CSCI567 Machine Learning (Spring 2021)

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Outline

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Bayes optimal classifier

Suppose $(\boldsymbol{x}, y)$ is drawn from a joint distribution p. The **Bayes optimal classifier** is

$$f^*(\boldsymbol{x}) = \operatorname*{argmax}_{c \in [\mathsf{C}]} p(c \mid \boldsymbol{x})$$

i.e. predict the class with the largest conditional probability.

p is of course unknown, but we can estimate it, which is *exactly a density estimation problem!*

A "naive" assumption

Naive Bayes assumption:
conditioning on a label, features are independent, which means

$$p(\boldsymbol{x} \mid y = c) = \prod_{d=1}^{\mathrm{D}} p(x_d \mid y = c)$$

Now for each d and c we have a simple 1D density estimation problem!

Is this a reasonable assumption? Sometimes yes, e.g.

- use $x = (\text{Height, Vocabulary})$ to predict $y = \text{Age}$
- Height and Vocabulary are dependent
- but condition on Age, they are independent!

More often this assumption is *unrealistic and "naive"*, but still Naive Bayes can work very well even if the assumption is wrong.

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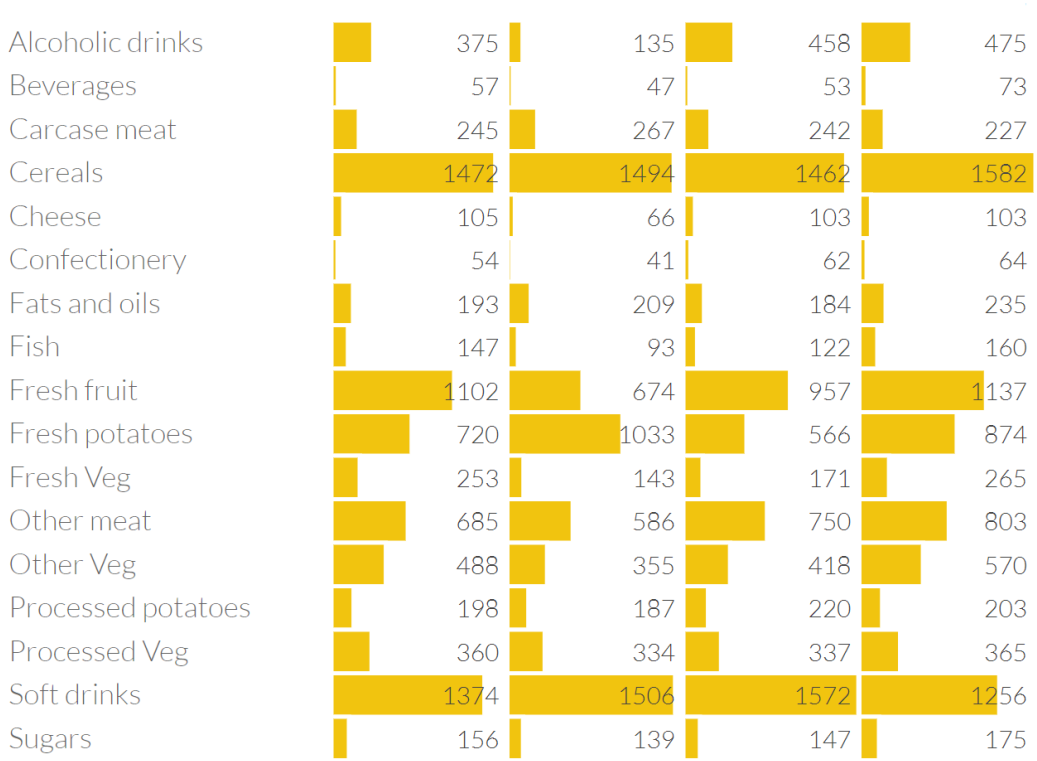
There are many approaches, we focus on a linear method:
Principal Component Analysis (PCA)

Example

picture from here

Consider the following dataset:

- 17 features, each represents the average consumption of some food



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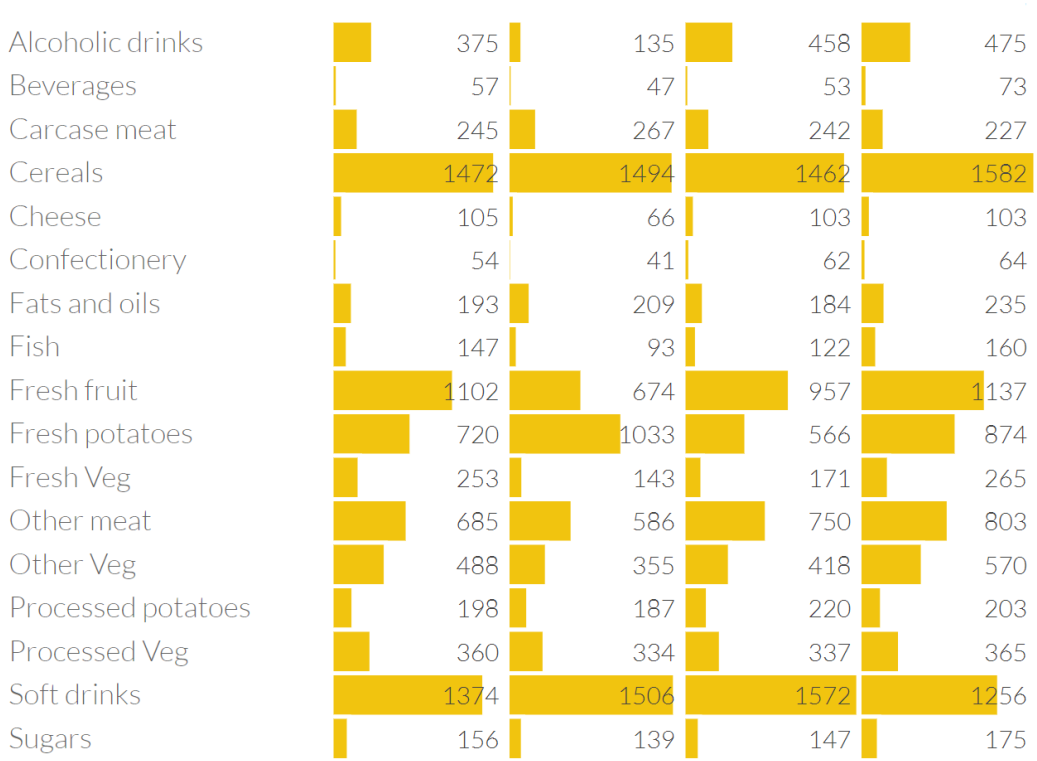

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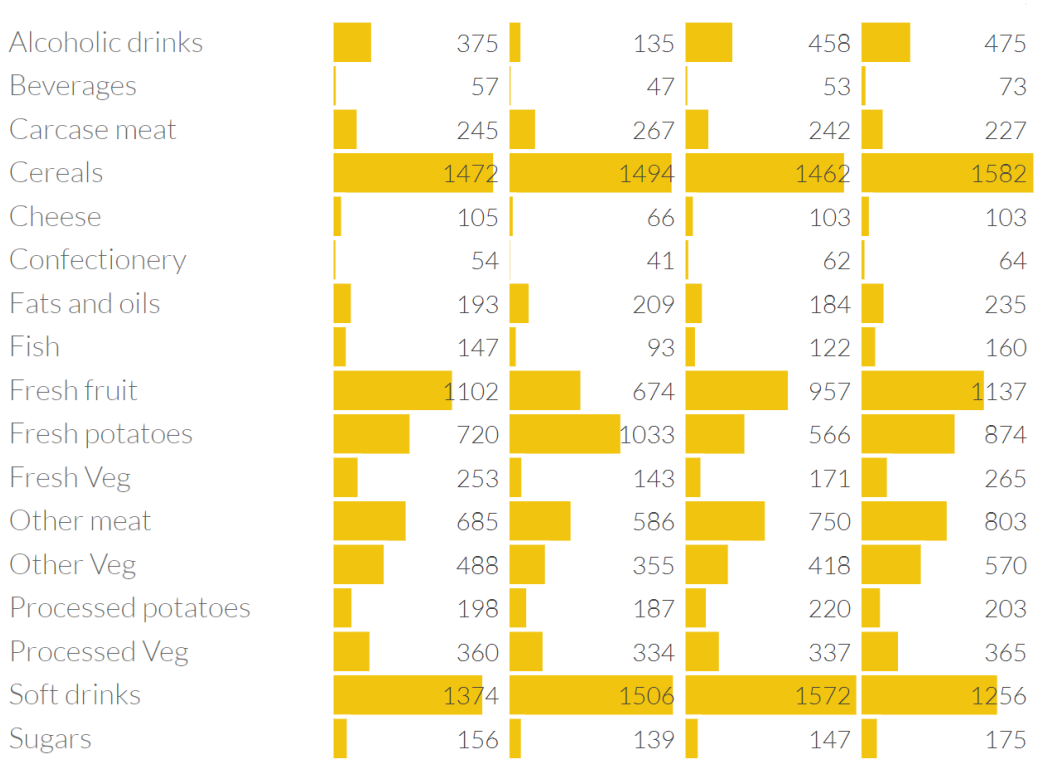

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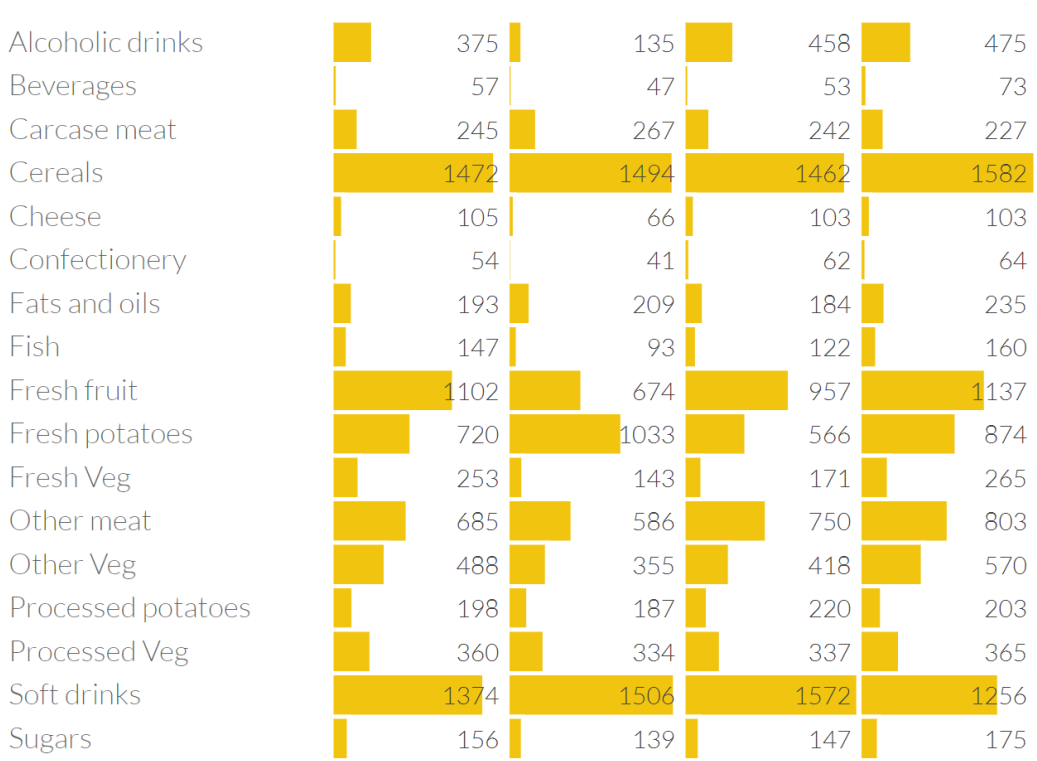

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Hard to say anything looking at all these 17 features.

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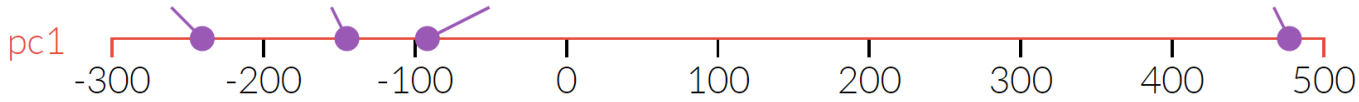

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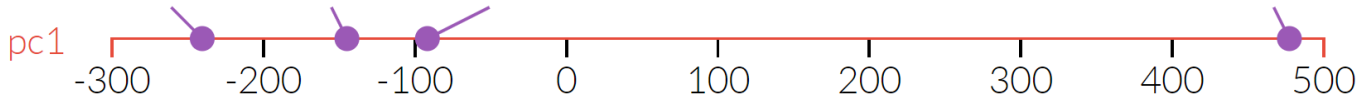

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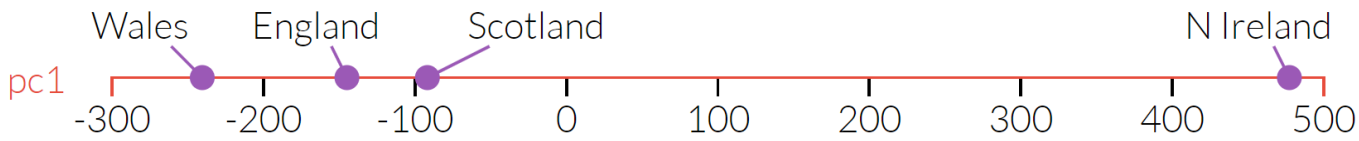

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That turns out to be data from Northern Ireland, *the only country not on the island of Great Britain out of the 4 samples.*

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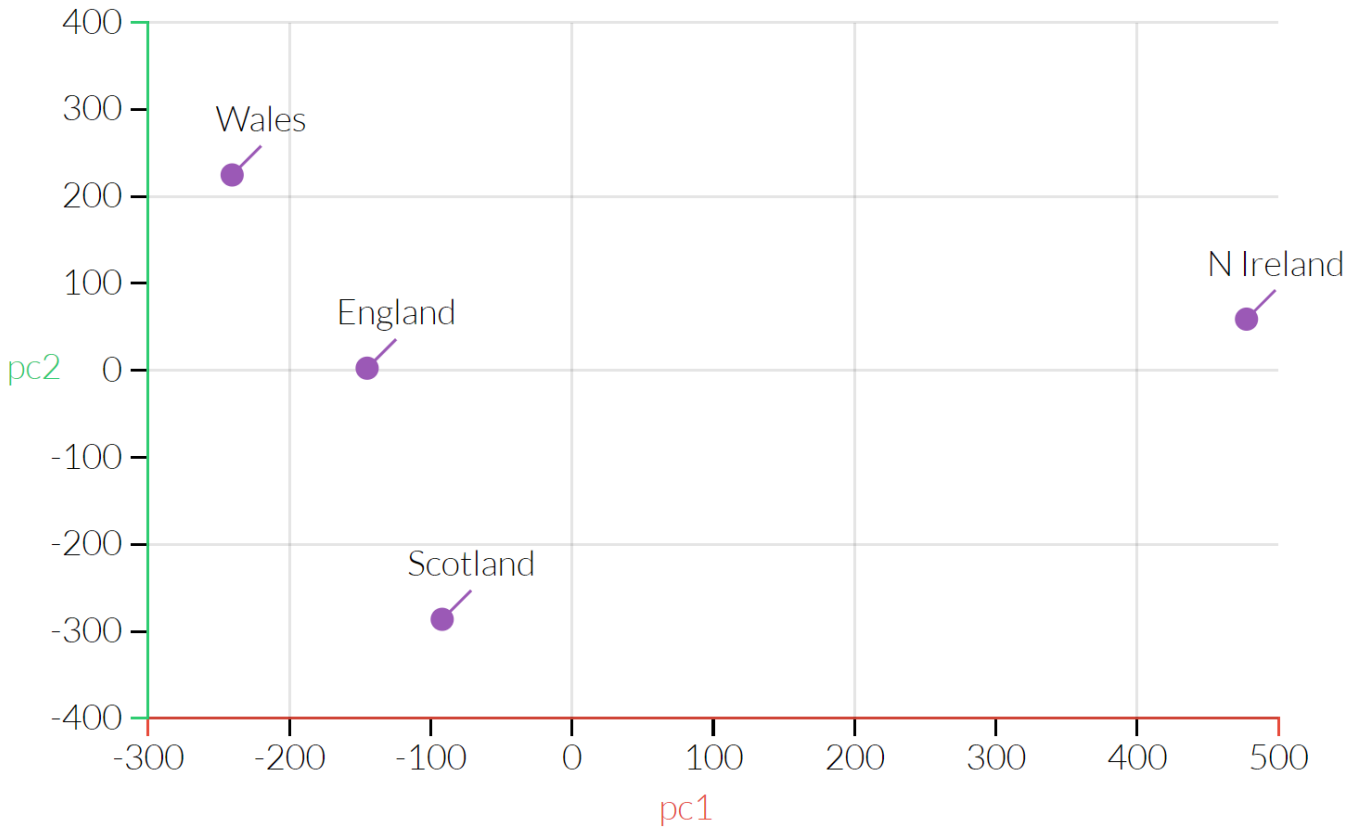
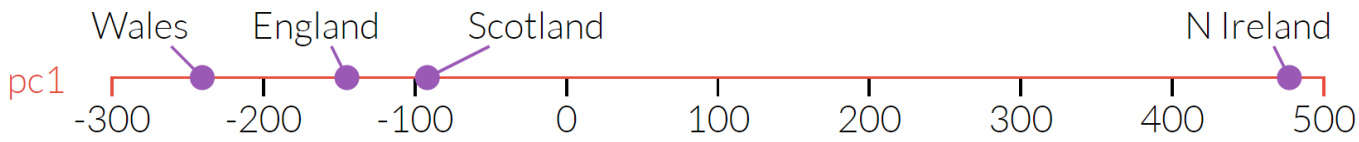
PCA can find the **second (and more) principal component** of the data too:



High level idea

How does PCA find these principal components (PC)?



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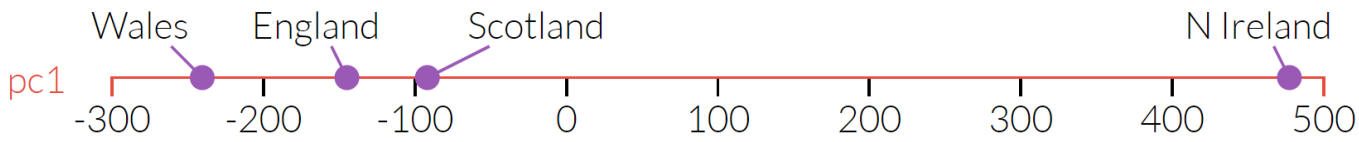

The first PC is in fact **the direction with the most variance**, i.e. the direction where the data is most spread out.

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- we will simply assume $\{\boldsymbol{x}_n\}$ is centered (to avoid notation $\boldsymbol{x}'_n$)

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With $\boldsymbol{X} \in \mathbb{R}^{N \times \mathrm{D}}$ being the data matrix, we want

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Conclusion: the first PC is the top eigenvector of the covariance matrix

Finding the other PCs

If v_1 is the first PC, then the **second PC** is found via

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Conclusion: the d-th principal component is the d-th eigenvector (sorted by the eigenvalue from largest to smallest).

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Step 3 Construct the new compressed dataset $\boldsymbol{X}\boldsymbol{V} \in \mathbb{R}^{N \times p}$

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For visualization, also often pick $p = 1$ or $p = 2$.

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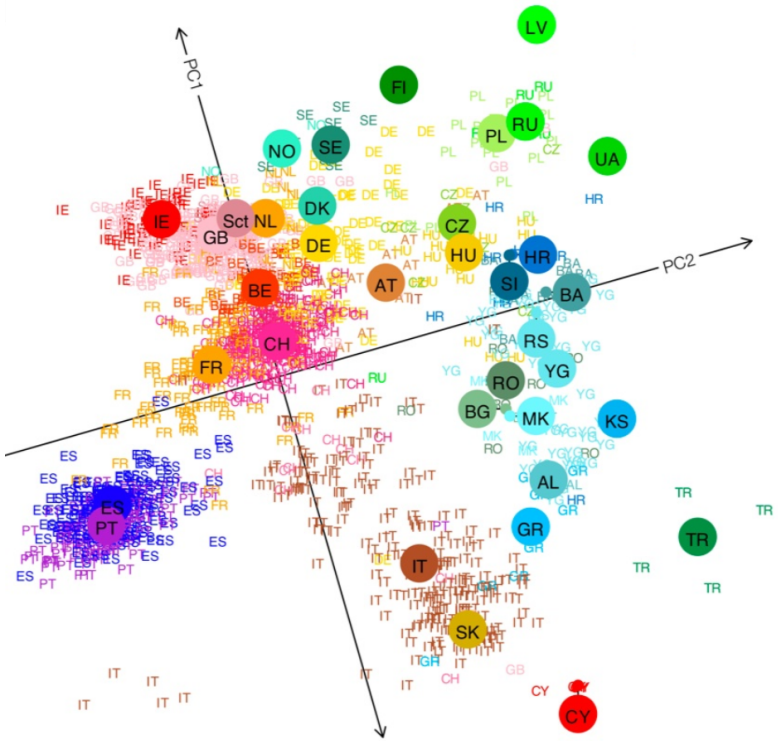

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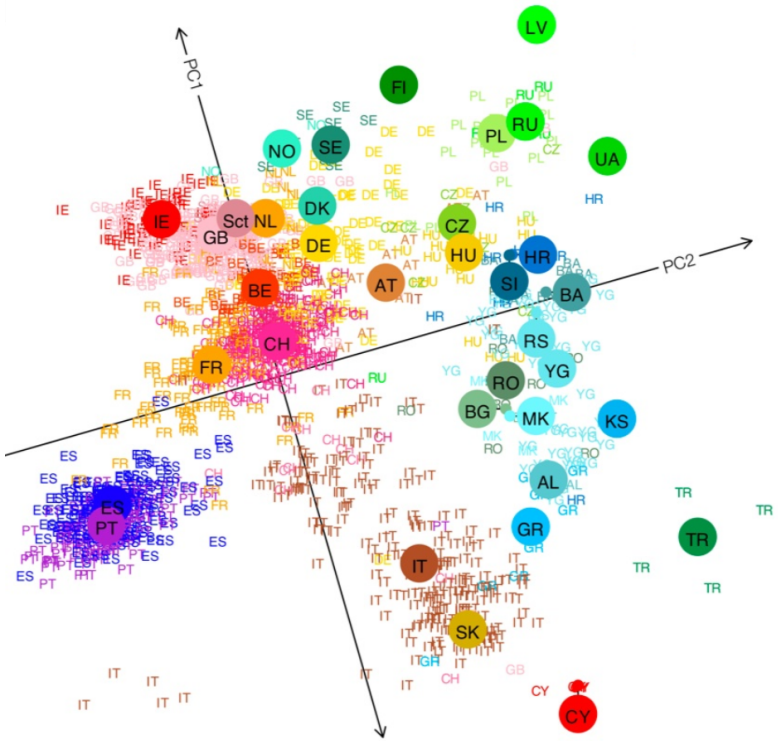

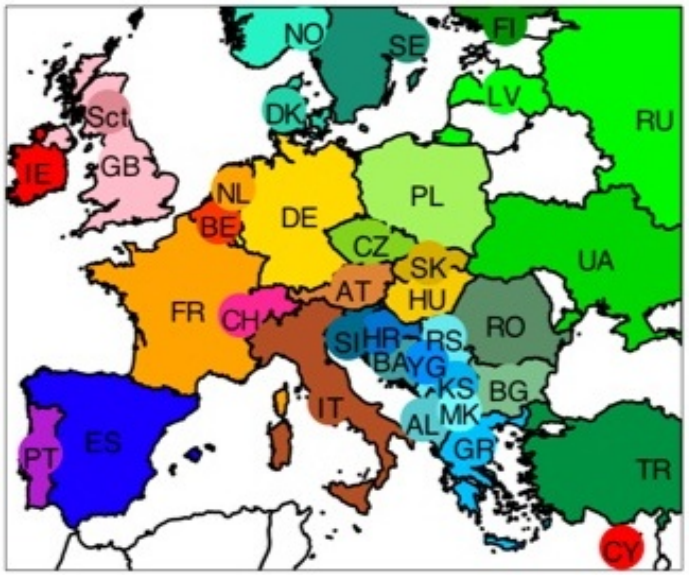

Does PCA always work?

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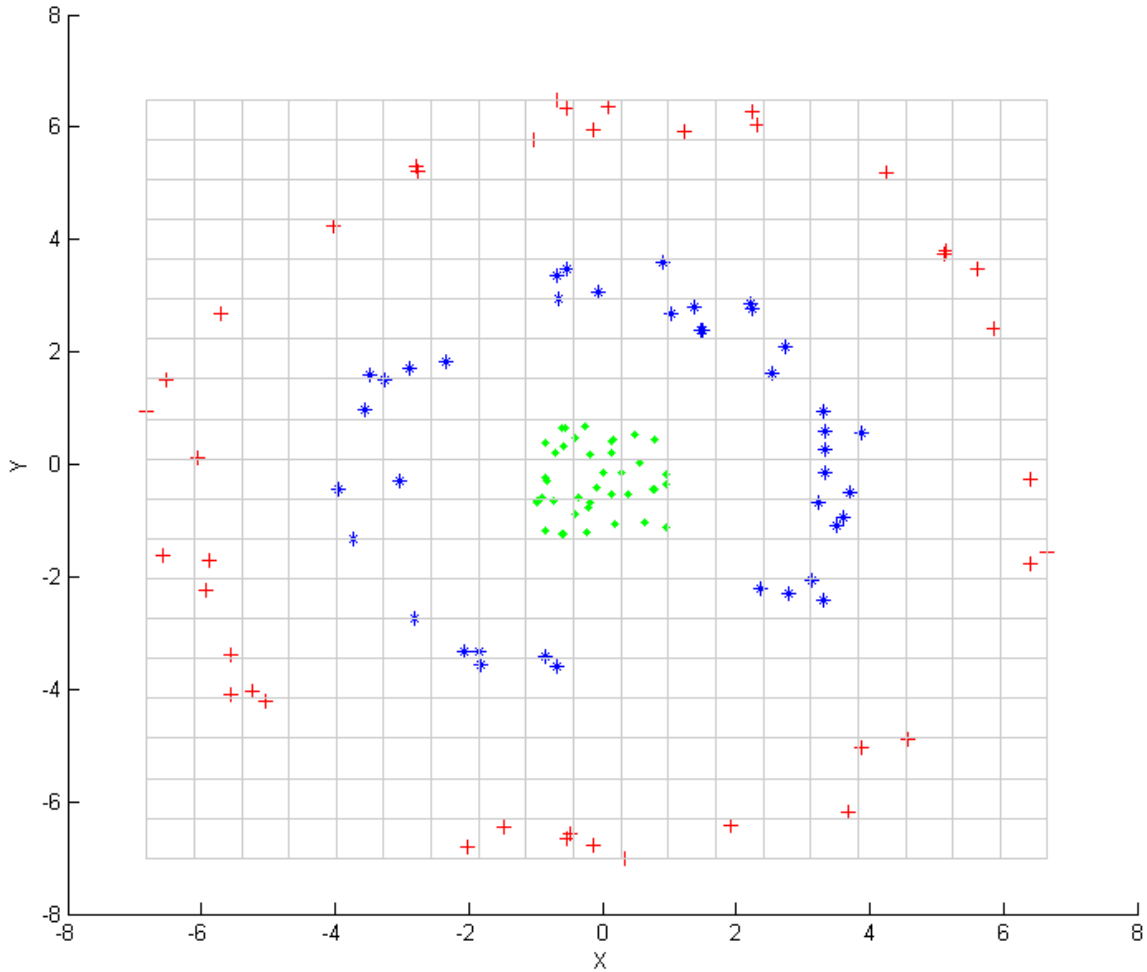
PCA is a **linear method** (recall the new dataset is $\boldsymbol{XV}$), it does not do much when every direction has similar variance.



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How to implement KPCA efficiently without actually working in $\mathbb{R}^{M}$?

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Plugging into $\boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} \boldsymbol{v} = \lambda \boldsymbol{v}$ gives

$$\boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\alpha} = \lambda \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\alpha}$$

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$$\boldsymbol{v} = \frac{1}{\lambda} \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} \boldsymbol{v} = \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\alpha}$$

for some $\boldsymbol{\alpha} \in \mathbb{R}^N$, i.e. it's a linear combination of data.

Plugging into $\boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} \boldsymbol{v} = \lambda \boldsymbol{v}$ gives

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Conclusion: KPCA is just finding top eigenvectors of the Gram matrix

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In other words, we in fact need to scale $\boldsymbol{\alpha}$ so that its L2 norm is $1/\sqrt{\lambda}$, where λ it's the corresponding eigenvalue.

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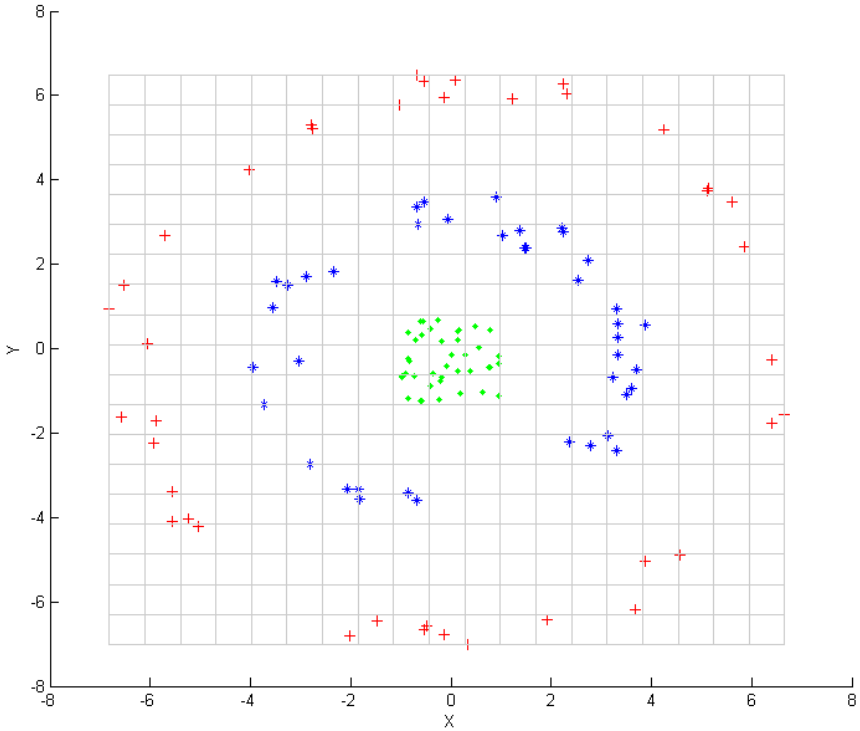
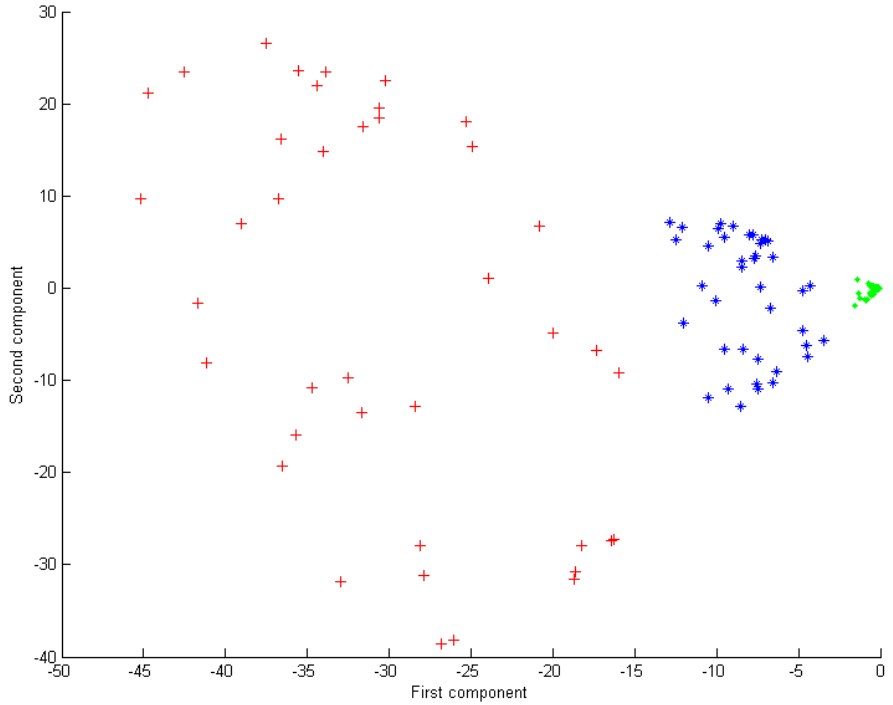
Step 3 Construct the new dataset $(\boldsymbol{\Phi} - \boldsymbol{E}\boldsymbol{\Phi})(\boldsymbol{\Phi} - \boldsymbol{E}\boldsymbol{\Phi})^{\mathrm{T}}\boldsymbol{A} = \bar{\boldsymbol{K}}\boldsymbol{A}$

Example

picture from Wikipedia

Applying kernel $k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}' + 1)^2$:

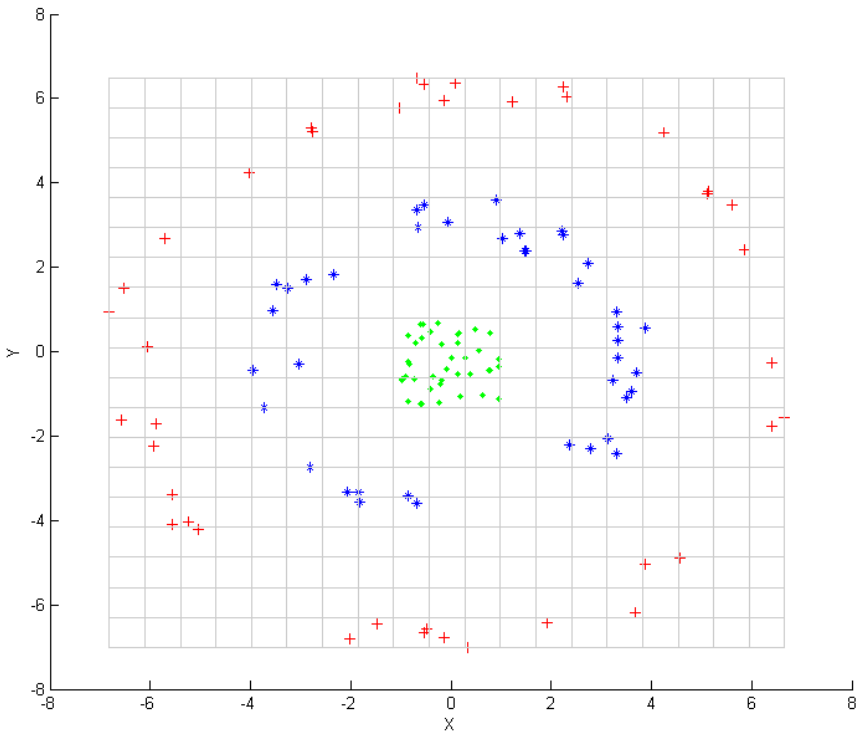


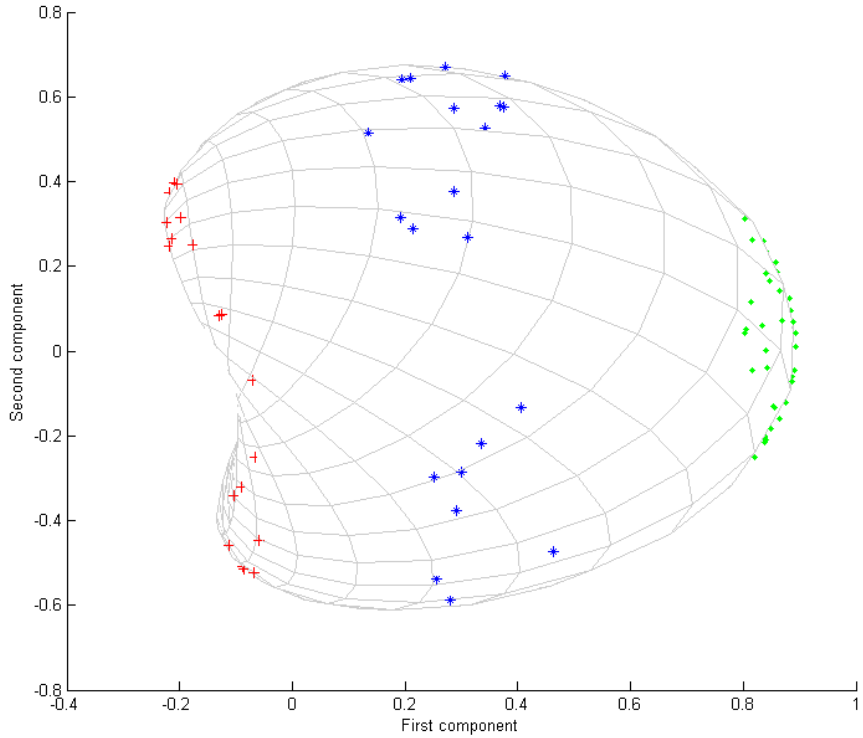


Example

picture from Wikipedia

Applying Gaussian kernel $k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(\frac{-\|\boldsymbol{x}-\boldsymbol{x}'\|^2}{2\sigma^2}\right)$:





Denoising via PCA

Original data

Data corrupted with Gaussian noise

Result after linear PCA

Result after kernel PCA, Gaussian kernel