Non-parametric density estimation

Gosia Migut

Slides credit: David Tax

TU Delft

Admin stuff

- Registrations on Brightspace: 800+
- Lab week 2 downloads: 309
- Questions asked on Thursday: 39

- Lab questions on the exam!

Recap last week

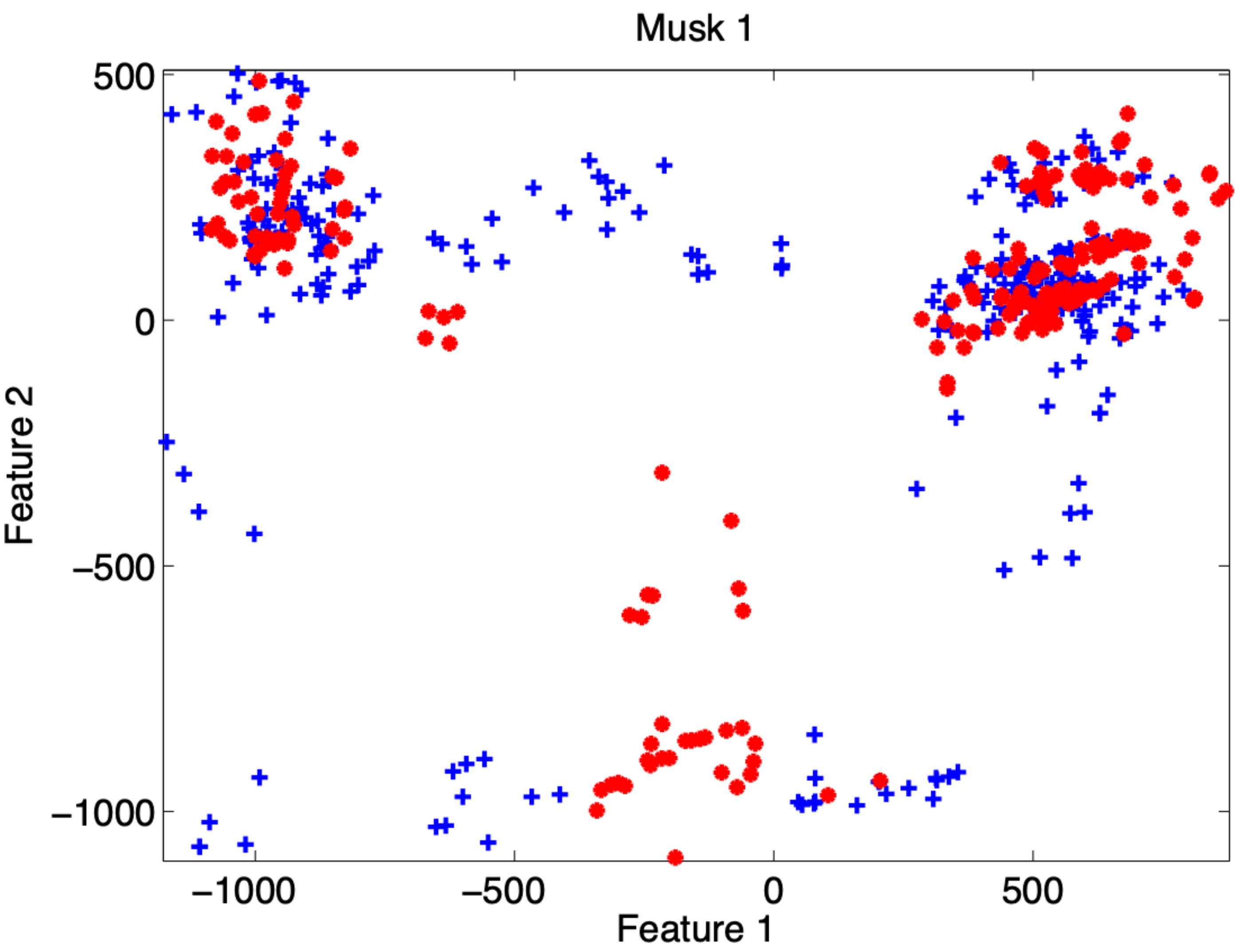
- Parametric density estimation
  - known distribution
  - estimate the parameters on training set
- Assume a single Gaussian distribution for each of the classes:

$$\hat{p}(x|y_i) = N(x|\mu_i, \Sigma_i)$$

$$N(x|\mu_i, \Sigma_i) = \frac{1}{(2\pi)^{p/2}|\Sigma_i|^{1/2}} \exp(\frac{1}{2}(x-\mu_i)^T {\Sigma_i}^{-1}(x-\mu_i))$$

TU Delft

But in real life…



Non-parametric density estimation

- Non-parametric
  - no knowledge on the distribution
  - manage the smoothness of the distribution

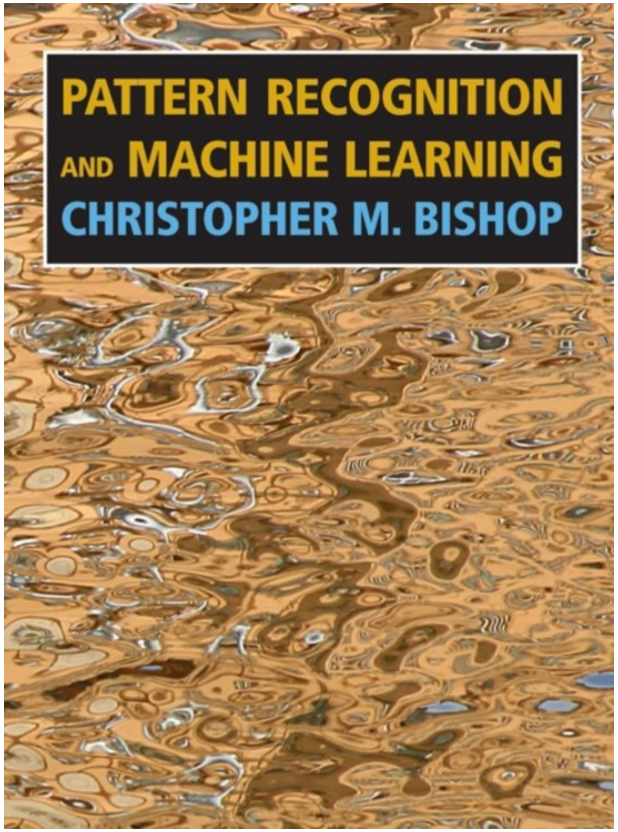
- Popular non-parametric algorithms are:
  - Parzen, k-Nearest Neighbors (today)
  - Naïve Bayes (Friday)

Literature

- Chapter 2 section 2.5 from:

  Bishop (2006). Pattern Recognition and Machine Learning. Springer, UK.

- Available online

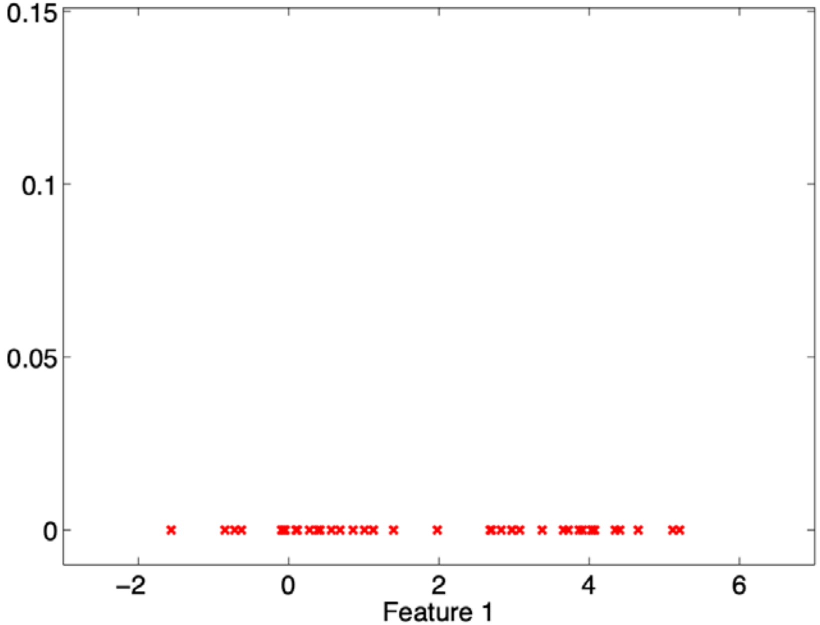


TU Delft

After practicing with the concepts of this lecture you should be able to:

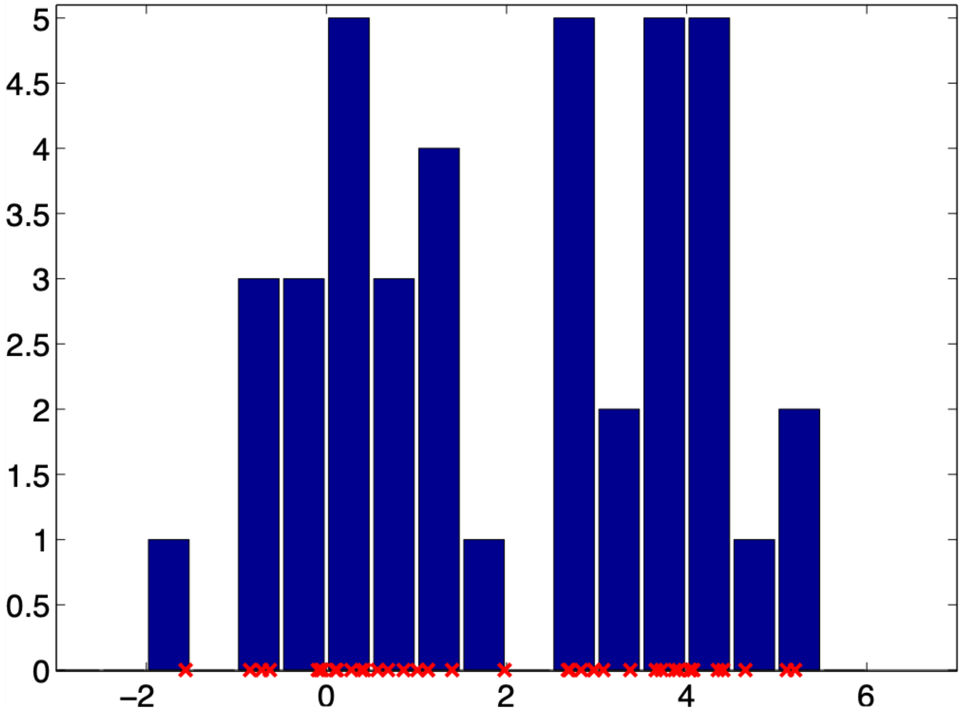
- Explain the difference between parametric and non-parametric density estimation
- Explain Parzen density estimation and classification
- Explain k-nn density estimation and classification
- Explain the advantages and disadvantages of Parzen and k-nn
- Implement k-nn classifier in Python

Histogram



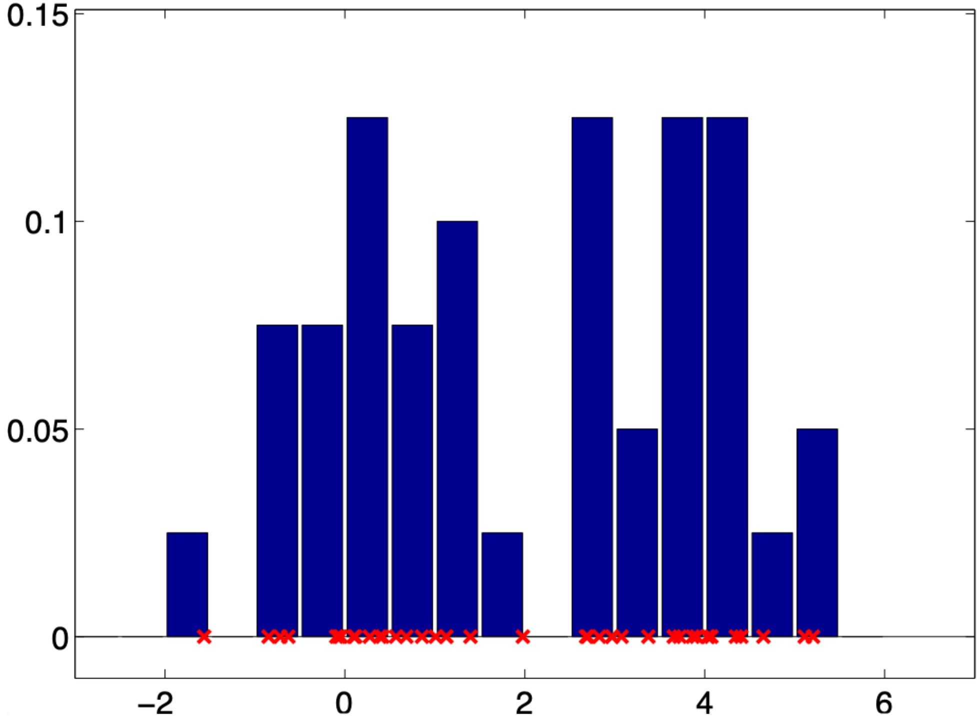
- Example: we have one feature
- We have 40 examples: how to estimate the probability density?

Histogram



- Split the feature in subregions: width h
- Count the number of objects in each region: k_N

Histogram method



- Probability density estimate: fraction of points/volume

$$\hat{p}(x) = \frac{1}{h} \frac{k_N}{N}$$

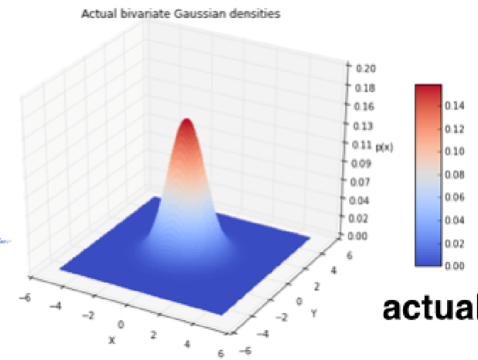
Histogram

- How many bins?
- For a reasonable precise approximation, h can’t be too large
- For a stable estimate, h cannot be too small
- Depends on the number of training examples
- In practice, two very related methods are used:
  – Parzen density estimate
  – k-Nearest-neighbor density estimate

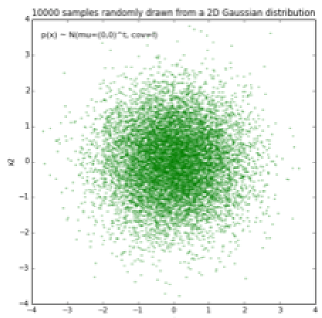
Parzen density estimation

Non-parametric density estimation

Our goal:

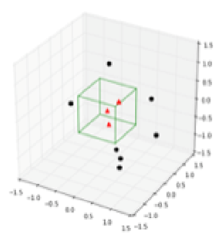


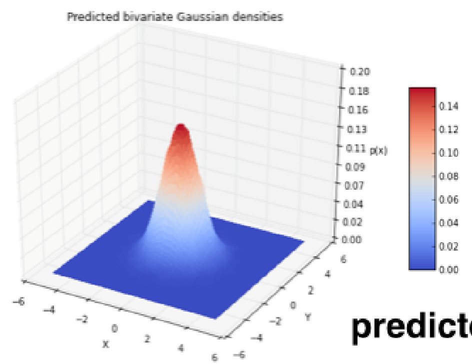
actual



Assuming we have samples drawn from a **unknown** distribution (here: bivariate Gaussian)

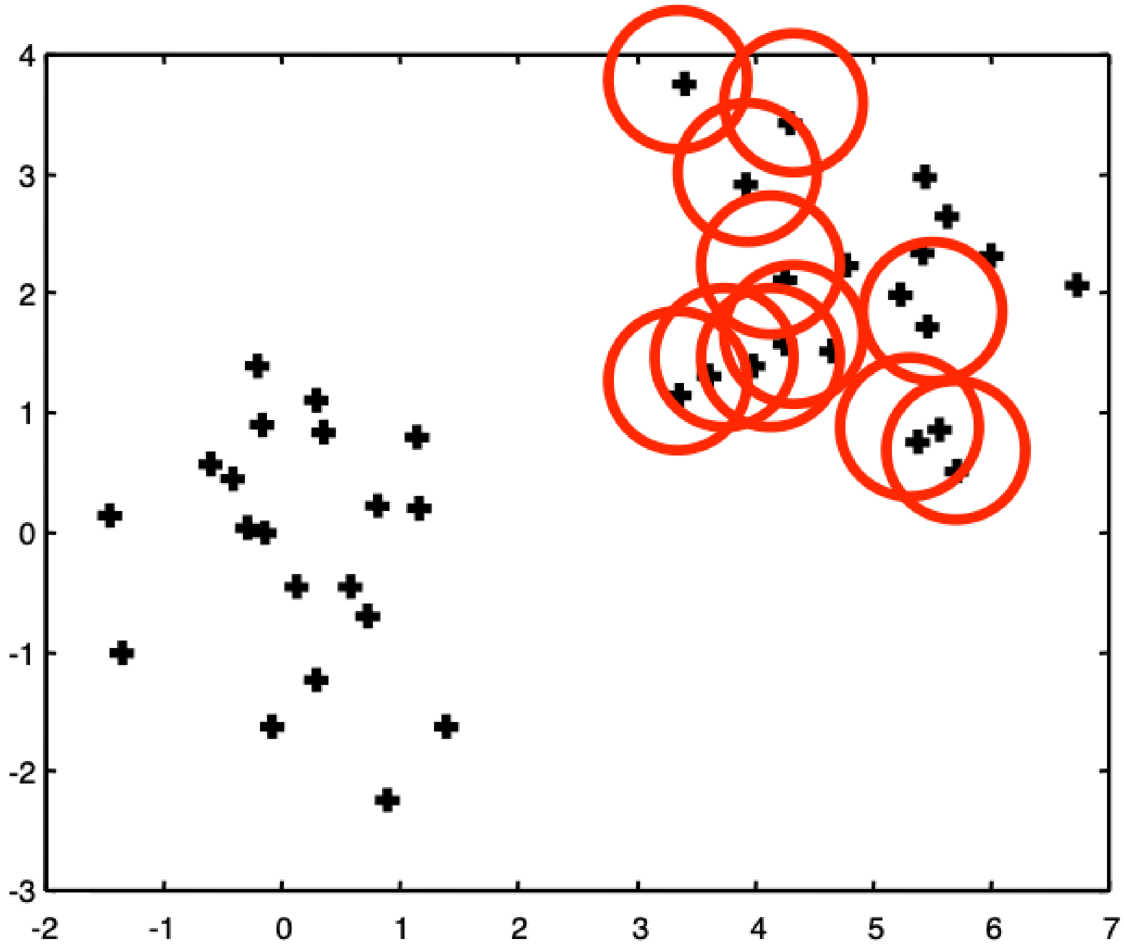
We want to **estimate** probability densities at certain points



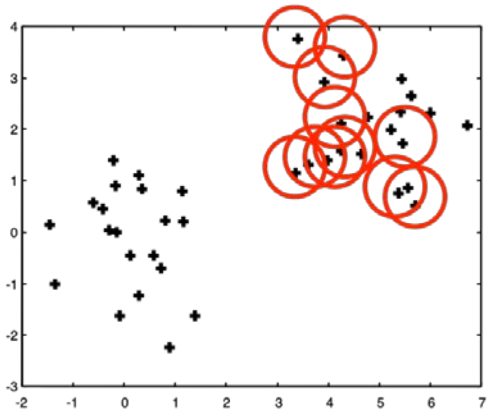


predicted

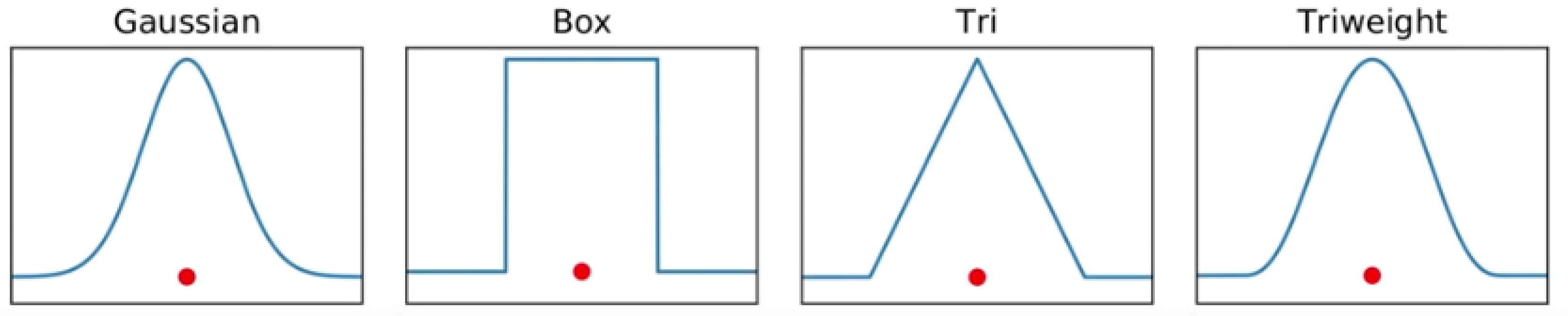
Parzen density estimation



Parzen density estimation



- Procedure:
  - Define cell shape (kernel) eg. Gaussian

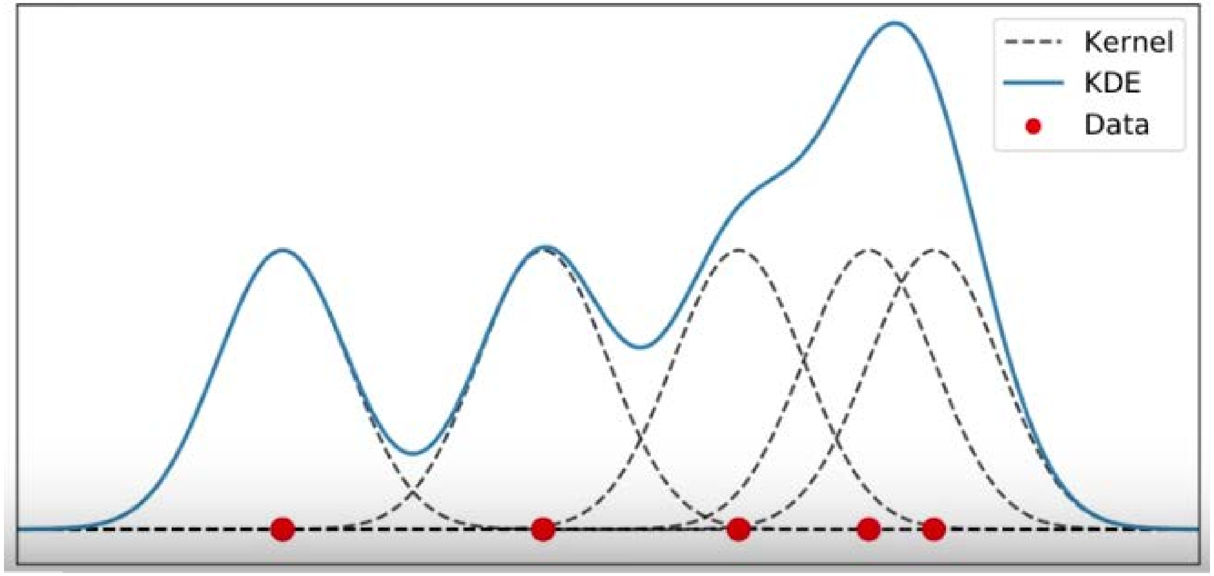


  - Fix size of cell (h)
  - Add contributions of cells

TUDelft

Parzen density estimation

- On every datapoint x_i place a kernel function K.



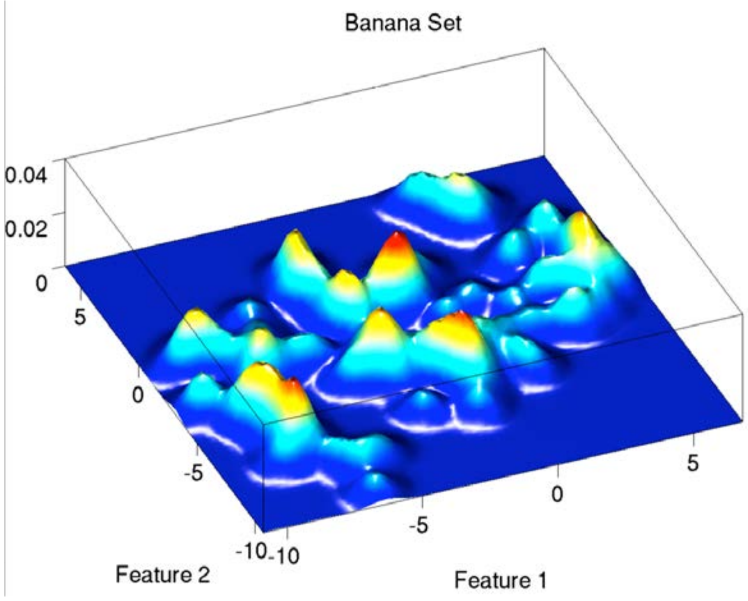
- Parzen density estimate is:

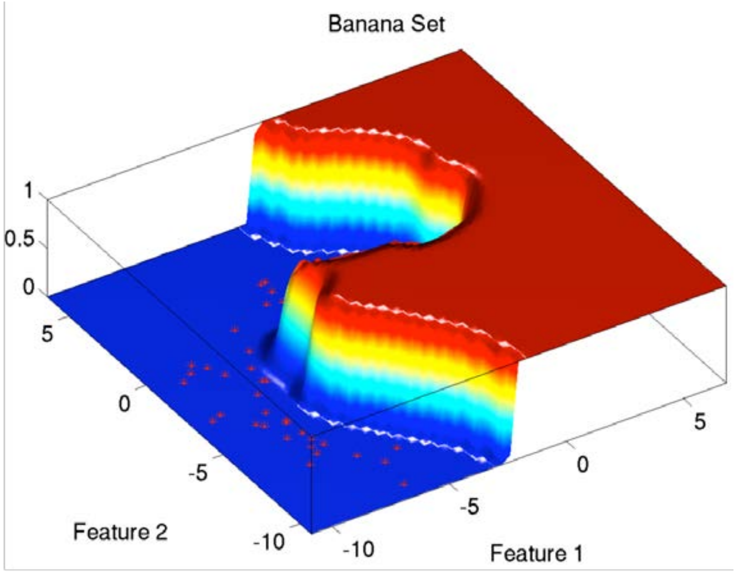
$$\hat{p}(x) = \frac{1}{nh}\sum_{i=1}^{n} K(\frac{x - x_i}{h})$$

Parzen classifier

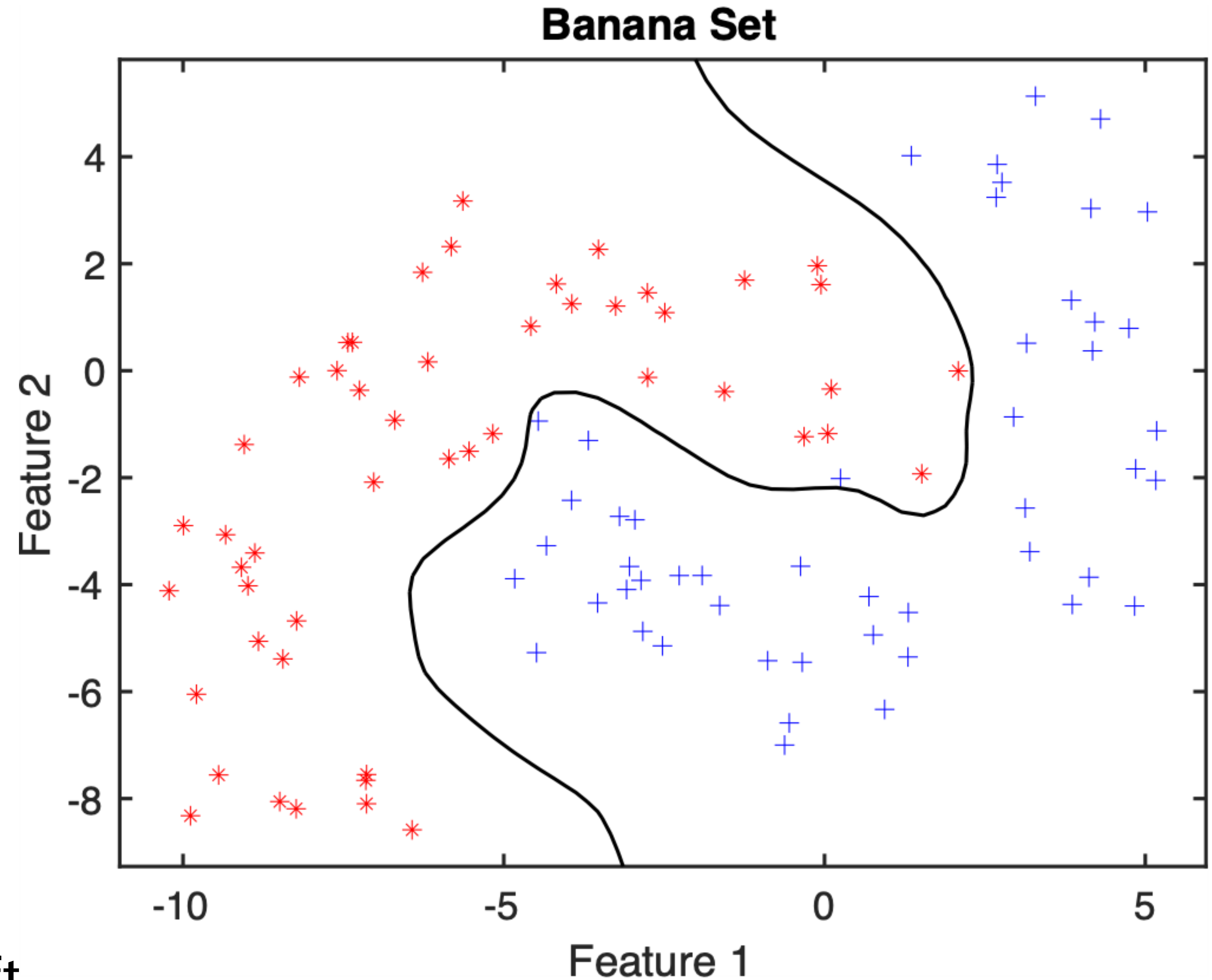
- Using Normal density

$$\hat{p}(x|y_i) = \frac{1}{n_i}\sum_{j=1}^{n_i} N(x|x_j^{(i)}, hI)$$

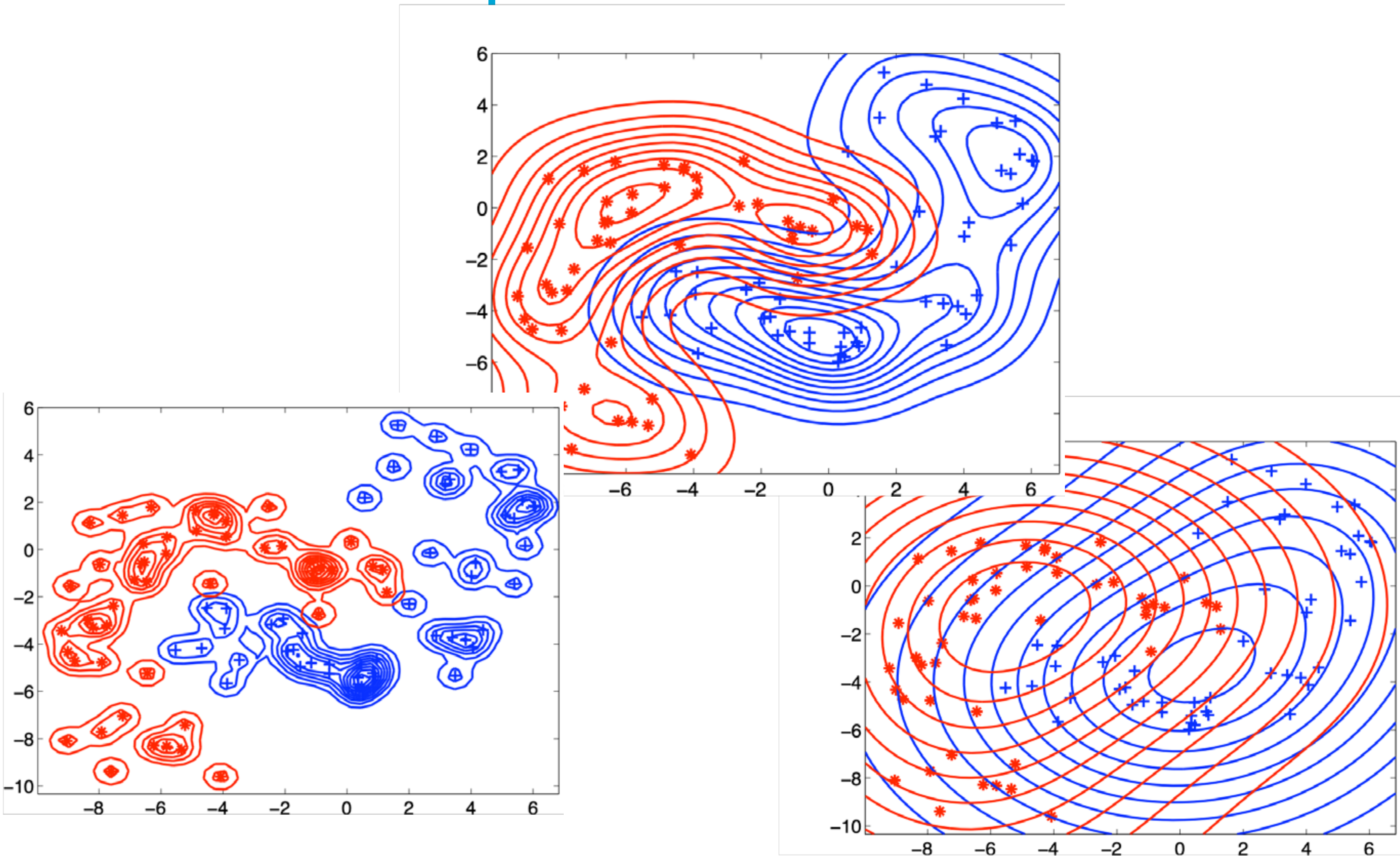




Parzen classifier



Parzen width parameter



Parzen width parameter

- The choice of h is important

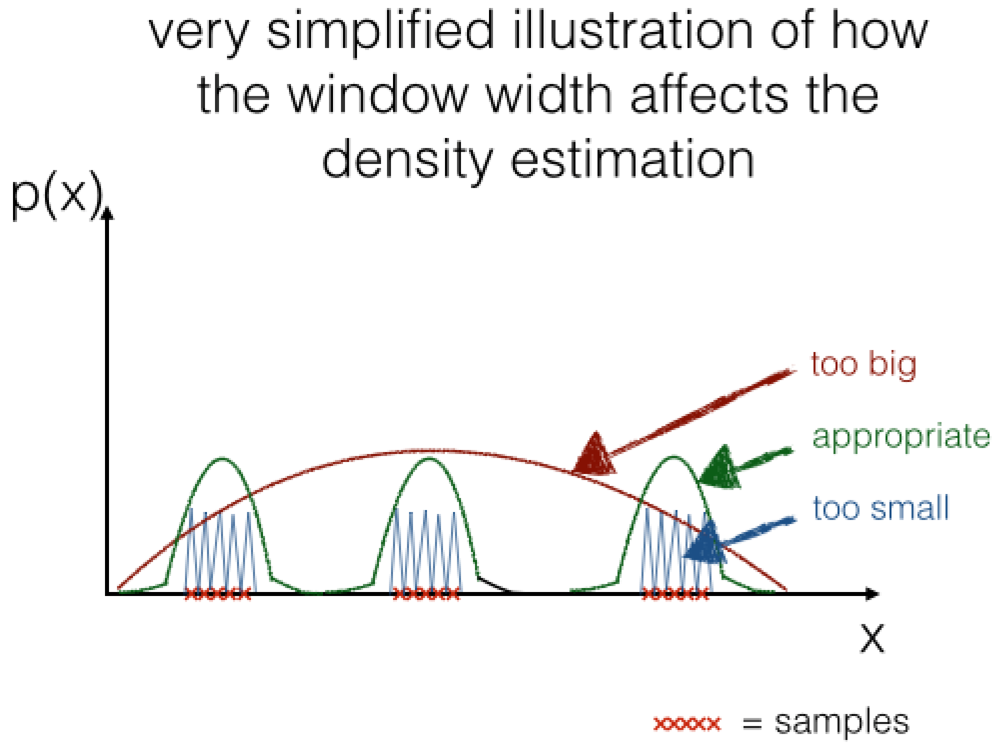


Figure by Sebastian Raschka

Optimization of h

- Use a heuristic

$$h = \sigma \left(\frac{4}{p+2}^{\frac{1}{p+4}} \right) n^{\frac{-1}{p+4}}$$

$$\sigma^2 = \frac{1}{p} \sum_{i=1}^{p} s_{ii}$$

- Optimize the likelihood

$$\prod_{i=1}^{n} \hat{p}(x_i)$$

- Use the average k-nearest neighbor distance
  (k=10 is suggested)

Question

- Given a set of five data points:

  $x_1 = 2, x_2 = 2.5, x_3 = 3, x_4 = 1, x_5 = 6,$

  find Parzen probability density function (pdf) estimates at $x = 3$,

  using the Gaussian function with $\sigma = 1$ as window function.

Solution

$$\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{(x_1 - x)^2}{2}\right)$$

$$= \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{(2 - 3)^2}{2}\right) = 0.2420$$

$$\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{(x_2 - x)^2}{2}\right)$$

$$= \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{(2.5 - 3)^2}{2}\right) = 0.3521$$

Solution

$$\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{(x_3-x)^2}{2}\right)=0.3989$$

$$\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{(x_4-x)^2}{2}\right)=0.0540$$

$$\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{(x_5-x)^2}{2}\right)=0.0044$$

so

$$p(x=3)=(0.2420+0.3521+0.3989$$

$$+0.0540+0.0044)/5 \quad =0.2103$$

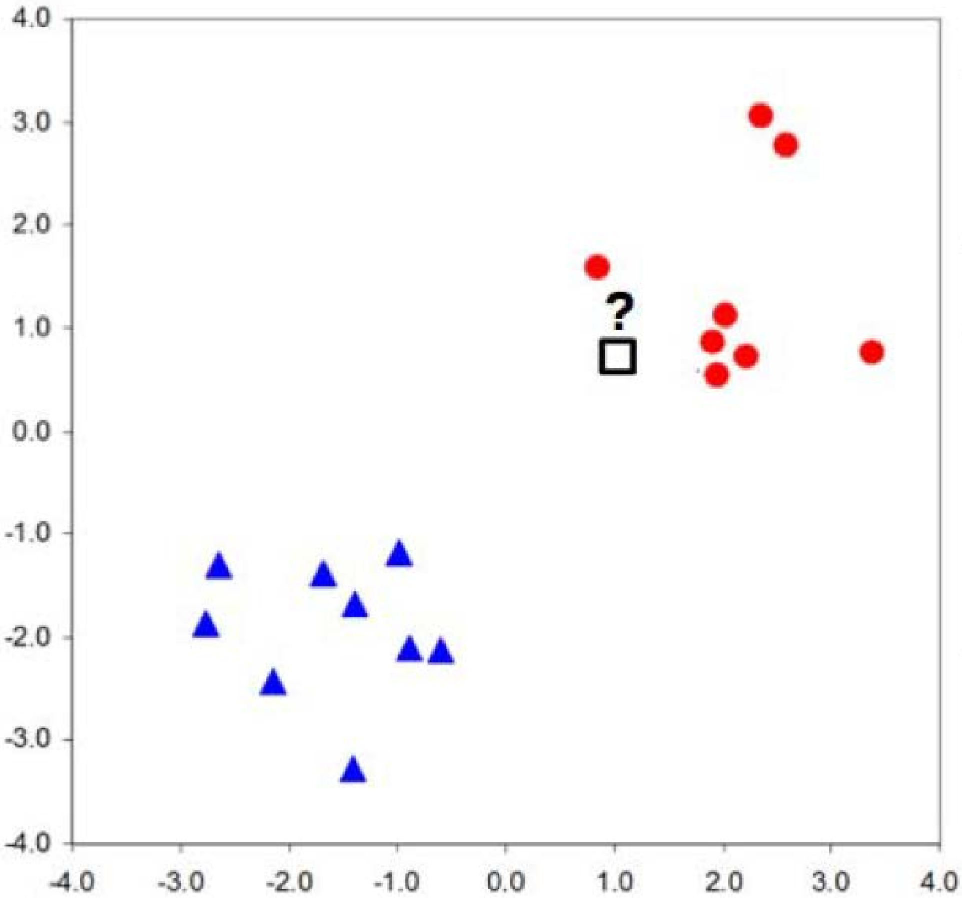
TU Delft

Parzen summary

- Estimates probability densities using kernel function
- Kernel funtion of fixed shape and size
- The choice of window shape and size is important

K-nearest Neighbours

K-nearest neighbour intuition

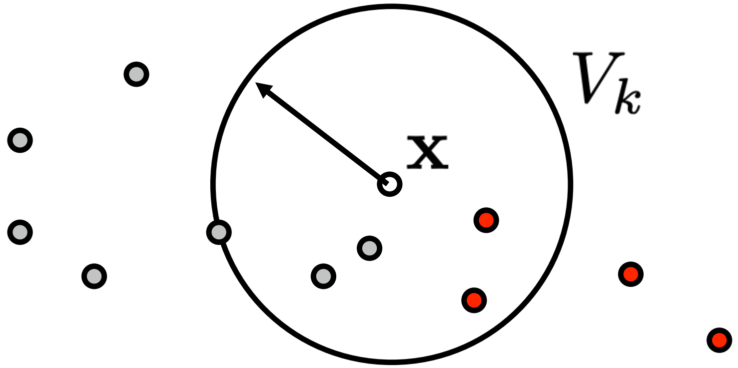


- Set of points (x_1, x_2)
  - Two classes
- Is the box red or blue?
- How did you do it?
- Nearby points are red
  - Use as a bias for a learning algorithm

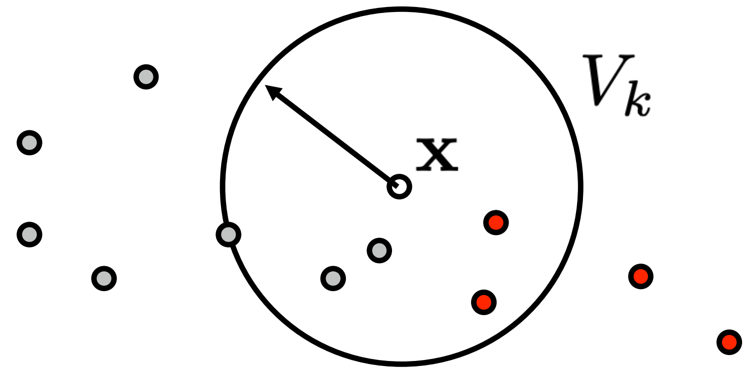
K nearest neighbor

- Use the intuition to classify a new point x:
  - Locate the cell on the new point x
  - Do **not** fix the volume of the cell:
    grow the cell until it covers k objects:
    find the k-th neighbors
  - predict the class y of new point x

k=5



K-nn density estimation

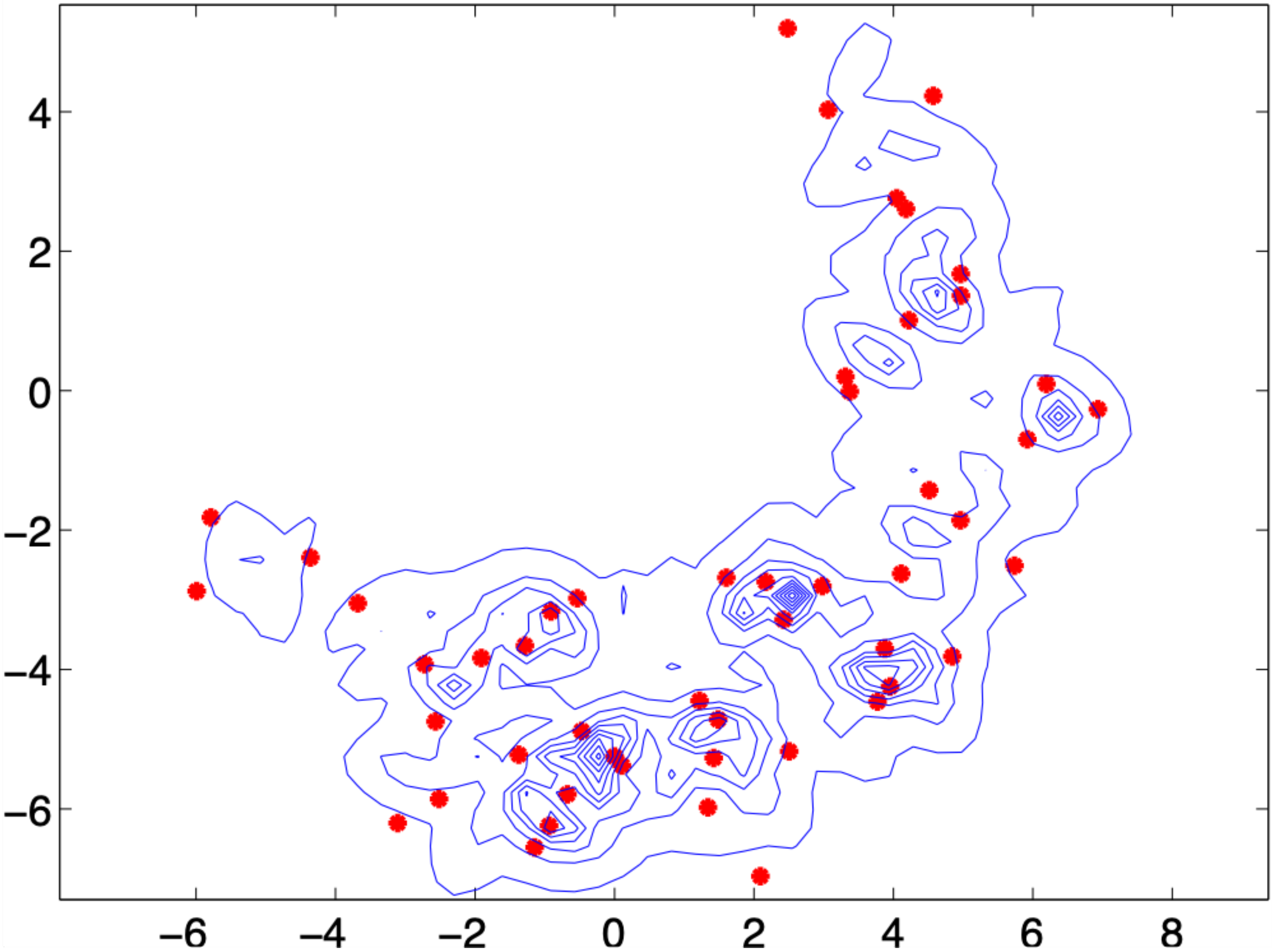


- $k = 5$
- $k_1 = 3$
- $k_2 = 2$

$$\hat{p}(x|y_i) = \frac{k_i}{n_i V_k}$$

- Where V_k is the volume of the sphere centered at x with radius r, being the distance to the k-th nearest neighbor
- Class priors: $\hat{p}(y_i) = \frac{n_i}{n}$
- Bayes: $\hat{p}(x|y_i)\hat{p}(y_i) > \hat{p}(x|y_j)\hat{p}(y_j) \rightarrow \ k_i > k_j$

K-nn density estimate

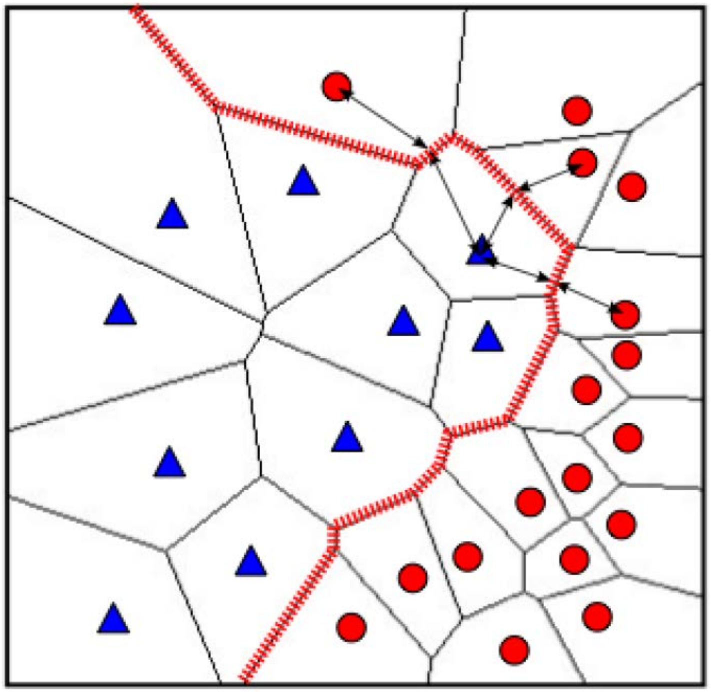


K-nn classification algorithm

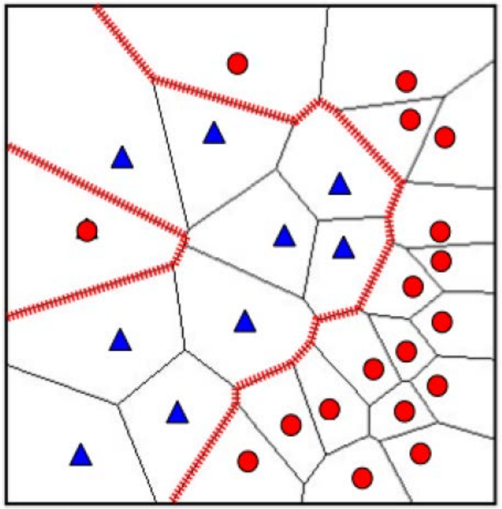
- Given:
  - training examples $\{x_i, y_i\}$
    - x_i attribute-value representation of examples
    - y_i class label: {male, female}, digit {0,1, ... 9} etc.
  - testing point x that we want to classify
- Algorithm:
  - compute distance $D(x, x_i)$ to every training example x_i
  - select k closest instances $x_{i1} \dots x_{ik}$ and their labels $y_{i1} \dots y_{ik}$
  - output the class y^* which is most frequent in $y_{i1} \dots y_{ik}$ **(majority vote)**

Decision boundary 1-nn

- Voronoi tessellation
  - partitions space into regions
  - boundary: points at same distance from two different training examples
- Classification boundary
  - non-linear, reflects classes well
  - impressive for simple method

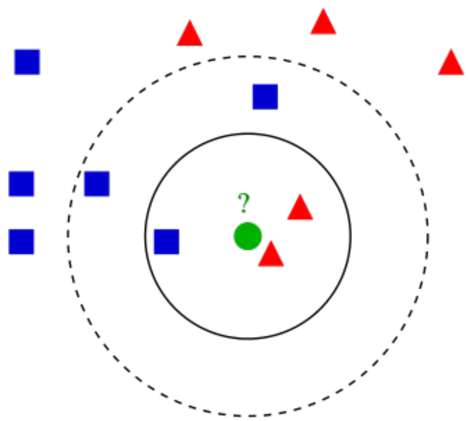


Nearest neighbout outliers



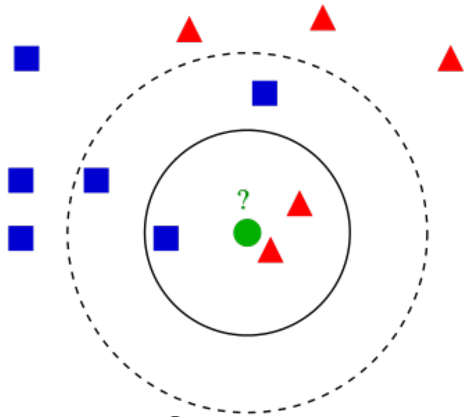
- Algorithm is sensitive to outliers
  - single mislabeled example dramatically changes boundary
- Idea:
  - use more than one nearest neighbor to make decision
  - count class labels in k most similar training examples
  - many "triangles" will outweigh single "circle" outlier

What is the influence of k?



- What is the largest/smallest value of k that you can choose?
  – What will be the classification error then?

What is the influence of k?

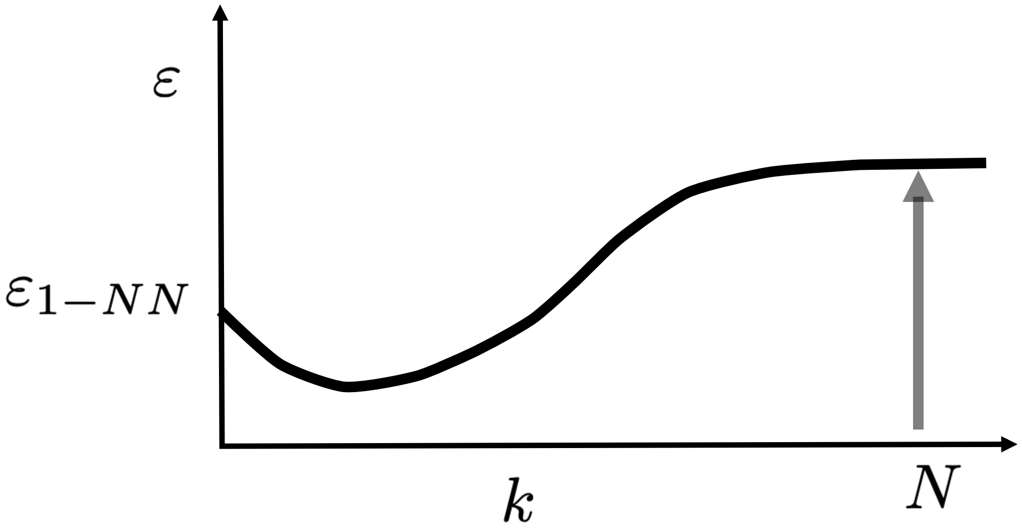


- Value of k has strong effect on k-nn performance
  - Large value ➔ everything classified as the most probable class
  - Small value ➔ highly variable, unstable decision boundaries
    - Small changes to training set➔ large changes to classification
  - affects “smoothness” of the boundary

TUDelft

Choosing the value of k

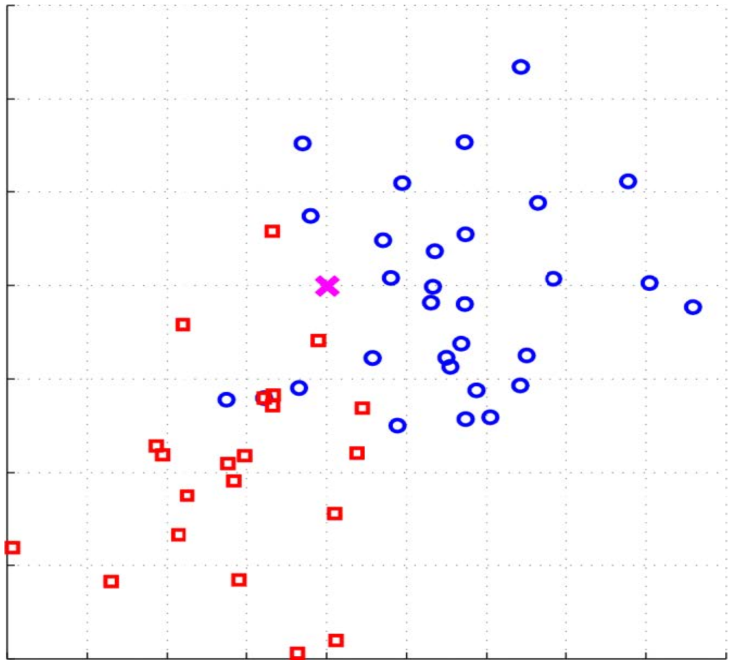
- Selecting the value of k
  - set aside a portion of the training data (validation set)
  - vary k
  - Pick k that gives best generalization performance



Question

- According to a k-NN classifier, to which class (red box or blue circle) does the new point **X** belong?

  1. If k=5 ?
  2. If k=2 ?



K-nn resolving ties

- Resolving ties:
  - equal number of positive/negative neighbours
  - use odd k (doesn't solve multi-class)
  - breaking ties:
    - random: flip the coin to decide positive/negative
    - prior: pick class with greater prior
    - nearest: use 1-nn classifier to decide

TU Delft

Distance measures

- The key component of the kNN algorithm
  - defines which examples are similar and which aren't
  - can have strong effect on performance

- Euclidean (numeric attributes):

$$D(x, x') = \sqrt{\sum_d |x_d - x'_d|^2}$$

  - symmetric, spherical, treats all dimensions equal
  - sensitive to extreme differences in single attribute

Distance measures

- Hamming (categorical attributes):
  - number of attributes where x, x' differ

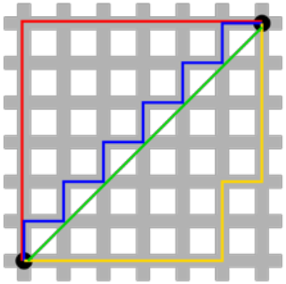
$$D(x, x') = \sum_{d} 1_{x_d \neq x'_d}$$

- Other
  - Kullback-Leibler (KL) divergence (for histograms)
  - Custom distance measures (BM25 for text)

Distance measures

- Minkowski distance (p-norm):

$$D(x, x') = \sqrt[p]{\sum_d |\, x_d - x'_d|^{\,p}}$$



  - $p = 2$: Euclidean
  - $p = 1$: Manhattan
  - $p = 0$: Hamming
  - $p = \infty$: $max_d |x_d - x'_d|$

Question

- Given a labeled two-dimensional data set:
  - Blue label: (1,4); (2,2); (3,3); (3,4);
  - Red label: (3,7); (5,7); (5,6); (6,5);
- Predict the label of a new point (4, 5) using 3-nn classifier with Manhattan distance.

TU Delft

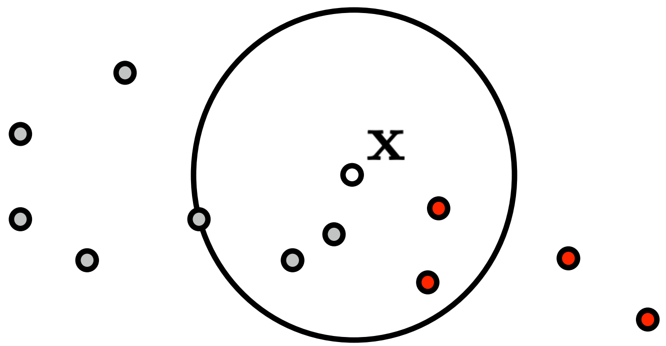
K-nn missing values

- Missing values
  - have to “fill in”, otherwise can't compute distance
  - keyconcern: should affect distances as little as possible
  - reasonable choice: average value across entire dataset

Why is k-nn slow?

- Find nearest neighbors of the new point X

- What you see:



- What algorithm sees:
  - Training set

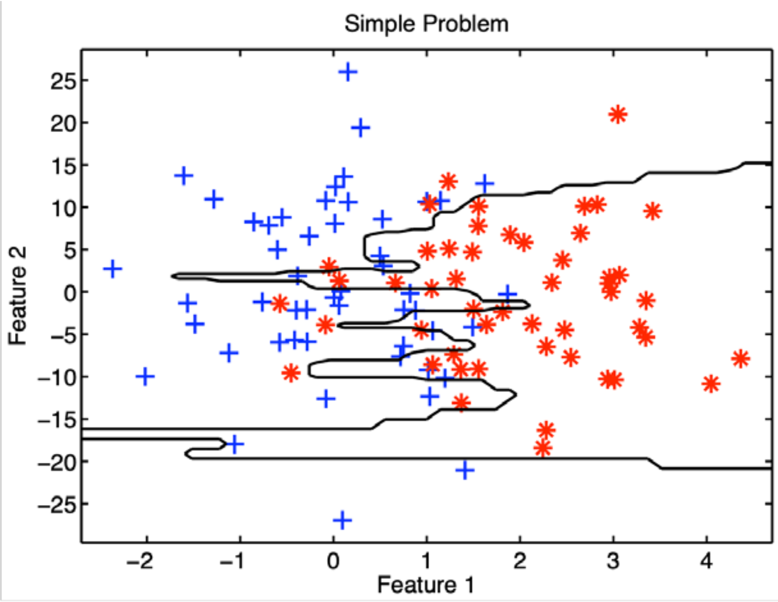
    {(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)}
  - Testing instance:

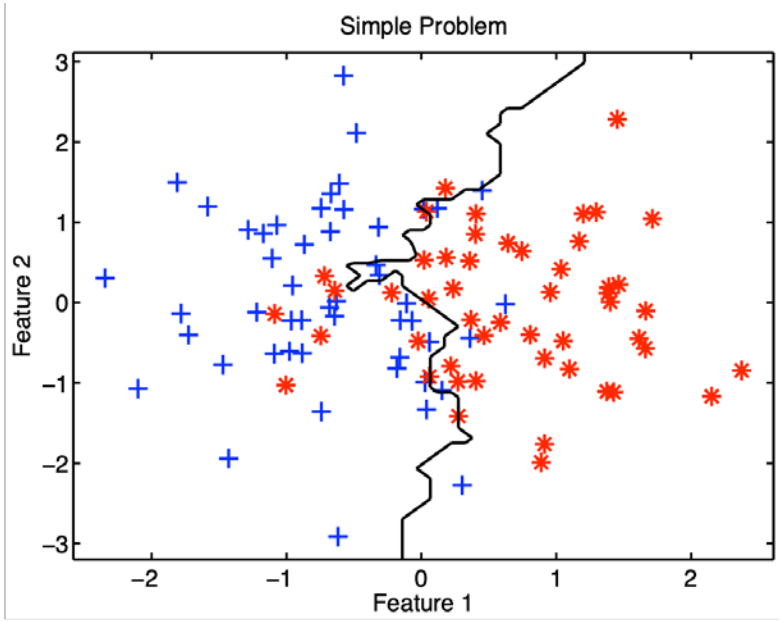
    (7, 4)
  - Nearest neighbors?

    compare one-by-one to each training instance

Sometimes strange results

- How is this possible?





Scale your features!

K-nn pros and cons

- Simple and flexible classifiers
- often a very good classification performance
- it is simple to adapt the complexity of the classifier

- relatively large training sets are needed
- the complete training set has to be stored
- distances to all training objects have to be computed
- the features have to be scaled sensibly
- the value for k has to be optimized

After practicing with the concepts of this lecture you should be able to:

- Explain the difference between parametric and non-parametric density estimation
- Explain Parzen density estimation and classification
- Explain k-nn density estimation and classification
- Explain the advantages and disadvantages of Parzen en k-nn
- Implement k-nn classifier in Python

Lab

- Starts at 13:45
- I will be at the lab today from 15:00