Lecture 14: Feature extraction
Introduction to Machine Learning

Sophie Robert

L3 MIASHS — Semestre 2

2023-2024

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis

Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

Introduction

Question

Do you remember what is the definition of feature extraction/projection ?

Motivation

Question

Do you remember what is the definition of feature extraction/projection ?

- Find a lower dimensional space to project the data in

Motivation

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

Question

Do you remember what is the definition of feature extraction/projection ?

- Find a lower dimensional space to project the data in
- While keeping as much information as possible

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

Motivation

Many methods exist in the literature:

Motivation

Many methods exist in the literature:

- **Linear transformations**: PCA, . . .

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

Motivation

Many methods exist in the literature:

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

Principal Component Analysis

Principal Component Analysis

Principal Component Analysis

Principal Component analysis is a feature projection method that consists in finding a **new coordinate system as a linear combination of the input features** to project the data: this system is orthogonal and a linear combination of the features that **maximizes the variance**.

Principal Component Analysis

Principal Component Analysis

Principal Component analysis is a feature projection method that consists in finding a **new coordinate system as a linear combination of the input features** to project the data: this system is orthogonal and a linear combination of the features that **maximizes the variance**.

The goal of PCA is to:

Principal Component Analysis

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis

Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

Principal Component Analysis

Principal Component analysis is a feature projection method that consists in finding a **new coordinate system as a linear combination of the input features** to project the data: this system is orthogonal and a linear combination of the features that **maximizes the variance**.

The goal of PCA is to:

- Find new axis more relevant to represent the data

Principal Component Analysis

Principal Component Analysis

Principal Component analysis is a feature projection method that consists in finding a **new coordinate system as a linear combination of the input features** to project the data: this system is orthogonal and a linear combination of the features that **maximizes the variance**.

The goal of PCA is to:

- Find new axis more relevant to represent the data
- Give us the importance of each axis

Principal Component Analysis

Principal Component Analysis

Principal Component analysis is a feature projection method that consists in finding a **new coordinate system as a linear combination of the input features** to project the data: this system is orthogonal and a linear combination of the features that **maximizes the variance**.

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

Lecture 14:
Feature
extraction

Sophie Robert

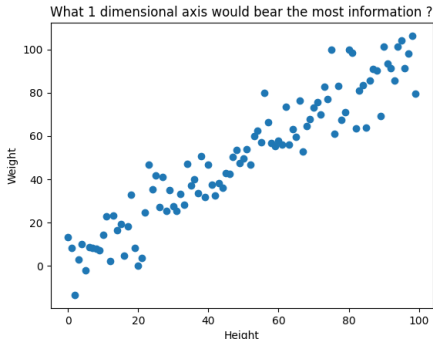Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

What 1 dimensional axis would bear the most information ?

Question

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

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis

Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

Principle

Possibility: $y = -x$

What 1 dimensional axis would bear the most information ?

Question

What would a projection on this new axis look like ?

Principle

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

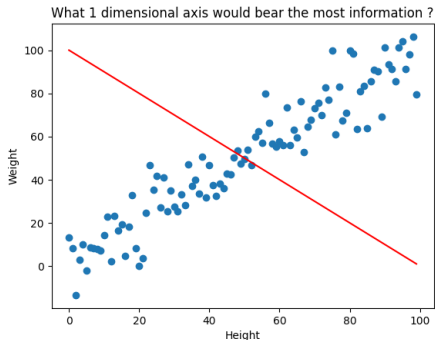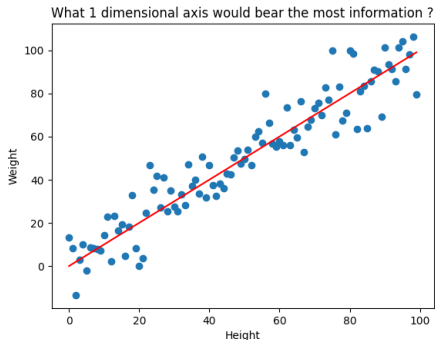t-SNE
Principle
Example
Advantages and
drawbacks

Possibility: $y = x$

Question

What would a projection on this new axis look like ?

Principle

We are looking for new axis that **maximize the variance** and are **uncorrelated**.

Principle

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

We are looking for new axis that **maximize the variance** and are **uncorrelated**.

It can be shown that these **principal components** are eigenvectors of the data's:

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis

Principle

Algorithm

Advantages and
drawbacks

t-SNE

Principle

Example

Advantages and
drawbacks

Principle

We are looking for new axis that **maximize the variance** and are **uncorrelated**.

It can be shown that these **principal components** are eigenvectors of the data's:

- Covariance matrix (**Centered PCA**)

We are looking for new axis that **maximize the variance** and are **uncorrelated**.

It can be shown that these **principal components** are eigenvectors of the data's:

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

Example dataset

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis

Principle

Algorithm

Advantages and
drawbacks

t-SNE

Principle

Example

Advantages and
drawbacks

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
4.9	3.1	1.5

Example dataset

Lecture 14:
Feature
extraction

Sophie Robert

Introduction
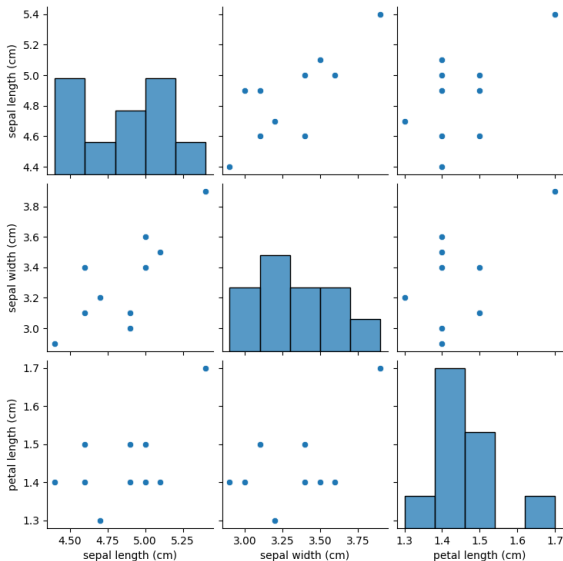
Principal
Component
Analysis

Principle

Algorithm

Advantages and
drawbacks

t-SNE

Principle

Example

Advantages and
drawbacks

Standardize matrix

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

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

Compute the correlation matrix

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

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

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis

Principle

Algorithm

Advantages and
drawbacks

t-SNE

Principle

Example

Advantages and
drawbacks

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

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
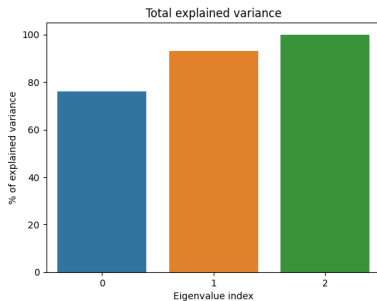Analysis

Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

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

Axis importance

The value of each eigenvalue is the **importance of the axis** and is used to select the number of axis to keep as a percentage of the explained variance.

Axis importance

The value of each eigenvalue is the **importance of the axis** and is used to select the number of axis to keep as a percentage of the explained variance.

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

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis

Principle
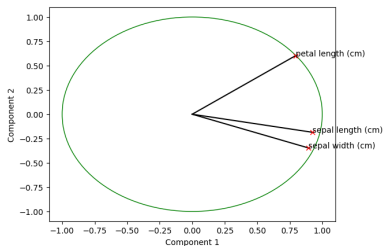
Algorithm

Advantages and
drawbacks

t-SNE

Principle

Example

Advantages and
drawbacks

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

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

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

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

Interpret results

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

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.

Advantages

Advantages

- Simple to implement

Advantages

- Simple to implement
- Simple to evaluate data loss because of transformation

Advantages

- Simple to implement
- Simple to evaluate data loss because of transformation

Drawbacks

- Features are transformed and lose interpretability of some results

Advantages

- Simple to implement
- Simple to evaluate data loss because of transformation

Drawbacks

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

t-SNE

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.

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.

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

Principle

We need two probability distributions:

Principle

We need two probability distributions:

- p_{ij}: measures the similarity between the individuals within the initial space.

Principle

We need two probability distributions:

- p_{ij}: measures the similarity between the individuals within the initial space.

- q_{ij}: measures the similarity between the individuals within the new space.

Principle

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

We need two probability distributions:

- p_{ij}: measures the similarity between the individuals within the initial space.

- q_{ij}: measures the similarity between the individuals within the new space.

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

Kullback-Leibler divergence

Kullback-Leibler divergence

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

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

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

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

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

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):

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

Probability distribution

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

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):

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

and set:

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2N}$$

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):

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

and set:

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2N}$$

In the new dimensional space, we set a heavy-tailed Student law:

Probability distribution

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

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):

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

and set:

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2N}$$

In the new dimensional space, we set a heavy-tailed Student law:

$$q_{ij} = \frac{(1 + \|\mathbf{q}_i - \mathbf{q}_j\|^2)^{-1}}{\sum_k \sum_{l \neq k} (1 + \|\mathbf{q}_k - \mathbf{q}_l\|^2)^{-1}}$$

Probability distribution

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
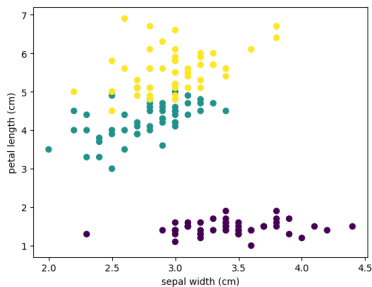Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

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):

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

and set:

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2N}$$

In the new dimensional space, we set a heavy-tailed Student law:

$$q_{ij} = \frac{(1 + \|\mathbf{q}_i - \mathbf{q}_j\|^2)^{-1}}{\sum_k \sum_{l \neq k} (1 + \|\mathbf{q}_k - \mathbf{q}_l\|^2)^{-1}}$$

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

Example: Iris dataset

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
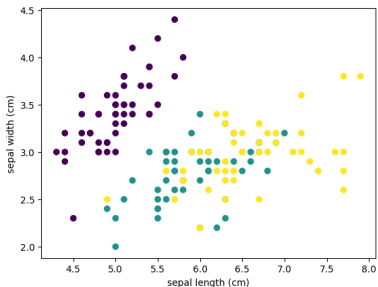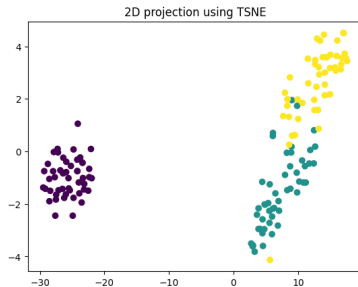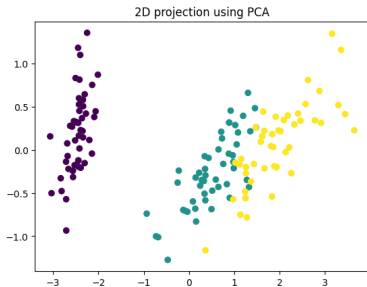Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

Data repartition without any transformation:

Example: Iris dataset

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

Advantages:

Advantages and drawbacks

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

Advantages:

- Usually visually nicer than PCA

Advantages and drawbacks

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis
Principle
Algorithm
Advantages and
drawbacks

t-SNE
Principle
Example
Advantages and
drawbacks

Advantages:

- Usually visually nicer than PCA
- Can find pattern in data that is non-linear

Advantages and drawbacks

Lecture 14:
Feature
extraction

Sophie Robert

Introduction

Principal
Component
Analysis

Principle
Algorithm
Advantages and
drawbacks

t-SNE

Principle
Example
Advantages and
drawbacks

Advantages:

- Usually visually nicer than PCA
- Can find pattern in data that is non-linear

Drawbacks:

Advantages:

- Usually visually nicer than PCA
- Can find pattern in data that is non-linear

Drawbacks:

- Many hyperparameters

Advantages:

- Usually visually nicer than PCA
- Can find pattern in data that is non-linear

Drawbacks:

- Many hyperparameters
- Only preserves local structure of the data

Advantages:

- Usually visually nicer than PCA
- Can find pattern in data that is non-linear

Drawbacks:

- Many hyperparameters
- Only preserves local structure of the data
- Stochastic results

Advantages:

- Usually visually nicer than PCA
- Can find pattern in data that is non-linear

Drawbacks:

- Many hyperparameters
- Only preserves local structure of the data
- Stochastic results
- Does not scale well

Advantages:

- Usually visually nicer than PCA
- Can find pattern in data that is non-linear

Drawbacks:

- Many hyperparameters
- Only preserves local structure of the data
- Stochastic results
- Does not scale well
- Hard to interpret

Advantages:

- Usually visually nicer than PCA
- Can find pattern in data that is non-linear

Drawbacks:

- Many hyperparameters
- Only preserves local structure of the data
- Stochastic results
- Does not scale well
- Hard to interpret
- Does not create new variables that can be understood

Questions ?