

Freie Universität Berlin



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Machine learning for data science

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1 Data science

Definition 1.0.1 (Study of data). *Data science is a study of data. It includes:*

- *Processing data*
- *Representation of data (compressed, understandable)*
- *Value extraction from data*
- *Knowledge extraction from data*

Definition 1.0.2 (Data-Driven science). *Data science as a tool scientific discovery, complement to hypothesis-drive science.*

1.1 Comparison

1.1.1 Hypothesis-Driven

In the **hypothesis-driven** experimentation, we first form an *hypothesis*, then we perform an *experiment* and in the end we *check* the results.

1.1.2 Data Science

Data-Driven science instead starts with taking *existing data*, performing an *analysis* on them and *observe* the result.

1.2 History

In the past, experimentation and data collection existed with separate purposes. When the **cost** of collection and accessing the data dropped dramatically (thanks to the internet and all the sensors), they started being implemented in science, since on the other hand the cost of an experiment was the same. Furthermore, computers are now able to process large amount of data.

Observation 1.2.1. The first and most important thing in data science is collecting the data and only later working on it.

The first example of data science can be found in a map made by John Snow in 1854 showing the clusters of cholera cases in London. With the map he noticed that there was a center place with a fountain/well and understood that the disease was transmitted via water and not air.

1.3 Sources of data

There are multiple sources of data:

- Physics equations: data generated artificially via simulation running multiple times with different parameters
- User content
- User activity: for example public GPS traces of OpenStreetMap, that enables to gain insights on mobility patterns (e.g. relation between location, mode of transportation, date and user).
- Historical books or artifacts: for example *De Sphaera Corpus*, the corpus of multiple editions of the cited textbook made available in digital form. It enables similar dataset-wide analysis, relating content, year and city of publications.
- Earth data
- Biomedical data: for example the National Cancer Institute in the USA and the UK Biobank data

Note 1.3.0.1. Data is often not intended for scientific use. It is often a by-product of an activity with a different purpose (e.g. clinical practice, accounting).

1.4 Usages

The outcome of a data science analysis can:

- be **insightful** and of interest by itself (and be published)
- inform on further experiments or investigations to be conducted in order to **verify a hypothesis**
- inform on whether it is **feasible** to build a system that accurately predicts the data

1.5 Examples

1.5.1 T-SNE analysis of TCGA high-dimensional omics data

We start by defining:

- x_i is the representation of i in the original measurement space (e.g. $x_i \in \mathbf{R}^{1000}$)
- d_{ij} is the distance between instance i and j in measurement space

$$d_{ij} = \|x_i - x_j\|$$

- y_i is the representation of instance i in low-dimensional space, usually \mathbf{R}^2
-

1.5.2 Planetary science

Can internal properties of a planet be predicted from a few observables? Yes, starting from predetermined parameters we then run tons of simulations via convection models and check the observables. In the end we try to build a model that can predicts them.

1.5.3 Digital humanities

The idea was to extract correlations between visual patterns and categorization of images.

1.6 Comparisons

1.6.1 Statistics

Statistics makes particular assumptions about the nature of the data whereas **data science** addresses the data as it occurs in real-world applications. Data science also addresses the technical challenge of processing the data.

1.6.2 Decision making

Data science focuses on extracting insightful structures and relations from the data and presenting them in an interpretable manner, while **Decision Making** focuses on learning good autonomous decisions so that repetitive tasks can be performed without human intervention.