CSCI567 Machine Learning (Fall 2021)

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Administration

Reminder: HW4 is due this Tue, 11/09

Outline

Outline

The K-means algorithm

Step 0 Initialize $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$

Step 1 Fix the centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$, assign each point to the closest center:

$$\gamma_{nk} = \mathbb{I}\left[k == \operatorname*{argmin}_c \|\boldsymbol{x}_n - \boldsymbol{\mu}_c\|_2^2\right]$$

Step 2 Fix the assignment $\{\gamma_{nk}\}$, update the centers

$$\boldsymbol{\mu}_k = \frac{\sum_n \gamma_{nk} \boldsymbol{x}_n}{\sum_n \gamma_{nk}}$$

Step 3 Return to Step 1 if not converged

K-means++

K-means++ is K-means with a better initialization procedure:

Start with a random data point as the first center $\boldsymbol{\mu}_1$

For $k = 2, \ldots, K$

- randomly pick the k-th center $\boldsymbol{\mu}_k$ such that

$$\Pr[\boldsymbol{\mu}_k = \boldsymbol{x}_n] \propto \min_{j=1,\ldots,k-1} \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|_2^2$$

Intuitively this *spreads out the initial centers*.

Applying EM to learn GMMs (a soft version of K-means)

EM for clustering:

Step 0 Initialize $\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$ for each $k \in [K]$

Step 1 (E-Step) update the "soft assignment" (fixing parameters)

$$\gamma_{nk} = p(z_n = k \mid \boldsymbol{x}_n) \propto \omega_k N\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)$$

Step 2 (M-Step) update the model parameter (fixing assignments)

$$\omega_k = \frac{\sum_n \gamma_{nk}}{N} \qquad \boldsymbol{\mu}_k = \frac{\sum_n \gamma_{nk} \boldsymbol{x}_n}{\sum_n \gamma_{nk}}$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

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General EM algorithm

Step 0 Initialize $\boldsymbol{\theta}^{(1)}$, $t = 1$

Step 1 (E-Step) **update the posterior of latent variables**

$$q_n^{(t)}(\cdot) = p(\cdot \mid \boldsymbol{x}_n \,; \boldsymbol{\theta}^{(t)})$$

and obtain **Expectation** of complete likelihood

$$Q(\boldsymbol{\theta} \,; \boldsymbol{\theta}^{(t)}) = \sum_{n=1}^{N} \mathbb{E}_{z_n \sim q_n^{(t)}} \left[\ln p(\boldsymbol{x}_n, z_n \,; \boldsymbol{\theta}) \right]$$

Step 2 (M-Step) **update the model parameter** via **Maximization**

$$\boldsymbol{\theta}^{(t+1)} \leftarrow \operatorname*{argmax}_{\boldsymbol{\theta}} Q(\boldsymbol{\theta} \,; \boldsymbol{\theta}^{(t)})$$

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- we have seen clustering already, will see more today
- these applications also *provide a way to measure quality of the density estimator*

Parametric methods: generative models

Parametric estimation assumes a generative model parametrized by $\boldsymbol{\theta}$:

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- Multinomial: a discrete variable with values in $\{1, 2, \ldots, K\}$ s.t.

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where $\boldsymbol{\theta}$ is a distribution over K elements.

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Size of $\boldsymbol{\theta}$ is independent of the training set size, so it's parametric.

Parametric methods: estimation

Again, we apply **MLE** to learn the parameters $\boldsymbol{\theta}$:

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For some other cases this admits a simple closed-form solution (e.g. multinomial).

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The solution is simply

$$\theta_k = \frac{z_k}{N} \propto z_k,$$

i.e. the fraction of examples with value k. (See HW4 Q1.1)

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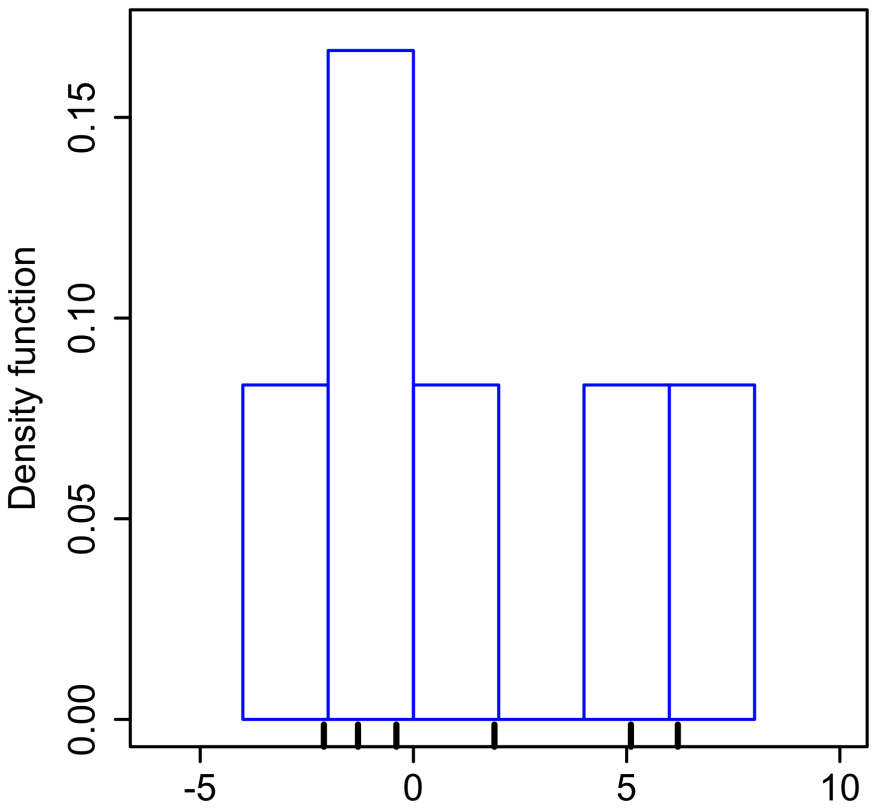
- here "kernel" means something different from what we have seen for "kernel function" (in fact it refers to several different things in ML)
- the approach is nonparametric: it keeps the entire training set
- we focus on the one-dimensional (continuous) case

High level idea

picture from Wikipedia

Construct something similar to a **histogram**:



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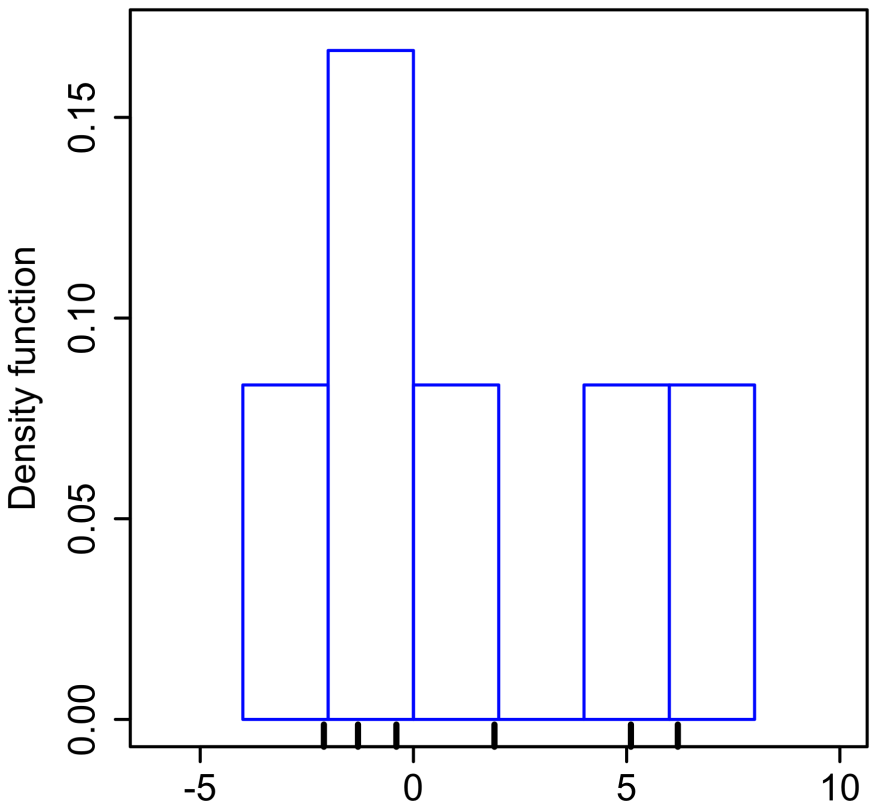
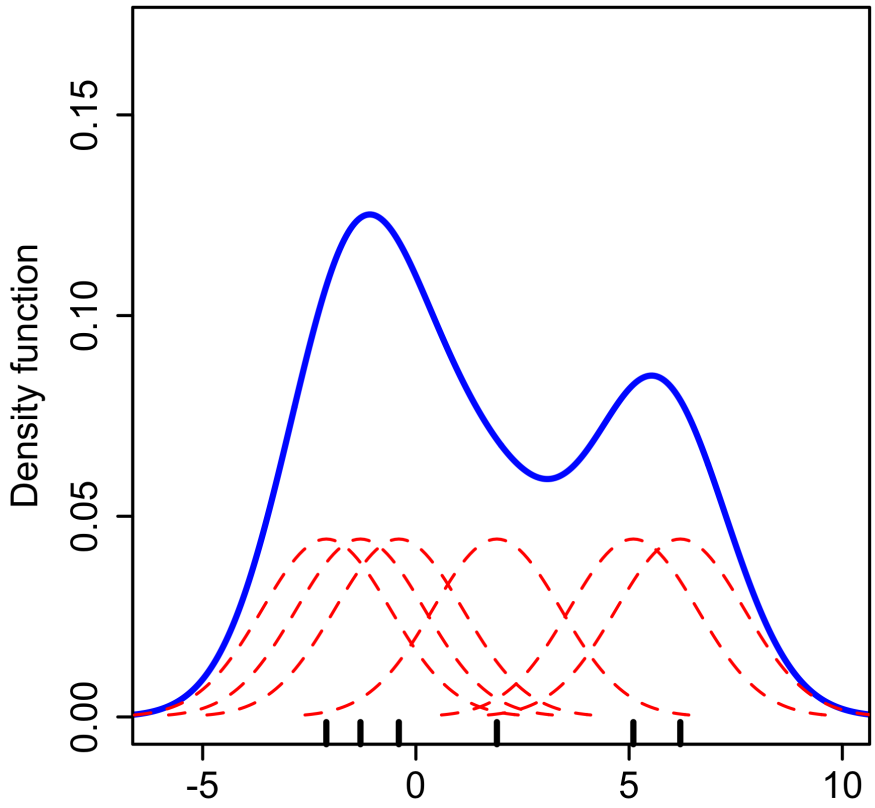
- for each data point, create a "bump" (via a Kernel)





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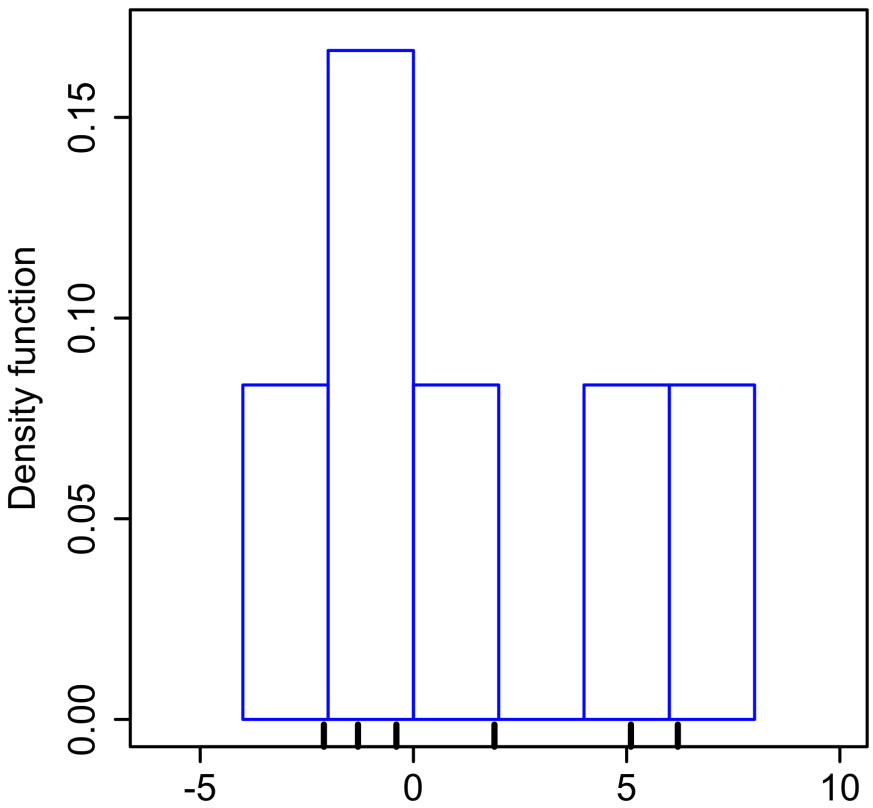
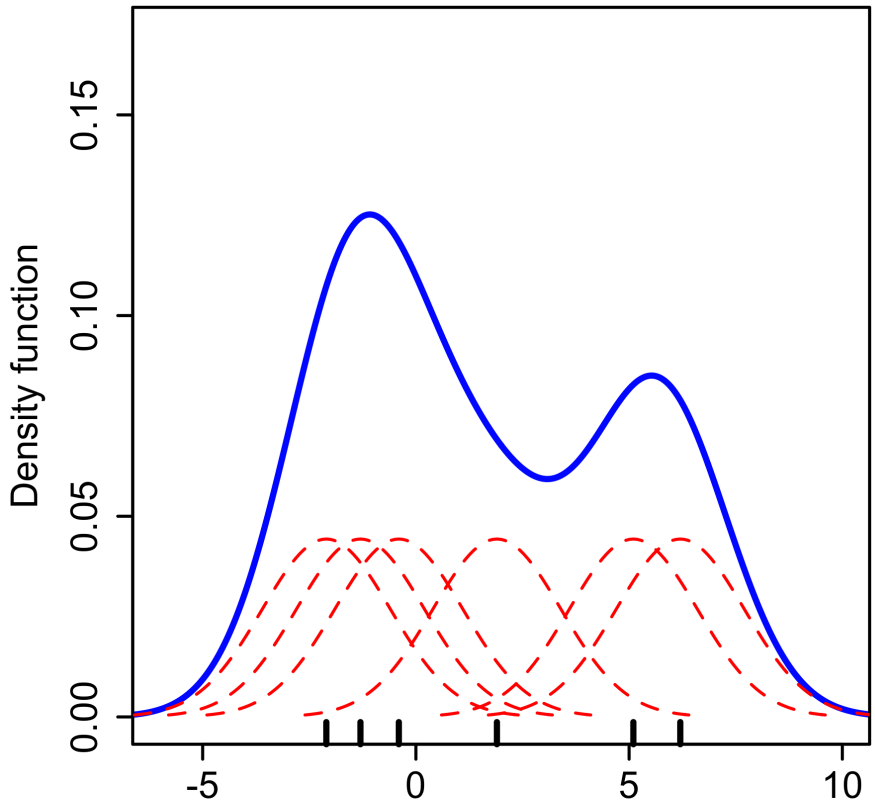
Construct something similar to a **histogram**:

- for each data point, create a "bump" (via a Kernel)
- sum up or average all the bumps

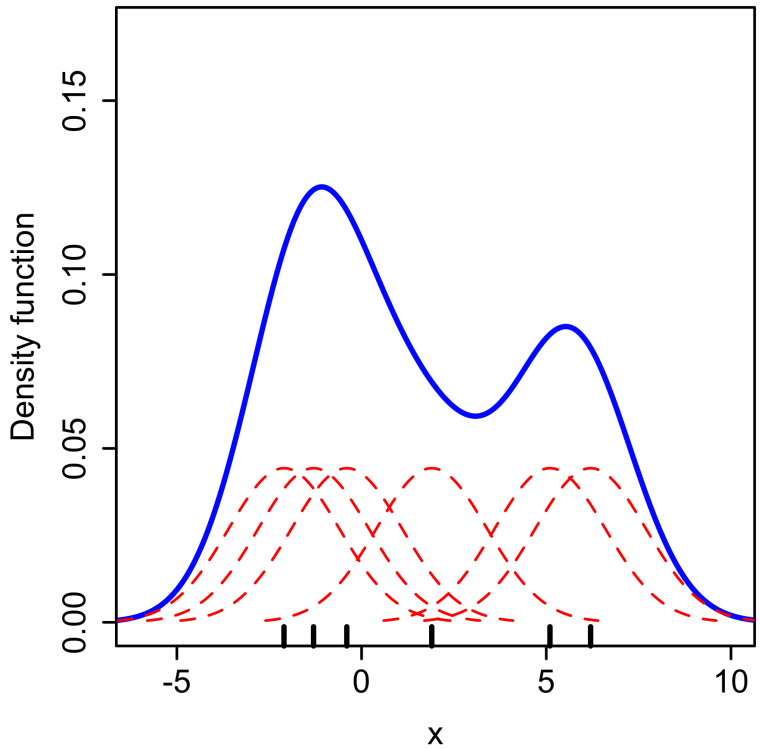




Kernel

KDE with **a kernel** K: $\mathbb{R} \to \mathbb{R}$:

$$p(x) = \frac{1}{N} \sum_{n=1}^{N} K\left(x - x_n\right)$$



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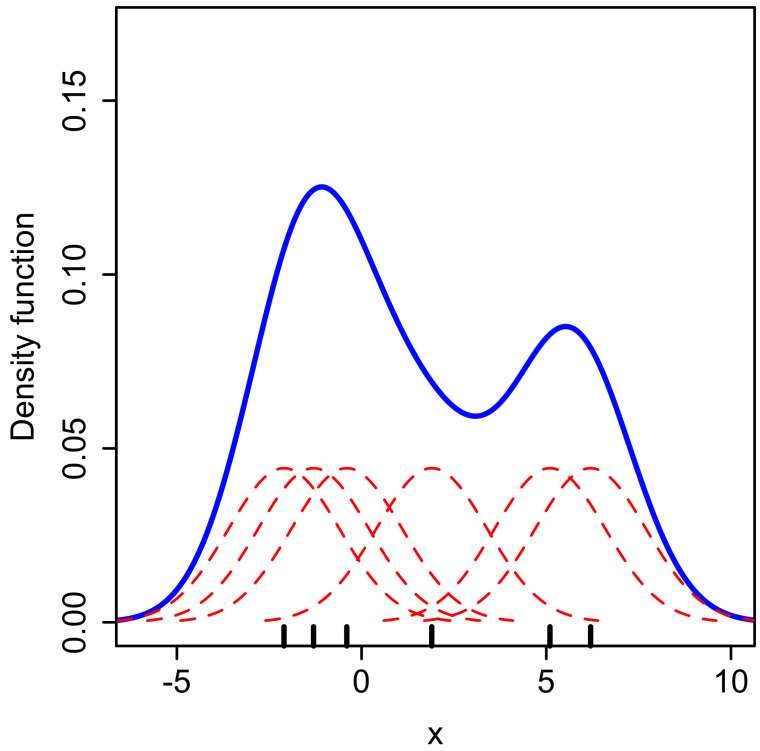

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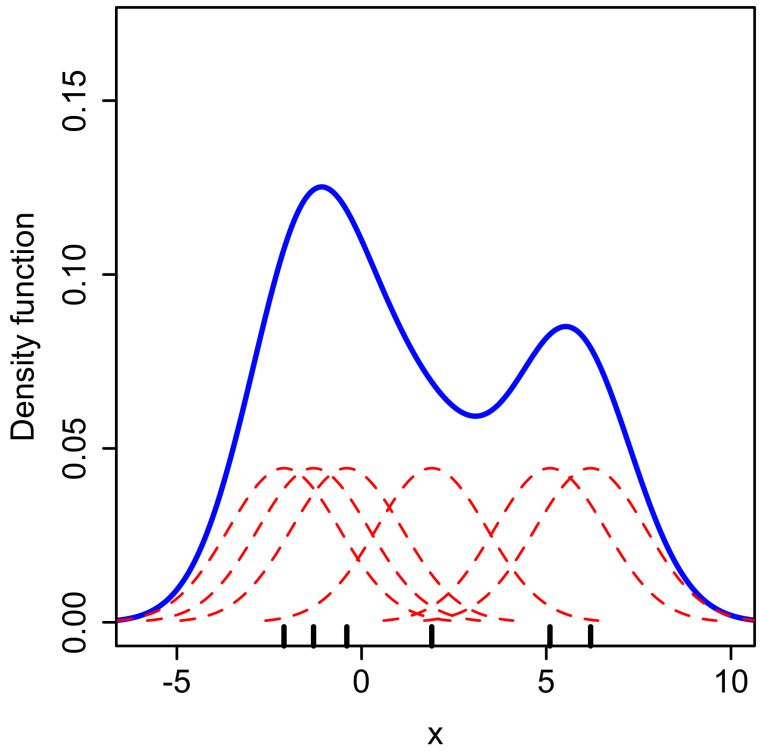

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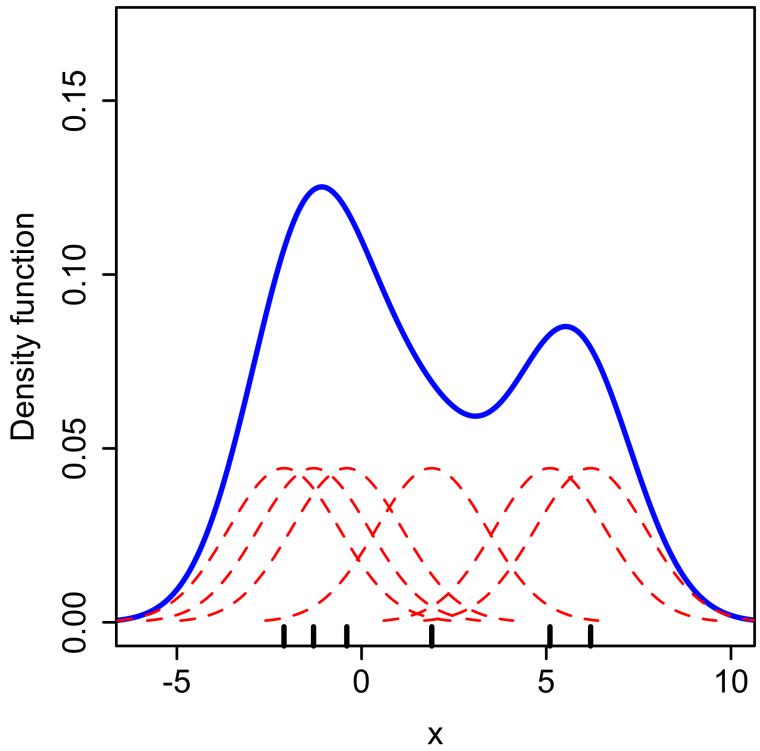
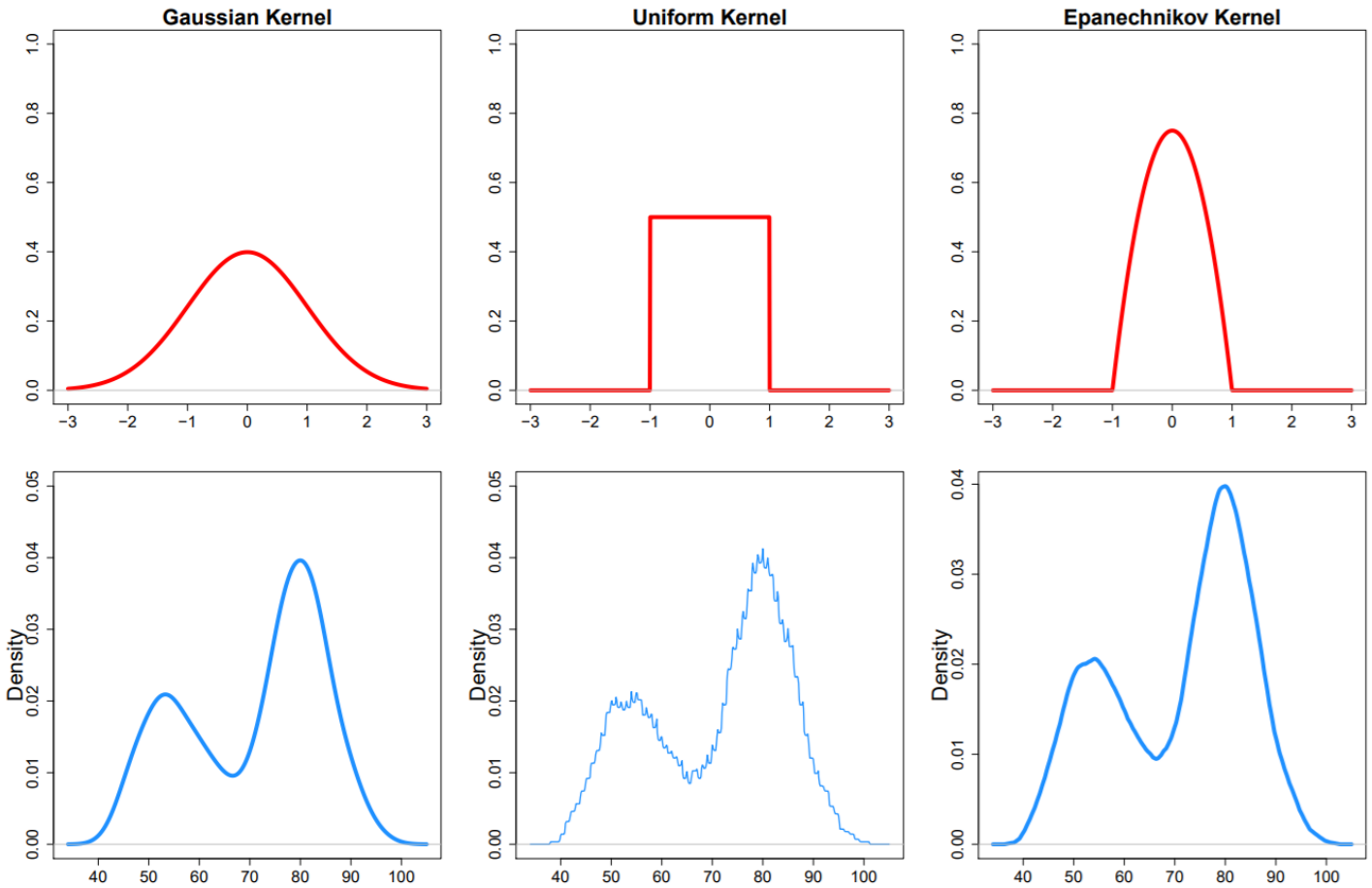
- $\int_{-\infty}^{\infty} K(u)du = 1$, makes sure p is a density function.



Different kernels $K(u)$

$$\frac{1}{\sqrt{2\pi}} e^{-\frac{u^2}{2}} \qquad \frac{1}{2}\mathbb{I}[|u| \leq 1] \qquad \frac{3}{4}\max\{1-x^2, 0\}$$



Bandwidth

If $K(u)$ is a kernel, then for any $h > 0$

$$K_h(u) \triangleq \frac{1}{h} K\left(\frac{u}{h}\right) \qquad \text{(stretching the kernel)}$$

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So general KDE is determined by both the kernel K and the bandwidth h

$$p(x) = \frac{1}{N} \sum_{n=1}^{N} K_h\left(x - x_n\right) = \frac{1}{Nh} \sum_{n=1}^{N} K\left(\frac{x - x_n}{h}\right)$$

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- x_n controls the center of each bump
- h controls the width/variance of the bumps

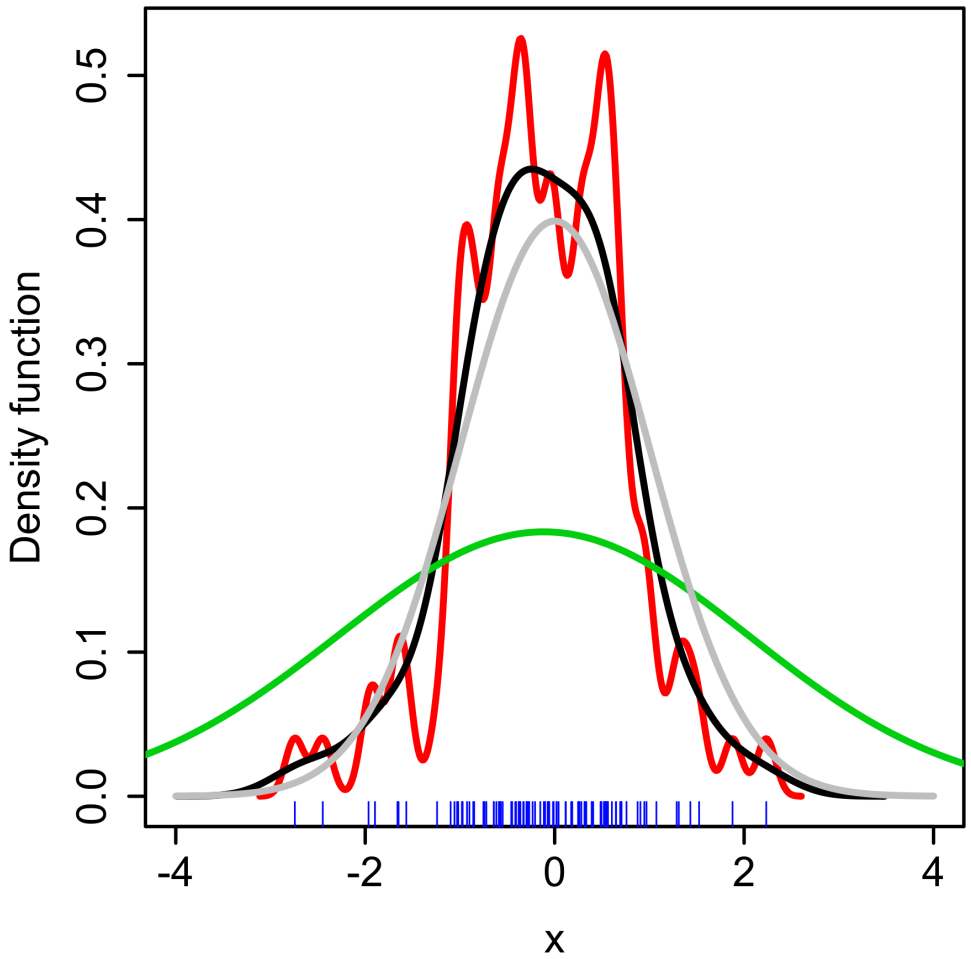
Effect of bandwidth

picture from Wikipedia

Larger h means larger variance and also smoother density

Gray curve is ground-truth

- Red: $h = 0.05$
- Black: $h = 0.337$
- Green: $h = 2$



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- one can also do cross-validation based on downstream applications

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- **density estimation** is one important part of the algorithm

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

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This is *not a 1D problem* in general.

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

Example: discrete features

Height: $\leq$3', 3'-4', 4'-5', 5'-6', $\geq$6'
Vocabulary: $\leq$5K, 5K-10K, 10K-15K, 15K-20K, $\geq$20K
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More formally

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For each possible value k of a discrete feature d,

$$p(x_d = k \mid y = c) = \frac{|\{n : x_{nd} = k, y_n = c\}|}{|\{n : y_n = c\}|}$$

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  where μ_{cd} and σ_{cd}^2 are the empirical mean and variance of feature d among all examples with label c.

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Continuous features

If the feature is continuous, we can do

- parametric estimation, e.g. via a Gaussian

$$p(x_d = x \mid y = c) = \frac{1}{\sqrt{2\pi}\sigma_{cd}} \exp\left(-\frac{(x - \mu_{cd})^2}{2\sigma_{cd}^2}\right)$$

  where μ_{cd} and σ_{cd}^2 are the empirical mean and variance of feature d among all examples with label c.

- or nonparametric estimation, e.g. via a Kernel K and bandwidth h:

$$p(x_d = x \mid y = c) = \frac{1}{|\{n : y_n = c\}|} \sum_{n:y_n=c} K_h(x - x_{nd})$$

How to predict?

After learning the model

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

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&= \operatorname*{argmax}_{c \in [\mathsf{C}]} \left(\ln p(y = c) + \sum_{d=1}^{\mathsf{D}} \ln p(x_d \mid y = c) \right)
\end{aligned}$$

Examples

For **discrete features**, plugging in previous MLE estimations gives

$$\begin{aligned}
&\operatorname*{argmax}_{c \in [\mathsf{C}]} \; p(y = c \mid \boldsymbol{x}) \\
&= \operatorname*{argmax}_{c \in [\mathsf{C}]} \left(\ln p(y = c) + \sum_{d=1}^{\mathsf{D}} \ln p(x_d \mid y = c) \right) \\
&= \operatorname*{argmax}_{c \in [\mathsf{C}]} \left(\ln |\{n : y_n = c\}| + \sum_{d=1}^{\mathsf{D}} \ln \frac{|\{n : x_{nd} = x_d, y_n = c\}|}{|\{n : y_n = c\}|} \right)
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For **continuous features** with a Gaussian model,

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which is *quadratic* in the feature $\boldsymbol{x}$.

What naive Bayes is learning?

Observe again for the case of continuous features with a Gaussian model, if we **fix the variance for each feature to be σ** (i.e. not a parameter of the model any more), then the prediction becomes

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where we denote $w_{c0} = \ln |\{n : y_n = c\}| - \sum_{d=1}^{\mathsf{D}} \frac{\mu_{cd}^2}{2\sigma^2}$ and $w_{cd} = \frac{\mu_{cd}}{\sigma^2}$.

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&= \operatorname*{argmax}_{c\in[\mathsf{C}]} \left(w_{c0} + \sum_{d=1}^{\mathsf{D}} w_{cd} x_d \right) = \operatorname*{argmax}_{c\in[\mathsf{C}]} \; \boldsymbol{w}_c^{\mathrm{T}} \boldsymbol{x} \qquad (\textit{linear classifier!})
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Moreover by similar calculation one can verify

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So what is different then? They **learn the parameters in different ways**:

- both via MLE, one on $p(y = c \mid \boldsymbol{x})$, the other on $p(\boldsymbol{x}, y)$
- solutions are different: logistic regression has no closed-form, naive Bayes admits a simple closed-form

Generative model v.s discriminative model

	Discriminative model	Generative model
Example	logistic regression	naive Bayes

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Remark		more flexible, can generate data after learning

Outline

Dimensionality reduction

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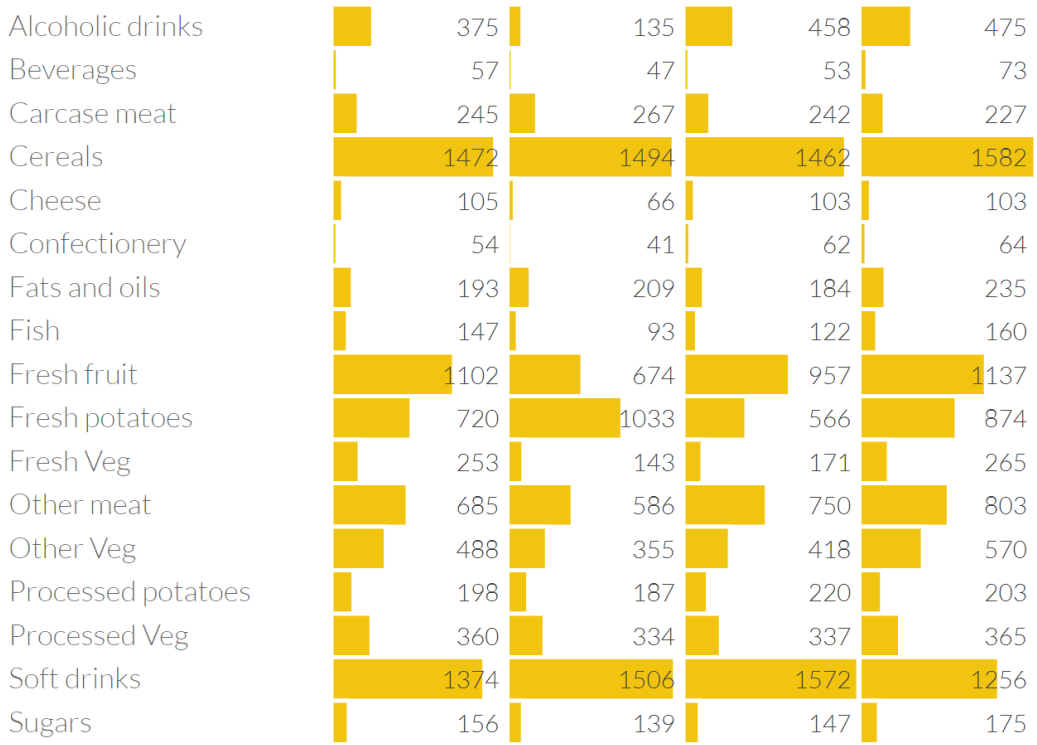
There are many approaches, we focus on a linear method:
Principal Component Analysis (PCA)

Example

picture from here

Consider the following dataset:

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



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Consider the following dataset:

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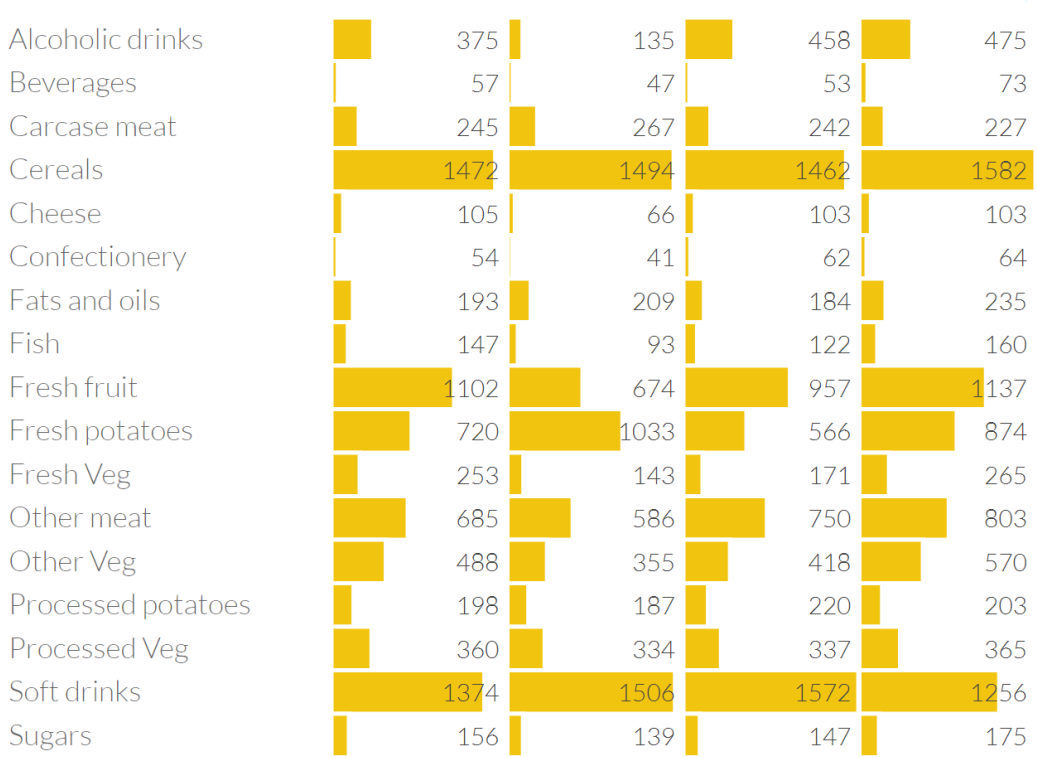

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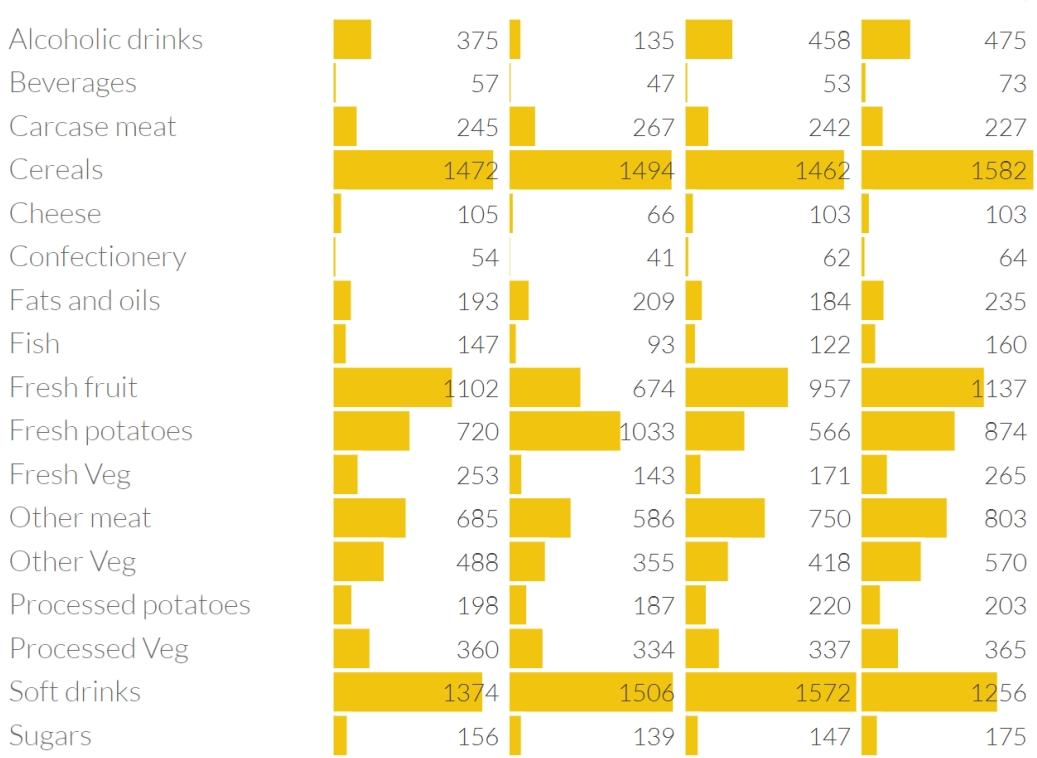

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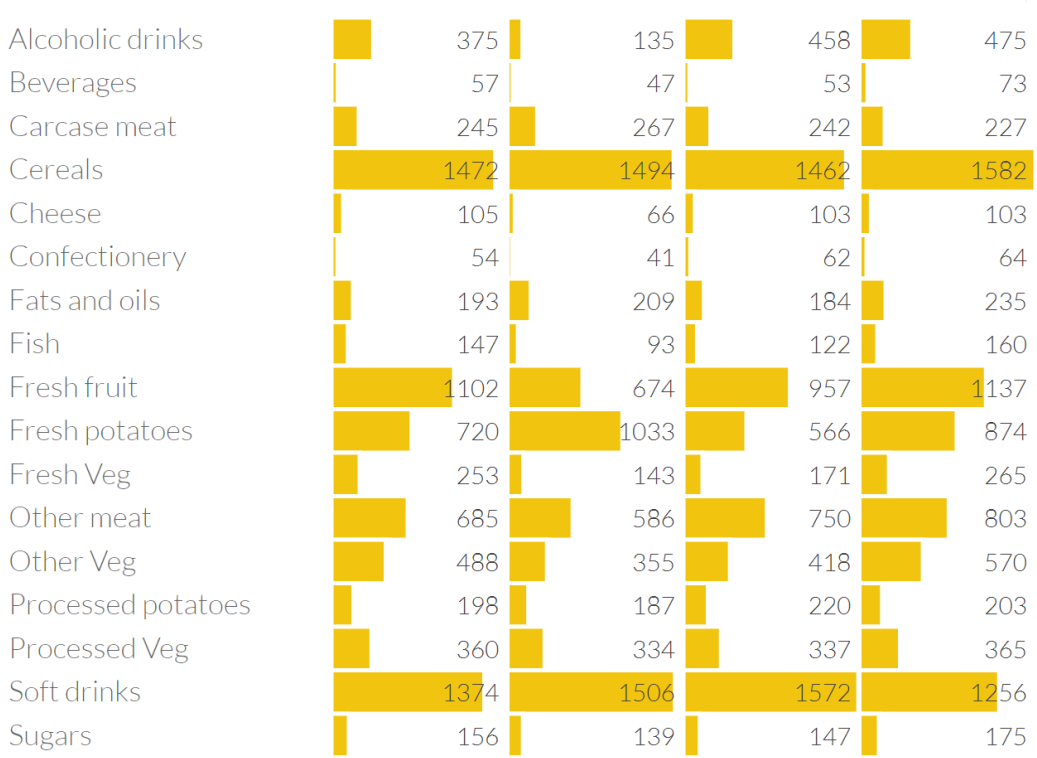


What can you tell?

Hard to say anything looking at all these 17 features.

Example

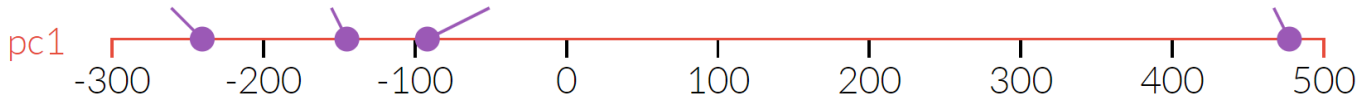
picture from here

PCA can help us!

Example

picture from here

PCA can help us! The first principal component of this dataset:



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Example

picture from here

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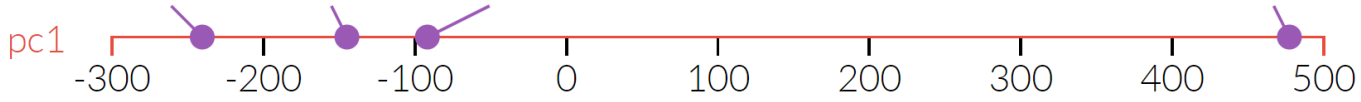

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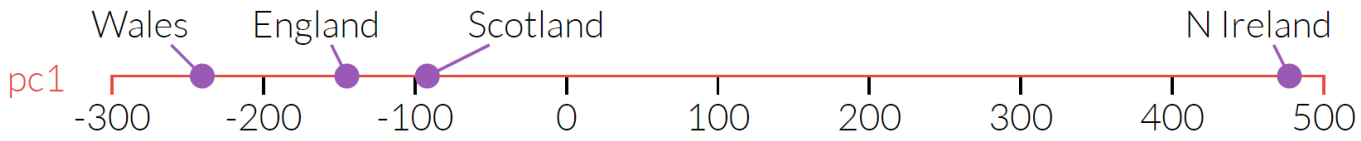

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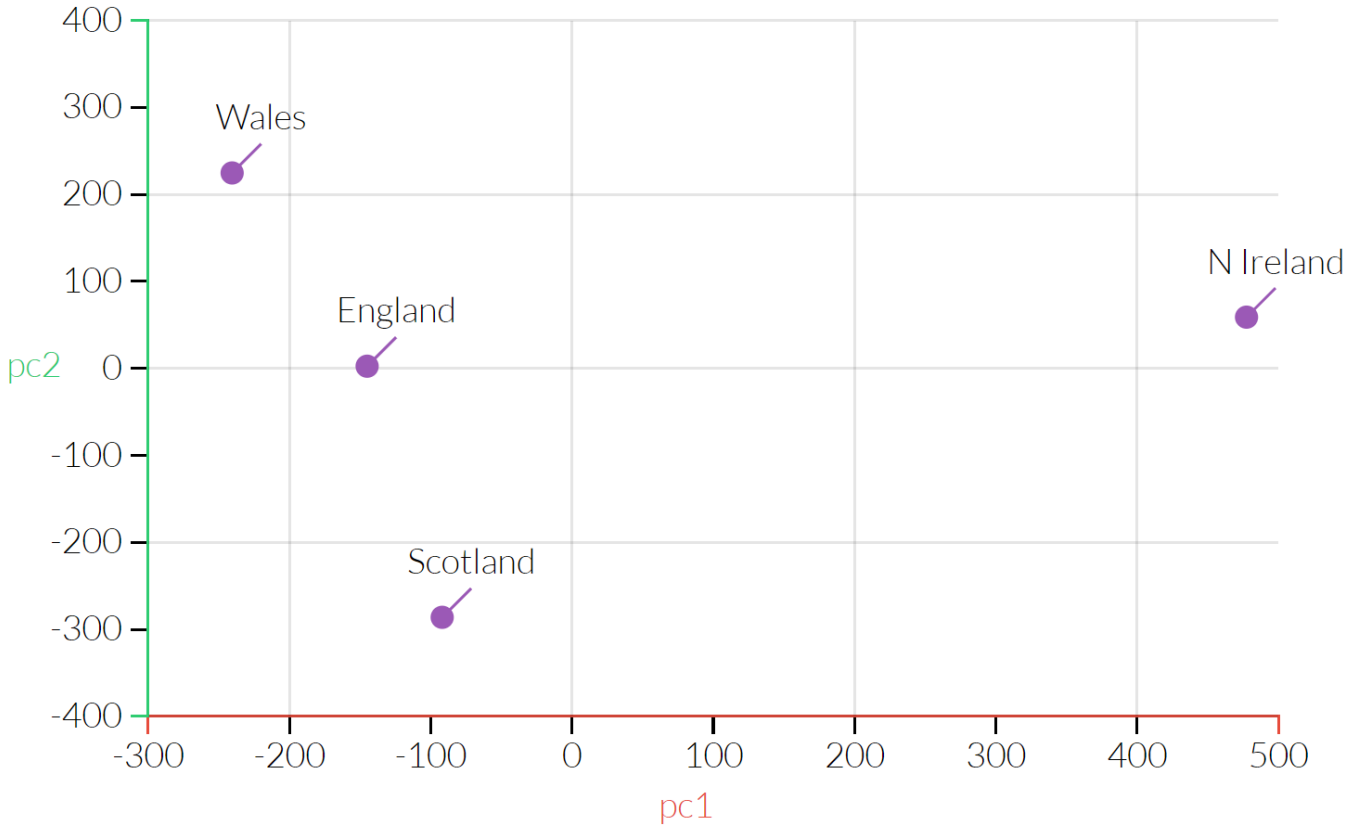
That turns out to be data from Northern Ireland, *the only country not on the island of Great Britain out of the 4 samples.*

Example

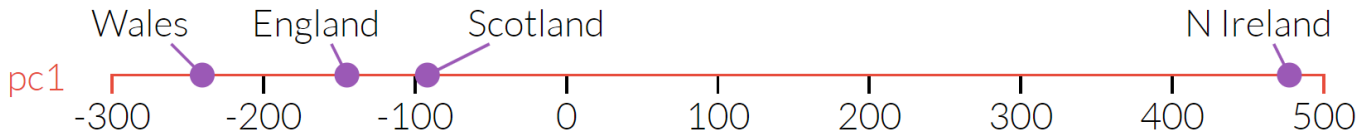
picture from here

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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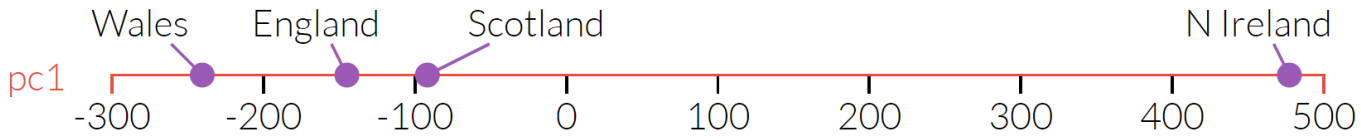

The first PC is in fact **the direction with the most variance**, i.e. the direction where the data is most spread out.

Finding the first PC

More formally, we want to find a direction $\boldsymbol{v} \in \mathbb{R}^{\mathsf{D}}$ with $\|\boldsymbol{v}\|_2 = 1$, so that the projection of the dataset on this direction has the most variance,

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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 (as in Lec 2), we want

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The stationary condition implies $\boldsymbol{X}^{\mathrm{T}} \boldsymbol{X} \boldsymbol{v} = \lambda \boldsymbol{v}$,

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The Lagrangian is

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

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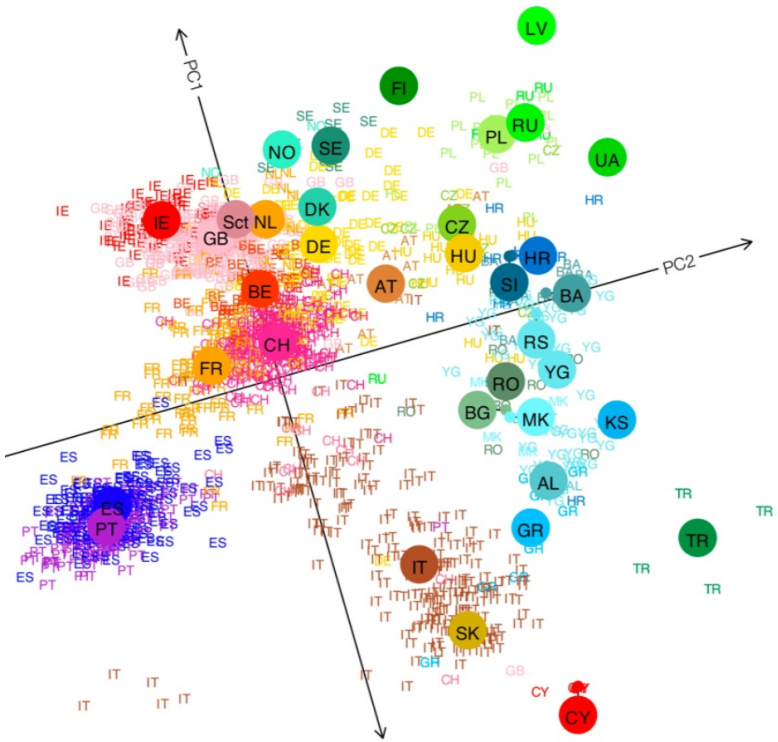

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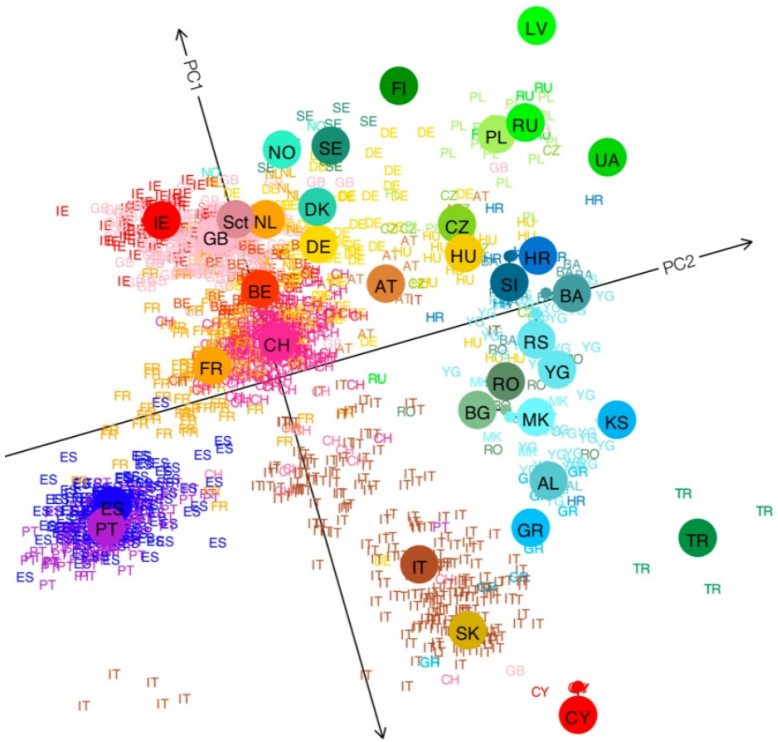

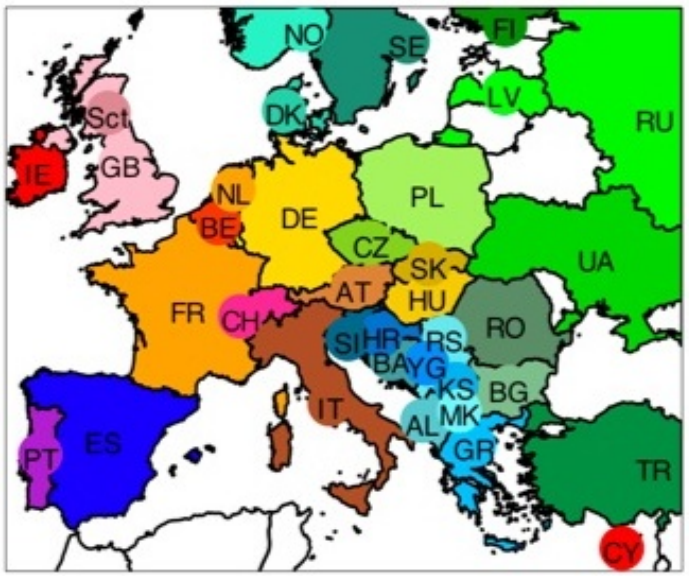

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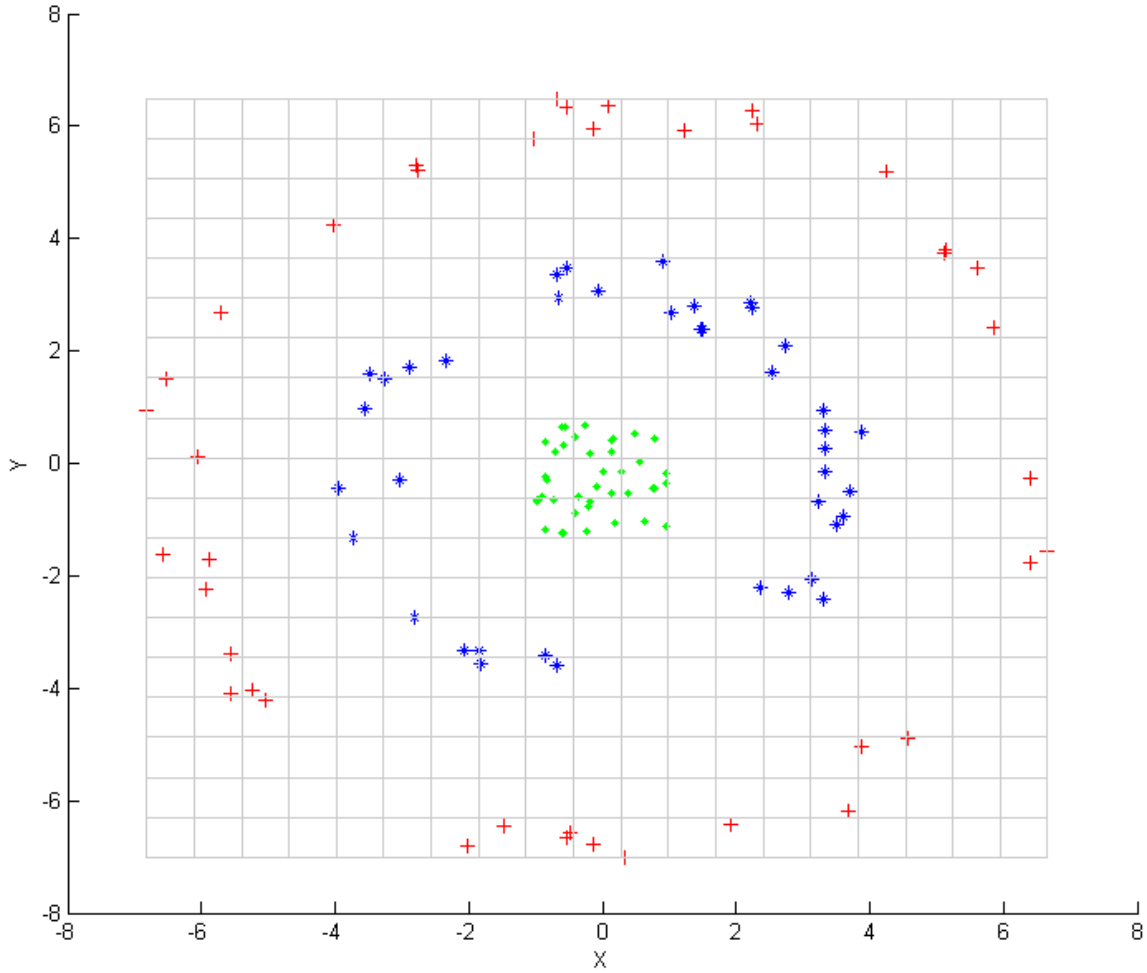
PCA is a **linear method** (recall the new dataset is $\boldsymbol{XV}$), it does not do much when every direction has similar variance.



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

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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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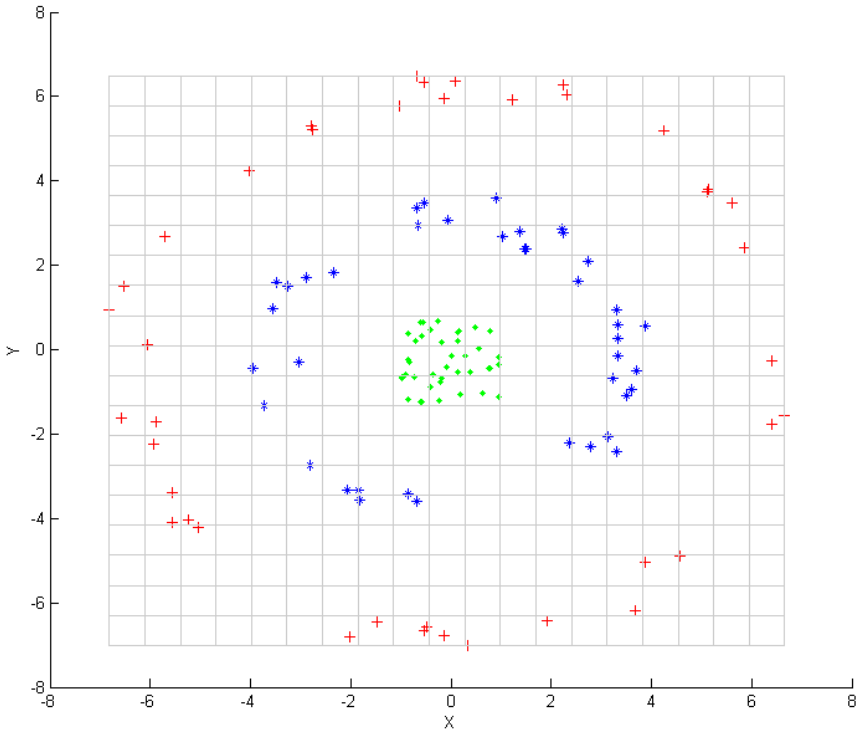
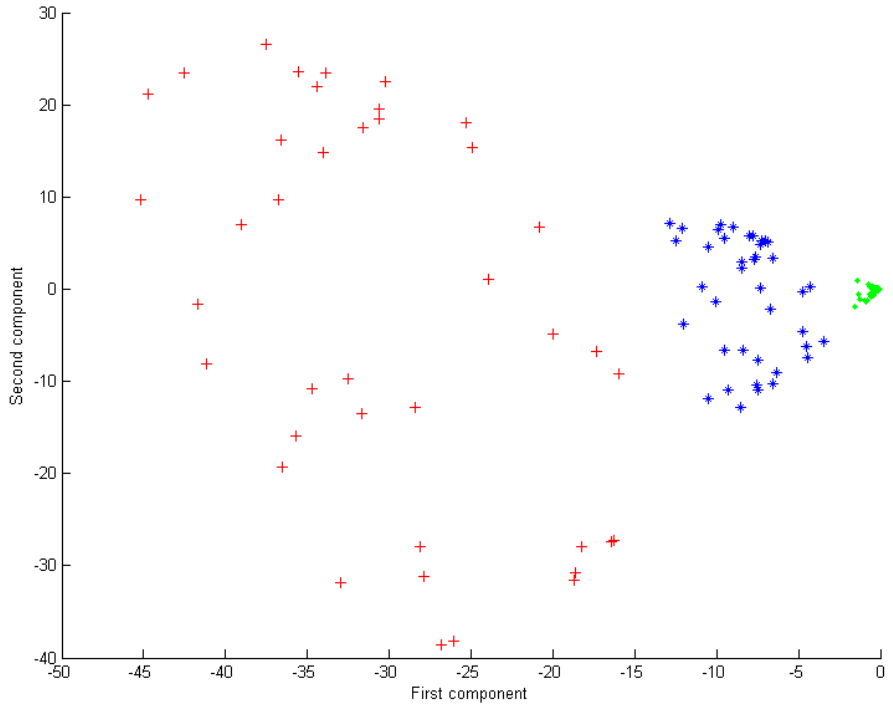
Example

picture from Wikipedia

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





Example

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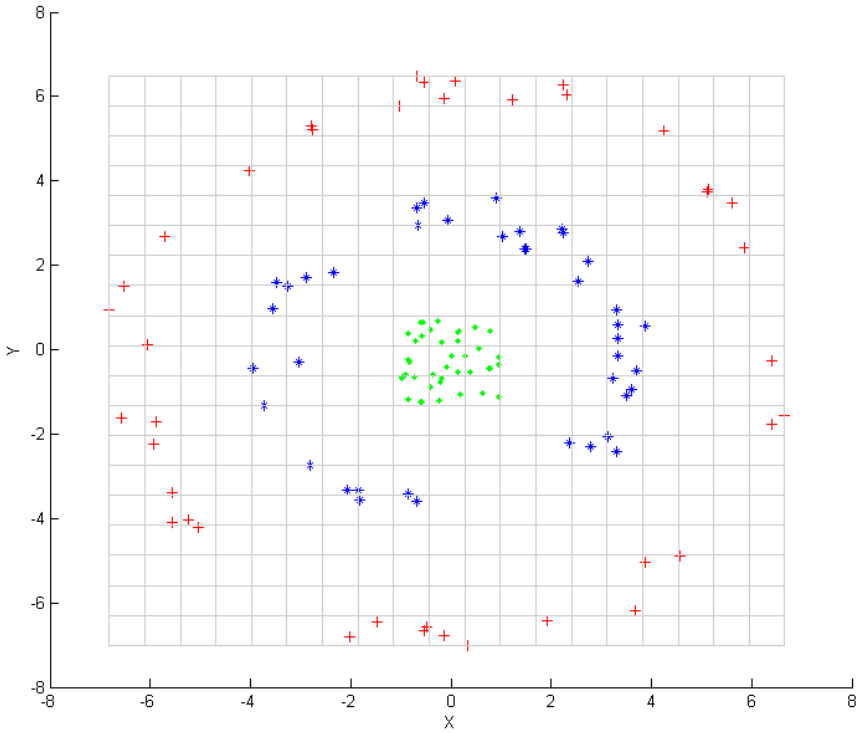
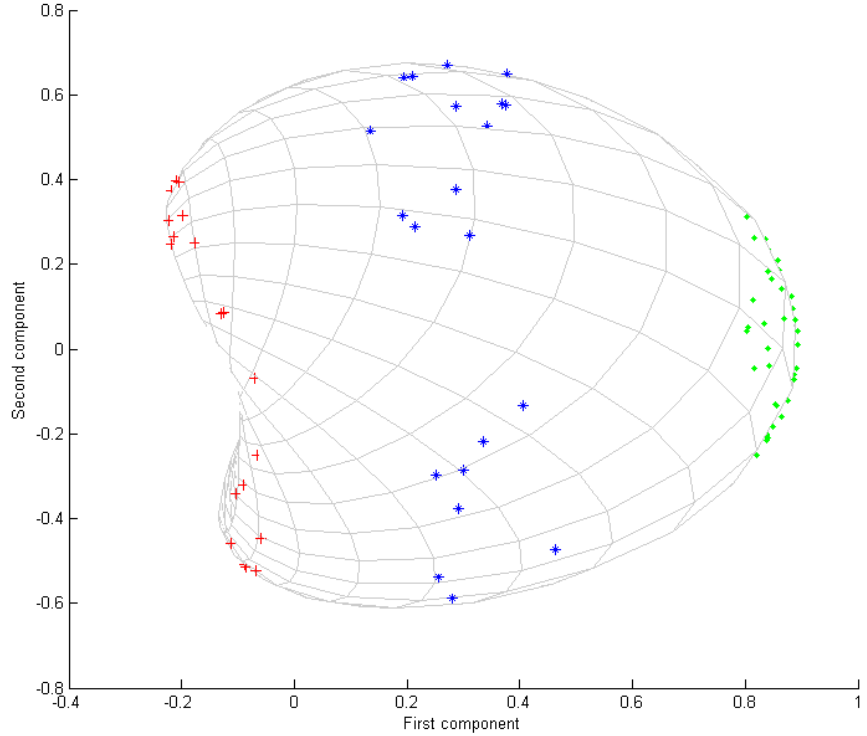
Applying Gaussian kernel $k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(\frac{-\|\boldsymbol{x}-\boldsymbol{x}'\|^2}{2\sigma^2}\right)$:





Denoising via PCA

Original data

Data corrupted with Gaussian noise

Result after linear PCA

Result after kernel PCA, Gaussian kernel