CSCI567 Machine Learning (Fall 2018)

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U of Southern California

Oct 31, 2018

Administration

HW3 solution is available, HW4 is due on Sunday (11/4)

Minor typo in P4 for the formula of multivariate Gaussian density, see Piazza pinned post as well as the updated P4.pdf.

- the comment in gmm.py:

  p = e^(-0.5(x-mean)*(inv(variance))*(x-mean)'/sqrt(c))

  should be

  p = e^(-0.5(x-mean)*(inv(variance))*(x-mean)')/sqrt(c)

Outline

1. Review of last lecture
2. (Hidden) Markov models
3. Principal Component Analysis (PCA)

Outline

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

Applying EM to learn GMMs

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)

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

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

Step 3 return to Step 1 if not converged

Outline

Markov Models

Markov models are powerful probabilistic tools to analyze **sequential data**:

- text or speech data
- stock market data
- gene data
- ...

Definition

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$$P(Z_{t+1} \mid Z_{1:t}) = P(Z_{t+1} \mid Z_t) \qquad \text{(Markov property)}$$

i.e. *the current state only depends on the most recent state* (notation $Z_{1:t}$ denotes the sequence $Z_1, \ldots, Z_t$).

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- $P(Z_1 = s) = \pi_s$
- $(\{\pi_s\}, \{a_{s,s'}\}) = (\boldsymbol{\pi}, \boldsymbol{A})$ are parameters of the model

Examples

- Example 1 (**Language model**)

  States $[S]$ represent a dictionary of words,

  $$a_{\text{ice,cream}} = P(Z_{t+1} = \text{cream} \mid Z_t = \text{ice})$$

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- Example 2 (**Weather**)

  States $[S]$ represent weather at each day

  $$a_{\text{sunny,rainy}} = P(Z_{t+1} = \text{rainy} \mid Z_t = \text{sunny})$$

High-order Markov chain

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Higher order Markov chains make it more reasonable, e.g.

$$P(Z_{t+1} \mid Z_{1:t}) = P(Z_{t+1} \mid Z_t, Z_{t-1}) \qquad \textbf{(second-order Markov)}$$

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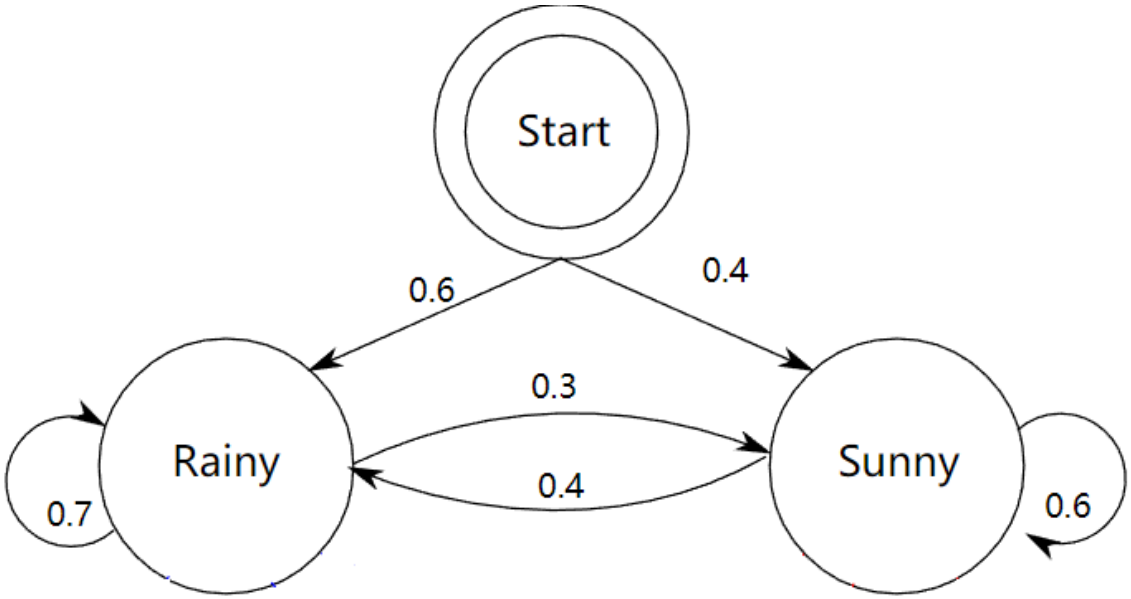
We only consider standard Markov chains.

Graph Representation

picture from Wikipedia

It is intuitive to represent a Markov model as a **graph**



Learning from examples

Now suppose we have observed N **sequences of examples**:

- $z_{1,1}, \ldots, z_{1,T}$
- $\ldots$
- $z_{n,1}, \ldots, z_{n,T}$
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- $z_{N,1}, \ldots, z_{N,T}$

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From these observations how do we *learn the model parameters* $(\boldsymbol{\pi}, \boldsymbol{A})$?

Finding the MLE

Same story, find the **MLE**.

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&= \sum_{s} \mathbb{I}[z_1 = s] \ln \pi_s + \sum_{s,s'} \left(\sum_{t=2}^{T} \mathbb{I}[z_{t-1} = s, z_t = s'] \right) \ln a_{s,s'}
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Finding the MLE

So MLE is

$$\underset{\boldsymbol{\pi}, \boldsymbol{A}}{\operatorname{argmax}} \sum_{s} (\textbf{\#initial states with value } s) \ln \pi_s + \sum_{s,s'} (\textbf{\#transitions from } s \textbf{ to } s') \ln a_{s,s'}$$

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We have seen this many times. The solution is:

$$\pi_s \propto \#\text{initial states with value } s$$
$$a_{s,s'} \propto \#\text{transitions from } s \text{ to } s'$$

Example

Suppose we observed the following 2 sequences of length 5

- sunny, sunny, rainy, rainy, rainy
- rainy, sunny, sunny, sunny, rainy

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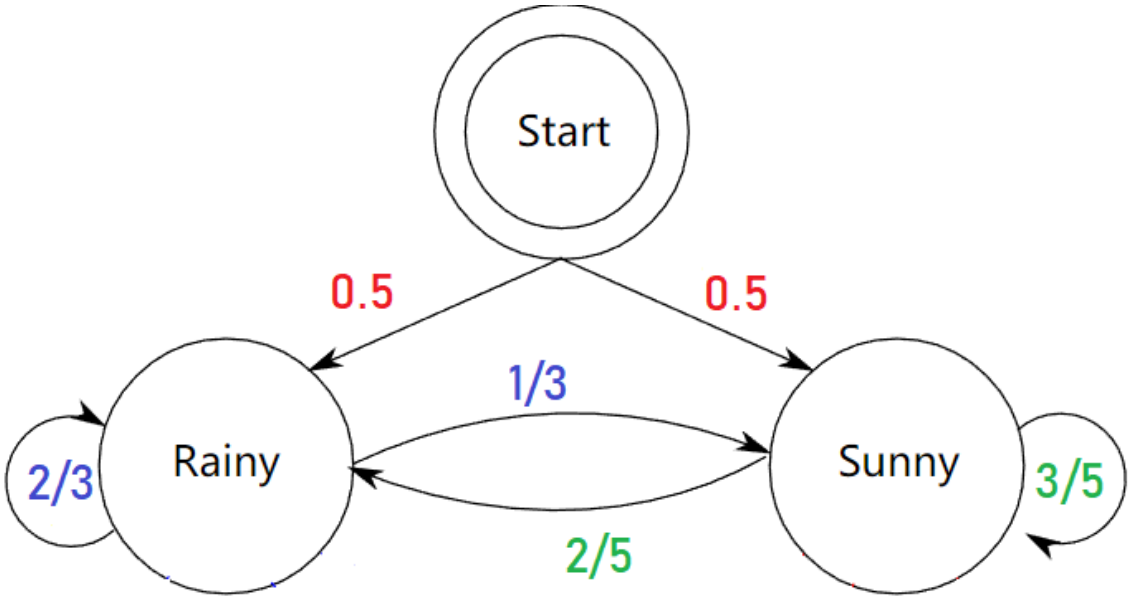
MLE is the following model



Markov Model with outcomes

Now suppose each state Z_t also "emits" some **outcome** $X_t \in [O]$ based on the following model

$$P(X_t = o \mid Z_t = s) = b_{s,o} \qquad \textbf{(emission probability)}$$

independent of anything else.

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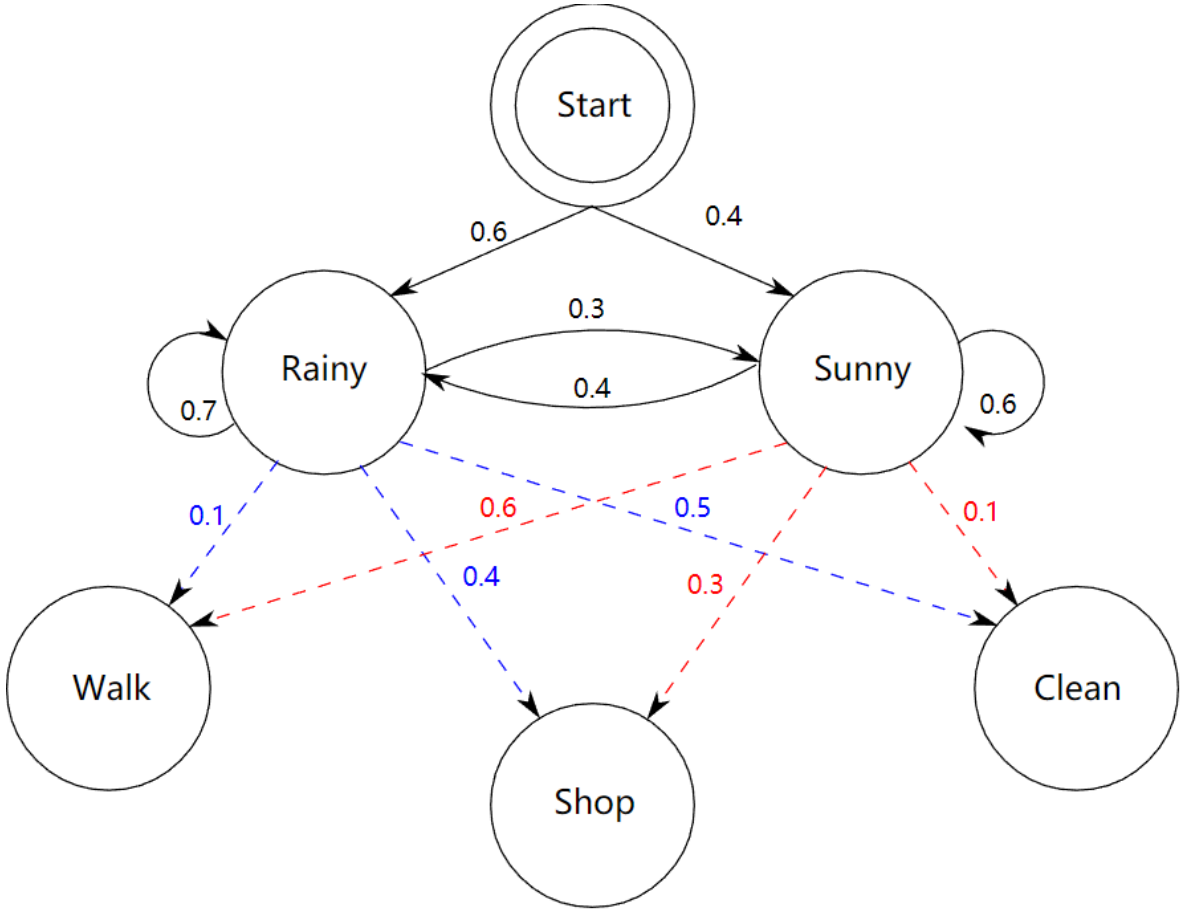
Now the model parameters are $(\{\pi_s\}, \{a_{s,s'}\}, \{b_{s,o}\}) = (\boldsymbol{\pi}, \boldsymbol{A}, \boldsymbol{B})$.

Another example

picture from Wikipedia

On each day, we also observe **Bob's activity: walk, shop, or clean**, which only depends on the weather of that day.



Joint likelihood

The joint log-likelihood of a state-outcome sequence $z_1, x_1, \ldots, z_T, x_T$ is

$$\ln P(Z_{1:T} = z_{1:T}, X_{1:T} = x_{1:T})$$

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&\qquad\qquad \text{(due to all the independence)} \\
&= \ln \pi_{z_1} + \sum_{t=2}^{T} \ln a_{z_{t-1}, z_t} + \sum_{t=1}^{T} \ln b_{z_t, x_t}
\end{aligned}$$

Learning the model

If we observe N state-outcome sequences: $z_{n,1}, x_{n,1}, \ldots, z_{n,T}, x_{n,T}$ for $n = 1, \ldots, N$, the MLE is again very simple (verify yourself):

$$\pi_s \propto \textbf{\#initial states with value } s$$
$$a_{s,s'} \propto \textbf{\#transitions from } s \textbf{ to } s'$$
$$b_{s,o} \propto \textbf{\#state-outcome pairs } (s, o)$$

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How to learn HMMs? **Roadmap**:

- first discuss how to **infer** when the model is known (key: dynamic programming)

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How to learn HMMs? **Roadmap**:

- first discuss how to **infer** when the model is known (key: dynamic programming)
- then discuss how to **learn** the model (key: EM)

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- **the probability of observing some sequence**

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- **the state at some point, given an observation sequence**

$$P(Z_t = s \mid X_{1:T} = x_{1:T})$$

  e.g. given Bob's activities for one week, how was the weather like on Wed?

What can we infer for a known HMM?

Knowing the parameter of an HMM, we can infer

- **the transition at some point, given an observation sequence**

$$P(Z_t = s, Z_{t+1} = s' \mid X_{1:T} = x_{1:T})$$

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- **most likely hidden states path, given an observation sequence**

$$\operatorname*{argmax}_{z_{1:T}} P(Z_{1:T} = z_{1:T} \mid X_{1:T} = x_{1:T})$$

e.g. given Bob's activities for one week, what's the most likely weather for this week?

Forward and backward messages

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$$\alpha_s(t) = P(Z_t = s, X_{1:t} = x_{1:t})$$

- **backward messages**: for each s and t

$$\beta_s(t) = P(X_{t+1:T} = x_{t+1:T} \mid Z_t = s)$$

Computing forward messages

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&= b_{s,x_t} \sum_{s'} a_{s',s} \alpha_{s'}(t-1) && \text{(recursive form!)}
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Base case: $\alpha_s(1) = P(Z_1 = s, X_1 = x_1) = \pi_s b_{s,x_1}$

Forward procedure

Forward procedure

For all $s \in [S]$, compute $\alpha_s(1) = \pi_s b_{s,x_1}$.

For $t = 2, \ldots, T$

- for each $s \in [S]$, compute

$$\alpha_s(t) = b_{s,x_t} \sum_{s'} a_{s',s} \alpha_{s'}(t-1)$$

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For all $s \in [S]$, compute $\alpha_s(1) = \pi_s b_{s,x_1}$.

For $t = 2, \ldots, T$

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$$\alpha_s(t) = b_{s,x_t} \sum_{s'} a_{s',s} \alpha_{s'}(t-1)$$

It takes $O(S^2T)$ time and $O(ST)$ space.

Computing backward messages

Again establish a recursive formula

$$\begin{aligned}&\beta_s(t)\\&= P(X_{t+1:T} = x_{t+1:T} \mid Z_t = s)\end{aligned}$$

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For $t = T-1, \ldots, 1$

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Again it takes $O(S^2T)$ time and $O(ST)$ space.

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This is true for any t; a good way to check correctness of your code.

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Another example: the conditional probability of transition s to s' at time t

$$\xi_{s,s'}(t) = P(Z_t = s, Z_{t+1} = s' \mid X_{1:T} = x_{1:T})$$

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The normalization constant is in fact again $P(X_{1:T} = x_{1:T})$

Finding the most likely path

Though can't use forward and backward messages directly to find the most likely path, it is very similar to the forward procedure.

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Though can't use forward and backward messages directly to find the most likely path, it is very similar to the forward procedure. Key: compute

$$\delta_s(t) = \max_{z_{1:t-1}} P(Z_t = s, Z_{1:t-1} = z_{1:t-1}, X_{1:t} = x_{1:t})$$

the probability of the most likely path for time $1:t$ ending at state s

Computing $\delta_s(t)$

Observe

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Exactly the same as forward messages except replacing "sum" by "max"!

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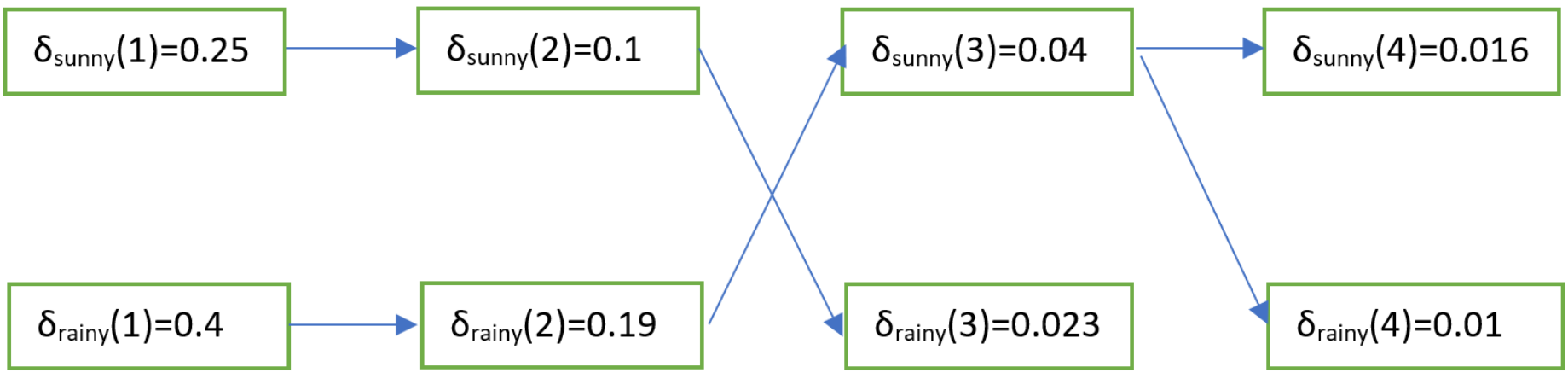
Output the most likely path $z_1^*, \ldots, z_T^*$.

Example

Arrows represent the "argmax", i.e. $\Delta_s(t)$.



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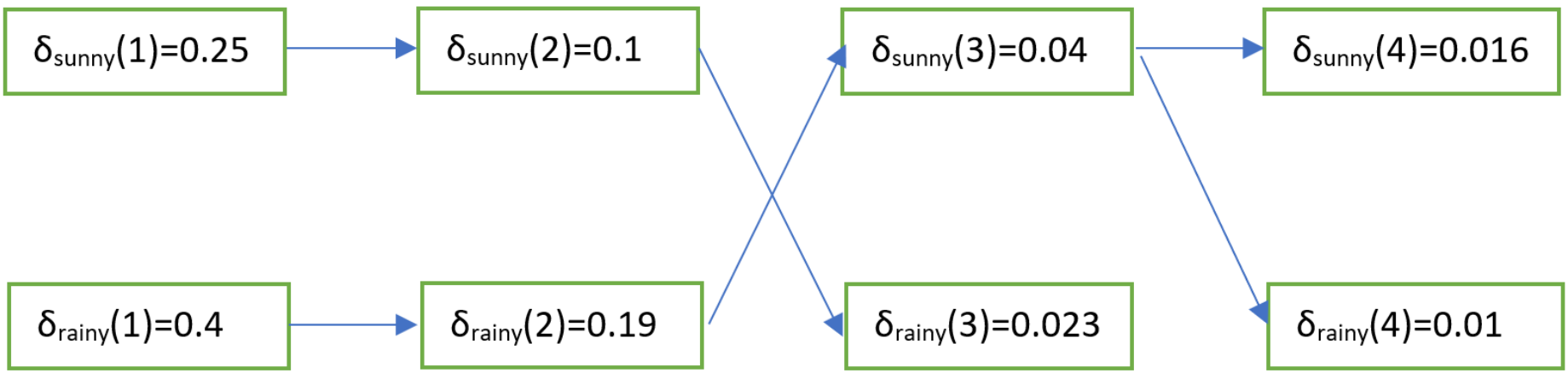

The most likely path is **"rainy, rainy, sunny, sunny".**

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All previous inferences depend on knowing the parameters $(\boldsymbol{\pi}, \boldsymbol{A}, \boldsymbol{B})$.

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Need to apply **EM** again! Known as the **Baum–Welch algorithm**.

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$$\begin{aligned}
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&= \mathbb{E}_{z_{1:T}\sim q}\left[\ln \pi_{z_1} + \sum_{t=1}^{T-1} \ln a_{z_t,z_{t+1}} + \sum_{t=1}^{T} \ln b_{z_t,x_t}\right] \\
&= \sum_s \gamma_s(1) \ln \pi_s + \sum_{t=1}^{T-1}\sum_{s,s'} \xi_{s,s'}(t) \ln a_{s,s'} + \sum_{t=1}^{T}\sum_s \gamma_s(t) \ln b_{s,x_t}
\end{aligned}$$

We have discussed how to compute

$$\begin{aligned}
\gamma_s(t) &= P(Z_t = s \mid X_{1:T} = x_{1:T}) \\
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Applying EM: M-Step

The maximizer of complete log-likelihood is simply doing **weighted counting** (compared to the unweighted counting on Slide 20):

$$\pi_s \propto \sum_n \gamma_s^{(n)}(1) = \mathbb{E}_q \left[\textbf{\#initial states with value } s \right]$$

$$a_{s,s'} \propto \sum_n \sum_{t=1}^{T-1} \xi_{s,s'}^{(n)}(t) = \mathbb{E}_q \left[\textbf{\#transitions from } s \textbf{ to } s' \right]$$

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Step 3 Return to Step 1 if not converged

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Several algorithms:

- forward and backward procedures
- inferring HMMs based on forward and backward messages
- Viterbi algorithm
- Baum–Welch algorithm

Outline

Dimensionality reduction

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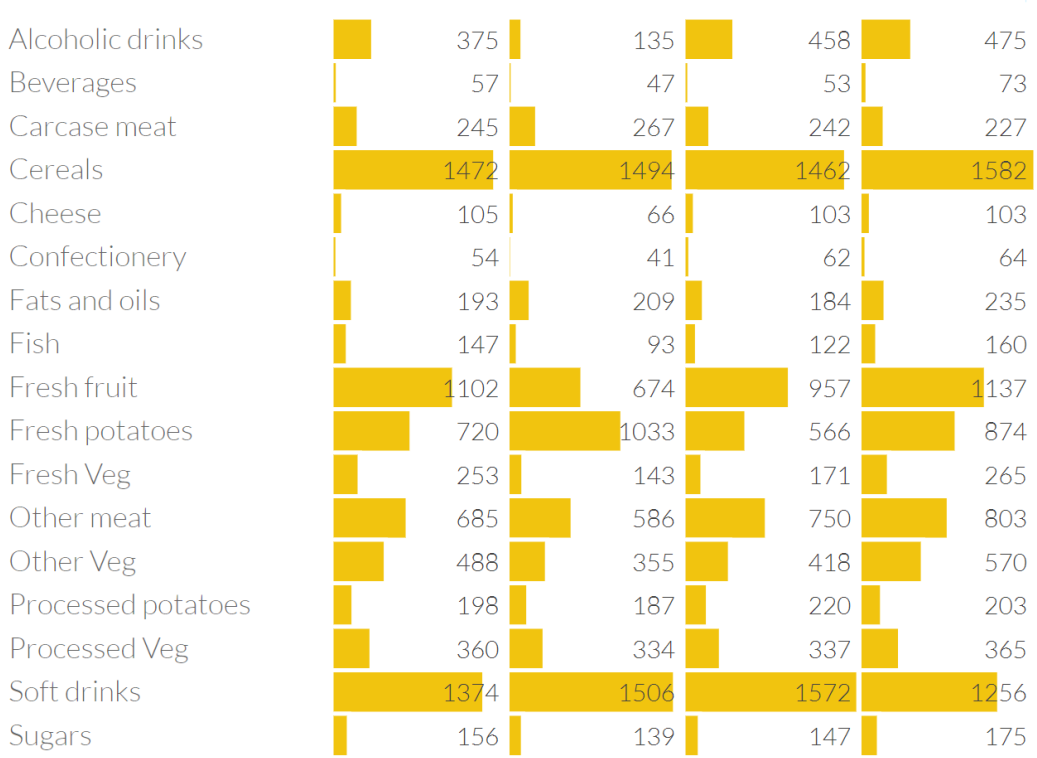
There are many approaches, we focus on a linear method:
Principal Component Analysis (PCA)

Example

picture from here

Consider the following dataset:

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



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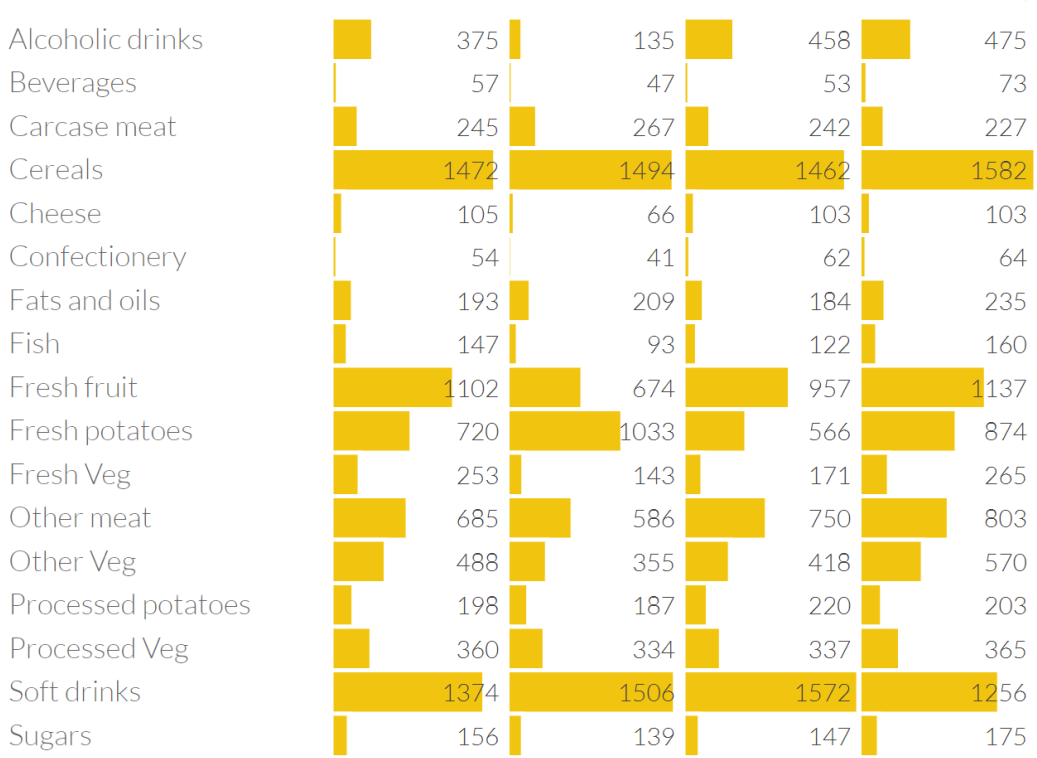

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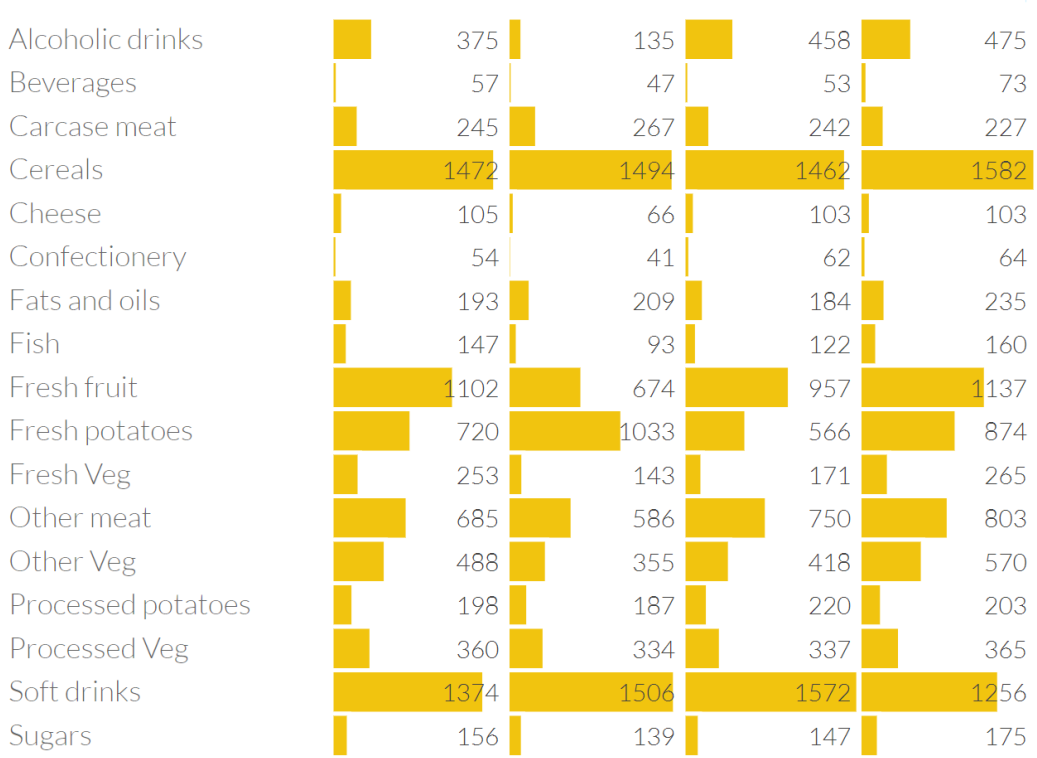

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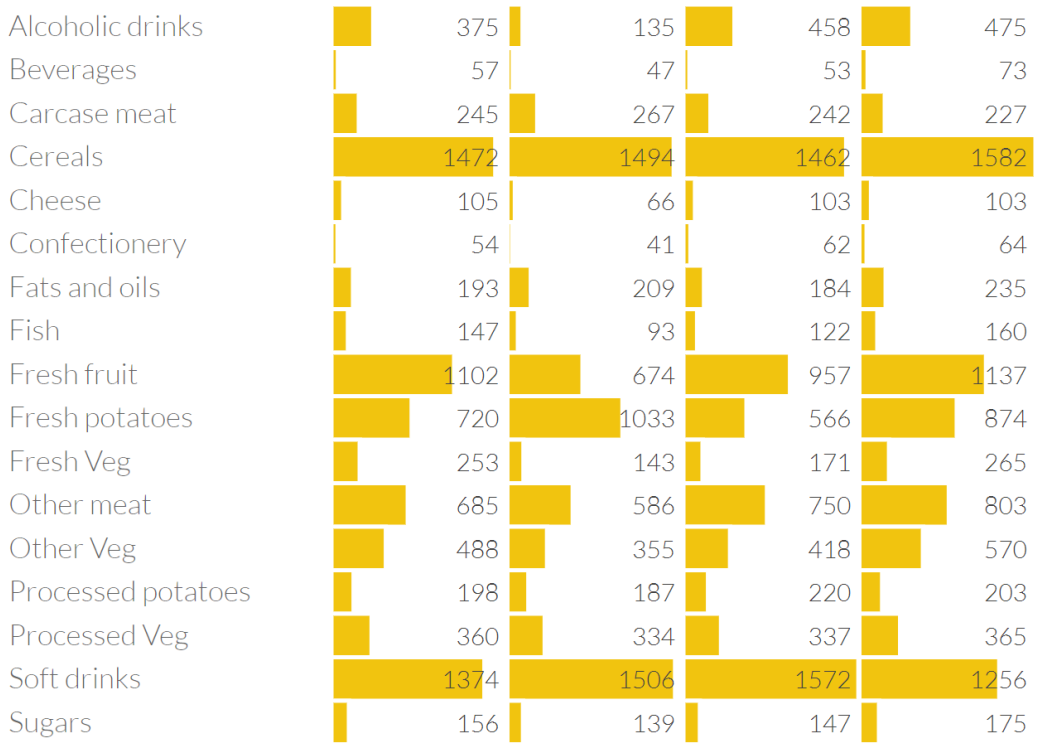

What can you tell?

Hard to say anything looking at all these 17 features.

Example

picture from here

PCA can help us!

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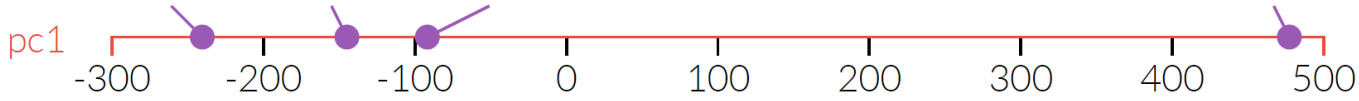
picture from here

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



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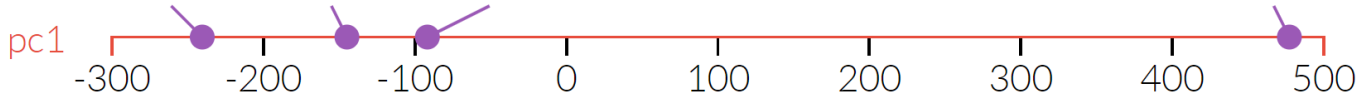

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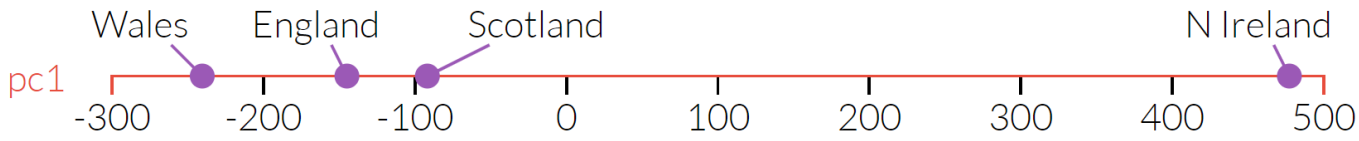

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That turns out to be data from Northern Ireland, *the only country not on the island of Great Britain out of the 4 samples.*

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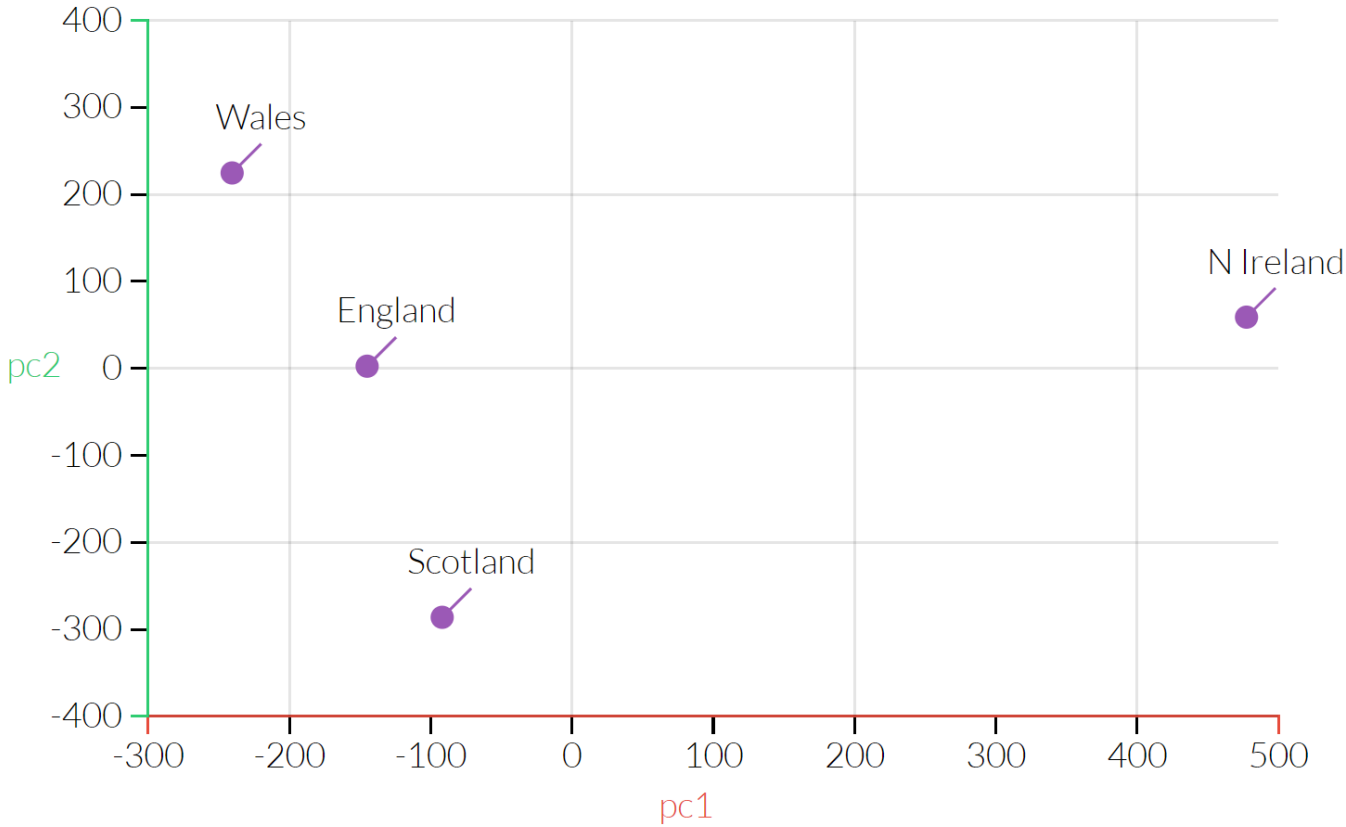
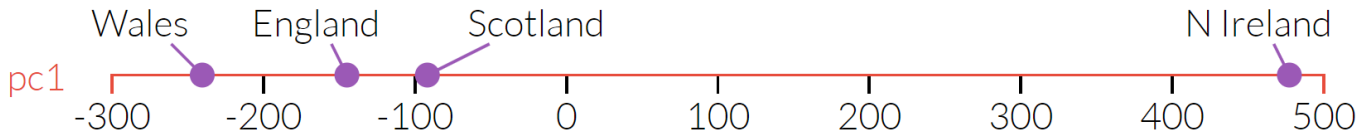
picture from here

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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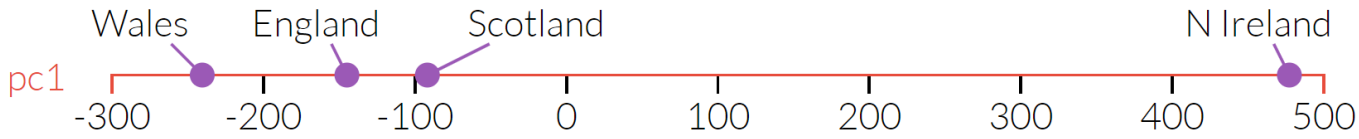

This is in fact **the direction with the most variance**, i.e. the direction where the data is most spread out.

Finding the first PC

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

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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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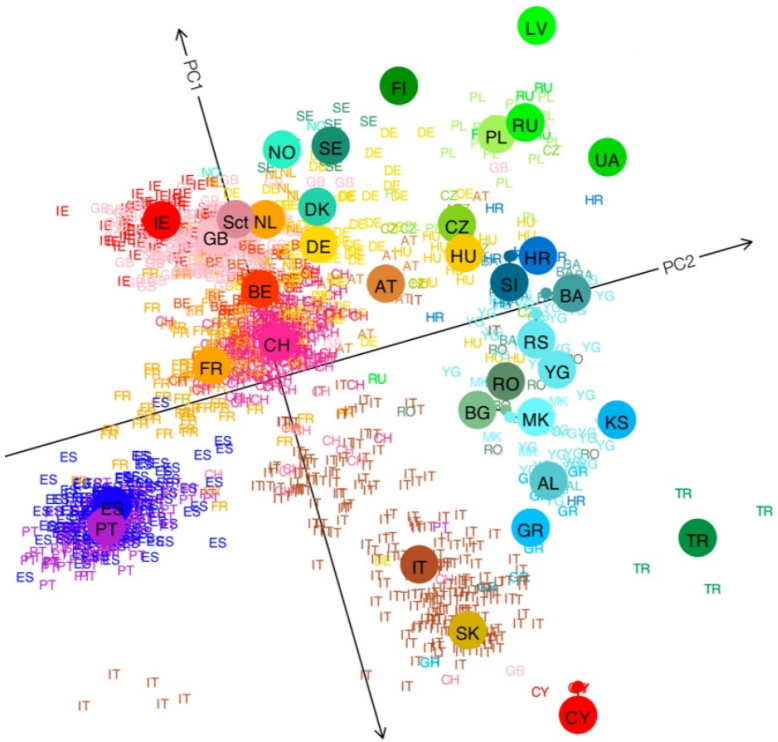

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- dataset: genomes of 1,387 Europeans
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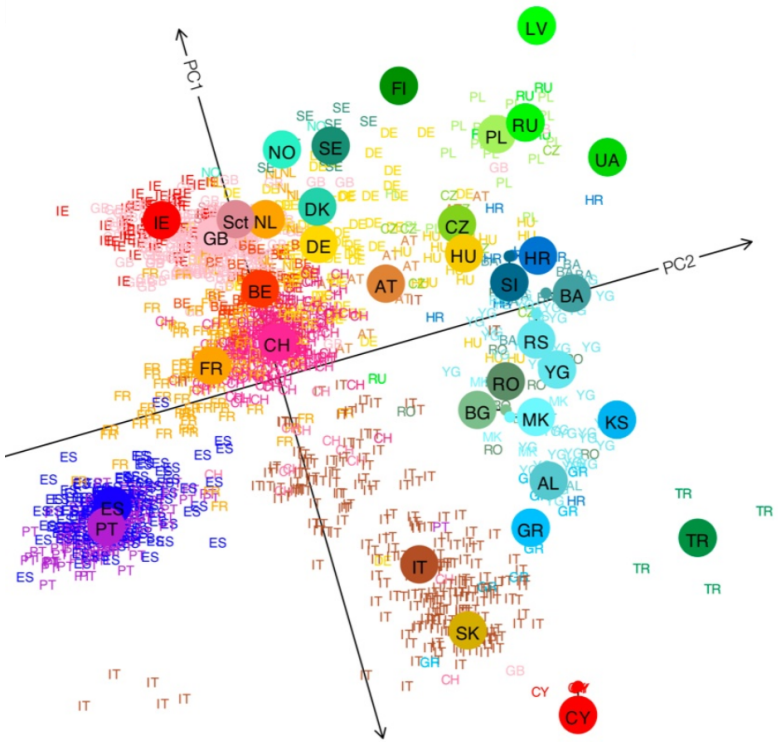

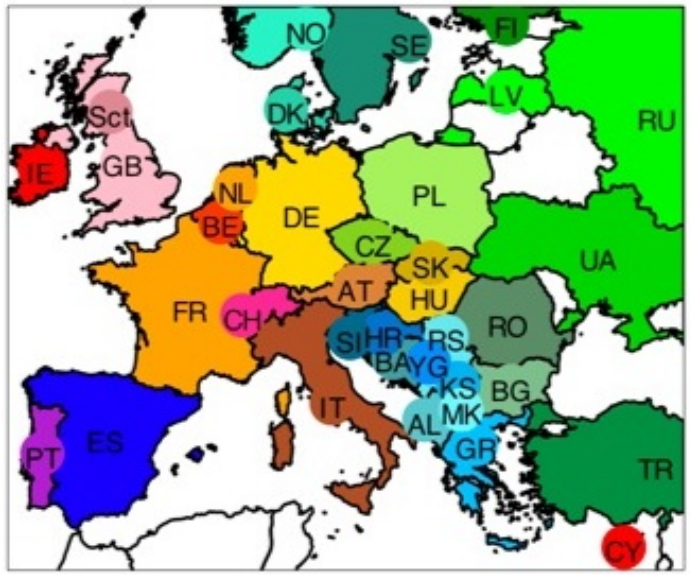

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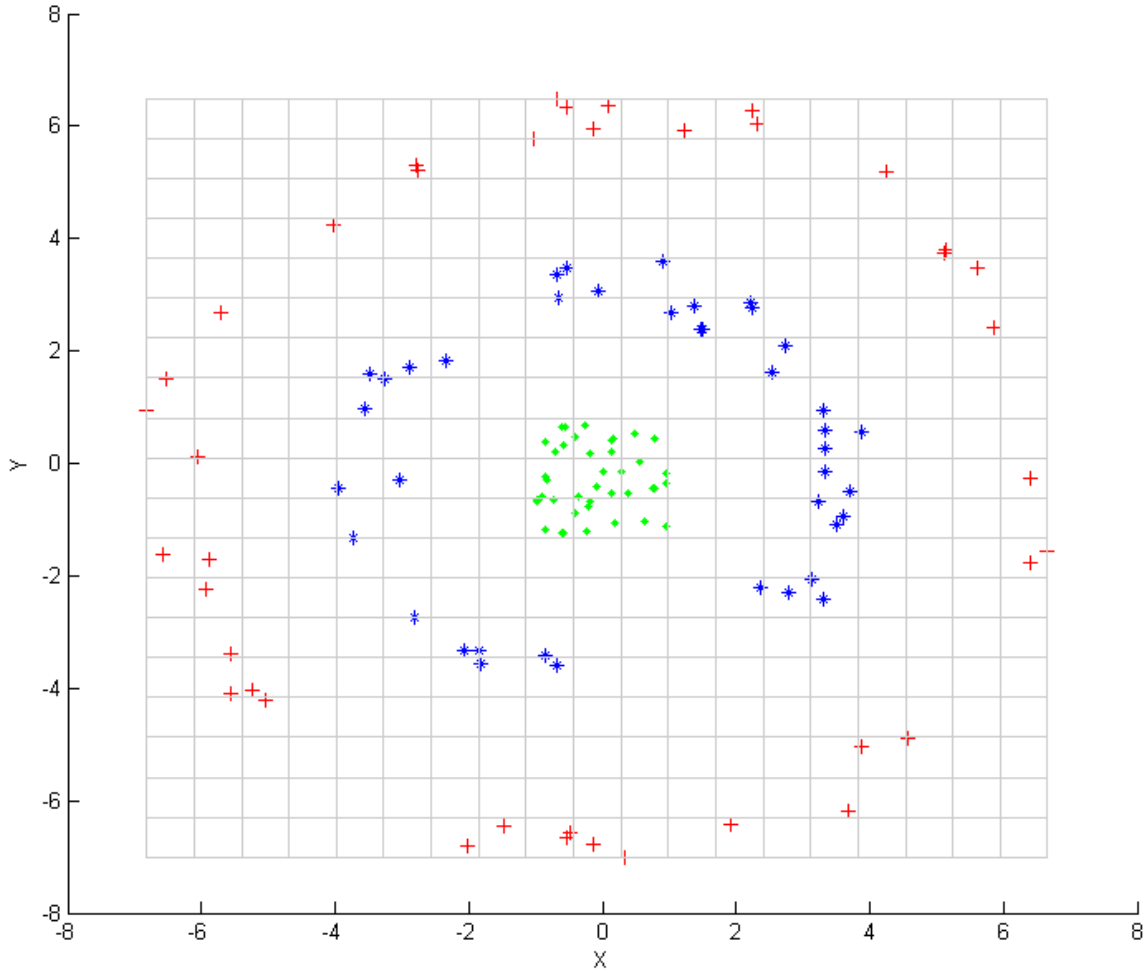
picture from Wikipedia

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 $\mathbb{R}^{M}$?

KPCA: finding the PCs

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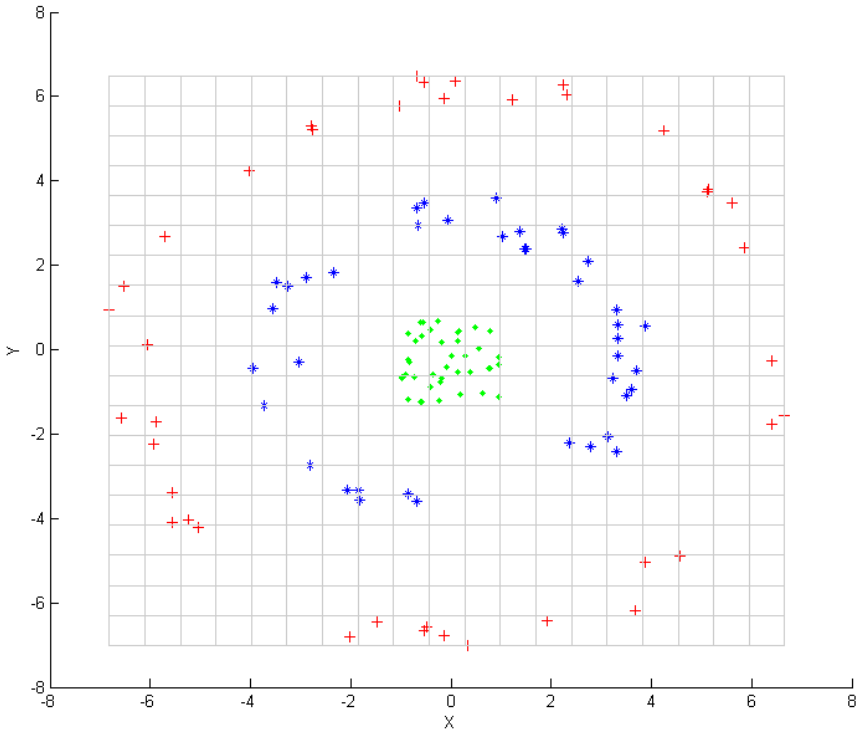
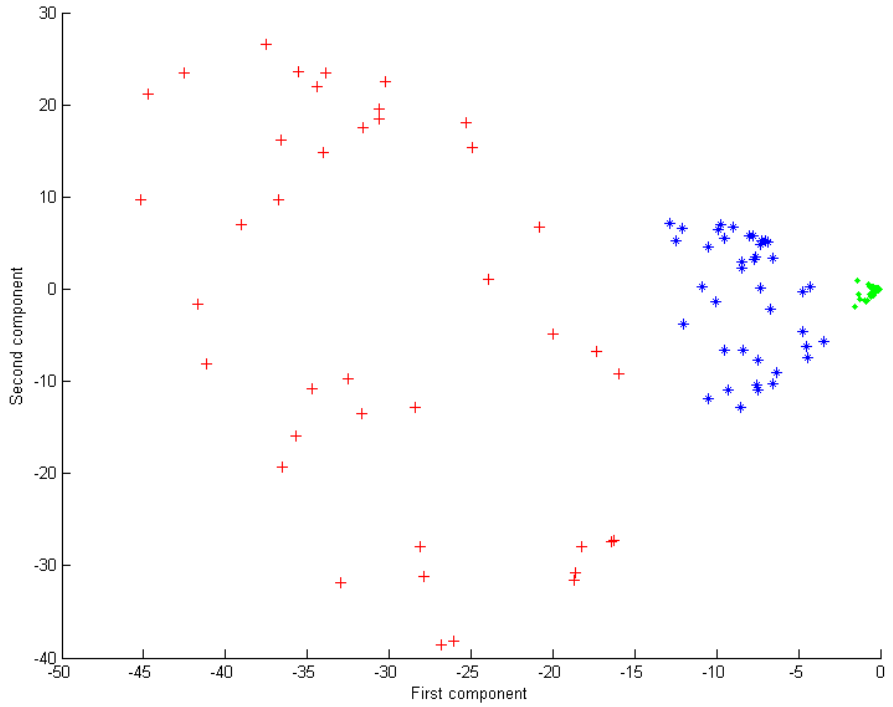
Step 3 Construct the new dataset $(\boldsymbol{\Phi} - \boldsymbol{E}\boldsymbol{\Phi})(\boldsymbol{\Phi} - \boldsymbol{E}\boldsymbol{\Phi})^{\mathrm{T}}\boldsymbol{A} = \bar{\boldsymbol{K}}\boldsymbol{A}$

Example

picture from Wikipedia

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





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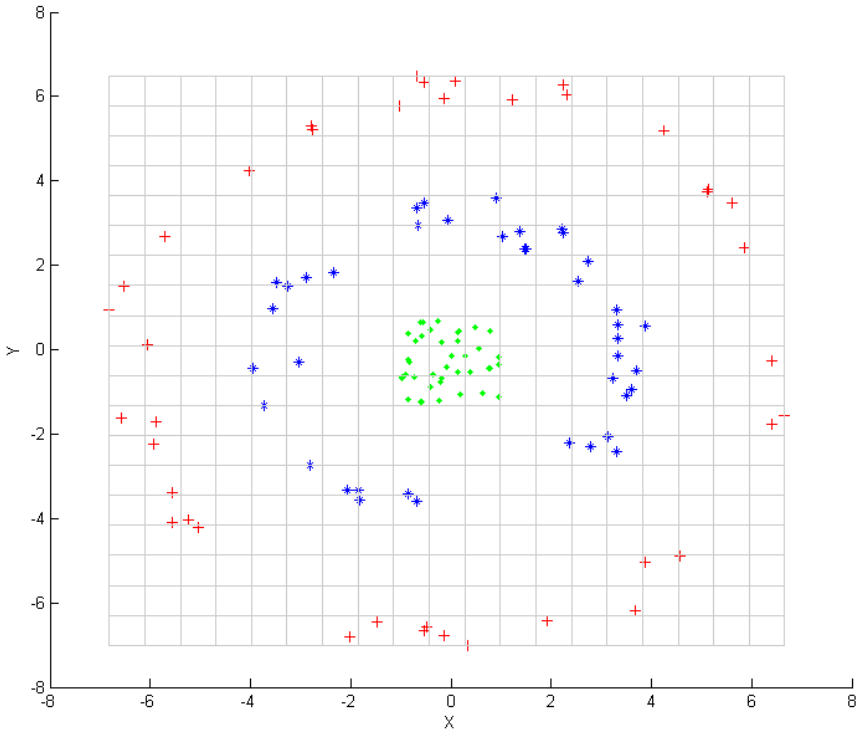
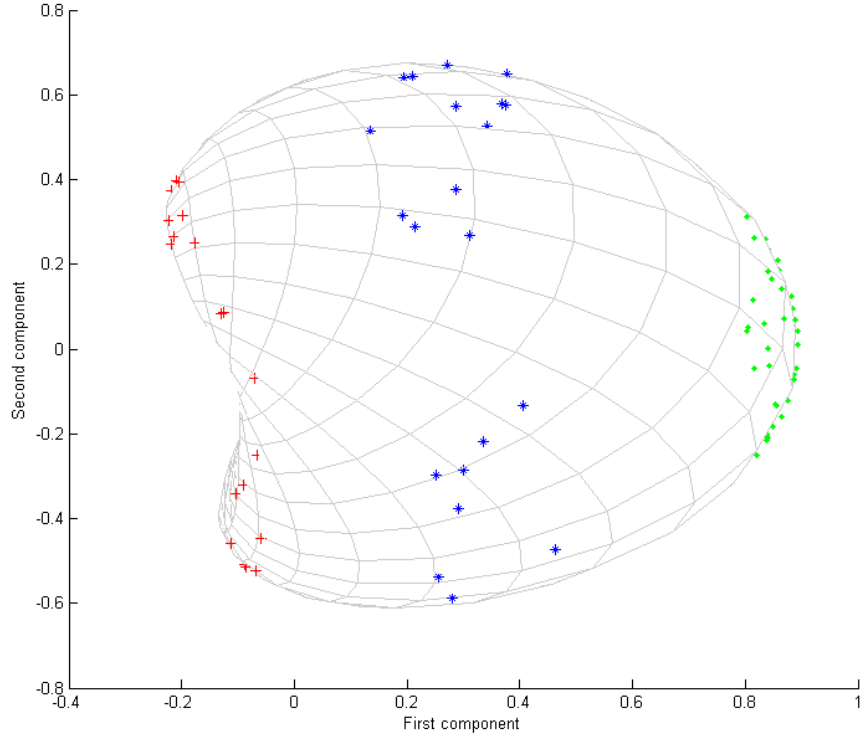
Applying Gaussian kernel $k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(\frac{-\|\boldsymbol{x}-\boldsymbol{x}'\|^2}{2\sigma^2}\right)$:





Denoising via PCA

Original data

Data corrupted with Gaussian noise

Result after linear PCA

Result after kernel PCA, Gaussian kernel