02450: Introduction to Machine Learning and Data Mining

Mixture models and density estimation

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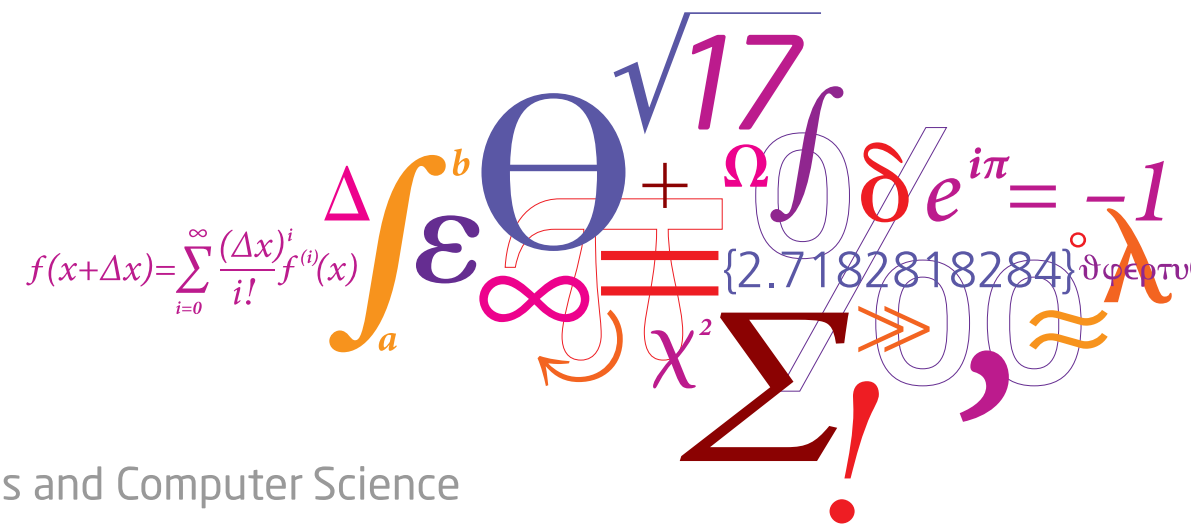
DTU Compute, Technical University of Denmark (DTU)



DTU Compute
Department of Applied Mathematics and Computer Science

Lecture Schedule

1. Introduction
   7 October: C1

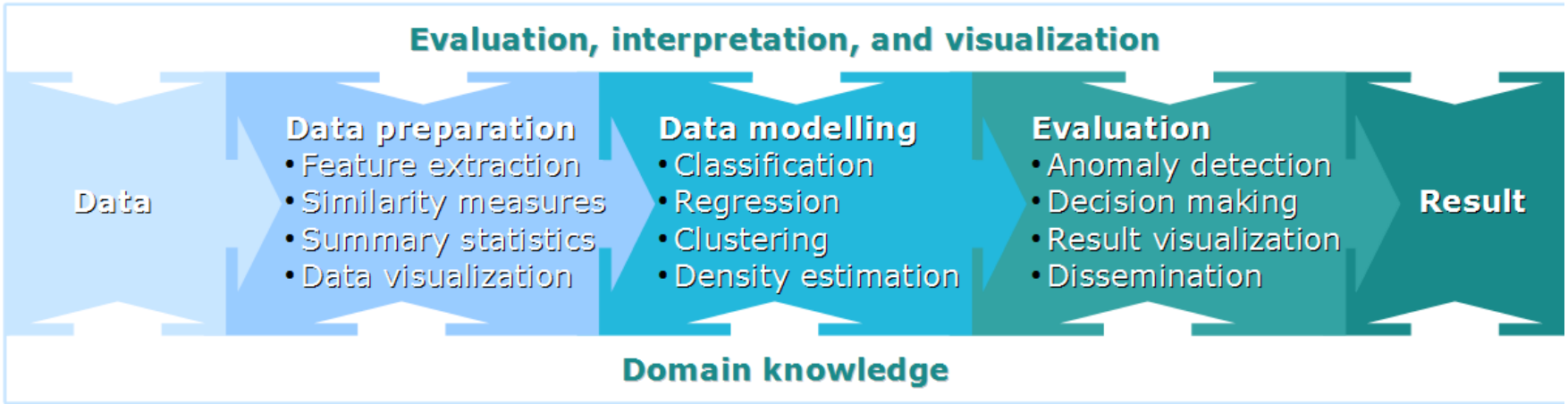
   Data: Feature extraction, and visualization
2. Data, feature extraction and PCA
   7 October: C2, C3
3. Measures of similarity, summary statistics and probabilities
   7 October: C4, C5
4. Probability densities and data Visualization
   7 October: C6, C7

   Supervised learning: Classification and regression
5. Decision trees and linear regression
   8 October: C8, C9
6. Overfitting, cross-validation and Nearest Neighbor
   8 October: C10, C12
7. Performance evaluation, Bayes, and Naive Bayes
   9 October: C11, C13
8. Artificial Neural Networks and Bias/Variance
   9 October: C14, C15
9. AUC and ensemble methods
   10 October: C16, C17

   Unsupervised learning: Clustering and density estimation
10. K-means and hierarchical clustering
    10 October: C18
11. **Mixture models and density estimation**
    11 October: C19, C20
12. Association mining
    11 October: C21

    Recap
13. Recap
    11 October: C1-C21

Piazza online help: `https://piazza.com/dtu.dk/fall2019/october2019`



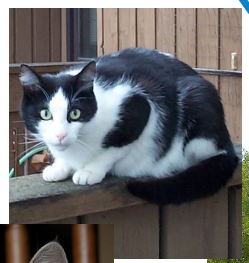
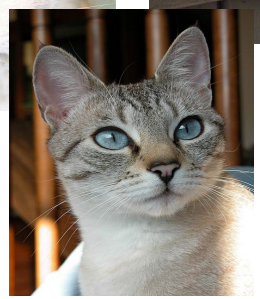
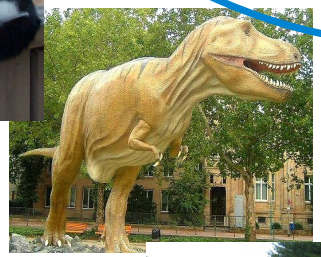
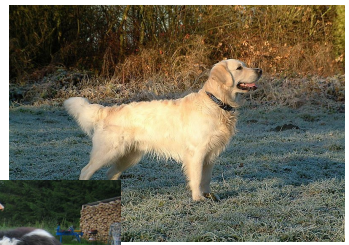
Learning Objectives

- Explain the role of the parameters in the Gaussian Mixture Model (GMM) and how the parameters are updated using the EM-algorithm
- Explain how cross-validation can be used for GMM
- Understand and apply kernel density, K-nearest neighbour density and average relative density estimation for outlier detection

Imagine you observe the world for the first time!

http://www.clipartlord.com/category/baby-clip-art/




We humans are skilled at dividing objects into groups (clustering), but how do we make computers do the same?

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http://commons.wikimedia.org/wiki/File:Cat_Eyes.jpg
http://commons.wikimedia.org/wiki/File:Black_white_cat_on_fence.jpg
http://commons.wikimedia.org/wiki/File:Golden_Retriever_Dukedestiny01.jpg
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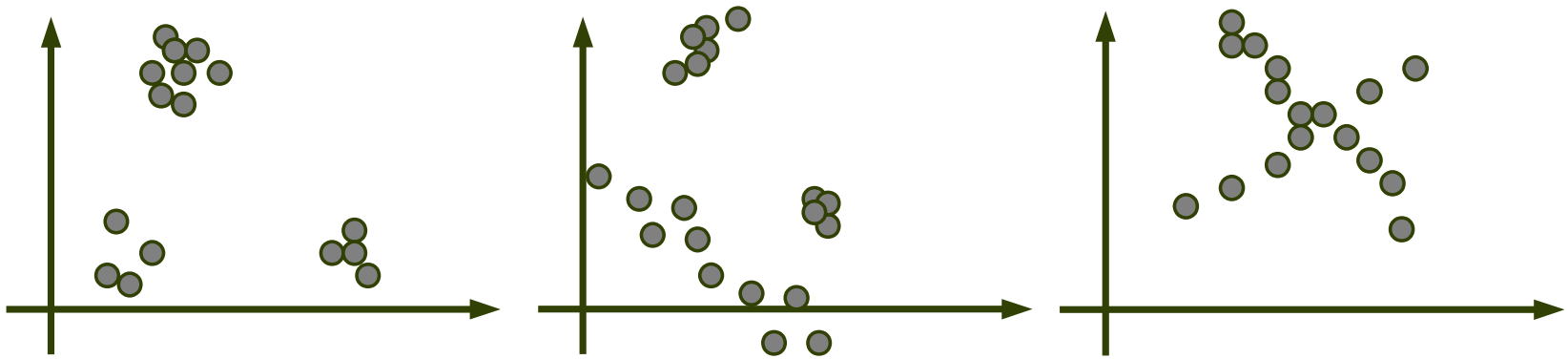
https://commons.wikimedia.org/wiki/Dog#/media/File:BluetickCoonhound.jpg
http://commons.wikimedia.org/wiki/File:Saurier2.jpg

- What are the clusters below and what characterize each cluster?
- Is **k-means** well suited for modeling the clusters below?
  - Will it always find the optimum solution?
  - Can it model the sizes of the clusters?
  - Can it model the shape of the clusters?
  - How can we determine the number of clusters?



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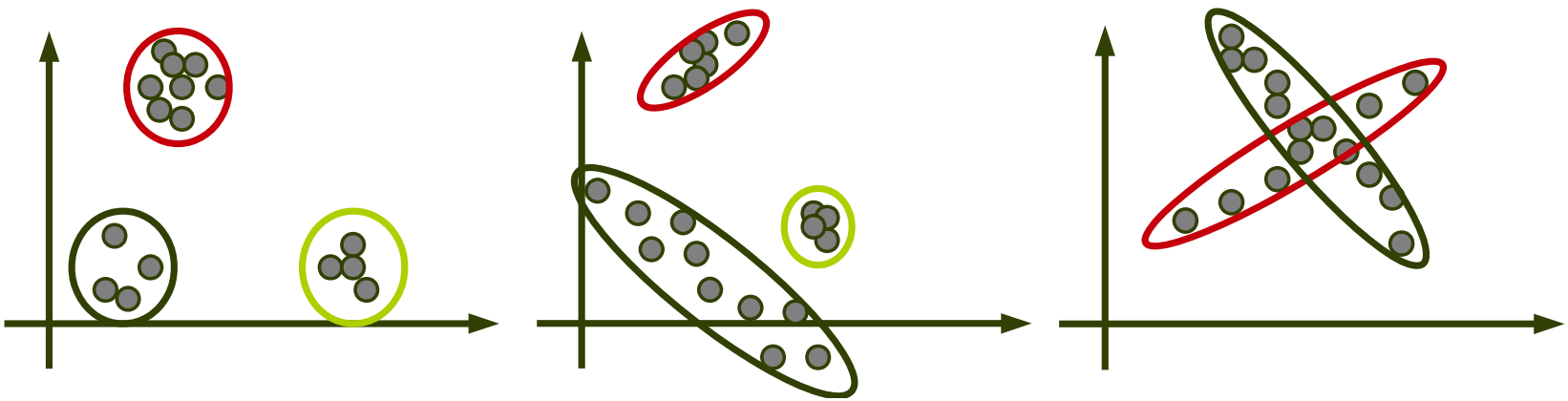
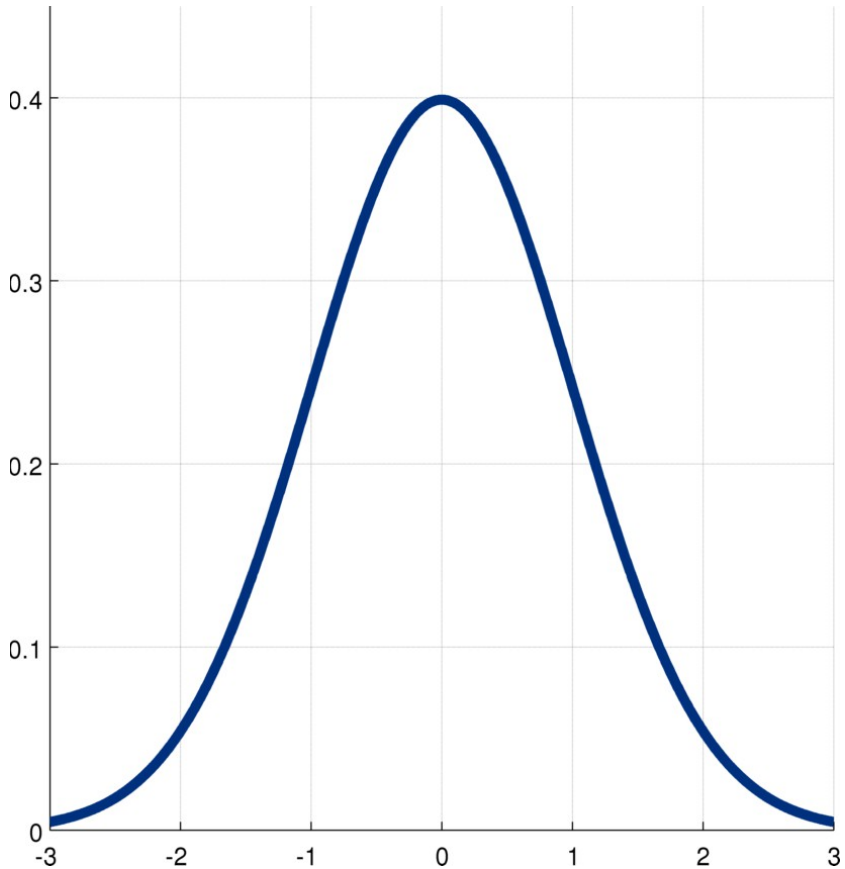


Normal distribution

- Probability density function describes the relative chance of a given value to occur

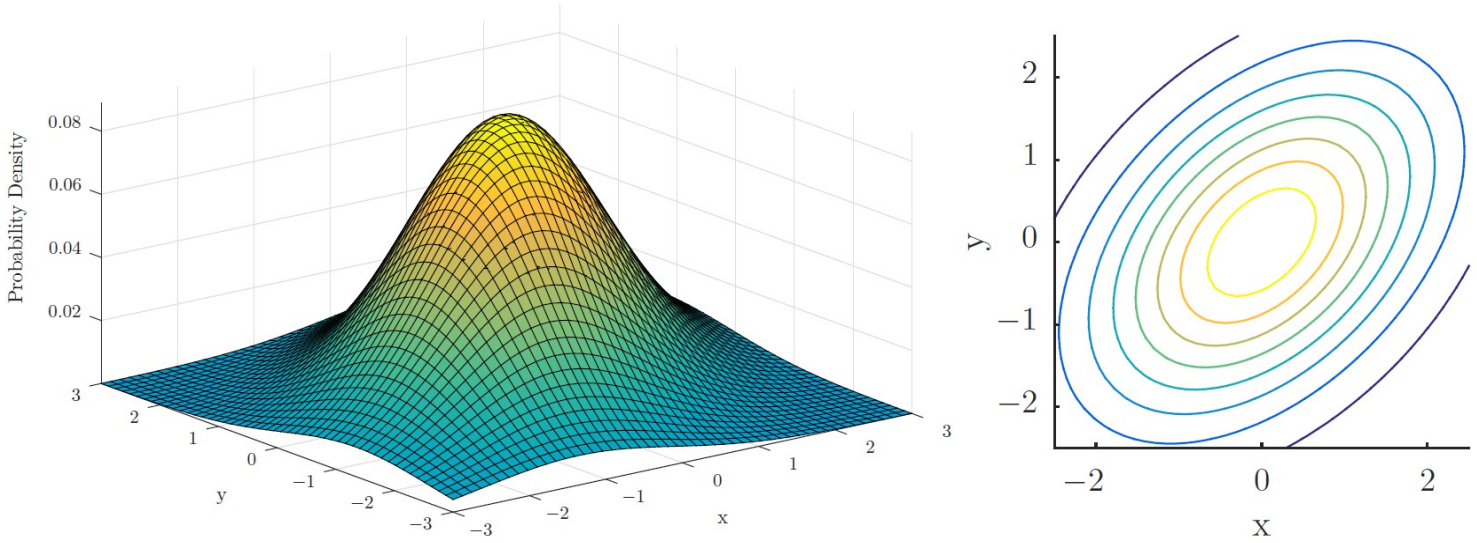
- Normal distribution characterized by
  - Mean
  - Variance

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



Multivariate Normal distribution

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^d|\boldsymbol{\Sigma}|}} e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}$$



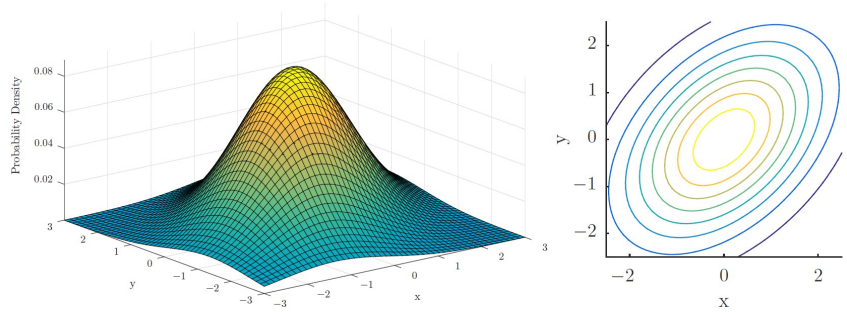
Multivariate Normal distribution

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^d|\boldsymbol{\Sigma}|}} e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}$$

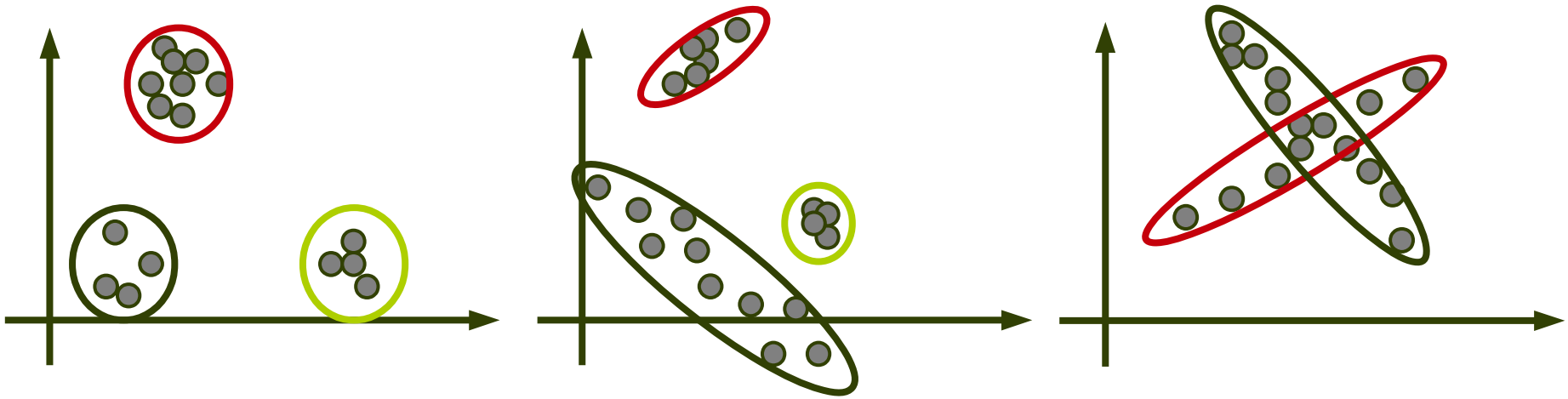
- Example: 2-dimensional Normal distribution

$$\mu = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} \mathrm{var}(x_1) & \mathrm{cov}(x_1, x_2) \\ \mathrm{cov}(x_2, x_1) & \mathrm{var}(x_2) \end{bmatrix}$$



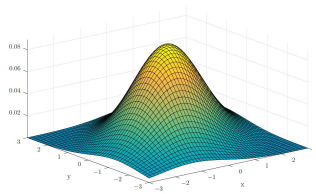
Prototypical mixture model



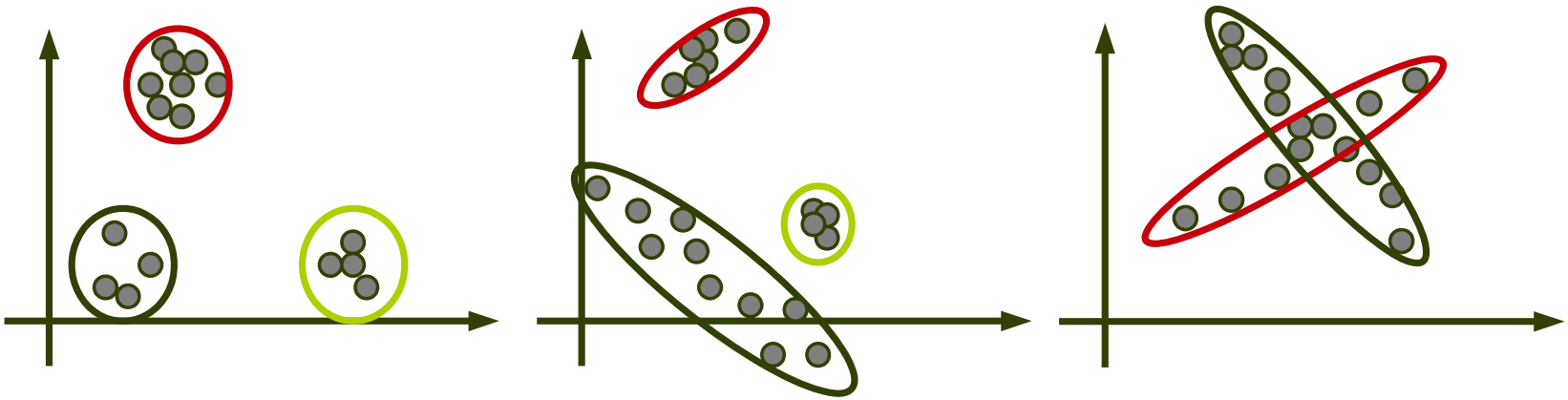
- We want a **density** $p(\boldsymbol{x})$ of our observations $\boldsymbol{x} \in \mathbb{R}^M$
- Suppose we have K clusters and let $z = k$ if $\boldsymbol{x}$ belongs to cluster k
- According to the the basic rules of probability:

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} p(\boldsymbol{x}, z = k) = \sum_{k=1}^{K} p(\boldsymbol{x}|z = k)p(z = k)$$

- If we specify $p(\boldsymbol{x}|z = k)$ and $p(z = k) = w_k$ we have a model



The Gaussian Mixture Model (GMM)



- Different locations $\boldsymbol{\mu}_{(k)}$
- Different shape $\boldsymbol{\Sigma}_{(k)}$
- Different sizes w_k

Data density

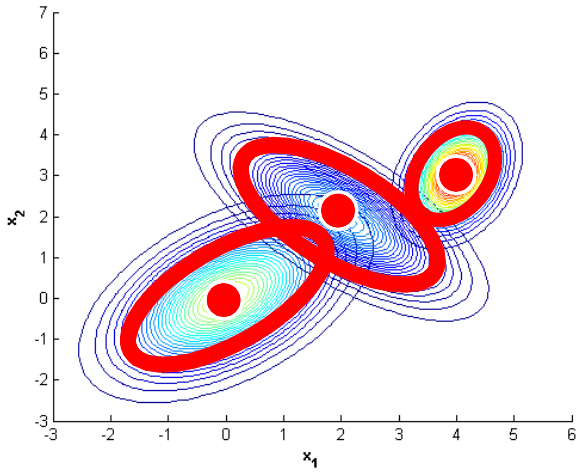
Sum of cluster specific densities assumed normal distributed

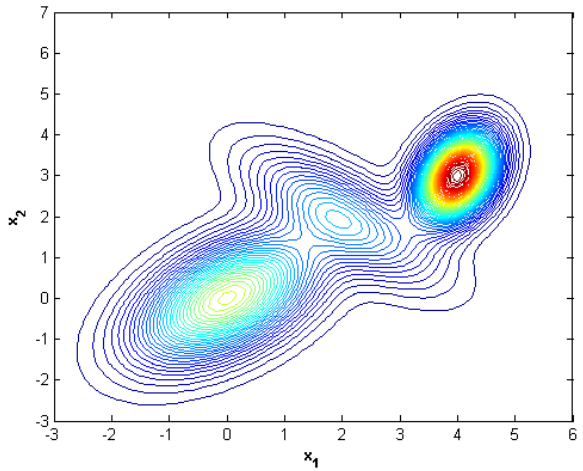
$$p(\mathbf{x}) = \sum_{k=1}^{K} w_k \mathcal{N}(\mathbf{x} \,|\, \mu_{(k)}, \boldsymbol{\Sigma}_{(k)})$$

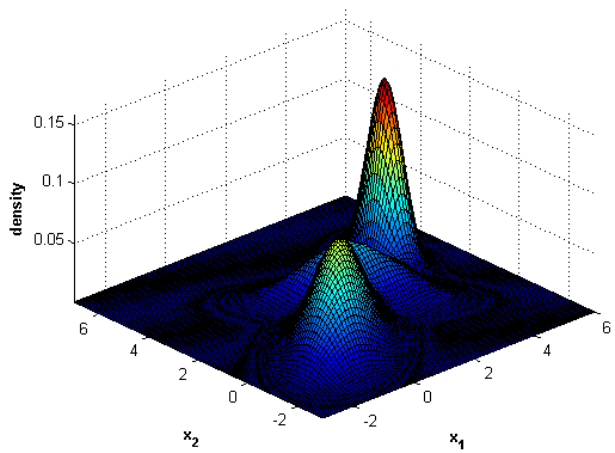
$$\text{s.t.} \sum_{k=1}^{K} w_k = 1, \; w_k \geq 0$$

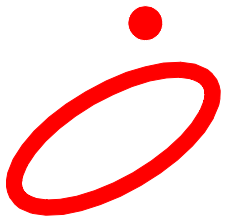
GMM example

$$p(\boldsymbol{x}) = 0.5\mathcal{N}(\boldsymbol{x}|\begin{bmatrix}0\\0\end{bmatrix},\begin{bmatrix}1 & 0.5\\0.5 & 1\end{bmatrix}) + 0.2\mathcal{N}(\boldsymbol{x}|\begin{bmatrix}2\\2\end{bmatrix},\begin{bmatrix}1 & -0.7\\-0.7 & 1\end{bmatrix}) + 0.3\mathcal{N}(\boldsymbol{x}|\begin{bmatrix}4\\3\end{bmatrix},\begin{bmatrix}0.2 & 0.1\\0.1 & 0.5\end{bmatrix})$$









$\boldsymbol{\mu}_{(k)}$: Cluster center (prototypical example in cluster)

$\boldsymbol{\Sigma}_{(k)}$: Shape of the cluster

w_k : Relative size/density of the cluster

Quiz 01 (please answer on Piazza): GMM

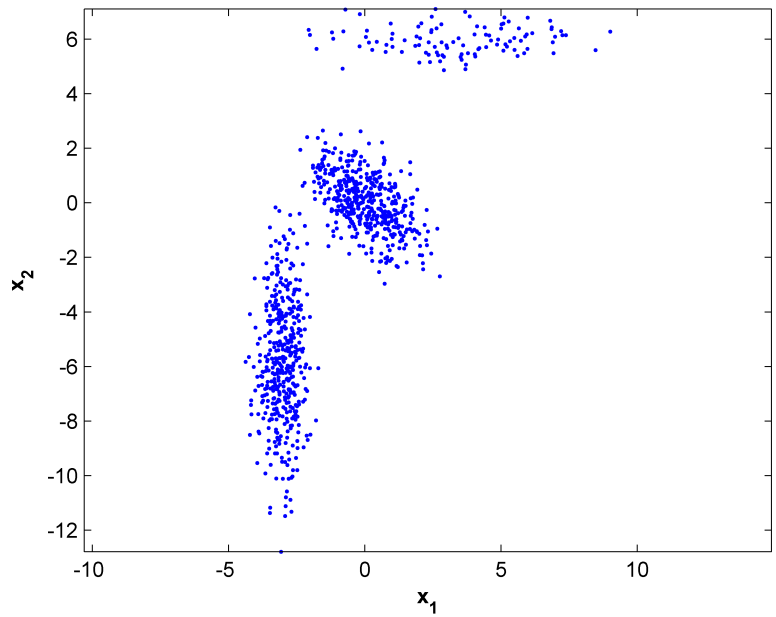


Figure 1: 1000 data observations drawn from a Gaussian Mixture Model (GMM) with three clusters.

In Figure 1 is shown 1000 observations drawn from a density defined by a Gaussian Mixture Model (GMM) with three clusters. Suppose $\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{2\pi|\boldsymbol{\Sigma}|}} \exp{(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}$ is the multivariate normal distribution, which one of the following GMM densities was used to generate the data?

A
$$p(x) = 0.1 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} 3 \\ 6 \end{bmatrix}, \begin{bmatrix} 5 & 0 \\ 0 & 0.25 \end{bmatrix}) + 0.45 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} -3 \\ -6 \end{bmatrix}, \begin{bmatrix} 0.25 & 0 \\ 0 & 5 \end{bmatrix}) + 0.45 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix})$$

B
$$p(x) = 0.45 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} 3 \\ 6 \end{bmatrix}, \begin{bmatrix} 5 & 0 \\ 0 & 0.25 \end{bmatrix}) + 0.1 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} -3 \\ -6 \end{bmatrix}, \begin{bmatrix} 0.25 & 0 \\ 0 & 5 \end{bmatrix}) + 0.45 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix})$$

C
$$p(x) = 0.1 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} 3 \\ 6 \end{bmatrix}, \begin{bmatrix} 0.25 & 0 \\ 0 & 5 \end{bmatrix}) + 0.45 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} -3 \\ -6 \end{bmatrix}, \begin{bmatrix} 5 & 0 \\ 0 & 0.25 \end{bmatrix}) + 0.45 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix})$$

D
$$p(x) = 0.1 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} 3 \\ 6 \end{bmatrix}, \begin{bmatrix} 0.25 & 0 \\ 0 & 5 \end{bmatrix}) + 0.45 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} -3 \\ -6 \end{bmatrix}, \begin{bmatrix} 5 & 0 \\ 0 & 0.25 \end{bmatrix}) + 0.45 \cdot \mathcal{N}(\boldsymbol{x}|\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix})$$

E Don't know.

Solution:

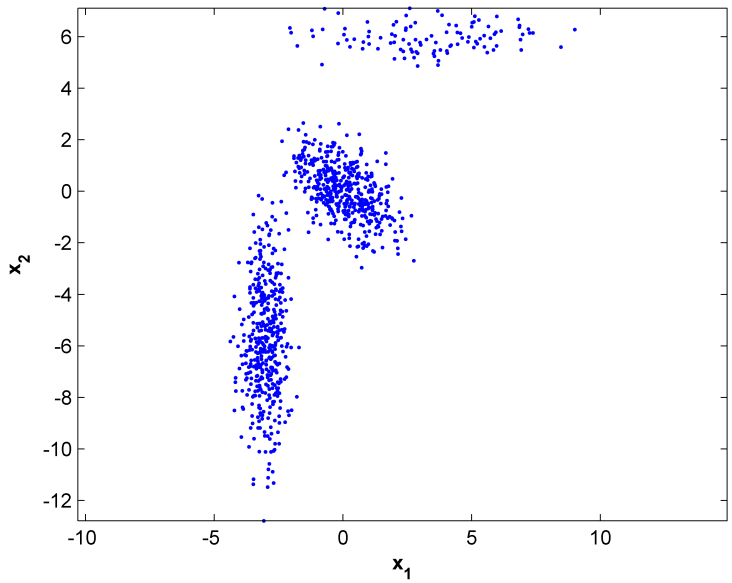


Figure 1: 1000 data observations drawn from a Gaussian Mixture Model (GMM) with three clusters.

The centroids of the clusters are $\begin{bmatrix} 3 \\ 6 \end{bmatrix}, \begin{bmatrix} -3 \\ -6 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. The cluster at $\begin{bmatrix} 3 \\ 6 \end{bmatrix}$ is not very dense and should therefore have the coefficient 0.1, it further has a large spread in the x_1 direction and small spread in the x_2 direction corresponding to a covariance matrix of $\begin{bmatrix} 5 & 0 \\ 0 & 0.25 \end{bmatrix}$, thus, answer option one is the only correct answer.

Sanity check time:

- Consider the Gaussian mixture model (GMM)

$$p(\mathbf{x}) = \sum_{k=1}^{K} w_k \mathcal{N}(\mathbf{x}|\, \mu_{(k)}, \mathbf{\Sigma}_{(k)}) \quad \text{s.t.} \sum_{k=1}^{K} w_k = 1,\ w_k \geq 0$$

- What is the value of the integral?

$$\int p(\mathbf{x}) \mathrm{d}\mathbf{x}$$

Gaussian mixture models, EM algorithm

Select an initial set of model parameters (mean and covariance for each cluster)

Repeat

- **Expectation**
  - For each object, calculate the probability of belonging to each distribution
- **Maximization**
  - For each probability distribution, estimate parameters by maximum likelihood

Until the parameters do not change

E-step

$$p(\boldsymbol{z}_n = k|\boldsymbol{x}_n) = \frac{w_k \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_{(k)}, \boldsymbol{\Sigma}_{(k)})}{\sum_{K=1}^{K} w_k \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_{(k)}, \boldsymbol{\Sigma}_{(k)})}$$

M-step

$$\begin{aligned}
N_k &= \sum_{n=1}^{N} p(\boldsymbol{z}_n = k|\boldsymbol{x}_n) \\
\boldsymbol{\mu}_{(k)} &= \frac{1}{N_k} \sum_{n=1}^{N} \boldsymbol{x}_n p(\boldsymbol{z}_n = k|\boldsymbol{x}_n) \\
w_k &= \frac{N_k}{N} \\
\boldsymbol{\Sigma}_{(k)} &= \frac{1}{N_k} \sum_{n=1}^{N} (\boldsymbol{x}_n - \boldsymbol{\mu}_{(k)})(\boldsymbol{x}_n - \boldsymbol{\mu}_{(k)})^\top p(\boldsymbol{z}_n = k|\boldsymbol{x}_n)
\end{aligned}$$

The GMM update rules approximately implements

$$w_k = p(z = k)$$
$$\mu_{(k)} = \mathbb{E}_{p(\boldsymbol{x}|z=k)}\left[\boldsymbol{x}\right]$$
$$\boldsymbol{\Sigma}_{(k)} = \mathbb{E}_{p(\boldsymbol{x}|z=k)}\left[(\boldsymbol{x} - \bar{\boldsymbol{x}})(\boldsymbol{x} - \bar{\boldsymbol{x}})^\top\right]$$

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E-step

$$p(\boldsymbol{z}_n = k|\boldsymbol{x}_n) = \frac{w_k \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_{(k)}, \boldsymbol{\Sigma}_{(k)})}{\sum_{K=1}^{K} w_k \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_{(k)}, \boldsymbol{\Sigma}_{(k)})}$$

$$\boldsymbol{\mu}_{(k)} = \frac{1}{N_k} \sum_{n=1}^{N} \boldsymbol{x}_n p(z_n = k|\boldsymbol{x}_n)$$

M-step

$$N_k = \sum_{n=1}^{N} p(\boldsymbol{z}_n = k|\boldsymbol{x}_n)$$
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$$w_k = \frac{N_k}{N}$$
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The GMM update rules approximately implements

$$
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w_k &= p(z = k) \\
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\end{aligned}
$$

Derivation:

$$
\begin{aligned}
w_k &= \frac{N_k}{N} \\
&= \sum_{n=1}^{N} p(z_n = k|\boldsymbol{x}_n)\frac{1}{N} \\
&= \sum_{n=1}^{N} p(z_n = k|\boldsymbol{x}_n)p(\boldsymbol{x}_n) \\
&= \sum_{n=1}^{N} p(z_n = k, \boldsymbol{x}_n) \\
&= p(z = k)
\end{aligned}
$$

The GMM update rules approximately implements

$$
\begin{aligned}
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\boldsymbol{\Sigma}_{(k)} &= \mathbb{E}_{p(\boldsymbol{x}|z=k)}\left[(\boldsymbol{x} - \bar{\boldsymbol{x}})(\boldsymbol{x} - \bar{\boldsymbol{x}})^\top\right]
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{\mu}_{(k)} &= \frac{1}{N_k}\sum_{n=1}^{N} \boldsymbol{x}_n p(z_n = k|\boldsymbol{x}_n) \\
&= \frac{1}{\frac{N_k}{N}}\sum_{n=1}^{N} \boldsymbol{x}_n p(z_n = k|\boldsymbol{x}_n)\frac{1}{N} \\
&= \sum_{n=1}^{N} \boldsymbol{x}_n \frac{p(z = k)p(\boldsymbol{x}_n)}{p(z = k)} \\
&= \sum_{n=1}^{N} \boldsymbol{x}_n \frac{p(z = k, \boldsymbol{x}_n)}{p(z = k)} \\
&= \sum_{n=1}^{N} \boldsymbol{x}_n p(\boldsymbol{x}_n|z = k)
\end{aligned}
$$

Gaussian mixture models, EM algorithm

Select an initial set of model parameters (mean and covariance for each cluster)

Repeat

- **Expectation**
  - For each object, calculate the probability of belonging to each distribution
- **Maximization**
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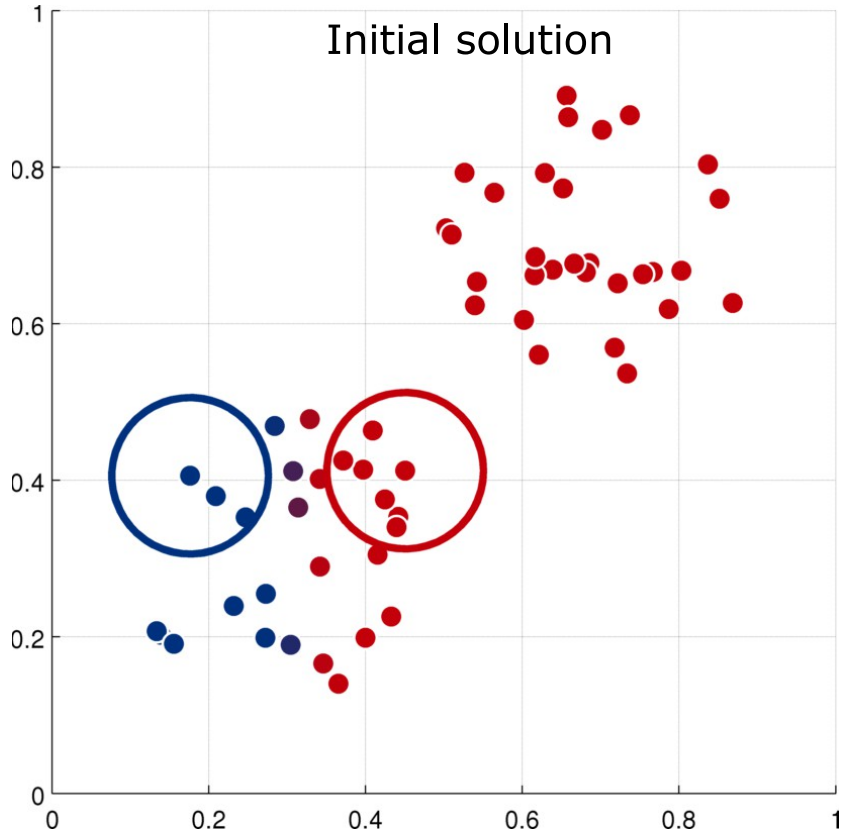
Until the parameters do not change



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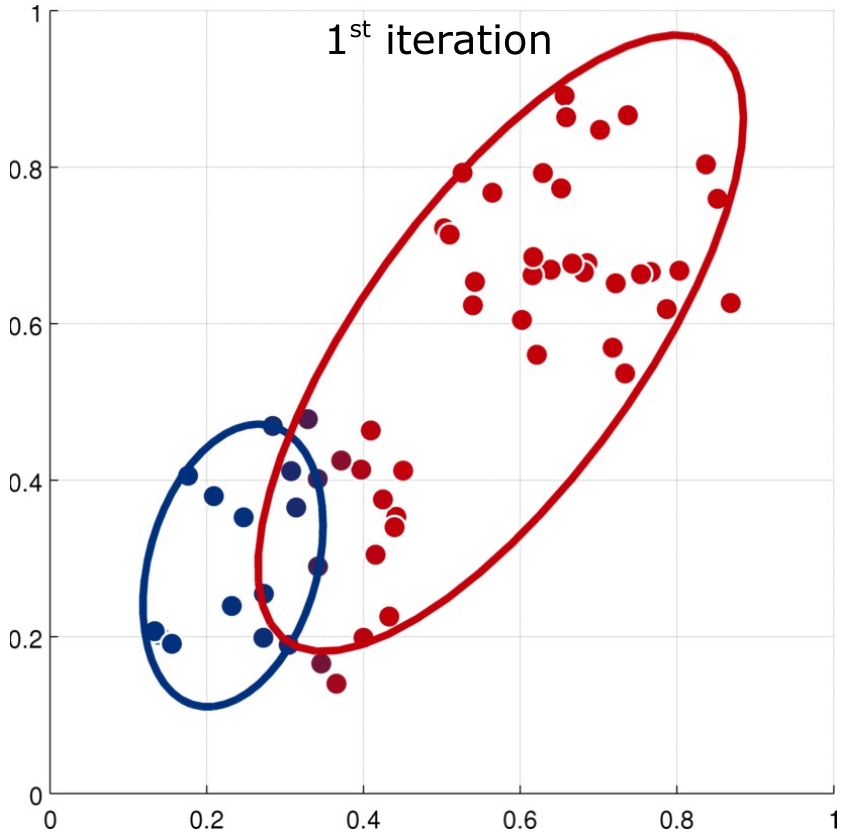

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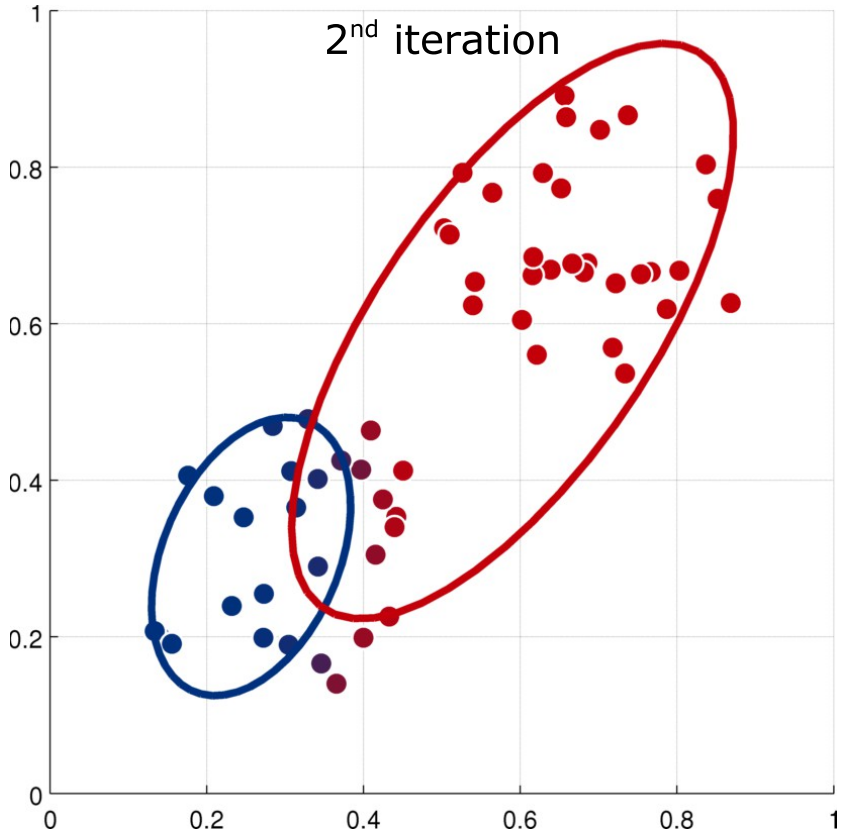
Until the parameters do not change



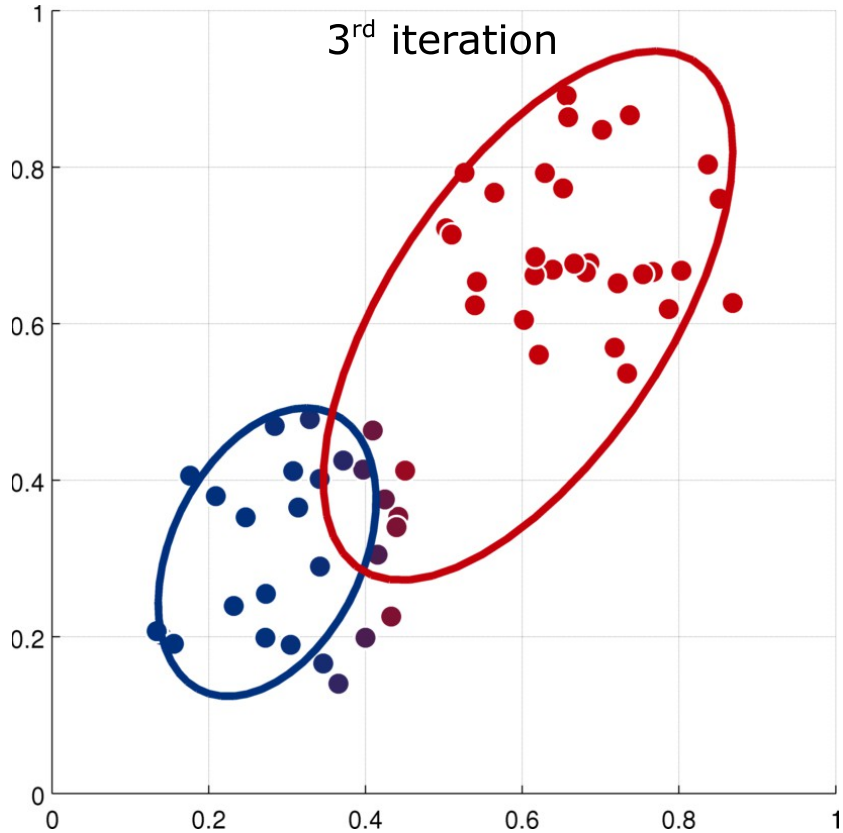
Gaussian mixture models, EM algorithm

Select an initial set of model parameters (mean and covariance for each cluster)

Repeat

- **Expectation**
  - For each object, calculate the probability of belonging to each distribution
- **Maximization**
  - For each probability distribution, estimate parameters by maximum likelihood

Until the parameters do not change



Gaussian mixture models, EM algorithm

Select an initial set of model parameters (mean and covariance for each cluster)

Repeat

- **Expectation**
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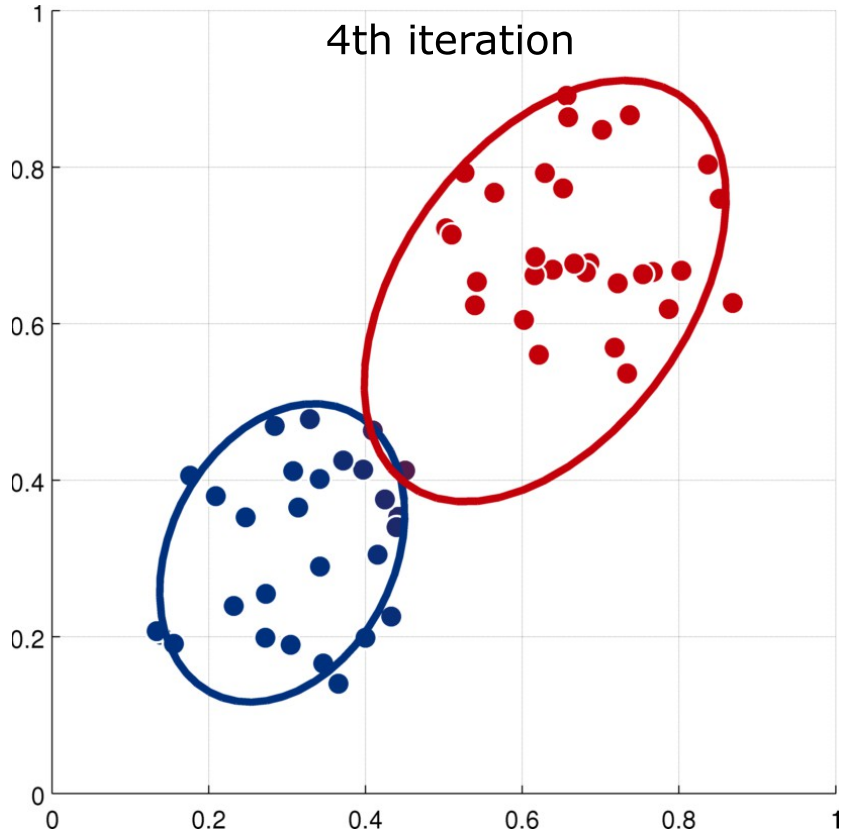
Until the parameters do not change



Gaussian mixture models, EM algorithm

Select an initial set of model parameters (mean and covariance for each cluster)

Repeat

- **Expectation**
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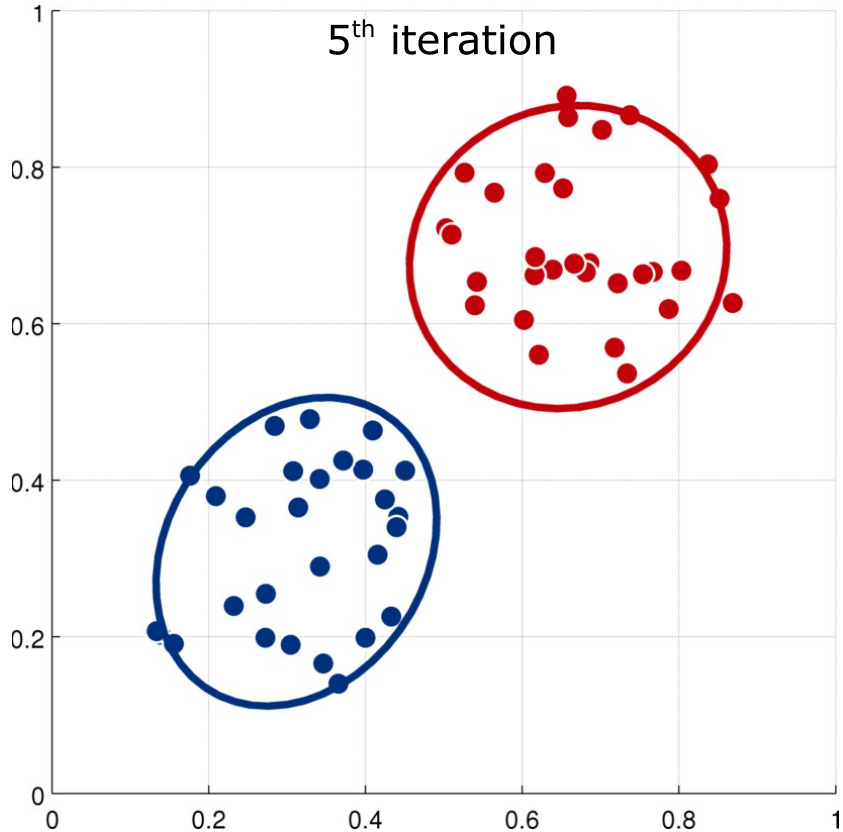
  - For each probability distribution, estimate parameters by maximum likelihood

Until the parameters do not change



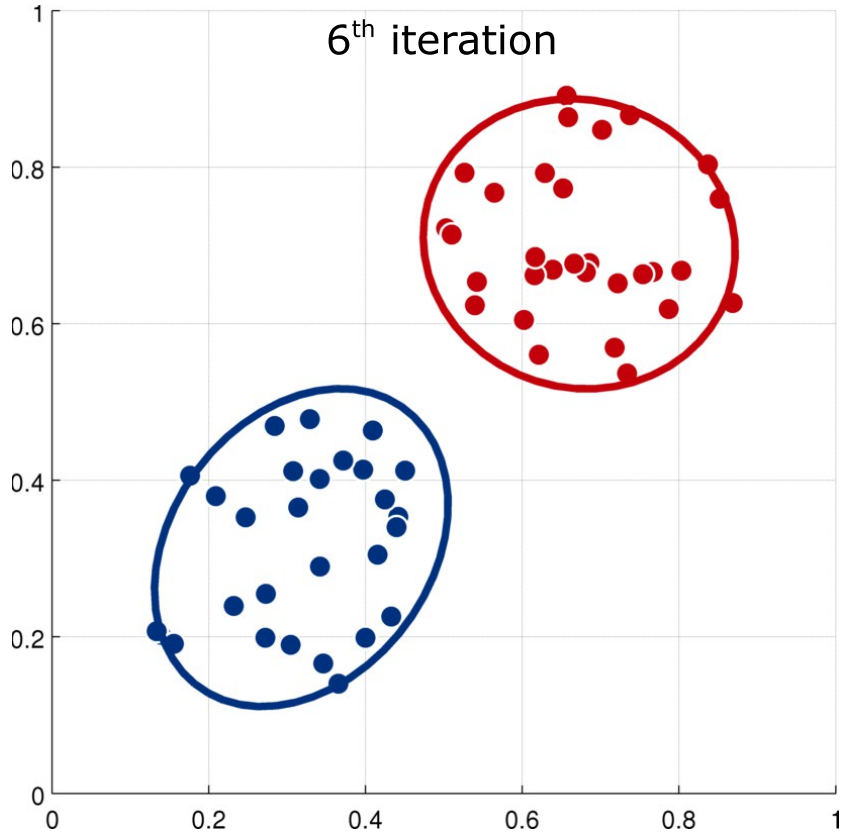
Gaussian mixture models, EM algorithm

Select an initial set of model parameters (mean and covariance for each cluster)

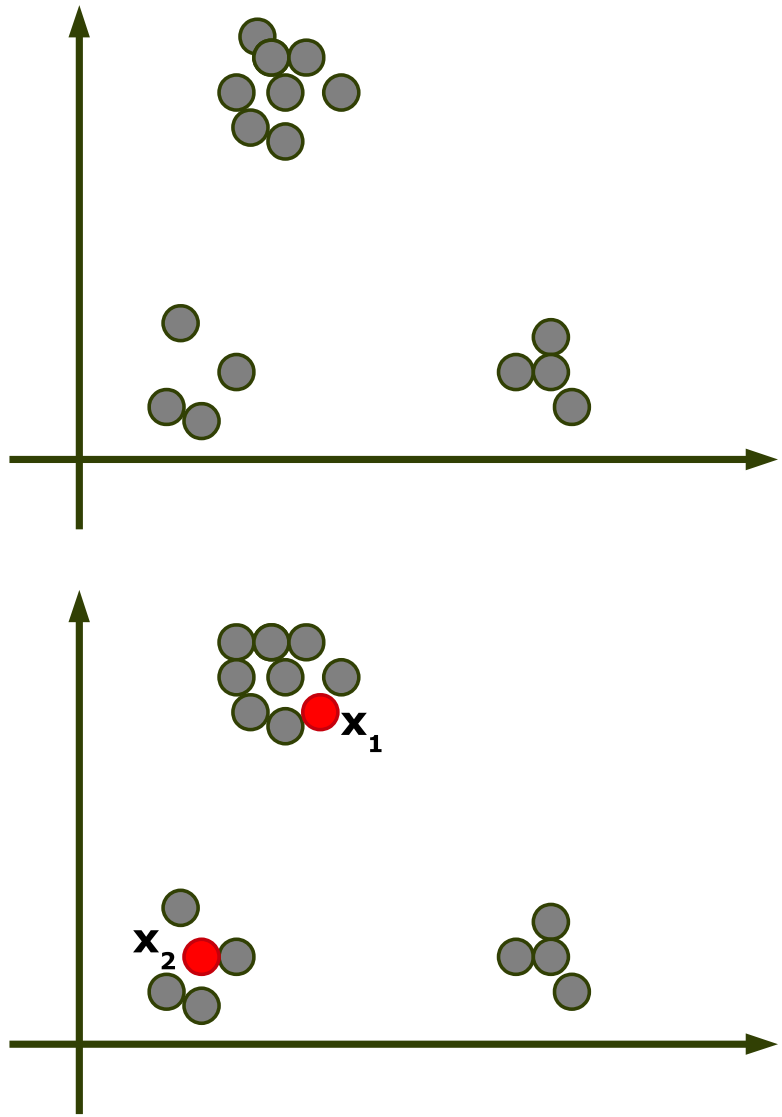
Repeat

- **Expectation**
  - For each object, calculate the probability of belonging to each distribution
- **Maximization**
  - For each probability distribution, estimate parameters by maximum likelihood

Until the parameters do not change

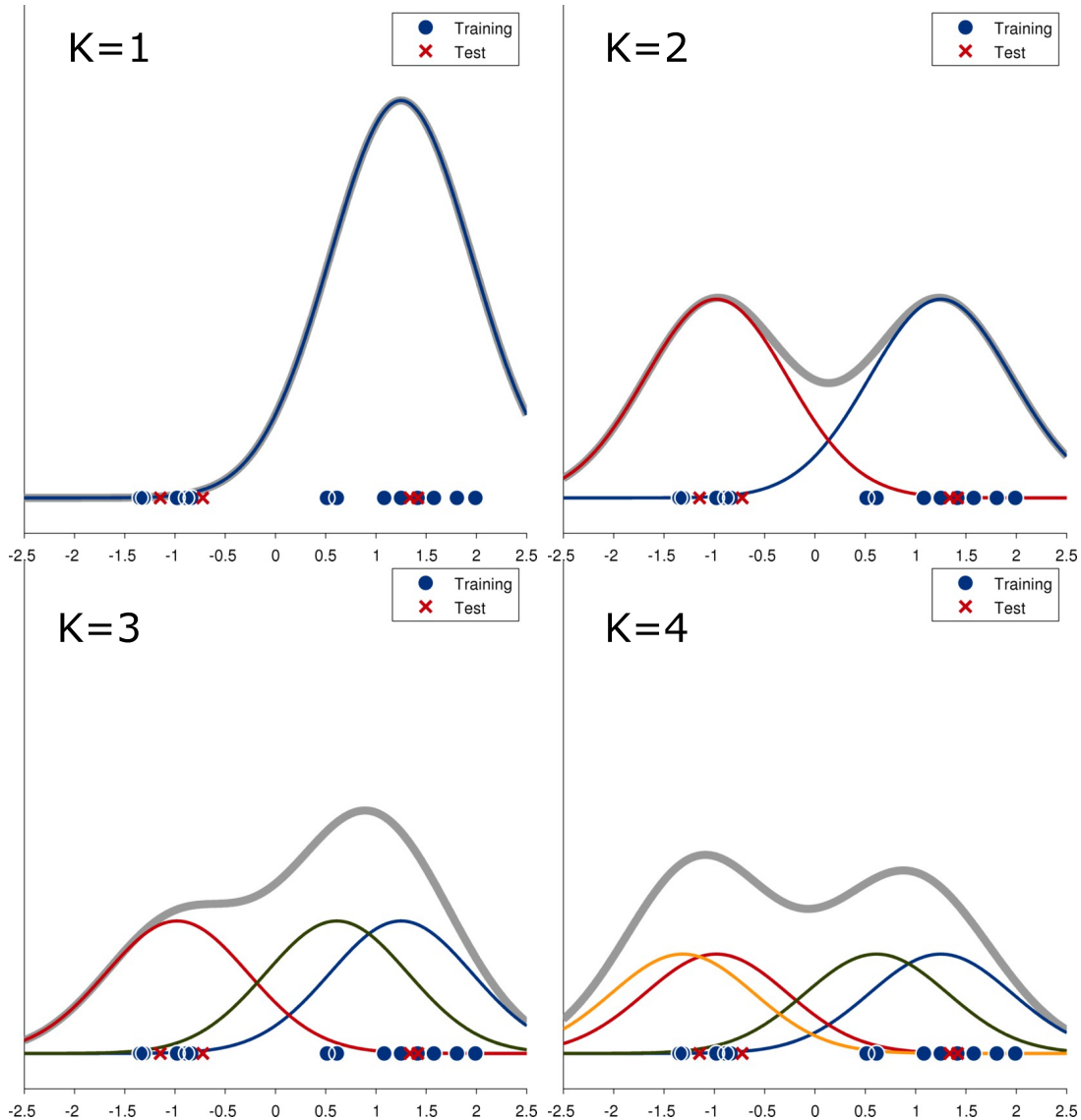


- Consider the data to the right with 16 observations.
  - What would ideally happen if we used a GMM with K=16 clusters to model the data?
- Imagine we have two **test observations** denoted $\mathbf{x}_1$ and $\mathbf{x}_2$ (red points) that are not used for training.
  - What happens to $p(\mathbf{x}_1)$ and $p(\mathbf{x}_2)$ if we use K=3 and K=16 clusters?



Mixture models

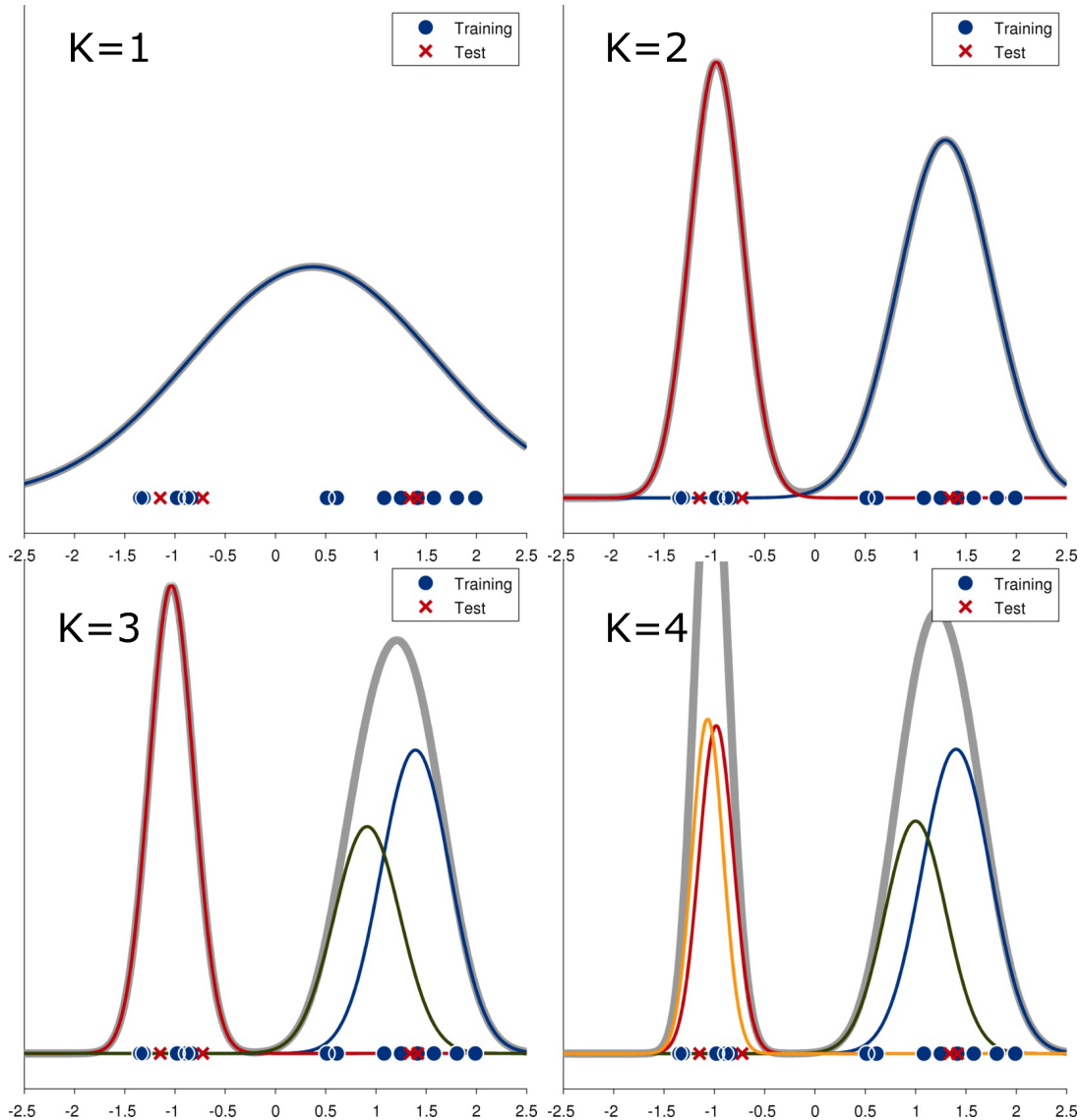
- Selecting complexity using crossvalidation



EM 1st iteration

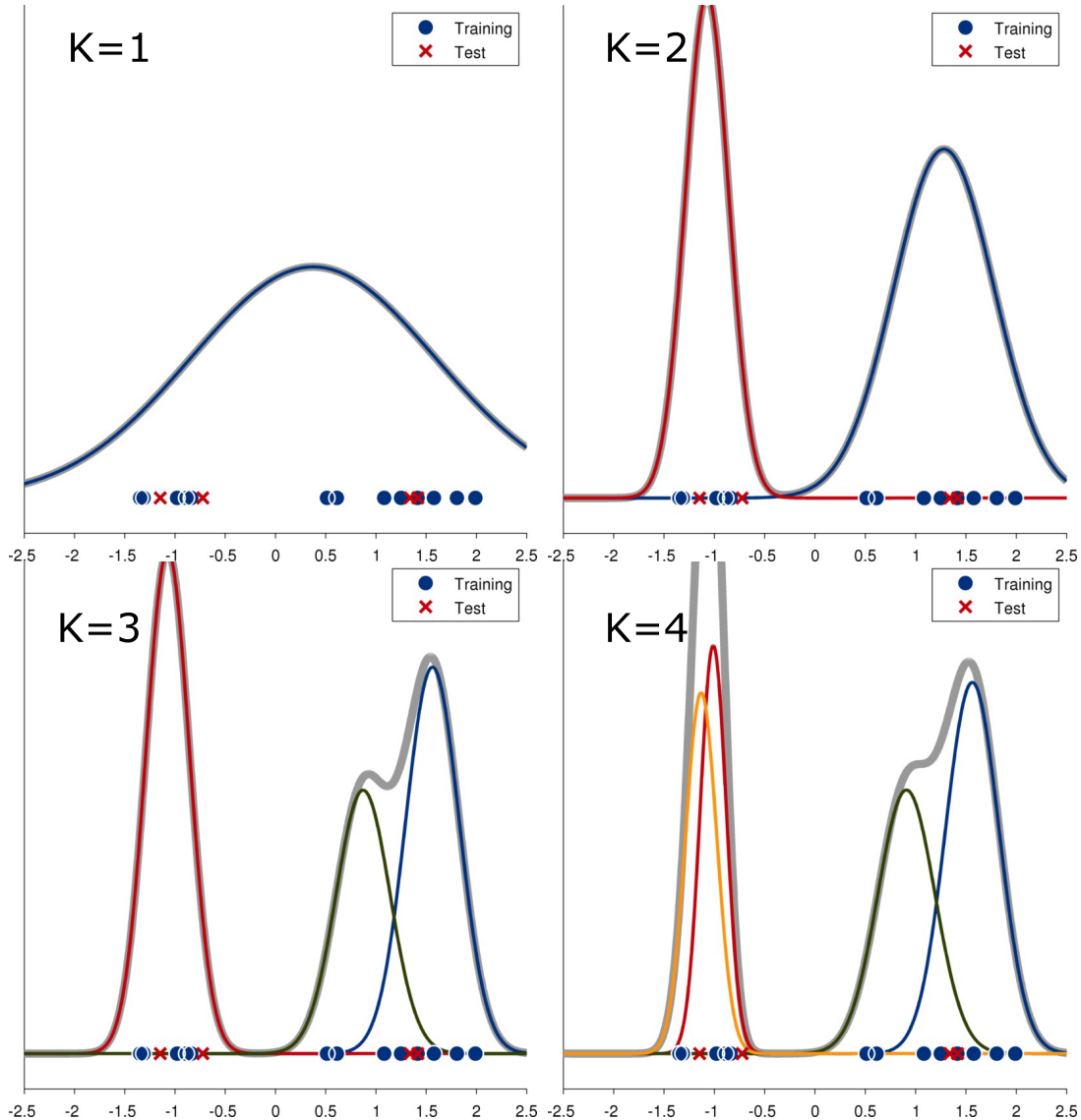
Mixture models

- Selecting complexity using crossvalidation



Mixture models

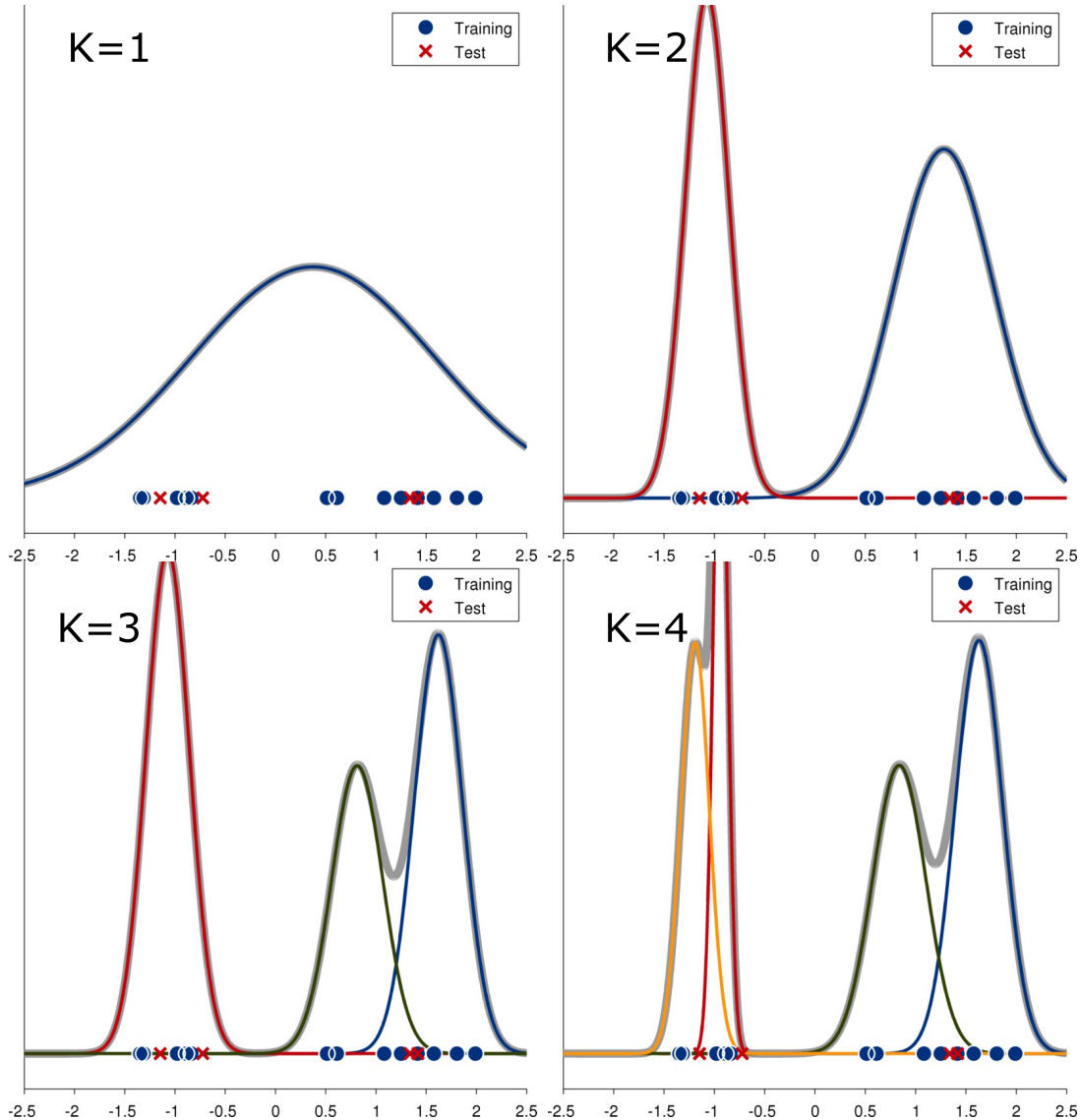
- Selecting complexity using crossvalidation



EM 3rd iteration

Mixture models

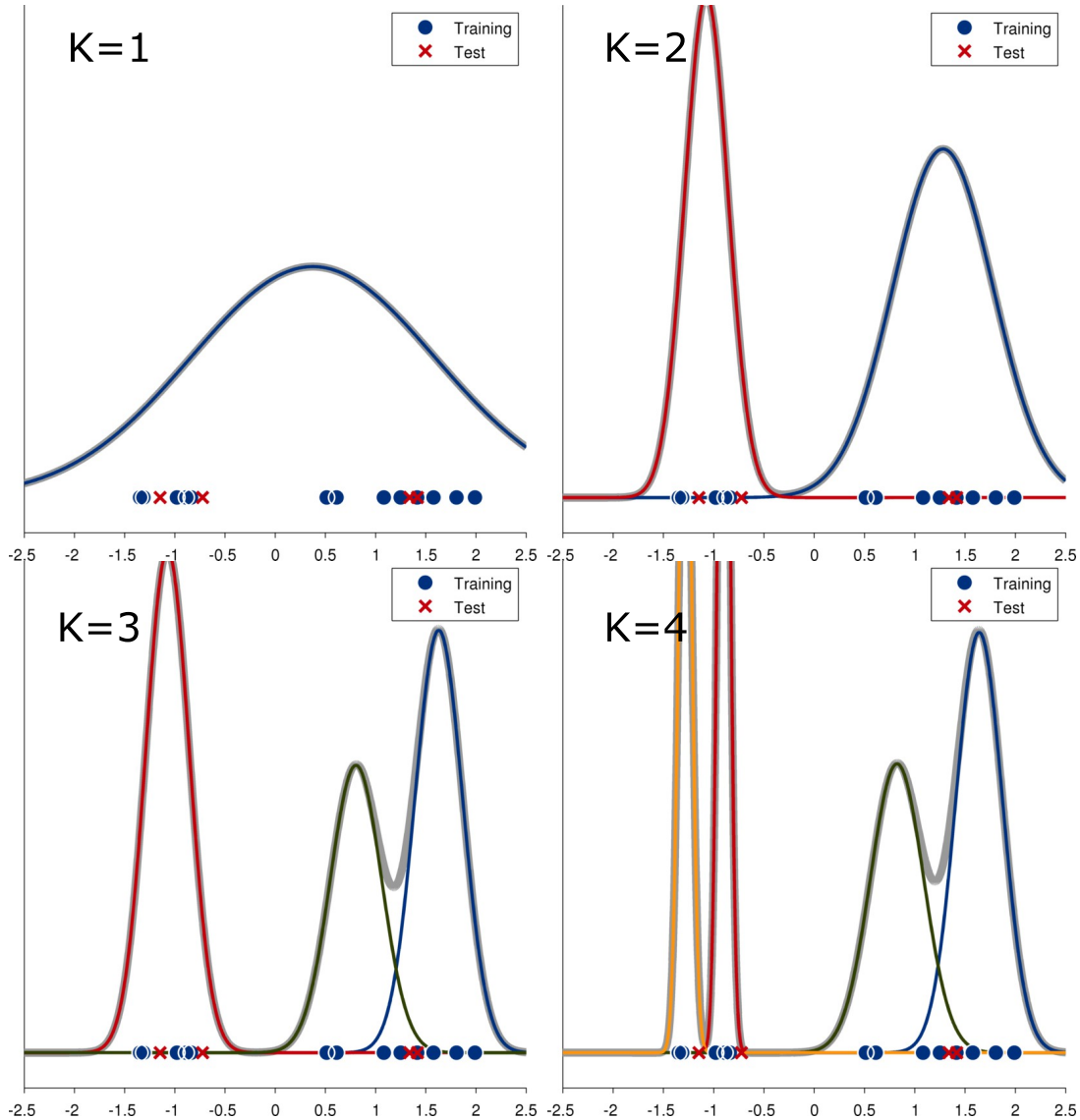
- Selecting complexity using crossvalidation



EM 4th iteration

Mixture models

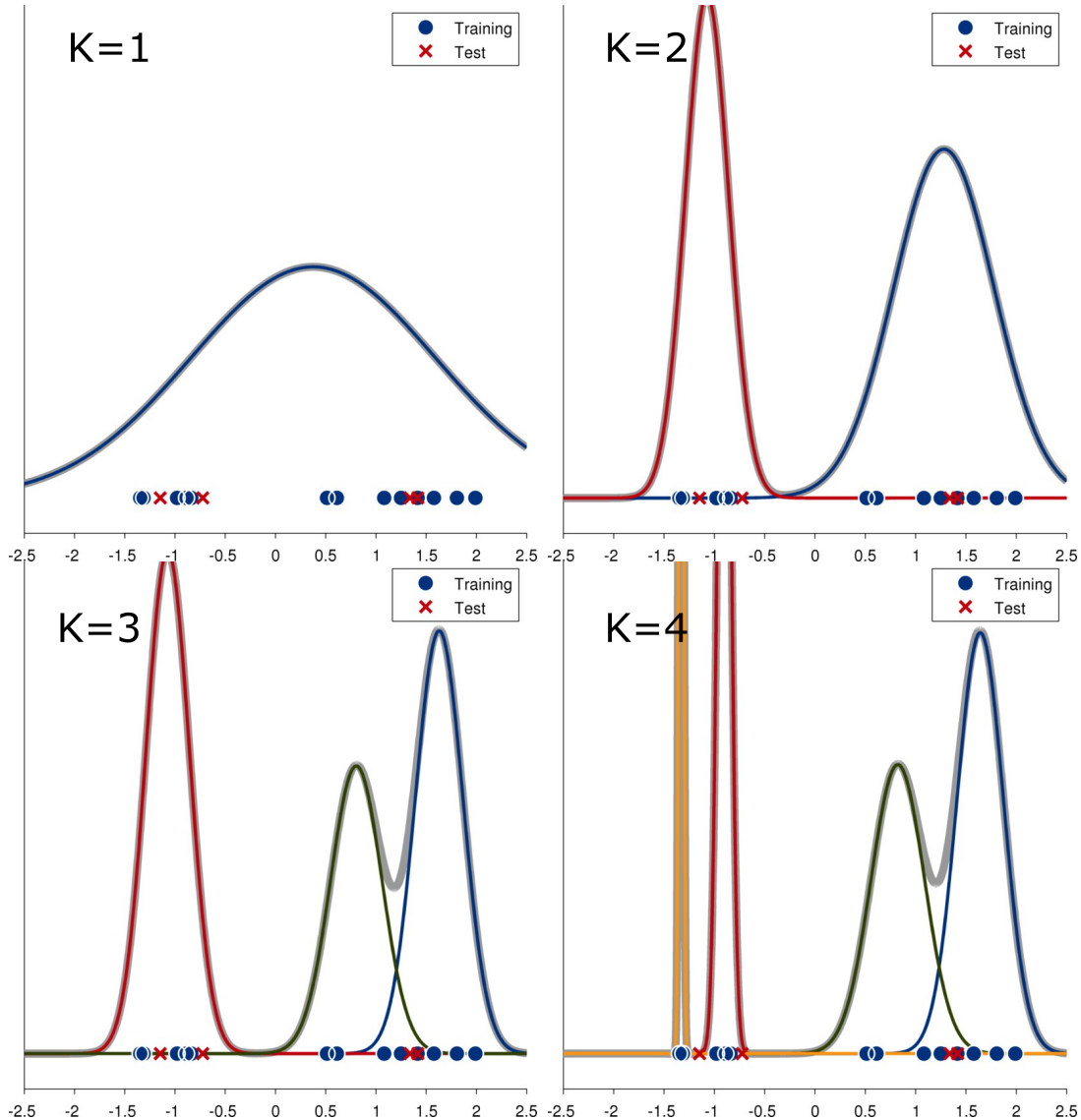
- Selecting complexity using crossvalidation



EM 5th iteration

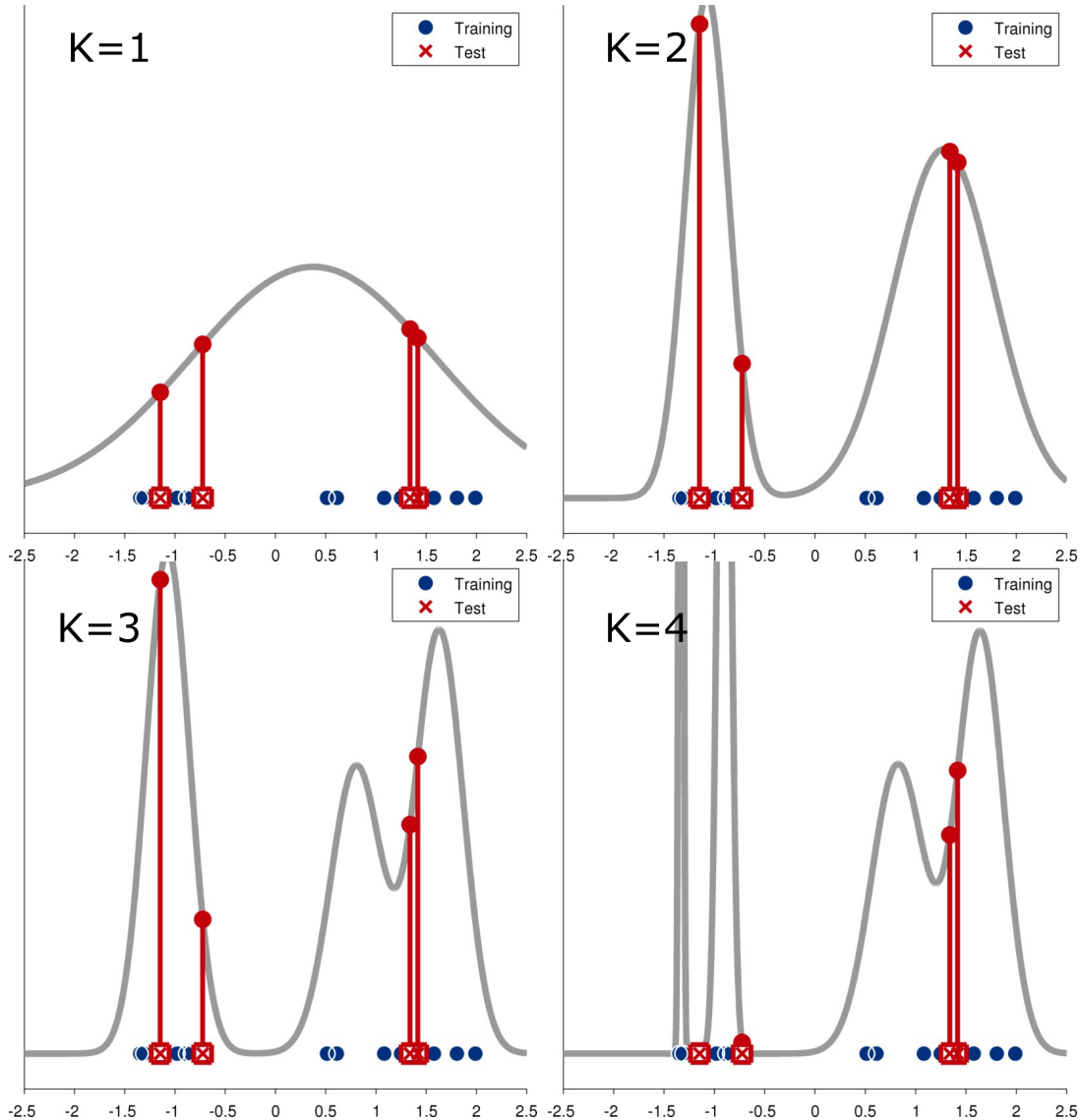
Mixture models

- Selecting complexity using crossvalidation



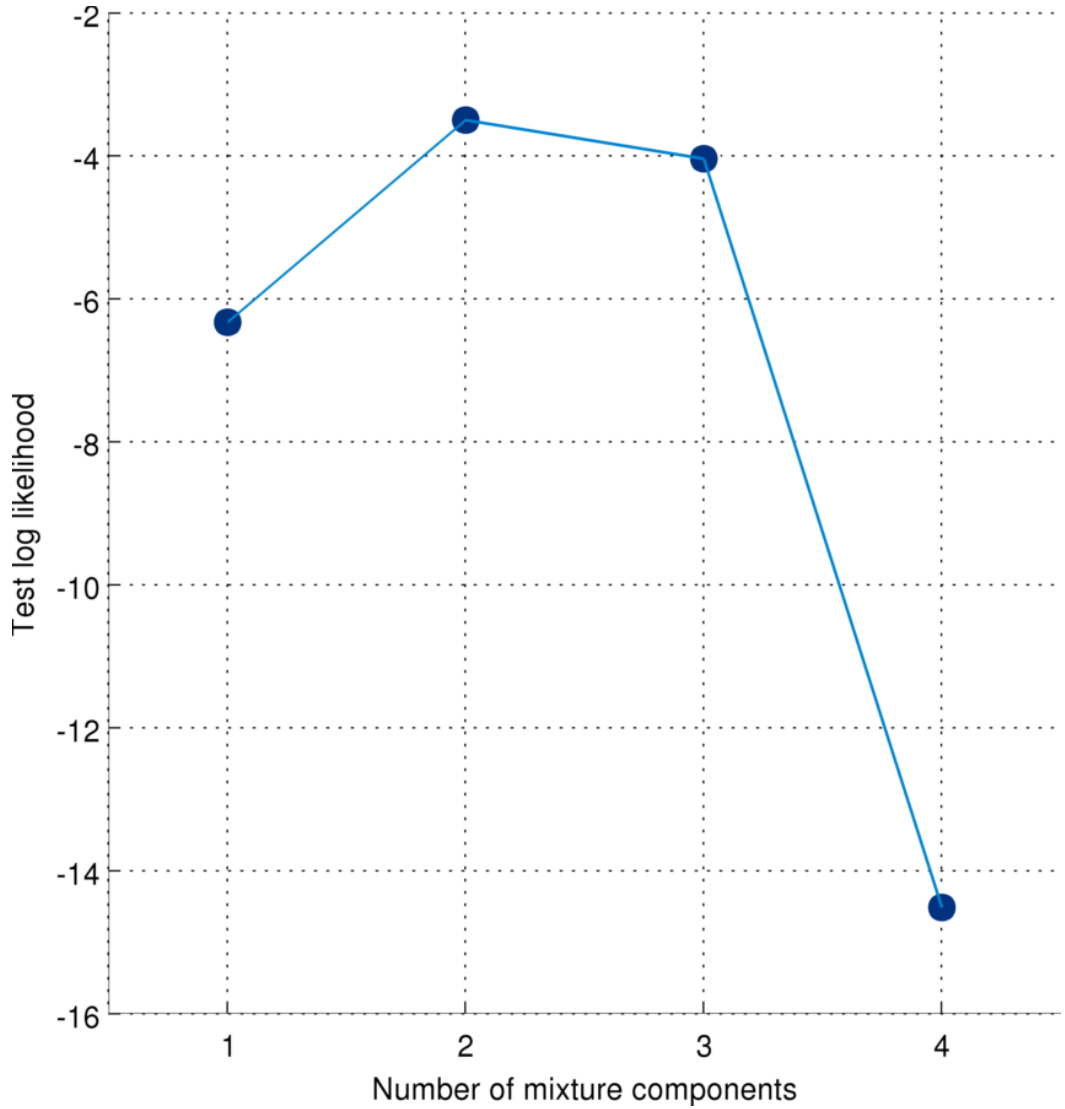
Mixture models

- Selecting complexity using crossvalidation



Mixture models

- Selecting complexity using crossvalidation



K-means versus GMM

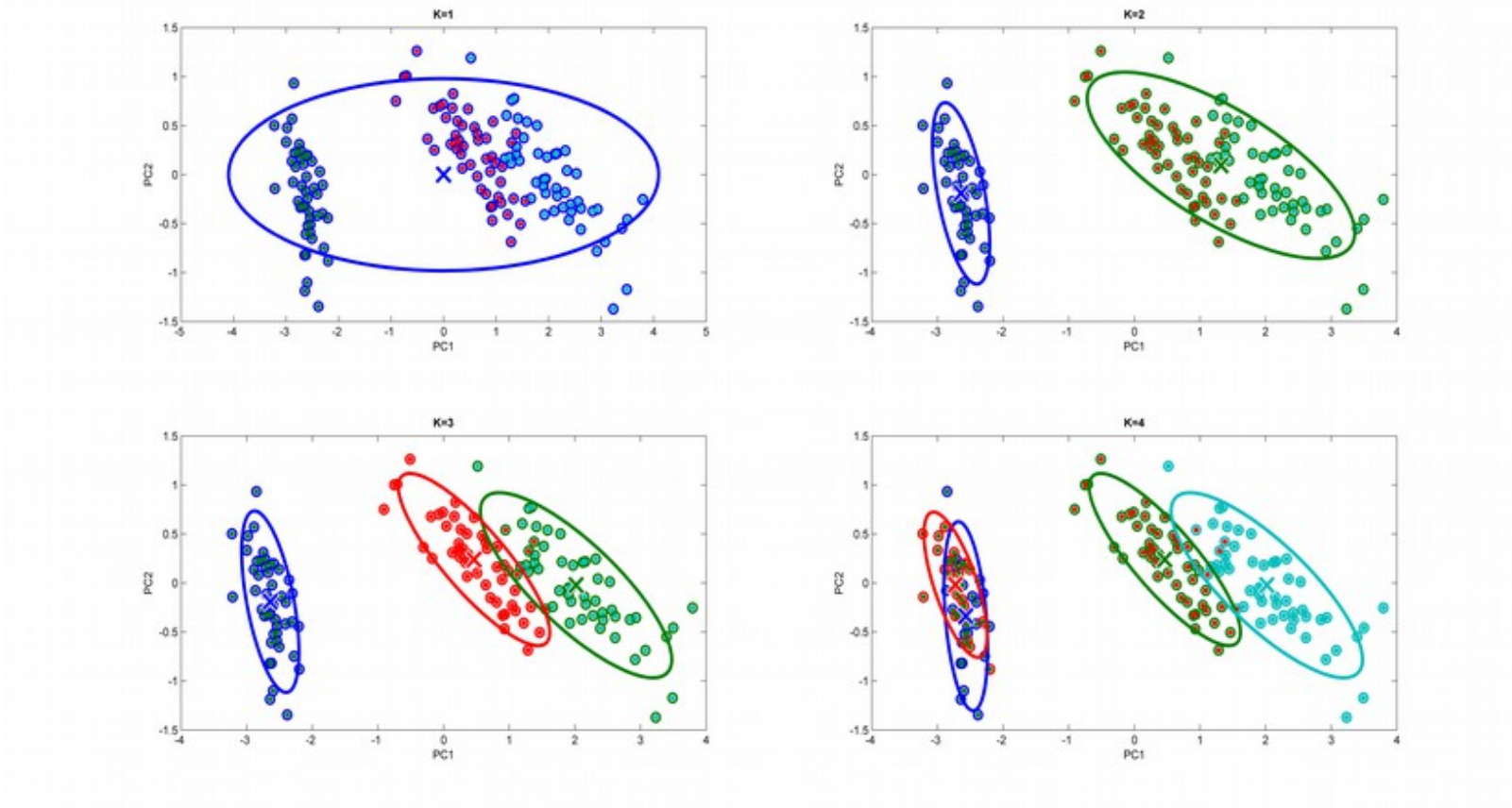
K-means

- No guarantee of optimal solution
- Does not model shape of clusters
- Does not model the size of clusters
- Difficult to assess the number of clusters to use particularly when there is no ground truth

Gaussian mixture model (GMM)

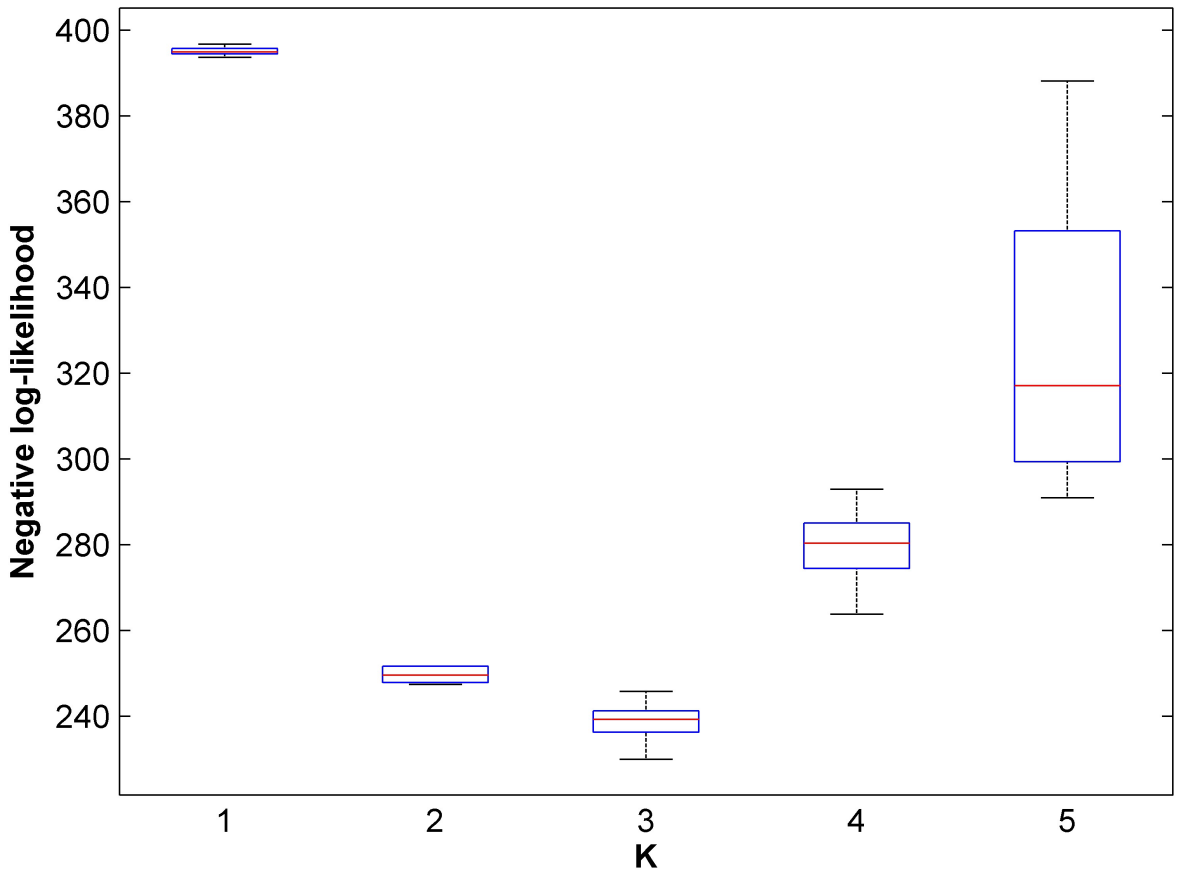
- No guarantee of optimal solution (even more local minima issues due to the additional model parameters)
- Models shape of cluster as ellipsoid
- Models the size of clusters
- Possible to estimate the number of components by cross-validation

GMM on Iris data using 1,2,3 and 4 components



Recap of GMM on Iris data

GMM 10 fold cross-validation on Iris data repeated five times where the five runs are plotted using box-plots.



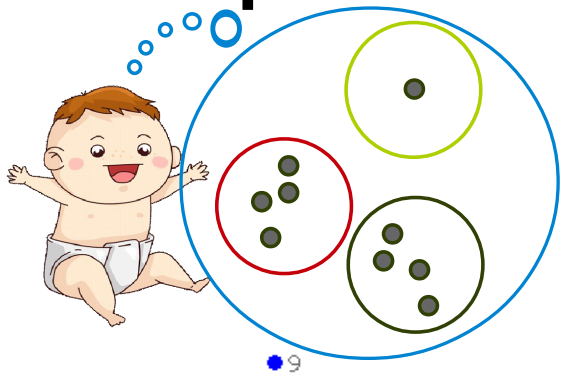
Anomaly detection: Definition

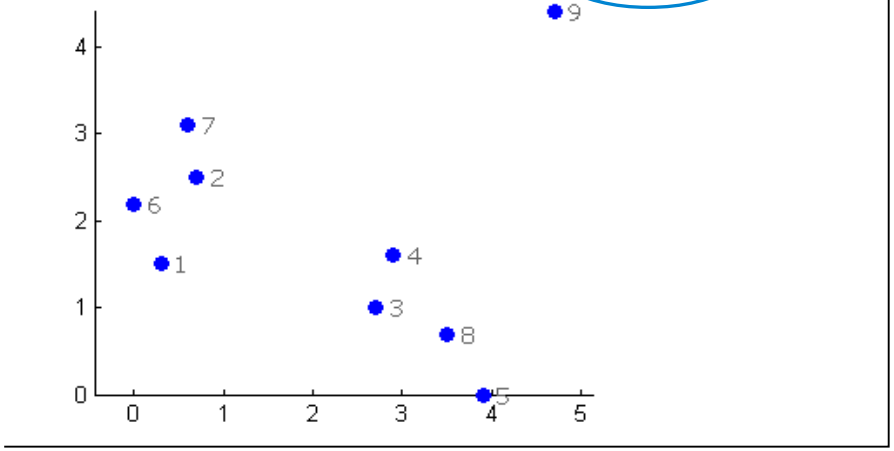
- Given a collection of data objects
  - Each object has associated a number of features
- Detect which objects **deviate from normal** behaviour

Anomaly detection: Example

- Credit card **fraud detection**
  - Recognize dubious credit card transactions based on the transaction history of the card holder
- Network **intrusion detection**
  - Detect hacker attacks, web crawlers etc.
- **Ecosystem disturbances**
  - Detect hurricanes, floods droughts, heat waves and fires
- **Health and medicine monitoring**
  - Detect abnormal behaviour in populations and patients
- **Fault detection in industry systems**
  - Detect when a wind turbine performs poorly due to ice coating on blades
- Detection of **outliers** in data measurements
  - Remove erroneous measurements due to misreading from an instrument

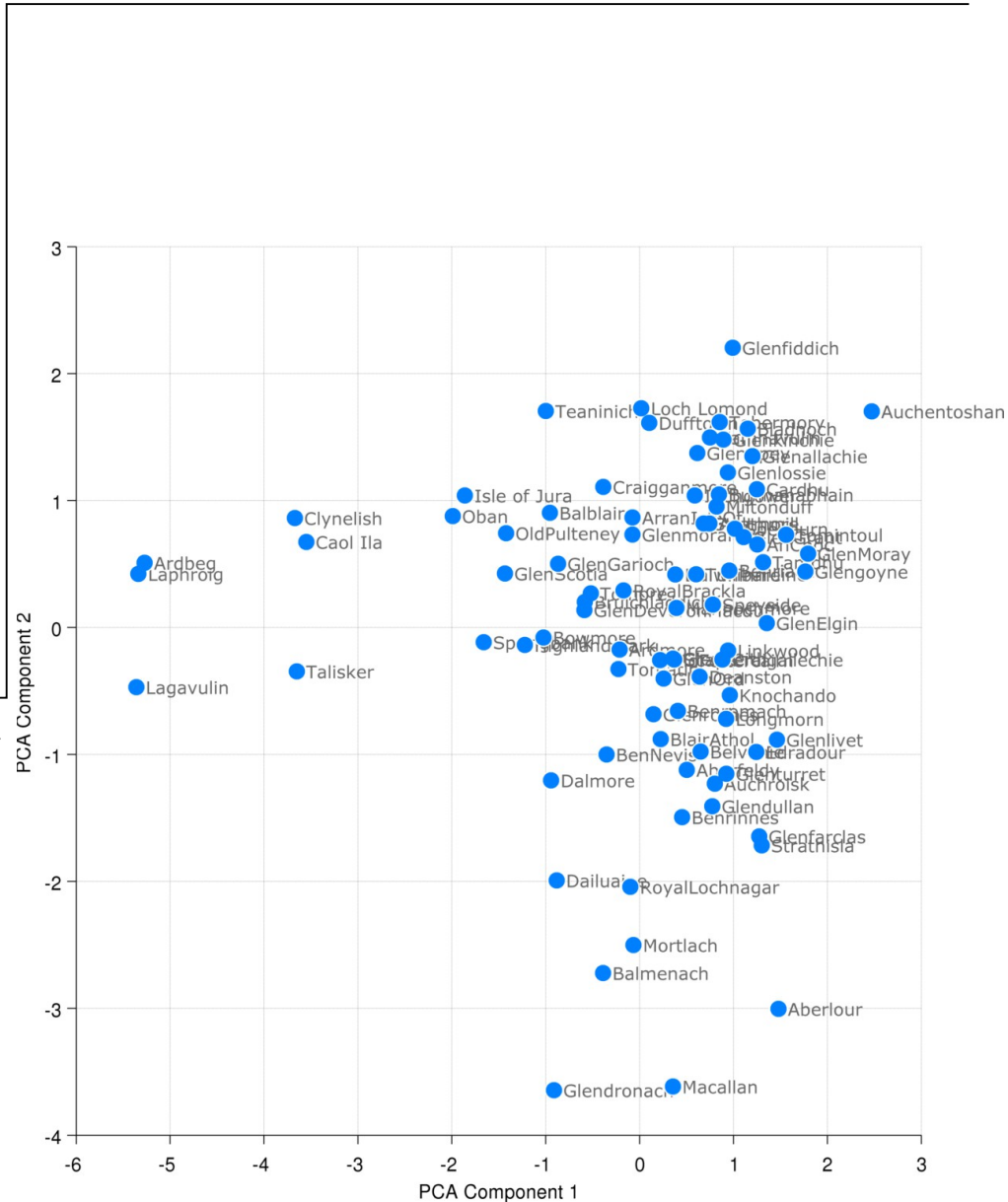
Data example I: Cats, Dogs and Dinosaurs



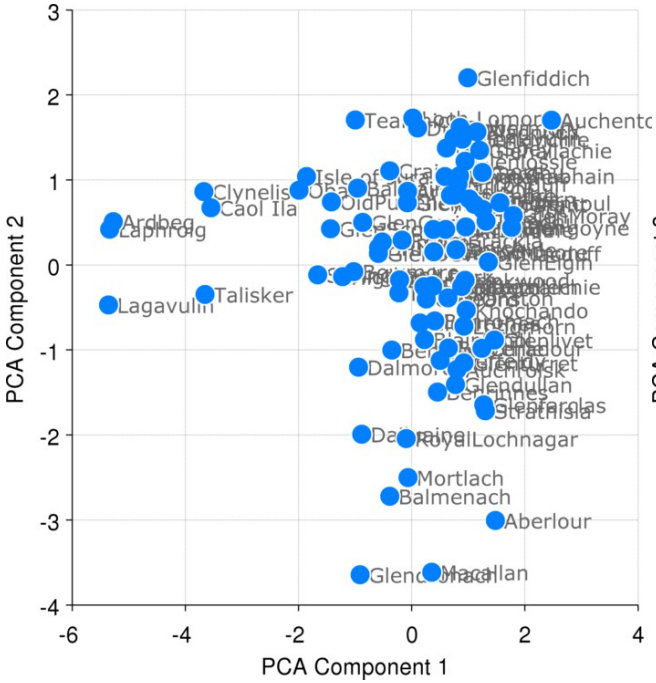


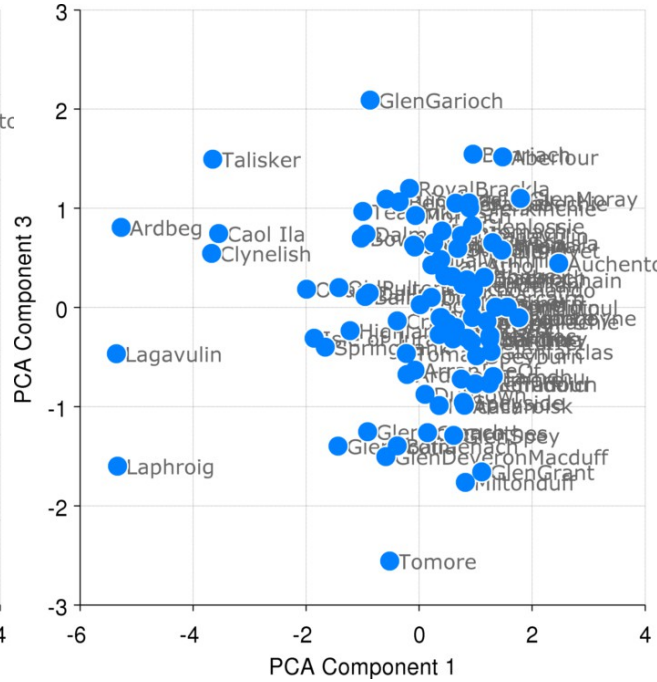
Data example II: Whisky

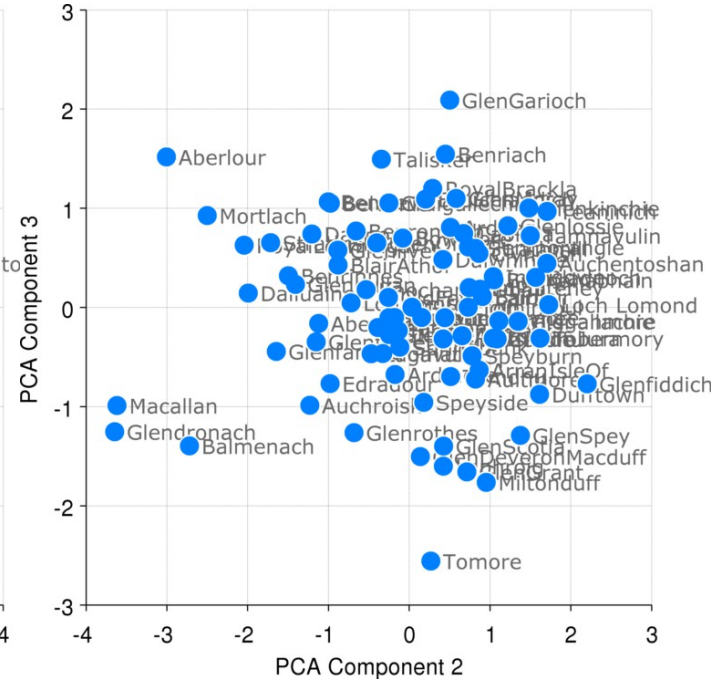
- 86 types of Scotch whisky
- Human ratings 1-5
- 12 taste categories
  - body, sweetness, smoky, medicinal, tobacco, honey, spicy, winey, nutty, malty, fruity, floral



PCA plot


Glenfiddich
Auchento
Clynelis
Caol Ila
Ardbeg
Laphroig
Talisker
Lagavulin
Dalmor
Glendullan
Strathisla
RoyalLochnagar
Mortlach
Balmenach
Aberlour
Macallan
PCA Component 2
PCA Component 1

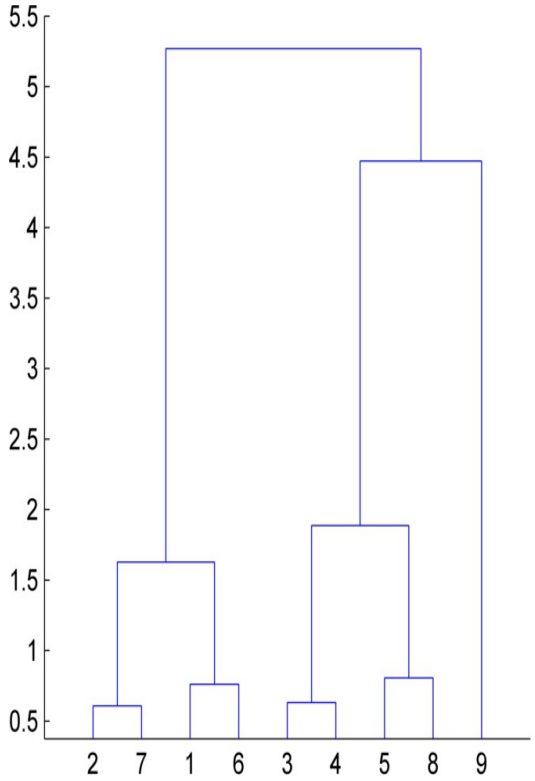

GlenGarioch
Talisker
Aberlour
Ardbeg
Caol Ila
Clynelish
Lagavulin
Laphroig
Tomore
PCA Component 3
PCA Component 1


GlenGarioch
Aberlour
Benriach
Mortlach
Edradour
Auchroisk
Speyside
Glenfiddich
Macallan
Glendronach
Balmenach
Glenrothes
GlenSpey
Tomore
PCA Component 3
PCA Component 2

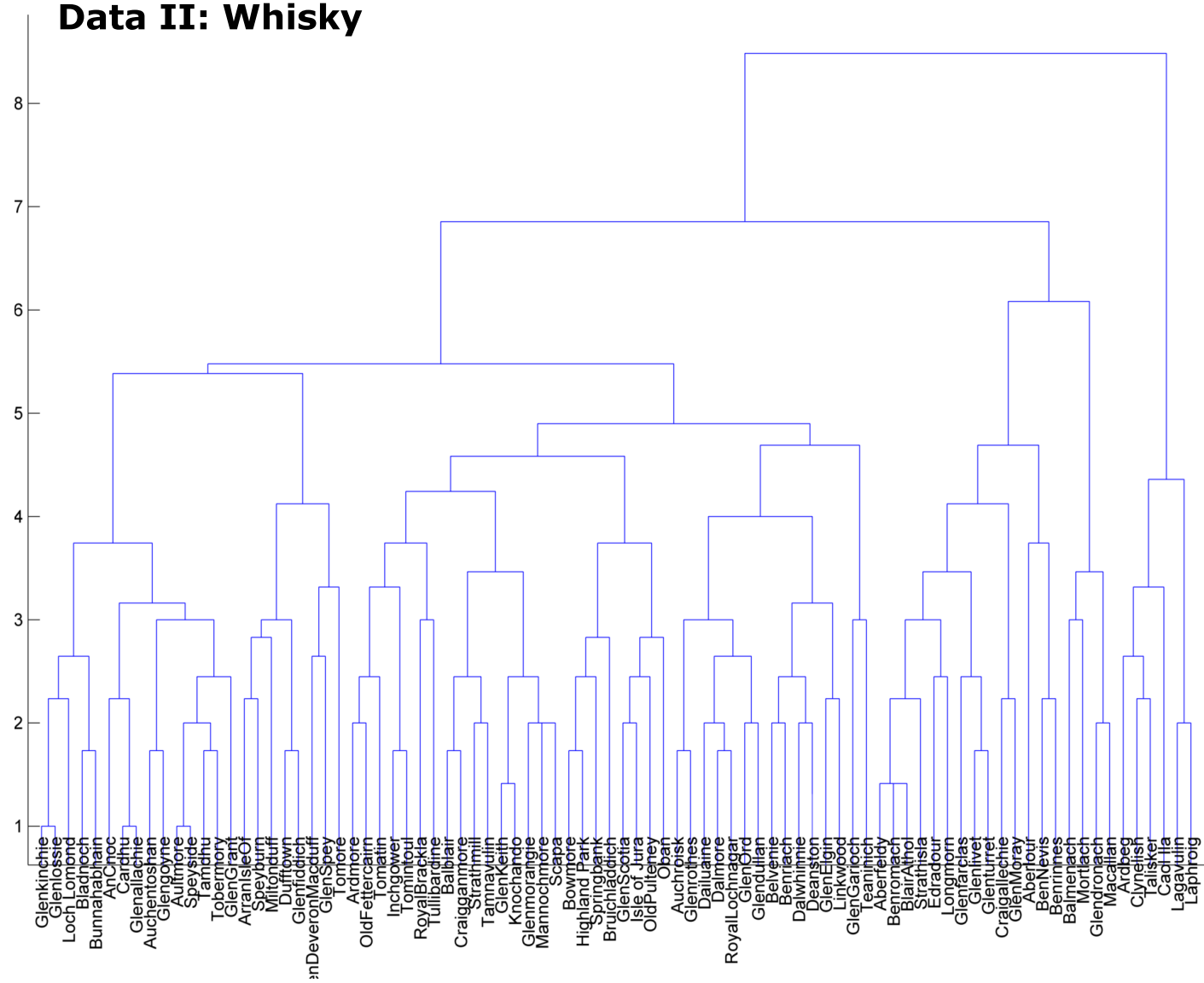
Dendrogram

- Dendrograms can be used to visualize relative distances between the observations

Data I: Cats, Dogs and Dinosaurs



Data II: Whisky



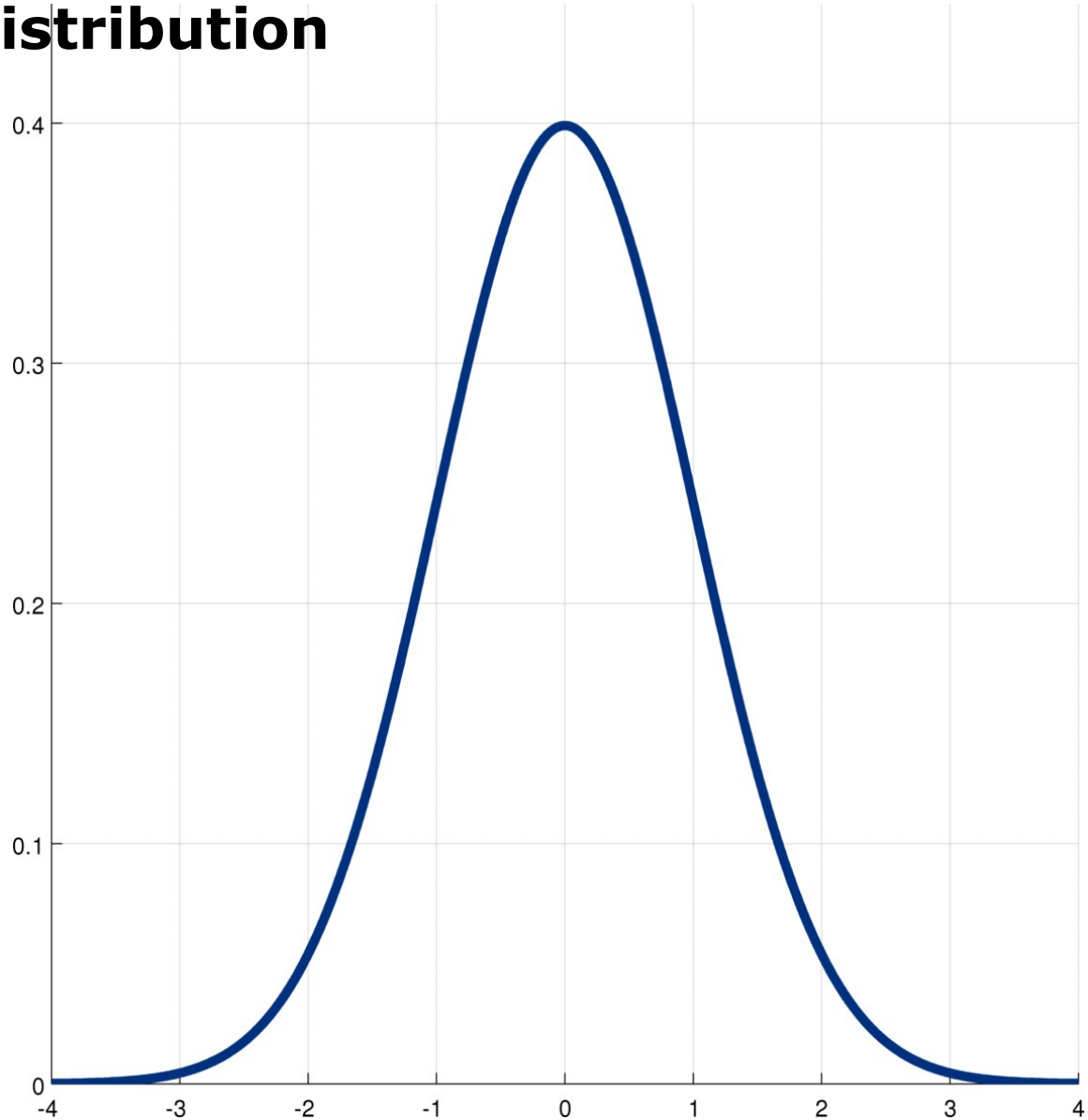
Density based techniques: Univariate normal distribution

- Map attribute to standard Normal variable

$$z = \frac{x - \mu}{\sigma}$$

- Choose a threshold

c	p(|z|>c)
1.0	0.3173
1.5	0.1336
2.0	0.0455
2.5	0.0124
3.0	0.0027
3.5	0.0005
4.0	0.0001



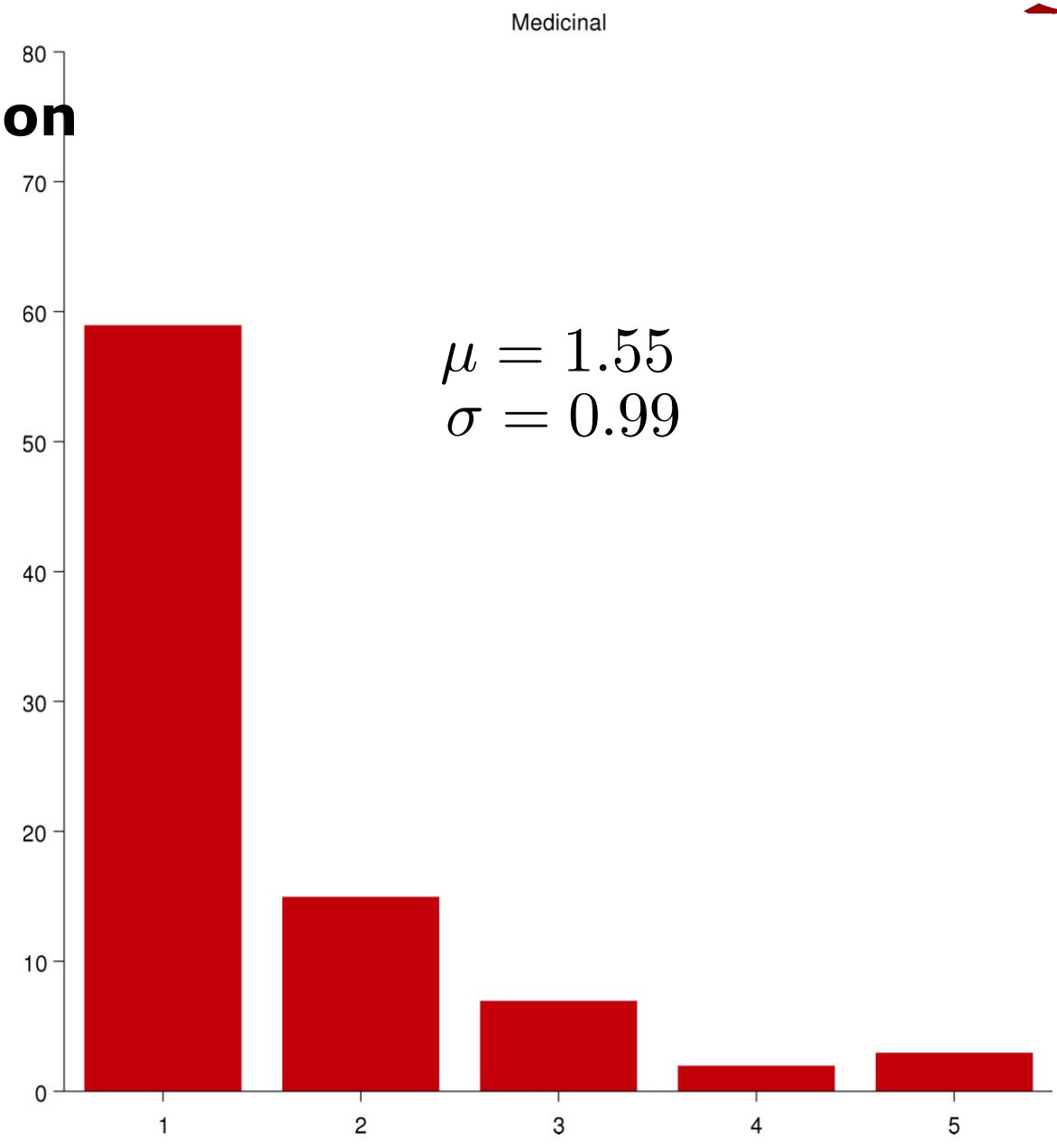
Normal distribution

- Map attribute to standard Normal variable

$$z = \frac{x - \mu}{\sigma}$$

- Choose a threshold

c	p(|z|>c)
1.0	0.3173
1.5	0.1336
2.0	0.0455
2.5	0.0124
3.0	0.0027
3.5	0.0005
4.0	0.0001



$$\mu = 1.55$$
$$\sigma = 0.99$$

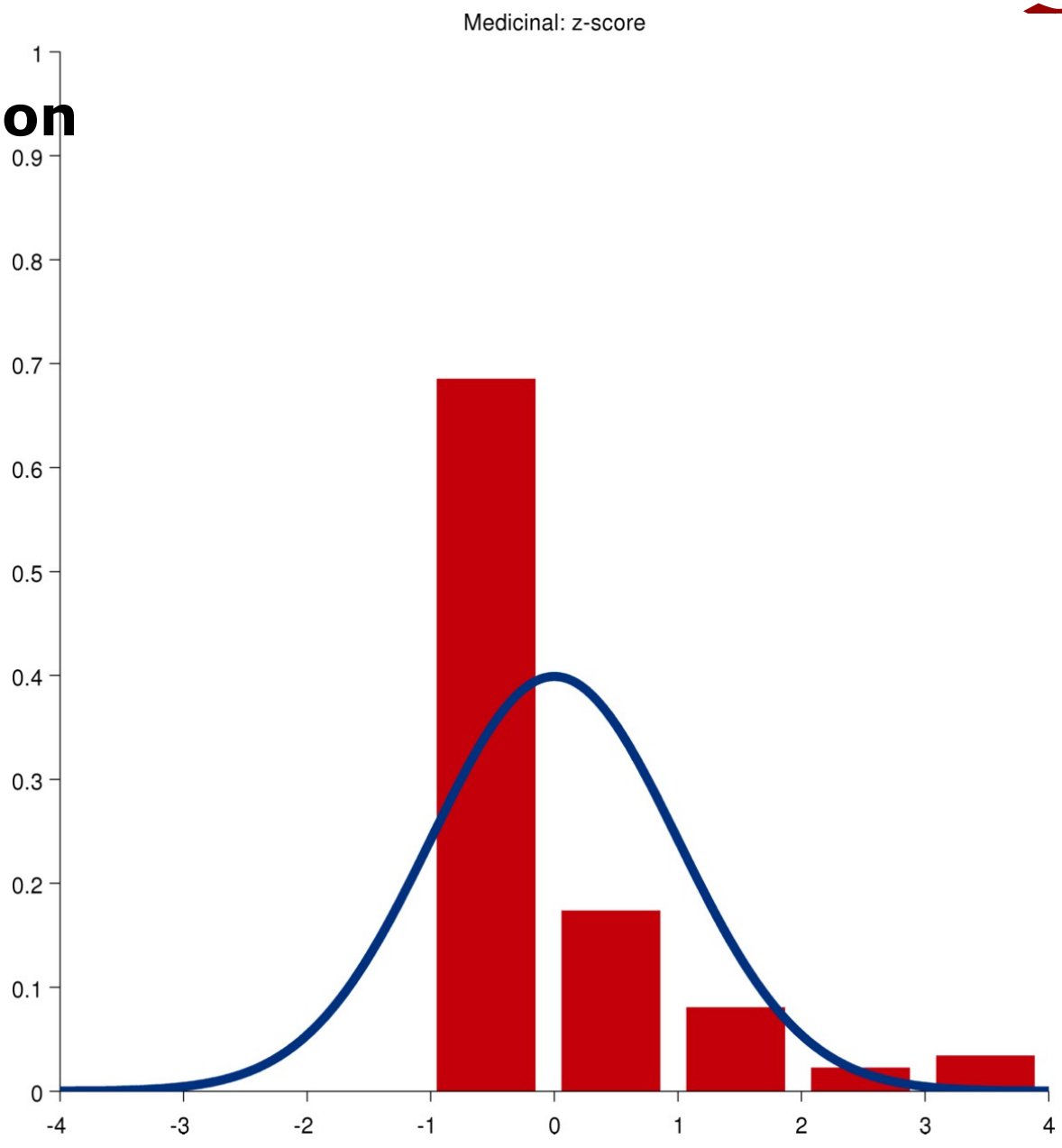
Normal distribution

- Map attribute to standard Normal variable

$$z = \frac{x - \mu}{\sigma}$$

- Choose a threshold

c	p(|z|>c)
1.0	0.3173
1.5	0.1336
2.0	0.0455
2.5	0.0124
3.0	0.0027
3.5	0.0005
4.0	0.0001



Normal distribution

- Map attribute to standard Normal variable

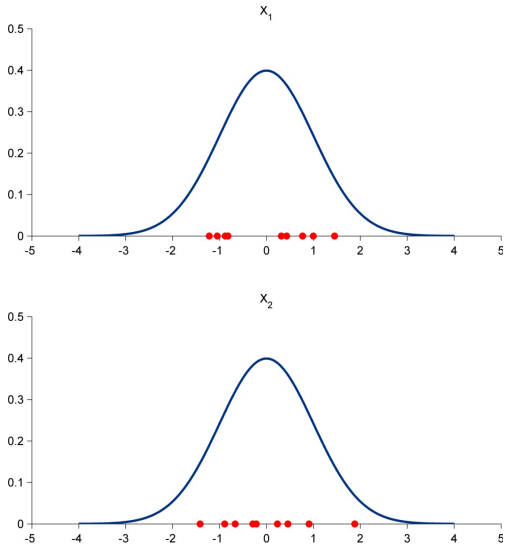
- Choose a threshold

$$z = \frac{x - \mu}{\sigma}$$

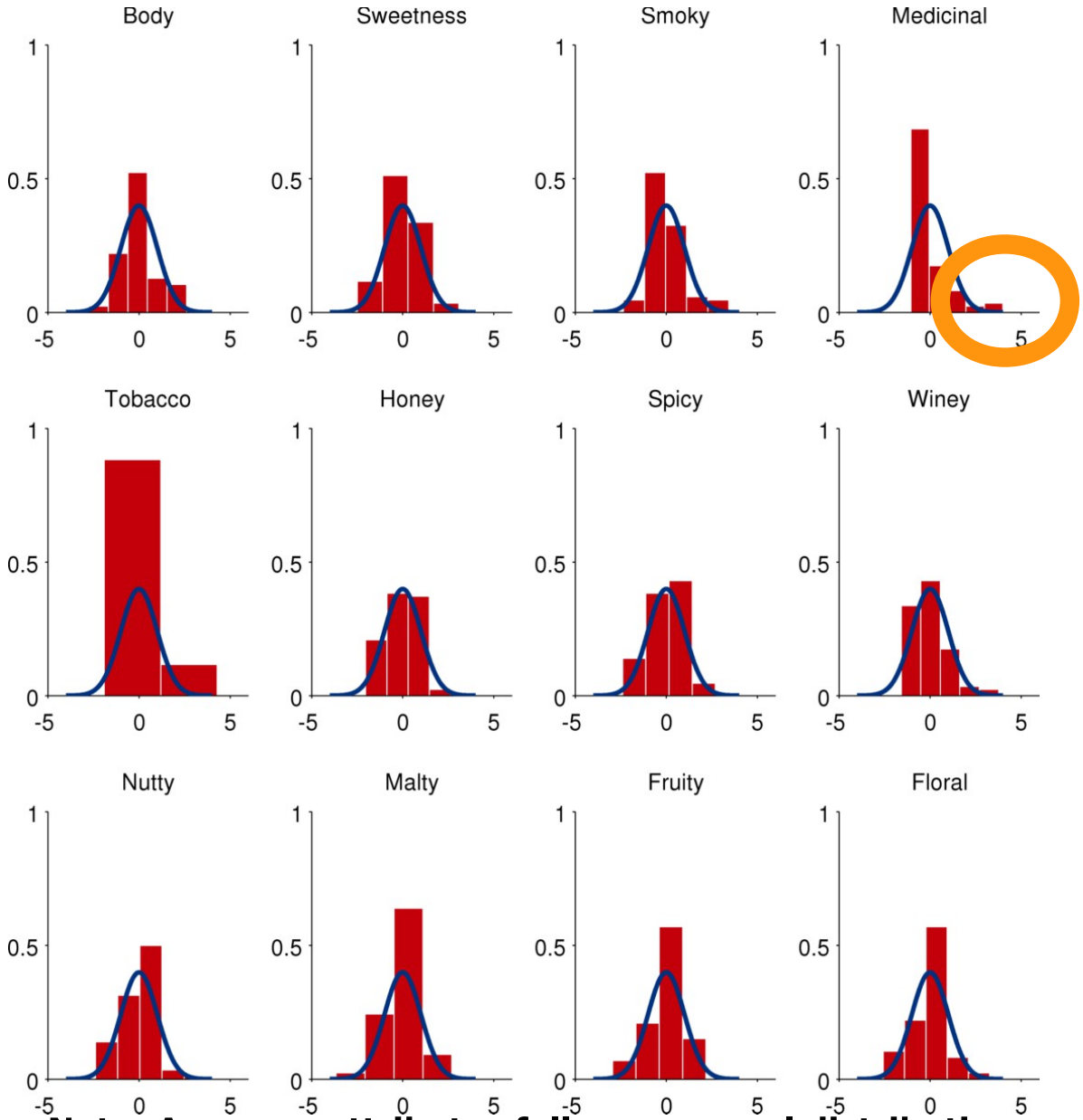
$$p(|z| > c) = 0.001$$

$$c = 3.2905$$

Data I: Cats, Dogs and Dinosaurs



Data II: Whisky



Note: Assumes attributes follow a normal distribution which may not be a valid assumption!

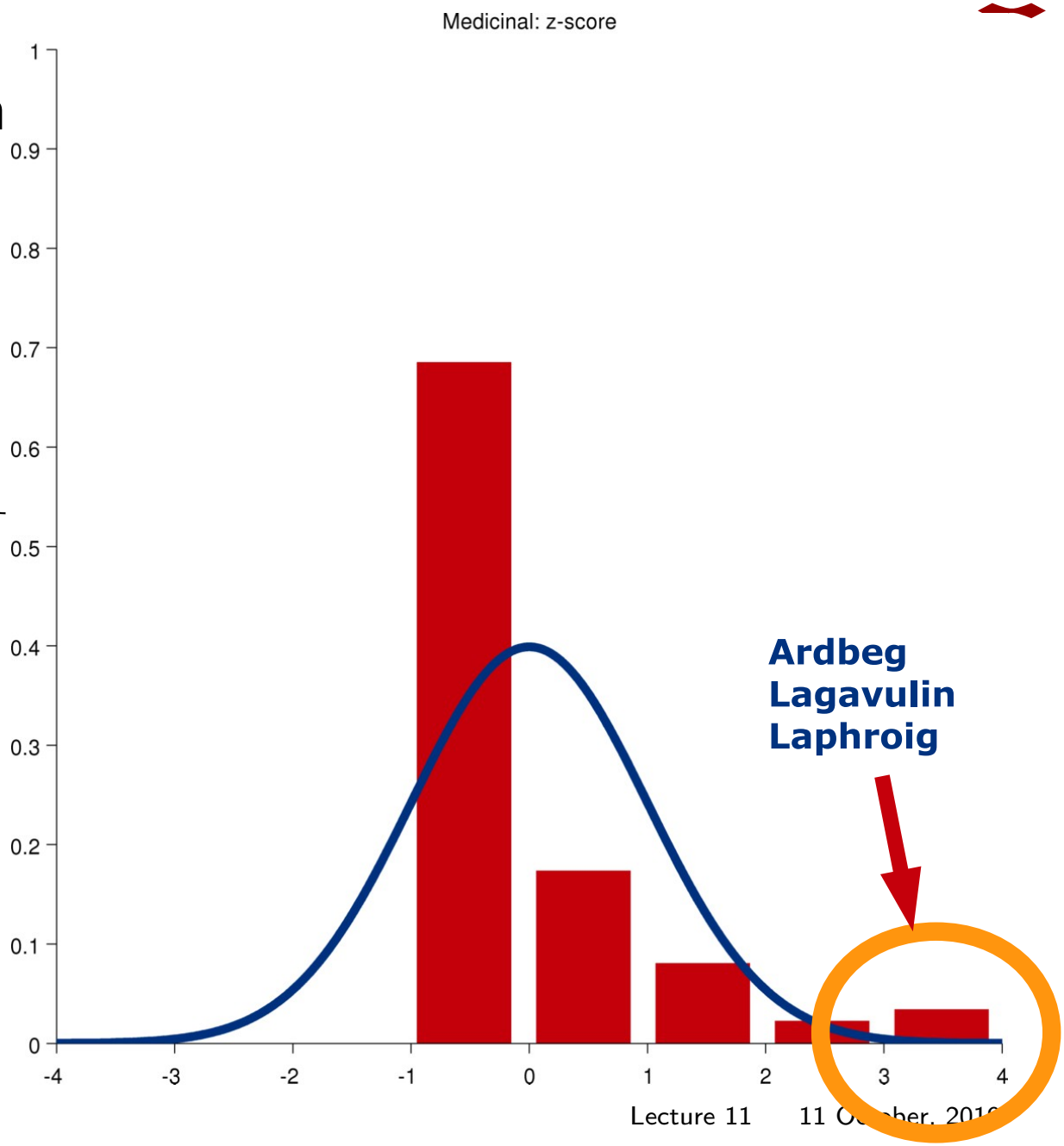
Normal distribution

- Map attribute to standard Normal variable

$$z = \frac{x - \mu}{\sigma}$$

- Choose a threshold

$$p(|z| > c) = 0.001$$
$$c = 3.2905$$



Approaches to anomaly detection

- **Density-based techniques**
  - Estimate the density of data objects
  - Outliers are:
    - Data objects in low density area

- **We can of course use the GMM to evaluate the density of test data.**
  - why not on the training data?

- **Approaches we will presently also consider**:
  - Kernel density estimation
  - Inverse average distance to K nearest neighbours (KNN density)
  - Average relative KNN density

Density based techniques: Kernel Density Estimator

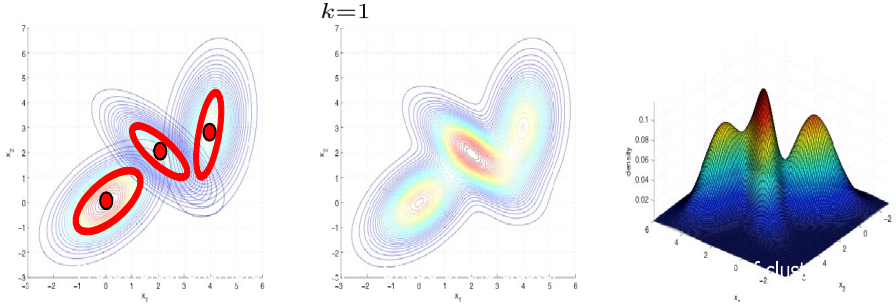
Recall the Gaussian Mixture Model (GMM)

Data density

Sum of cluster specific densities assumed normal distributed

$$p(\boldsymbol{x}) = \sum_{K=1}^{K} w_k \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_{(k)}, \boldsymbol{\Sigma}_{(k)})$$

$$(s.t. \sum_{k=1}^{K} w_k = 1, \quad w_k \geq 0)$$

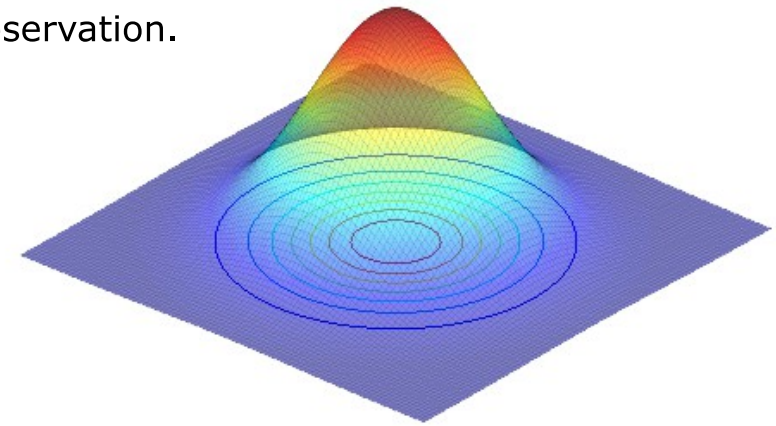


$\boldsymbol{\mu}_{(k)}$: Cluster center (prototypical example in cluster)

$\boldsymbol{\Sigma}_{(k)}$: Shape of the cluster

w_k : Relative density of the cluster

Kernel Density estimation based on Gaussian Kernel: Consider the GMM and define a Gaussian with mean $\boldsymbol{x}_n$ and co-variance $\sigma^2 I$ around each Observation.



Let all observation weight the same, i.e. $w_n = 1/N$

$$p(\mathbf{x}) = \sum_{n=1}^{N} \frac{1}{N} \mathcal{N}(\mathbf{x}|\mathbf{x}_n, \sigma^2 \mathbf{I})$$

Only free parameter σ^2!

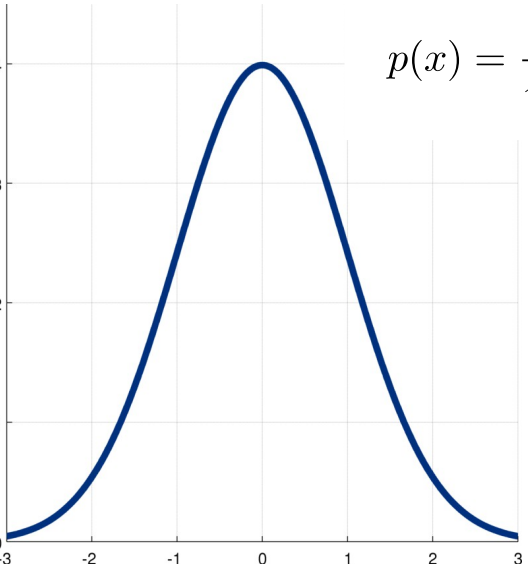
There is nothing special about the normal distribution. For a general mixture distribution p the general form of kernel density estimator is:

$$p(\mathbf{x}) = \sum_{n=1}^{N} \frac{1}{N} p(\mathbf{x}|\mathbf{x}_n, \theta)$$

This may be useful if x is discrete or non-negative.

Piazza quiz 03: Kernel density (Spring 2013)

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



Consider five observations of an attribute x given by

$$\boldsymbol{X} = \{2, 3, 5, 10, 12\}.$$

Based on the five observations, what is the Gaussian kernel density estimate at $x = 4$ using $\sigma^2 = 4$?

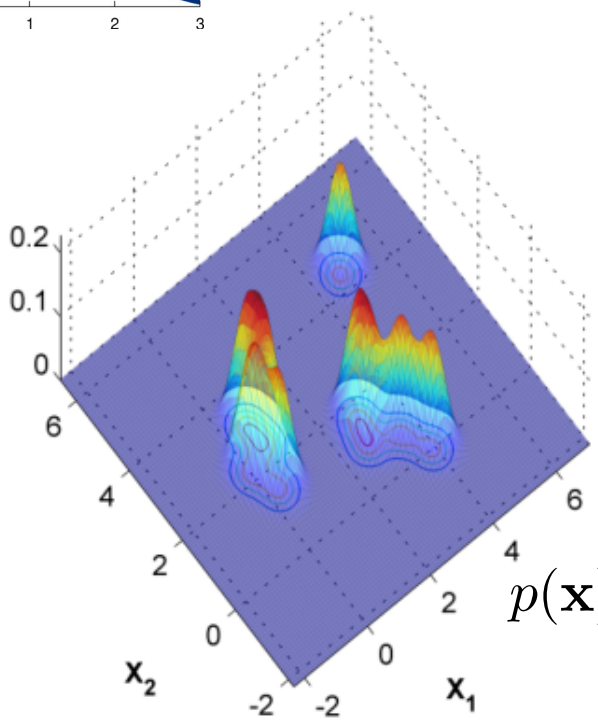
A. $\frac{1}{\sqrt{8\pi}^5} \exp(-\frac{53}{4})$

B. $\frac{1}{5\sqrt{8\pi}} \exp(-\frac{53}{4})$

C. $\frac{1}{5\sqrt{8\pi}}(\exp(-\frac{1}{2})+2\cdot\exp(-\frac{1}{8})+\exp(-\frac{9}{2})+\exp(-8))$

D. $\frac{1}{5\sqrt{8\pi}}(\exp(-1)+2\cdot\exp(-\frac{1}{4})+\exp(-9)+\exp(-16))$

E. Don't know.



$$p(\mathbf{x}) = \sum_{n=1}^{N} \frac{1}{N} \mathcal{N}(\mathbf{x}|\mathbf{x}_n, \sigma^2\mathbf{I})$$

n

Solution:

When inserting $\sigma^2 = 4$ the Gaussian kernel density is given by

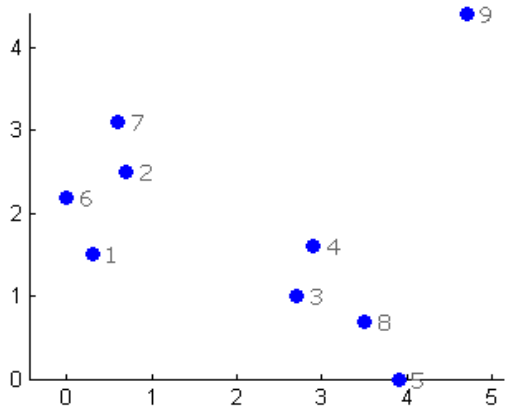
$$p(x) = \frac{1}{N}\sum_{n=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\tfrac{(x-x_n)^2}{2\sigma^2}) = \frac{1}{5\sqrt{8\pi}}(\exp(-\tfrac{(x-2)^2}{2\cdot 4}) + \exp(-\tfrac{(x-3)^2}{2\cdot 4}) + \exp(-\tfrac{(x-5)^2}{2\cdot 4}) + \exp(-\tfrac{(x-10)^2}{2\cdot 4}) + \exp(-\tfrac{(x-12)^2}{2\cdot 4})).$$

Evaluating the density at $x = 4$ we obtain

$$p(x=4) = \frac{1}{N}\sum_{n=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\tfrac{(x-x_n)^2}{2\sigma^2}) = \frac{1}{5\sqrt{8\pi}}(\exp(-\tfrac{(2)^2}{2\cdot 4}) + \exp(-\tfrac{(1)^2}{2\cdot 4}) + \exp(-\tfrac{(-1)^2}{2\cdot 4}) + \exp(-\tfrac{(-6)^2}{2\cdot 4}) + \exp(-\tfrac{(-8)^2}{2\cdot 4})) = \frac{1}{5\sqrt{8\pi}}(\exp(-\tfrac{1}{2}) + 2\cdot(\exp(-\tfrac{1}{8}) + \exp(-\tfrac{9}{2}) + \exp(-8)).$$

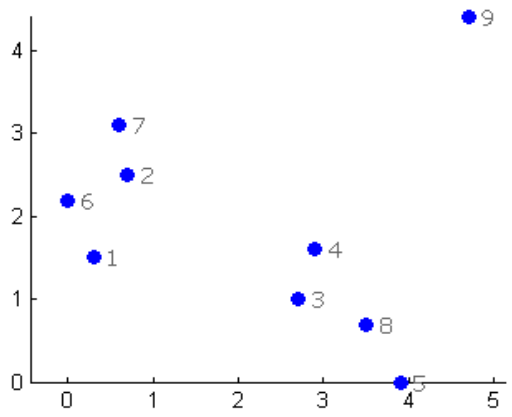
How do we determine σ^2?

Data I: Cats, Dogs and Dinosaurs

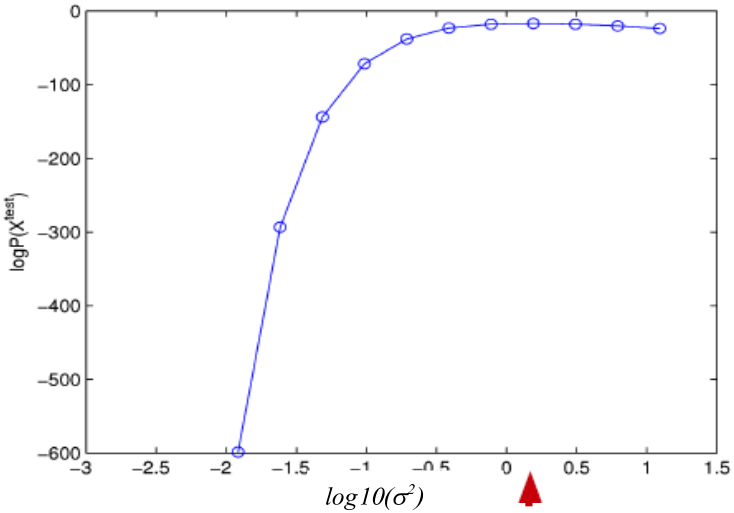


How do we determine σ^2? Crossvalidation!

Data I: Cats, Dogs and Dinosaurs

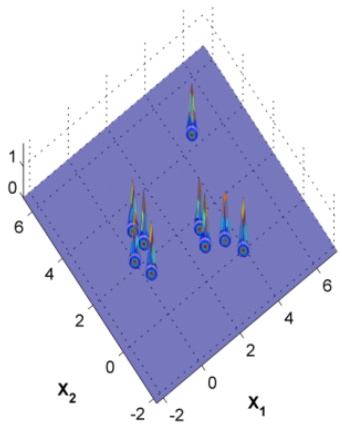


Density of test set based on leave-one-out cross validation

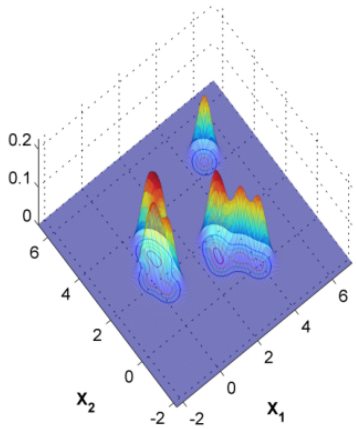


Optimal $\sigma^2=1.55$

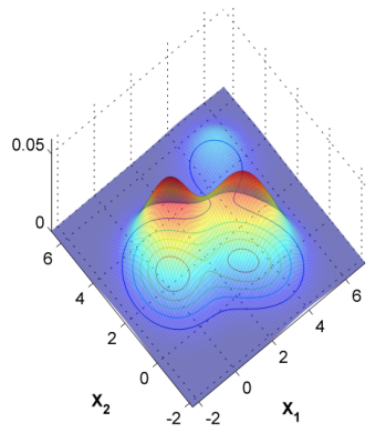
$\sigma^2=0.01$



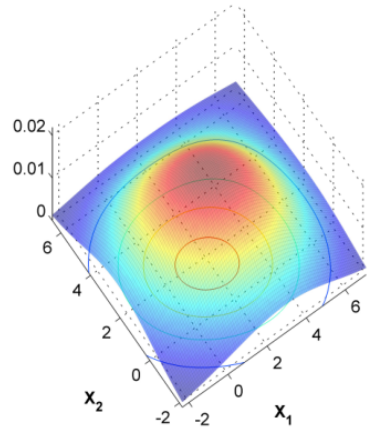
$\sigma^2=0.1$



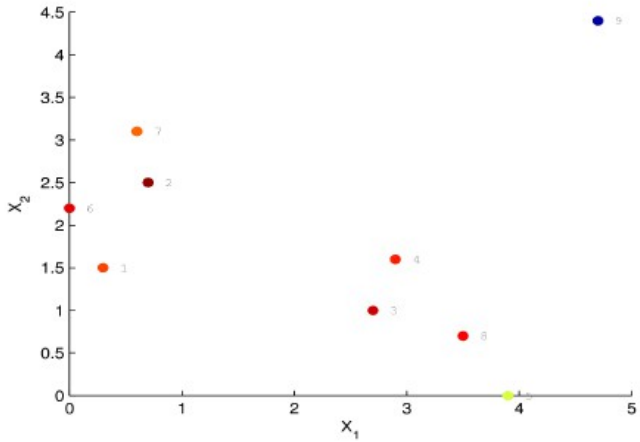
$\sigma^2=1$

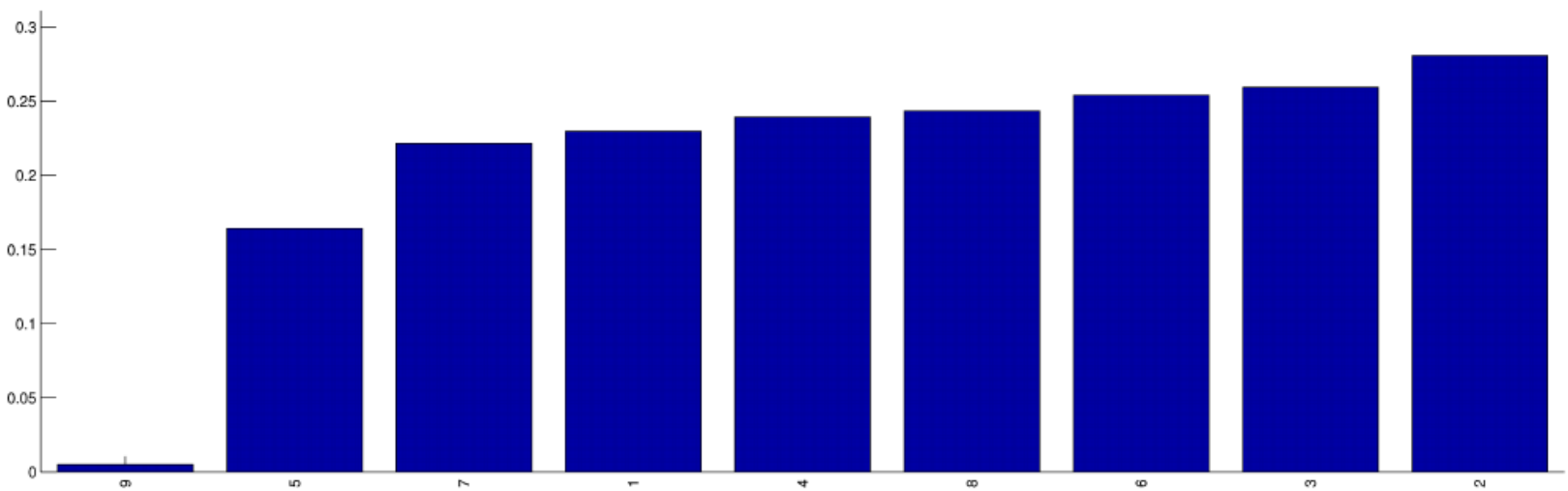


$\sigma^2=5$



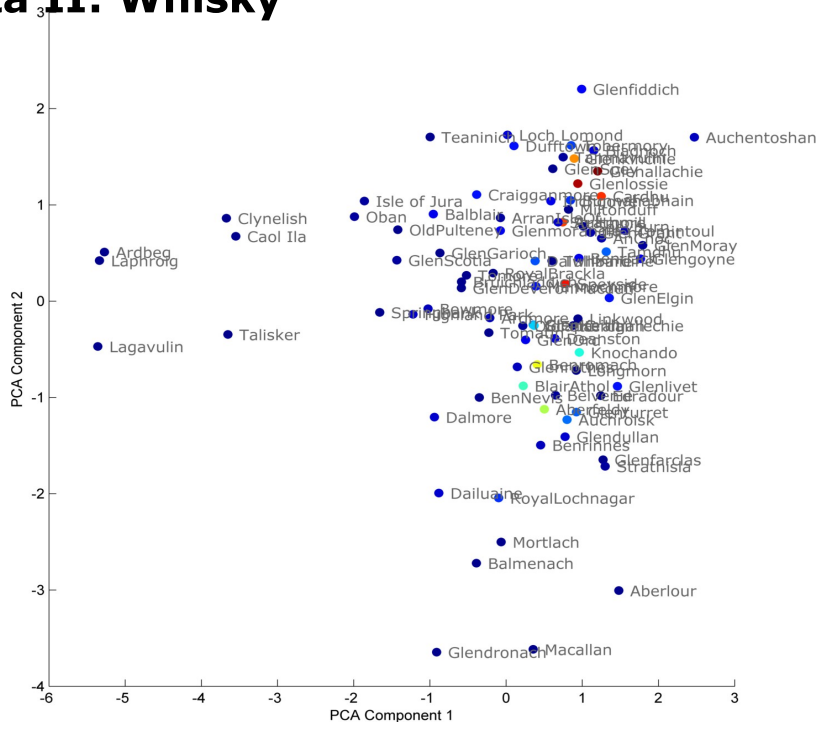
Etimated leave-one-out density evaluated at each observation



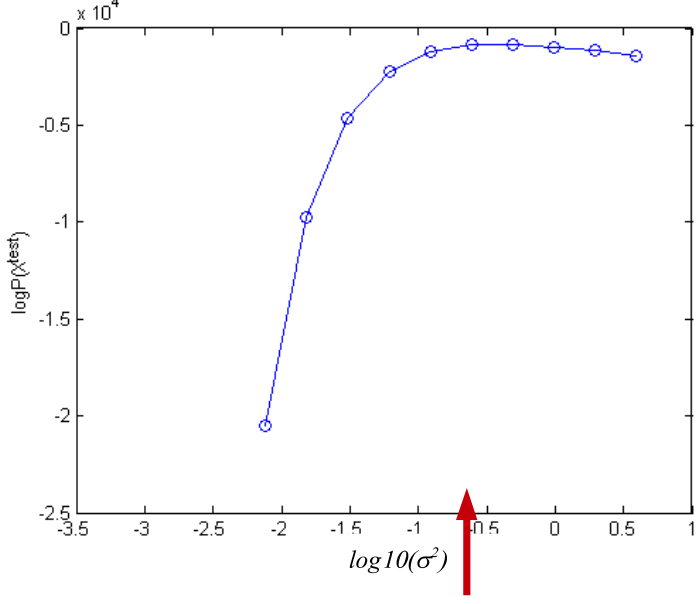


Etimated density evaluated at each observation

Data II: Whisky

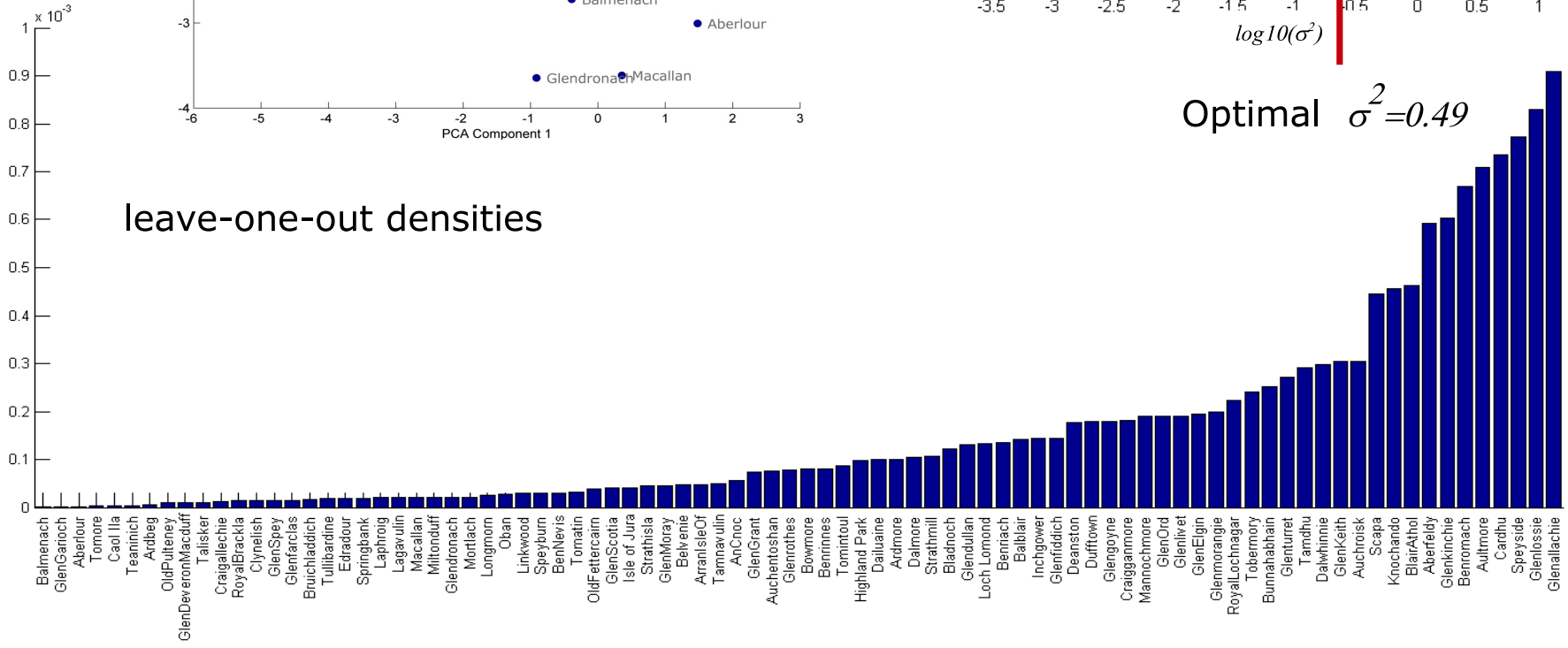


Density of test set based on leave-one-out cross validation



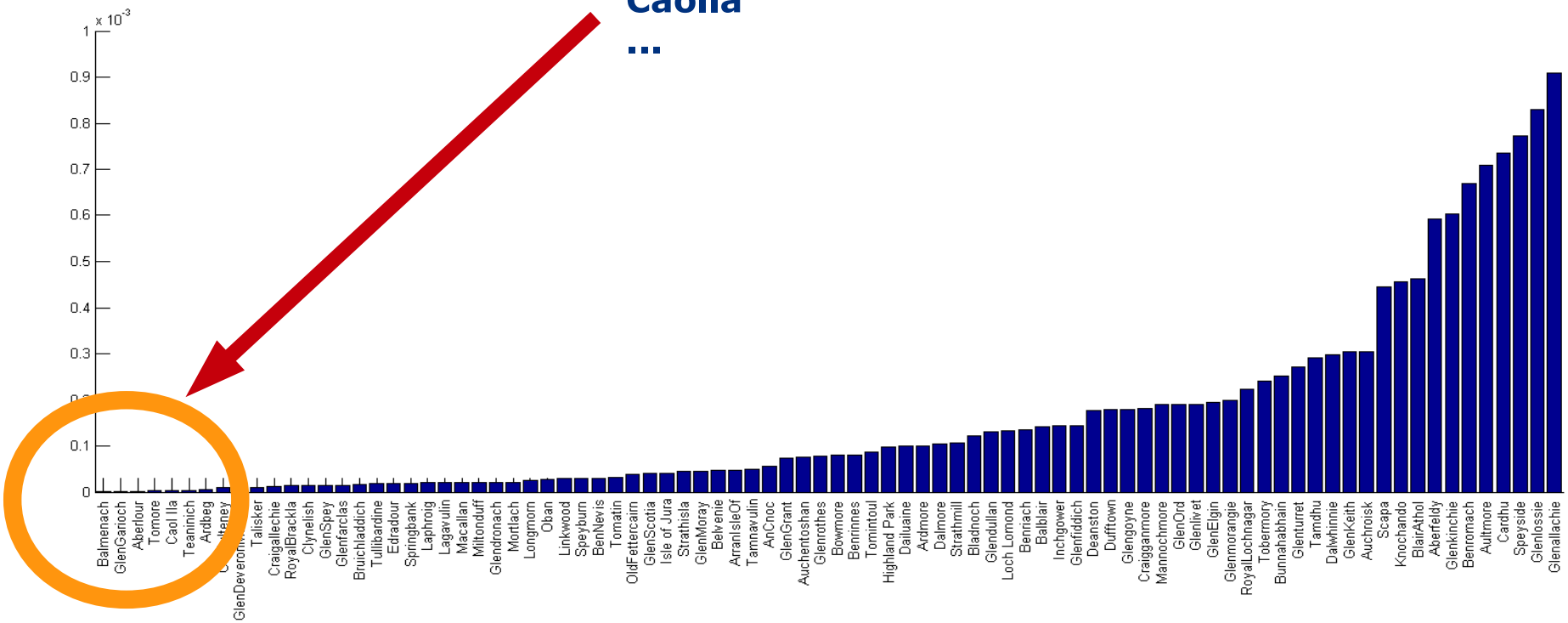
Optimal $\sigma^2 = 0.49$

leave-one-out densities



Data II: Whisky

Balmenach
Glen Garioch
Aberlour
Tomore
Caolla
...



Inverse distance density estimation

- **Distance based measure of density**
  - Density is inverse proportional to avereage distance to k nearest neighbors
  - Density is low if nearest neighbors are far away

$$\text{density}_{\boldsymbol{X}_{\setminus i}}(\boldsymbol{x}_i, K) = \frac{1}{\frac{1}{K}\sum_{\boldsymbol{x}' \in N_{\boldsymbol{X}_{\setminus i}}(\boldsymbol{x}_i, K)} d(\boldsymbol{x}_i, \boldsymbol{x}')}$$

- **Relative density**
  - Density compared to density at nearest neighbors

$$\text{ard}_{\boldsymbol{X}}(\boldsymbol{x}_i, K) = \frac{\text{density}_{\boldsymbol{X}_{\setminus i}}(\boldsymbol{x}_i, K)}{\frac{1}{K}\sum_{\boldsymbol{x}_j \in N_{\boldsymbol{X}_{\setminus i}}(\boldsymbol{x}_i, K)} \text{density}_{\boldsymbol{X}_{\setminus j}}(\boldsymbol{x}_j, K)}$$

$$N_{\boldsymbol{X}}(\boldsymbol{x}, K) = \{\text{The } K \text{ observations in } \boldsymbol{X} \text{ which are nearest to } \boldsymbol{x}\}$$

$$\boldsymbol{X}_{\setminus i}^T = \left[\boldsymbol{x}_1\ \boldsymbol{x}_2 \cdots \boldsymbol{x}_{i-2}\ \boldsymbol{x}_{i-1}\ \boldsymbol{x}_{i+1}\ \boldsymbol{x}_{i+2} \cdots\ \boldsymbol{x}_N\right]$$

These measures are taken from:
"Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, Vipin Kumar

Piazza quiz 4: ARD (Spring 2015)

	O1	O2	O3	O4	O5	O6	O7	O8	O9	O10
O1	0	393.5	68.1	165.4	271.8	200.6	210.9	206.1	166.3	365.0
O2	393.5	0	411.3	361.8	478.6	490.9	409.2	382.3	391.1	37.4
O3	68.1	411.3	0	119.8	208.4	136.6	152.8	154.3	111.1	387.1
O4	165.4	361.8	119.8	0	137.5	130.8	62.1	44.7	32.5	346.2
O5	271.8	478.6	208.4	137.5	0	99.0	76.8	101.0	116.4	468.5
O6	200.6	490.9	136.6	130.8	99.0	0	100.1	124.0	100.5	473.8
O7	210.9	409.2	152.8	62.1	76.8	100.1	0	29.5	45.2	396.8
O8	206.1	382.3	154.3	44.7	101.0	124.0	29.5	0	44.6	370.1
O9	166.3	391.1	111.1	32.5	116.4	100.5	45.2	44.6	0	375.1
O10	365.0	37.4	387.1	346.2	468.5	473.8	396.8	370.1	375.1	0

Table 1: Pairwise Euclidean distance between the 10 first observations in the PM10 (air polution) dataset. Red/green observations corresponds to high/low pollution levels.

We suspect that observation O1 in Table 1 may be an outlier. In order to assess if this is the case we will calculate the average relative density (ARD) based on the distances in the table using the definitions:

$$\text{density}(\boldsymbol{x}, K) = \left(\frac{1}{K}\sum_{\boldsymbol{y}\in N(\boldsymbol{x},K)} distance(\boldsymbol{x},\boldsymbol{y})\right)^{-1},$$

$$\text{a.r.d.}(\boldsymbol{x}, K) = \frac{\text{density}(\boldsymbol{x},K)}{\frac{1}{K}\sum\limits_{\boldsymbol{y}\in N(\boldsymbol{x},K)} \text{density}(\boldsymbol{y},K)},$$

where $N(\boldsymbol{x}, K)$ is the set of K nearest neighbors of observation $\boldsymbol{x}$ and a.r.d$(\boldsymbol{x}, K)$ is the average relative density of $\boldsymbol{x}$ using K nearest neighbors. What is ARD for observation O1 for $K = 2$ nearest neighbors?

A. 0.01

B. 0.02

C. 0.23

D. 0.46

E. Don't know.

Solution:

	O1	O2	O3	O4	O5	O6	O7	O8	O9	O10
O1	0	393.5	68.1	165.4	271.8	200.6	210.9	206.1	166.3	365.0
O2	393.5	0	411.3	361.8	478.6	490.9	409.2	382.3	391.1	37.4
O3	68.1	411.3	0	119.8	208.4	136.6	152.8	154.3	111.1	387.1
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O9	166.3	391.1	111.1	32.5	116.4	100.5	45.2	44.6	0	375.1
O10	365.0	37.4	387.1	346.2	468.5	473.8	396.8	370.1	375.1	0

Table 1: Pairwise Euclidean distance between the 10 first observations in the PM10 (air polution) dataset. Red/green observations corresponds to high/low pollution levels.

The intermediate computations are:

$$\text{density}(\boldsymbol{x}_{O1}, 2) = (\frac{1}{2} \cdot (68.1 + 165.4))^{-1} = 0.0086$$

$$\text{density}(\boldsymbol{x}_{O3}, 2) = (\frac{1}{2} \cdot (68.1 + 111.1))^{-1} = 0.0112$$

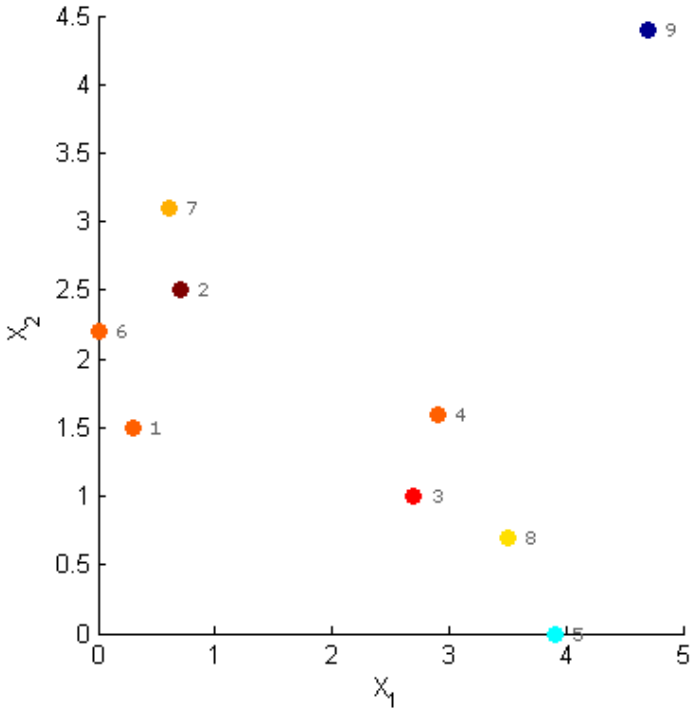
$$\text{density}(\boldsymbol{x}_{O4}, 2) = (\frac{1}{2} \cdot (32.5 + 44.7))^{-1} = 0.0259$$

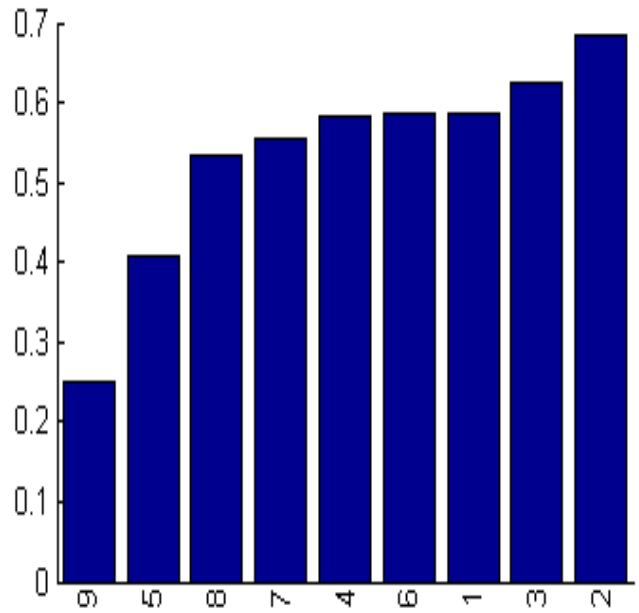
$$\begin{aligned}\text{a.r.d.}(\boldsymbol{x}, K) &= \frac{\text{density}(\boldsymbol{x}_{O1}, 2)}{\frac{1}{2}(\text{density}(\boldsymbol{x}_{O3}, 2) + \text{density}(\boldsymbol{x}_{O4}, 2))} \\ &= \frac{0.0086}{\frac{1}{2} \cdot (0.0112 + 0.0259)} = 0.46\end{aligned}$$

Inverse distance density estimation

- KNN density (5 nearest neighbors)

Data I: Cats , dogs and dinosaurs

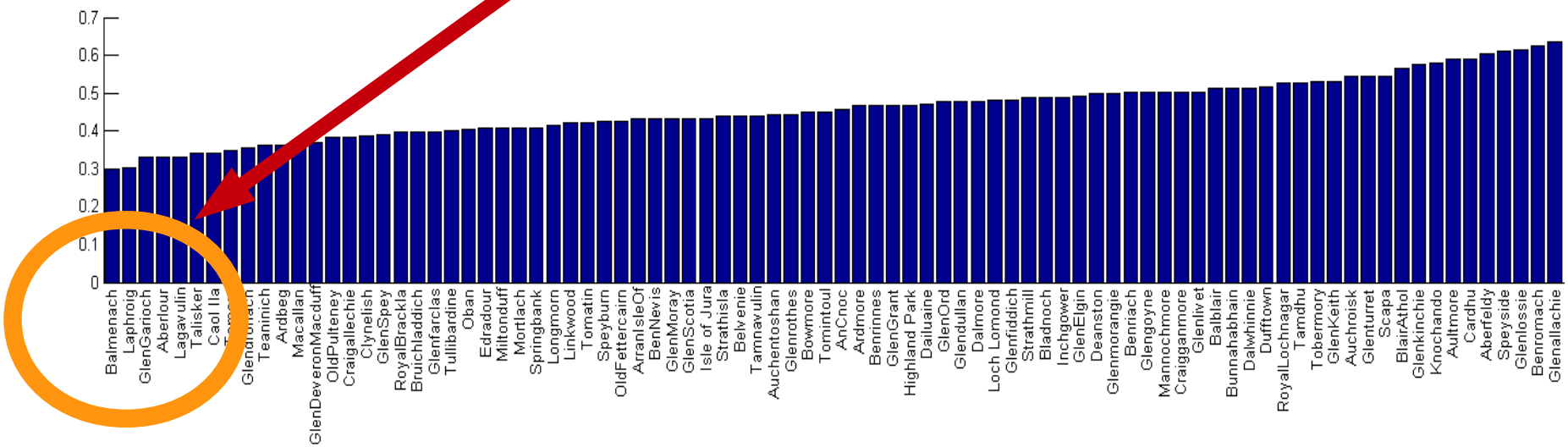




Inverse distance density estimation

- KNN density (5 nearest neighbors)

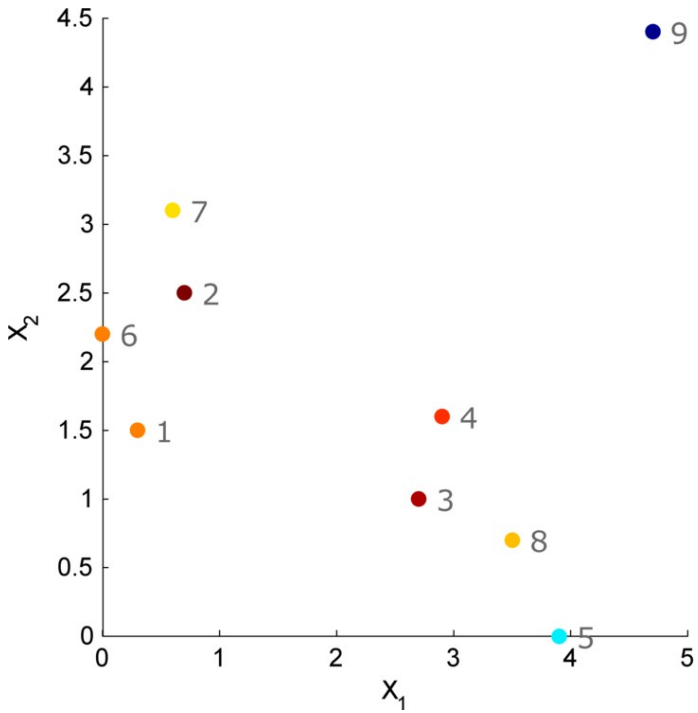
Balmenach
Laphroig
GlenGarioch
Aberlour
Lagevulin
...

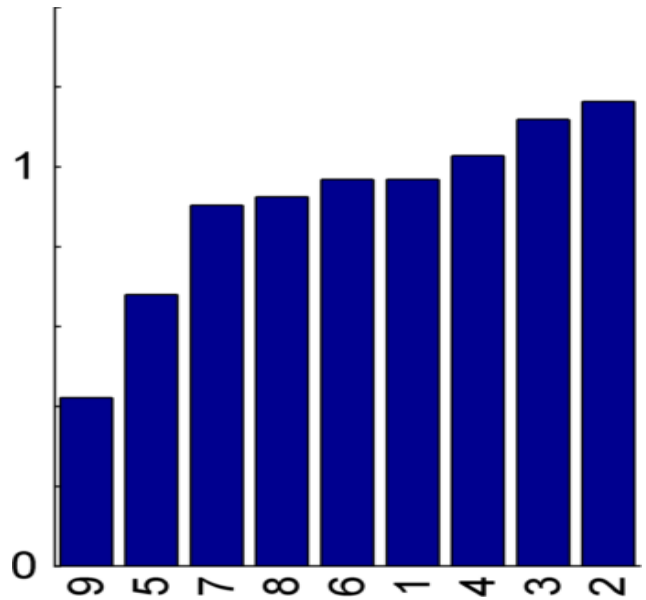


Average Relative density

- Average Relative KNN density (5 nearest neighbors)

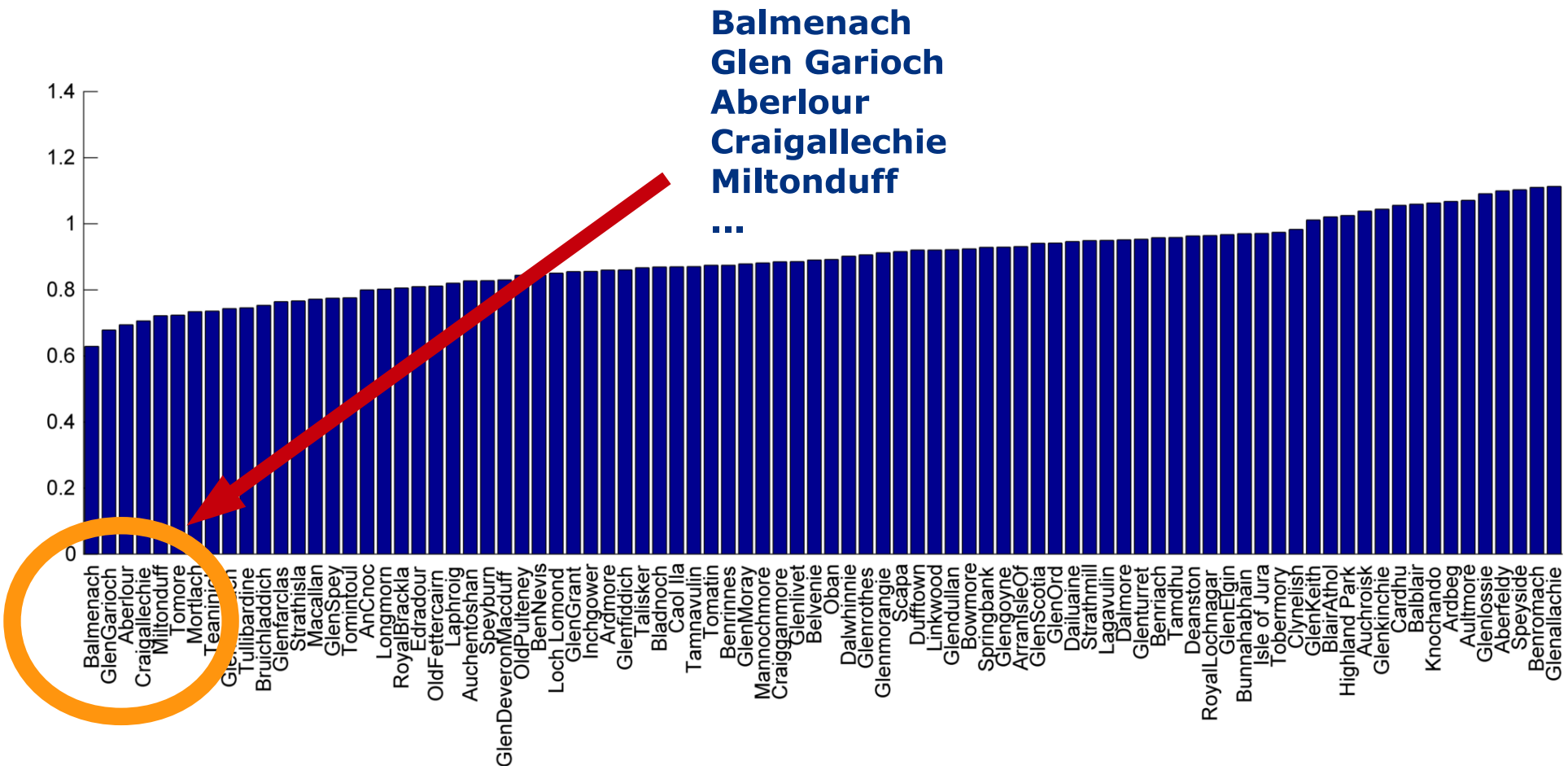
Data I: Cats , dogs and dinosaurs





Average relative density

- Average relative KNN density (5 nearest neighbors)



Results using different methods

- **Kernel Density Estimation**
  - Balmenach
  - Glen Garioch
  - Aberlour
  - Tomore
  - Caolla
- **KNN density**
  - Balmenach
  - Laphroig
  - Glen Garioch
  - Aberlour
  - Lagavulin
- **KNN average relative density**
  - Balmenach
  - Glen Garioch
  - Aberlour
  - Craigallechie
  - Miltonduff

Common: Balmenach, Glen Garioch, Aberlour

Resources