Applied statistics and Machine learning in Python with subsurface applications

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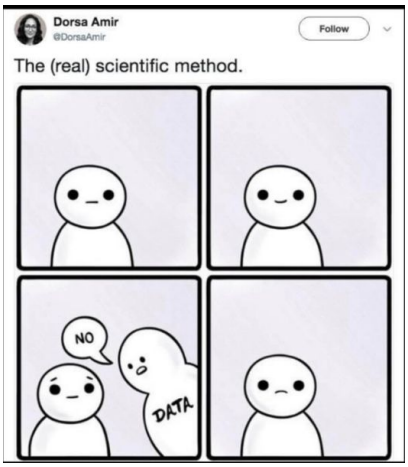
Data properties



Representation

A representation should **capture** the nature of the subject being studied.

Example: If you want to evaluate the 3D structure of a wind turbine, a set of descriptors an be:

1. Blade length
2. Turbine height
3. Geographical position
4. Output power
5. Wind direction

which are two decimal numbers, a 2d tuple, a 1D time series and a 2D time series (or 3D even).

Comparability

Same meaning **represenations** for different objects (inputs).

Discussion point!

How do we compare two wind turbines accounting for the 5 variables previously introduced?

Data properties

- All starts from data: what are data-properties?
- Are there such things as good data and bad data?

Life lesson (or exam question, same thing ;))

- Data DO NOT always have value.

- TRASH in TRASH out

Data structures

Given a representation, it is then needed to decide on a suitable **data structure** for the problem.

Definition

A data structure is a way of storing and organising data in a computer so that it can be used effectively.

Typical data structures used in data analysis are:

- Data points
- Arrays (vectors, matrices, N-mode (way) arrays)
- Graphs (trees)
- Databases

Workflow

Data has to be prepared with these steps in mind

1. Plan experiments: Use experimental design to set up experiments in a *systematic* way
2. Pre-processing: Is there systematic variation in the data which should be removed Can cross-checking/validation procedures be designed?
3. Examine the data: Look at data (tables and plots). Strange behaviours? Smooth behaviour? WARNING!
4. Define desired model outcomes (speed, accuracy, false positive/negatives rate)
5. Estimate and validate model: What do the results tell us? Is the generated model general (valid for future sampling)?
6. Apply model to unknown samples

Spatial and Temporal Data

Statistics is collecting, organising, and interpreting data

Spatial and temporal statistics is a branch of applied statistics that emphasises:

1. the geo context of the data
2. the spatial and time dependent relationship between data
3. the different relative value and precision of the data.

Actual data

The data matrix is an extremely common data structure.

$$X = \begin{bmatrix} 95 & 89 & 82 \\ 23 & 76 & 44 \\ 61 & 46 & 62 \\ 49 & 2 & 79 \end{bmatrix}$$

In python these can be saved as

- lists (vanilla python)
- numpy.arrays
- pandas dataframes

Nomenclature

There are different conventions. Commonly we will construct data matrix such that:

- Rows are called instances, objects or samples.
- Columns are called features, variables.

One can think of each row to be an experiment, and the rows its properties. Each row (experiment, object, sample, ...) is thus a list of values, one for property.

Note

Mathematically speaking, this is just a notation. As long as one keeps track and is consistent, columns can be used as rows and vice versa.

A quick example

Environmental measurements of rivers. Features (properties):

- pH
- Temperature
- Concentration of pollutants
- Flow rate
- water speed

The instances/experiments/observations/sample:

- Po
- Danube
- Rio delle Amazzoni
- Sjoa
- Atna

Data into Machine Learning algorithms: normalisation

Different measurements can lead to different data distribution and numerical values.

When fed to numerical recipes, data is just a set of numbers.

For faster computations, data can be **normalized**: i.e. rescaled to the same numerical interval.

Normalisation

The procedure simplifies the numerical recipes work, but it also loses information

As it is not possible to complete sample any distribution, data might be disproportionately handled depending upon data collection (i.e. this can be an error source).

Classification types

There are two main types of classification methods for analysis of a set of objects stored in matrix X:

Unsupervised classification

- Only the X data is used
- "Natural" classes/clusters/groupings in X are discovered

Supervised classification

- We know the class/group/cluster membership of every object/sample
- Class information is stored in an Y matrix

Classification types

Several approaches can be found in classification tasks:

Unsupervised classification

- Principal component analysis (PCA)
- Agglomerative (hierarchical) cluster analysis.
- k-means cluster analysis
- Fuzzy c-means cluster analysis
- Self organising feature maps (SOFM)

Supervised classification

- Linear discriminant analysis (LDA)
- k-nearest neighbours (kNN)
- Discriminant partial least squares
- Soft independent modelling of class analogies (SIMCA)
- Support vector machine (SVM)

Limitations of unsupervised classification

- Do "natural" clusters in a data set exist and/or have any meaning?
- First we must have a definition of what is a cluster. To do this we

must define what we mean by similar or dissimilar objects.

- Objects that are close have low dissimilarity and high similarity.

A metric system is required.

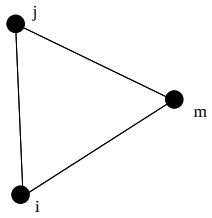
Proximity: Continuous variables

Triangle inequality

Considering a vectors in an N-dimensional space, to be a distance it must satisfy the triangle inequality:

$$d_{ij} + d_{im} \geq d_{jm}$$

If also $d_{jj} = 0$, if $i = j$ and $d_{jj} - d_{ii} = 0$, then we call it a *metric*.



Proximity: Continuous measures

Common metrics:

- Euclidean.

$$d_{ij}^{(E)} = \left[\sum_{k=1}^{N} (x_{ik} - x_{jk})^2 \right]^{\frac{1}{2}}$$

- Manhattan

$$d_{ij}^{(M)} = \sum_{k=1}^{N} \|x_{ik} - x_{jk}\|$$

- Minkowski

$$d_{ij}^{(M(p))} = \left[\sum_{k=1}^{N} (x_{ik} - x_{jk})^p \right]^{\frac{1}{p}}$$

Proximity: Categorical variables

- Many applications consist of binary vectors, typical is "yes" and "no" answers to a lot of tests
- It is tempting to use distance between binary vectors to signify distance. However that is *by far* not optimal.

Lets look at an example:

- $\mathbf{v}_1 = [1\ 1\ 0\ 0\ 0\ 0]$
- $\mathbf{v}_2 = [0\ 0\ 1\ 1\ 0\ 0]$
- $\mathbf{v}_3 = [1\ 1\ 1\ 1\ 1\ 1]$

It makes NO SENSE to compute the Euclidean distances between these vectors

Proximity: Categorical variables: Binary matching

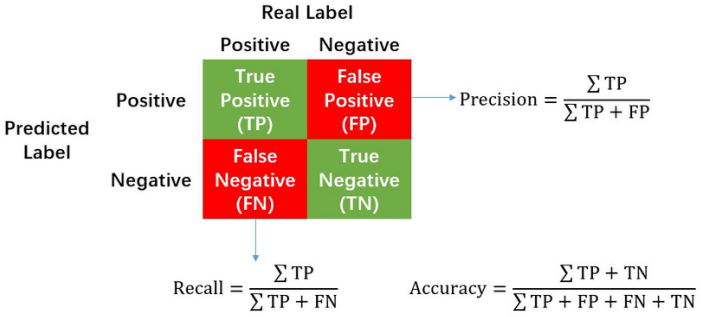
	Object B value 1	*Object B* value 0
Object A value 1	a	b
Object A value 0	c	d

Example

a = [0 0 0 1]
b = [1 1 0 1]

- $c = 2$: two places where A has 0 and B has 1.
- $d = 1$: one place where A and B are equal to 0.
- $a = 1$: one place where A and B are equal to 1.

Classification metric



Unsupervised learning

Unsupervised learning, a term that resonates with the autonomy of machine intelligence, operates on the principle of identifying patterns and structures in datasets without labelled responses.

This branch of machine learning is distinguished by its lack of explicit guidance, where algorithms are tasked with uncovering hidden structures from unlabeled data.

The most common clustering strategies are :

- filtering
- clustering
- dimensionality reduction
- association learning

Application of unsupervised learning

It is a bit of a holy grail: a computer that finds patterns without guidance. (Yes, it doesn't work, most of the time)

Still, it has been shown efficient for:

- Computer vision
- Anomaly detection
- Exploratory data analysis

Main challenge

The right result is quite undefined, Uncertain goal.

Goals

Finding a pattern in data does not mean to find something useful.

Relevant is not the same as causal.

Correlation is not causation.

As we do not have a 'truth', or a supervision, we can look for data-patterns by

- grouping strategy according to some properties analogy
- reducing variance within groups.

Note: these approaches will (almost) always converge or provide information. Which is a better outcome, strategy or model parameter can be, at the end, only evaluated with domain expertise.

Common approaches

The number of unsupervised approach is tremendous, yet, the most common are the following:

- k-means (rigid clustering)
- Gaussian mixed model (soft clustering)
- Hierarchical clustering (grouping into trees/dendrograms)
- Principal component analysis (PCA) (Principal components identifications,)
- Auto-encoders (data compression)

We will discuss a few of them.

k-means cluster analysis

With the rise of Machine Learning, one of the most popular approaches is k-means.

The algorithm consists of:

1. Select the number of clusters $K \leq K_{max}$ to look for
2. Start by creating K random cluster centres $\mathbf{m}_k$
3. For each object $\mathbf{x}_j$ assign it to the cluster centre it is nearest to
4. Re-compute centre points $\mathbf{m}_k$ for the new clusters and re-iterate towards convergence

This procedure minimises the within-cluster variance

Optimal no of clusters

In k-means cluster analysis we assume a **true** number of clusters.

To estimate the optimal no. of clusters K^* from data we may do as follows:

1. Compute k means for $K \in [1, 2, \cdots, K_{max}]$
2. Compute the mean within cluster variance W_K for each selection of $K \in [1, K_{max}]$
3. The variances $[W_1, W_2, \cdots, W_{max}]$ generally decrease with increasing K. This will even be the case for an independent test set such that cross-validation cannot be used.

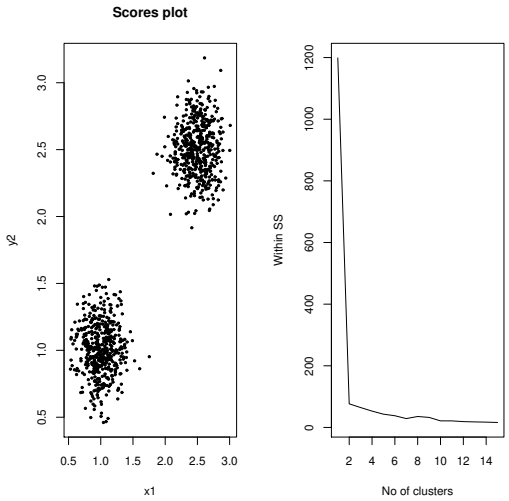
Optimal no of clusters

1. Intuitively, when $K < K^*$ we expect that an additional cluster will lower the within cluster variance: $W_{K+1} \ll W_K$.
2. When $K > K^*$ the decrease of the variance will be less evident.

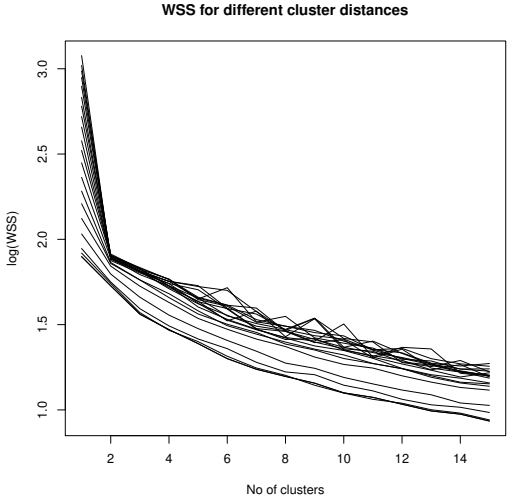
Optimal *n_clusters*

This means there will be flattening of the W_j curve. A sharp drop in the variance may be used to identify the optimal no. of clusters.

Optimal no of clusters, example



Optimal no of clusters, example



Gaussian Mixture Model (GMM)

Gaussian Mixture is a probabilistic model that tries to split the data into clusters.

Each cluster is represented by a centre (its mean) and a Gaussian distribution around it with different variance for the different dimensions.

To each datapoint, a belonging probability to each cluster is assigned.

Assumption

Data points are generated from a mixture of a finite number of Gaussian distributions with unknown parameters.

Limitations

The method is rather powerful, but it has quite significant drawbacks:

- The method can be rather unstable and not converge for 'poor' data.
- Iterative procedure is usually needed and convergence depends on initial guest.
- Interpretability of the results might be rather poor.
- High dimensionality limitations.
- Computationally expensive

GMM model development

$$p(x) = \sum_{k=1}^{K} w_k f_k(x, \theta_k)$$

where

- $p(x)$ is the overall density or mass function of the mixture model.
- K is the number of distributions to be considered
- $g_k(x, \theta_k)$ is the density mass function of the k-th component
- θ_k are the parameters for the $g_k()$ distribution

and where a Gaussian is:

$$g(x) = \frac{1}{\sigma\sqrt{(2\pi)}} exp(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2})$$

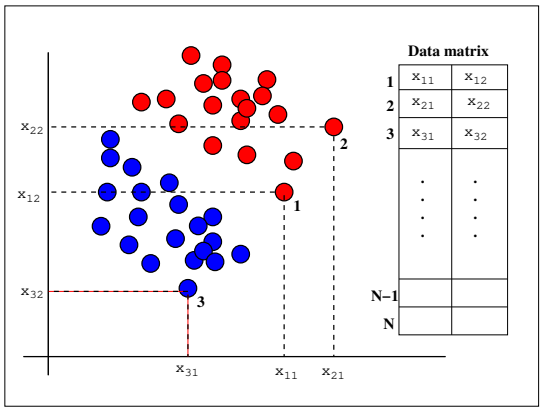
GMM usage example

GMM is used in a large span of fields:

- Clustering: GMMs can identify clusters with different shapes and sizes due to their probabilistic nature, making them suitable for more complex datasets.
- Anomaly Detection: By modelling the normal behaviour of data through its distribution, GMMs can be used to detect outliers or anomalous events.
- Image Segmentation: In computer vision, GMMs can be used for image segmentation, where the goal is to partition an image into segments based on the colours or textures.
- Speech Recognition: GMMs have been used in speech recognition systems to model the distribution of audio features.
- Bioinformatics: GMMs are used in bioinformatics for tasks such as modelling gene expression data or protein structure. They can help in identifying biological patterns or clusters within the data that are not immediately apparent.
- Astronomy: GMMs are used in astronomy to classify celestial objects and to estimate the distribution of stars or galaxies

PCA

Central in any data analysis is the use of a *data matrix*



PCA base

Question:

How can we understand the information contained in such a data matrix?

- The geometry of the "object cloud" in N dimensions is used to understand relations

Geometrical insights

Plotting provides **geometrical insights** and observation of **hidden data structures** and **patterns**

Correlated variables

Problem

How can we use plotting if we have more than 3 variables?

Solution

1. Seek for **correlated variables** in the data matrix
2. Seek for latent variable
3. Give up (use AI)

Correlated variables

- Correlated variables contain approximately the same information.
- Several correlated variables suggests:
  - the same **phenomenon** is manifested in different way
  - an **underlying phenomenon** more fundamental exists

Let's assume the latter:

Linear combinations

Assuming the latent variables to be a **linear combinations** of the original variables, i.e.:

$$\text{LV} = a_1x_1 + a_2x_2 + \cdots + a_nx_n$$

Latent variables

A new coordinate system

1. Latent variables are based on creating a new coordinate system based on linear combination of the original variables
2. Objects are projected from a higher dimensional

data space onto this new (lower dimensional) coordinate system

1. The new coordinate system improves interpretation and prediction.

Principal component analysis (PCA) can automatically create useful latent variables

PCA

Originally invented in 1901 by Karl Pearson and re-invented several times. The PCA method is also referred to as:

1. Singular value decomposition (numerical analysis)
2. Karhunen-Loeve expansion (electric engineering)
3. Eigenvector analysis (physical sciences)
4. Hotelling transform (image analysis/statistics)
5. Correspondence analysis (double scaled version of PCA)

Karl Pearson

PCA

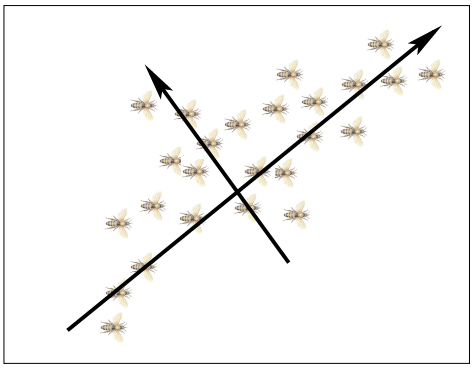
Goals of PCA:

1. Simplification.
2. Data reduction and data compression
3. Modeling
4. Outlier detection
5. Variable selection
6. Classification
7. Prediction
8. ... world peace ...

PCA

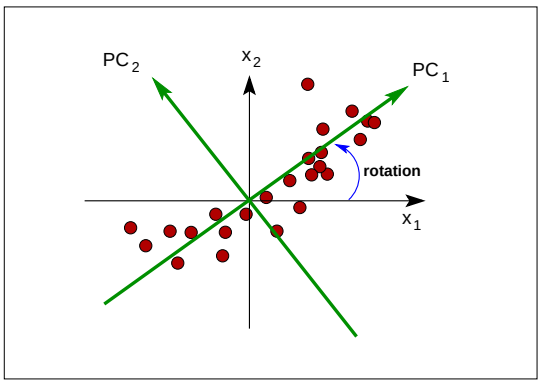
Rotation of the coordinate system

In PCA the original coordinate system is rotated such that the new latent variable axes point in the direction of max variance



PCA

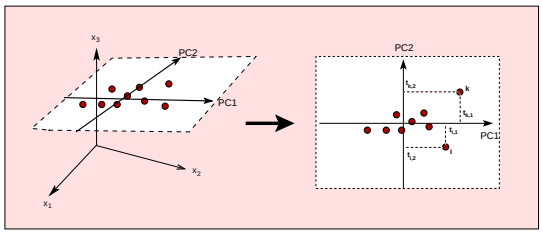
Rotation of the coordinate system



PCA

Scores are new coordinates

Scores are the coordinates of objects in the **new** coordinate system



Data = Model + Noise

Data matrix	=	Model matrix	+	Residual matrix

PCA Model

$$X = M_1 + M_2 + \ldots\ldots + M_{Aopt} + E$$

$$X = \mathbf{t_1}\mathbf{p_1} + \mathbf{t_2}\mathbf{p_2} + \ldots\ldots + \mathbf{t_{Aopt}}\mathbf{p_{Aopt}} + E$$