Lecture 14: Feature extraction

Introduction to Machine Learning

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L3 MIASHS — Semestre 2

2022-2023

Motivation

Question

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- While keeping as much information as possible

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- **Linear transformations**: PCA, ...
- **Non-linear transformations**: t-distributed stochastic neighbourhood embedding (**t-SNE**), Uniform Manifold Approximation and Projection (**UMAP**) ...

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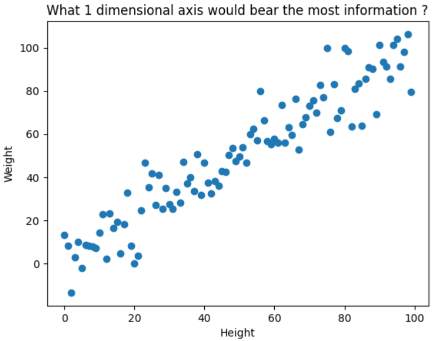
The goal of PCA is to:

- Find new axis more relevant to represent the data
- Give us the importance of each axis
- Remove unimportant axis and reduce dimension

Principle

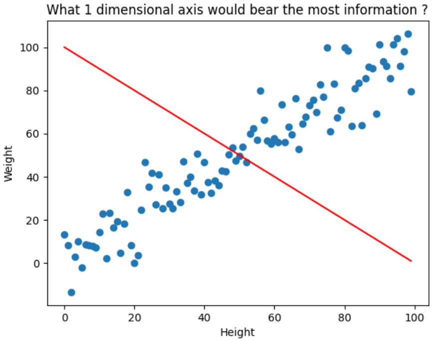


Question

What would be an adequate axis to project the data on to reduce to a single axis ?

Principle

Possibility: $y = -x$



Question

What would a projection on this new axis look like ?

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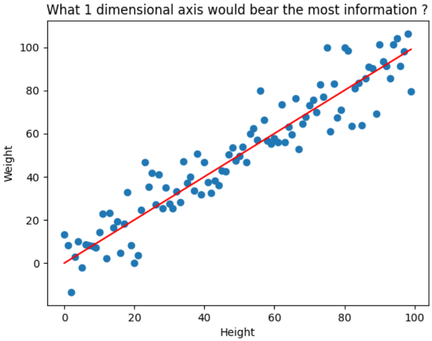

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- Covariance matrix (**Centered PCA**)
- Correlation matrix (**Normed PCA**)

Example dataset

The **Iris dataset** D:

sepal length (cm)	sepal width (cm)	petal length (cm)
5.1	3.5	1.4
4.9	3.0	1.4
4.7	3.2	1.3
4.6	3.1	1.5
5.0	3.6	1.4
5.4	3.9	1.7
4.6	3.4	1.4
5.0	3.4	1.5
4.4	2.9	1.4
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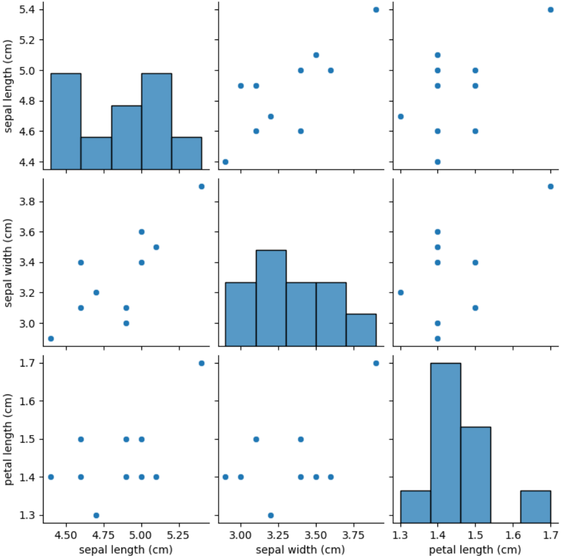
Example dataset



Standardize matrix

For **centered PCA**, center matrix.
For **normed PCA**, standardize matrix (remove mean and divide by standard error): Z.

Compute the correlation matrix

Compute correlation matrix C.

With Z the standardized matrix and n the number of individuals within the dataset,
$C = \frac{1}{n} Z^t Z$

	Sepal length	width	Petal length
Sepal length	1.00	0.79	0.60
width	0.79	1.00	0.52
Petal length	0.60	0.52	1.00

Find eigenvalues and eigenvectors

Eigen values (sorted) of the correlation matrix are: $[2.27, 0.51, 0.20]$

Eigen vectors matrix P (sorted by eigen values) is:

Feature	Component 0	Component 1	Component 2
S. length	0.61	-0.26	0.75
Width	0.59	-0.48	-0.65
P. length	0.53	0.84	-0.14

Project matrix into new space

Multiply the standardized matrix Z by the eigenvectors to have the matrix Z^* in the new projected space $Z^* = ZP$: **this is the projection of the individuals in the new feature space**.

ID	Component 0	Component 1	Component 2
0	0.66	-0.95	0.30
1	-0.80	0.07	0.87
2	-1.35	-0.90	0.02
3	-0.74	1.00	-0.31
4	0.64	-1.02	-0.20
5	3.68	0.57	-0.20
6	-0.65	-0.31	-0.83
7	0.75	0.13	0.11
8	-2.11	0.70	-0.26
9	-0.08	0.72	0.51

Select number of axis

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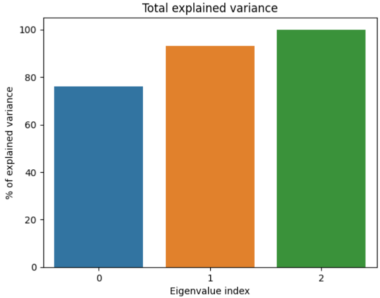
Usually, compute the cumulated sum of $\frac{\lambda_i}{\sum_{i=0}^{n} \lambda_i}$ for the i-th eigenvalue λ_i: the selected value is the **total explained variance of the dataset**.

Select number of axis

Here the cumulated sum is: $[0.76, 0.93, 1]$



We select **two axis**.

Final projection

We have our final projection for each individual within the reduced space:

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0	0.66	-0.95
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Interpret results

A possible interpretation is the plot of the **correlation circle**.

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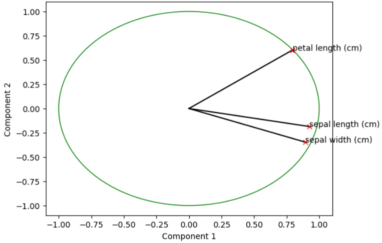
Correlation circle

The correlation circle consists in computing **the correlation of the original features with the new components** and deducing from it the contribution of each variable to the axis.



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- Simple to evaluate data loss because of transformation

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- Features are transformed and lose interpretability of some results
- Sensitive to outliers

t-distributed Stochastic Neighbor Embedding

t-SNE

t-distributed Stochastic neighbor embedding (t-SNE) is a nonlinear feature reduction method that consists in associating for each pair of individual **the probability of being close** to each other in the new space by relying on a probability distribution in the original space.

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Given a matrix X with k individuals and n features, find a matrix Q with k individuals and d features, with $d << n$

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The divergence between these probability distributions **needs to minimized**.

Kullback-Leibler divergence

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The **Kullback-Leibler divergence** is a statistical similarity that measures how one probability distribution P is different from a distribution Q.

$$D_{KL}(P||Q) = \sum_{x \in \mathcal{X}} P(x) log(\frac{P(x)}{Q(x})$$

In the case of t-SNE we want to minimize:

$$KL(P||Q) = \sum_{i \neq j} p_{ij} log(\frac{p_{ij}}{q_{ij}})$$

Probability distribution

We define the conditional probability of j being the neighbor of i as a Gaussian around x_i (σ_i measures the density around x_i and should be estimated):

$$p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2/2\sigma_i^2)}$$

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and set:

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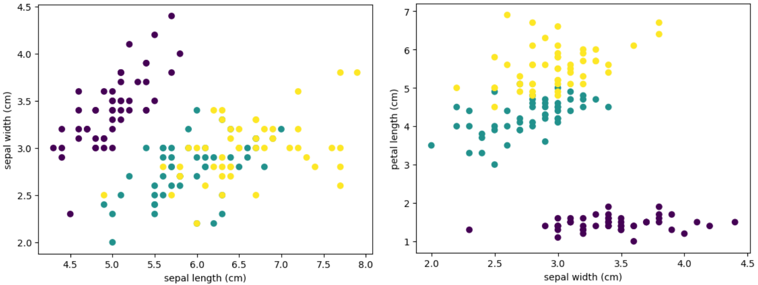
and use gradient descent to **minimize the KL divergence**.

Example: Iris dataset

Data repartition without any transformation:



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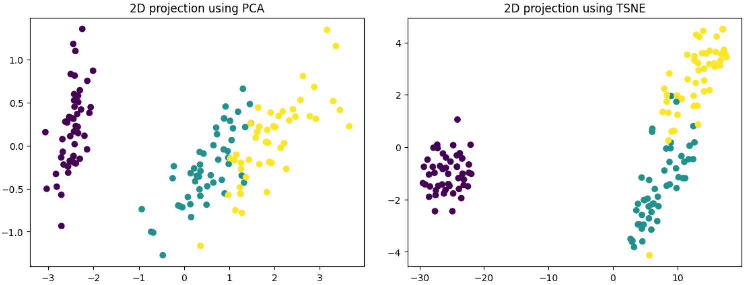
Projection in 2-D using t-SNE and PCA:



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