Lecture 1: Introduction & Data

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

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

Today's lecture

What this course is about...

Who am I?

Course modalities

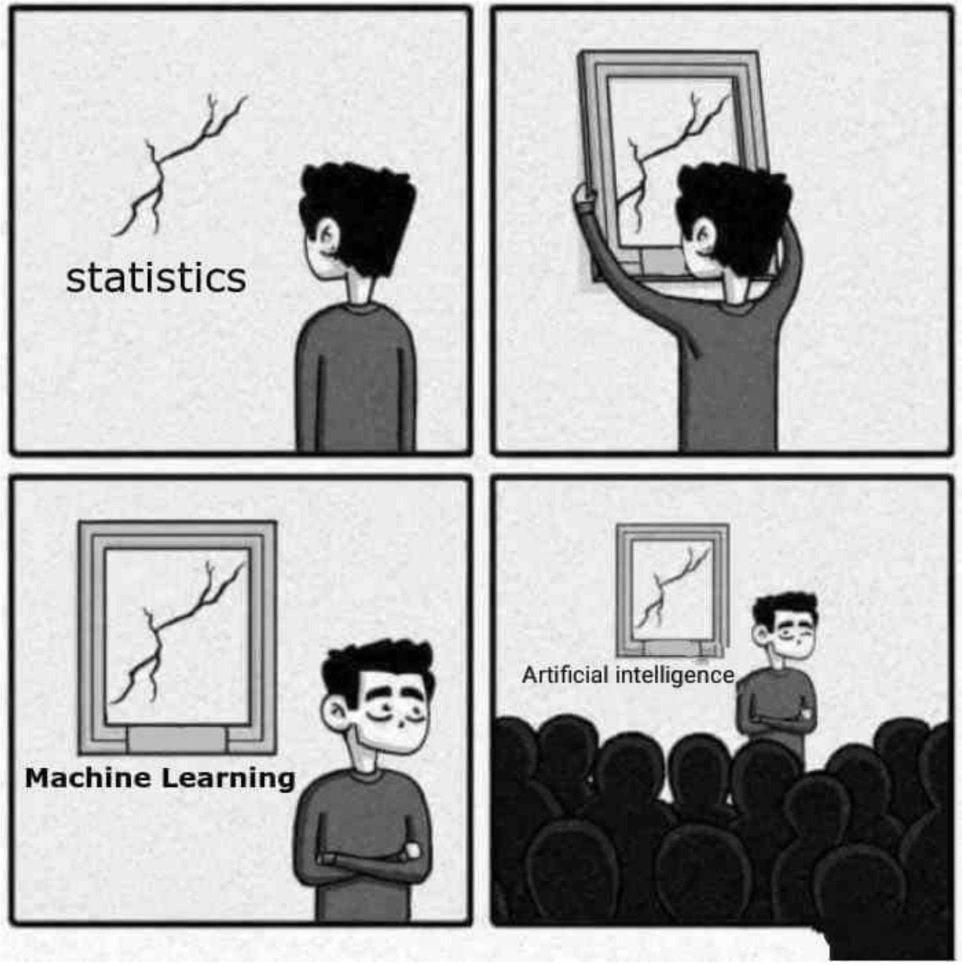
Course syllabus

Types of data

Features and feature engineering

Data scaling

What this course is about...



sandserif

Mapping terminology

Mapping terminology

Artificial Intelligence

Systems that perceive their environment and take actions to maximize their chances of achieving their goals.

Mapping terminology

Statistics

Data science

Mathematics

Artificial Intelligence

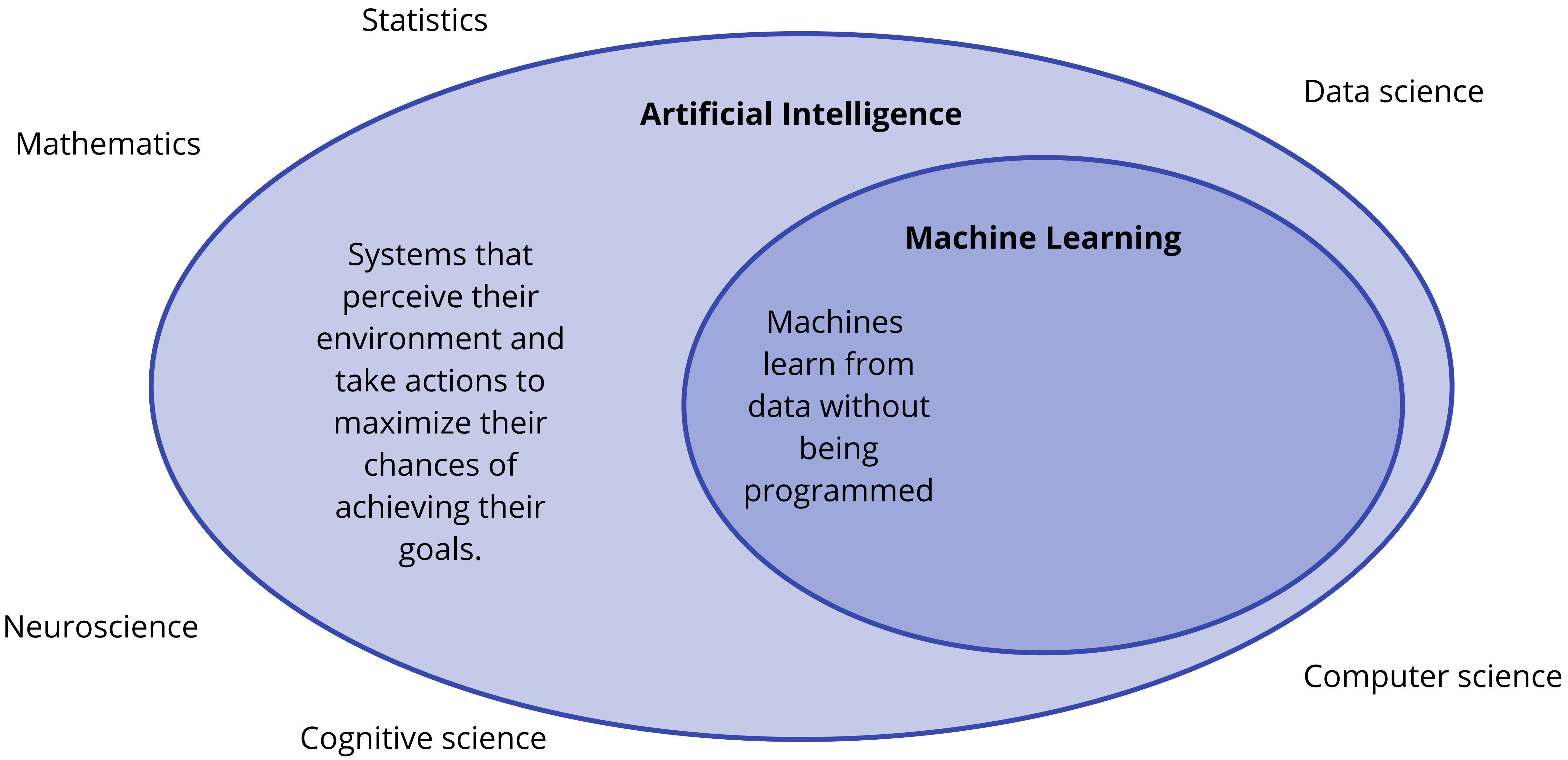
Systems that perceive their environment and take actions to maximize their chances of achieving their goals.

Neuroscience

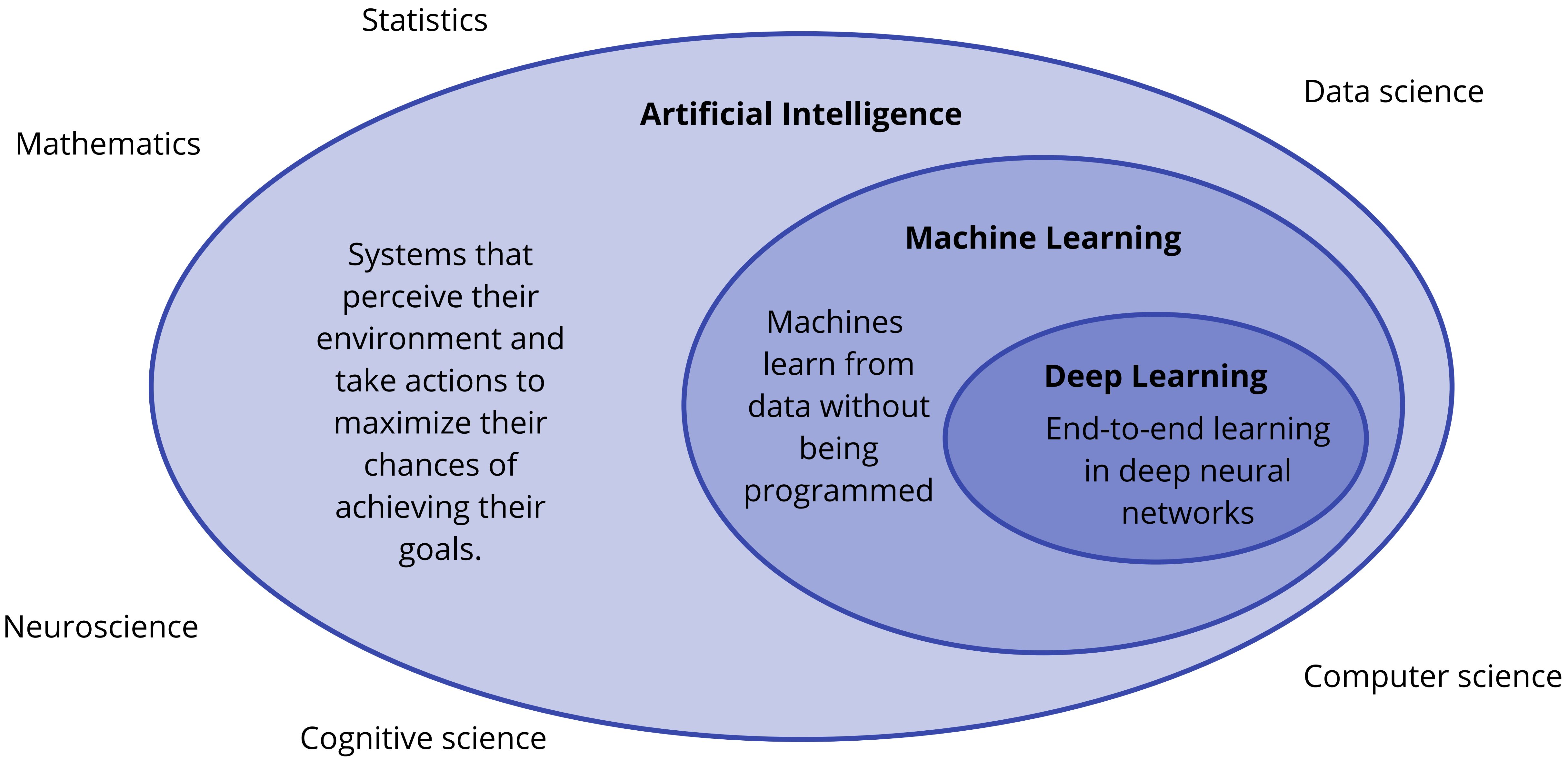
Computer science

Cognitive science

Mapping terminology



Mapping terminology



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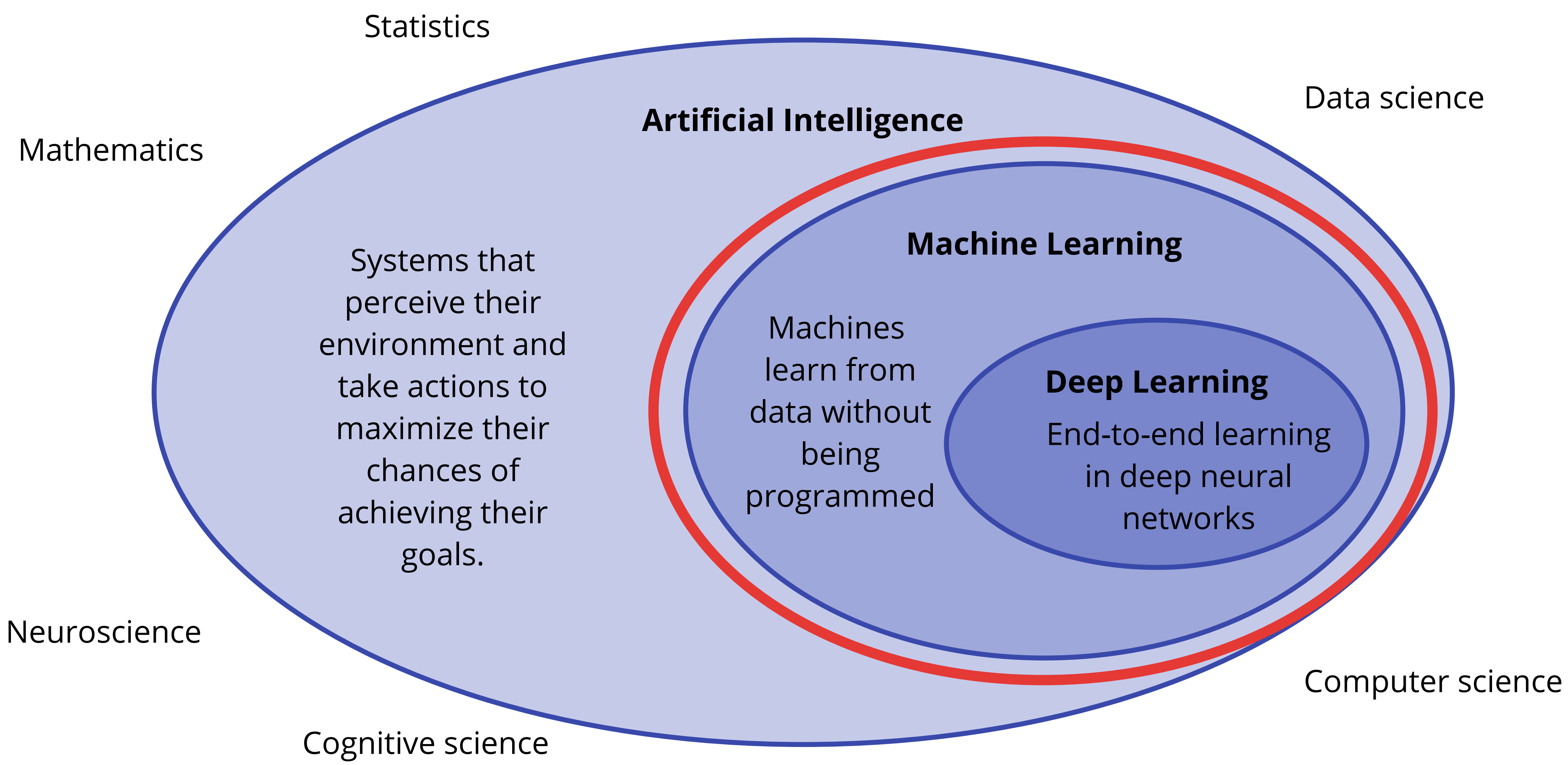


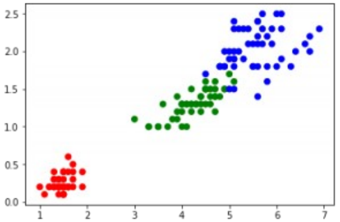
What is Machine Learning (ML)?

> *"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.

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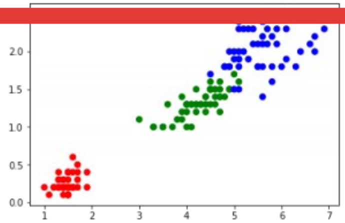

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Supervised ML

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General goal for supervised problems:
Find a function (“task”) that relates input data ($\boldsymbol{x}$) to output data ($\boldsymbol{y}$) such that: $f(\boldsymbol{x}) = \boldsymbol{y}$

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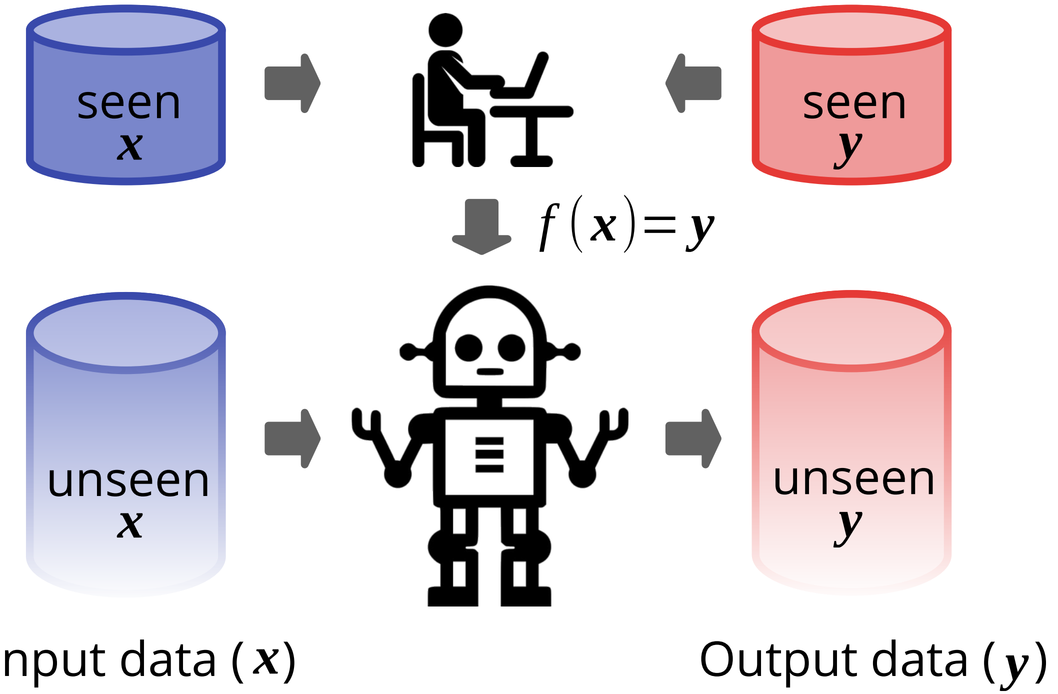
Traditional (Rule-based) Approach:



Supervised ML

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

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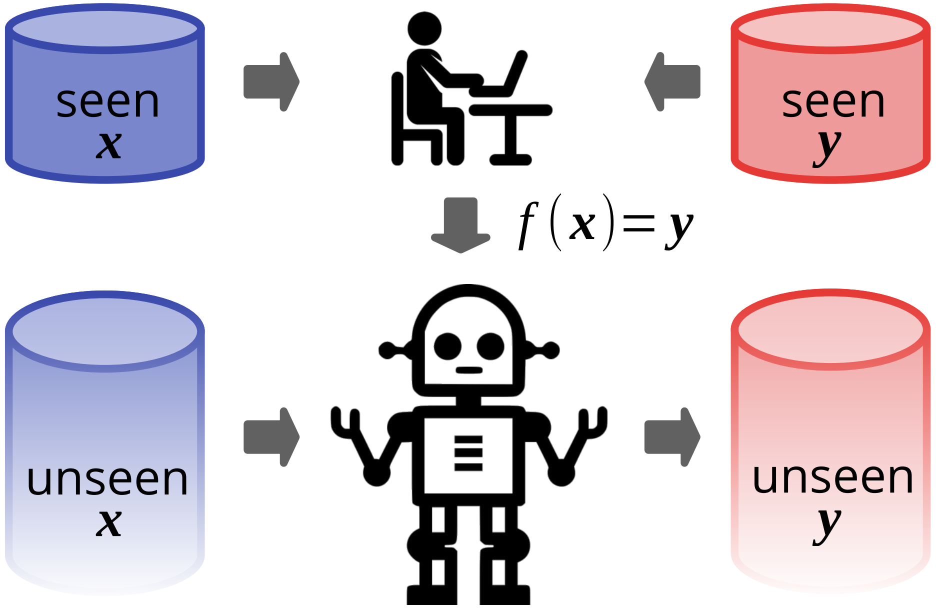
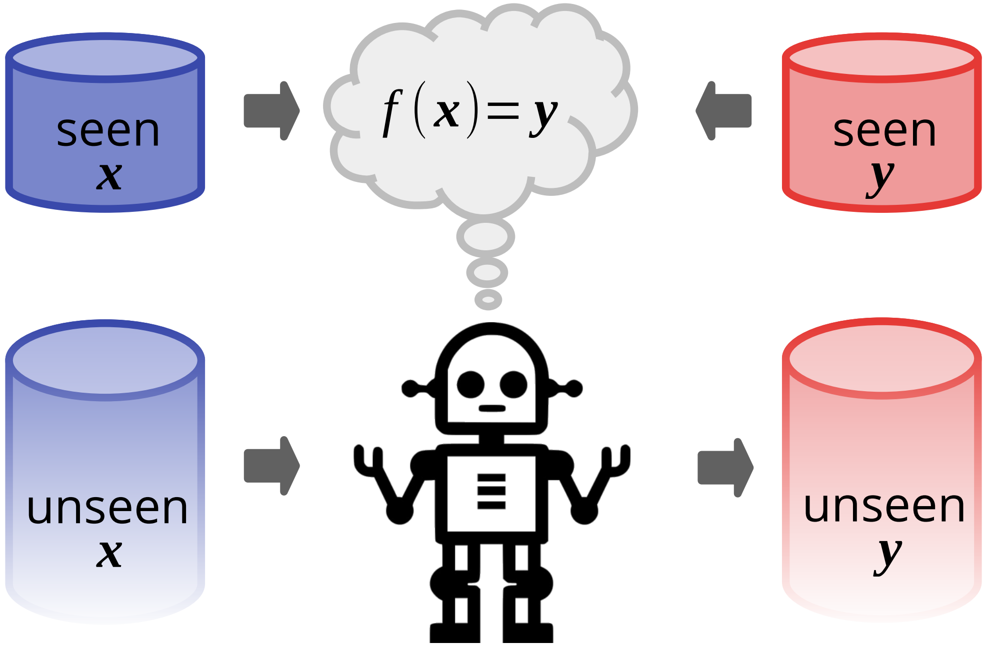


Input data (x) Output data (y)

Machine-Learning Approach:



Input data (x) Output data (y)

Who am I?

About myself

About myself

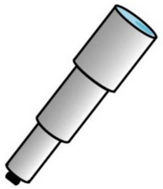
UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

Physics

2009

About myself

About myself



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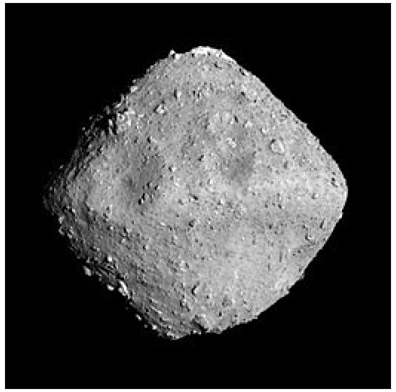

Gerald Rhemann

Deutsches Zentrum für Luft- und Raumfahrt
German Aerospace Center

Northern Arizona University

Universität Heidelberg
Zukunft seit 1386

Freie Universität Berlin

Lowell Observatory
125 years | 1894 - 2019

Physics

Dr. rer. nat.
(Earth Sciences)

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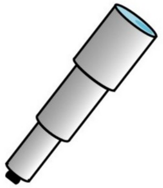
About myself



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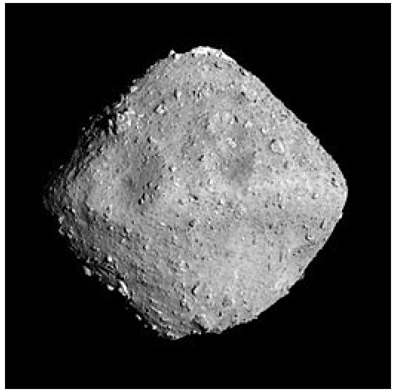

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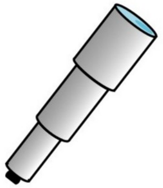

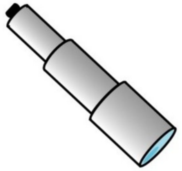

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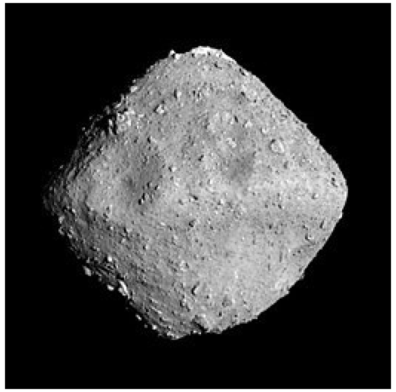

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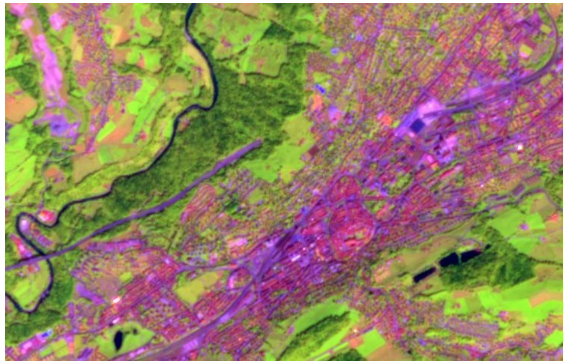

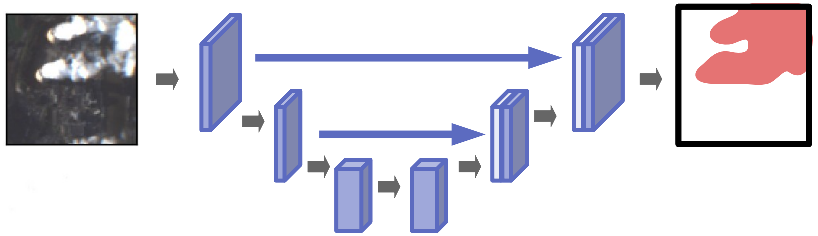

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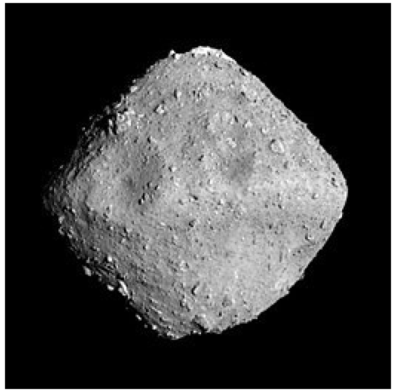

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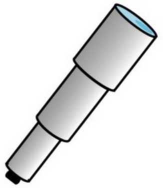

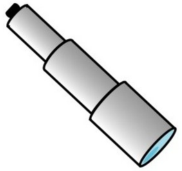

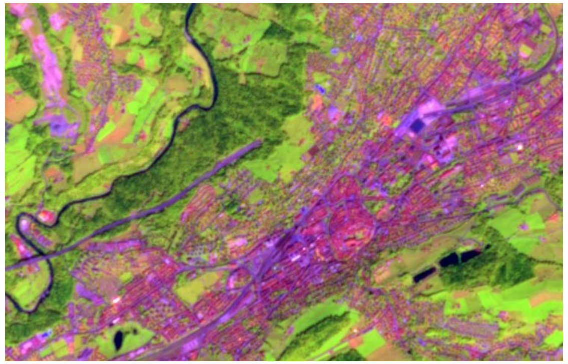

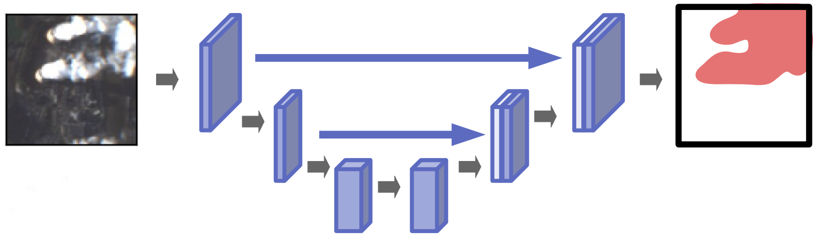

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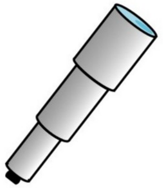

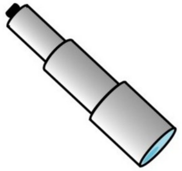

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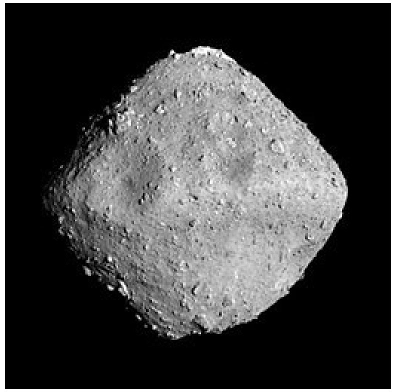

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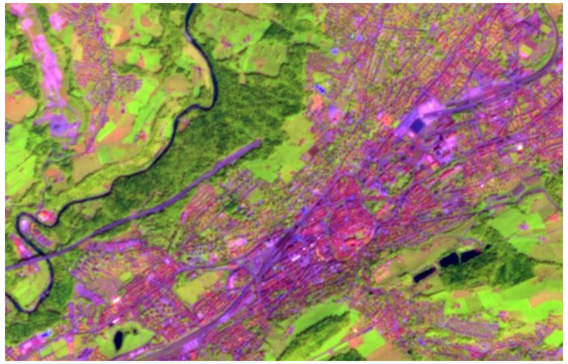

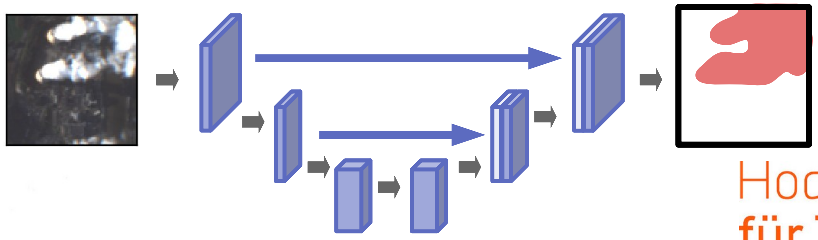

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- 2024: Prof. AI in Remote Sensing

What I work on...

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

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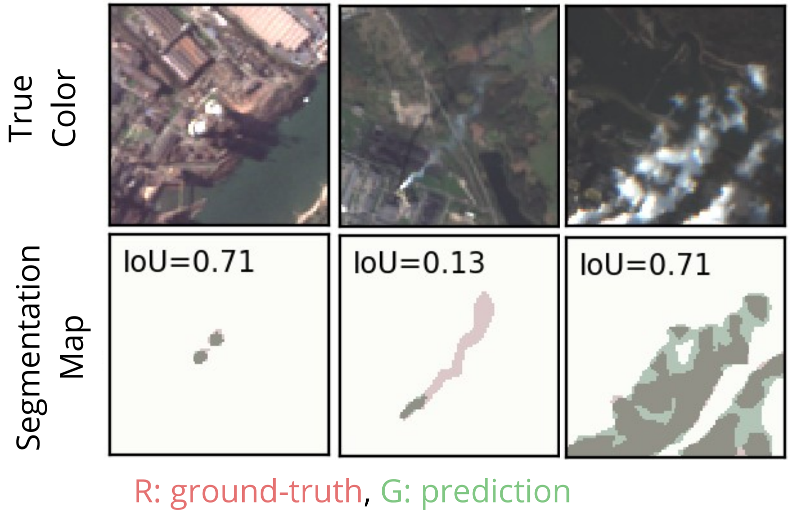
Characterization of Plumes and Estimation of Power Generation from Remote Sensing Data
(*Mommert et al. 2020, Hanna et al. 2023*)



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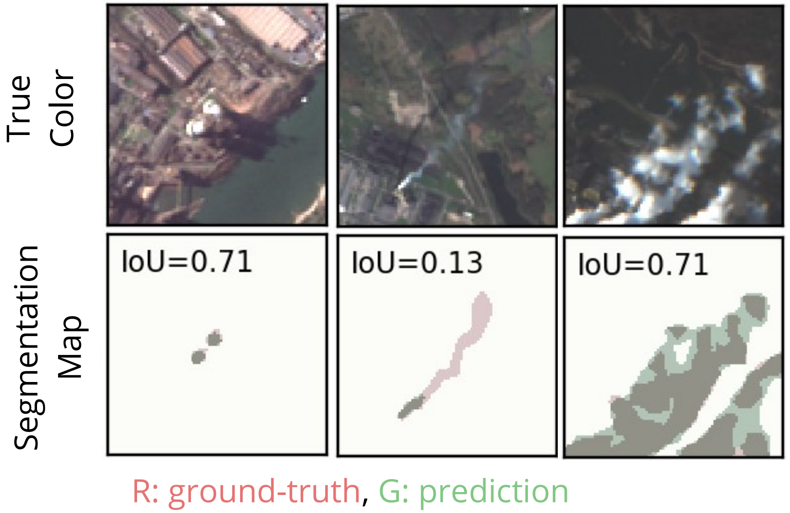

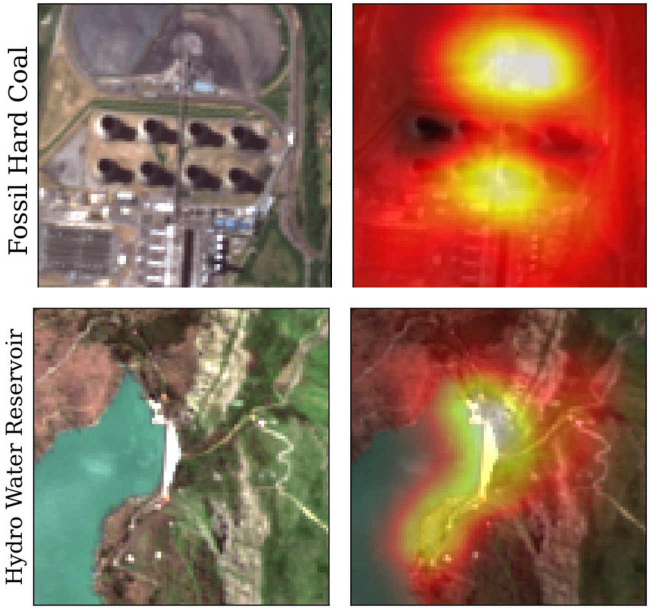

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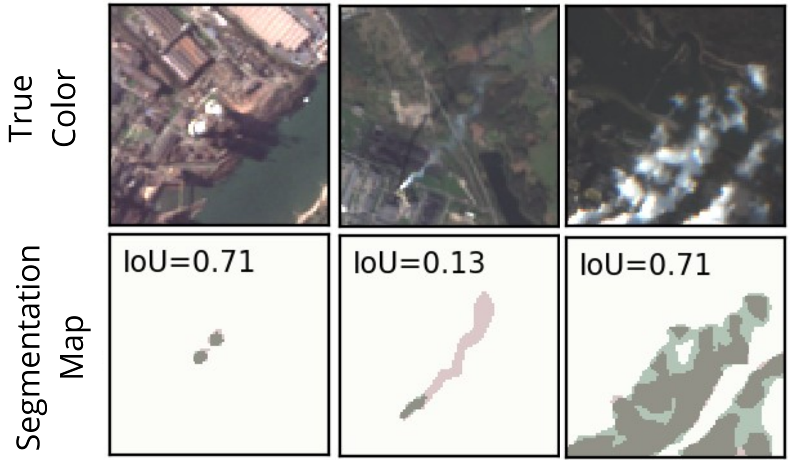
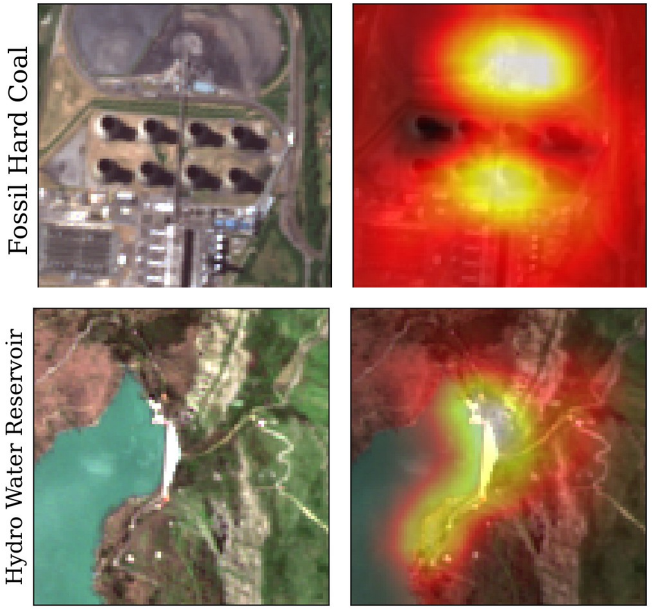


R: ground-truth, G: prediction



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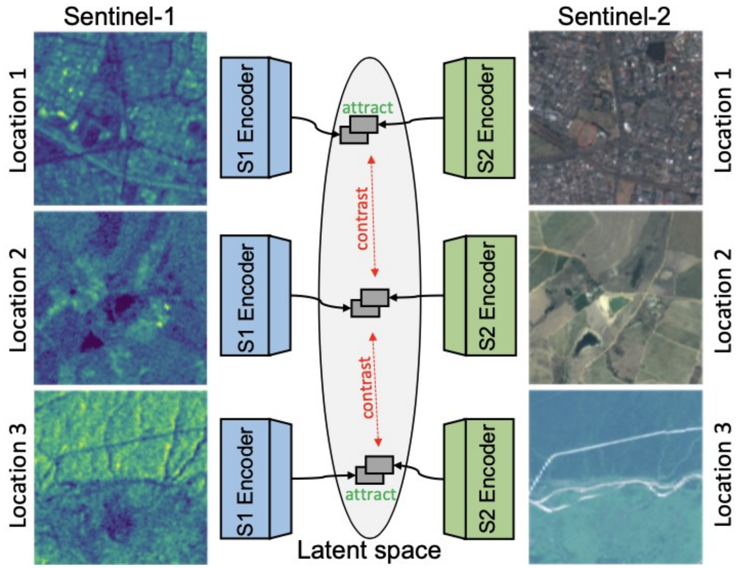
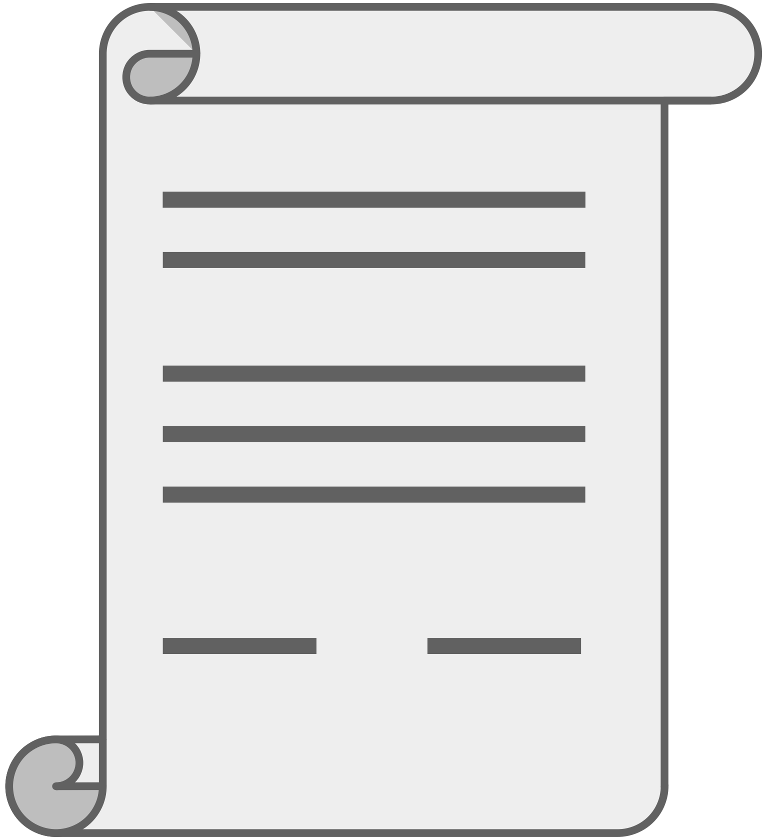
Contrastive Self-supervised data fusion for Satellite Imagery
(Scheibenreif et al. 2022)



Course modalities

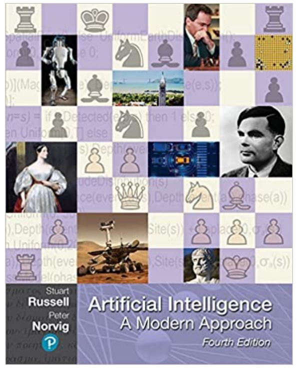


Course modalities

- **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!

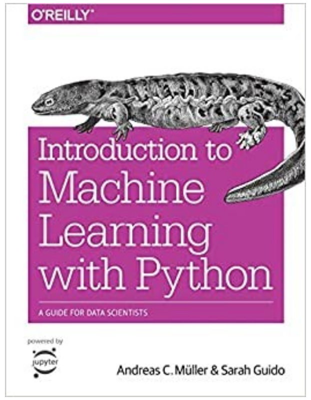
Literature resources

- 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

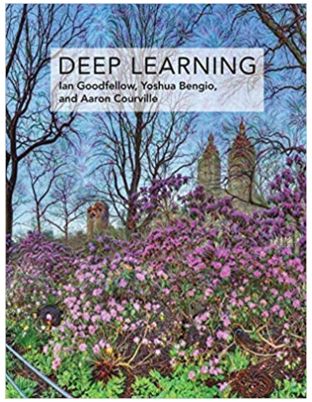


ebook@HSG

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

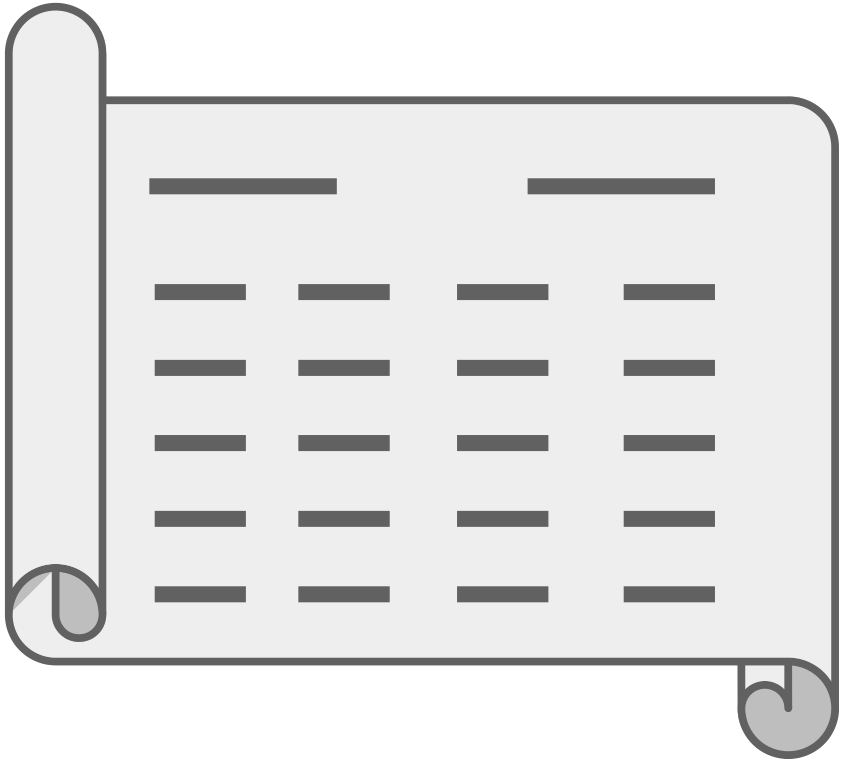


- Ian Goodfellow, Yoshua Bengio, Aaron Courville: **Deep Learning** (2016, MIT Press)
  All you need to know about Deep Learning



free online

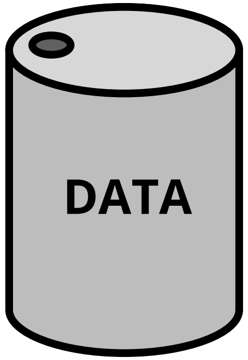
Course syllabus



Content

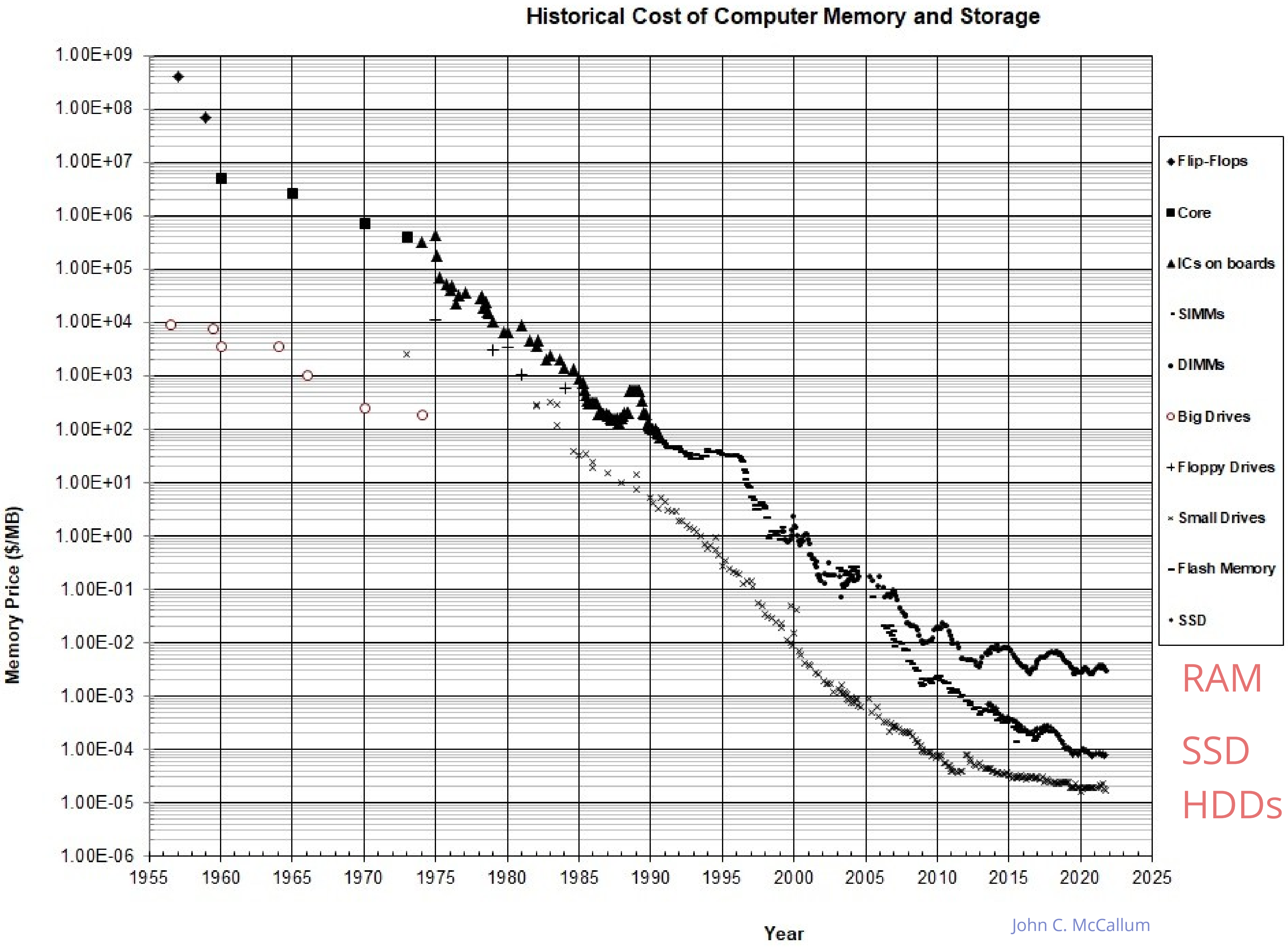
Slot	Wednesday	Thursday
09:00 - 10:30	**Intro & Data**	**Neural Networks**
10:30 – 10:45	Break	Break
10:45 – 12:15	**Supervised ML: Concepts**	**Convolutional Neural Networks & Computer Vision**
12:15 – 13:45	Lunch break	Lunch break
13:45 – 15:15	**Supervised ML: Methods**	**Lab: Neural Networks**
15:15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



John C. McCallum

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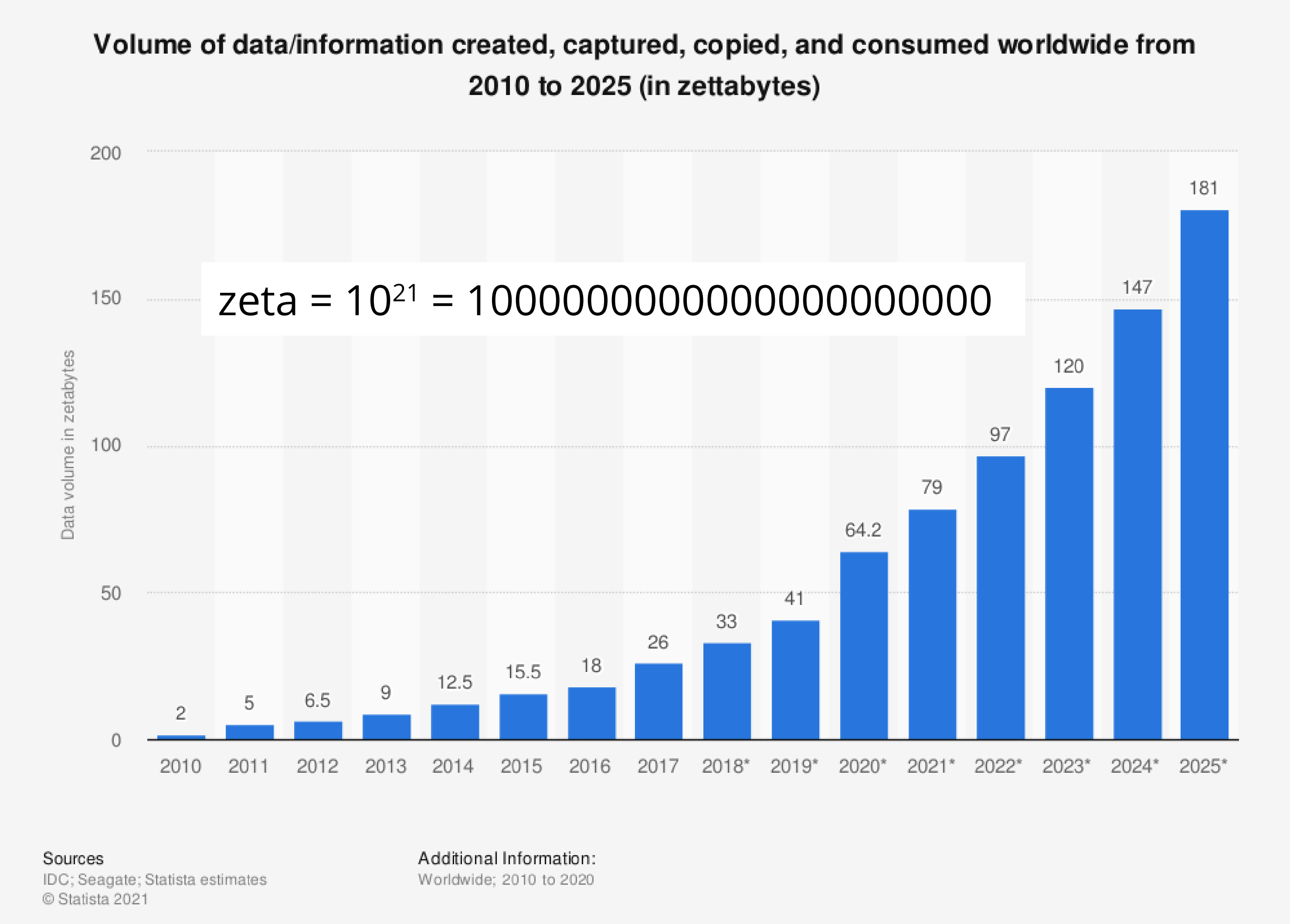


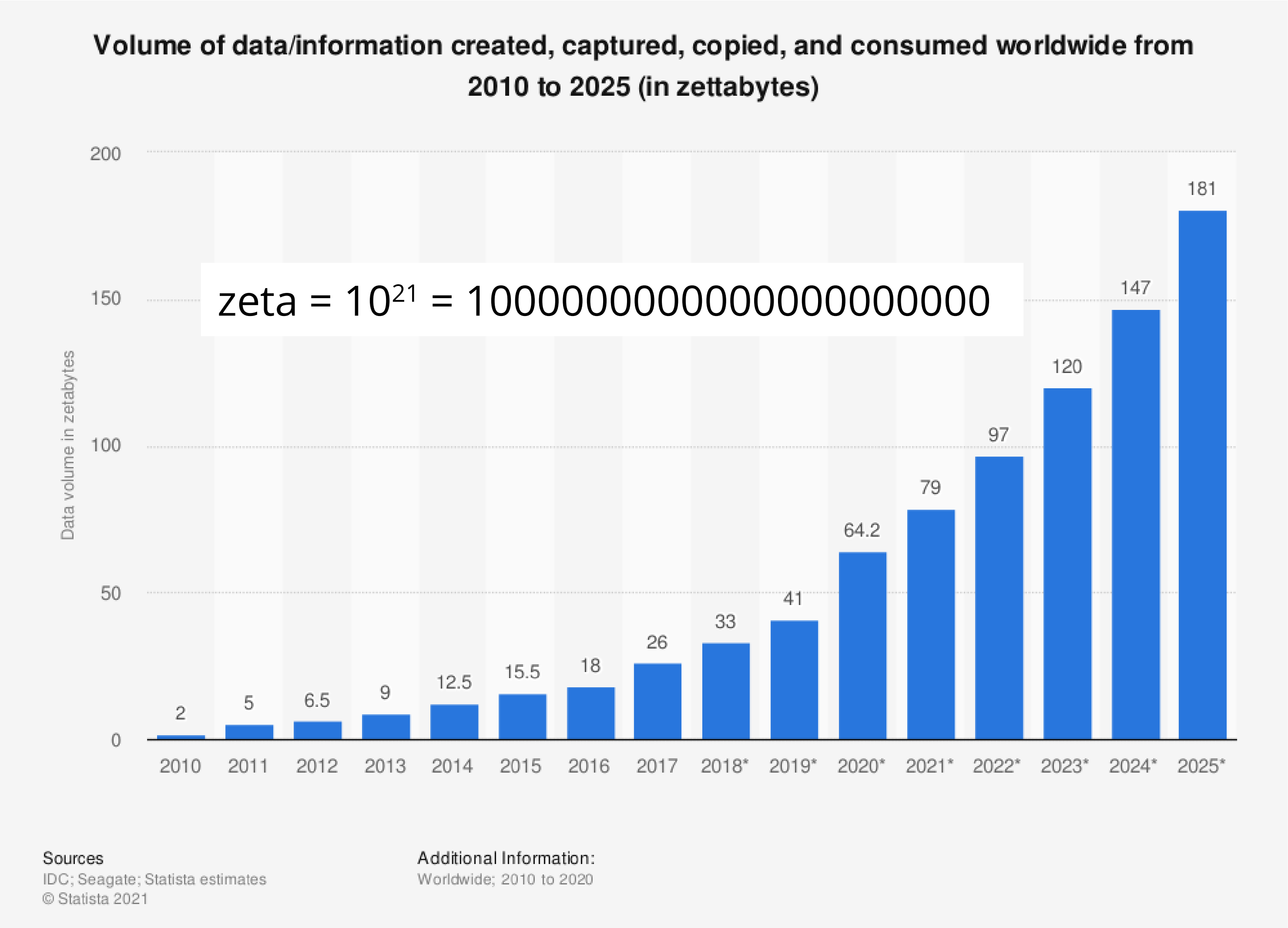
Statista

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...)



Statista

Structured vs unstructured data

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Structured data

Preprocessed and formatted data that is easily queryable.

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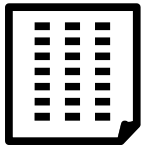
Quantitative data



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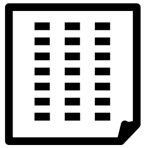

Unstructured data

Unprocessed and unformatted data is not easily queryable.

Structured vs unstructured data

Structured data

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Quantitative data

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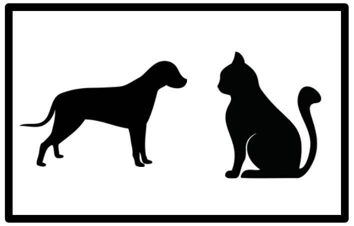
Qualitative data

Image data



Video data

Textual data

Data stream

Audio data

Structured vs unstructured data

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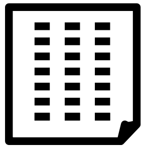

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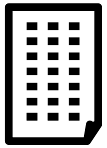
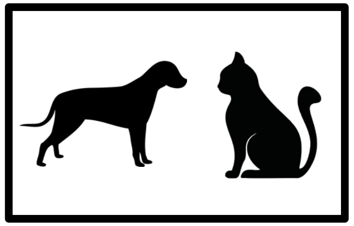
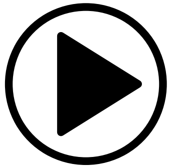


Image data

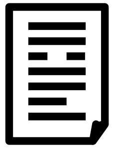


Video data



Data complexity

Textual data



Data stream

Audio data

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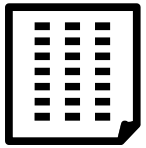


Most data analysis techniques require data to be available in a structured form for easier processing.

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.

Qualitative data

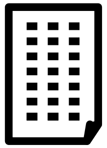
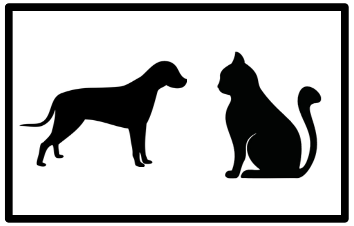
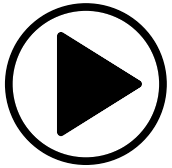


Image data

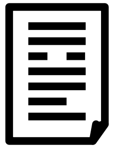


Video data



Data complexity

Textual data



Data stream

Audio data

Structured vs unstructured data

Structured data

Preprocessed and formatted data that is easily queryable.

Quantitative data

Unstructured data

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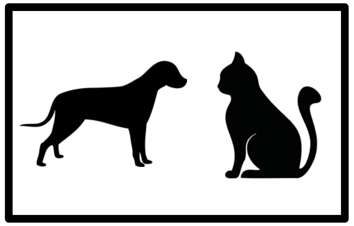
Qualitative data

Image data



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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).

Quantitative and qualitative data

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

Quantitative and qualitative data

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

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Continuous data

Real-valued numbers; potentially within a given range

Examples:
- Temperatures
- A person’s height
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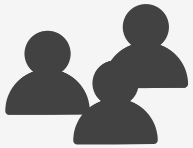
Discrete data

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



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

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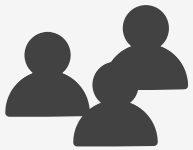

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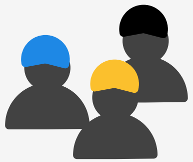
Nominal data

Labels for different categories without ordering



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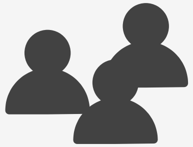

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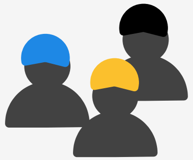

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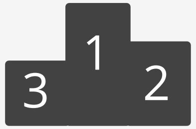
Ordinal data

Labels for different categories following an inherent ranking scheme.



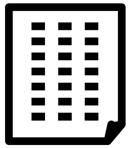
Examples:
- Rank in a competition
- Grades
- Day of the week

Turning unstructured data into structured data

Structured data

Preprocessed and formatted data that is easily queryable.

Quantitative



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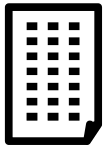

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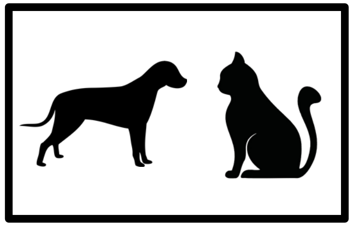

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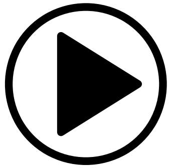

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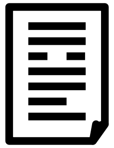

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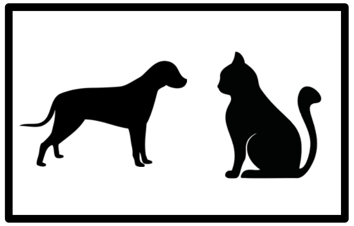

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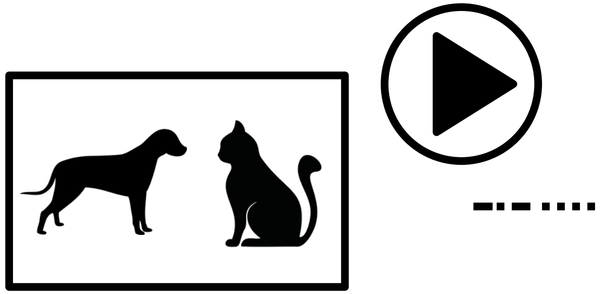
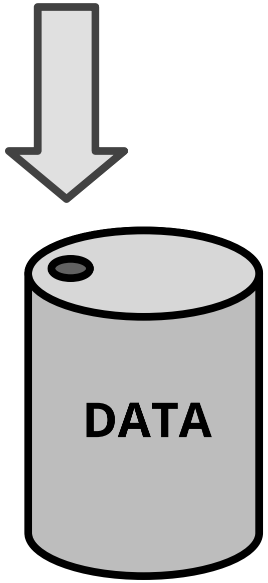
Before ML methods can be applied to unstructured data, we have to process those and extract useful features from them.

This process is called **feature engineering**.



Features and Feature Engineering



What are features?

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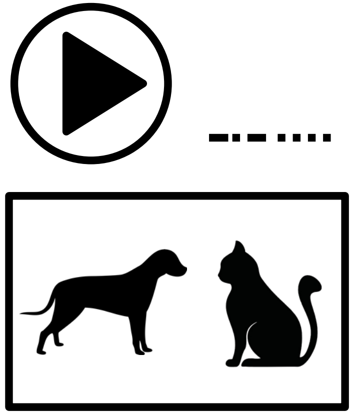

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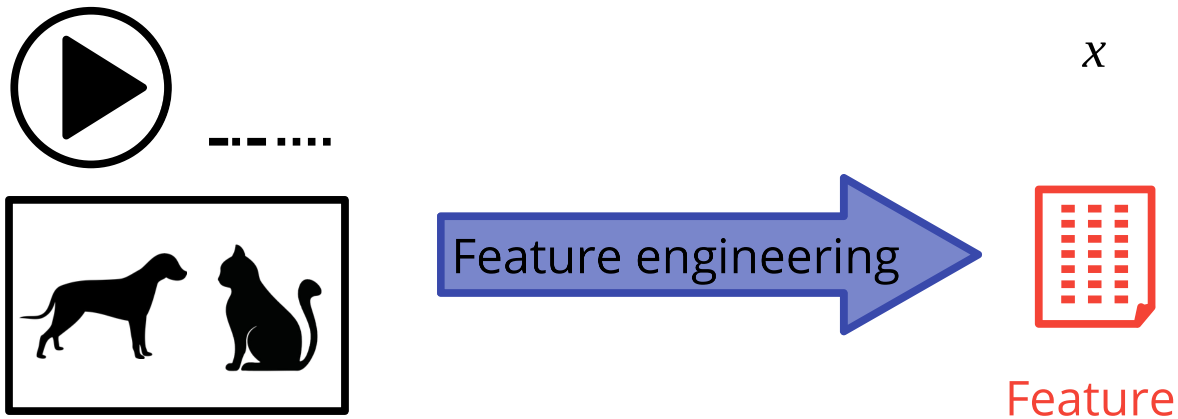

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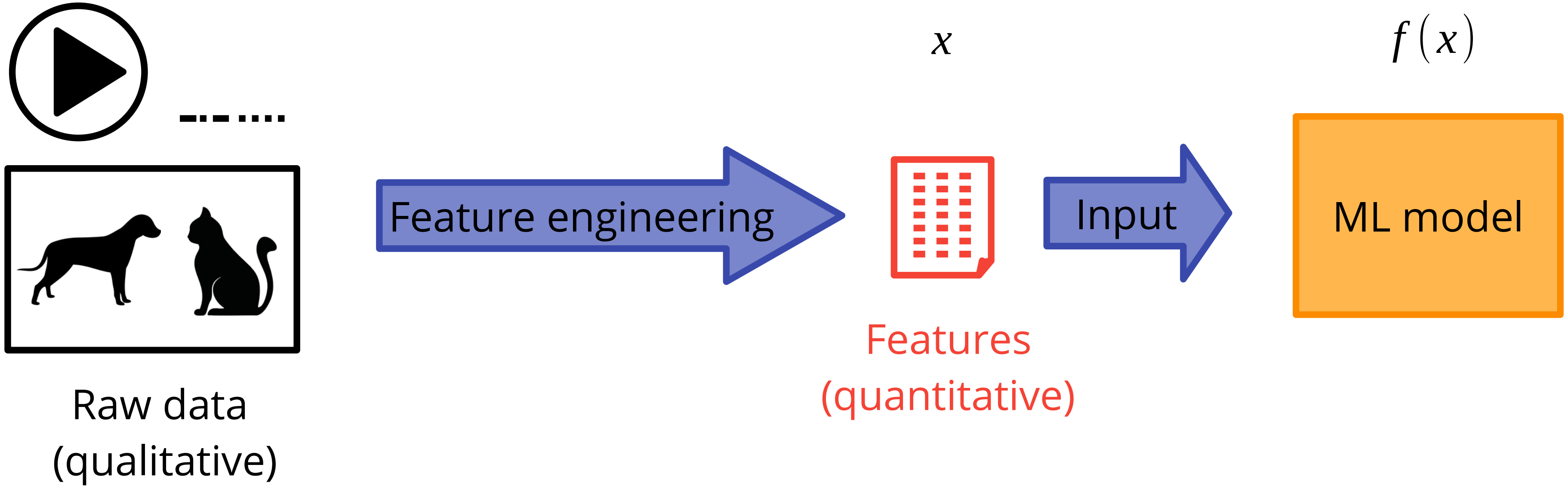

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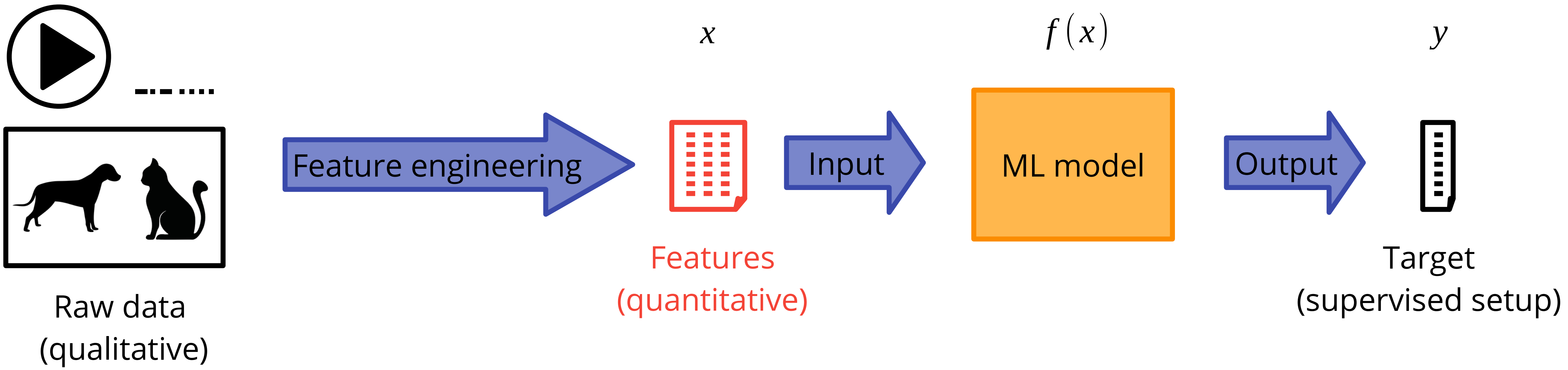
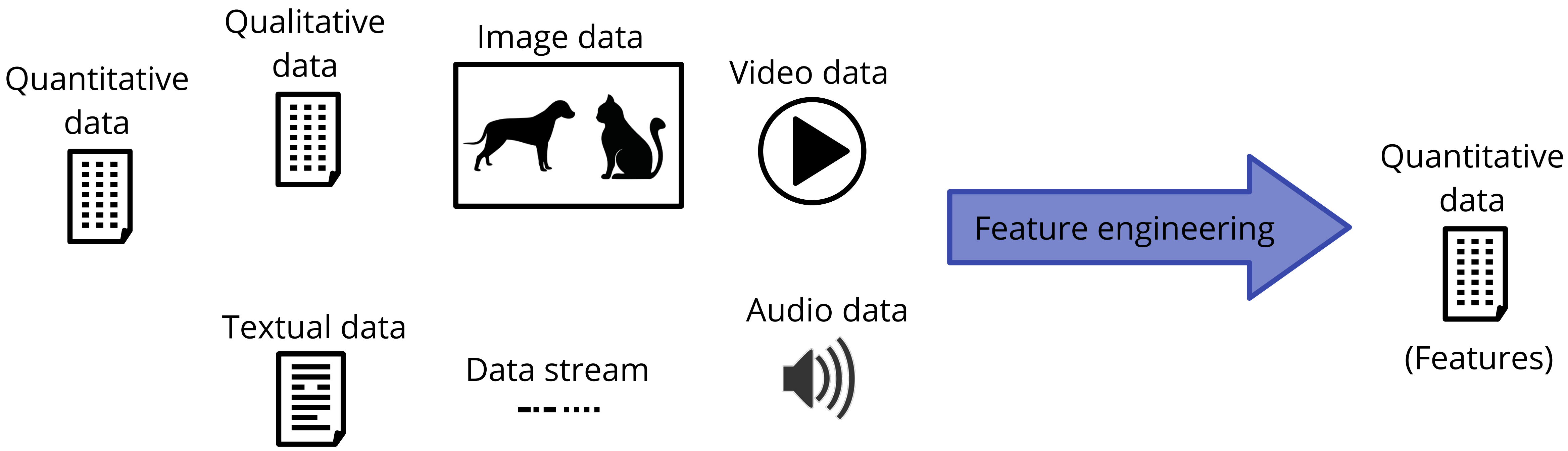


Feature engineering

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).



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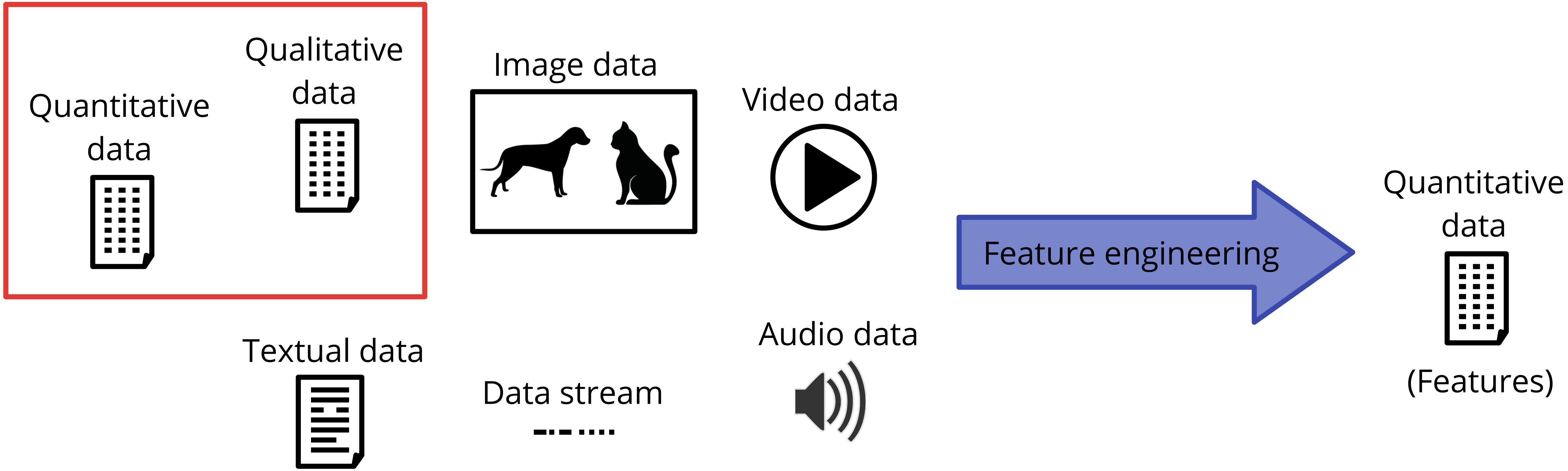

Feature engineering – quantitative data

Create meaningful features through mathematical transformations.

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

Transformation:

$$\delta = x_1 - x_2$$

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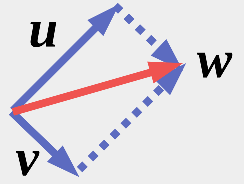
Geometric Transformations

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

Transformation:

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



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  - Cloudiness scale: [clear, mostly clear, partly cloudy, mostly cloudy] → [0, 1, 2, 3]
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(Caveat: Label encoding can also be used if a large number of classes is present)

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  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" →
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balcony	cellar	fireplace	jacuzzi
1	0	0	0
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(Caveat: if too many classes present, use label encoding instead; see *curse of dimensionality*)

Final data set nomenclature

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

Example:

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
...	...	...	...	...

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

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

Ground-Truth

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Ground-Truth

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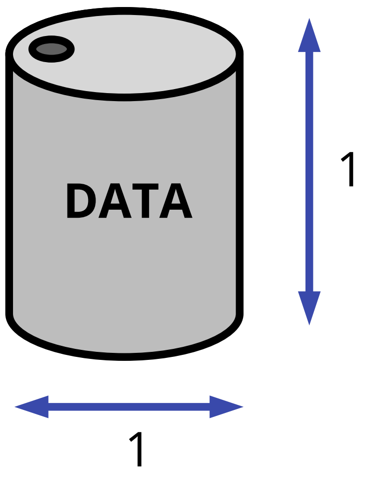
false	rhinoceros
false	chimera
...	...

classes of label "Type"

Data Types: continuous, continuous, binary, discrete, ordinal; binary, categorical (multi-class)

Data scaling



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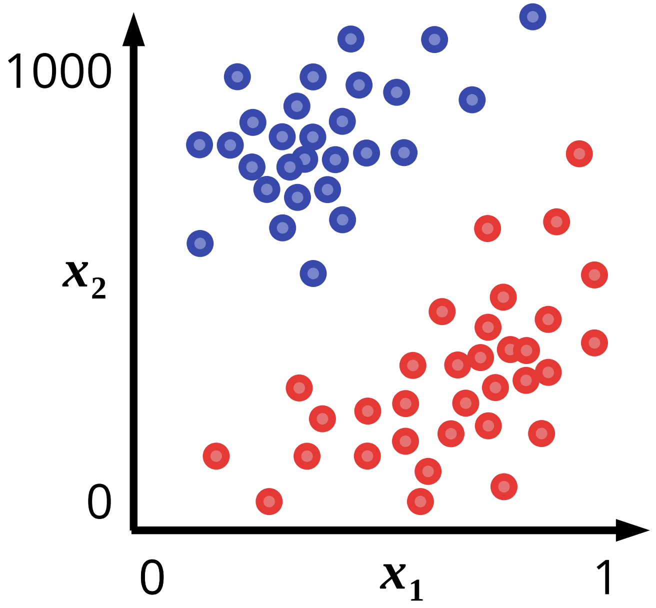

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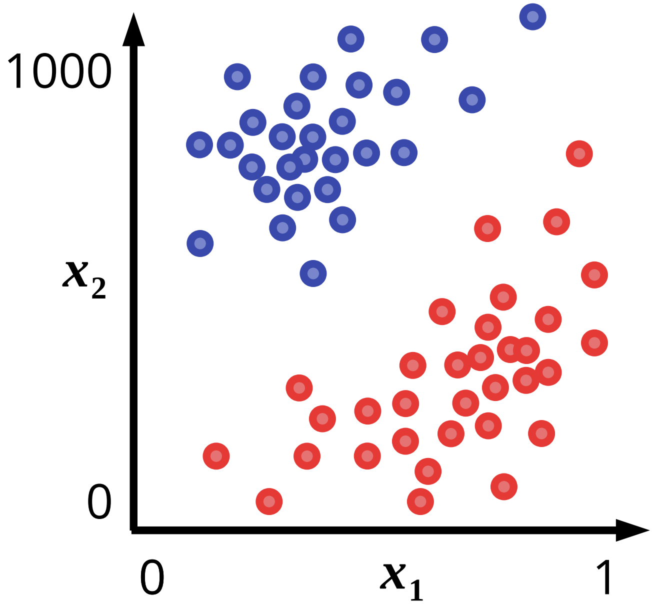

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Euclidean distance metric

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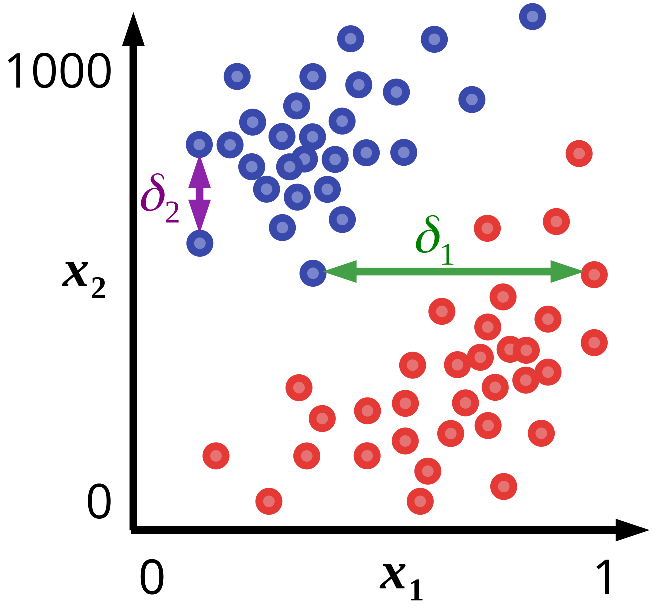

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Euclidean distance metric

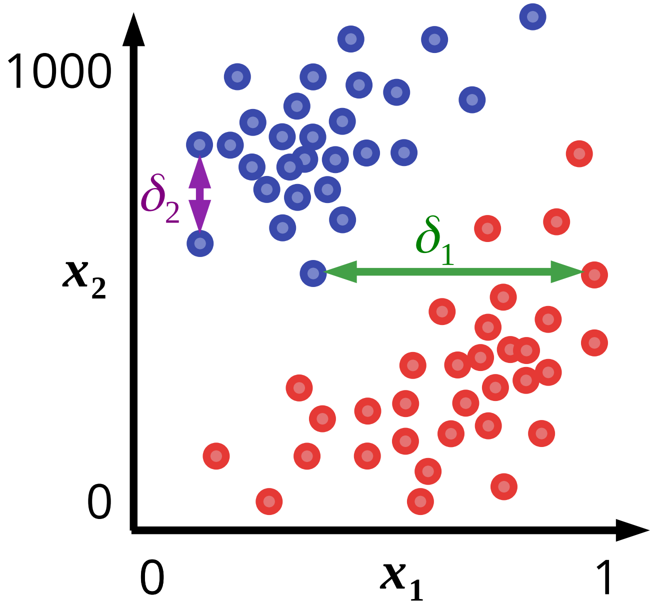
$$\delta_1 \ll \delta_2$$

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.



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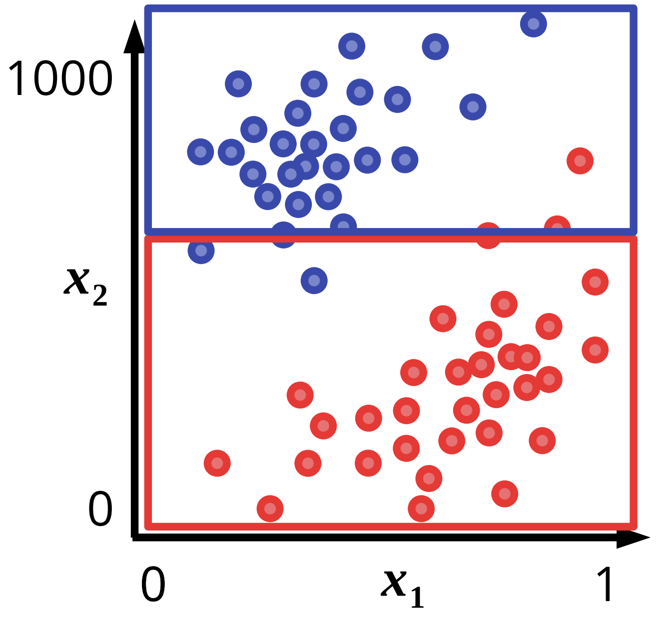

Decision regions of a hypothetical distance-based classifier.

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

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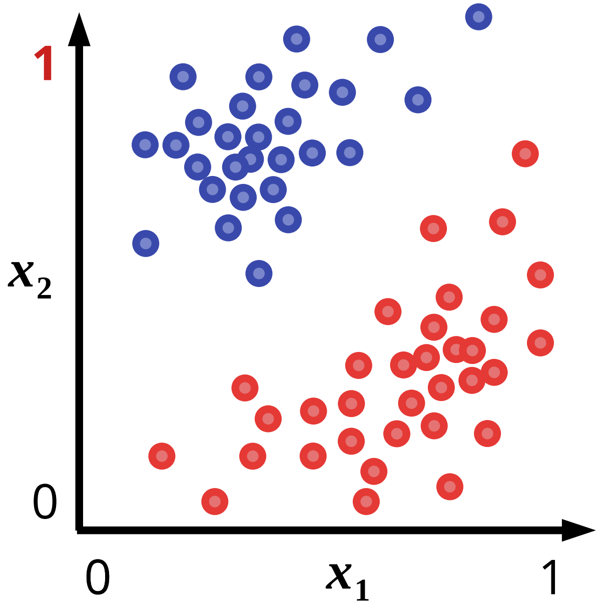

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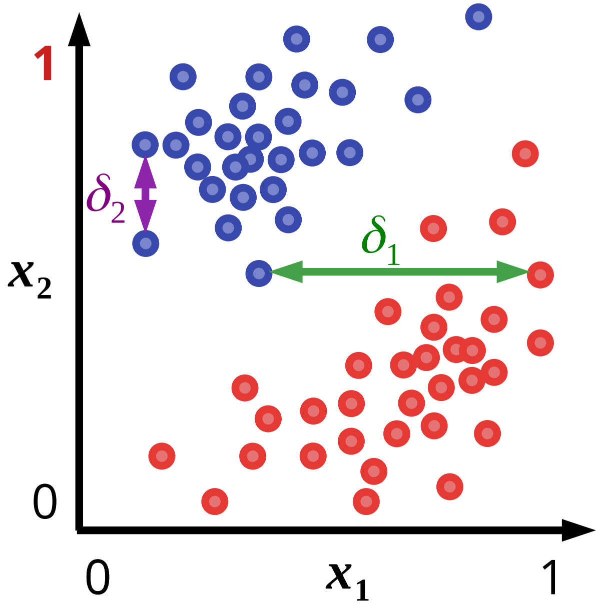

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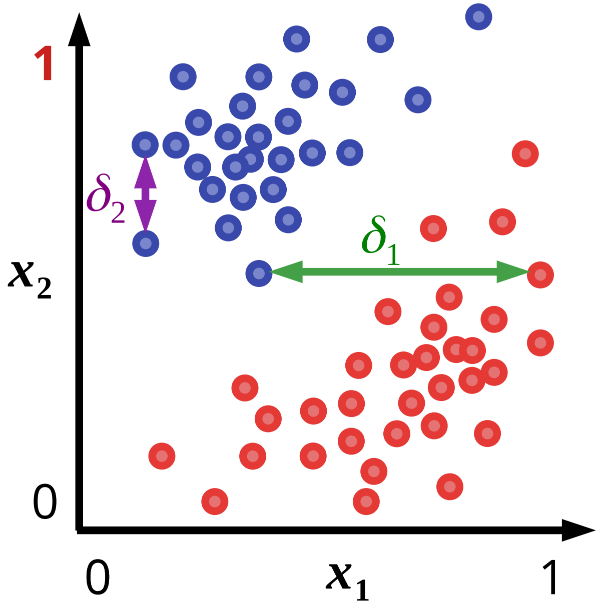

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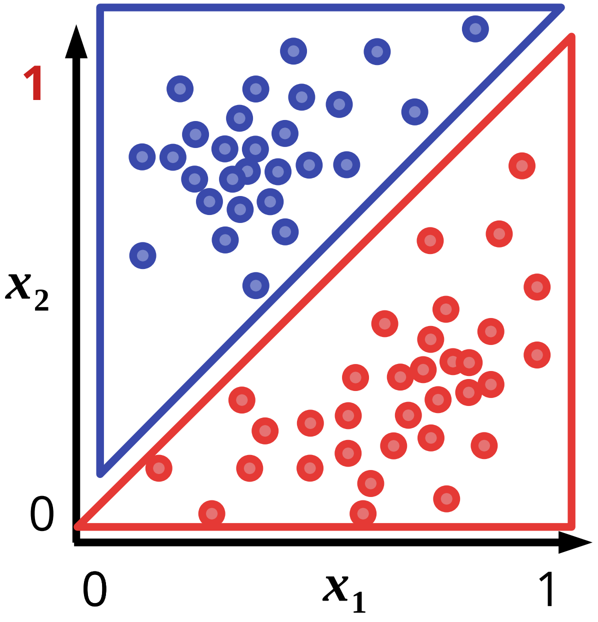

Decision regions of a hypothetical distance-based classifier.

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.

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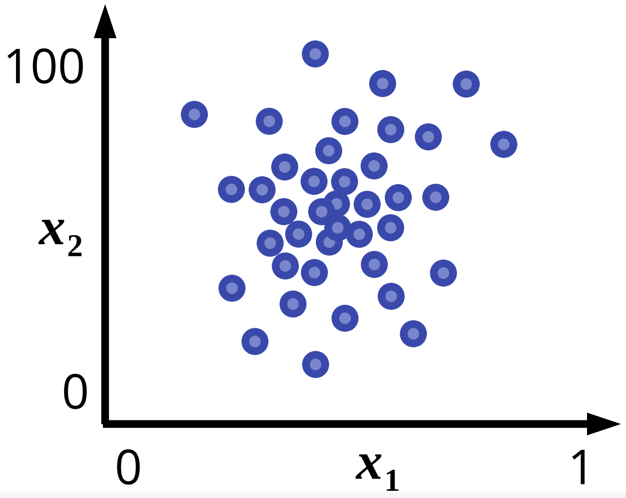

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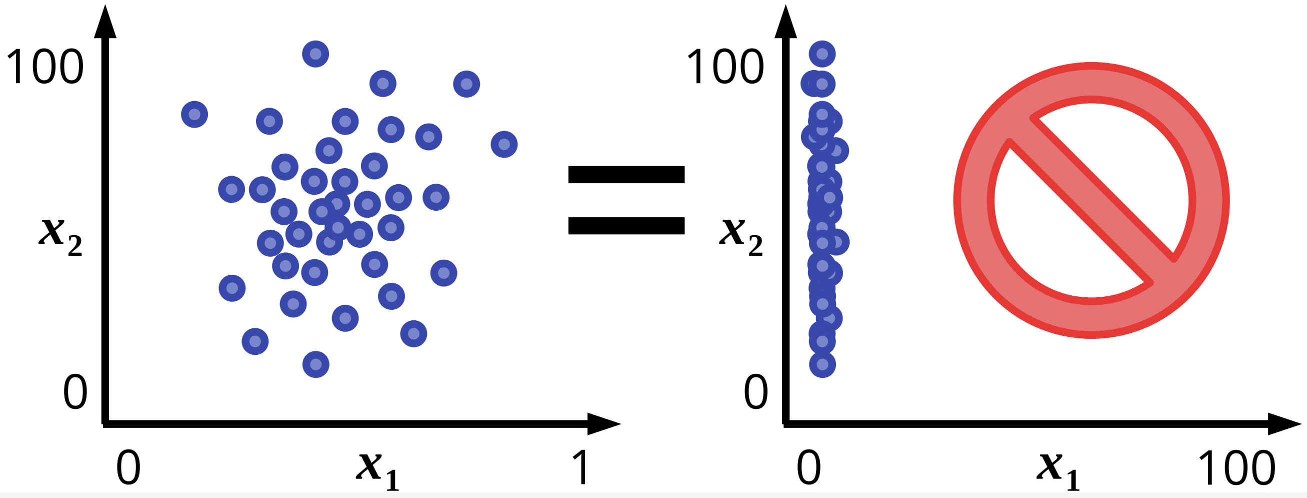

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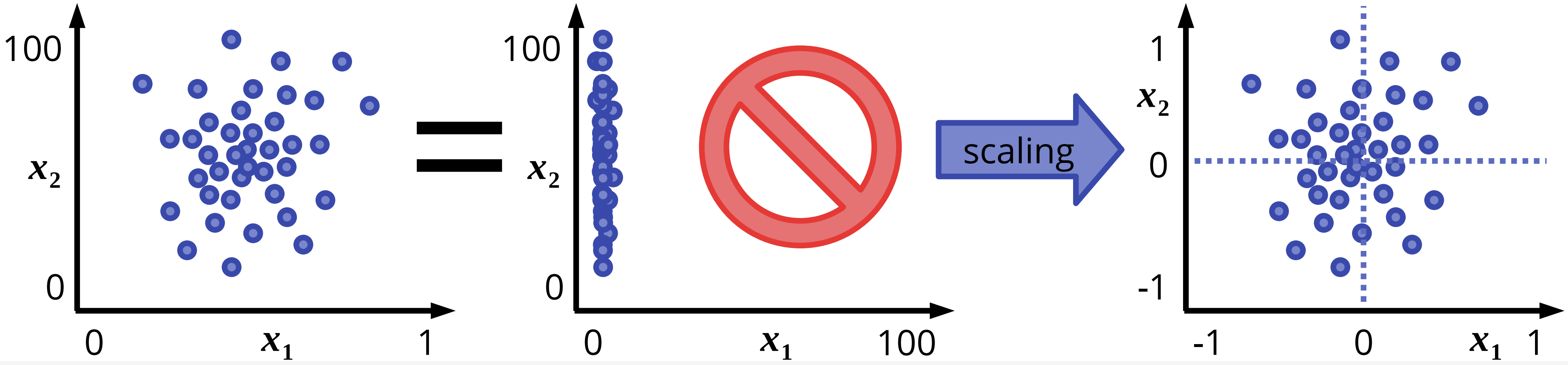

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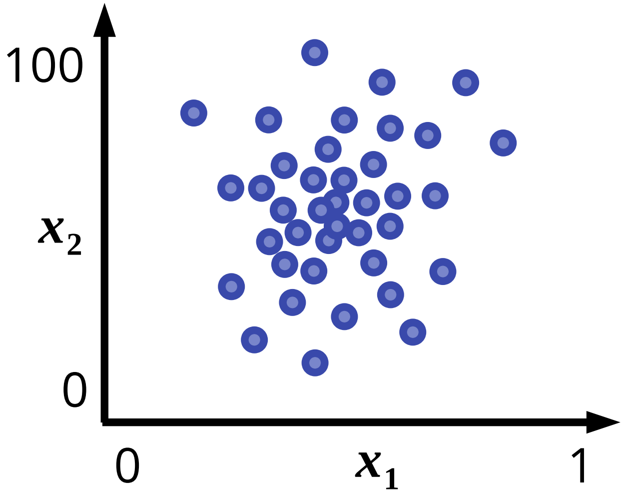
How to scale data?

- 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.



$x_i \in \boldsymbol{X}_i$

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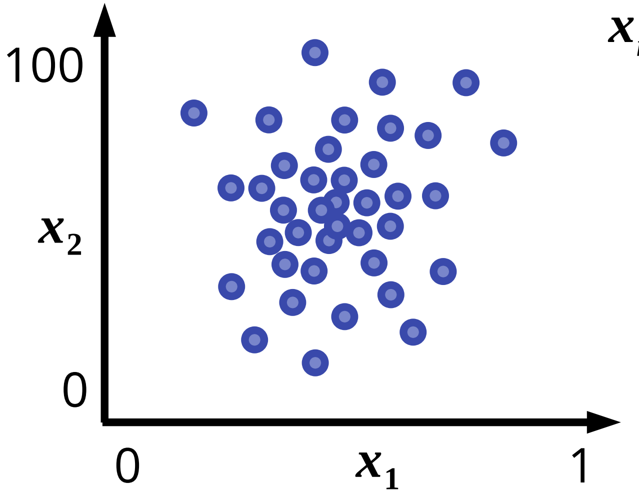

$$x_i' = \frac{x_i - min(X_i)}{max(X_i) - min(X_i)}$$

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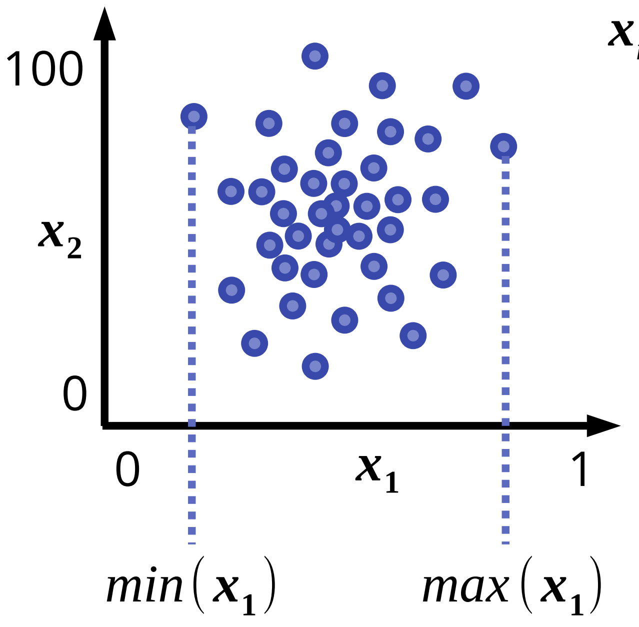

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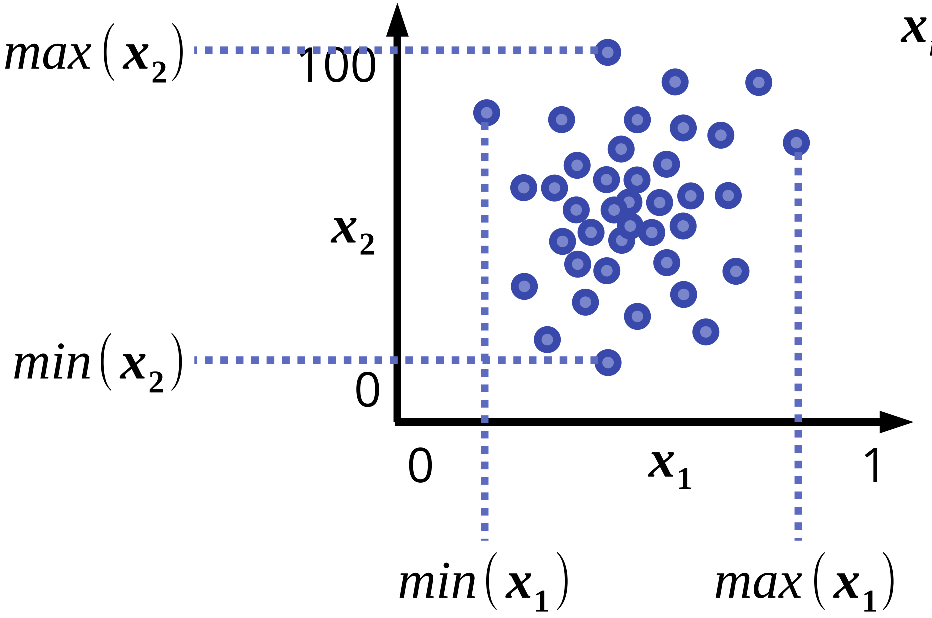

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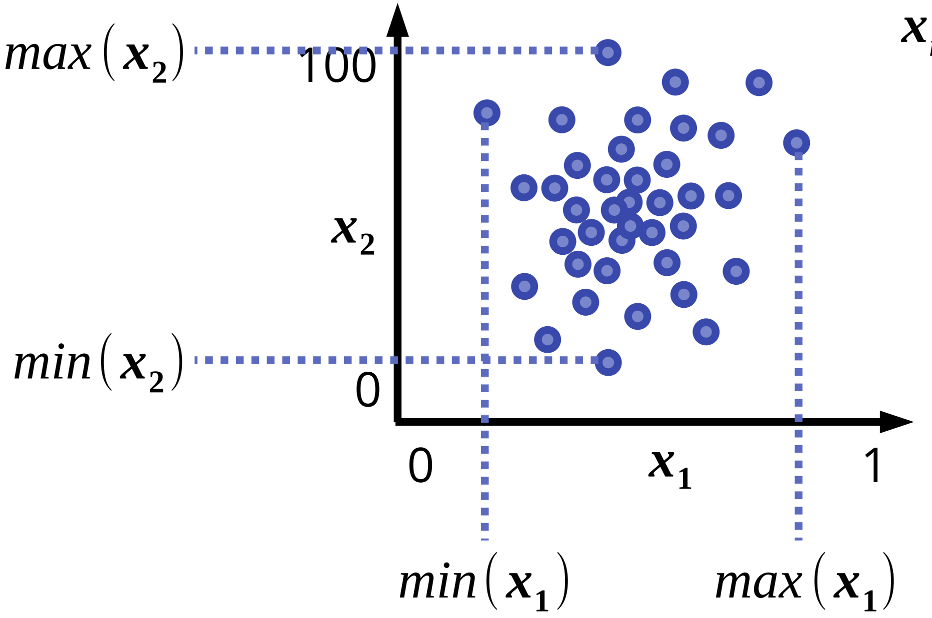

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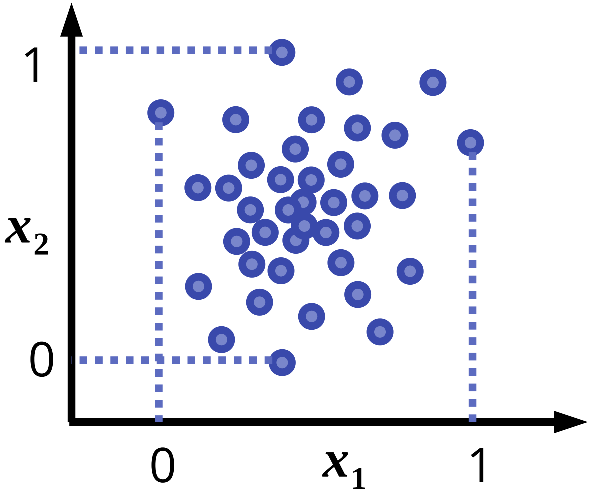
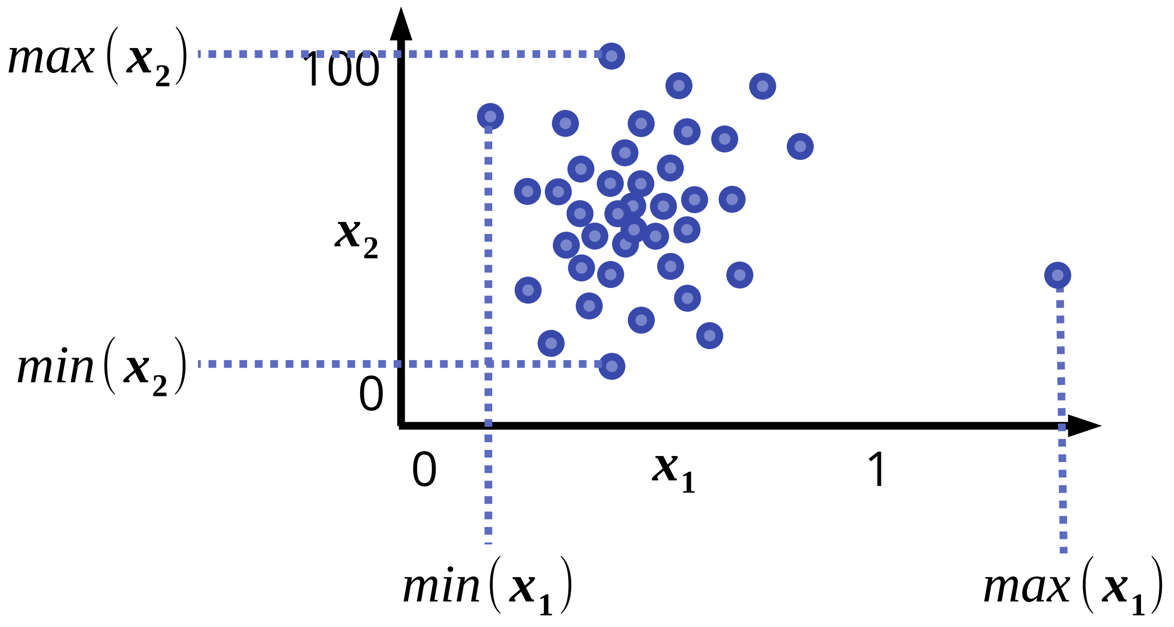


Data scaling – MinMax scaler

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.



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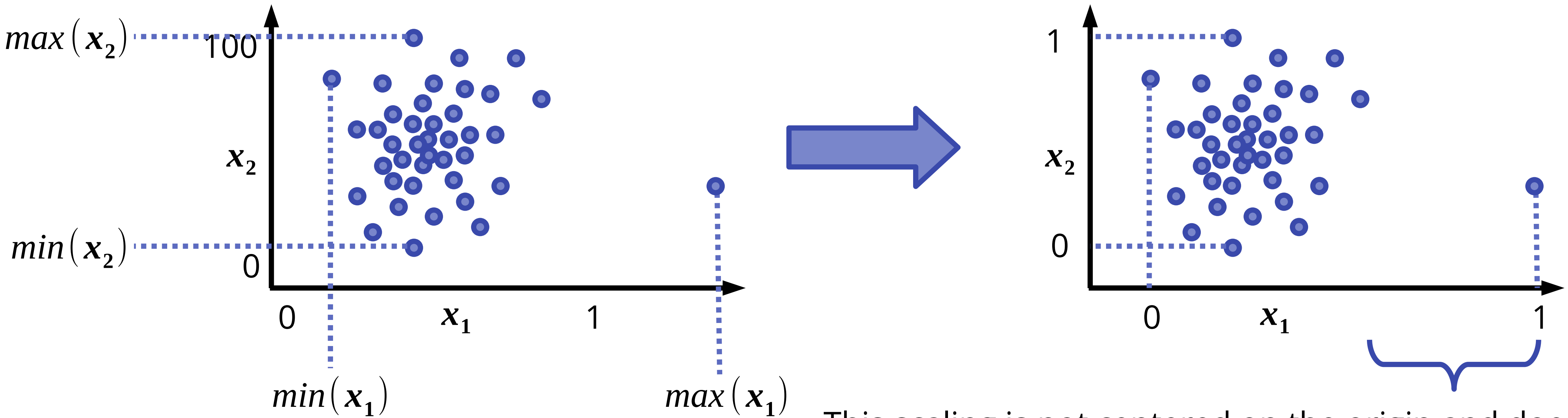
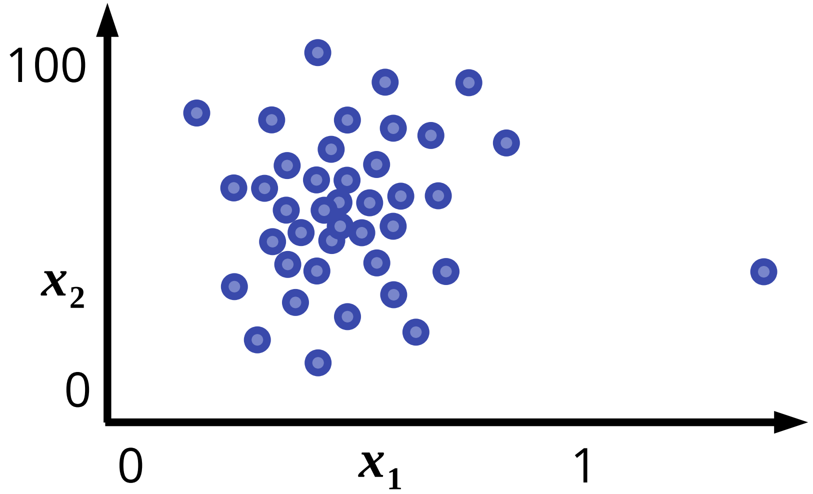


This scaling is not centered on the origin and does not describe the data distribution well.

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.



$x_i \in \boldsymbol{X_i}$

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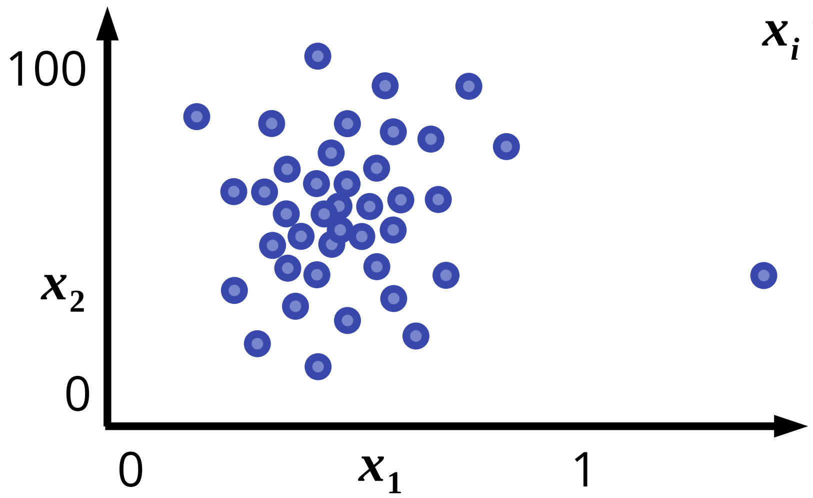

$$\boldsymbol{x_i}' = \frac{\boldsymbol{x_i} - mean(\boldsymbol{X_i})}{\sigma(\boldsymbol{X_i})}$$

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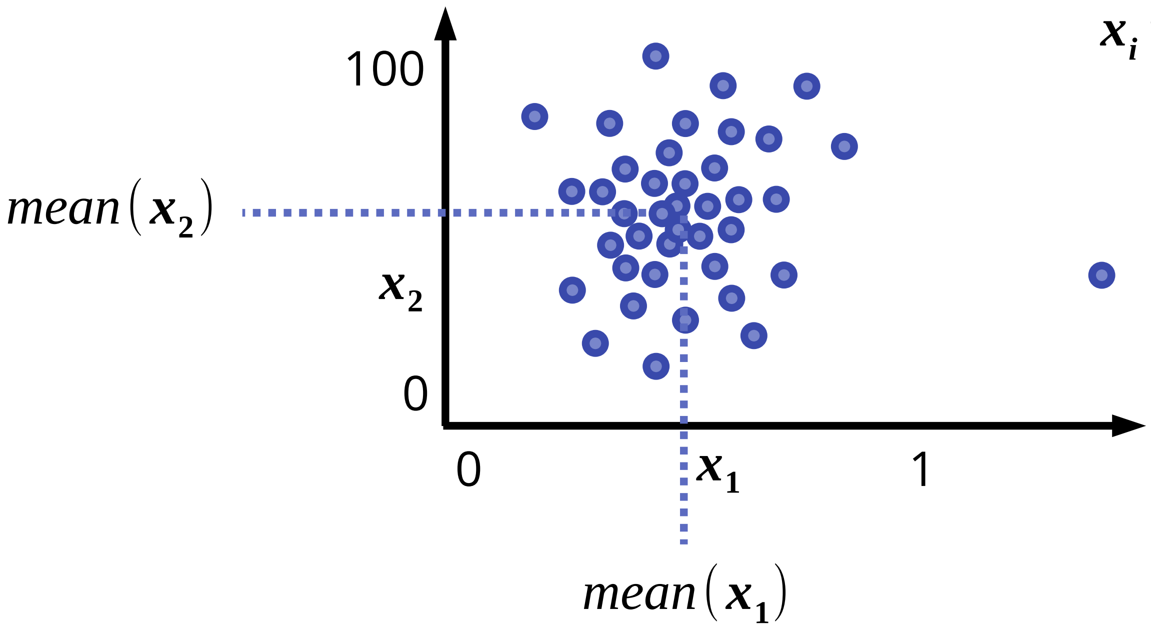

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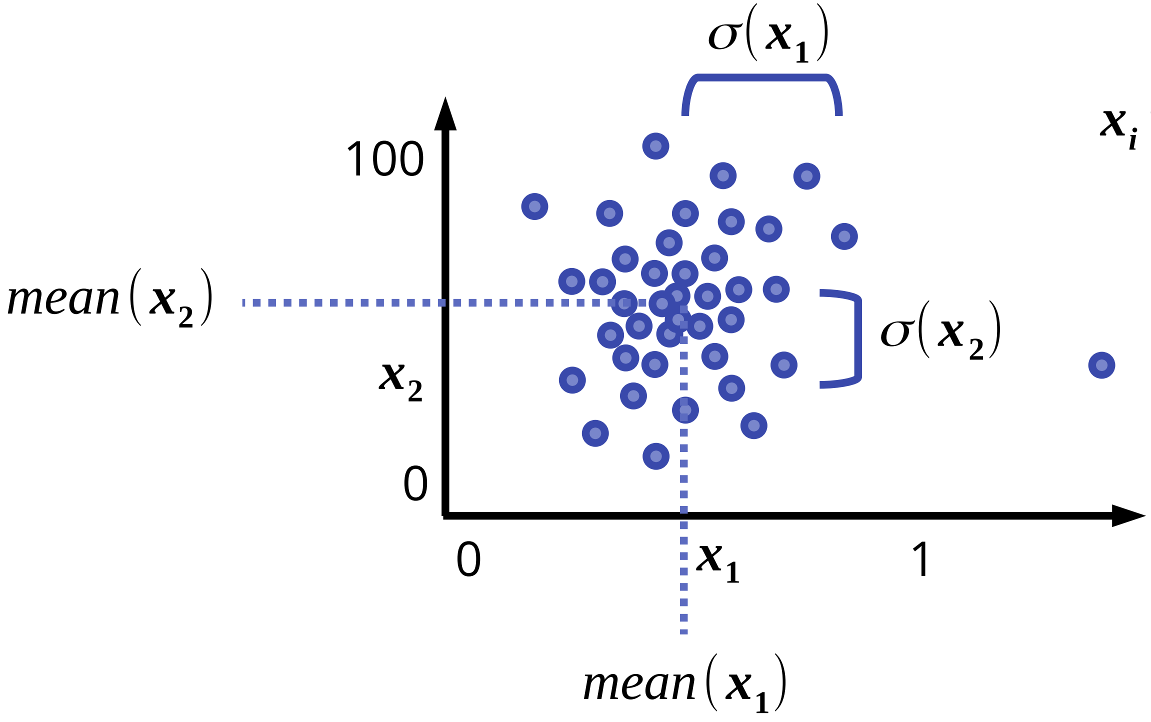

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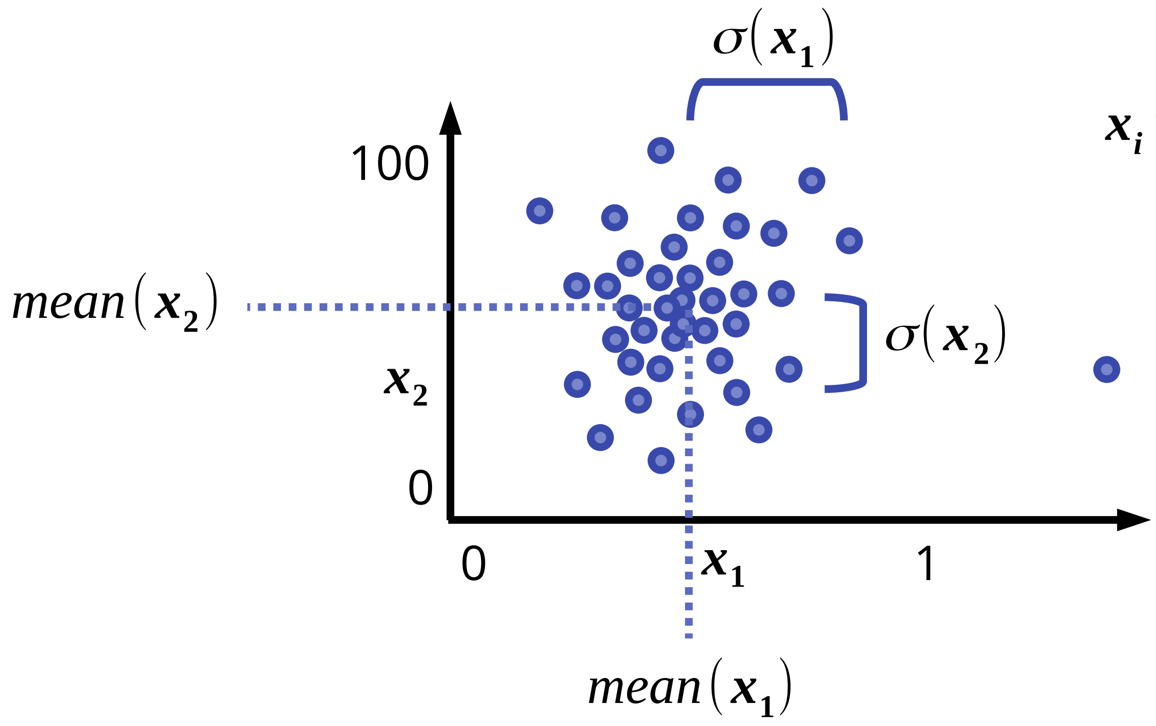

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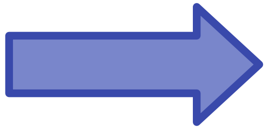

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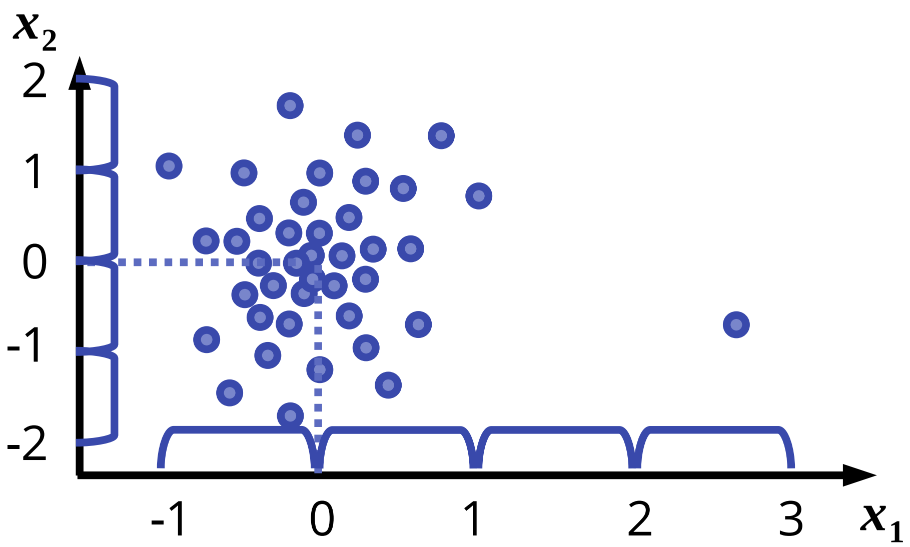
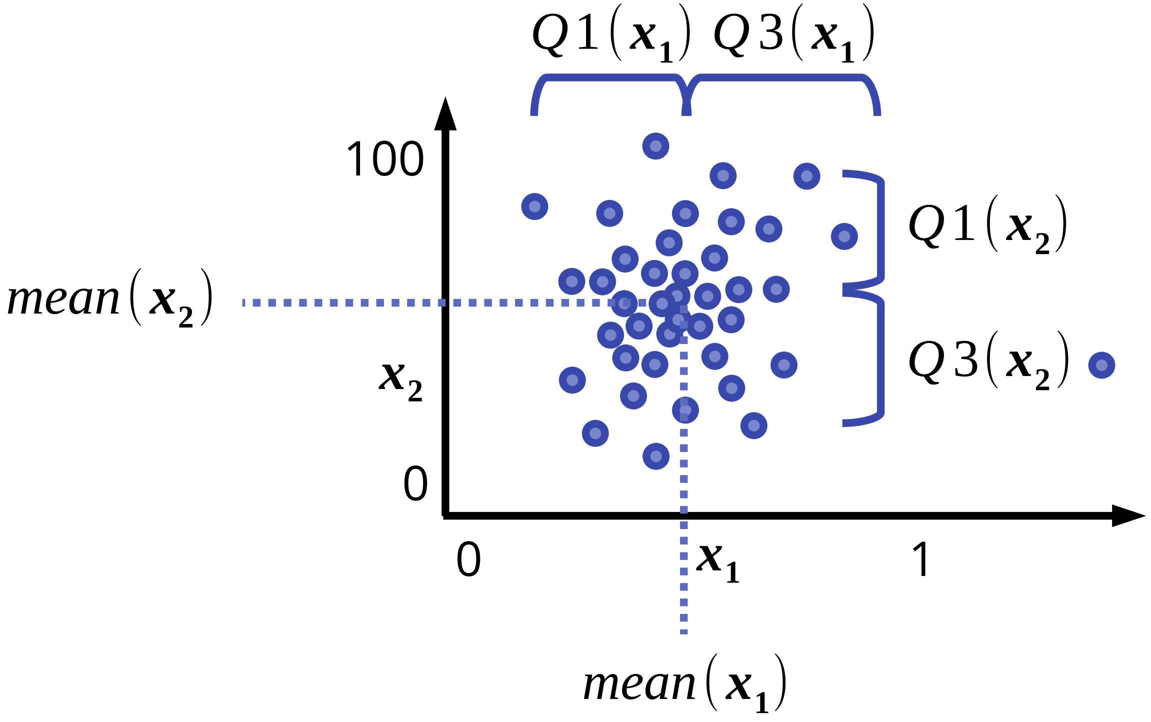


This scaling is centered on the origin but is still prone to outliers to some extent.

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.



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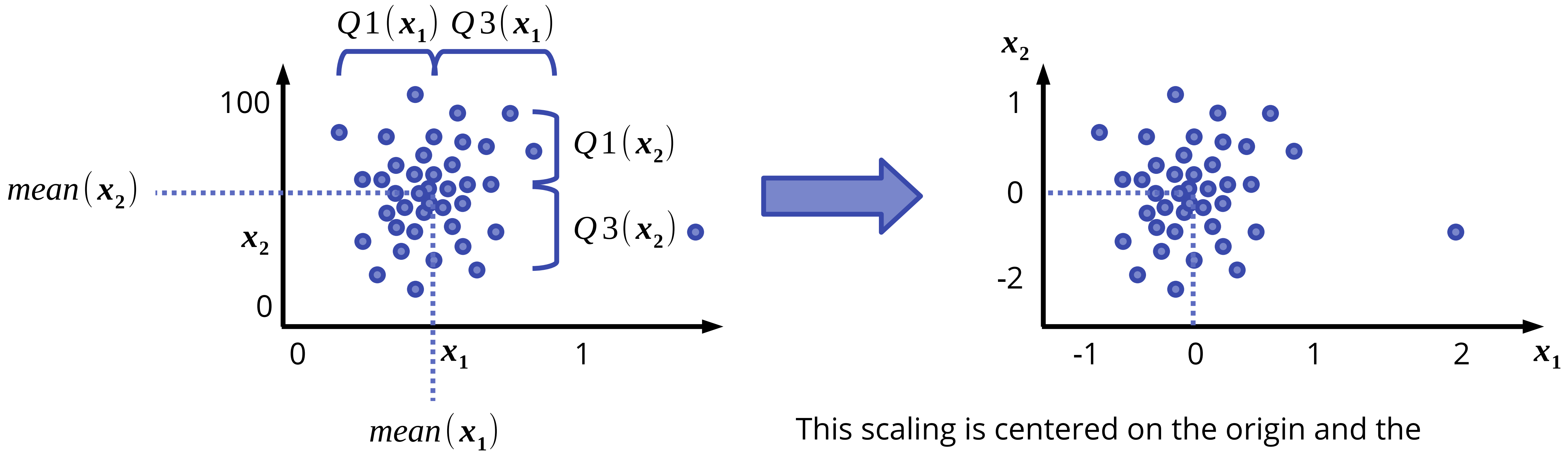

This scaling is centered on the origin and the resulting distribution is less affected by outliers

That’s all folks!