Lecture 1: Introduction & Data

KI-Workshop
(HFT Stuttgart, 8-9 Nov 2023)

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University of St. Gallen (soon-to-be HFT Stuttgart)

Today's lecture

What this course is about...

Who am I?

Course modalities

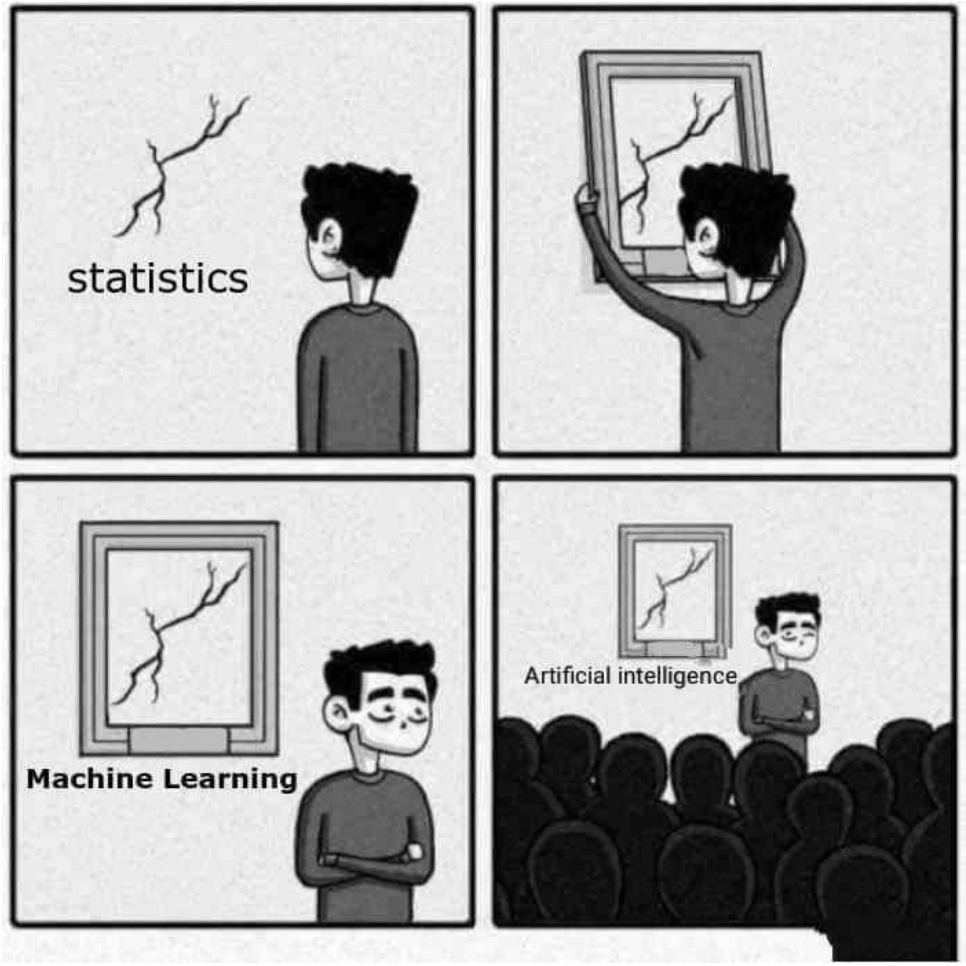
Course syllabus

Types of data

Features and feature engineering

Data scaling

What this course is about...



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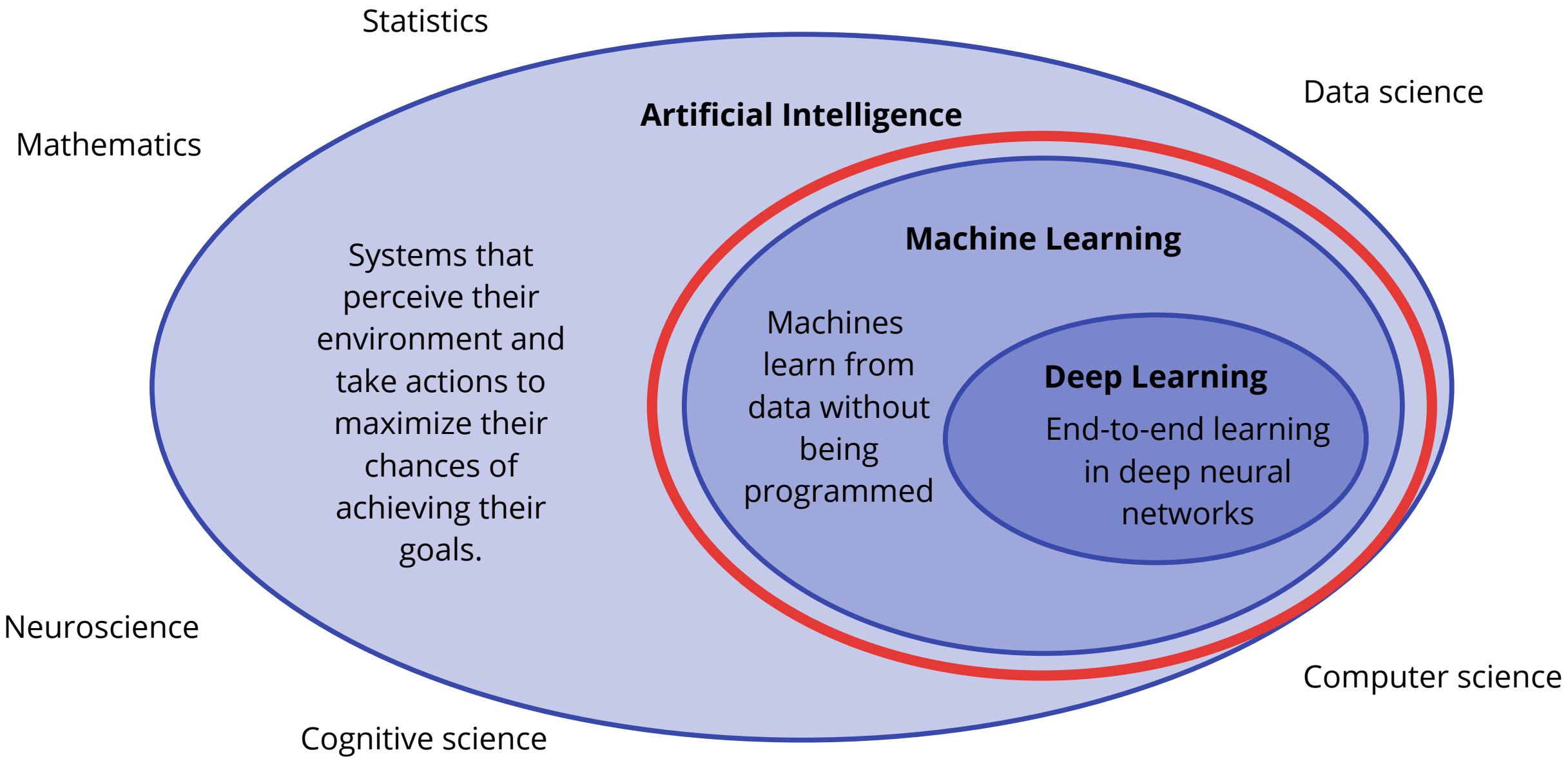
Mapping terminology



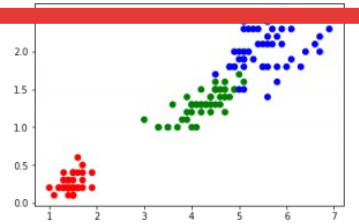
What is Machine Learning (ML)?

> *"The field of study that gives computers the ability to learn without being explicitly programmed."*
> - Arthur Samuel (1959)

Different approaches:

Iris Versicolor

- **Supervised learning**
  Find a function that relates input data to output data by learning a specific task.



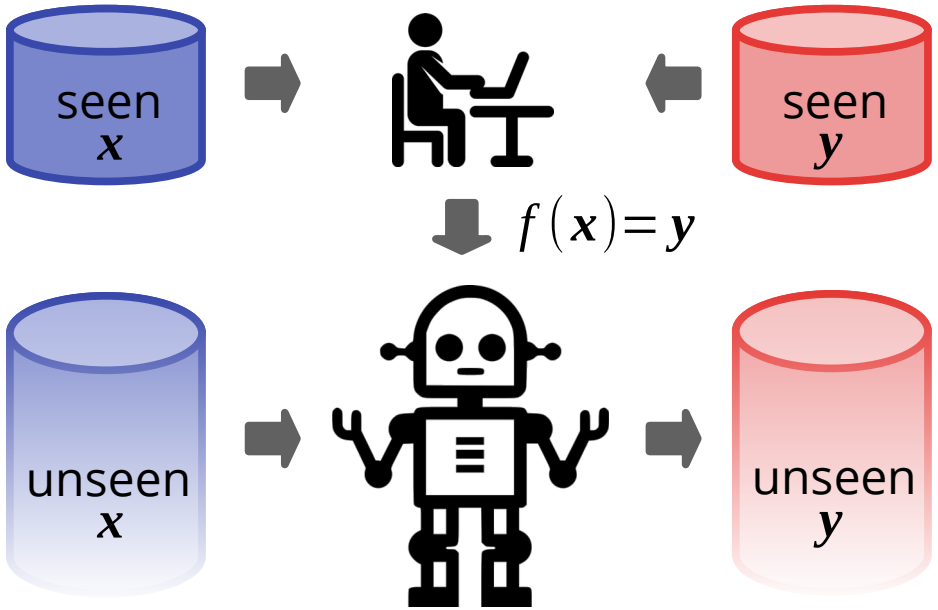
- **Unsupervised learning**
  Find structure within a data set.

- **Reinforcement learning**
  Learn a task in a dynamic and responsive environment.

Supervised ML

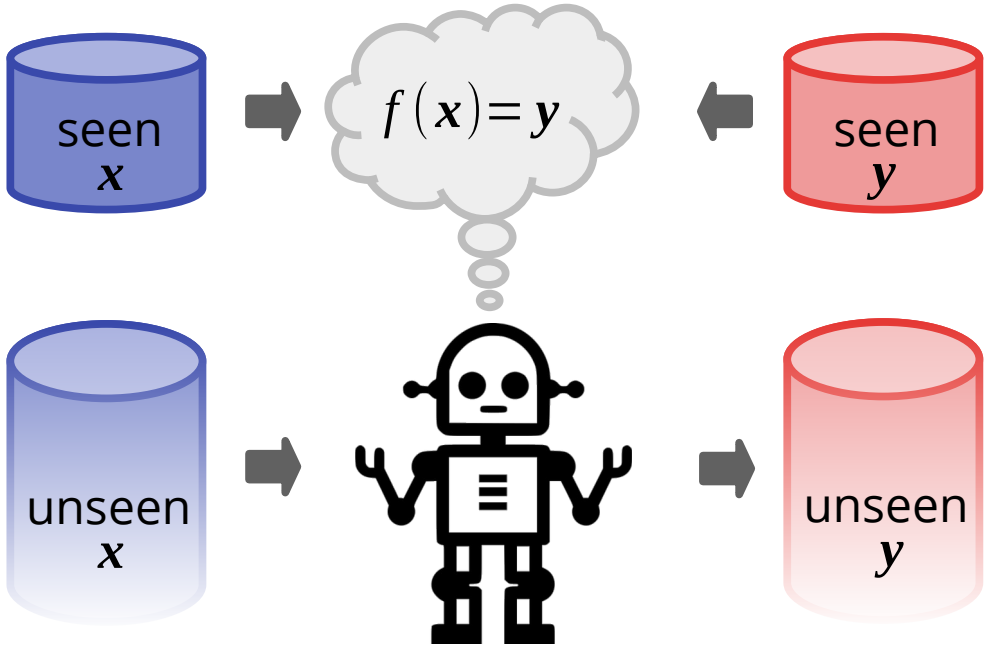
General goal for supervised problems:
Find a function ("task") that relates input data (x) to output data (y) such that: $f(x)=y$

Traditional (Rule-based) Approach:



Input data (x) Output data (y)

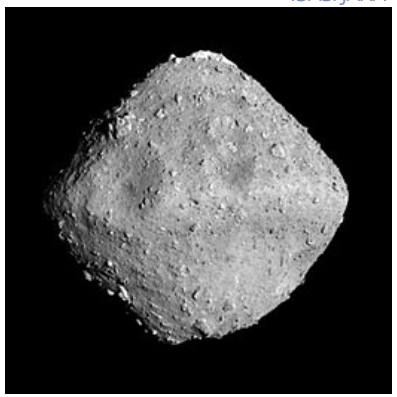
Machine-Learning Approach:



Input data (x) Output data (y)

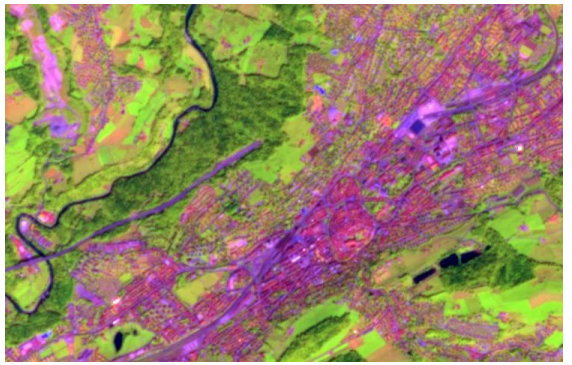
Who am I?

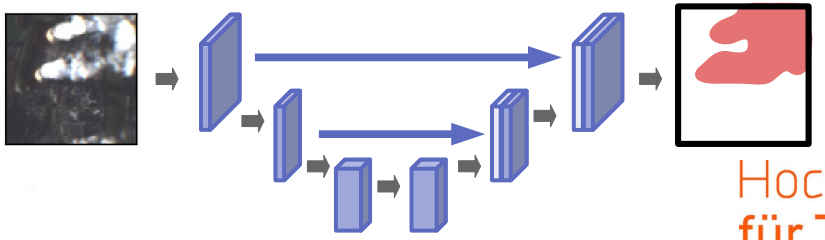
About myself



ISAS/JAXA

Gerald Rhemann





Deutsches Zentrum für Luft- und Raumfahrt
German Aerospace Center

Freie Universität Berlin

NAU NORTHERN ARIZONA UNIVERSITY

LOWELL OBSERVATORY
125 YEARS | 1894 - 2019

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

Universität St.Gallen

Hochschule für Technik Stuttgart

Physics

Dr. rer. nat. (Earth Sciences)

Postdoc @HSG-AIML

Asst. Prof. Computer Vision

Prof. AI in Remote Sensing

2009

2013

2020

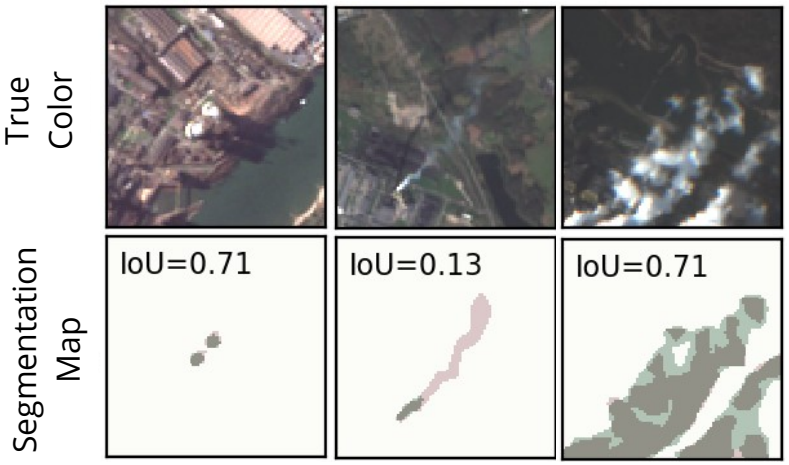
2022

2024

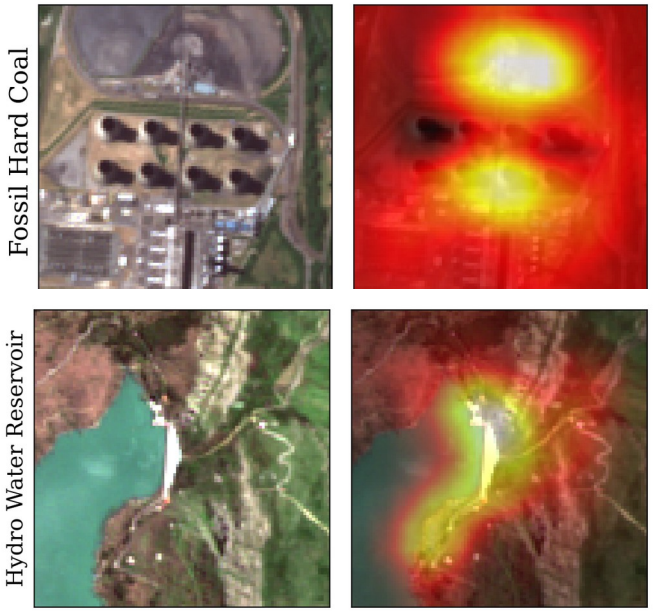
What I work on...

Commercial Vehicle Traffic Monitoring
(*Blattner et al. 2021*)

Characterization of Plumes and Estimation of Power Generation from Remote Sensing Data
(*Mommert et al. 2020, Hanna et al. 2023*)

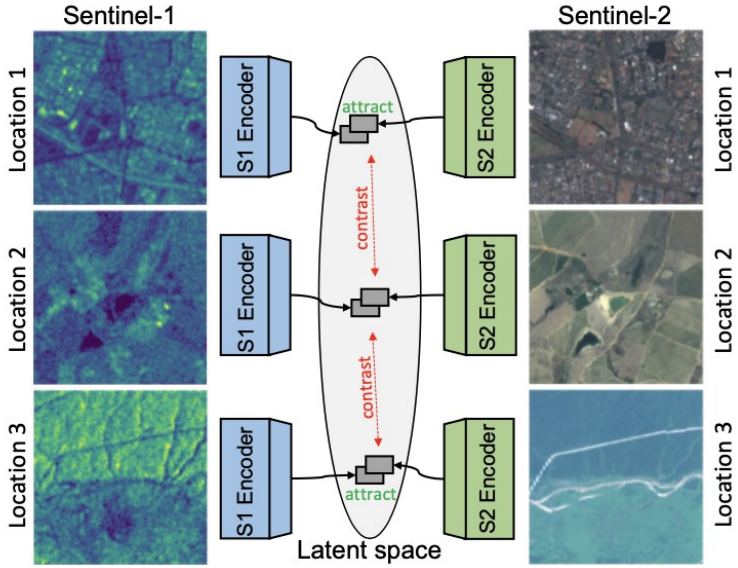


R: ground-truth, G: prediction

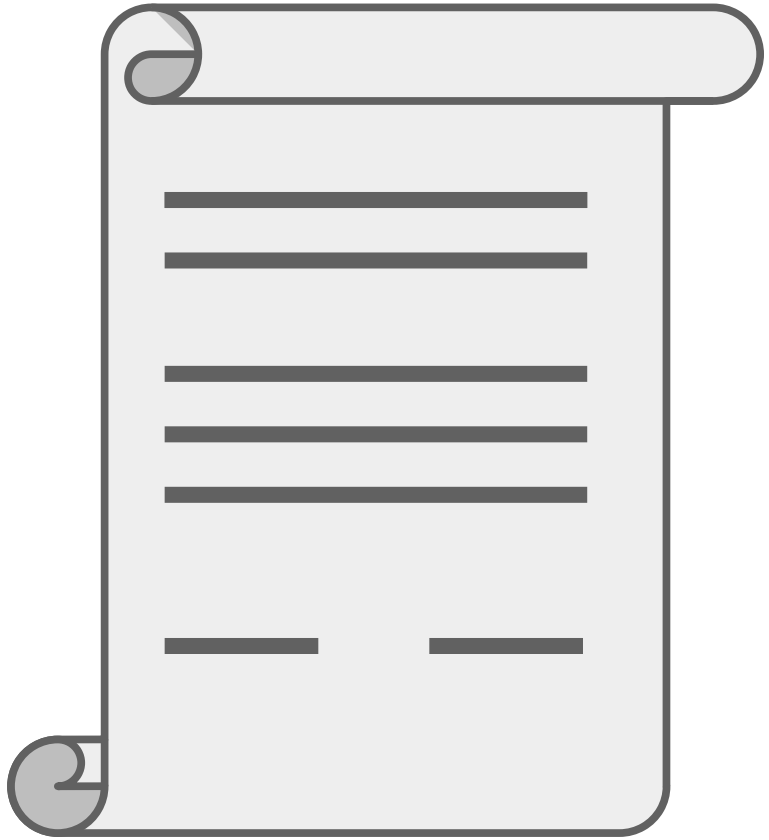


Power Plant Classification from Remote Imaging with Deep Learning
(*Mommert et al. 2021*)

Contrastive Self-supervised data fusion for Satellite Imagery
(Scheibenreif et al. 2022)



Course modalities

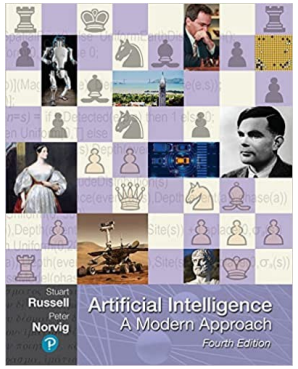


Course modalities

- **Goal** of this course:
  To understand and be able to implement and utilize supervised traditional Machine Learning and Deep Learning models.
- **Setup**: Combination of lectures and voluntary hands-on lab courses
- **Lecture mode**: This course is supposed to be bi-directional: let me know if anything is unclear, ask questions anytime!
- We will use **Google Colab** for running our Lab Notebooks (they offer free GPUs!). If you don't have a Google account, please let me know as soon as possible!

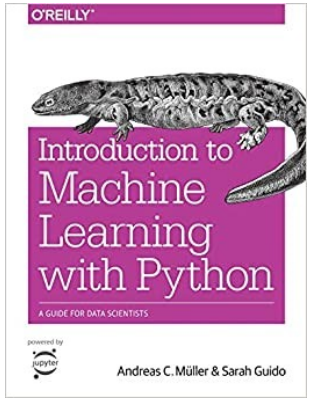
Literature resources

- Stuart Russell, Peter Norvig: **Artificial Intelligence: A Modern Approach** (2020 and earlier versions, MIT Press)
  Part V ("Learning") is especially relevant to this course and provides good introductions

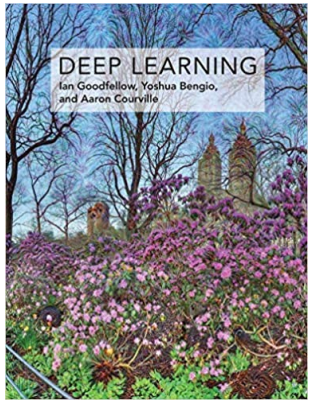


ebook@HSG

- Andreas Müller & Sarah Guido: **Introduction to Machine Learning with Python** (2017, O'Reilly)
  Easy-to-understand introduction to Python for ML, uses scikit-learn

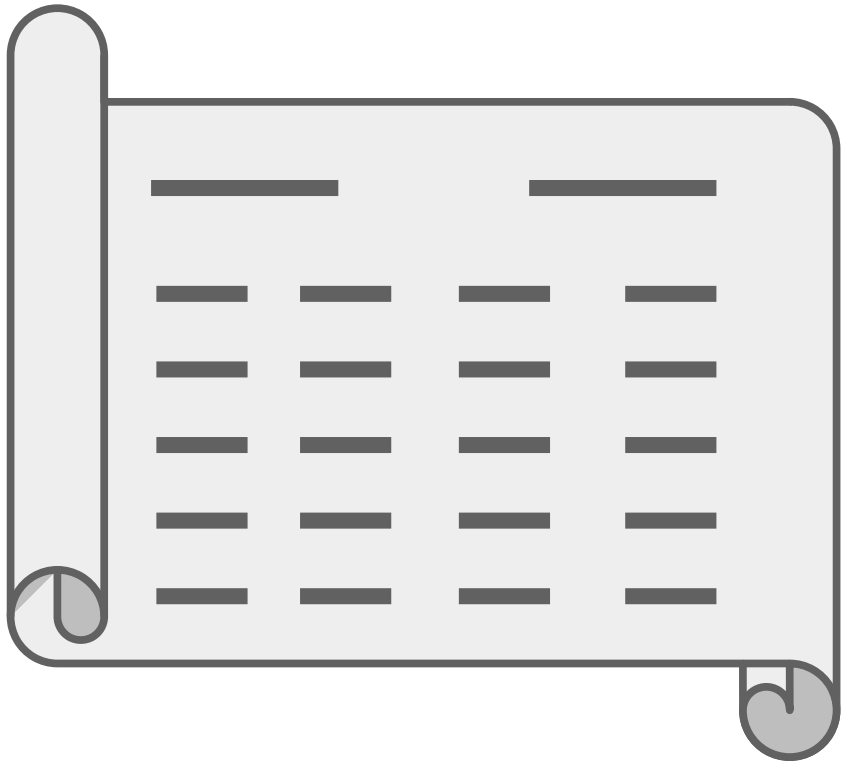


- Ian Goodfellow, Yoshua Bengio, Aaron Courville: **Deep Learning** (2016, MIT Press)
  All you need to know about Deep Learning



free online

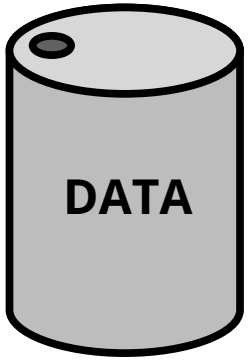
Course syllabus



Content

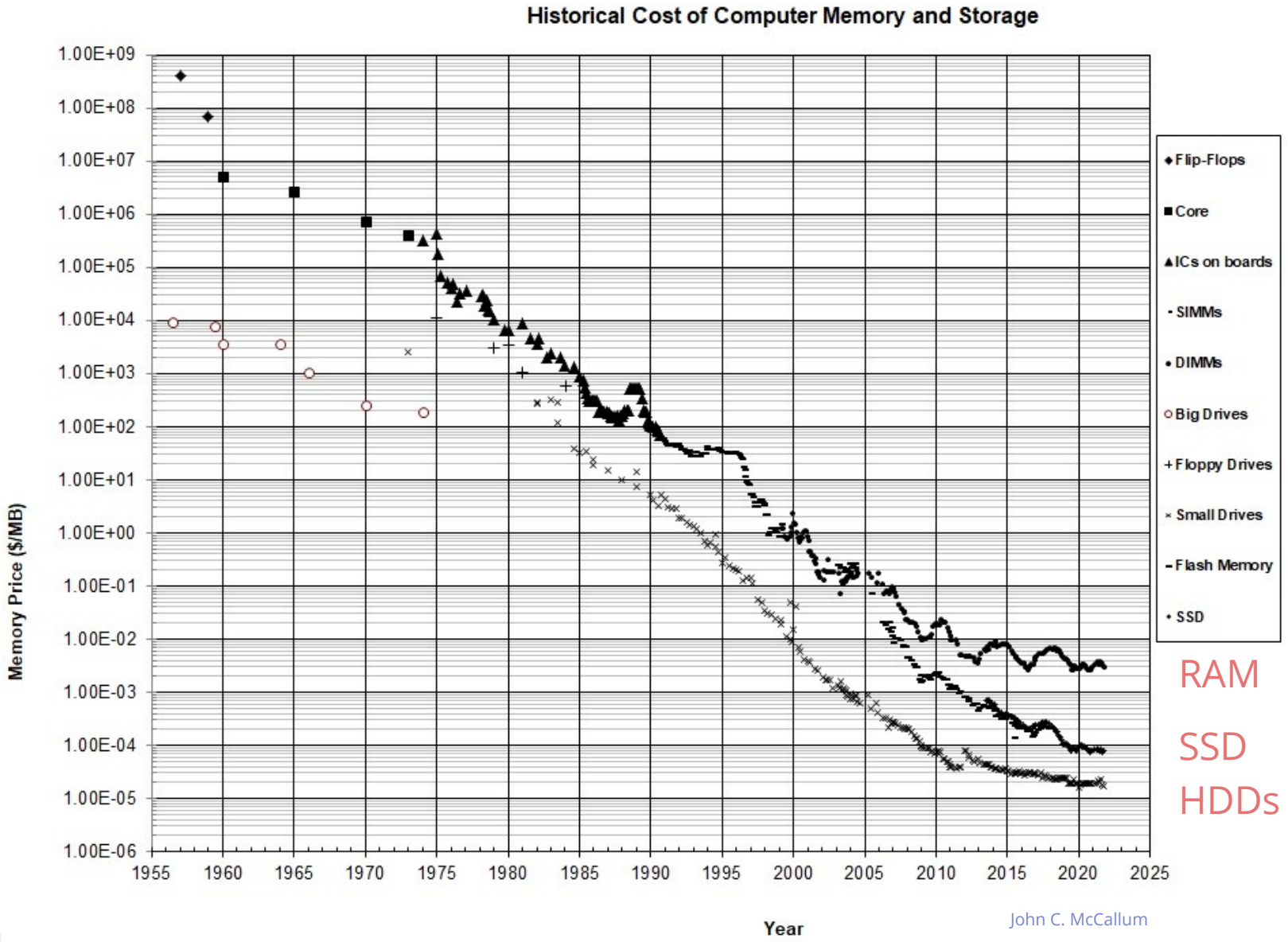
Slot	Wednesday	Thursday
09:00 - 10:30	**Intro & Data**	**Neural Networks**
10:30 – 10:45	Break	Break
10:45 – 12:15	**Supervised ML: Concepts**	**Convolutional Neural Networks & Computer Vision**
12:15 – 13:45	Lunch break	Lunch break
13:45 – 15:15	**Supervised ML: Methods**	**Lab: Neural Networks**
15:15 – 15:30	Break	Break
15:30 – 17:00	**Lab: Supervised ML**	**Advanced Deep Learning**

Data



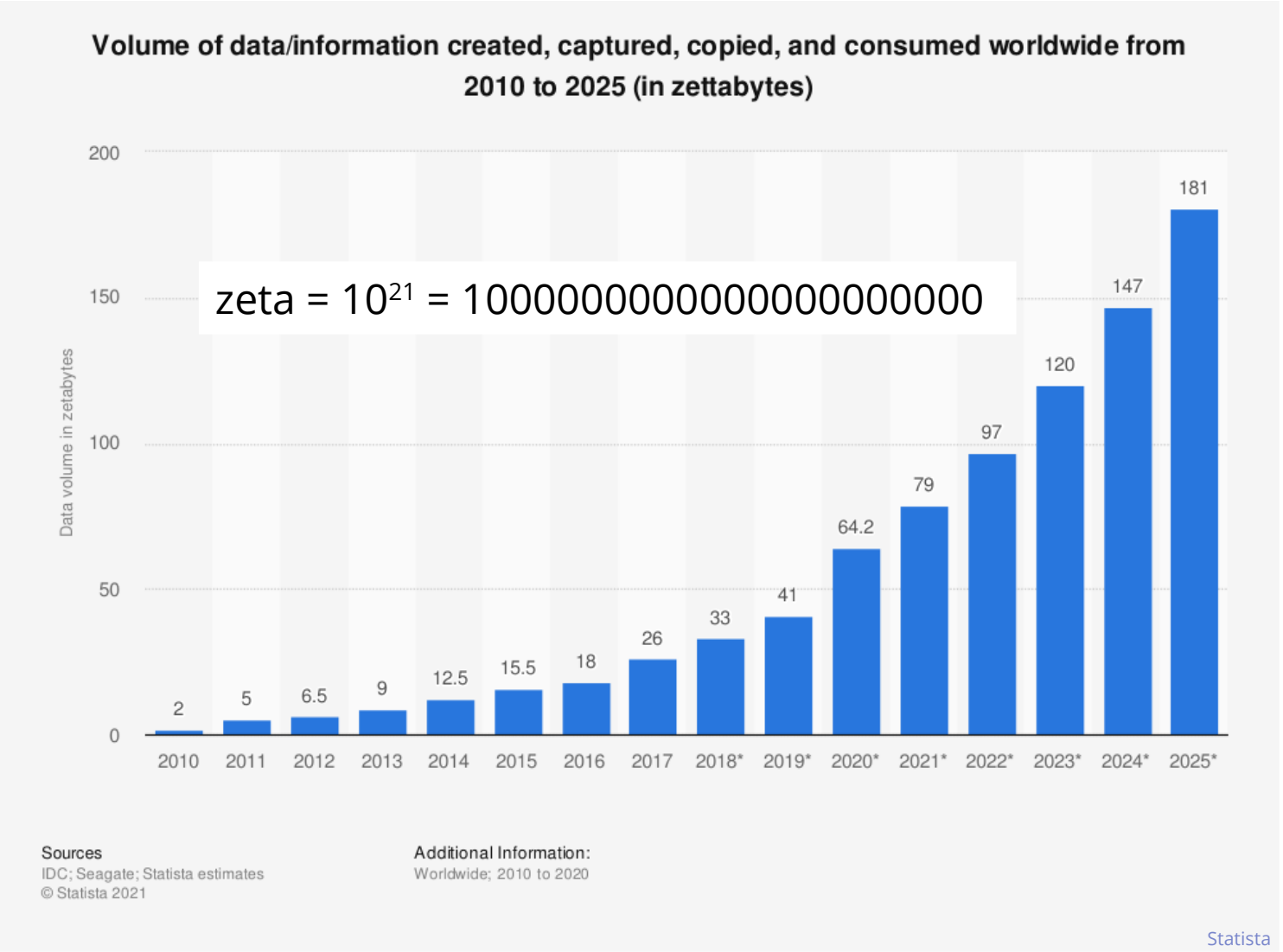
Data storage

- Data storage used to be a bottleneck – not anymore!



Data storage

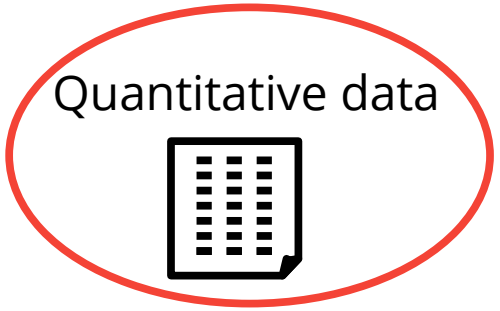
- Data storage used to be a bottleneck – not anymore!
- Vast amounts of data can now be stored easily
- Is all this data technically accessible for analysis?
  (of course not, since most of it is privately owned, but…)



Structured vs unstructured data

Structured data

Preprocessed and formatted data that is easily queryable.

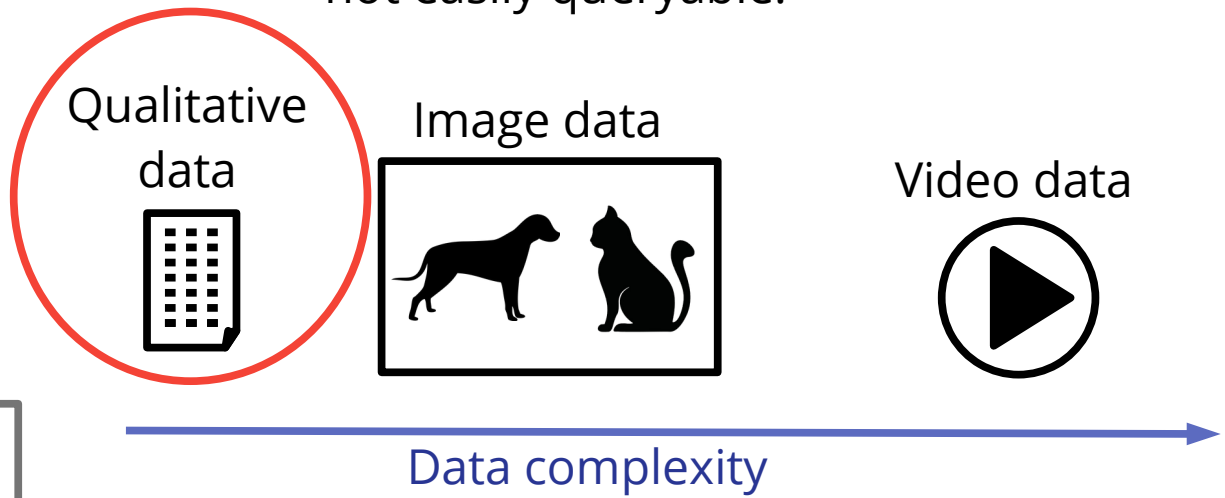


Most data analysis techniques require data to be available in a structured form for easier processing.

Structured data can always be represented in a database **schema** (e.g., a table in 2 dimensions).

Unstructured data

Unprocessed and unformatted data is not easily queryable.



Quantitative and qualitative data

Quantitative data
(can be measured; distances can be defined)

Qualitative (categorical) data
(cannot be measured; distances not defined)

Continuous data

Real-valued numbers; potentially within a given range

Examples:
- Temperatures
- A person's height
- Prices

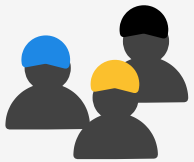
Discrete data

Discrete numbers; whole numbers or real numbers, potentially within a given range

Examples:
- Number of people in a room
- Inventory counts

Nominal data

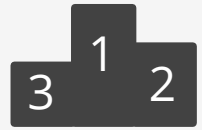
Labels for different categories without ordering



Examples:
- Color of hair
- Names of persons
- Types of fruit

Ordinal data

Labels for different categories following an inherent ranking scheme.



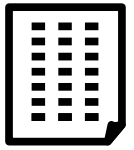
Examples:
- Rank in a competition
- Grades
- Day of the week

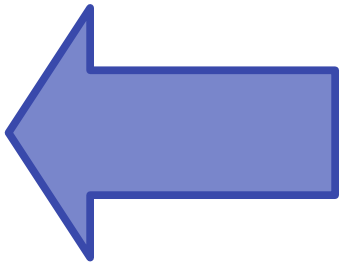
Turning unstructured data into structured data

Structured data

Preprocessed and formatted data that is easily queryable.

Quantitative





Unstructured data

Unprocessed and unformatted data is not easily queryable.

Qualitative data

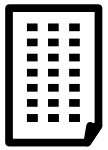
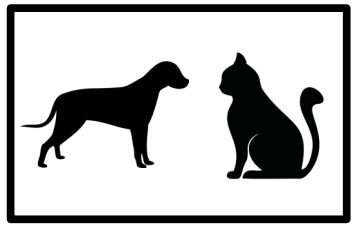


Image data



Video data

Textual data

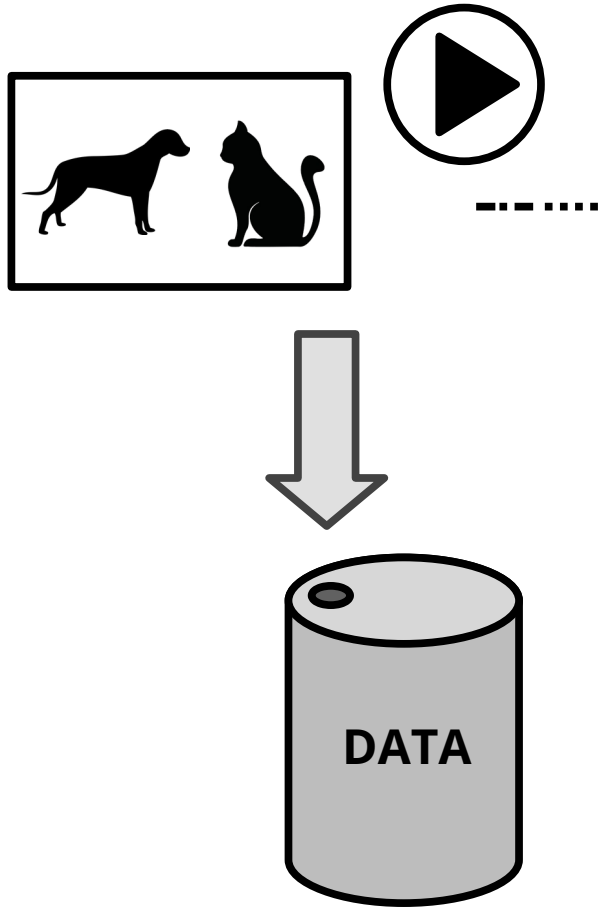
Data stream

Audio data

Before ML methods can be applied to unstructured data, we have to process those and extract useful features from them.

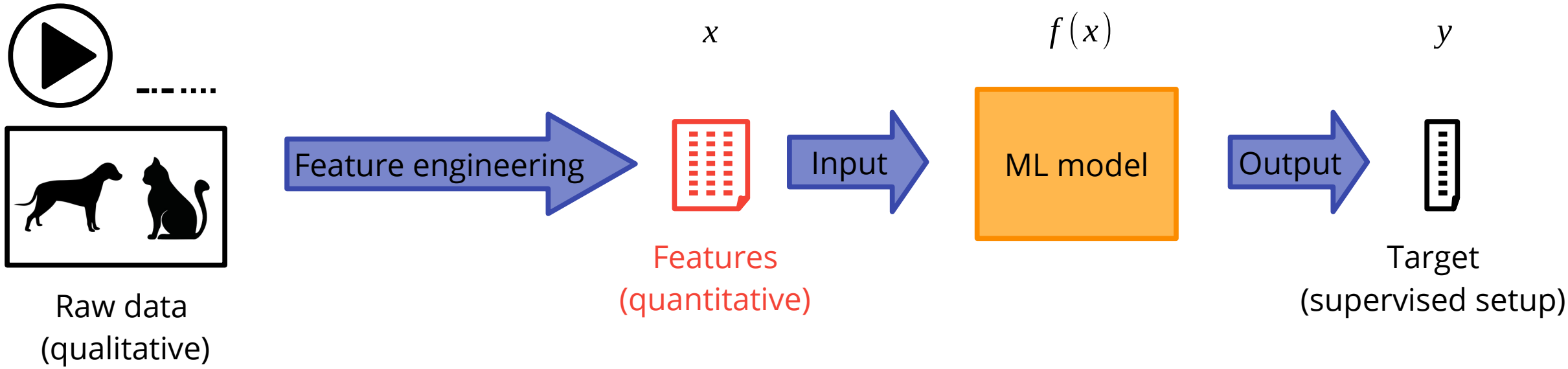
This process is called **feature engineering**.

Features and Feature Engineering



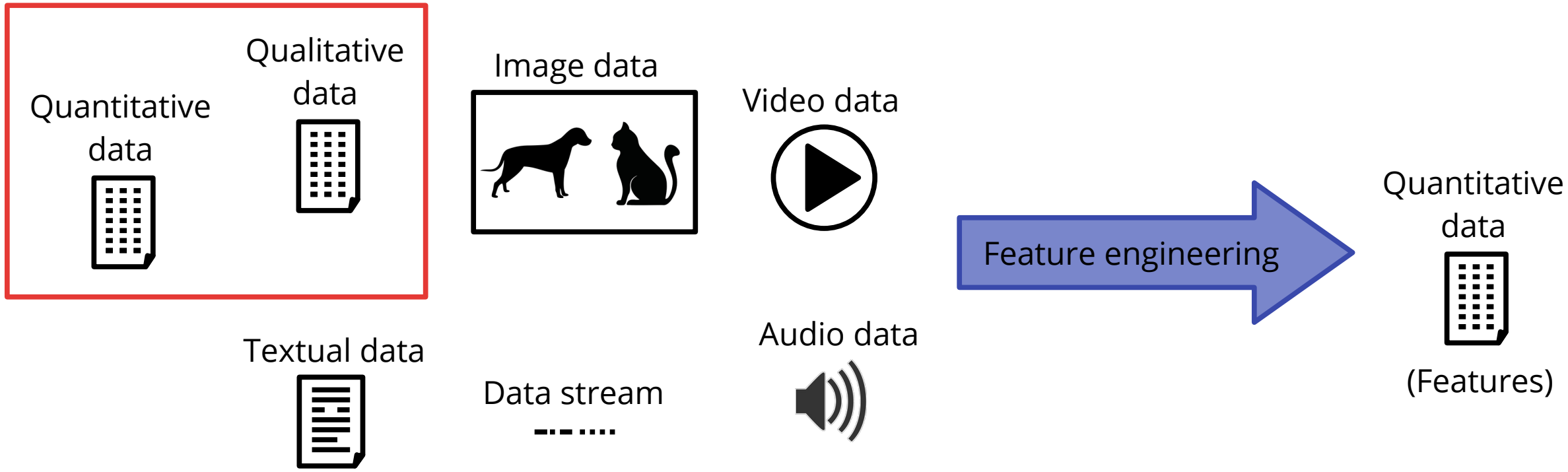
What are features?

Features are quantitative and independent variables based on which our ML models learn.



Feature engineering

Extract or create features that may provide a ML model with rich information on its task based on **domain knowledge**. Feature engineering can be applied to raw data, resulting in quantitative data that can be directly fed into the ML model (features).



Feature engineering – quantitative data

Create meaningful features through mathematical transformations.

Examples:

Arithmetic

Situation: You have two variables, x_1 and x_2, but you are more interested in their difference, δ.

Transformation:

$$\delta = x_1 - x_2$$

Aggregation of Features

Situation: You have results from different business units, x_i, but your ML model should not consider the results separately, but as an aggregated overall result, x.

Transformation:

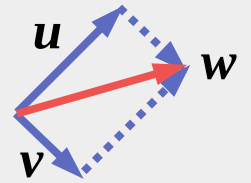
$$x = \sum_i x_i$$

Geometric Transformations

Situation: To identify common wind speed patterns, you have measurements of two orthogonal wind speed components, u and v. Since only the magnitude of the resulting wind vector, w, matters, you can utilize its magnitude, $|w|$.

Transformation:

$$|w| = \sqrt{u^2 + v^2}$$



Feature engineering – qualitative data

Qualitative (categorical) data cannot be fed into ML models directly, they have to be turned into quantitative data first. There are two common methods available, depending on the data type:

- **Label encoding**: ordinal (ranked) data → discrete quantitative data
  The intuition is that the ranking/order of the classes is conserved in a discrete numerical schema and a "distance" can be defined.

  Examples:

  - Competition ranks: [1st, 2nd, 3rd, 4th, 5th] → [1, 2, 3, 4, 5]
  - Cloudiness scale: [clear, mostly clear, partly cloudy, mostly cloudy] → [0, 1, 2, 3]
  - Quality scale: [very good, good, satisfying, sufficient, insufficient] → [0, 1, 2, 3, 4]
  - Days of the week: [Mon, Tue, Wed, Thu, Fri, Sat, Sun] → [1, 2, 3, 4, 5, 6, 7]

  ← be careful: day of week is cyclical!

  (Caveat: Label encoding can also be used if a large number of classes is present)

Feature engineering – qualitative data

Qualitative (categorical) data cannot be fed into ML models directly, they have to be turned into quantitative data first. There are two common methods available, depending on the data type:

- **Label encoding**: *ordinal (ranked) data → discrete quantitative data*
- **One-hot encoding**: *nominal (unranked) data → binary coding of labels*
  For each possible class in a feature, a binary feature is introduced; for each sample, all one-hot features are zero, only those that match have a value of one.
  Examples:
  - House properties: [balcony, cellar, fireplace, jacuzzi] →
    samples: house 1: “balcony” →
    house 2: ”fireplace” →
    Multi-class feature: house 3: ”balcony and jacuzzi” →
    house 4: “cellar, fireplace and jacuzzi” →

balcony	cellar	fireplace	jacuzzi
1	0	0	0
0	0	1	0
1	0	0	1
0	1	1	1

(Caveat: if too many classes present, use label encoding instead; see *curse of dimensionality*)

Final data set nomenclature

Feature engineering results in a compilation of features that we can use to train our ML models.

Example:

Features/Attributes (input variables, x) $f(x) = y$ **Targets**/Labels (output variables, y)

Samples/Instances

Weight	Height	Wings	Legs	Cuteness
0.1	0.1	true	2	1
3.5	0.3	false	4	1
12.0	0.7	false	4	1
500	1.8	false	4	2
800	3.0	true	4	3
...	...	...	...	...

Ground-Truth

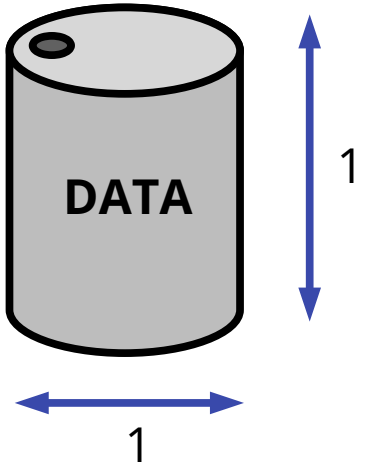
Pet	Type
true	bird
true	cat
true	dog
false	rhinoceros
false	chimera
...	...

classes of label "Type"

Data Types:

continuous	continuous	binary	discrete	ordinal	binary	categorical (multi-class)

Data scaling

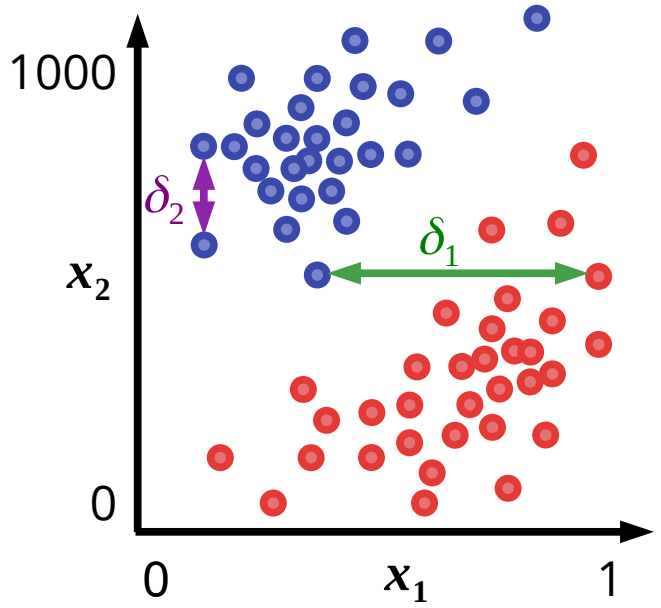


Data scaling

Data scaling means to linearly transform your data in order to normalize them.

Why scale data?

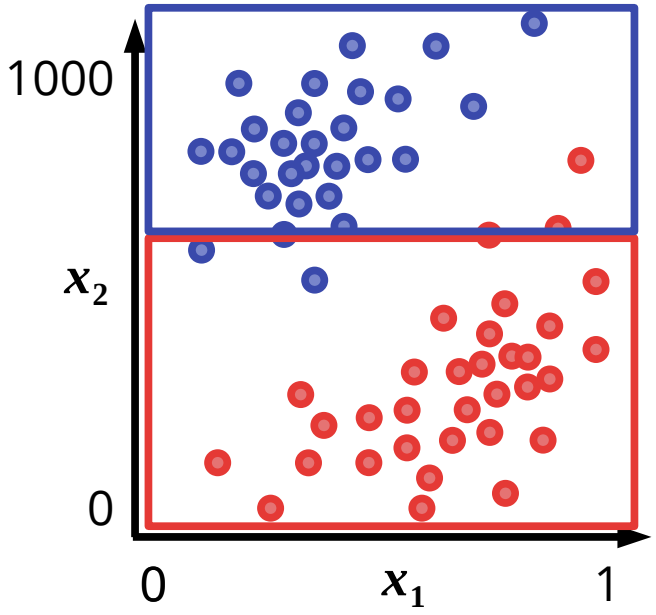
- Many ML models are based on a notion of "distance" between samples; improperly scaled data may jeopardize the learning capability of such models.



$$\delta = \sqrt{x_1^2 + x_2^2}$$

Euclidean distance metric

$$\delta_1 \ll \delta_2$$



Decision regions of a hypothetical distance-based classifier.

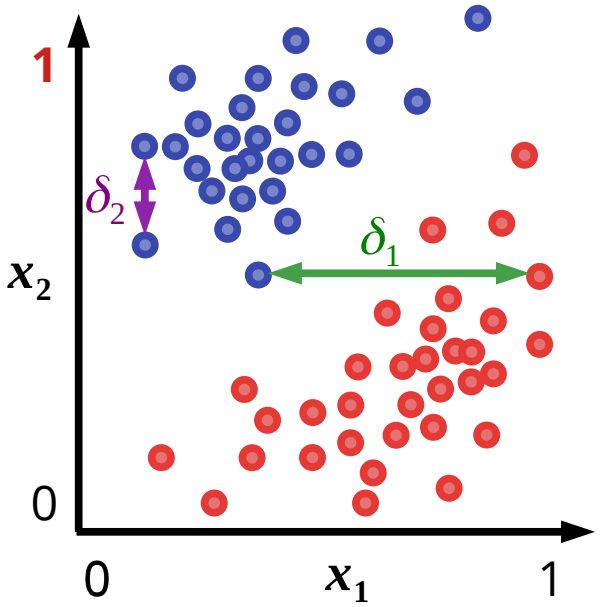
Results are ok-ish, but could be much better…

Data scaling

Data scaling means to linearly transform your data in order to standardize them.

Why scale data?

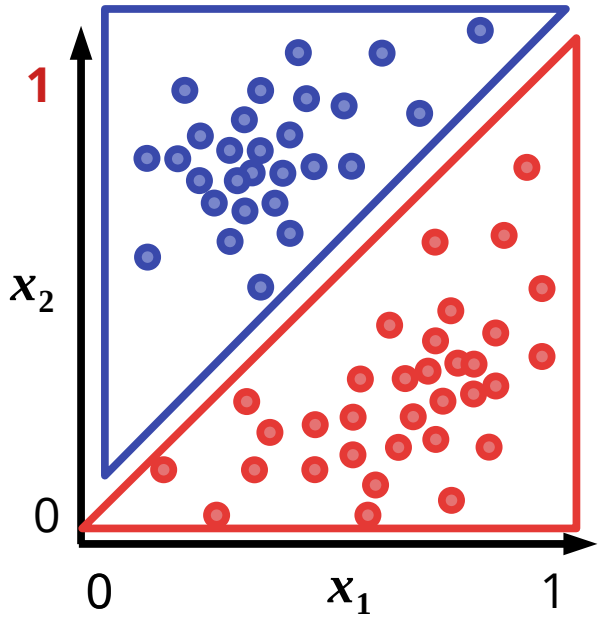
- Many ML models are based on a notion of "distance" between samples; improperly scaled data may jeopardize the learning capability of such models.



$$\delta = \sqrt{x_1^2 + x_2^2}$$

Euclidean distance metric

$\delta_1 > \delta_2$



Decision regions of a hypothetical distance-based classifier.

This is much better!

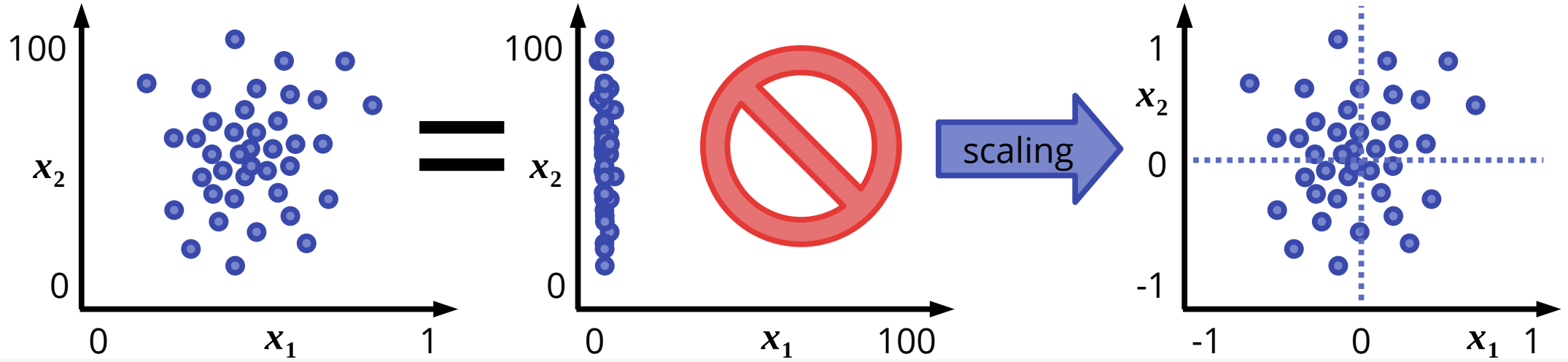
Data should be scaled!

Data scaling

Data scaling means to linearly transform your data in order to standardize them.

Why scale data?

- Many ML models are based on a notion of “distance” between samples; improperly scaled data may jeopardize the learning capability of such models.
- Some ML models intrinsically presume that data are distributed following a Gaussian fashion with similar variances along all features; high variance along one feature leads to bias.



Data scaling

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Why scale data?

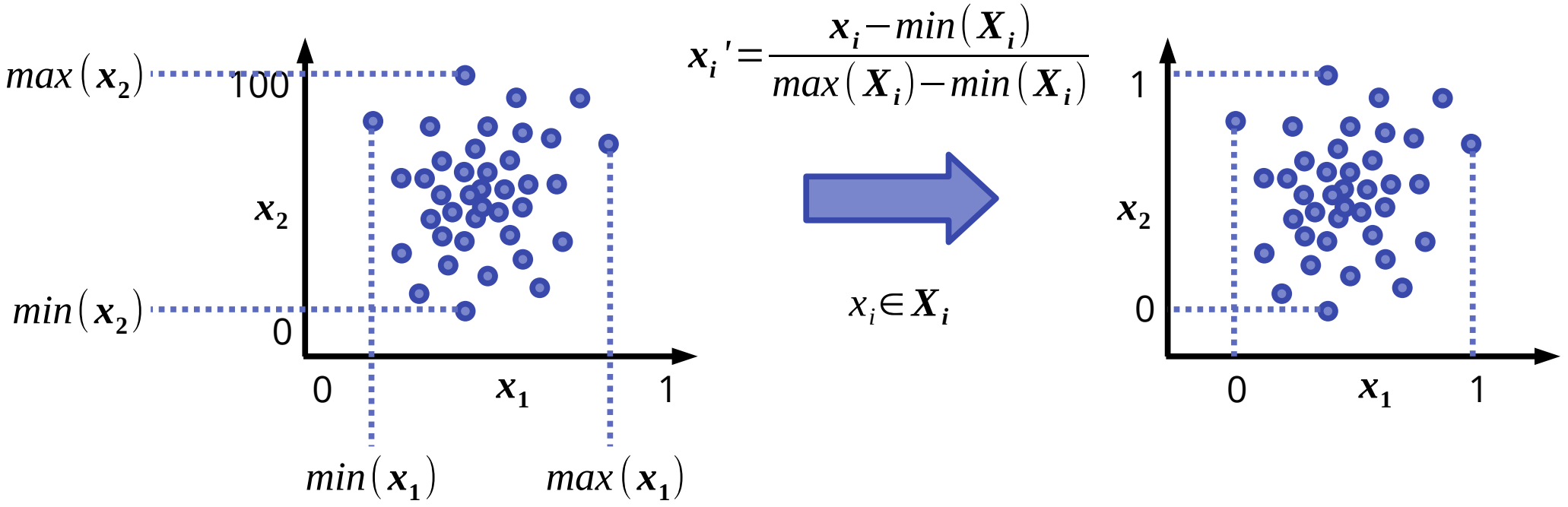
- Many ML models are based on a notion of “distance” between samples; improperly scaled data may jeopardize the learning capability of such models.
- Some ML models intrinsically presume that data are distributed following a Gaussian fashion with similar variances along all features; high variance along one feature leads to bias.

How to scale data?

- Normalize feature variances (to give similar weights to the different features)
- Normalize feature mean values (assumed by a number of ML models)

Data scaling – MinMax scaler

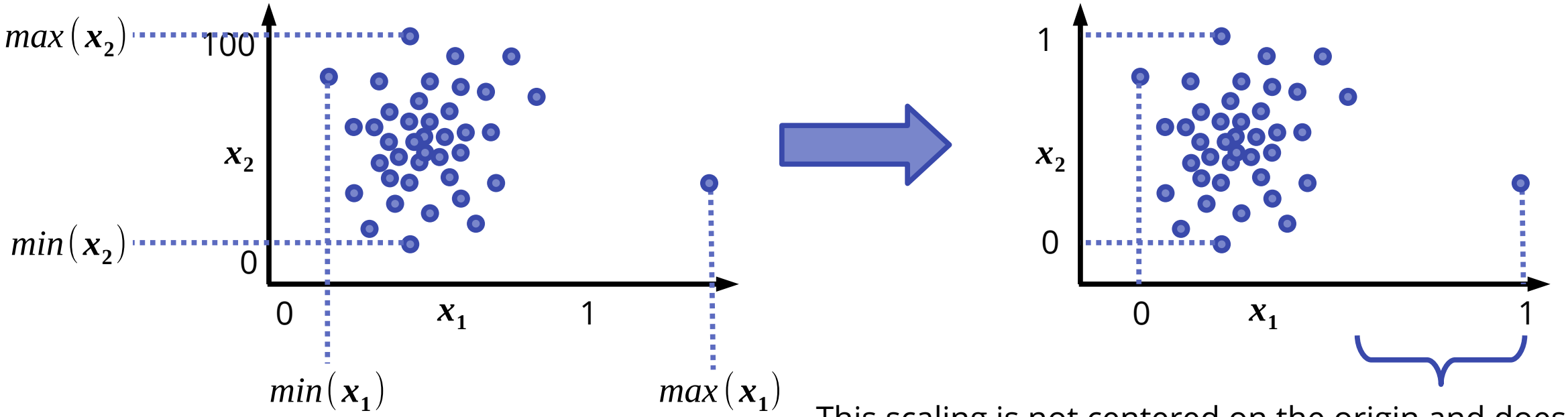
Scale every feature onto a range from 0 to 1 based on the minimum and maximum of the underlying distribution.



Data scaling – MinMax scaler

Scale every feature onto a range from 0 to 1 based on the minimum and maximum of the underlying distribution.

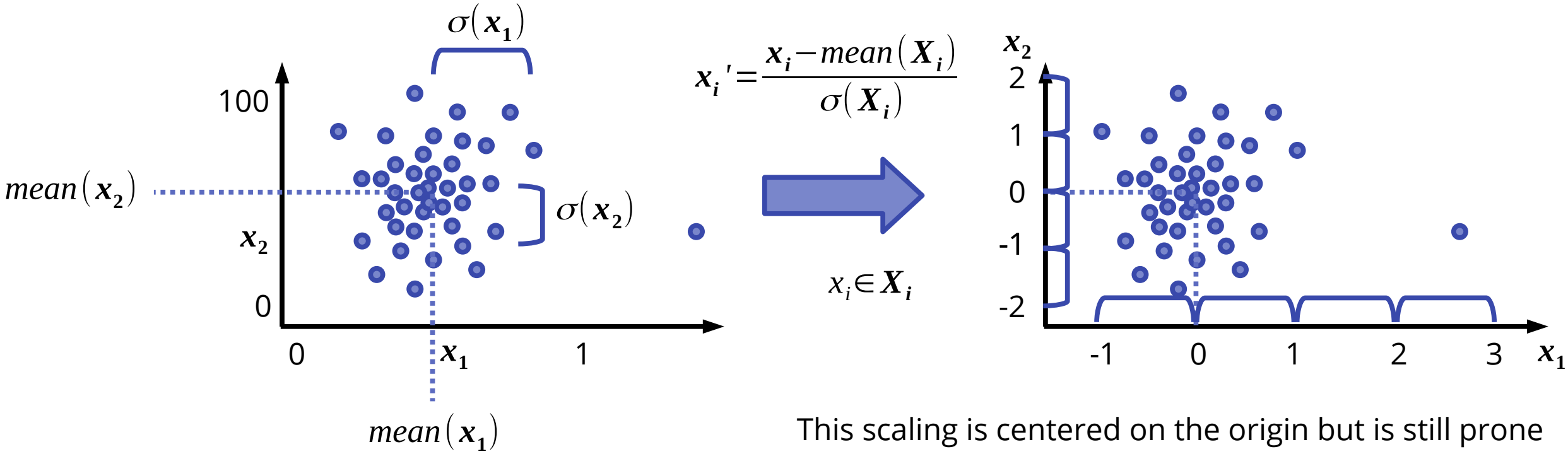
Disadvantage: the MinMax scaler is prone to outliers and does not center the distribution in the origin.



This scaling is not centered on the origin and does not describe the data distribution well.

Data scaling – Standard scaler

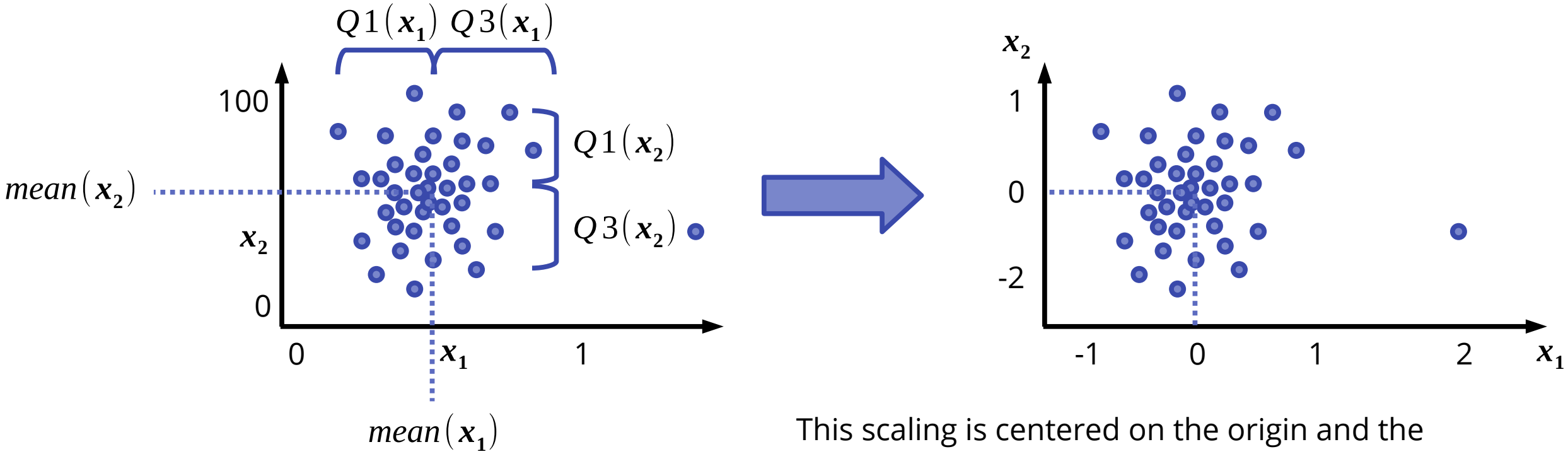
Scale every feature onto a range from -1 to 1 based on the mean and standard deviation of the underlying distribution.



This scaling is centered on the origin but is still prone to outliers to some extent.

Data scaling – Robust scaler

Scale every feature onto a range from -1 to 1 based on the mean and the quantiles of the underlying distribution.



This scaling is centered on the origin and the resulting distribution is less affected by outliers

That’s all folks!