Nonparametric Density Estimation
Nearest Neighbors , KNN

k-Nearest Neighbors

- Recall the generic expression for density estimation

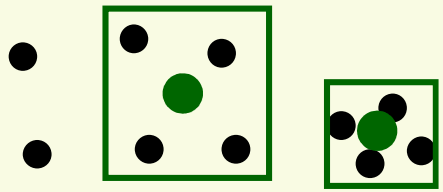
$$p(x) \approx \frac{k / n}{V}$$

- 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***

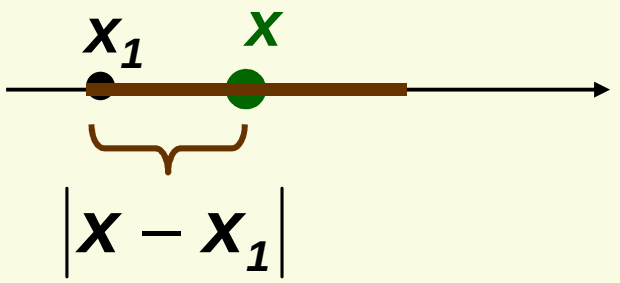


- 2 possibilities can occur:
  - Density is high near *x*; therefore the cell will be small which provides a good resolution
  - Density is low; therefore the cell will grow large and stop until higher density regions are reached

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. $n = 1$

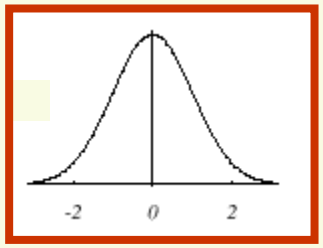
$$p(x) \approx \frac{k/n}{V} = \frac{1}{2|x - x_1|}$$

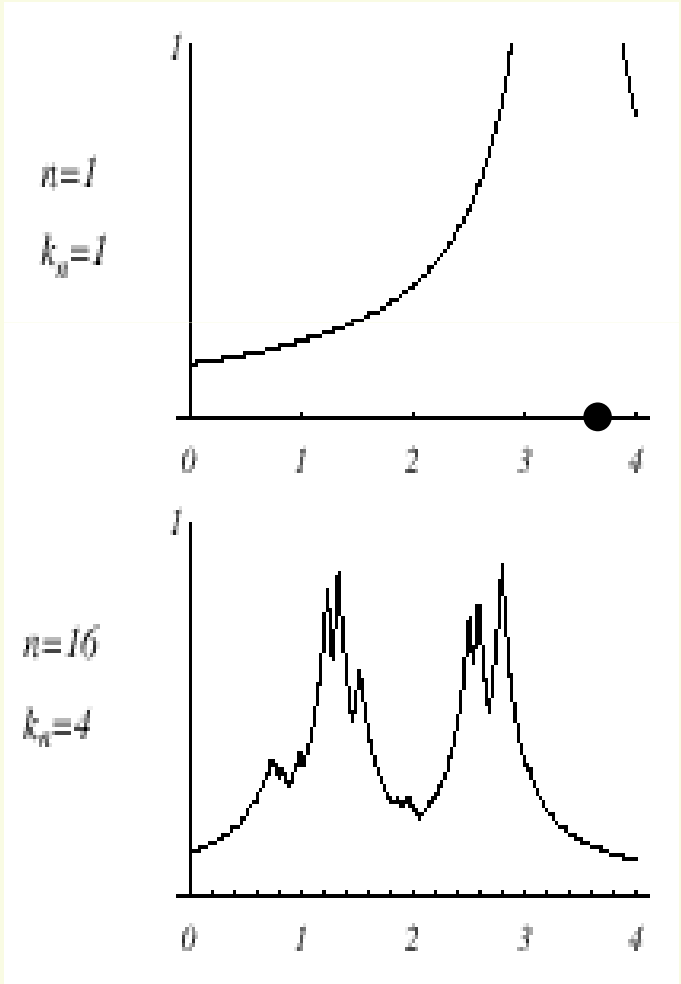


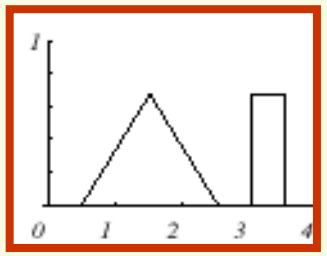
- But the estimated $p(x)$ is not even close to a density function:

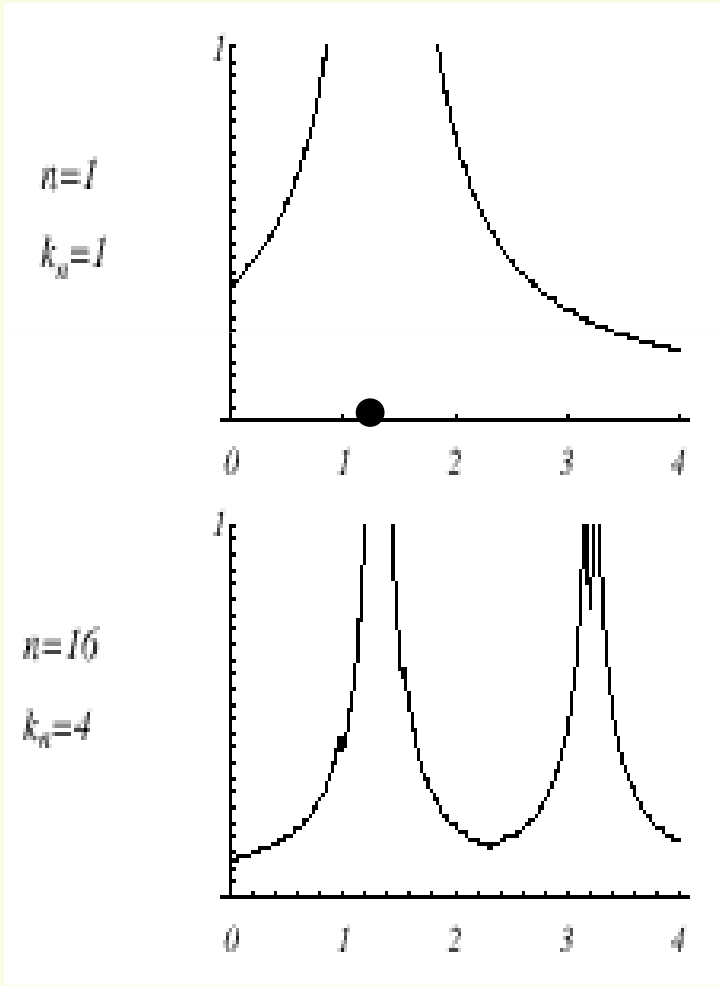
$$\int_{-\infty}^{\infty} \frac{1}{2|x - x_1|} dx = \infty \neq 1$$

k-Nearest Neighbor: Density estimation









k-Nearest Neighbor

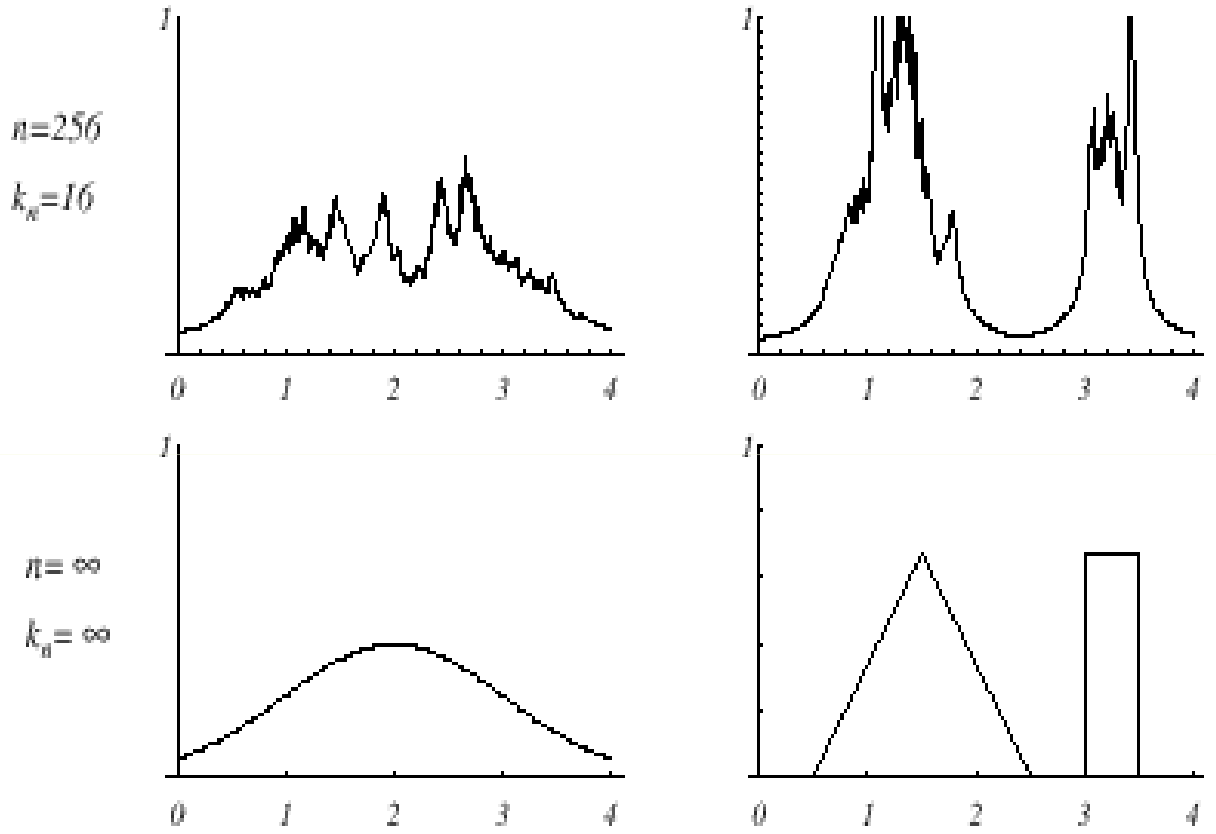


FIGURE 4.12. Several *k*-nearest-neighbor estimates of two unidimensional densities: a Gaussian and a bimodal distribution. Notice how the finite *n* estimates can be quite "spiky." From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

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*

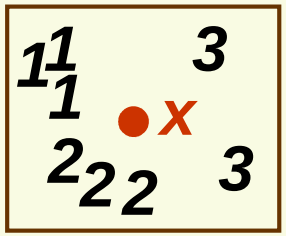
k-Nearest Neighbor

- 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

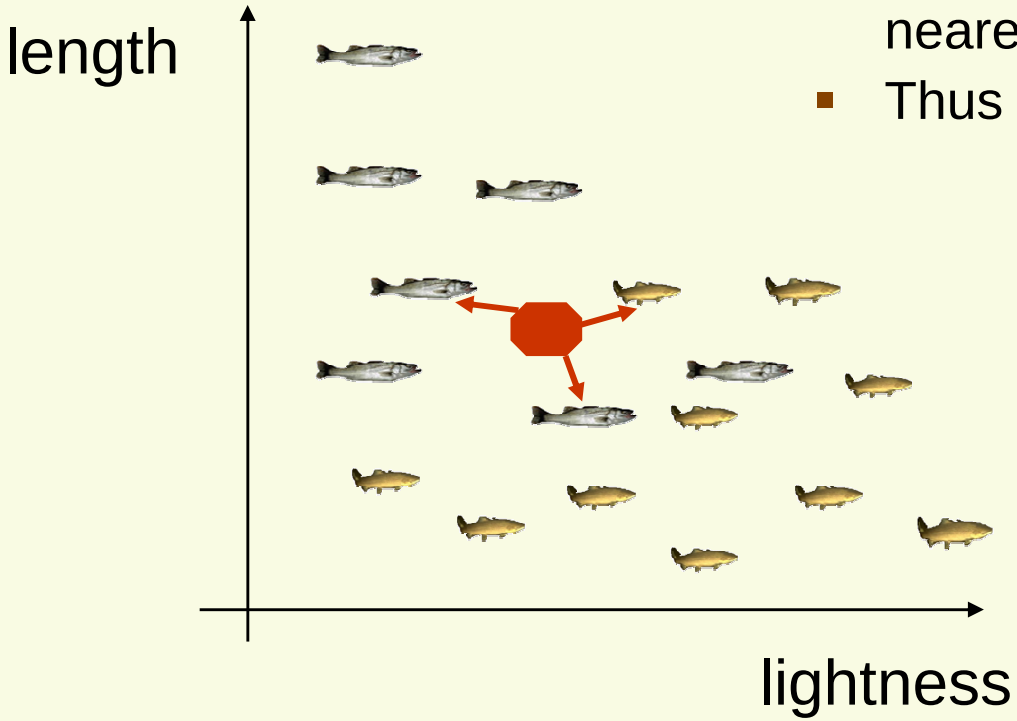
- Thus our estimate of posterior is just the fraction of samples which belong to class c_i:

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

- 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

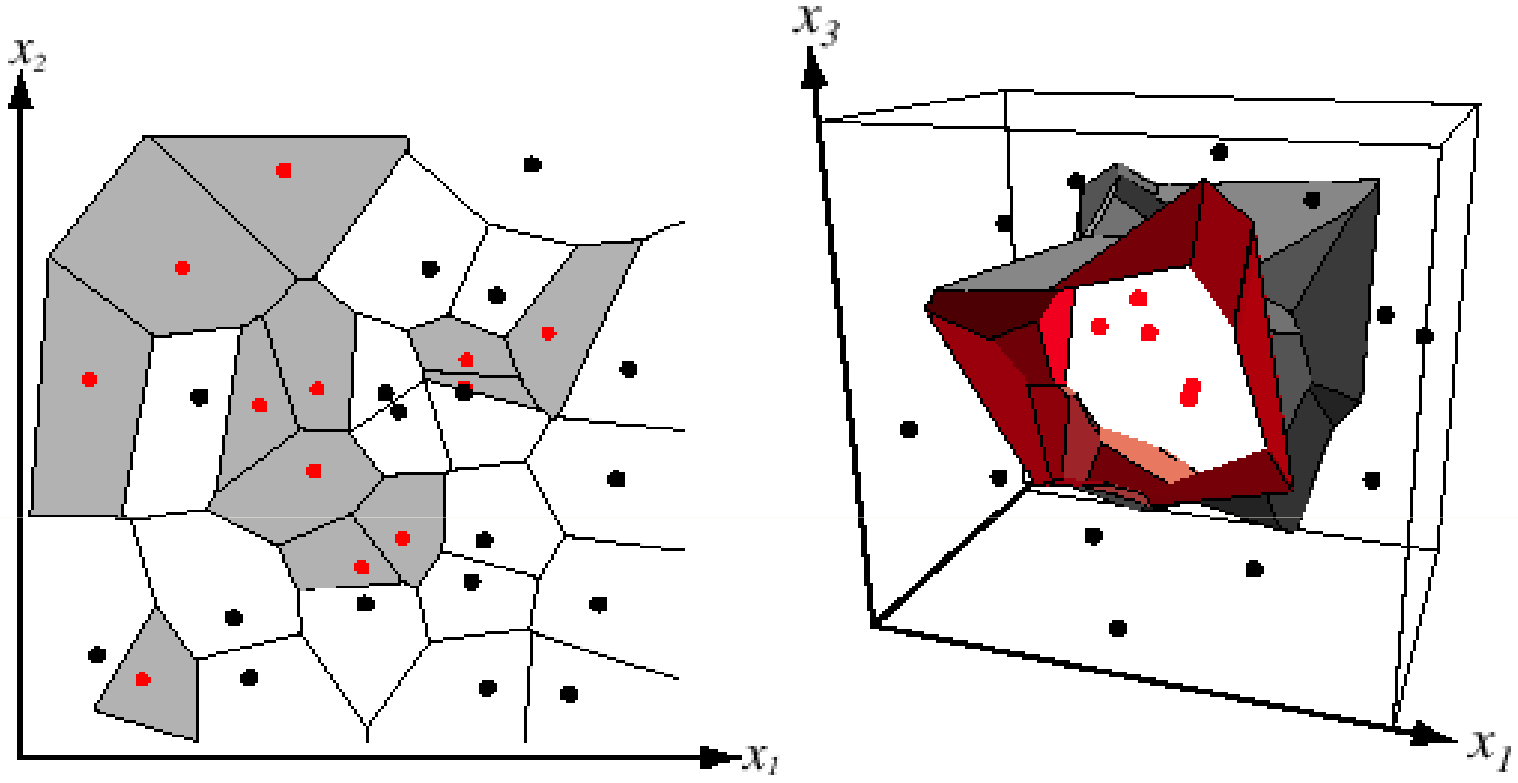
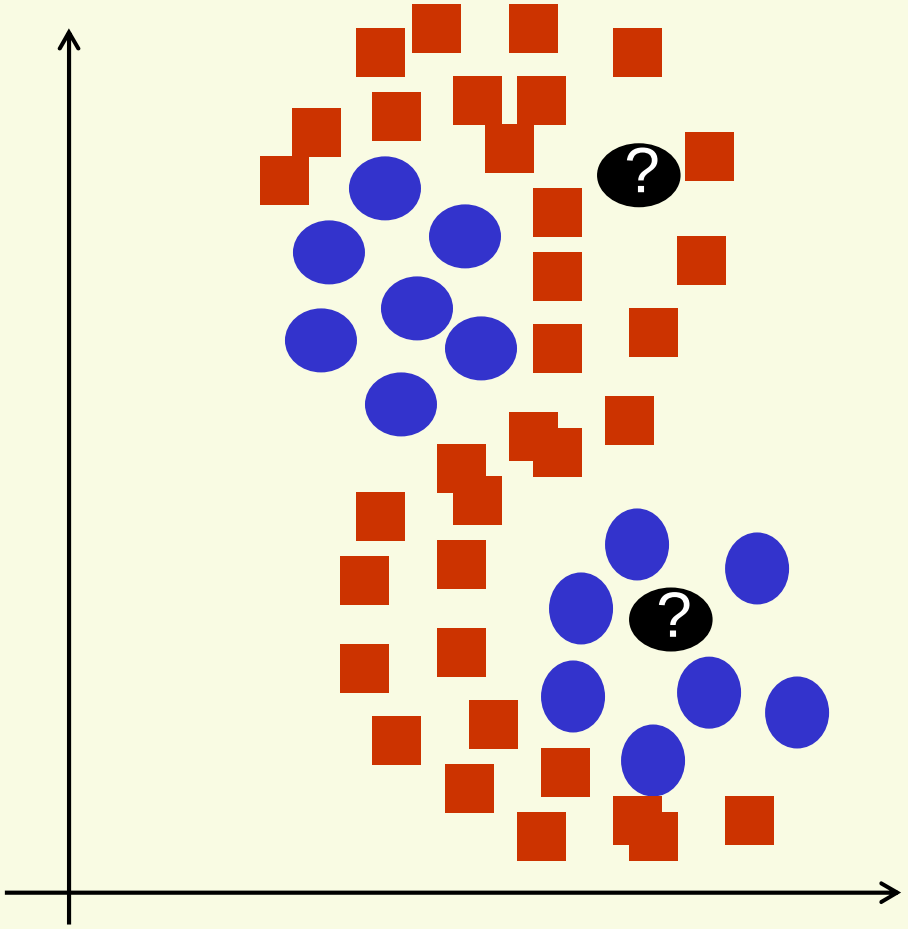


FIGURE 4.13. In two dimensions, the nearest-neighbor algorithm leads to a partitioning of the input space into Voronoi cells, each labeled by the category of the training point it contains. In three dimensions, the cells are three-dimensional, and the decision boundary resembles the surface of a crystal.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



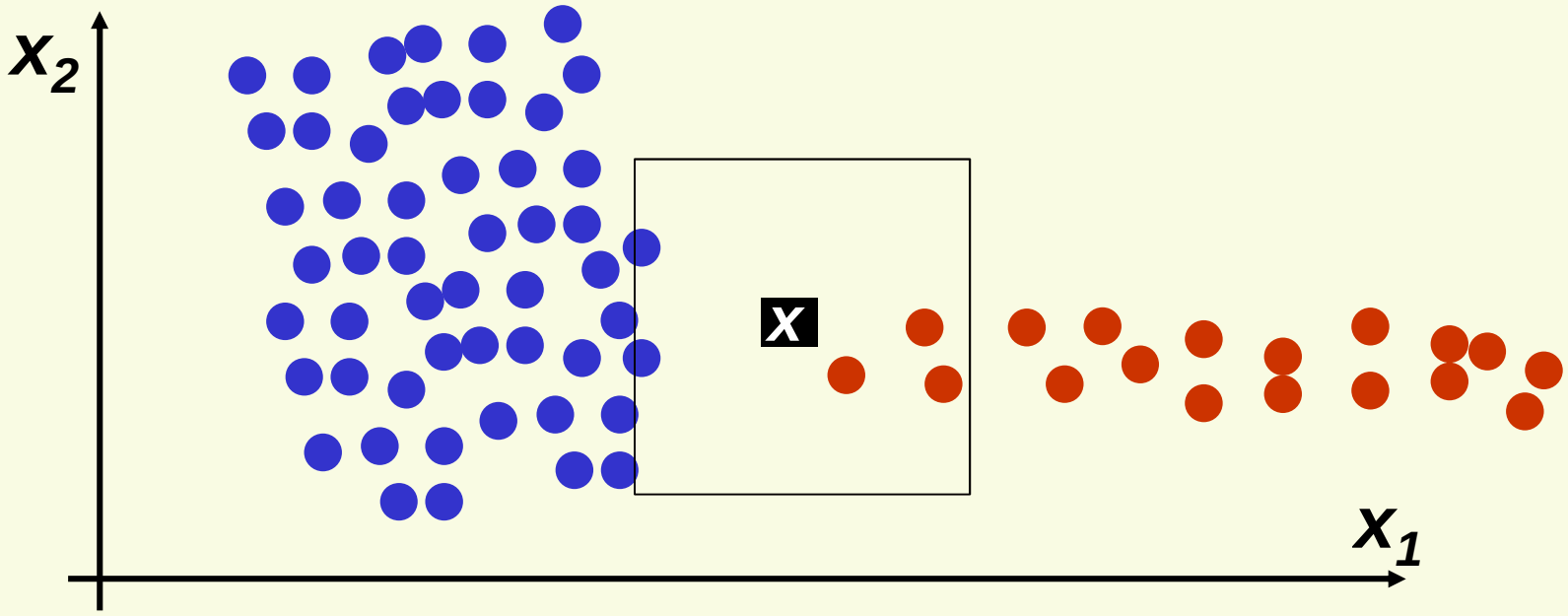
kNN: How to Choose k?

- 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?



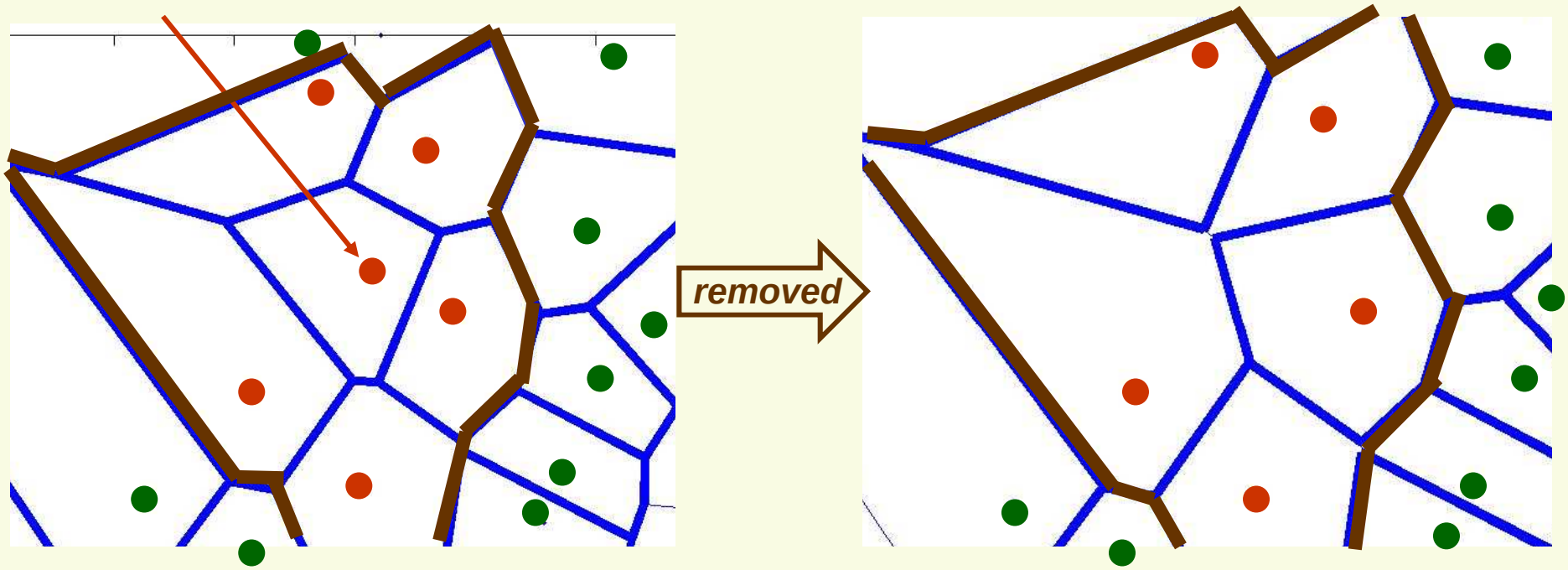
- For ***k*** = 1, …,5 point ***x*** gets classified correctly
  - red class
- For larger ***k*** classification of ***x*** is wrong
  - blue class

kNN: Computational Complexity

- Basic ***kNN*** algorithm stores all examples. Suppose we have ***n*** examples each of dimension ***d***
  - ***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:



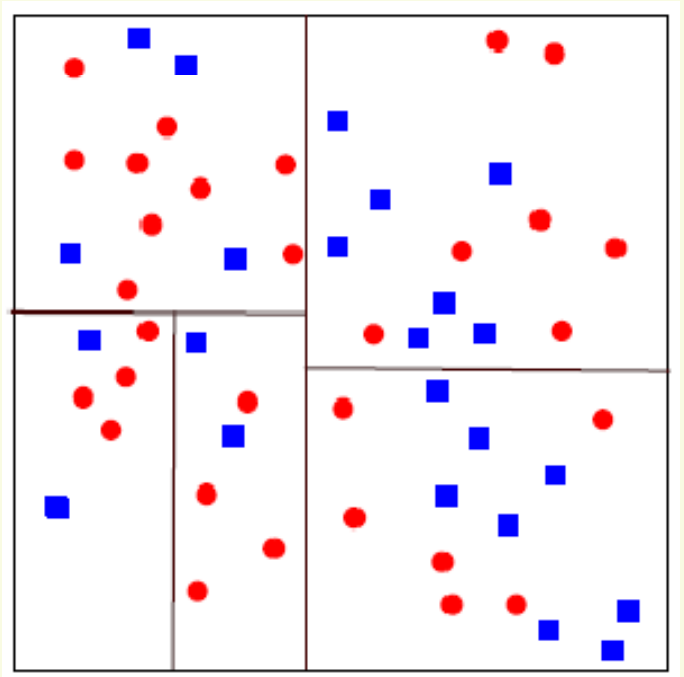
- Number of samples decreases
- We are guaranteed that the decision boundaries stay the same

Reducing the complexity of KNN

- Idea: Partition space recursively and search for NN only close to the test point
- Preprocessing: Done prior to classification process.

Axis-parallel tree construction:

1. Split space in direction of largest ‘spread’ into two equi-numbered cells
2. Repeat procedure recursively for each subcell,until some stopping criterion is achieved



Reducing the complexity of KNN

- Classification:

  1. Propagate a test point down the tree. Classification is based on NN from the final leaf reached.

  2. If NN (within leaf) is further than nearest boundary - retrack

- Notes:
  - Clearly log n layers (and distance computations) suffice.
  - Computation time to build tree: O(dn log n) (offline)
  - Many variations and improvements exist (e.g. diagonal splits)
  - Stopping criterion: often ad-hoc (e.g. number of points in leaf region is k, region size, etc.)

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)

- Euclidian distance treats each feature as equally important

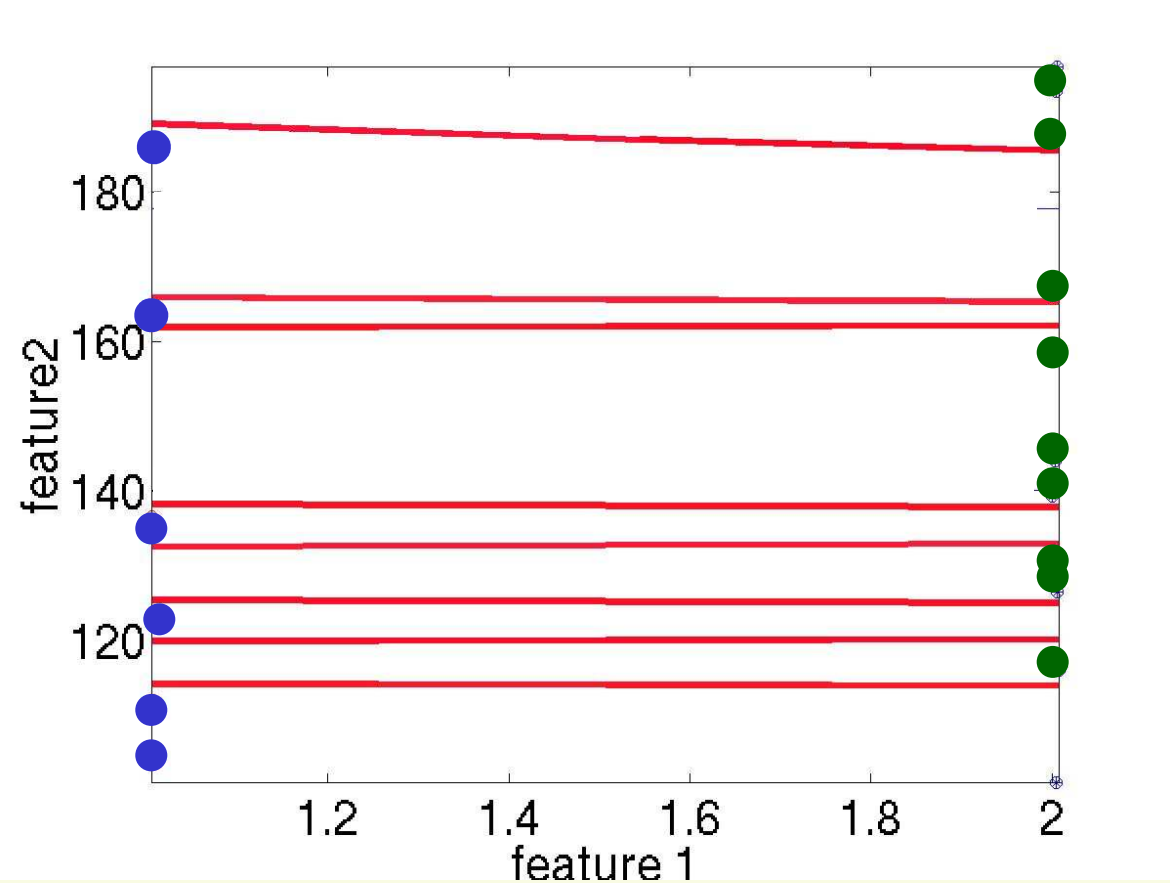
kNN: Selection of Distance

- 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]

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

- 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

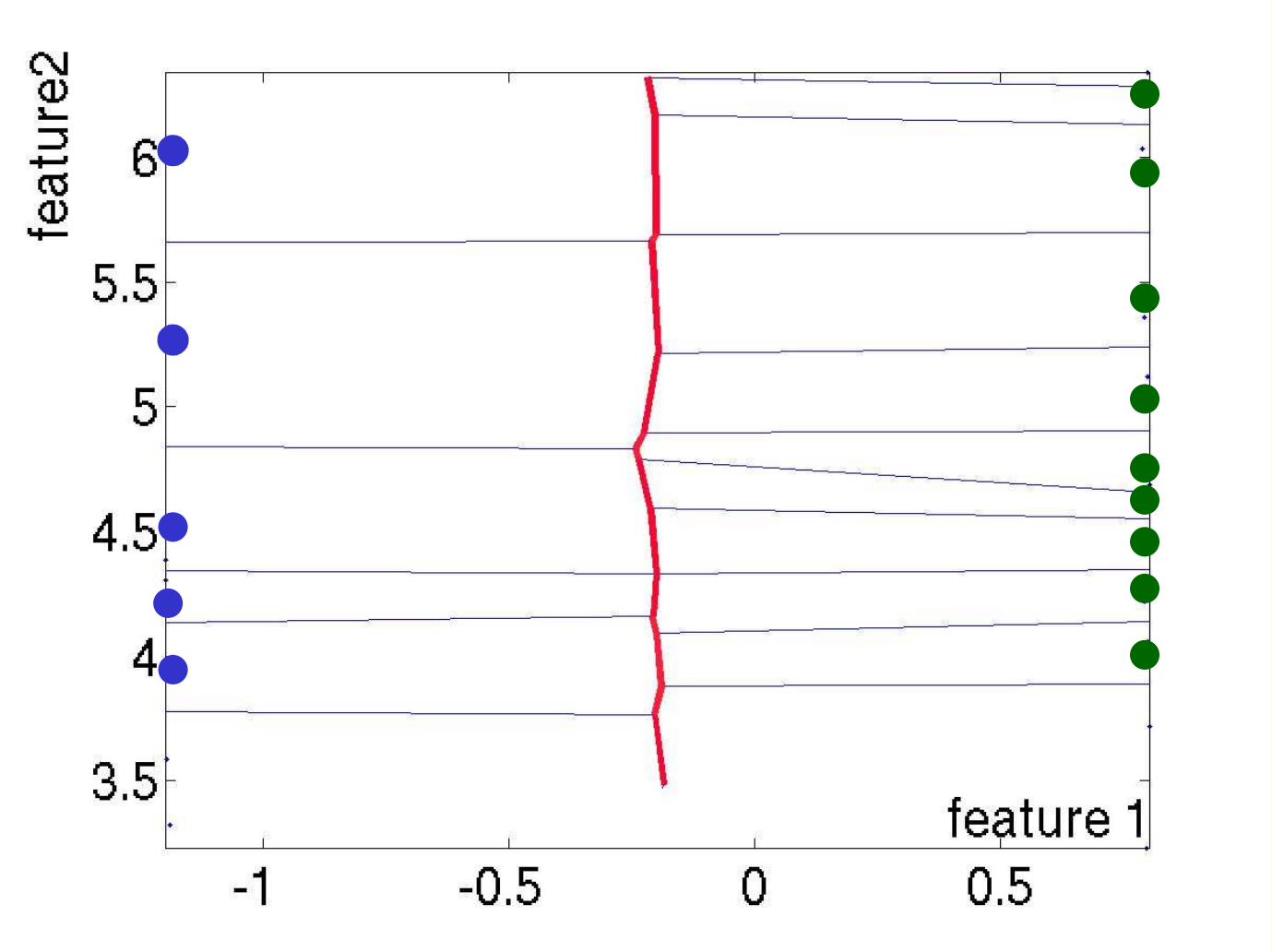


- decision boundaries for blue and green classes are in red
- These boundaries are really bad because
  - feature 1 is discriminative, but it's scale is small
  - feature 2 gives no class information (noise) but its scale is large

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

$$D(a,b) = \sqrt{\sum_k (a_k - b_k)^2} = \sqrt{\sum_i (a_i - b_i)^2 + \sum_j (a_j - b_j)^2}$$

discriminative feature ***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

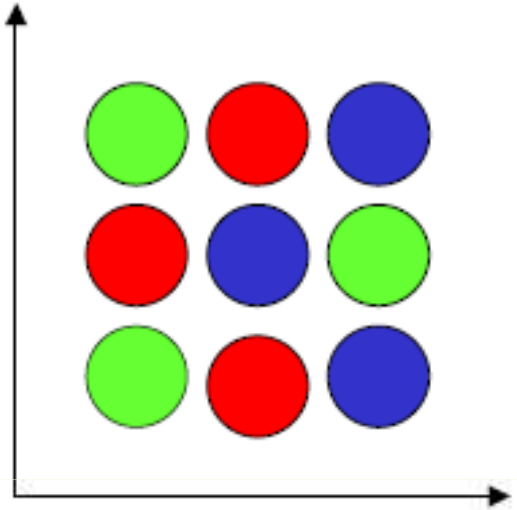
- Scale each feature by its importance for classification

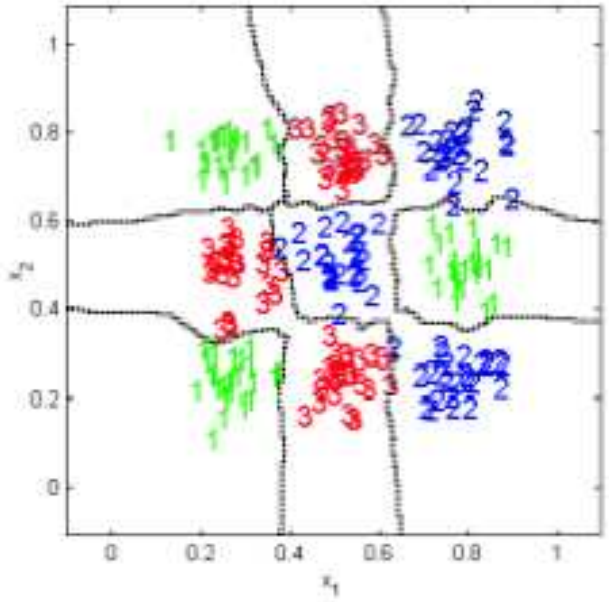
$$D(a,b) = \sqrt{\sum_k w_k (a_k - b_k)^2}$$

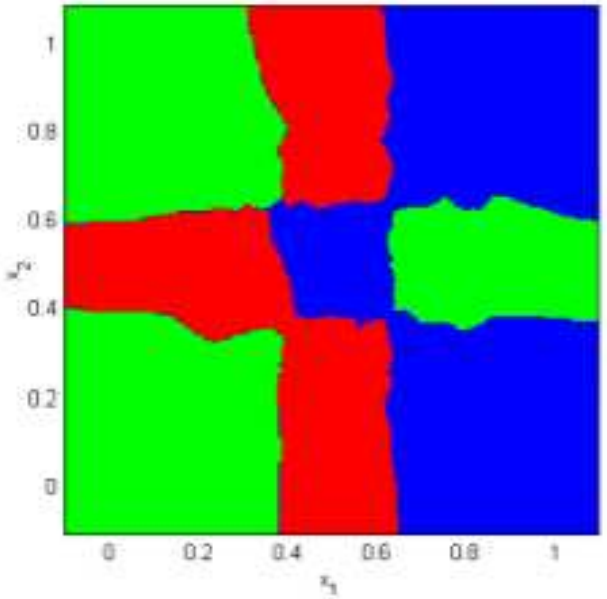
- Can learn the weights w_k from the validation data
  - Increase/decrease weights until classification improves

k-NNR in action: example 1

- We have generated data for a 2-dimensional 3-class problem, where the class-conditional densities are multi-modal, and non-linearly separable, as illustrated in the figure
- We used the k-NNR with
  - k = five
  - Metric = Euclidean distance
- The resulting decision boundaries and decision regions are shown below

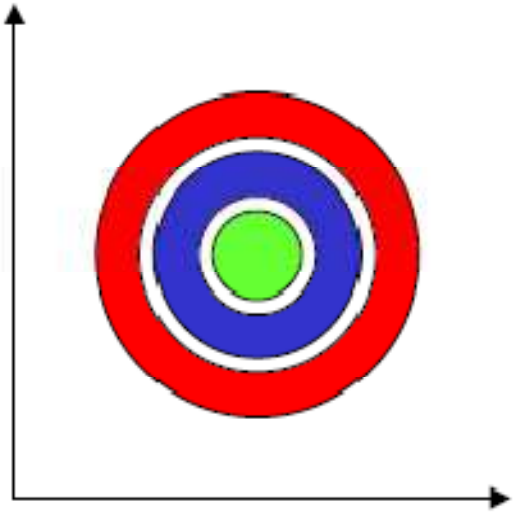


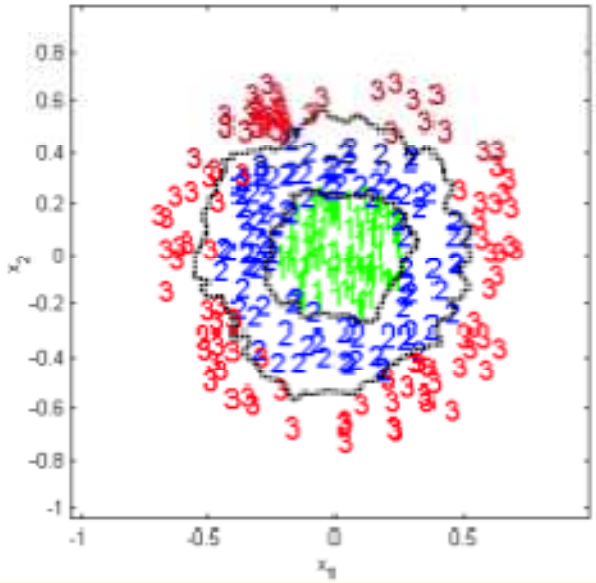


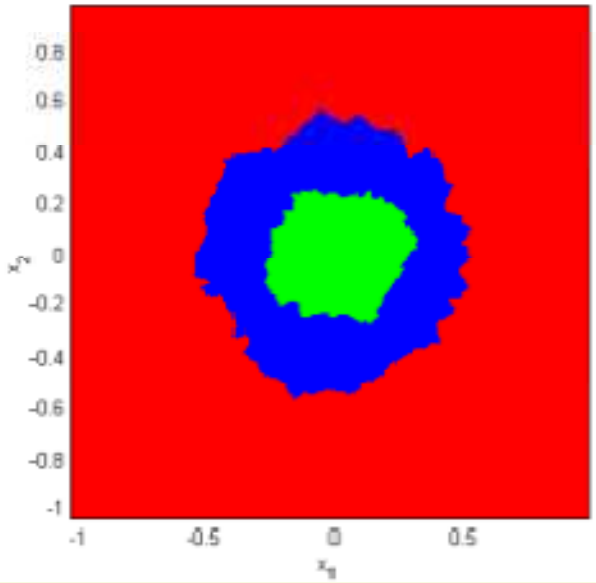


k-NNR in action: example 2

- We have generated data for a 2-dimensional 3-class problem, where the class-conditional densities are unimodal, and are distributed in rings around a common mean. These classes are also non-linearly separable, as illustrated in the figure
- We used the k-NNR with
  - k = five
  - Metric = Euclidean distance
- The resulting decision boundaries and decision regions are shown below







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