CSCI567 Machine Learning (Fall 2023)

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Outline

1. Review of last lecture
2. Density estimation
3. Naive Bayes
4. Principal Component Analysis (PCA)

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4. Principal Component Analysis (PCA)

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**

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

Step 3 $t \leftarrow t + 1$ and return to Step 1 if not converged

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    - Parametric methods
    - Nonparametric methods
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Useful for many downstream applications

- we have seen clustering already, will see more today

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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.

  $$p(x = k\ ; \boldsymbol{\theta}) = \theta_k$$

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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 $\boldsymbol{\theta}$:

$$\underset{\boldsymbol{\theta}}{\operatorname{argmax}} \sum_{n=1}^{N} \ln p(x_n \; ; \boldsymbol{\theta})$$

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

MLE for multinomial

The log-likelihood is

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where $z_k = |\{n : x_n = k\}|$ is **the number of examples with value k**.

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where $z_k = |\{n : x_n = k\}|$ is **the number of examples with value k**.

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)

Nonparametric methods

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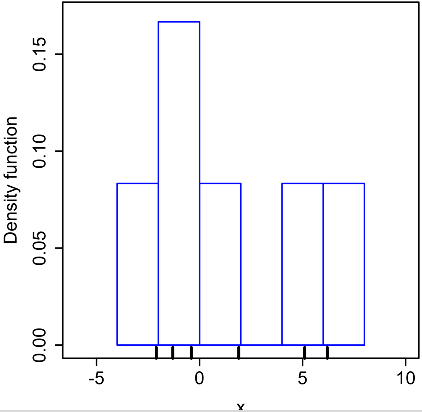
Yes, **kernel density estimation (KDE)** is a common approach

- 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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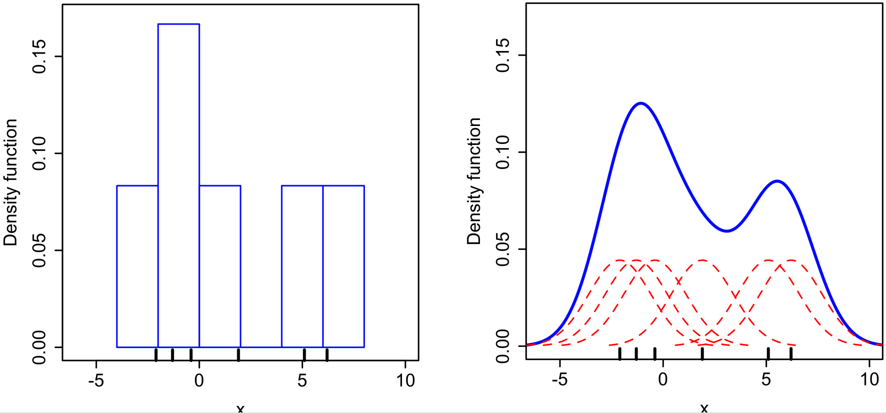
Construct something similar to a **histogram**:

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



High level idea

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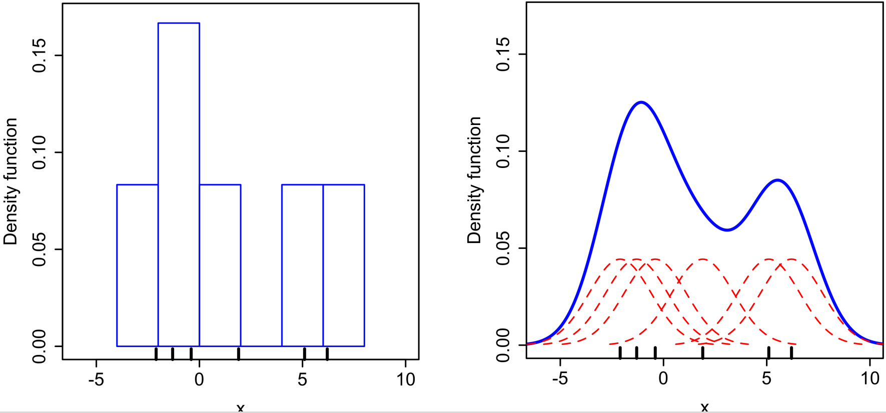
Construct something similar to a **histogram**:

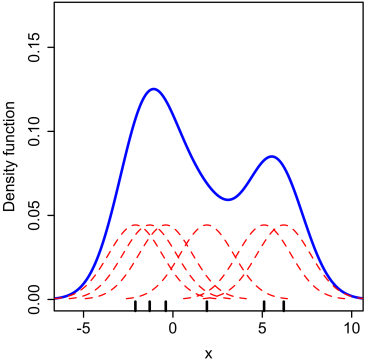
- for each data point, create a "bump" (via a Kernel)
- sum up or average all the bumps



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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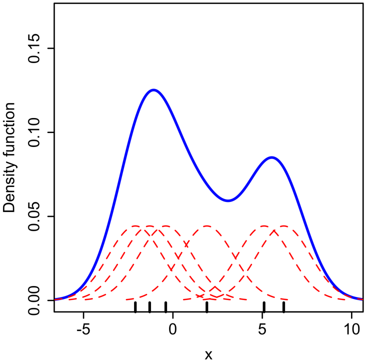

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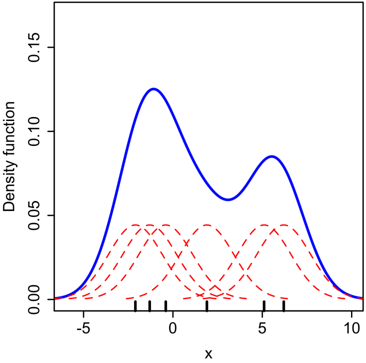

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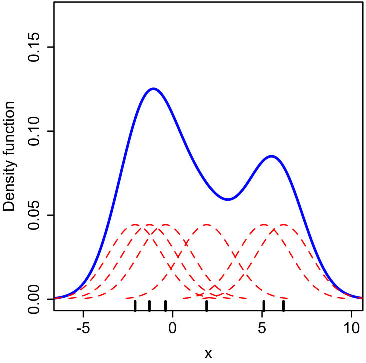
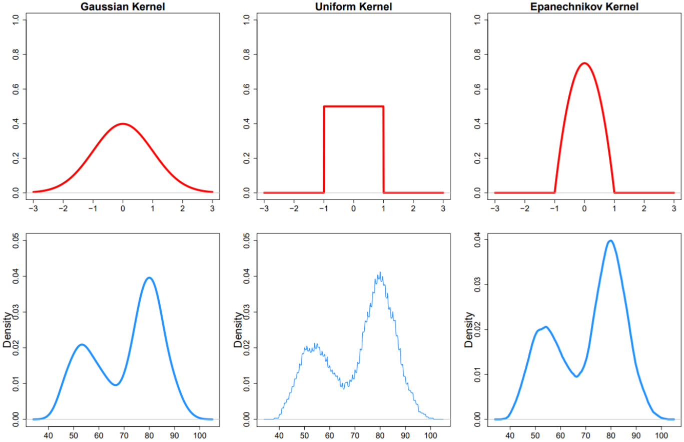
Kernel needs to satisfy:

- symmetry: $K(u) = K(-u)$
- $\int_{-\infty}^{\infty} K(u) du = 1$, 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 $h > 0$

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

can be used as a kernel too (verify the two properties yourself)

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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

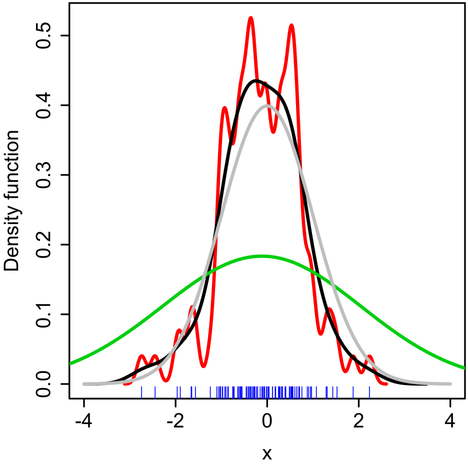
Effect of bandwidth

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: $h = 2$



Bandwidth selection

Selecting h is a deep topic

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- there are theoretically-motivated approaches
- one can also do cross-validation based on downstream applications

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1. Review of last lecture
2. Density estimation
3. Naive Bayes
    - Setup and assumption
    - Estimation and prediction
    - Connection to logistic regression
4. Principal Component Analysis (PCA)

Naive Bayes

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- a simple yet surprisingly powerful **classification** algorithm
- **density estimation** is one important part of the algorithm

Bayes optimal classifier

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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
Age: $\leq$5, 5-10, 10-15, 15-20, 20-25, $\geq$25

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$$p(\text{Height} = \text{5'-6'} \mid \text{Age} = \text{10-15}) \\ = \frac{\#\text{examples with height 5'-6' and age 10-15}}{\#\text{examples with age 10-15}}$$

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

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

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the **prediction** for a new example $\boldsymbol{x}$ is

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

How to predict?

After learning the model

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

the **prediction** for a new example $\boldsymbol{x}$ is

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\end{aligned}$$

Examples

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

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\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)
\end{aligned}
$$

Examples

For **continuous features** with a Gaussian model,

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\end{aligned}$$

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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\end{aligned}$$

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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

1. Review of last lecture
2. Density estimation
3. Naive Bayes
4. Principal Component Analysis (PCA)
    - PCA
    - Kernel PCA

Dimensionality reduction

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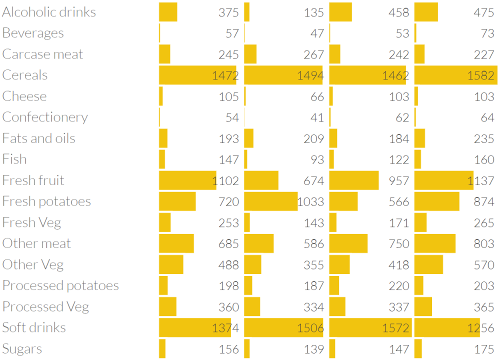
There are many approaches, we focus on a linear method: **Principal Component Analysis (PCA)**

Example

picture from here

Consider the following dataset:

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



Alcoholic drinks	375	135	458	475
Beverages	57	47	53	73
Carcase meat	245	267	242	227
Cereals	1472	1494	1462	1582
Cheese	105	66	103	103
Confectionery	54	41	62	64
Fats and oils	193	209	184	235
Fish	147	93	122	160
Fresh fruit	1102	674	957	1137
Fresh potatoes	720	1033	566	874
Fresh Veg	253	143	171	265
Other meat	685	586	750	803
Other Veg	488	355	418	570
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Processed Veg	360	334	337	365
Soft drinks	1374	1506	1572	1256
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Consider the following dataset:

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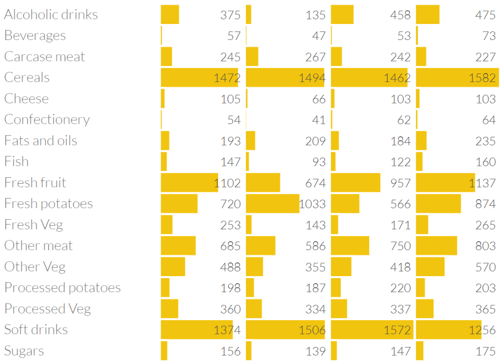

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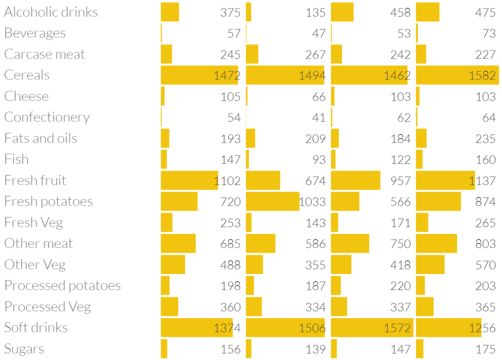

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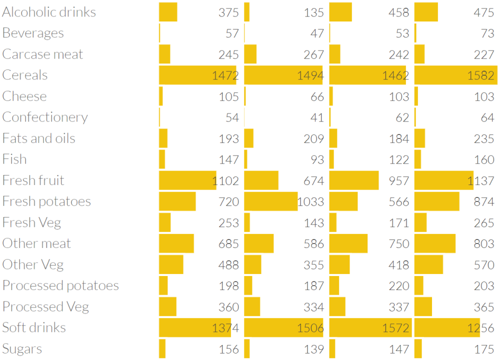

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Hard to say anything looking at all these 17 features.

Example

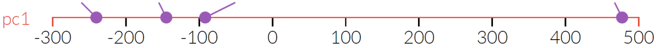
picture from here

PCA can help us!

Example

picture from here

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



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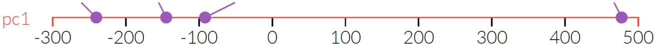

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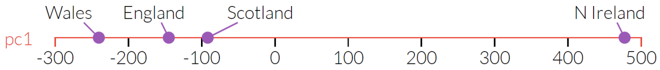

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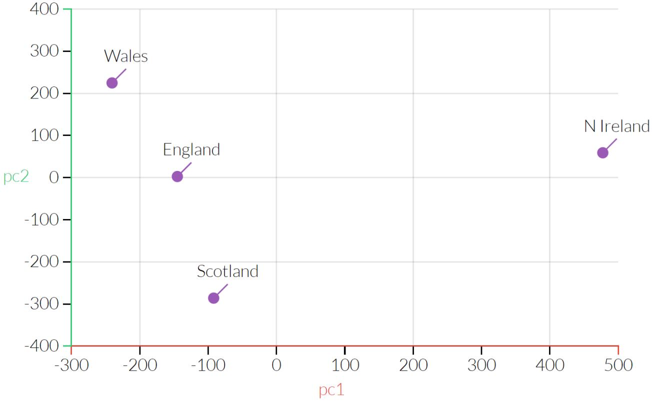
That turns out to be data from Northern Ireland, *the only country not on the island of Great Britain out of the 4 samples.*

Example

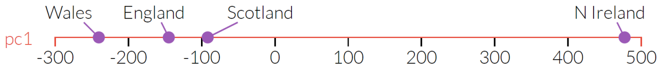
picture from here

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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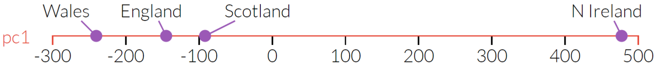

The first PC is in fact **the direction with the most variance**, i.e. the direction where the data is most spread out.

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 $\boldsymbol{X} \in \mathbb{R}^{N \times \mathsf{D}}$ being the data matrix (as in Lec 2), 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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For visualization, also often pick $p = 1$ or $p = 2$.

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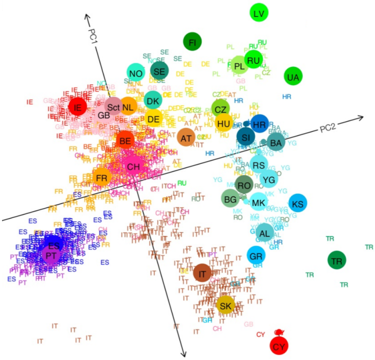

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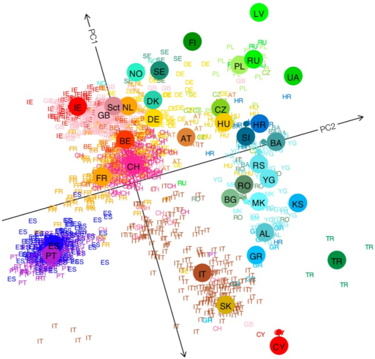

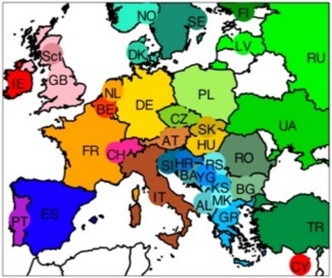

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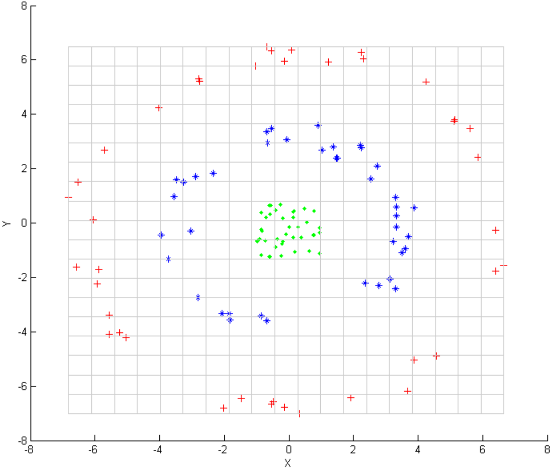
PCA is a **linear method** (recall the new dataset is $\boldsymbol{XV}$), it does not do much when every direction has similar variance.



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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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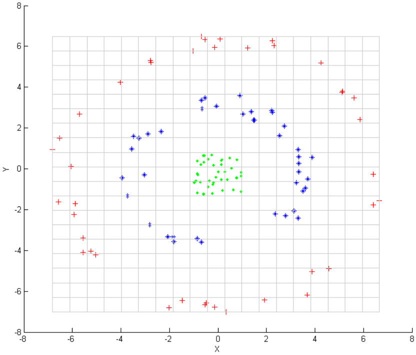
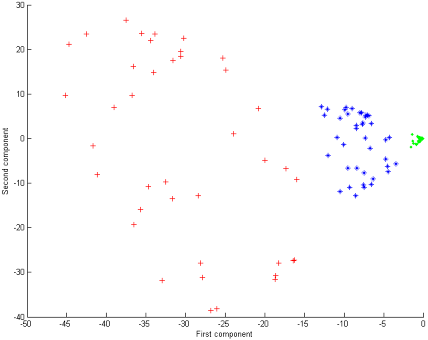
Example

picture from Wikipedia

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





Example

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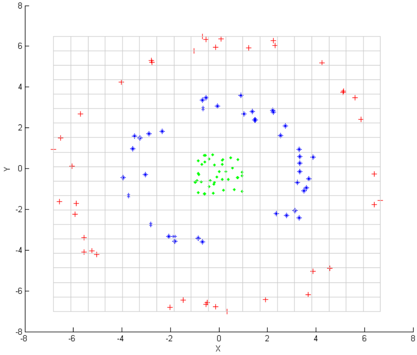
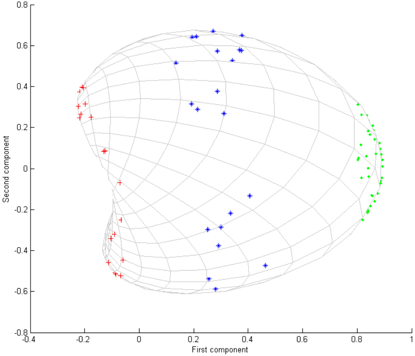
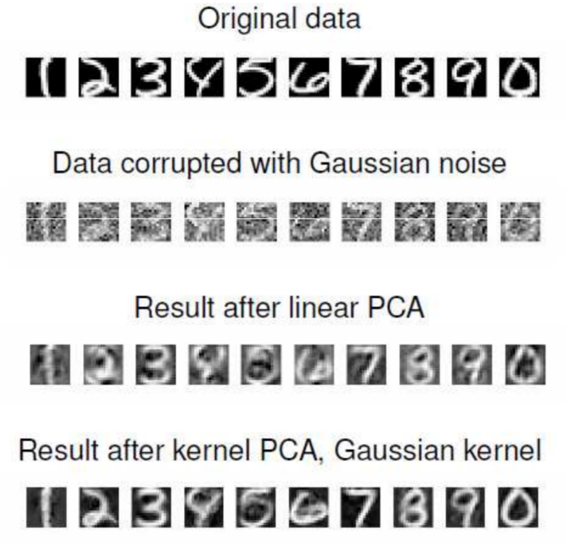
Applying Gaussian kernel $k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(\frac{-\|\boldsymbol{x}-\boldsymbol{x}'\|^2}{2\sigma^2}\right)$:





Denoising via PCA



Original data

Data corrupted with Gaussian noise

Result after linear PCA

Result after kernel PCA, Gaussian kernel