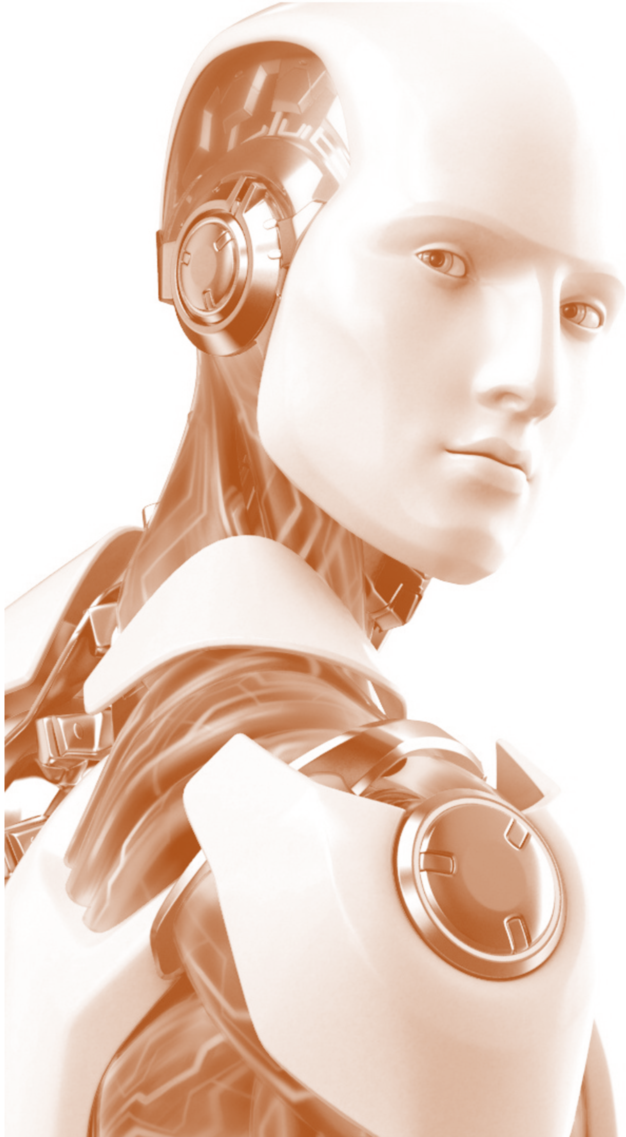

Machine Learning

Lecture 2 - Machine Learning Fundamentals

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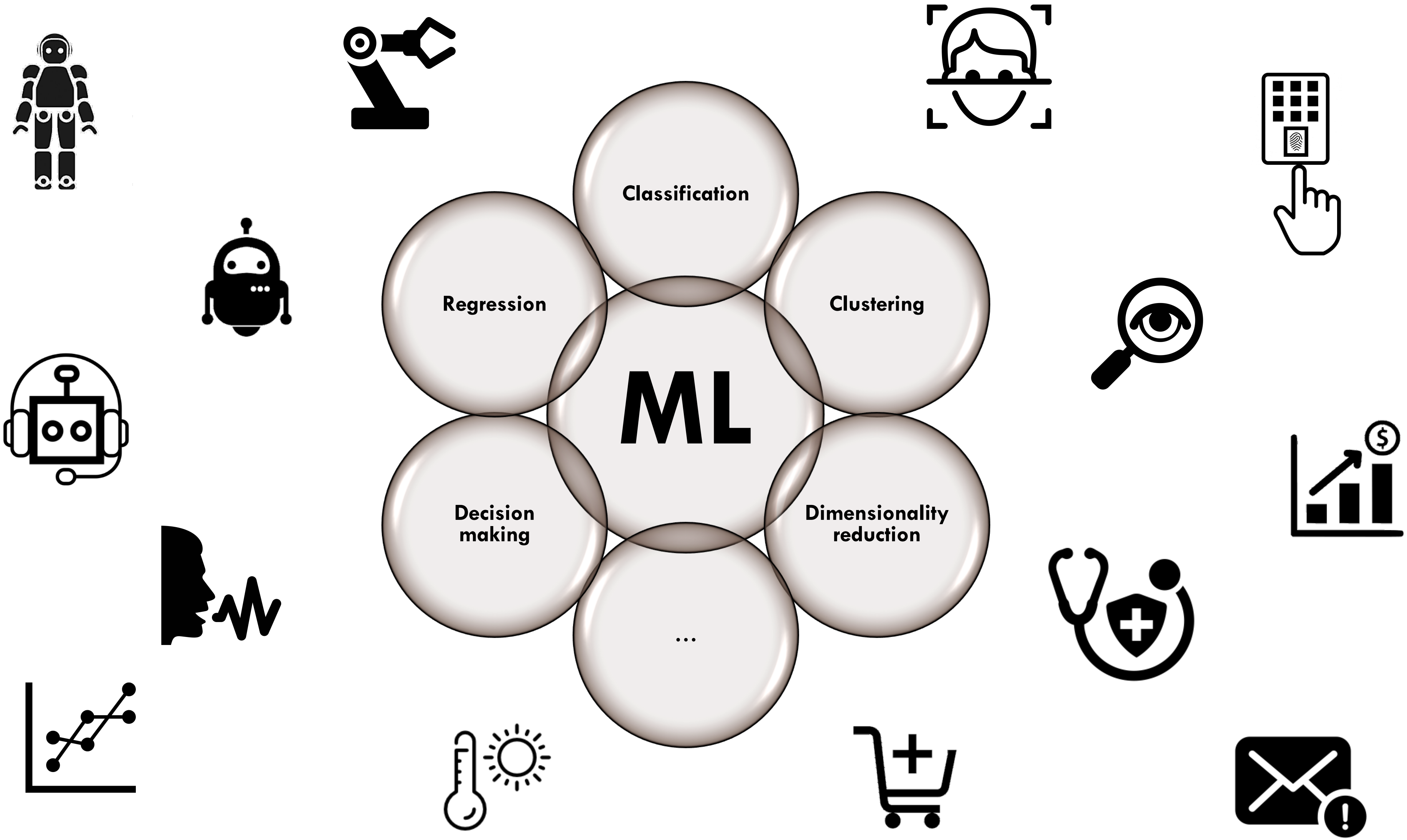
Summary

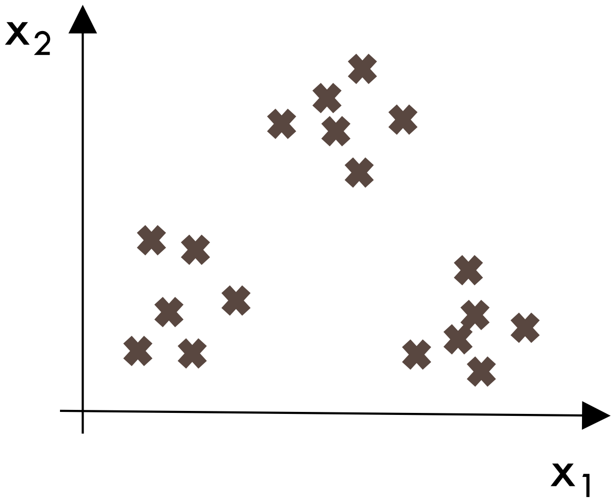
- ML typical tasks:
  - Regression
  - Clustering
  - Classification
  - Dimensionality reduction
  - Decision making
- Model training, performance and evaluation basic concepts:
  - Generalization
  - Underfitting
  - Overfitting
  - Data splitting
  - Cross-validation
  - Training early stopping
  - Data normalization

ML Typical Tasks

ML typical tasks



- Given some (typically unlabeled) data points, the goal is to group these points in such a way that points in the same group (or cluster) can be, **in some sense, more similar to each other** than points in other groups
- Common measures: distance between cluster members, density of clusters, statistical distribution...



Clustering

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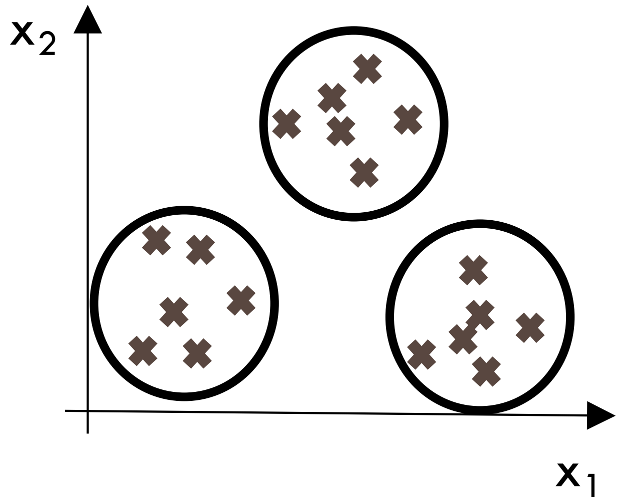
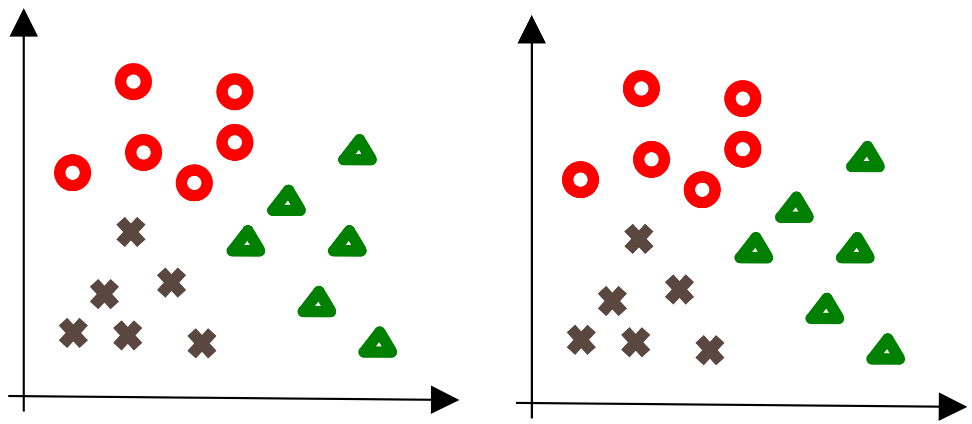


Classification

- Given a set of input data points and the classes they belong (labels), the goal is **to identify to which class a new observation belongs**



- Most of the classification methods look to establish **decision boundaries** to separate the different classes

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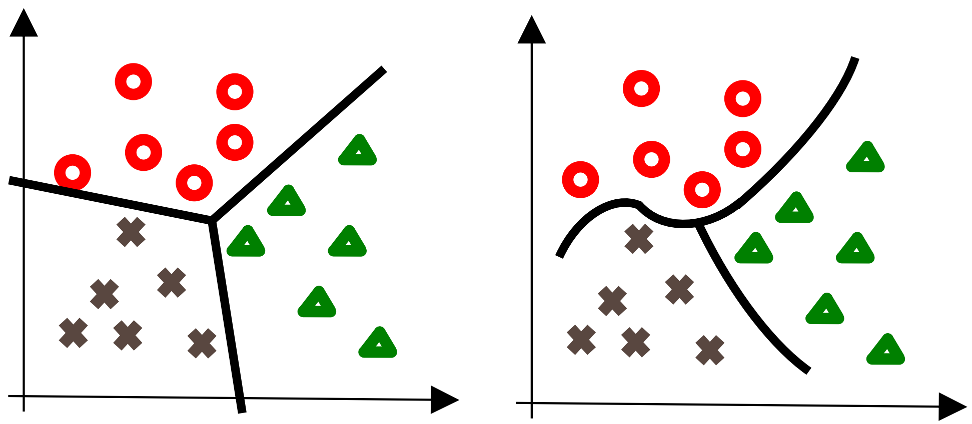

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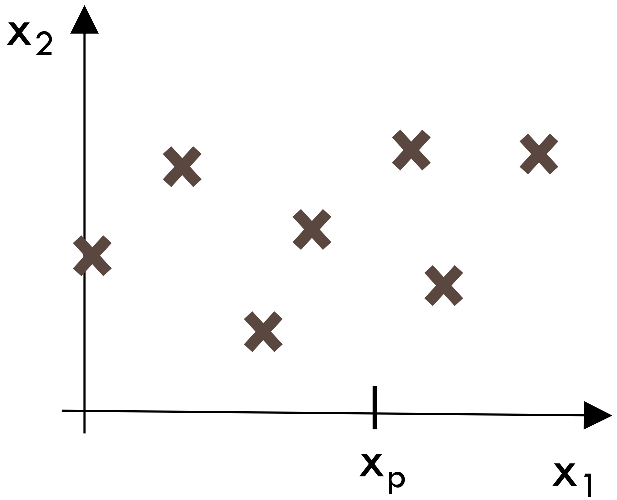
- Given some data points, the goal is to learn a **mathematical model** capable to fit data with a **curve,** so that the curve passes as close as possible to all of the data points
- This approach allows to **predict** the output for points that were not part of the original data



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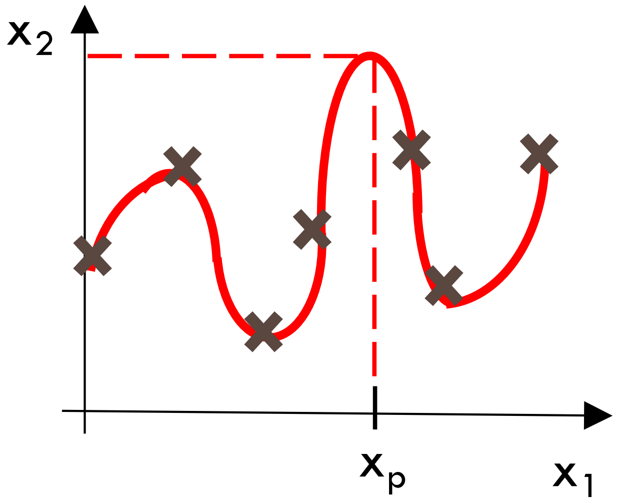
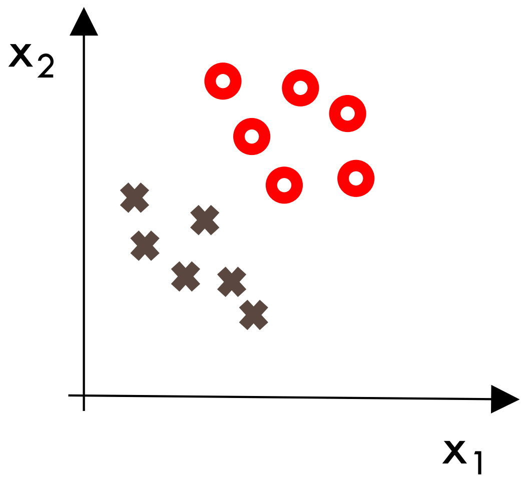


- Given a set of data points in a high number of dimensions (features or attributes), the goal is **to reduce the number of dimensions under consideration**
- Benefits: lower data volume, less computing required, shorter analysis time…



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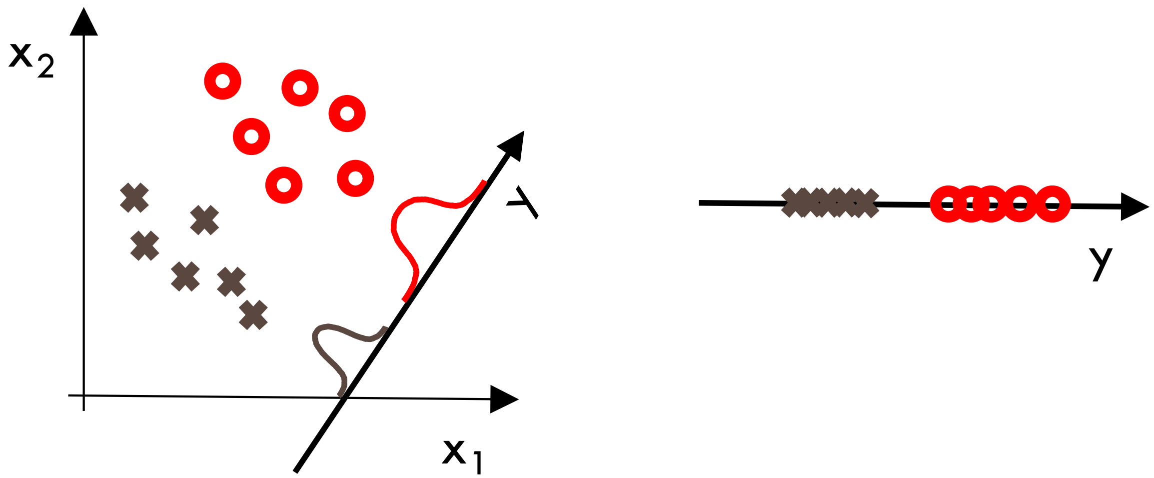

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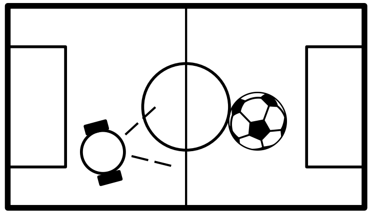

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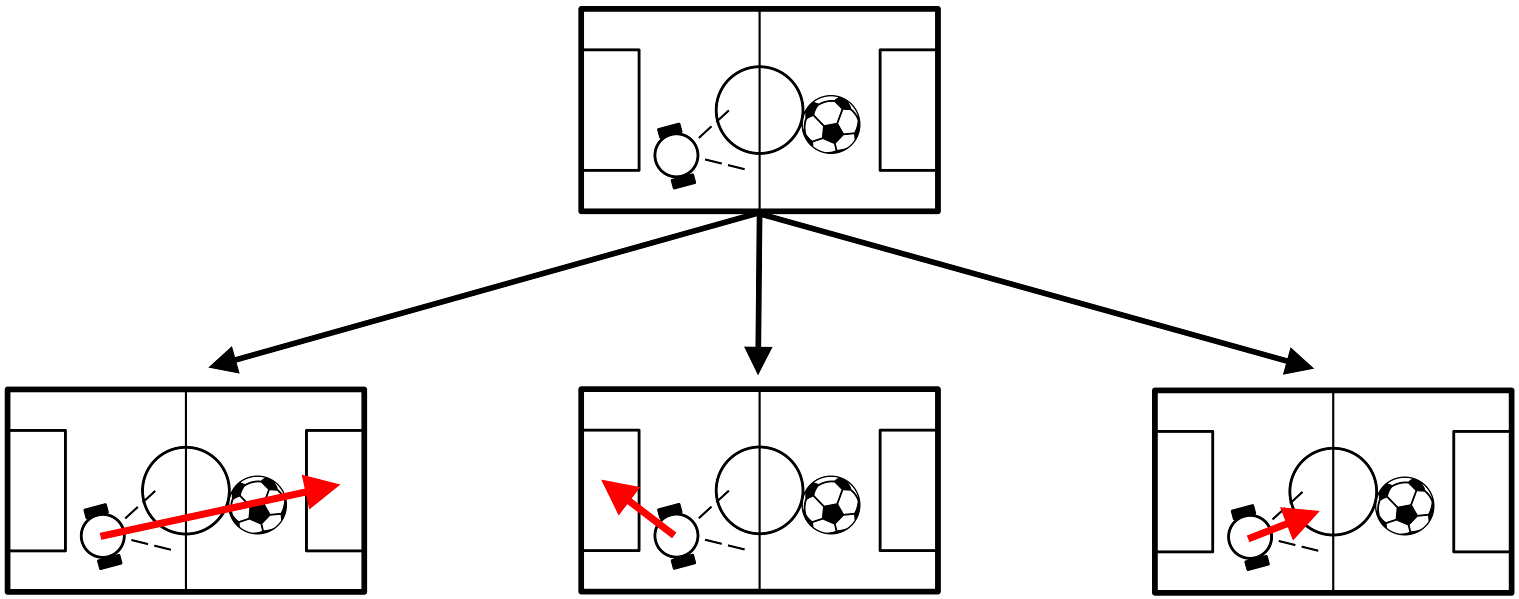
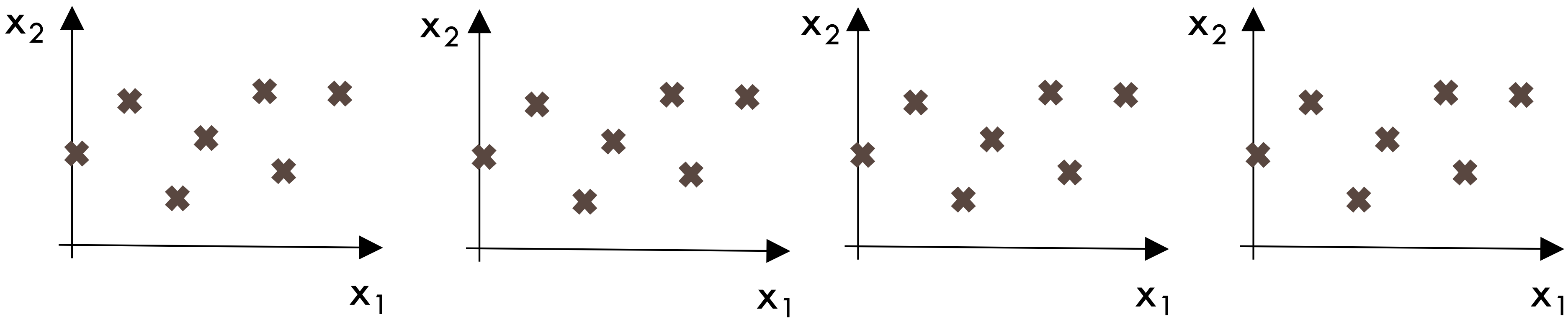


Fundamental concepts

Generalization

- Which function best describes the data?



- In learning process, we are concerned with:
  1. Learning functions/models/concepts that will give us the correct outputs for the data present in the training set
  2. Learning functions/concepts/models that can **generalize** to instances similar, but not identical, to those in the training set
- **Generalization:** capacity to correctly predict values for unseen data

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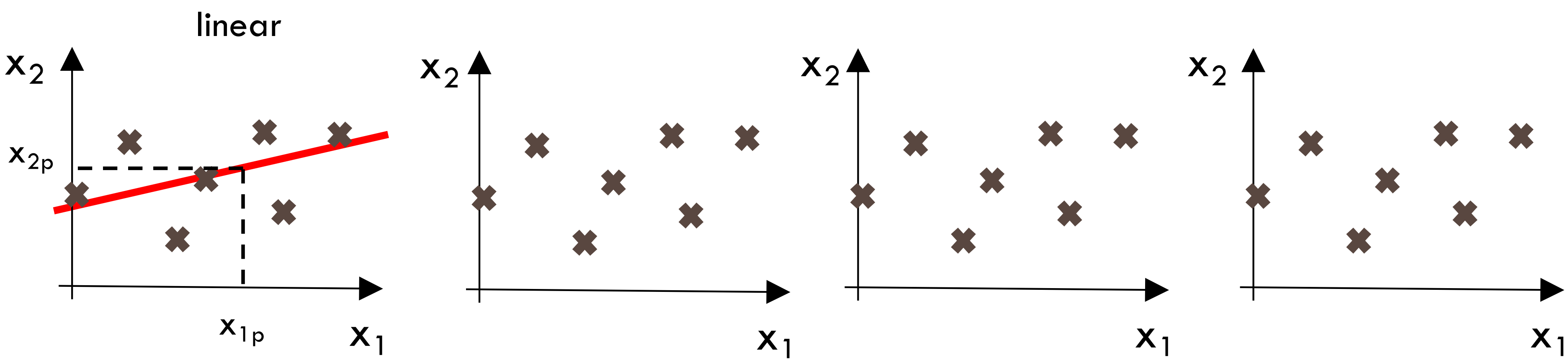

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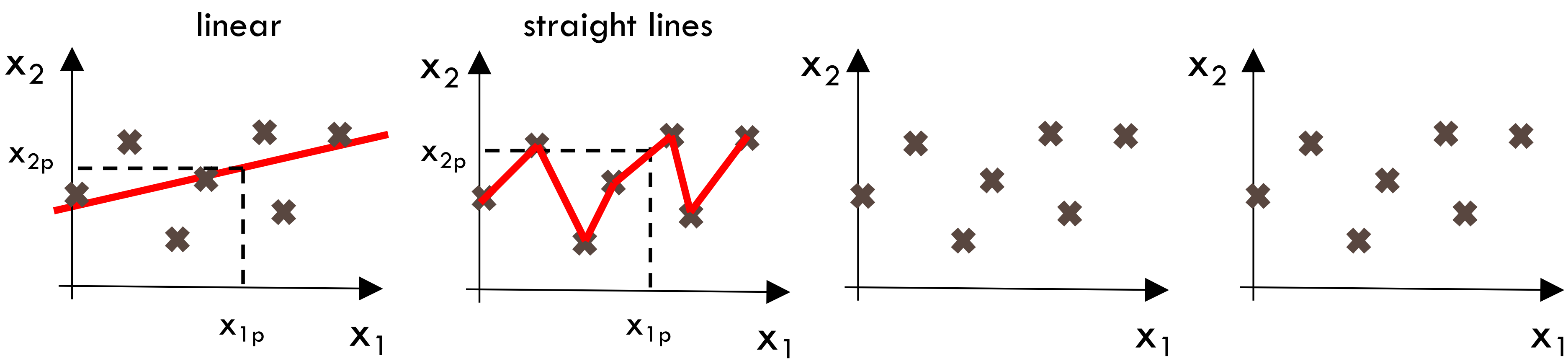

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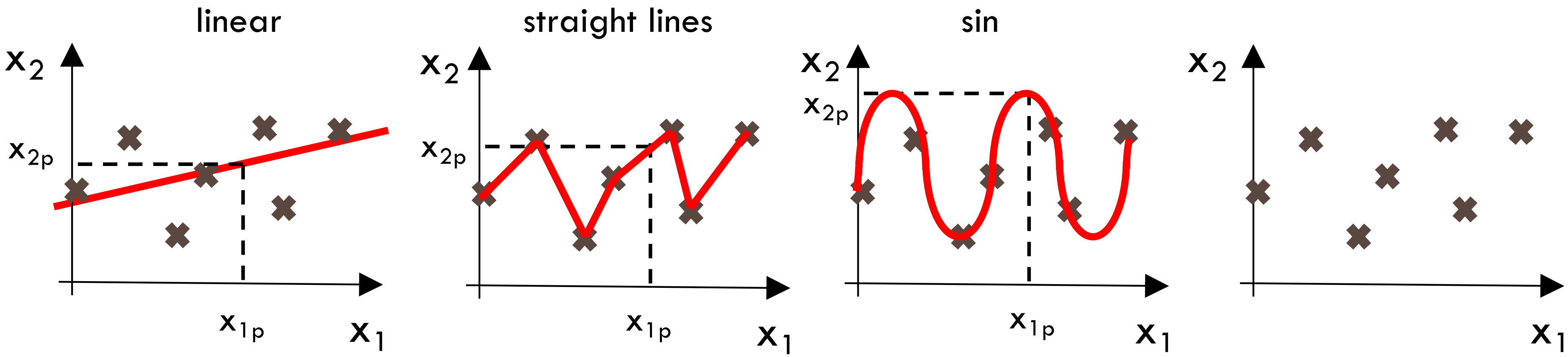

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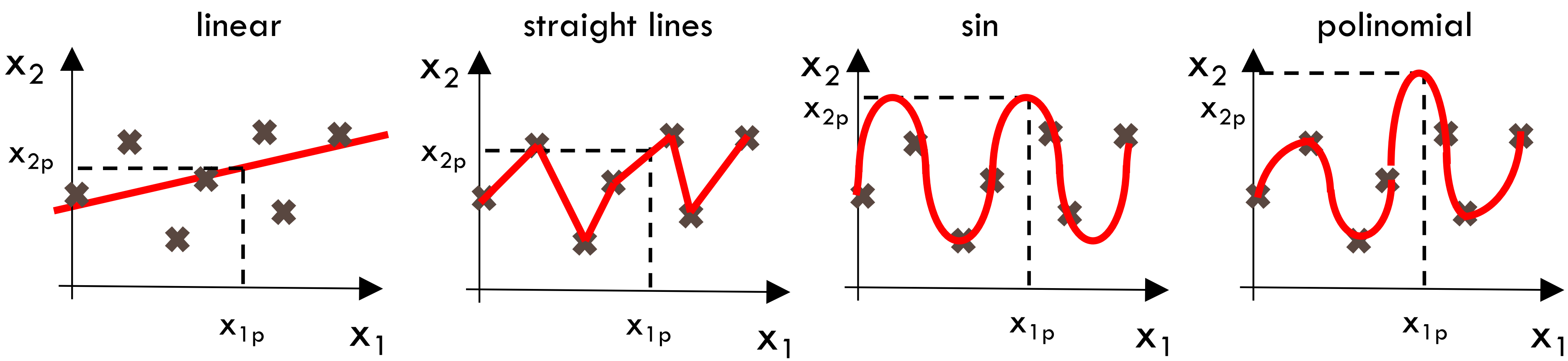

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Underfitting

- Occurs when a model is **not capable** of adequately represent the training data ($\uparrow e_{training}$) nor generalize to new data
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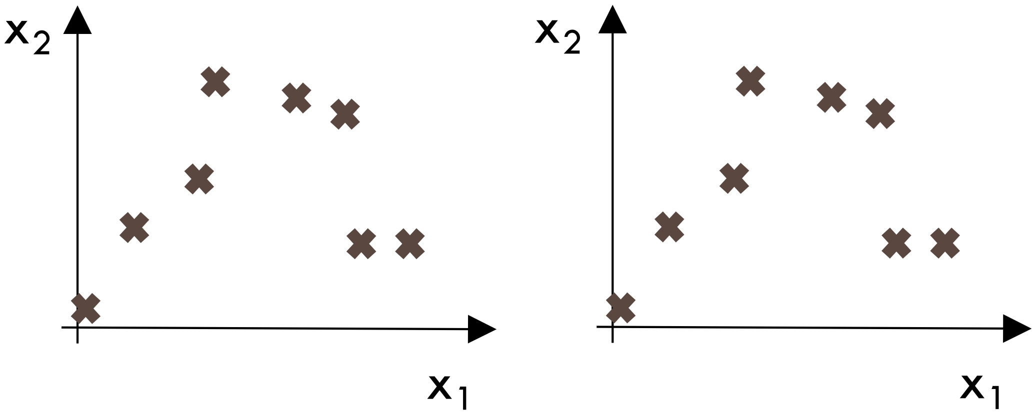

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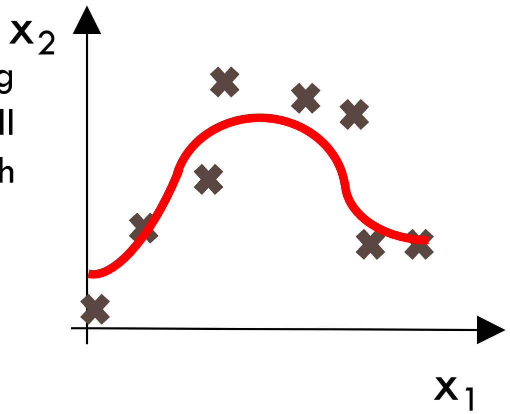

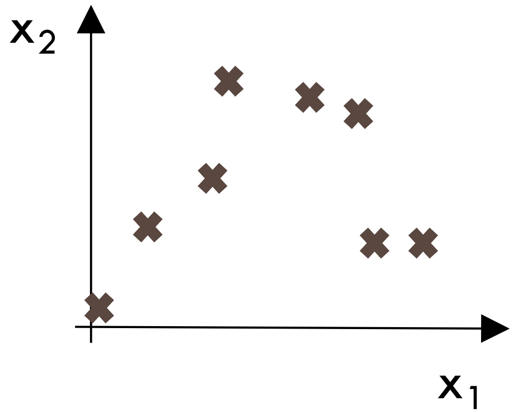

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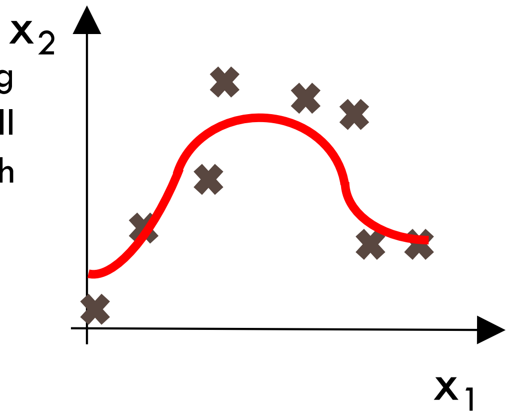
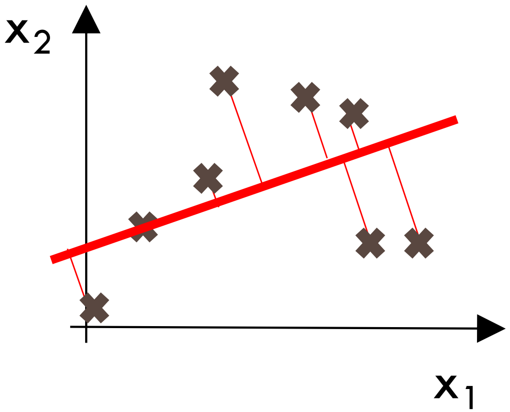
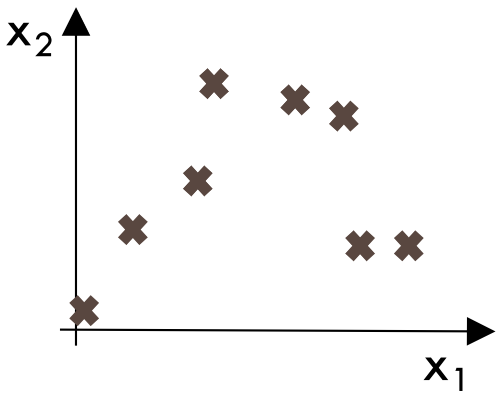
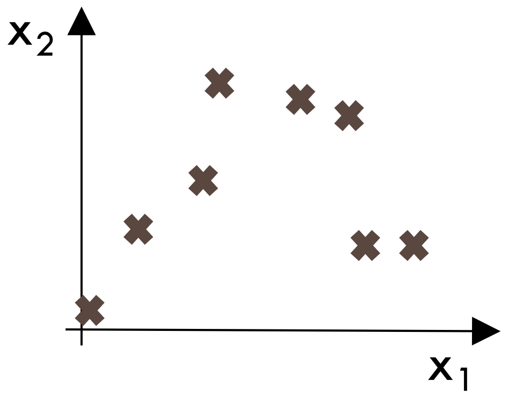




A first order model that may not be suitable for representing the data ($e_{training}$ typically will not decrease with more training)

- In well trained systems, typically curves will tend to fit **the overall trend** of the data ($e_{training}$>0)
- If the system is **trained for too long,** it tends to learn the noise and inaccuracies of the data. Models that are more complex than necessary will be learned, generating lower training errors (eventually $e_{training}$=0), but reducing the performance of the system with new data (↑$e_{generalization}$). This situation is called **overfitting.**





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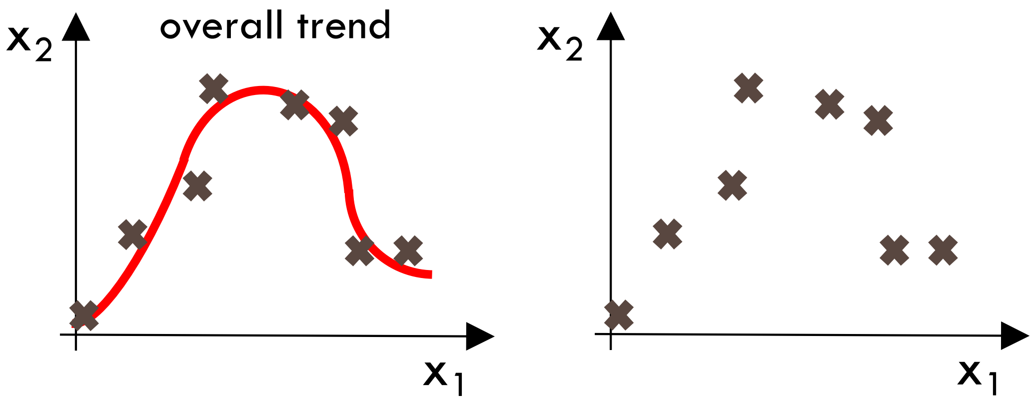

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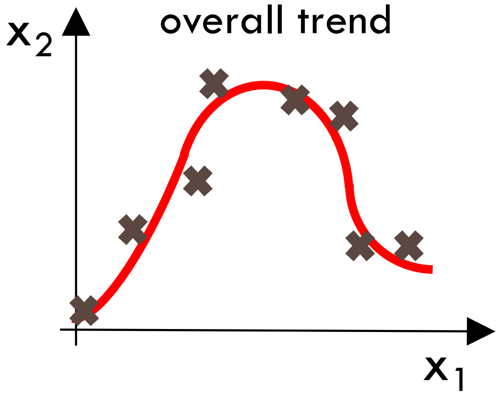
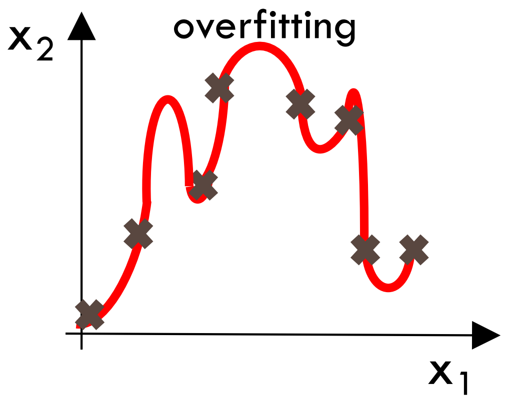
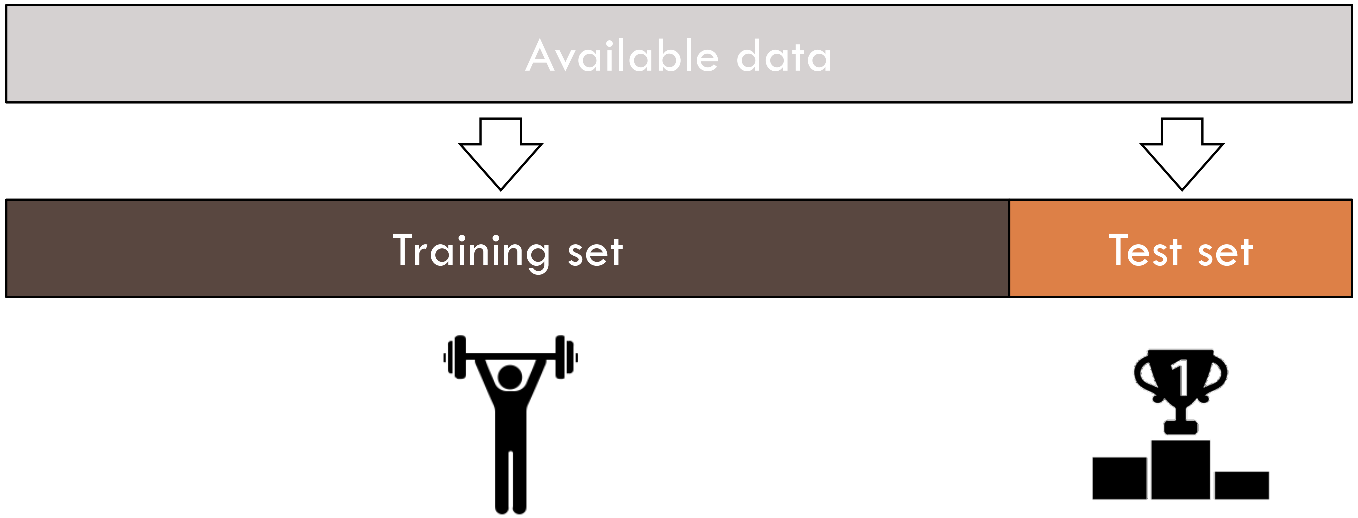




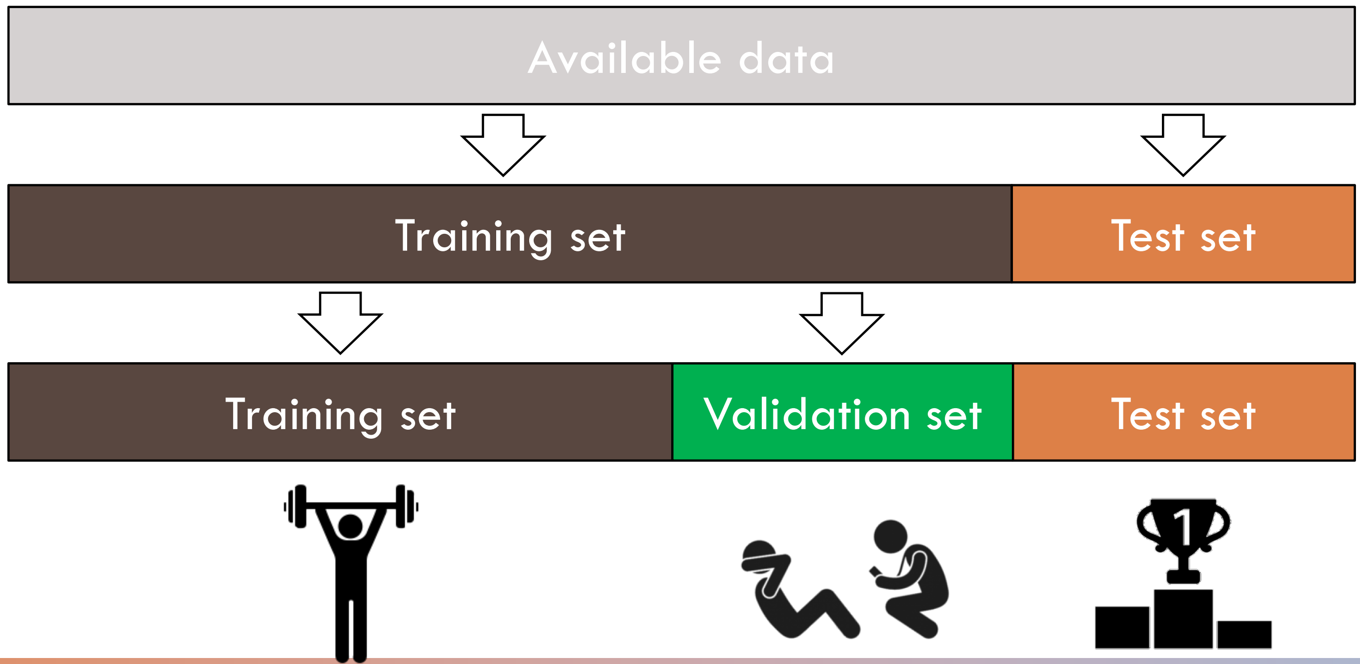
Data splitting

- A common strategy in learning systems is to split the data set in two subsets:
  - **Training set:** data used to train system (adjust the free parameters of the model)
  - **Test set:** data used to evaluate system (learned model). This data should never be used until the end of training!

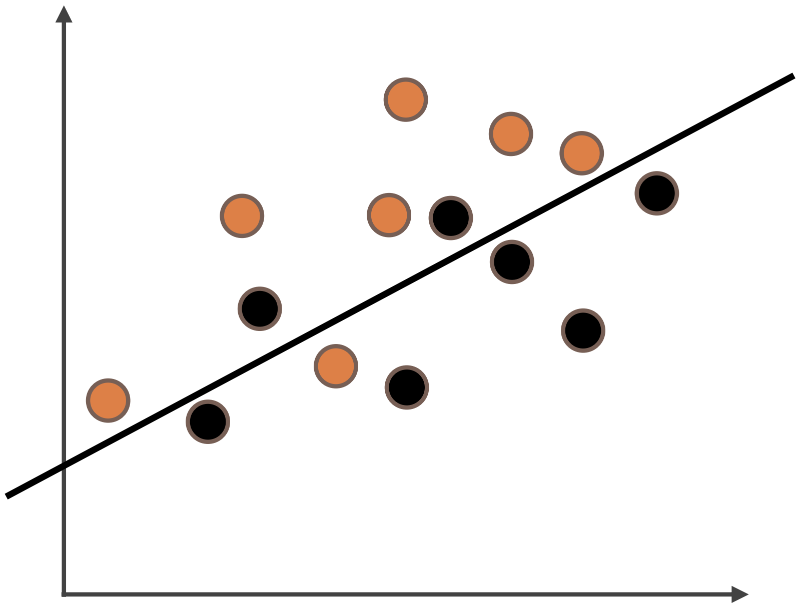


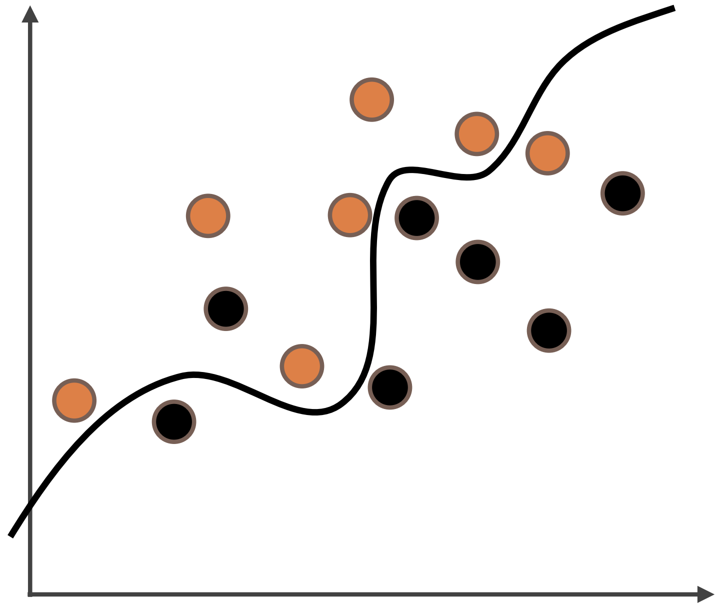
Cross-validation

- Strategy to estimate **how good is the model generalization** in the training phase and eventually to **stop training**
- **Validation set:** data set (not used in training phase) that will be eventually used to evaluate training
- A suitable **proportion** between sets must be defined. Usual practical values are: 50:25:25 or 60:20:20 (if you have plenty of data) until 90:5:5 (few data)

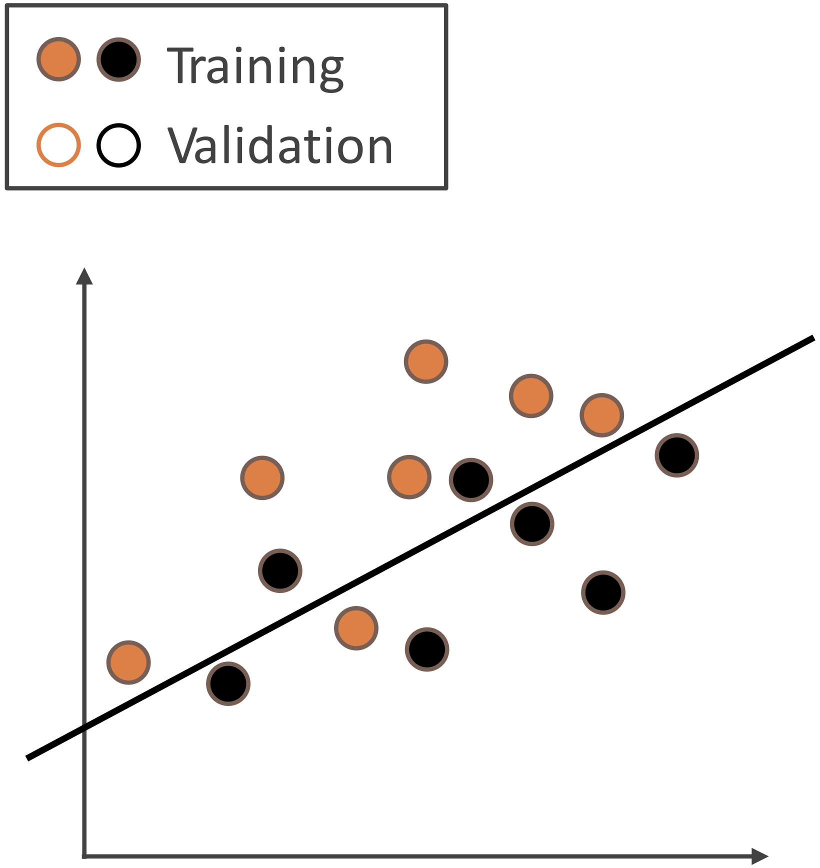


Which model is better?





Why validating?



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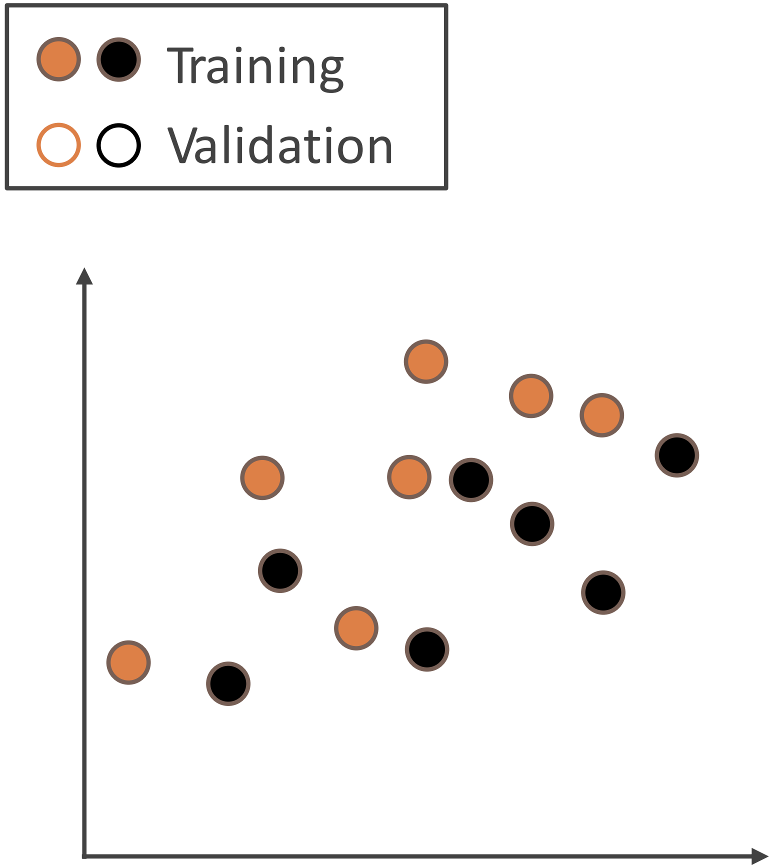

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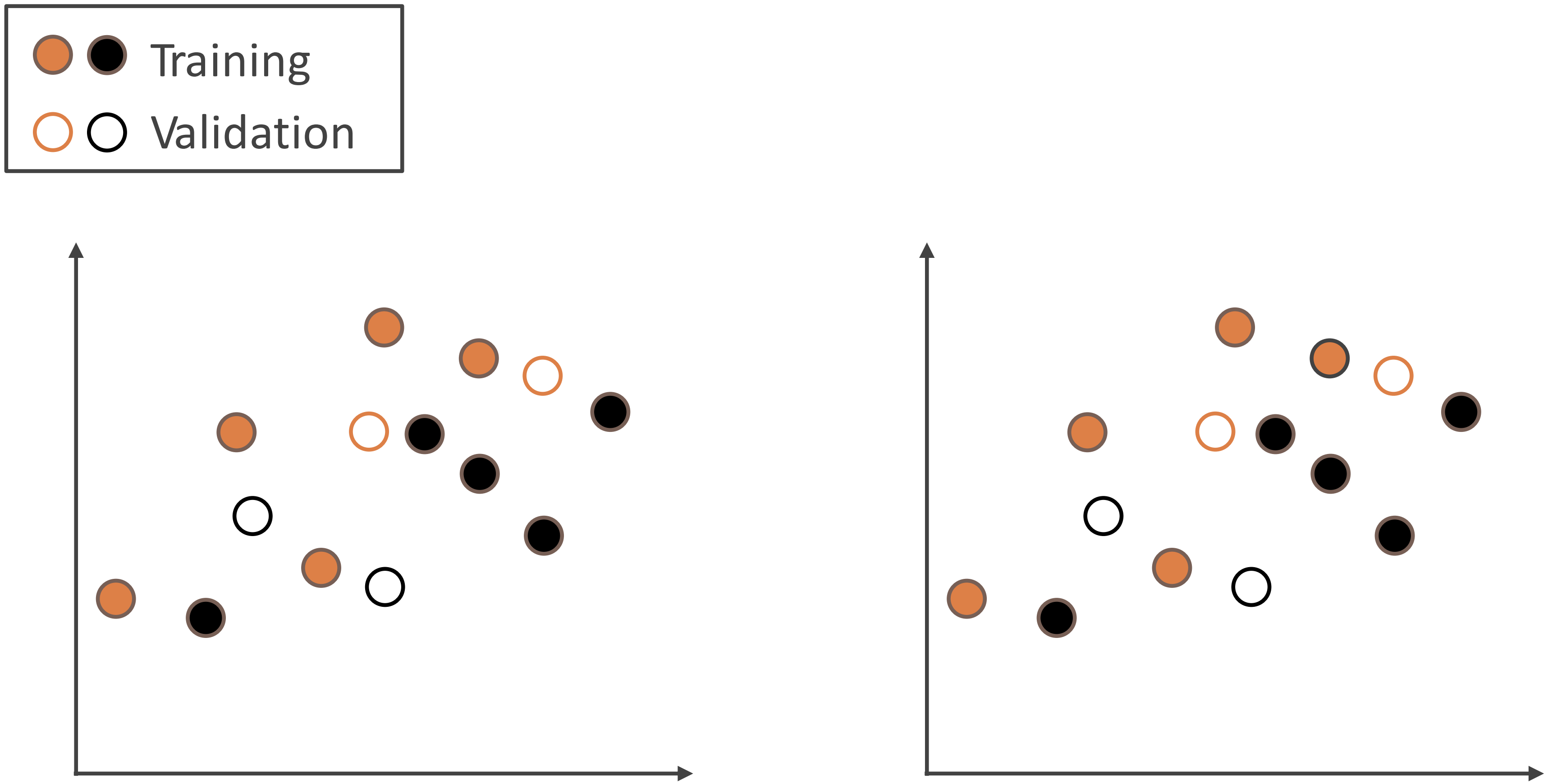

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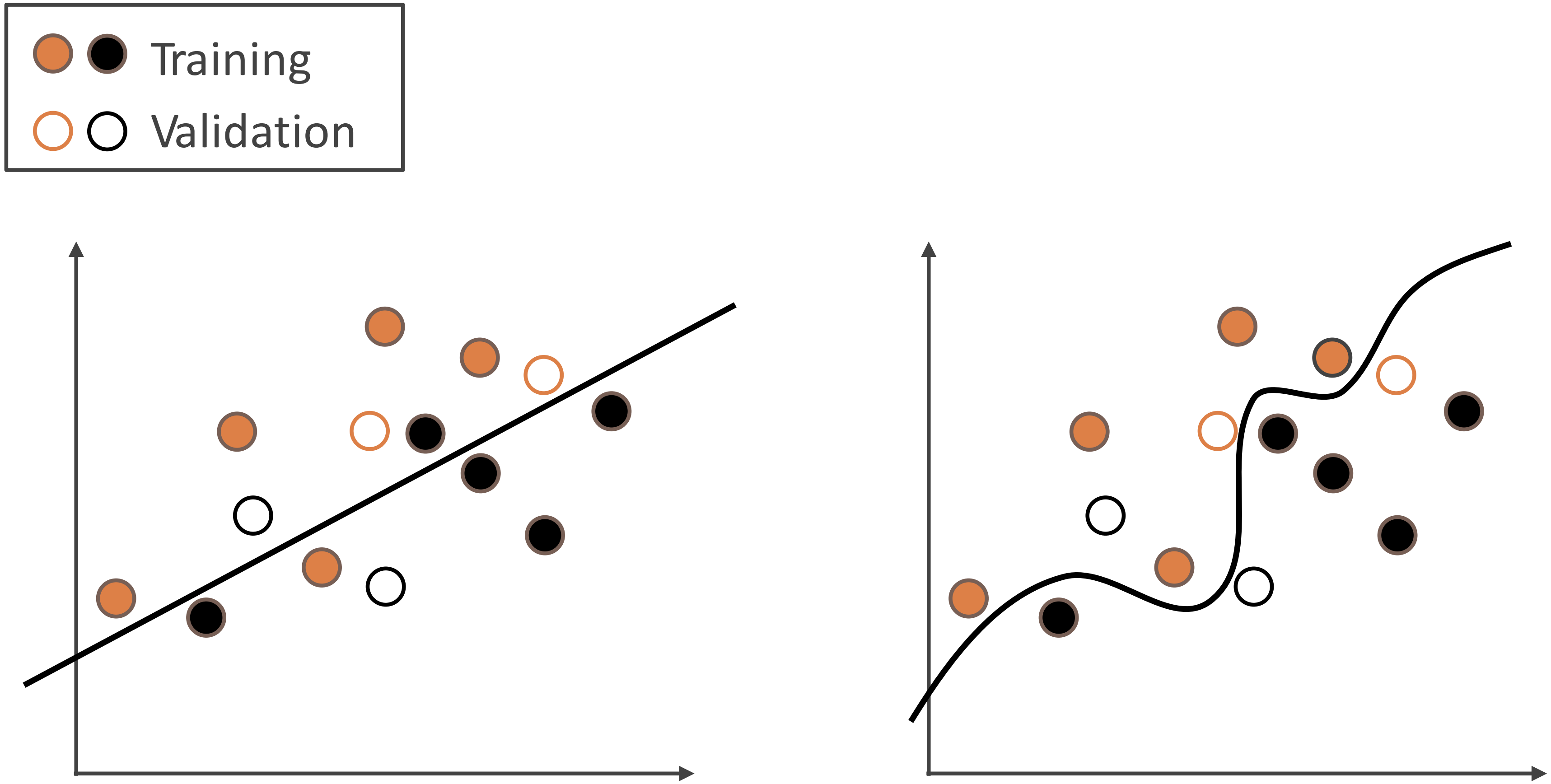

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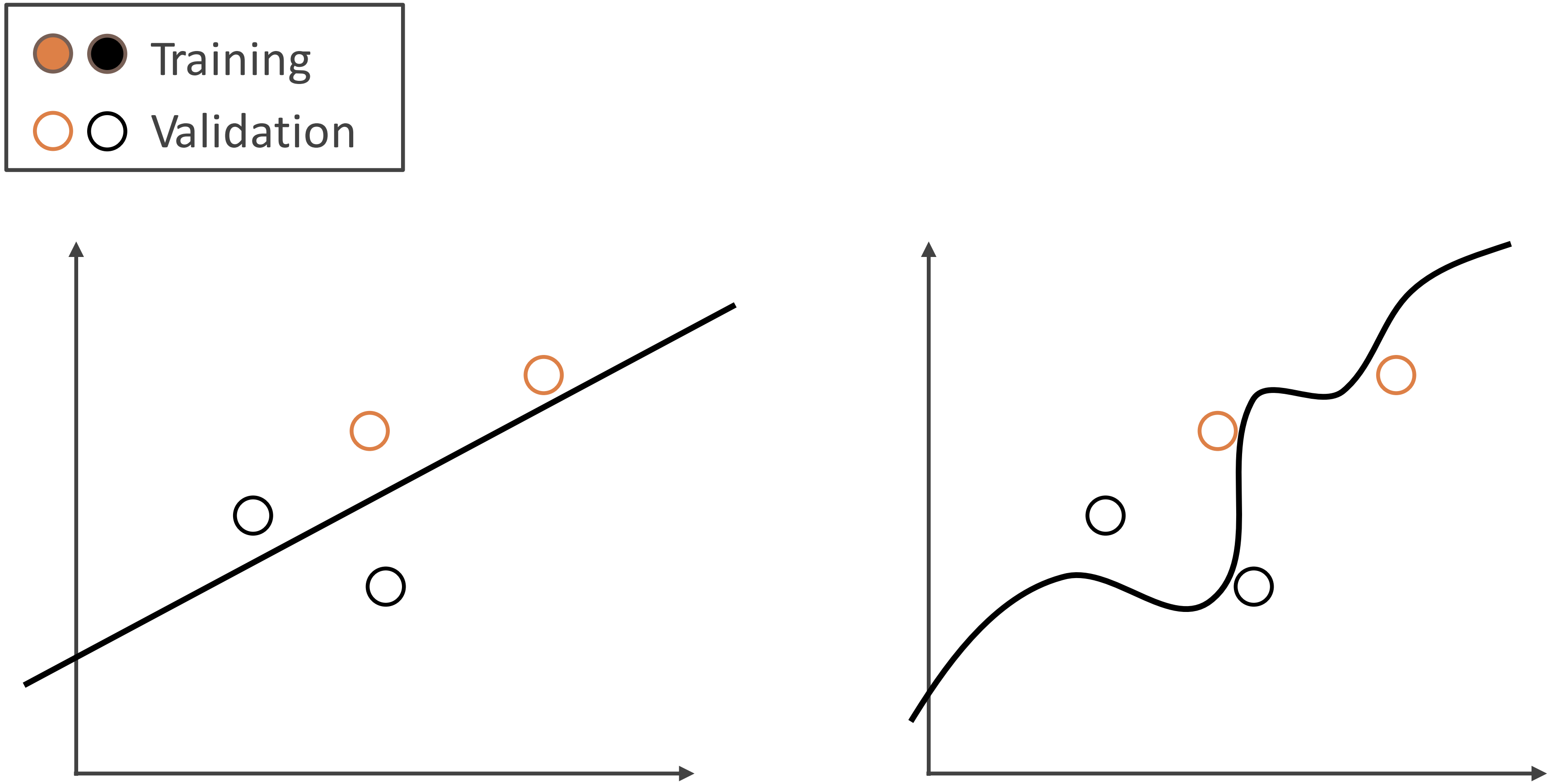

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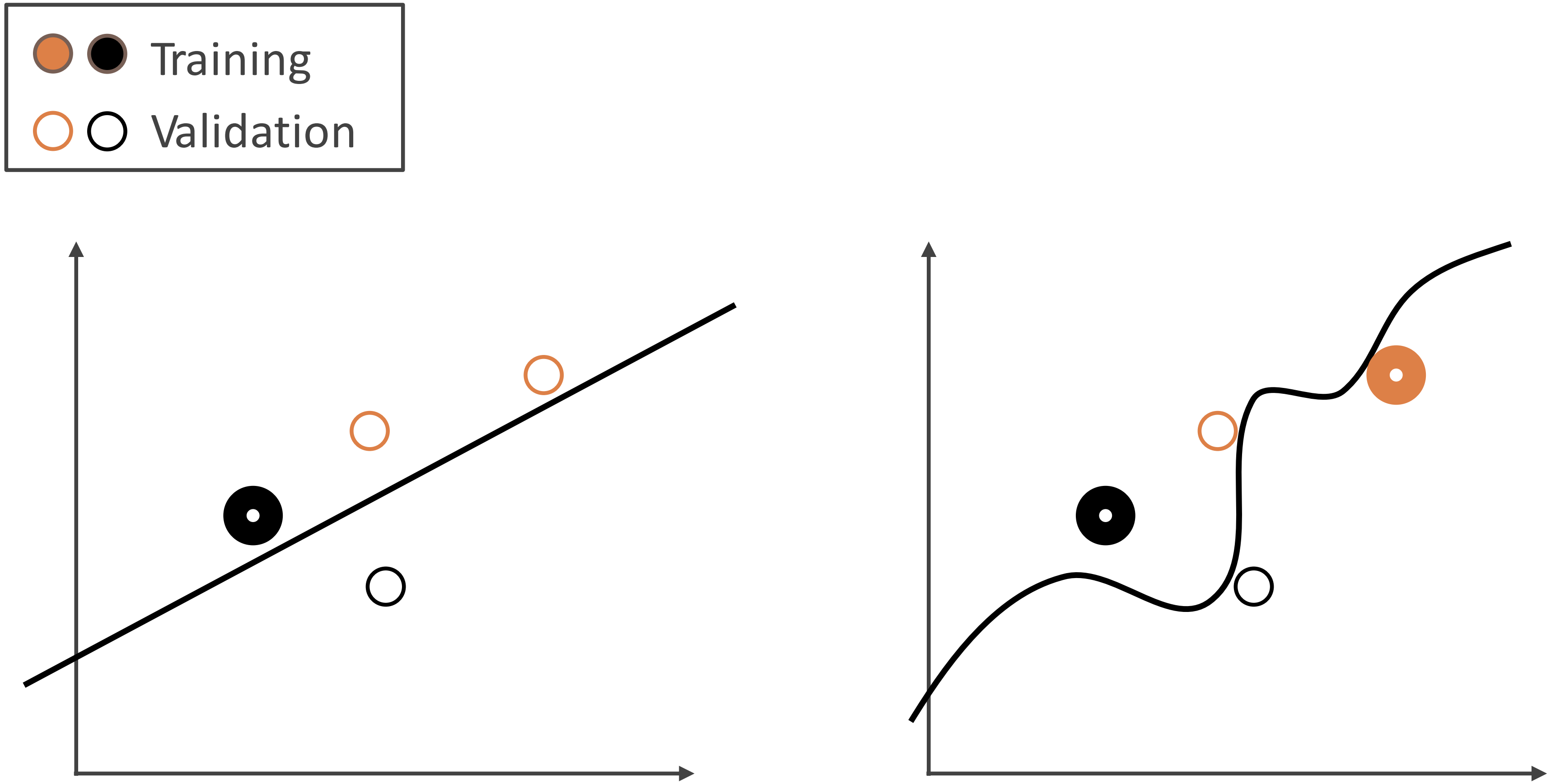

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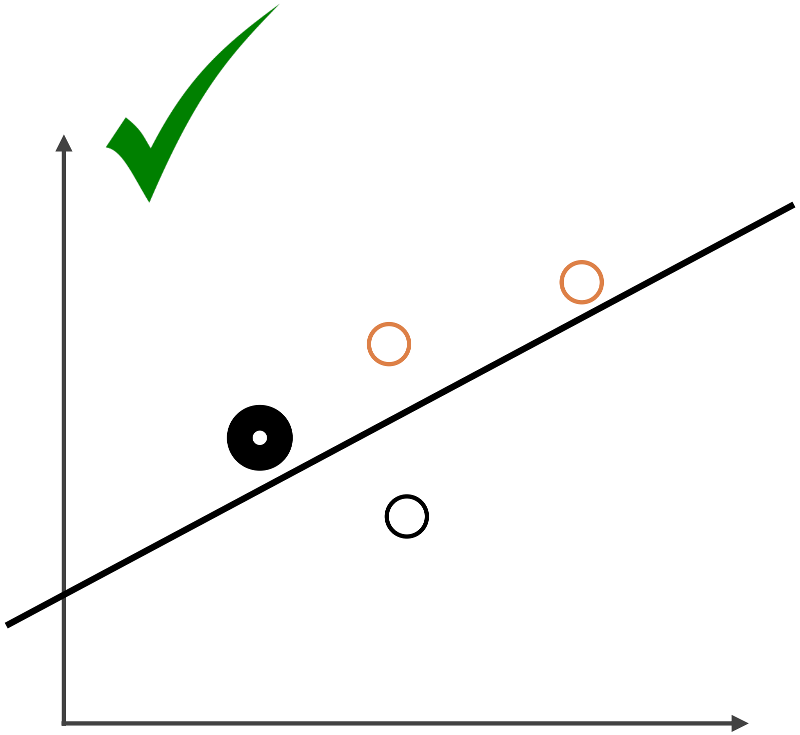
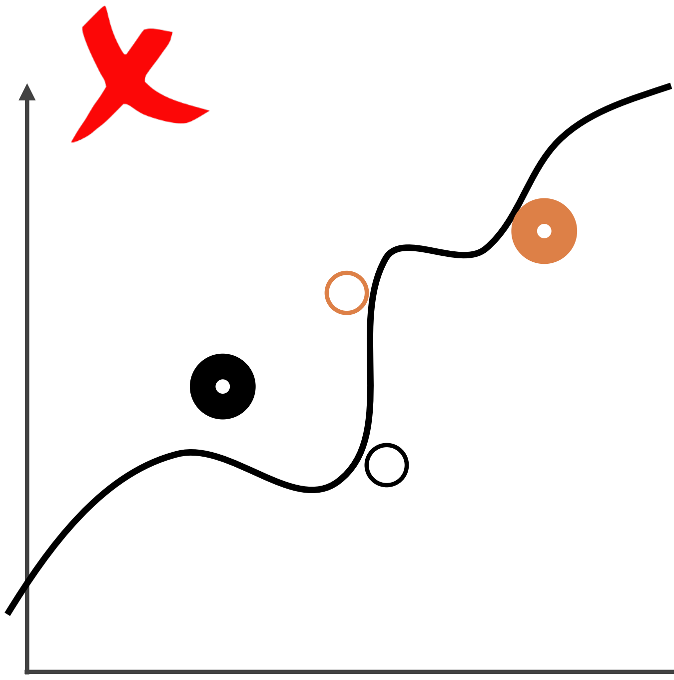
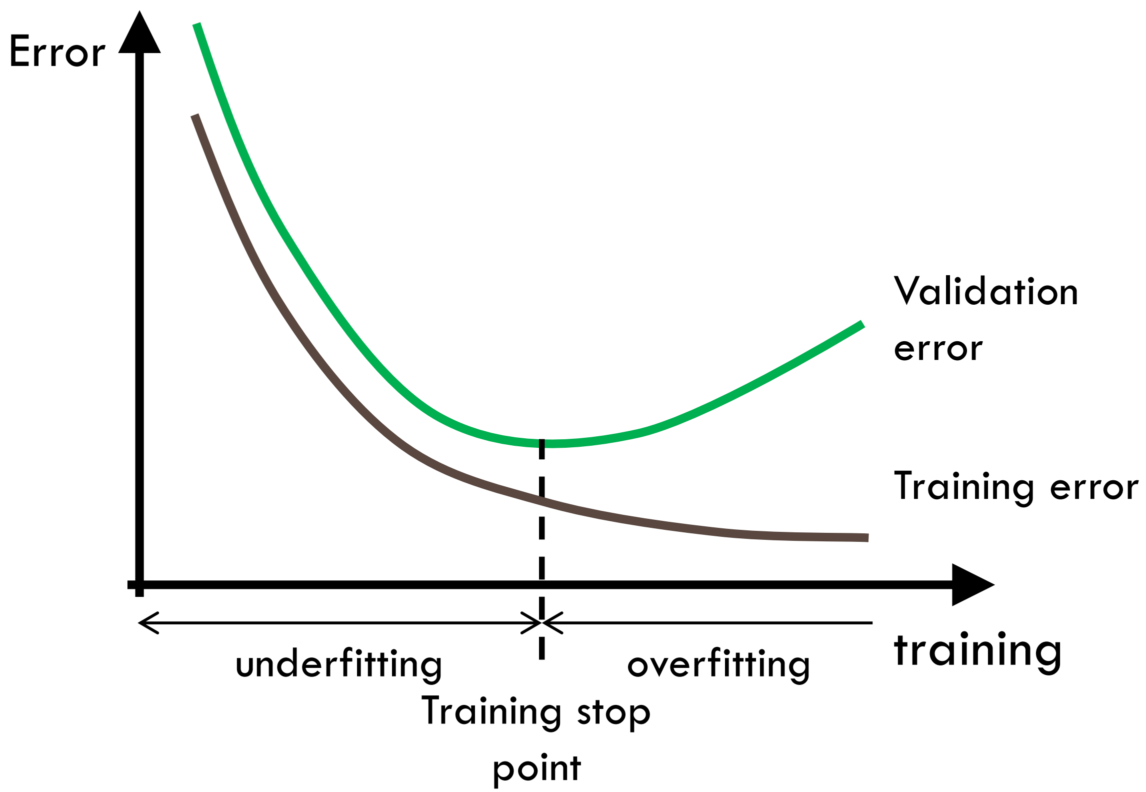




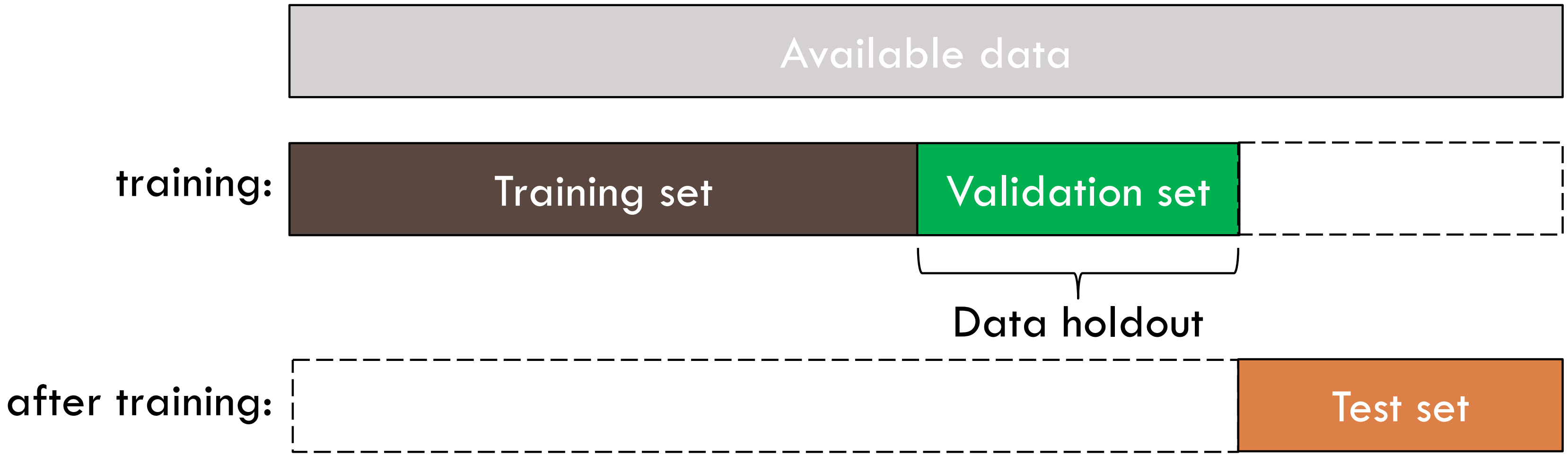
Training early-stopping

- In training, the early-stopping must occur to avoid *underfitting* and *overfitting*



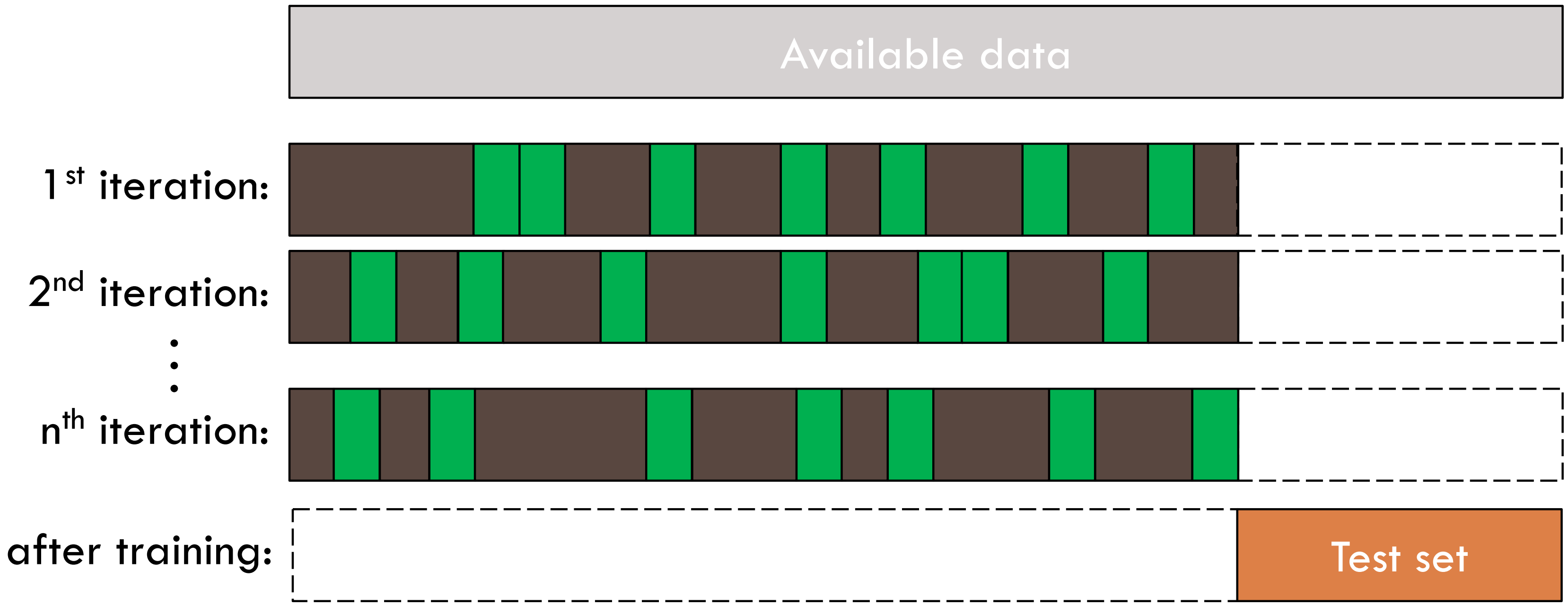
Data splitting strategies

- Holdout method:



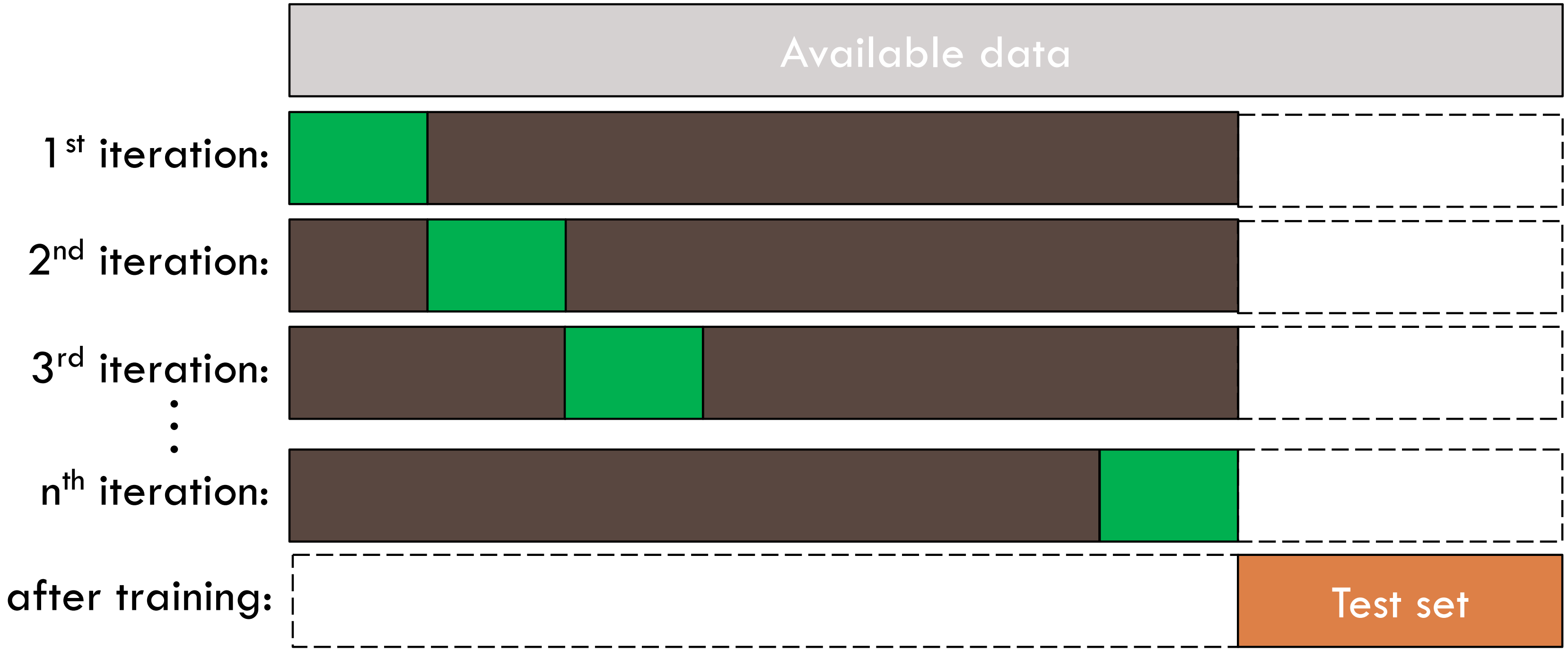
- Remarks:
  - Less data available to training
  - If training and validation sets have different data distribution, results can be distorted

- Repeated holdout method:



- Remark:
  - If some examples are selected more (or less) than others for the training or validation sets, results can be distorted

- K-Fold:

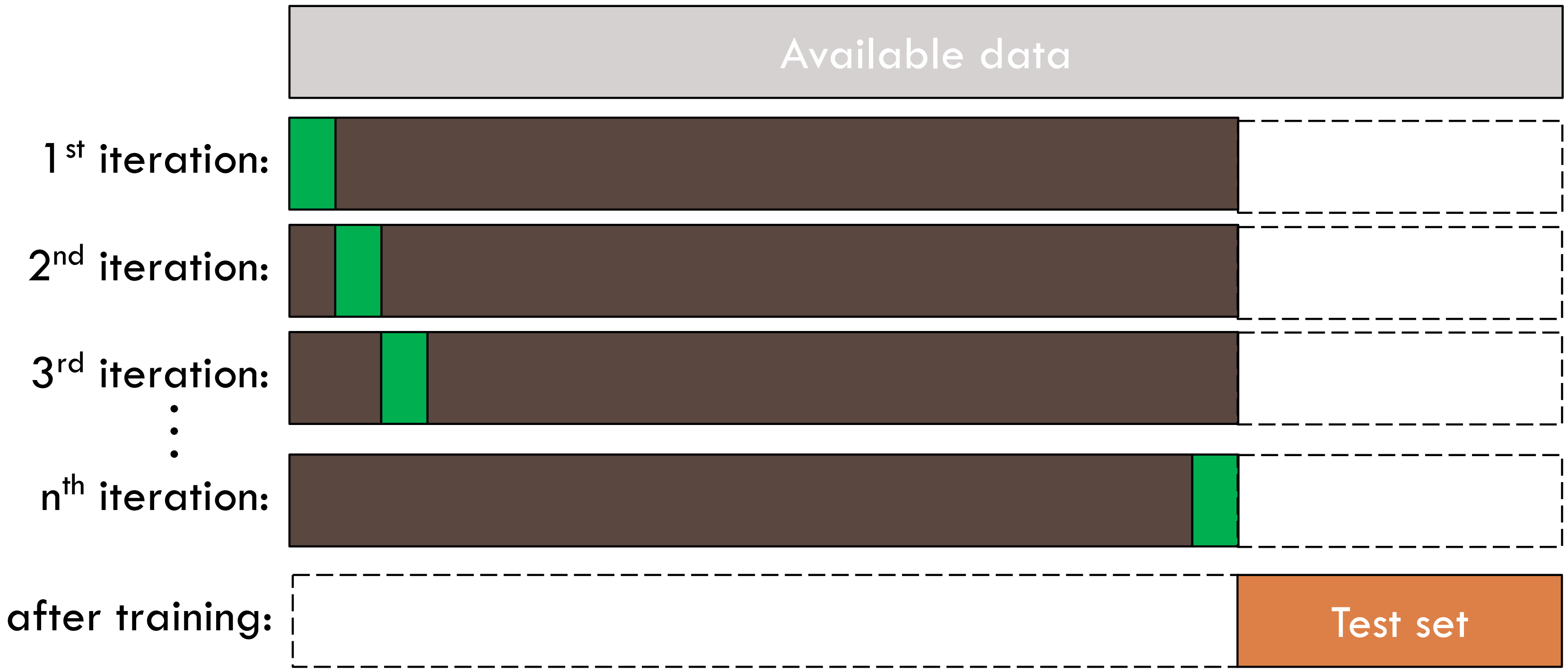


- Remarks:
  - This strategy has a more structured way to divide the available data between training and validation sets
  - Very common approach in practice

$$CV_{(K)} = \sum_{k=1}^{K} \frac{n_k}{n} \text{Error}_k$$

Data splitting strategies

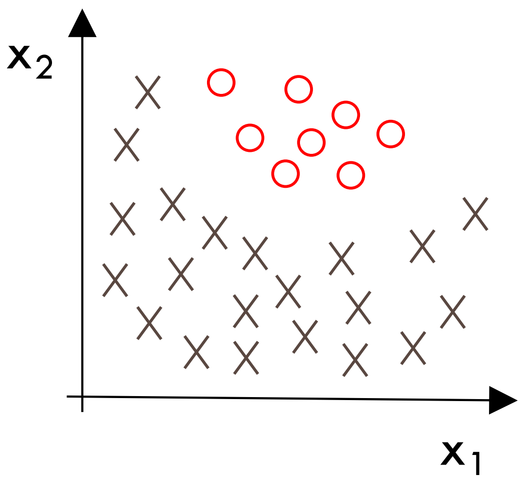
- Leave-one-out:

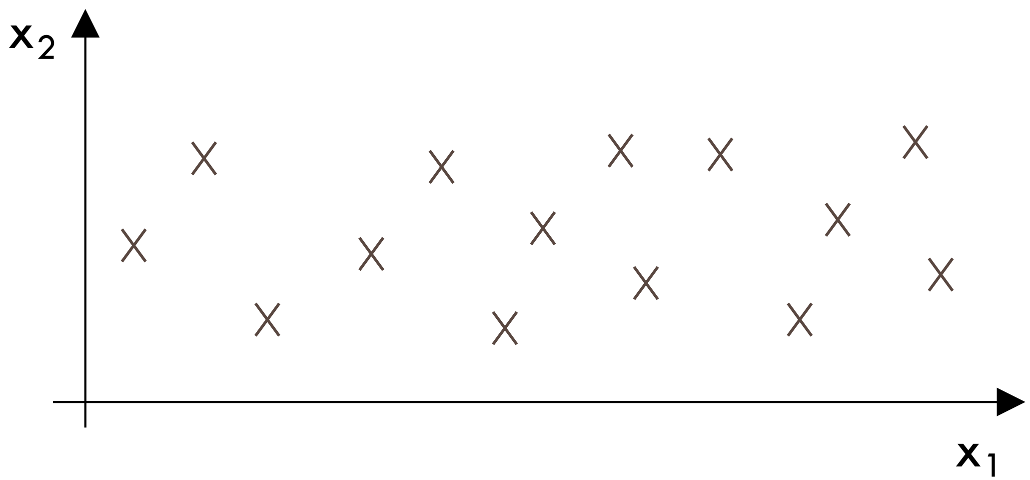


- Remarks:
  - Particular case of K-Fold with just one sample at the validation set

Input data distribution

- Ideally, sampling in all datasets (training, validation and test) must have the **same data distribution than the total available data.** Particularly:
  1. Sets must preserve the same relation of the number of samples from each class present in original data
  2. Sets must contain samples spread over all regions of the domain





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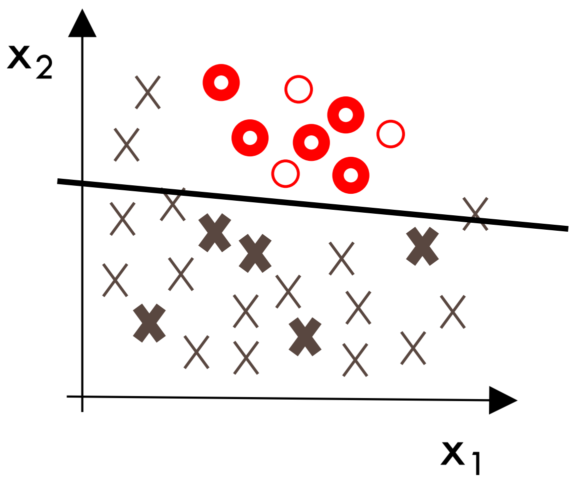

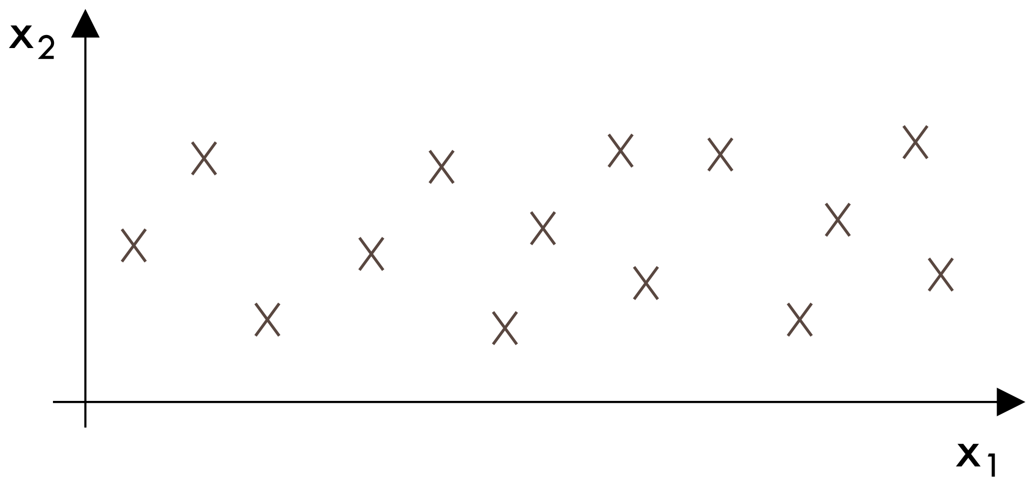

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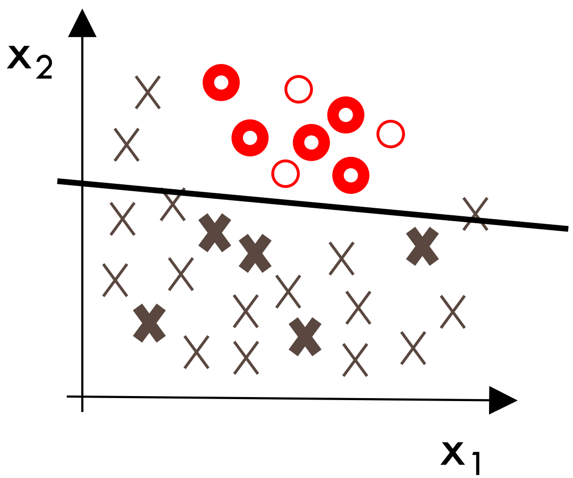
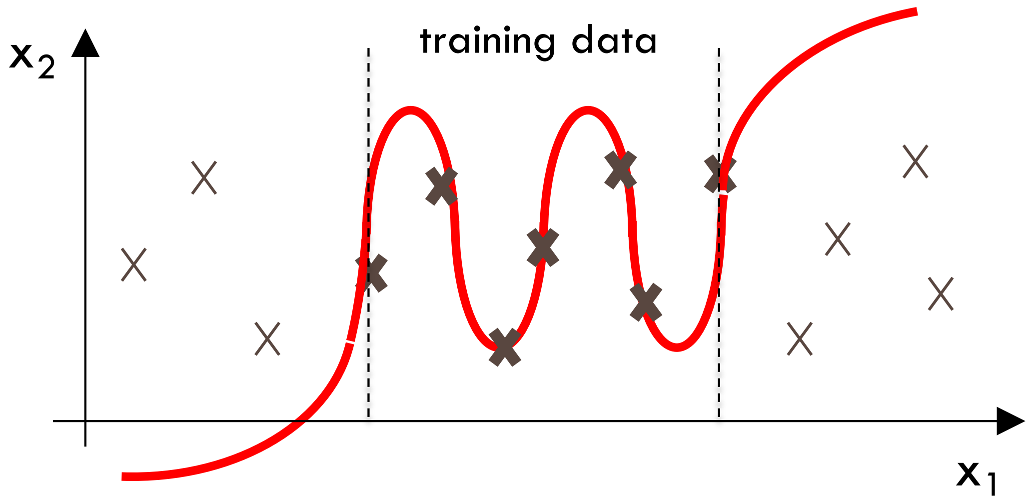
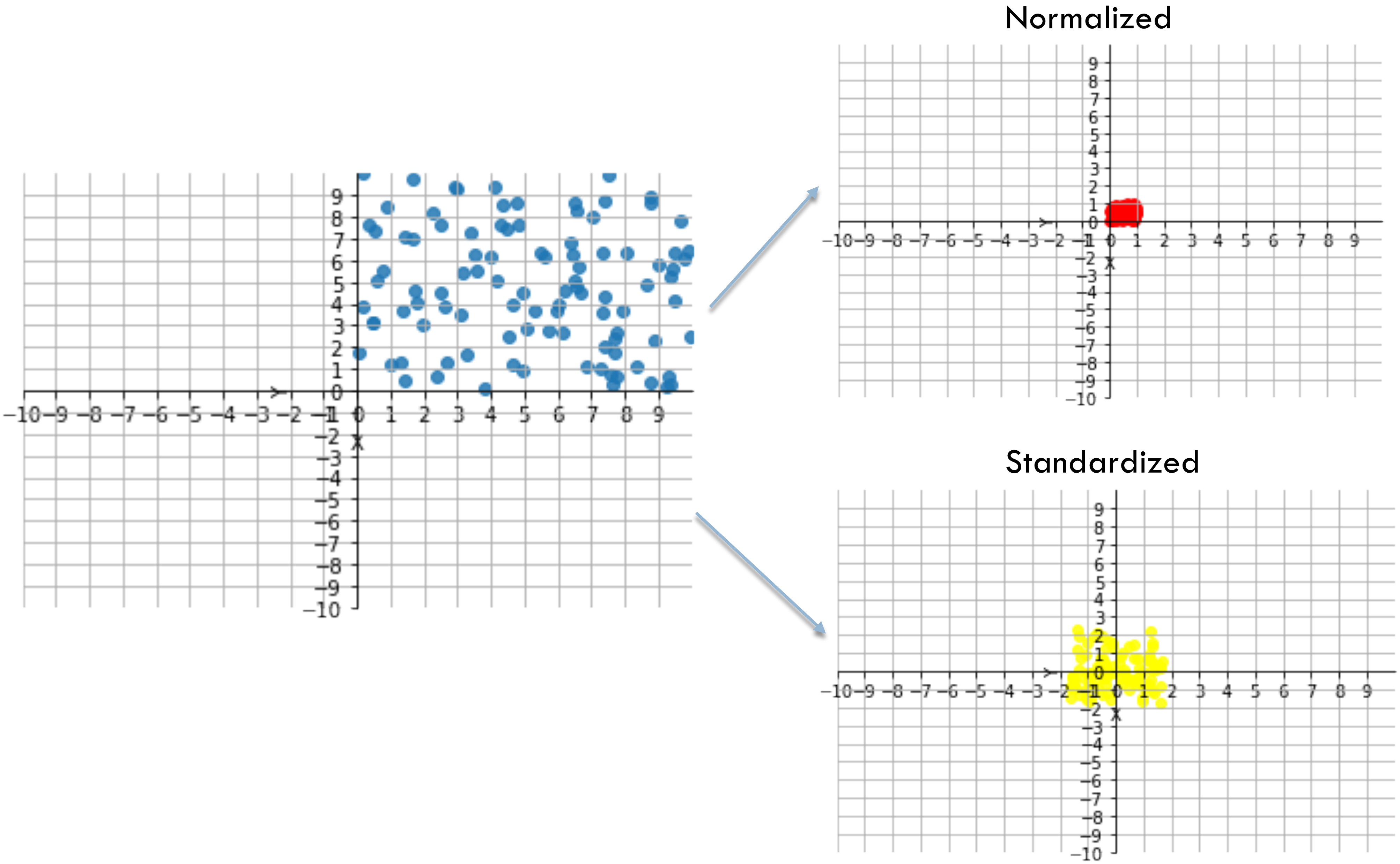




Feature scaling

- **Feature scaling** is a method used to normalize the range of independent variables or features of data
  - It is also known as data **normalization** and is generally performed during the data preprocessing step
  - In **normalization**, the range of your data changes. Normalization means adjusting values measured on different scales to a common scale
    - typically, between [0,1] or [-1,1]
  - In **standardization** the shape of the distribution of your data changes
    - typically means rescaling data to have a mean of 0 and a standard deviation of 1 (unit variance)
- Why use these pre-processing steps?
  - the range of values of raw data varies widely
  - some machine learning algorithms will not work properly without normalization
  - For example, methods that calculate the distance between two points using the Euclidean distance
    - If one of the features has a broad range of values, the distance will be governed by this particular feature

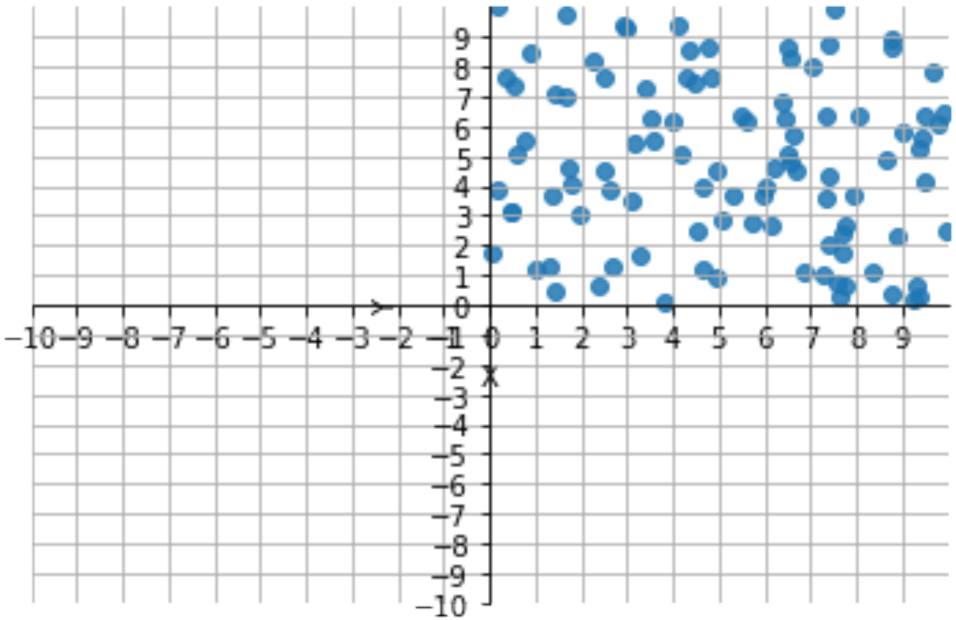
Feature scaling



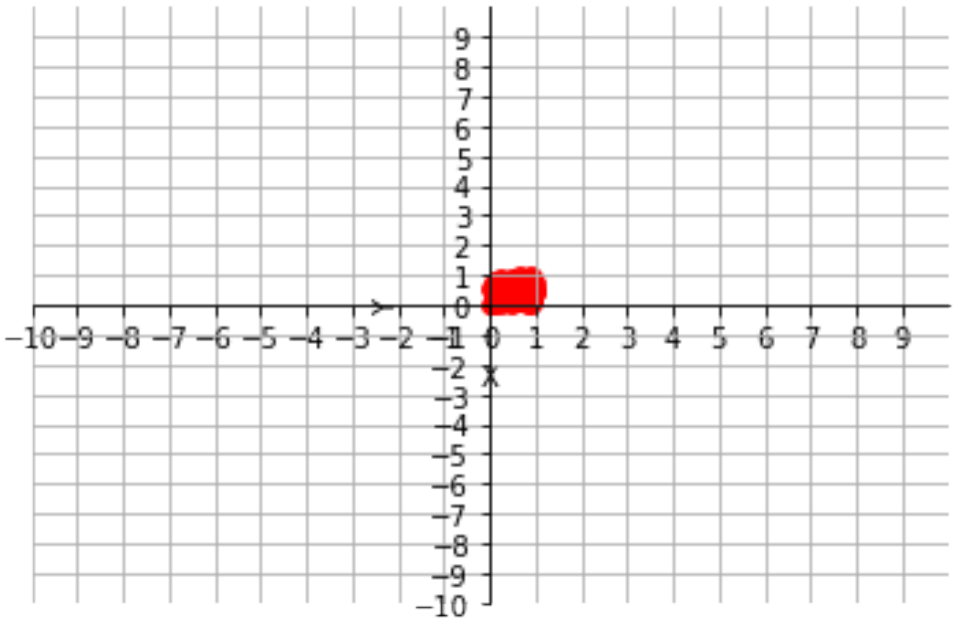
Feature scaling

Types

- Min-Max Scaler (MinMaxScaler)
  - Transform features by scaling each feature to a given range



mean: [4.64091733 4.71477069]
std: [2.92323848 2.93324495]
min: [0.02917744 0.07193049]
max: [9.97337705 9.99855761]

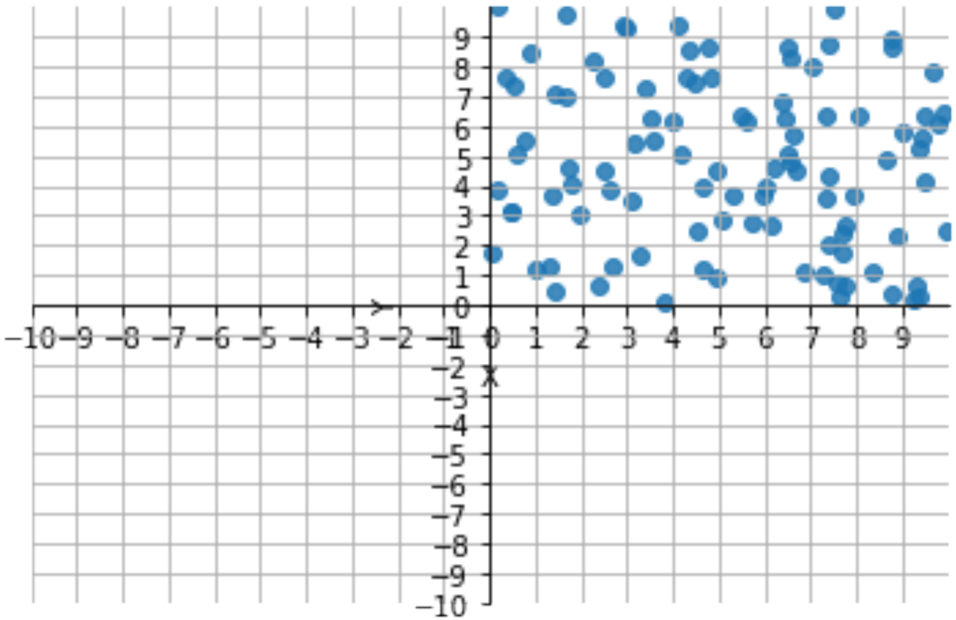


mean: [0.52228216 0.50308238]
std: [0.30594303 0.26681954]
min: [0. 0.]
max: [1. 1.]

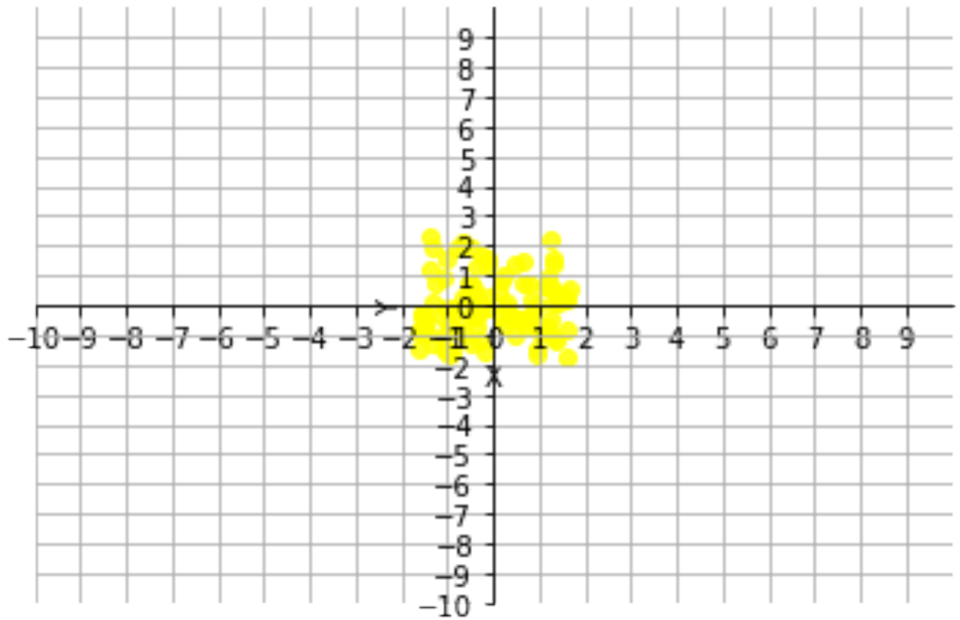
Feature scaling

Types

- Standard Scaler (StandardScaler)
  - Standardize features by removing the mean and scaling to unit variance

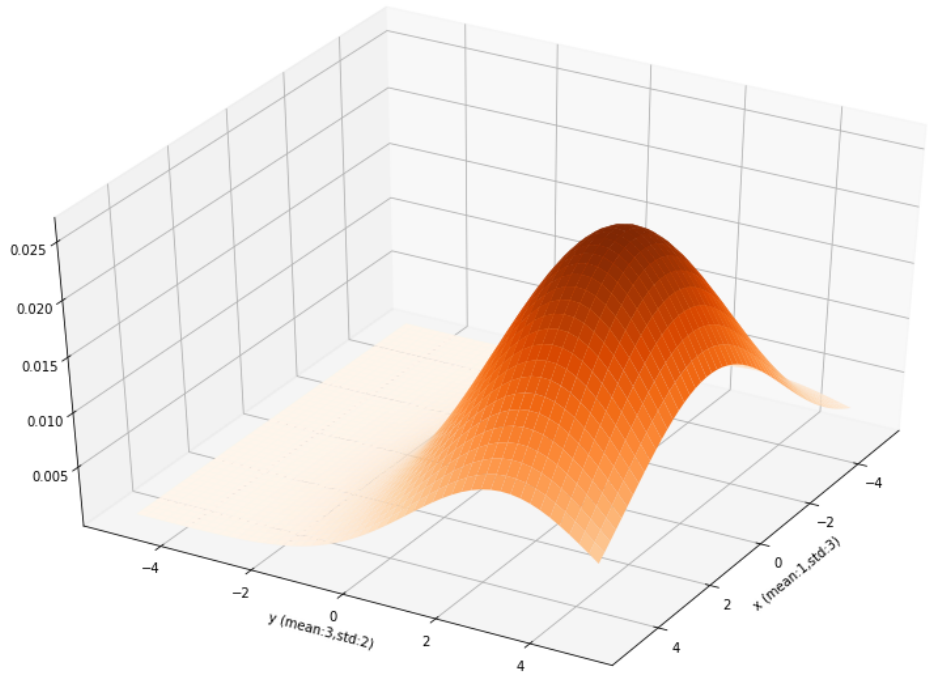


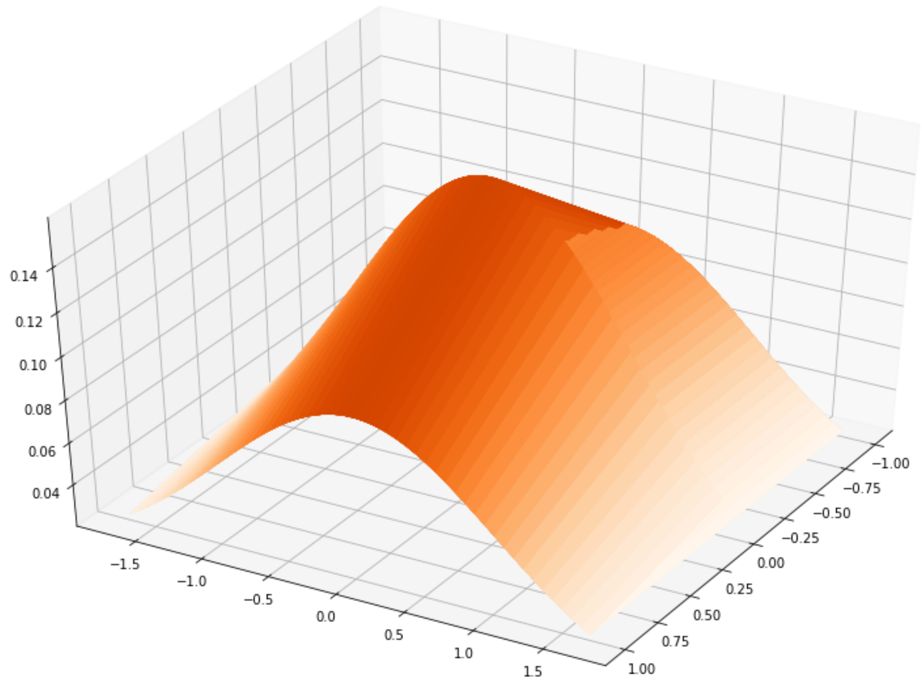
mean: [4.64091733 4.71477069]
std: [2.92323848 2.93324495]
min: [0.02917744 0.07193049]
max: [9.97337705 9.99855761]



mean: [0.52228216 0.50308238]
std: [0.30594303 0.26681954]
min: [0. 0.]
max: [1. 1.]

- Standard Scaler (StandardScaler) – 3d
  - Standardize features by removing the mean and scaling to unit variance

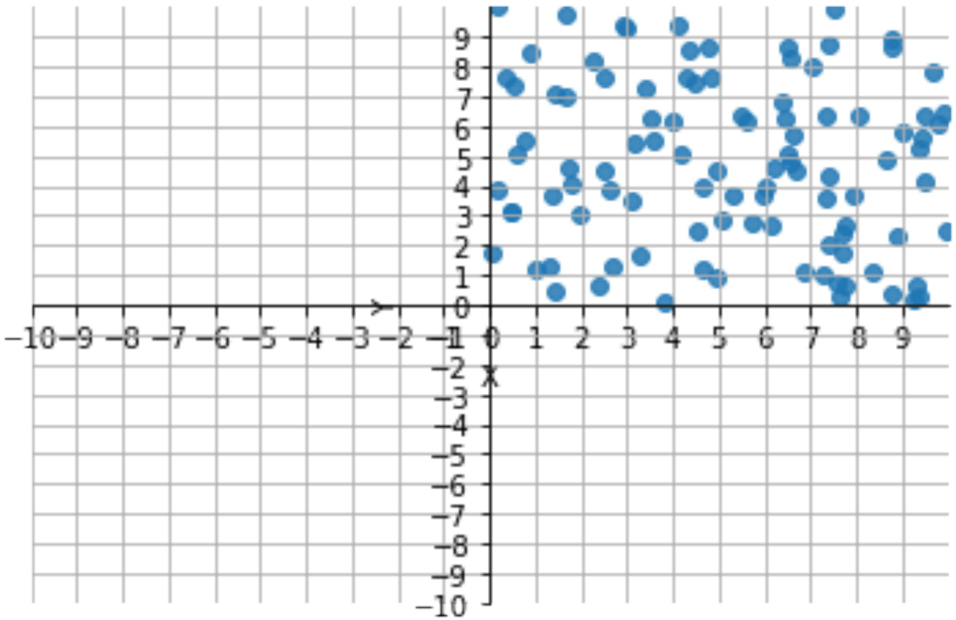




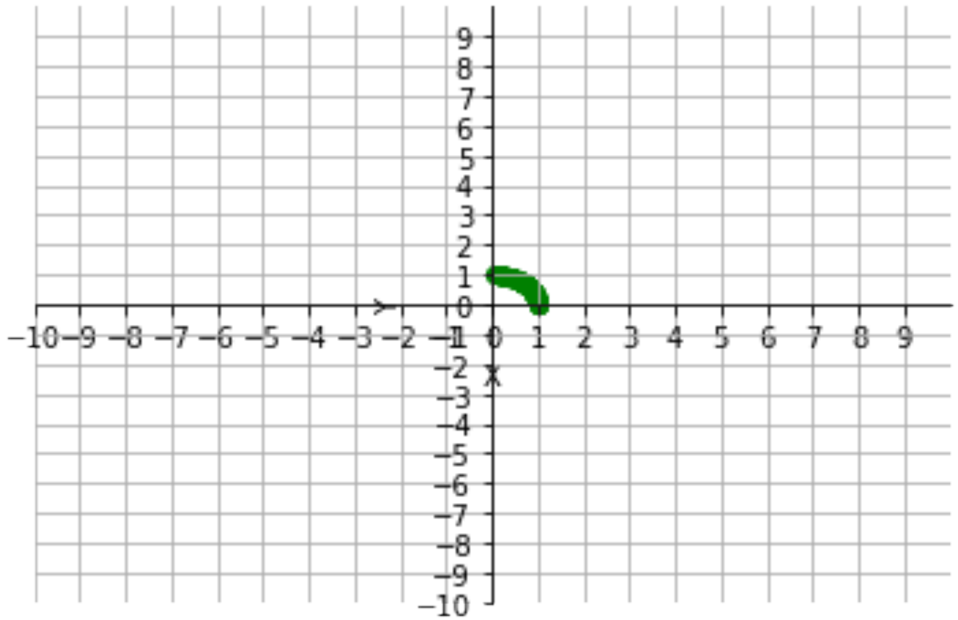
Feature scaling

Types

- Unit Vector Scaler (Normalizer)
  - Normalize samples individually to unit norm.



mean: [5.24874418 4.65066746]
std: [3.03272127 3.02536061]
min: [0.01605648 0.07731266]
max: [9.93963622 9.76344994]



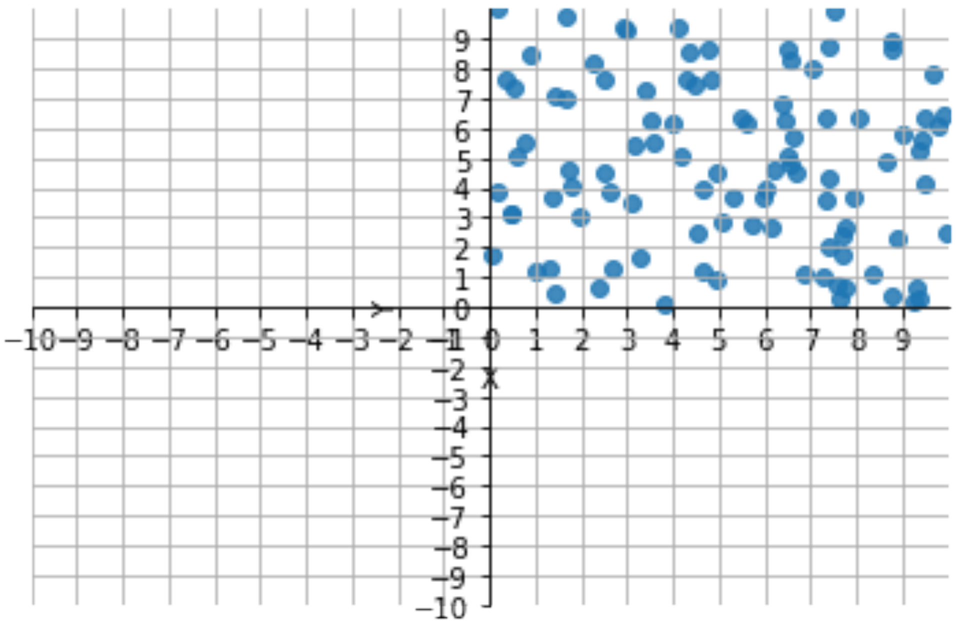
mean: [0.67938241 0.59354895]
std: [0.30042037 0.3096559]
min: [0.00180982 0.05084794]
max: [0.99870641 0.99999836]

Feature scaling

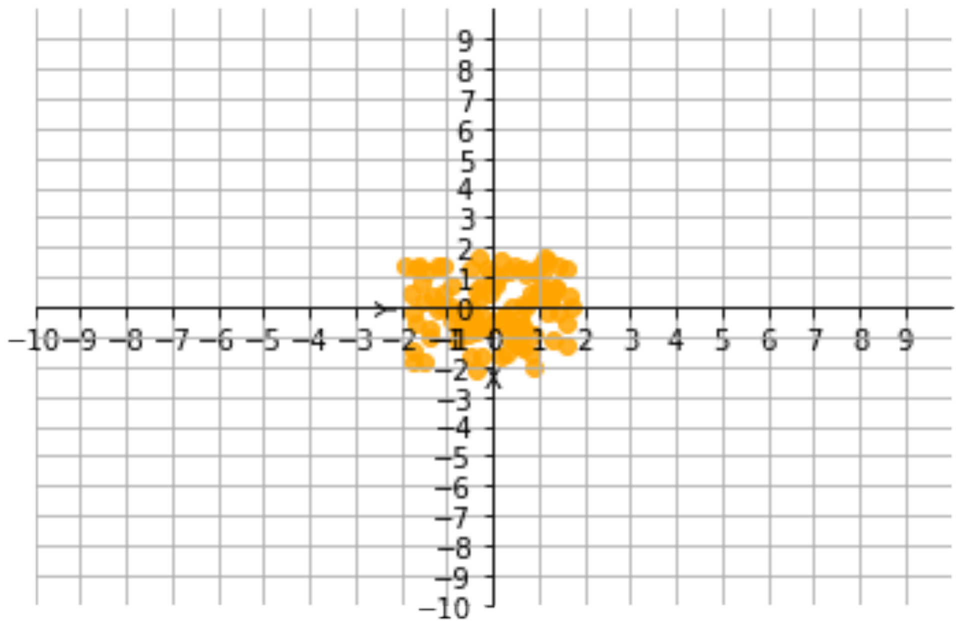
Types

Power Transformer Scaler (PowerTransformer)

- Apply a power transform featurewise to make data more Gaussian-like.



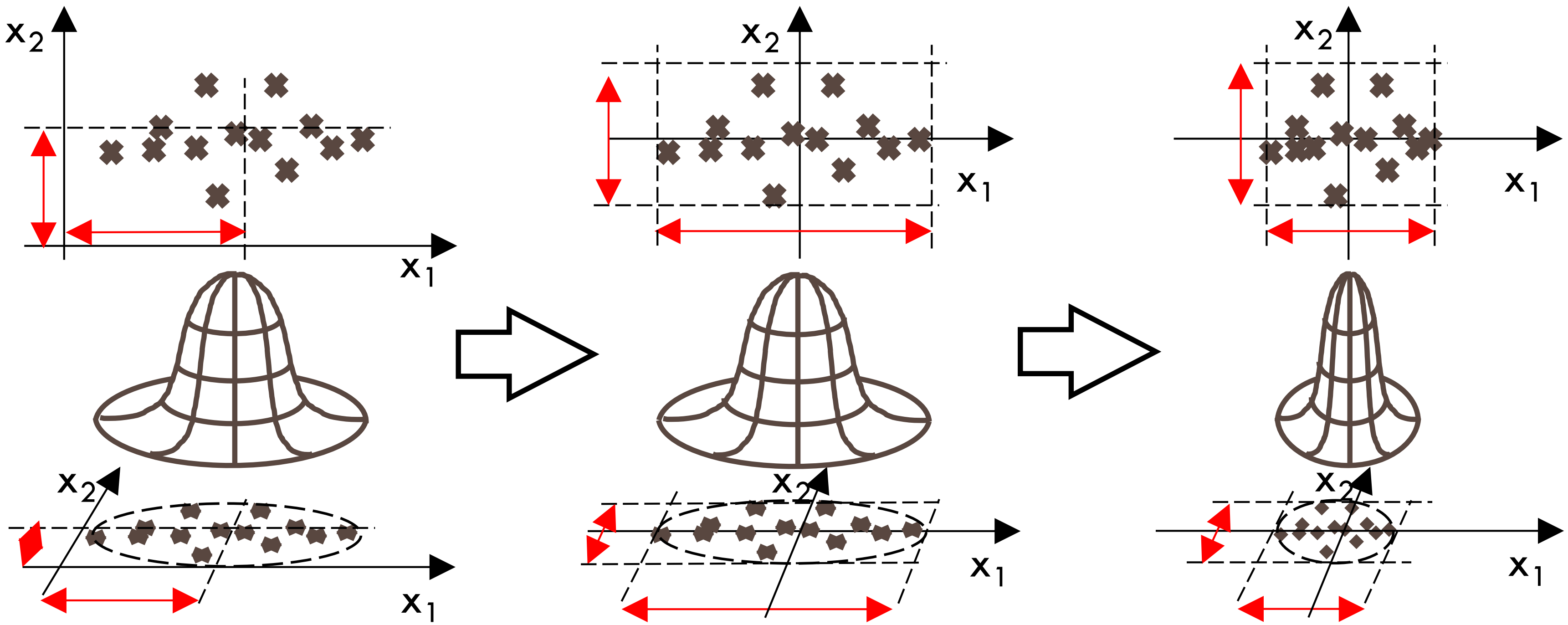
mean: [5.00643671 5.14637406]
std: [2.7285058 2.73460667]
min: [0.07036322 0.0115435]
max: [9.99080893 9.87448843]



mean: [-2.44249065e-17 -7.73617281e-16] std: [1. 1.]
min: [-1.92383512 -2.07521871]
max: [1.74245717 1.63357549]

Input data normalization

- Adjust of measured values (probability distribution):



Zero mean adjustment:

$$\mu_d = \frac{1}{n}\sum_{i=1}^{n} x_{id}$$

$$x_{id} := x_{id} - \mu_d$$

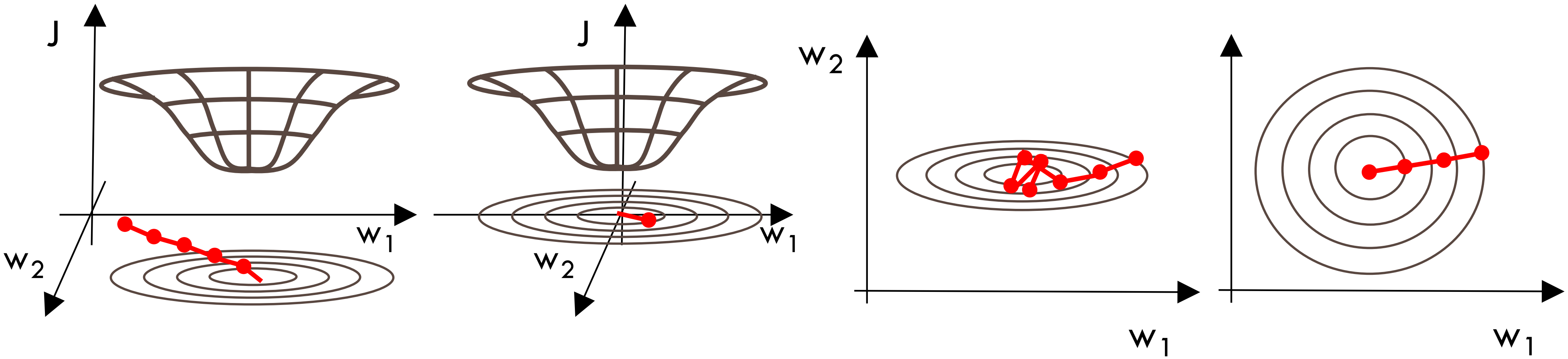
Variance normalization:

$$\sigma_d{}^2 = \frac{1}{n}\sum_{i=1}^{n} (x_{id} - \mu_d)^2$$

$$x_{id} := \frac{x_{id}}{\sigma_d{}^2}$$

Why normalize input data?

- Input data distribution has implications in the **shape of the cost function** used in some learning processes. Although most of the learning algorithms are able to learn over unnormalized data:
  - If data distribution has **zero mean,** it will probably require less learning steps to tune variables in models
  - In a **symmetrical cost function,** the step size (learning rate) tends to be more effective to find the center of the function



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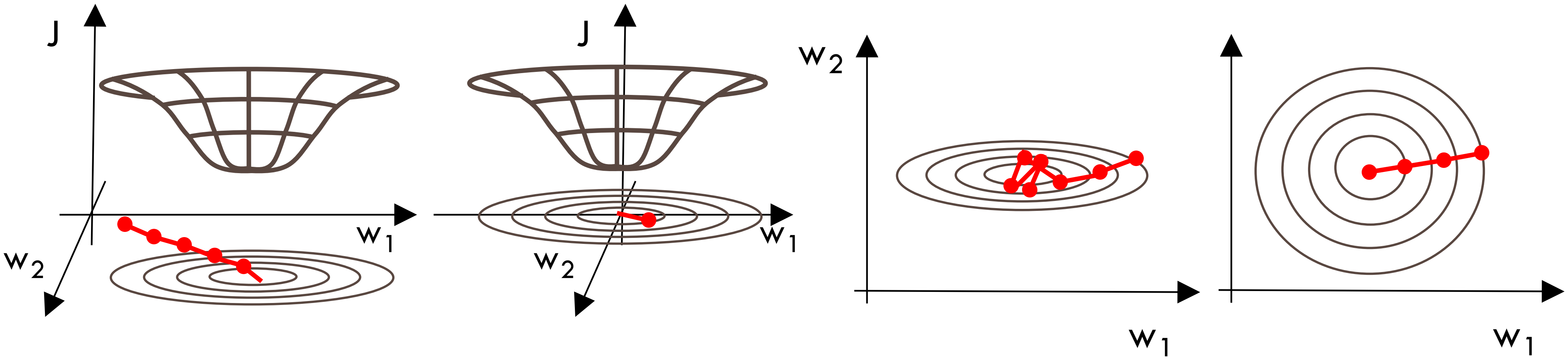

Extra-class activities

Lecture 2

- Activities
  - Quis 2
    - Fundamental of ML
  - Reading:
    - Python for ML

References

Lecture 2

- MARSLAND, S. Machine Learning: an algorithm perspective. CRC Press, 2nd edition, 2015.
- ALPAYDIN, E. Introduction to Machine Learning. MIT Press, 3rd edition, 2014.
- SILVA, I. N.; SPATTI, D. H.; FLAUZINO, R. A. Redes Neurais Artificiais para engenharia e ciências aplicadas. Curso prático. Artliber Editora, 2010.
- SUTTON, R. S.; BARTO, A. G. Reinforcement learning: an introduction. MIT Press, Cambridge, MA, 2nd edition in progress, 2017.

This material is part of the Machine Learning Course
By Esther Colombini and Alexandre Simões

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