HANDS-ON AI I

Tabular Data, Dimensionality Reduction and Clustering

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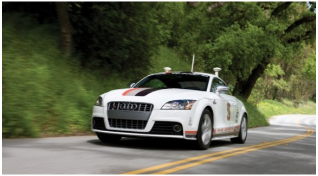
Copyright Statement

Content of Unit 1

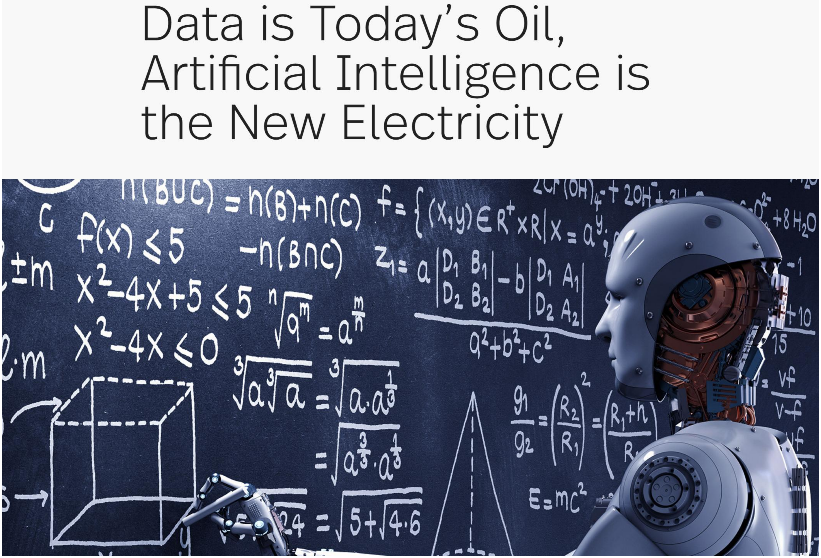
- Short motivation
- First data source: tabular data
- Dimensionality reduction
- Clustering

AI is Ubiquitous

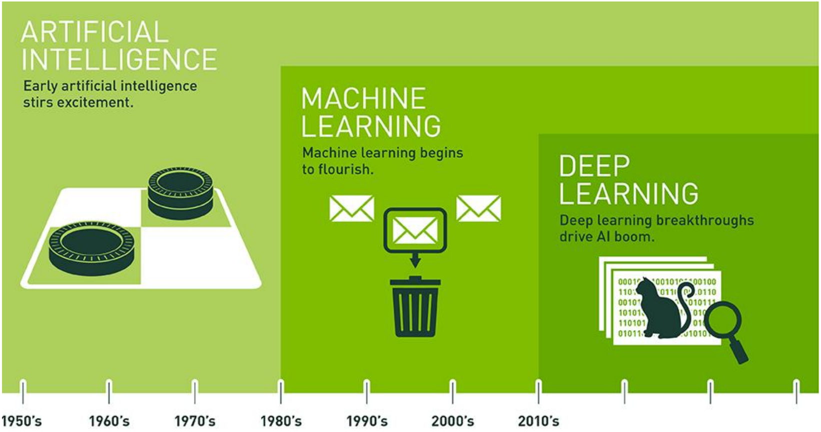
- AI **pervades commercial applications** in an unprecedented manner and is fundamentally changing how businesses operate across **virtually all sectors**:
  - Information technology
  - Manufacturing and supply chains
  - Medicine and healthcare
  - Education
  - Financial, legal and tax services
  - News and publishing
  - Transportation
  - ...
  - Science



Golden Age of AI



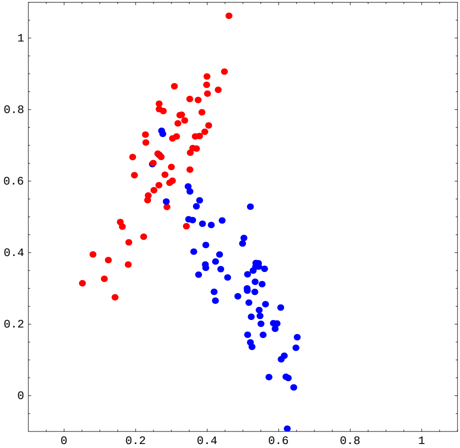
AI is a Broad Field



Data


Geographical
Transport
Cultural
Natural
Scientific
Types of Data
Meteorological
Financial
Statistical

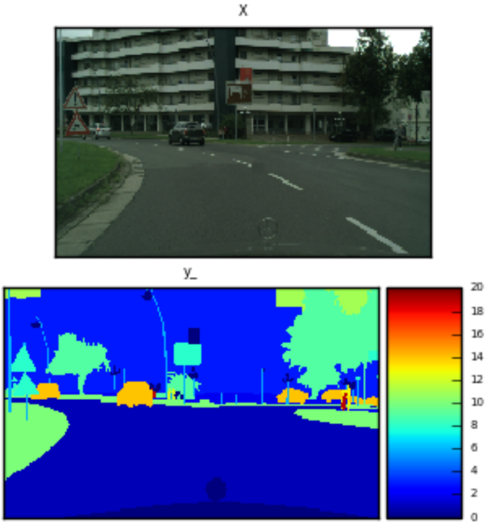
Example Data (1)



Example Data (2)

0.99516	0.890813	0.933726	0.793397	0.826405	0.236946	-1
0.853206	0.611647	0.317486	0.633609	0.411492	0.985231	+1
0.387494	0.459847	0.815049	0.394526	0.678227	0.031886	-1
0.733515	0.640438	1.19068	0.639685	0.0793674	0.160503	+1
0.274817	0.261054	1.20056	0.689895	0.401913	0.277955	-1
0.329943	0.241299	0.848705	0.721673	0.973852	0.795238	-1
0.334784	0.350487	0.315131	0.928277	0.816343	0.558292	-1
0.481578	0.738839	0.0925513	0.294667	0.612725	0.573062	-1
0.0940846	0.278992	0.451819	0.900141	0.220497	0.541176	+1
0.360569	0.638554	1.0307	0.260456	0.00658296	0.380672	+1
0.0857518	0.3775	0.386551	0.570562	0.15437	0.102717	+1
0.755808	0.1362	0.544536	0.848888	0.874862	0.307479	-1
0.421025	0.785714	0.449038	0.920612	0.420418	0.749187	-1
0.939446	0.0468747	0.15846	0.625944	0.198894	0.176125	+1
0.845362	0.767883	0.824993	0.725803	0.808218	0.63495	-1
0.484793	0.129329	0.0783719	0.465347	0.291457	0.254278	+1
0.399041	0.751829	0.763511	0.894785	0.47902	0.15156	-1
0.643232	0.615629	0.430261	0.0458972	0.446513	0.844081	+1
...	...	...	...	...	...	...

Example Data (3)



What is Data?

- Etymologically, data is the plural of datum in Latin, which means “given”.
- Data is typically **generated from a real world process** (e.g., measurements), but **synthetic** data also exists.

One Example

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- We now present the process of varying changes in the air pressure as zeros and ones.
- **Binary representation** of data is the **basis of computerized data processing** at present.

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- Each column and row is uniquely numbered.
- Tabular data has a virtually infinite range for mass data storage (can always add rows).
- Tabular databases include the following key properties:
  - Share the same set of properties per record, i.e., every row has the same column titles.
  - Each column is (usually) assigned with a header title (metadata).
  - Access through identifiers, i.e., each object can be retrieved by a query through key values.

Example: Iris Data Set

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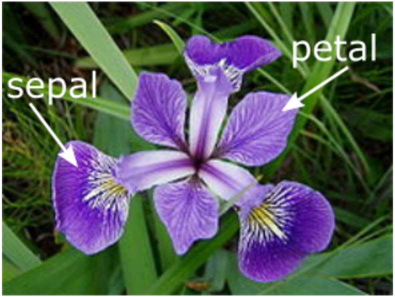
- It is also sometimes called **Anderson's Iris data set** since biologist Edgar Anderson collected the data.
- The data set consists of 50 samples from each of three species of the **Iris flower**:
  - Iris setosa
  - Iris virginica
  - Iris versicolor

Example: Iris Data Set

We have the following $d = 4$ **features**:

- Sepal length in cm
- Sepal width in cm
- Petal length in cm
- Petal width in cm



Terminology

sep-len	sep-width	pet-len	pet-width	species
6.7	3.1	4.7	1.5	versicolor
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6.5	3.2	5.1	2.0	virginica
5.0	3.6	1.4	0.2	setosa
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- Every sample lists the species/class via its **label**, e.g.: $y =$ versicolor.

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- The analysis determined the quantities of 13 constituents found in each of the three types of wines.
- The data set consists of 178 samples with 13 features (13 constituents).

Example: Wine Data Set

We have the following $d = 13$ **features**:

- Alcohol
- Malic acid
- Ash
- Alcalinity of ash
- Magnesium
- Total phenols
- Flavanoids
- Nonflavanoid phenols
- Proanthocyanins
- Color intensity
- Hue
- OD280/OD315 of diluted wines
- Proline

VISUALIZATION

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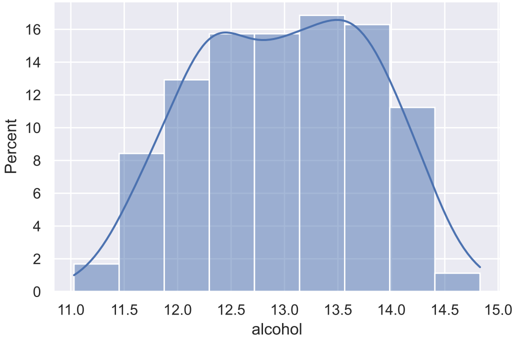
  - Time series data: line plots
  - Labeled data $\rightarrow$ separation into classes: combined plots with class-color encoding
  - etc.

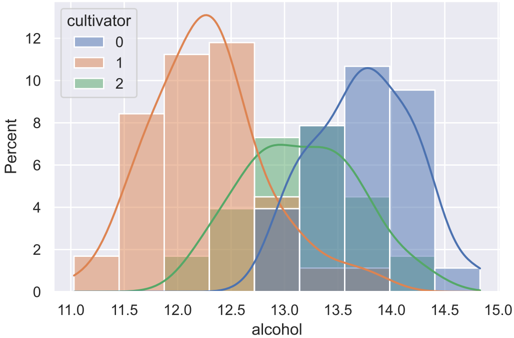
Example: Wine Data Set

- Visualize the feature `alcohol` via a histogram:



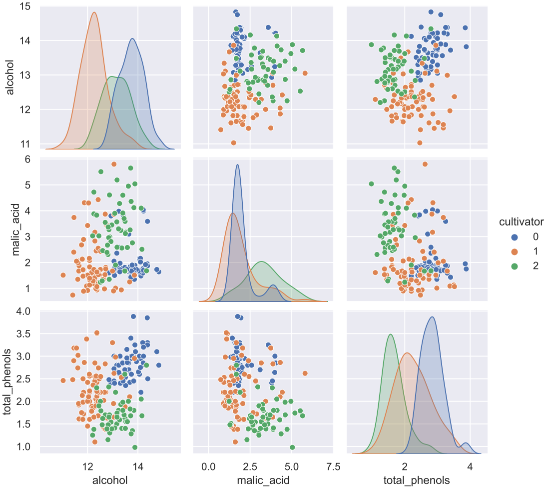
Example: Wine Data Set

- Visualize the feature `alcohol` via a histogram and separate the three cultivators (classes):



Example: Wine Data Set

- Visualize multiple features simultaneously by always comparing pairs of features (including class separation):



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- What about bigger data sets? Let's say 500 features?
  - Of course, we could still look at all features individually or compare features pair-wise.
  - Would probably take a "couple" of minutes ...

DIMENSIONALITY REDUCTION

Dimensionality Reduction

- Problem: Too many features to see anything in the data.
- Often, data is described with hundreds (or thousands) of features $\rightarrow$ visualization is a common problem.
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- Popular algorithms are **PCA** (principal component analysis) or **t-SNE** (t-distributed stochastic neighbor embedding).
- Can reduce n-dimensional data to, e.g., 2-dimensional data $\rightarrow$ can be easily visualized.

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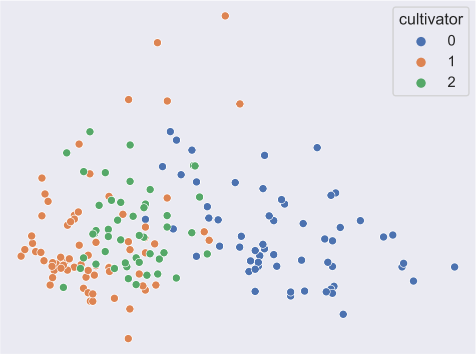

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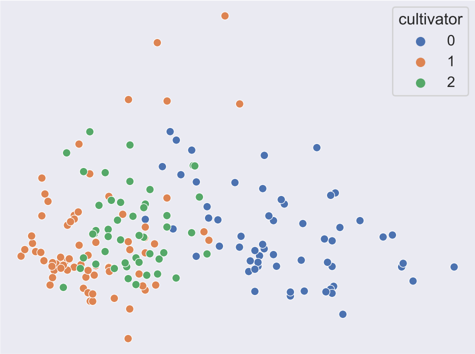

- While we lose some information, we quickly gain interesting insights: Samples from the same cultivar form a so called **cluster** (close to each other in space).

CLUSTERING

Clustering Algorithms

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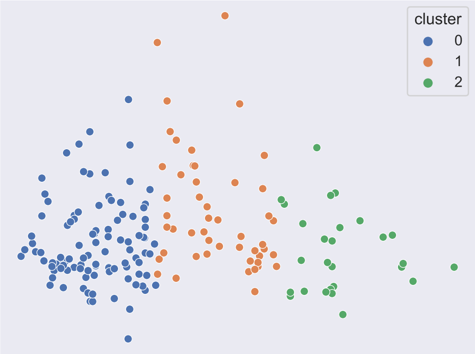
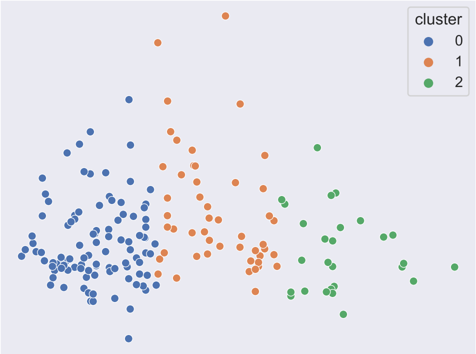
- So far, all our data was labeled.
- Imagine now that the data is unlabeled and we still want to find out which data belongs together.
- We can now use so-called **clustering algorithms** that try to group samples into "similar" and "dissimilar" samples.[1]



[1] What is considered "similar" highly depends on the algorithm.

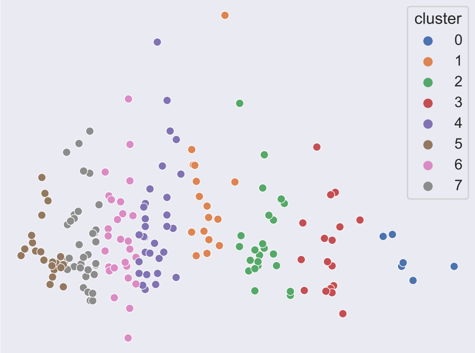
k-means

- In the k-means clustering algorithm, k is the most important parameter.
- k determines how many clusters the algorithm should search for.
- k is set by the user.



Affinity Propagation

- For affinity propagation, the number of clusters does not have to be specified.
- For the wine data set, affinity propagation determines 8 cluster centers and assigns points to them.



Notes on Clustering

- Clustering is **not** classification (which we will discuss in later units).
- On the contrary, the clustering algorithms we pass our data to do not have any knowledge about the classes/labels, they just receive the raw features of the samples (unlabeled data).

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- On the contrary, the clustering algorithms we pass our data to do not have any knowledge about the classes/labels, they just receive the raw features of the samples (unlabeled data).
- This also means that we often do not really know whether the identified clusters are “correct” $\rightarrow$ must inspect again (e.g., with the help of visualization) to see if they make sense.

SUMMARY

Summary

- Tabular data is very common.
- Data is structured in a tabular form.
- Data elements are arranged in columns (features, labels) and rows (samples).
- Visualization is a powerful tool to gain insights into the data.
- High-dimensional data can be handled with dimensionality reduction techniques.
- Clustering allows to find samples “close” to each other.
- Note: The described methods like dimensionality reduction or clustering can also be applied to other forms of data.