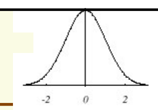


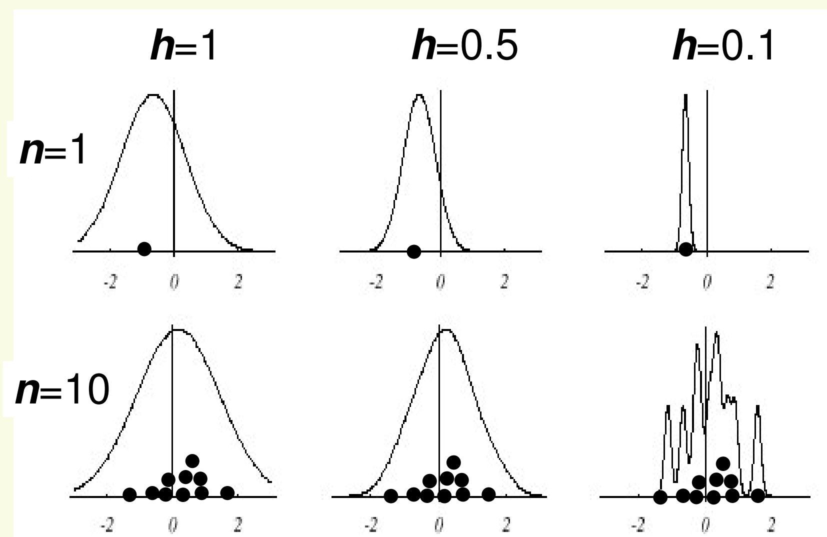
***N*(*0*,*1*)**



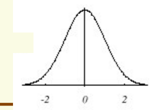
triangle and uniform mixture

Parzen Windows: True Density N(0,1)





Parzen Windows: True Density N(0,1)



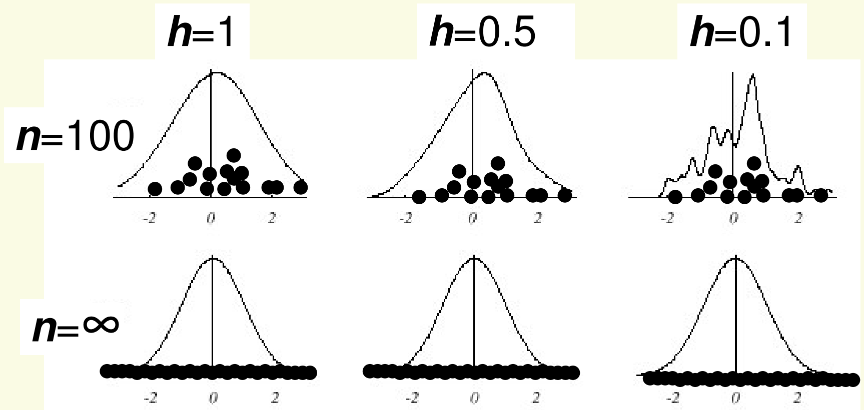
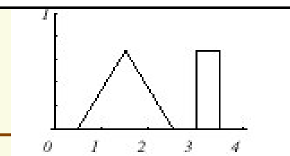
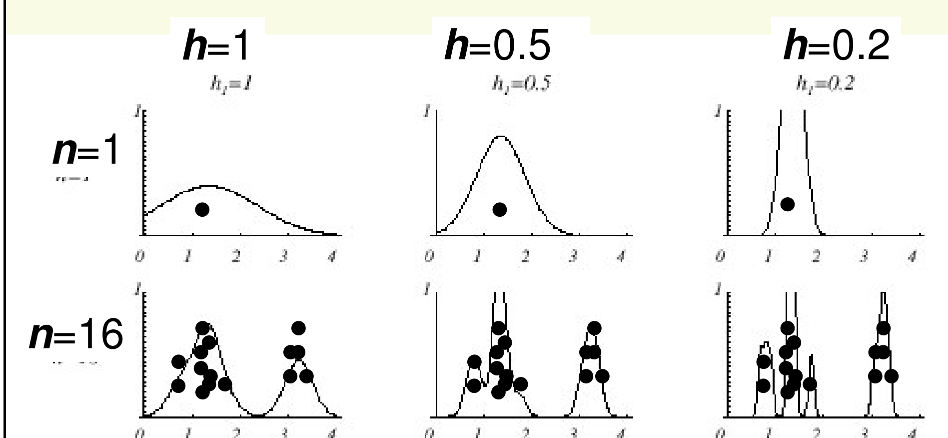


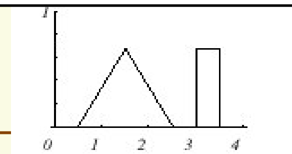
FIGURE 4.5. Parzen-window estimates of a univariate normal density using different window widths and numbers of samples. The vertical axes have been scaled to best show the structure in each graph. Note particularly that the $n = \infty$ estimates are the same (and match the true density function), regardless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



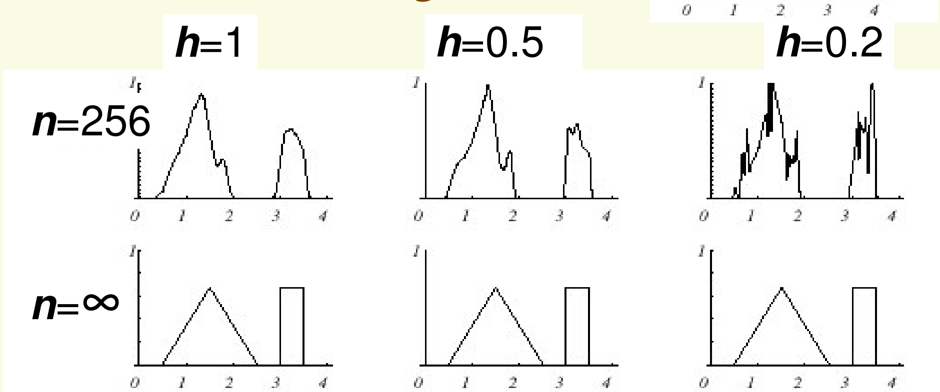
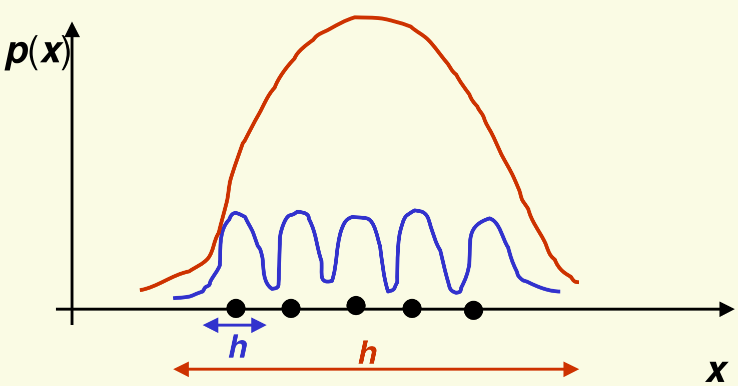


FIGURE 4.7. Parzen-window estimates of a bimodal distribution using different window widths and numbers of samples. Note particularly that the $n = \infty$ estimates are the same (and match the true distribution), regardless of window width. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern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

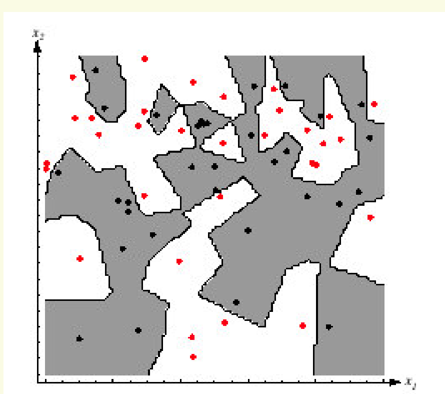
Learning window width *h* From Labeled Data

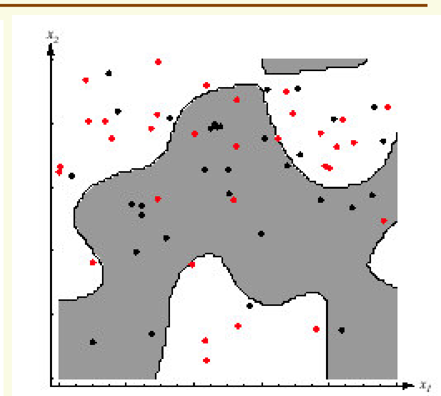
- Divide labeled data into *training* set, *validation* set, *test* set
- For a range of different values of *h* (possibly using binary search), construct density estimate p(x) using Parzen windows
- Test the classification performance on the ***validation*** set for each value of *h* you tried
- For 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* is classification on training data is be 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

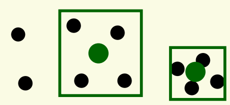
- Advantages
  - Can be applied to the data from any distribution
  - In theory can be shown to converge as the number of samples goes to infinity
- Disadvantages
  - Number of training data is limited in practice, and so choosing the appropriate window size ***h*** is difficult
  - May need large number 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!**

k-Nearest Neighbors

- Recall the generic expression for density estimation
$$p(x) \approx \frac{k/n}{V}$$
- In Parzen windows estimation, we fix V and that determines k, the number of points inside V
- In k-nearest neighbor approach we fix k, and find V that contains k points inside

k-Nearest Neighbors

- kNN approach seems a good solution for the problem of the "best" window size
  - Let the cell volume be a function of the training data
  - Center a cell about x and let it grows until it captures ***k*** samples
  - ***k*** are called the ***k*** nearest-neighbors of ***x***

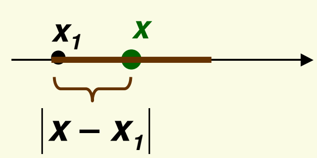


- 2 possibilities can occur:
  - Density is high near *x*; therefore the cell will be small which provides a good resolution
  - Density is low; therefore the cell will grow large and stop until higher density regions are reached

k-Nearest Neighbor

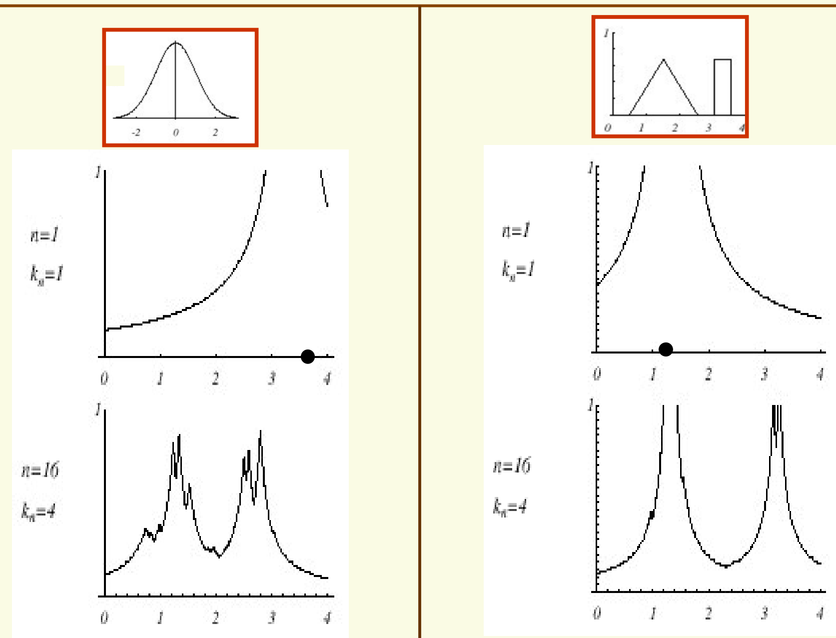
- Of course, now we have a new question
  - How to choose ***k***?
- A good "rule of thumb" is ***k*** = $\sqrt{n}$
  - Can prove convergence if **n** goes to infinity
  - Not too useful in practice, however
- Let's look at 1-D example
  - we have one sample, i.e. ***n*** = 1

$$p(x) \approx \frac{k/n}{V} = \frac{1}{2|x - x_1|}$$



- But the estimated ***p***(***x***) is not even close to a density function: $\int_{-\infty}^{\infty} \frac{1}{2|x - x_1|} dx = \infty \neq 1$

k-Nearest Neighbor: Density estimation



k-Nearest Neighbor

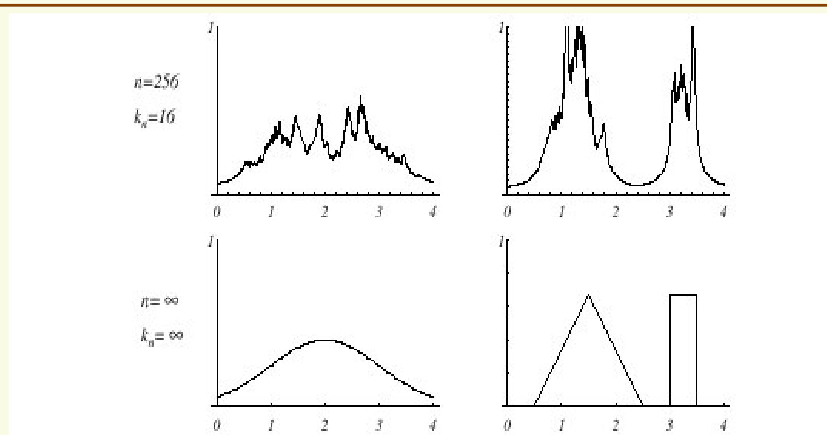


FIGURE 4.12. Several k-nearest-neighbor estimates of two unidimensional densities: a Gaussian and a bimodal distribution. Notice how the finite n estimates can be quite "spiky." From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*.

k-Nearest Neighbor

- Thus straightforward density estimation $\boldsymbol{p}(\boldsymbol{x})$ does not work very well with kNN approach because the resulting density estimate
  1. Is not even a density
  2. Has a lot of discontinuities (looks very spiky, not differentiable)
  3. Even for large regions with no observed samples the estimated density is far from zero (tails are too heavy)
- *Notice in the theory, if infinite number of samples is available, we could construct a series of estimates that converge to the true density using kNN estimation. However this theorem is not very useful in practice because the number of samples is always limited*

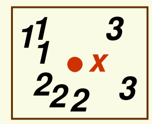
k-Nearest Neighbor

- However we shouldn't give up the nearest neighbor approach yet
- Instead of approximating the density $\boldsymbol{p}(\boldsymbol{x})$, we can use kNN method to approximate the posterior distribution $\boldsymbol{P}(\boldsymbol{c_i}|\boldsymbol{x})$
  - We don't need $\boldsymbol{p}(\boldsymbol{x})$ if we can get a good estimate on $\boldsymbol{P}(\boldsymbol{c_i}|\boldsymbol{x})$

k-Nearest Neighbor

- How would we estimate $P(c_i \mid x)$ from a set of n labeled samples?
- Recall our estimate for density: $p(x) \approx \frac{k/n}{V}$
- Let's place a cell of volume V around x and capture k samples
  - k_i samples amongst k labeled c_i then:

$$p(c_i, x) \approx \frac{k_i/n}{V}$$



- Using conditional probability, let's estimate posterior:

$$p(c_i \mid x) = \frac{p(x, c_i)}{p(x)} = \frac{p(x, c_i)}{\sum_{j=1}^{m} p(x, c_j)} \approx \frac{k_i/n}{V \sum_{j=1}^{m} \frac{k_j/n}{V}} = \frac{k_i}{\sum_{j=1}^{m} k_j} = \frac{k_i}{k}$$

k-Nearest Neighbor Rule

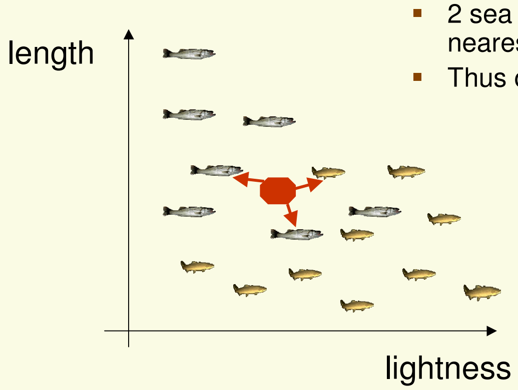
- Thus our estimate of posterior is just the fraction of samples which belong to class c_i:

$$p(c_i \mid x) = \frac{k_i}{k}$$

- This is a very simple and intuitive estimate
- Under the zero-one loss function (MAP classifier) just choose the class which has the largest number of samples in the cell
- Interpretation is: given an unlabeled example (that is x), find k most similar labeled examples (closest neighbors among sample points) and assign the most frequent class among those neighbors to x

k-Nearest Neighbor: Example

- Back to fish sorting
  - Suppose we have 2 features, and collected sample points as in the picture
  - Let k = 3



- 2 sea bass, 1 salmon are the 3 nearest neighbors
- Thus classify as sea bass

kNN: How Well Does it Work?

- kNN rule is certainly simple and intuitive, but does it work?
- Assume we have an unlimited number of samples
- By definition, the best possible error rate is the Bayes rate E^*
- Nearest-neighbor rule leads to an error rate greater than E^*
- But even for k =1, as $n \to \infty$, it can be shown that nearest neighbor rule error rate is smaller than $2E^*$
- As we increase k, the upper bound on the error gets better and better, that is the error rate (as $n \to \infty$) for the ***kNN*** rule is smaller than cE^*,with smaller c for larger k
- If we have a lot of samples, the kNN rule will do very well !

1NN: Voronoi Cells

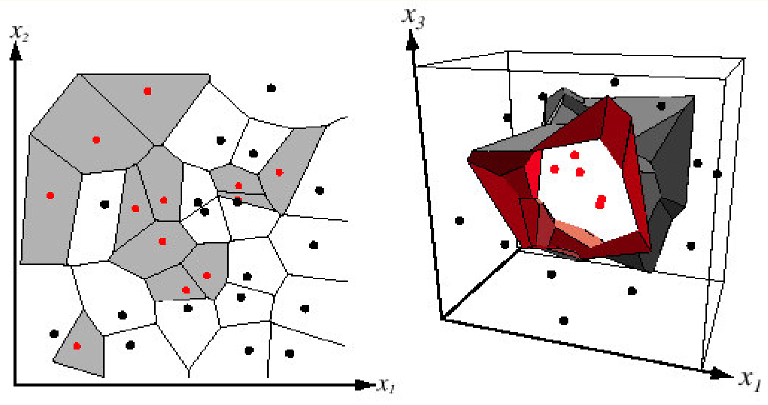
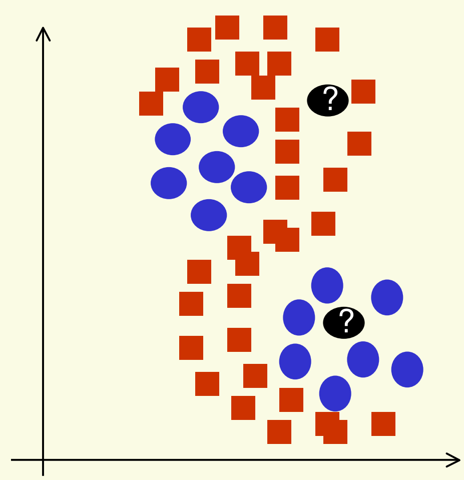


FIGURE 4.13. In two dimensions, the nearest-neighbor algorithm leads to a partitioning of the input space into Voronoi cells, each labeled by the category of the training point it contains. In three dimensions, the cells are three-dimensional, and the decision boundary resembles the surface of a crystal. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

kNN: Multi-Modal Distributions

- Most parametric distributions would not work for this 2 class classification problem:
- Nearest neighbors will do reasonably well, provided we have a lot of samples



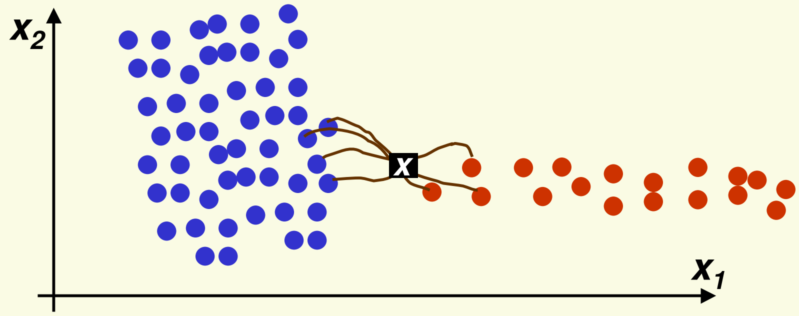
kNN: How to Choose k?

- In theory, when the infinite number of samples is available, the larger the ***k***, the better is classification (error rate gets closer to the optimal Bayes error rate)
- But the caveat is that all ***k*** neighbors have to be close to ***x***
  - Possible when infinite # samples available
  - Impossible in practice since # samples is finite

kNN: How to Choose k?

- In practice
  1. ***k*** should be large so that error rate is minimized
     - ***k*** too small will lead to noisy decision boundaries
  2. ***k*** should be small enough so that only nearby samples are included
     - ***k*** too large will lead to over-smoothed boundaries
- Balancing ***1*** and ***2*** is not trivial
  - This is a recurrent issue, need to smooth data, but not too much

kNN: How to Choose k?



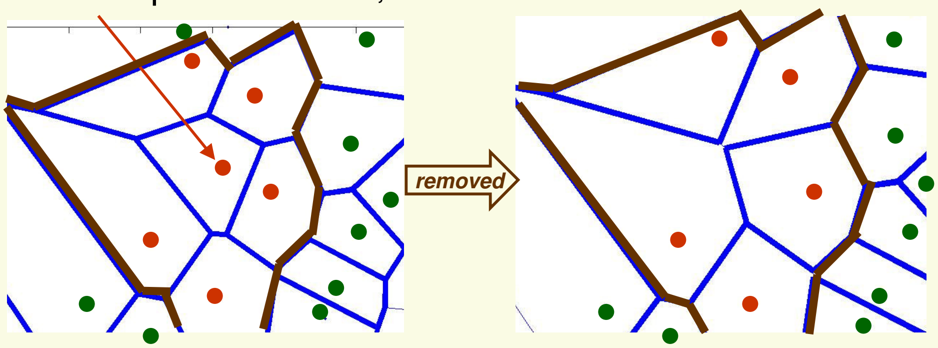
- For k = 1, …,7 point x gets classified correctly
  - red class
- For larger k classification of x is wrong
  - blue class

kNN: Computational Complexity

- Basic ***kNN*** algorithm stores all examples. Suppose we have n examples each of dimension k
  - $O(d)$ to compute distance to one example
  - $O(nd)$ to find one nearest neighbor
  - $O(knd)$ to find k closest examples examples
  - Thus complexity is $O(knd)$
- This is prohibitively expensive for large number of samples
- But we need large number of samples for ***kNN*** to work well!

Reducing Complexity: Editing 1NN

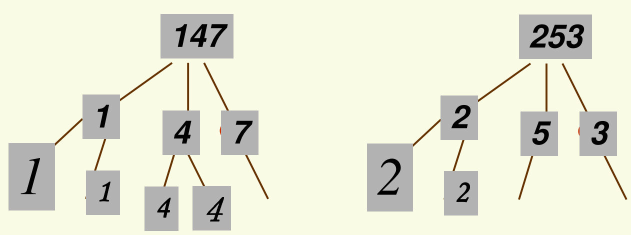
- If all voronoi neighbors have the same class, a sample is useless, we can remove it:



- Number of samples decreases
- We are guaranteed that the decision boundaries stay the same

Reducing Complexity: kNN prototypes

- Explore similarities between samples to represent data as search trees of *prototypes*



- Advantages: Complexity decreases
- Disadvantages:
  - finding good search tree is not trivial
  - will not necessarily find the closest neighbor, and thus **not** guaranteed that the decision boundaries stay the same

kNN: Selection of Distance

- So far we assumed we use Euclidian Distance to find the nearest neighbor:

$$D(a,b) = \sqrt{\sum_k (a_k - b_k)^2}$$

- However some features (dimensions) may be much more discriminative than other features (dimensions)
- Eucleadian distance treats each feature as equally important

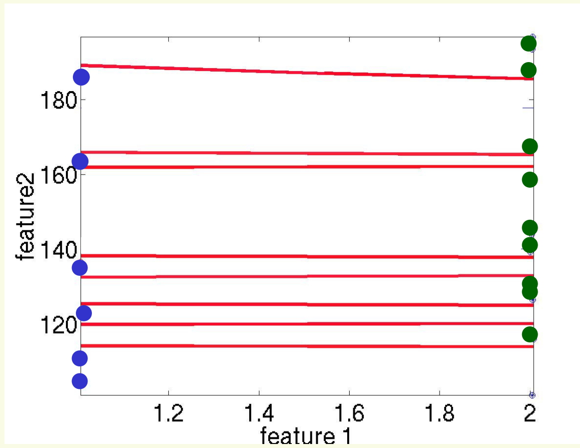
kNN: Selection of Distance

- Extreme Example
  - feature 1 gives the correct class: 1 or 2
  - feature 2 gives irrelevant number from 100 to 200
- Suppose we have to find the class of x=[1 100] and we have 2 samples [1 150] and [2 110]

$$D(\begin{bmatrix}1\\100\end{bmatrix},\begin{bmatrix}1\\150\end{bmatrix}) = \sqrt{(1-1)^2 + (100-150)^2} = 50 \qquad D(\begin{bmatrix}1\\100\end{bmatrix},\begin{bmatrix}2\\110\end{bmatrix}) = \sqrt{(1-2)^2 + (100-110)^2} = 10.5$$

- x = [1 100] is misclassified!
- The denser the samples, the less of the problem
  - But we rarely have samples dense enough

kNN: Extreme Example of Distance Selection

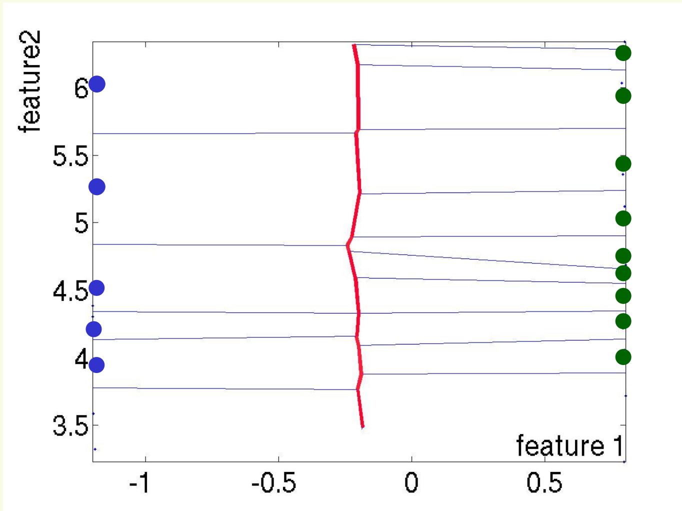


- decision boundaries for blue and green classes are in red
- These boundaries are really bad because
  - feature 1 is discriminative, but it's scale is small
  - feature 2 gives no class information (noise) but its scale is large

kNN: Selection of Distance

- Notice the 2 features are on different scales:
  - feature 1 takes values between 1 or 2
  - feature 2 takes values between 100 to 200
- We could normalize each feature to be between of mean 0 and variance 1
- If $\boldsymbol{X}$ is a random variable of mean μ and varaince σ^2, then $(\boldsymbol{X} - \mu)/\sigma$ has mean 0 and variance 1
- Thus for each feature vector $\boldsymbol{x}_i$, compute its sample mean and variance, and let the new feature be $[\boldsymbol{x}_i - \text{mean}(\boldsymbol{x}_i)]/\text{sqrt}[\text{var}(\boldsymbol{x}_i)]$
- Let's do it in the previous example

kNN: Normalized Features



- The decision boundary (in red) is very good now!

kNN: Selection of Distance

- However in high dimensions if there are a lot of irrelevant features, normalization will not help

$$D(a,b) = \sqrt{\sum_k (a_k - b_k)^2} = \sqrt{\underbrace{\sum_i (a_i - b_i)^2}_{\text{discriminative feature}} + \underbrace{\sum_j (a_j - b_j)^2}_{\text{noisy features}}}$$

- If the number of discriminative features is smaller than the number of noisy features, Euclidean distance is dominated by noise

kNN: Feature Weighting

- Scale each feature by its importance for classification

$$D(a,b) = \sqrt{\sum_k w_k (a_k - b_k)^2}$$

- Can learn the weights w_k from the validation data
  - Increase/decrease weights until classification improves

kNN Summary

- Advantages
  - Can be applied to the data from any distribution
  - Very simple and intuitive
  - Good classification if the number of samples is large enough
- Disadvantages
  - Choosing best k may be difficult
  - Computationally heavy, but improvements possible
  - Need large number of samples for accuracy
    - Can never fix this without assuming parametric distribution