

HFT Summer School 2025

Fundamentals of Machine Learning

Michael Mommert

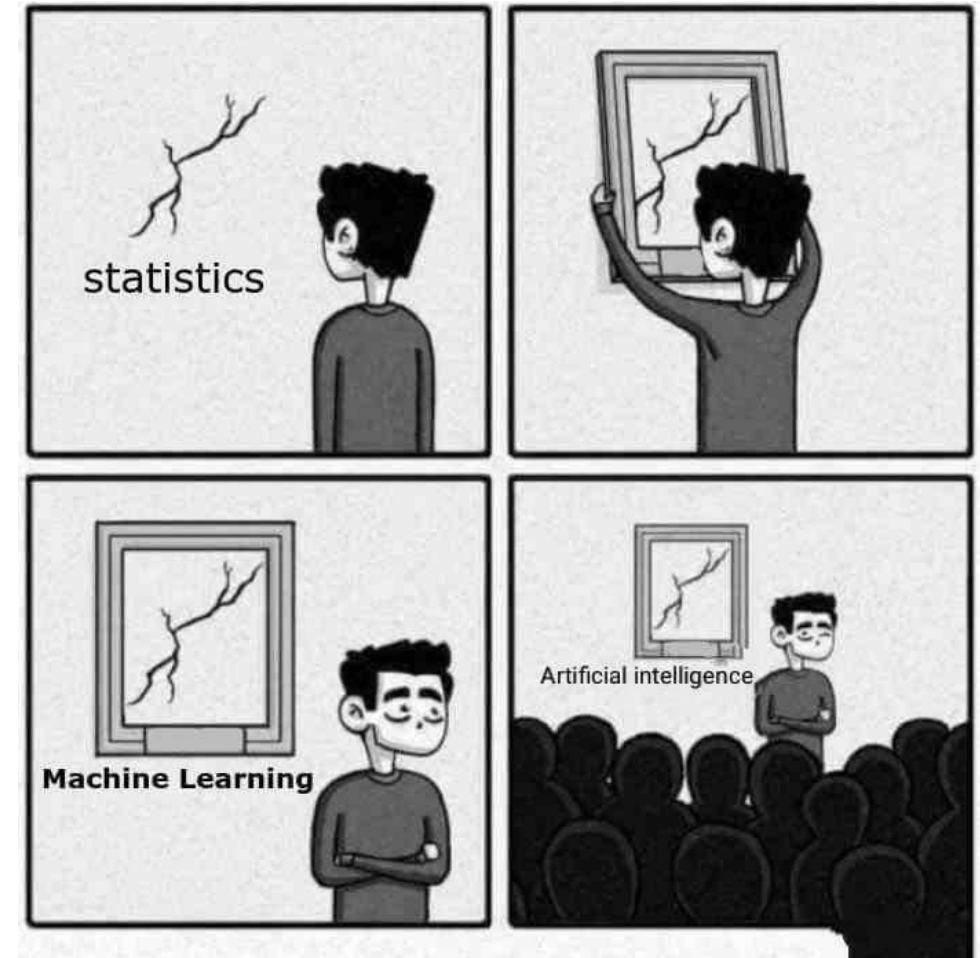
Stuttgart University of Applied Sciences

Learning Objectives

In this lecture you will learn the following:

- What is machine learning?
- What is supervised learning?
- What is feature engineering?
- What is overfitting, underfitting and generalization?
- How to benchmark machine learning models?
- How to use a linear regression model?
- How to use a k-Nearest Neighbor classifier?

What is Machine Learning?

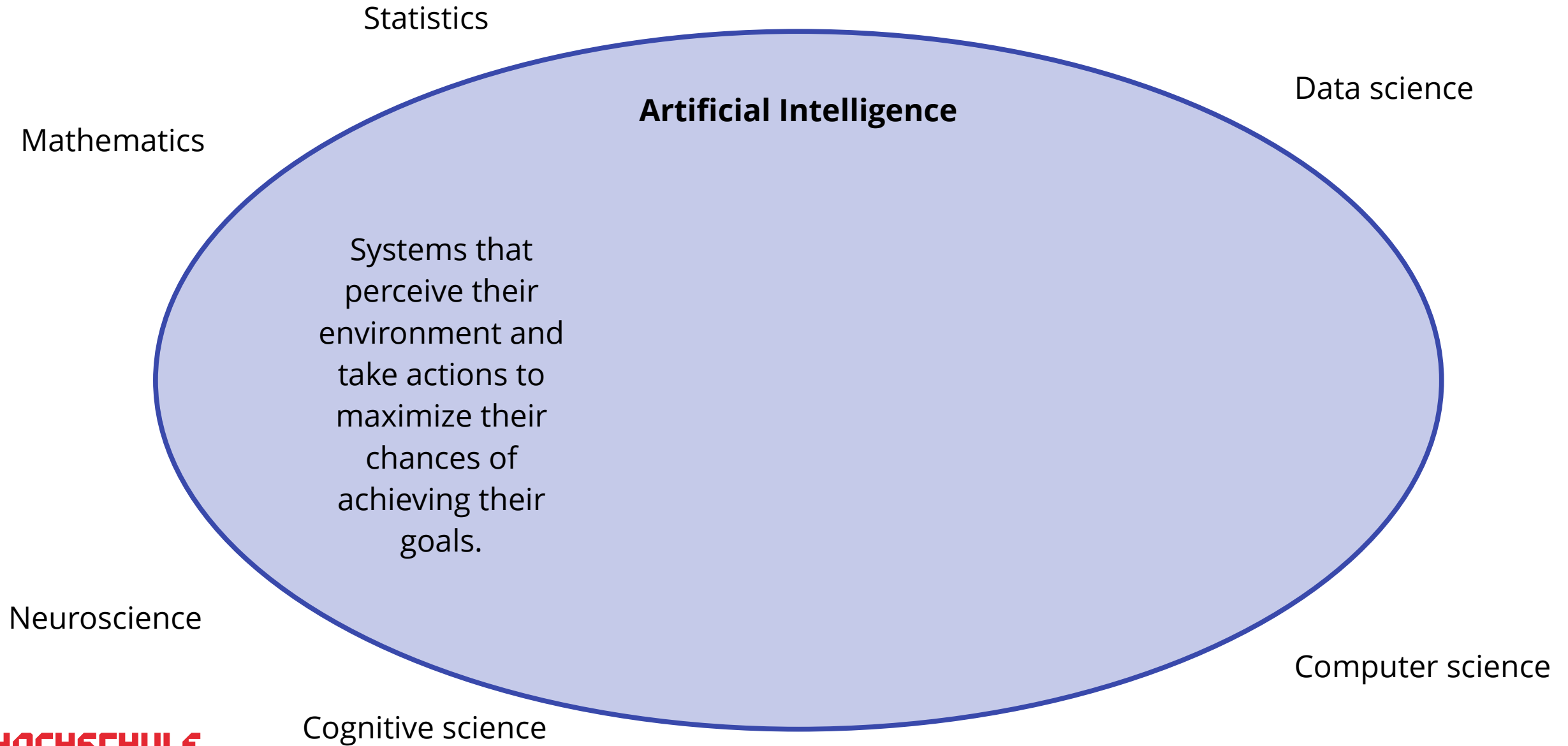


Mapping terminology

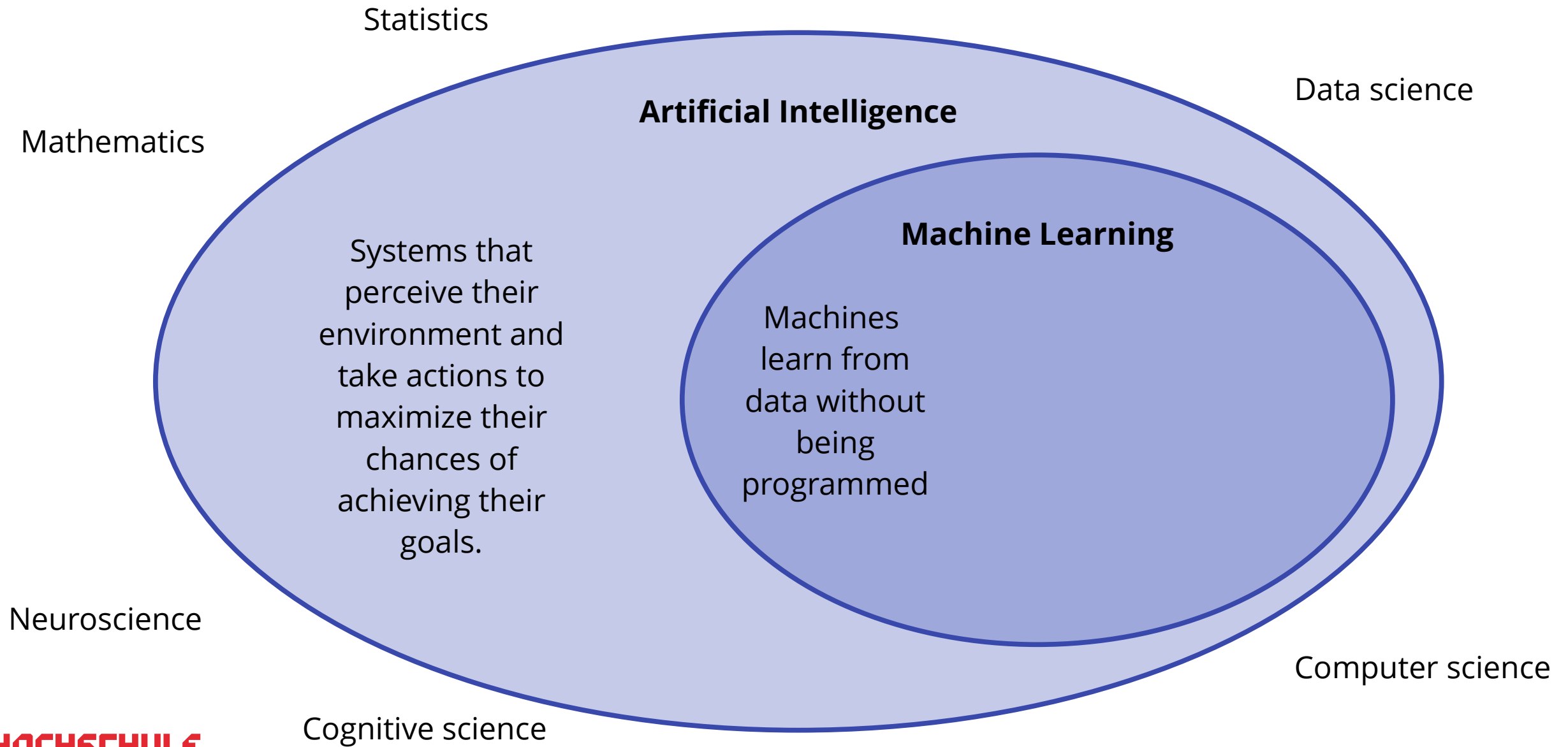
Artificial Intelligence

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

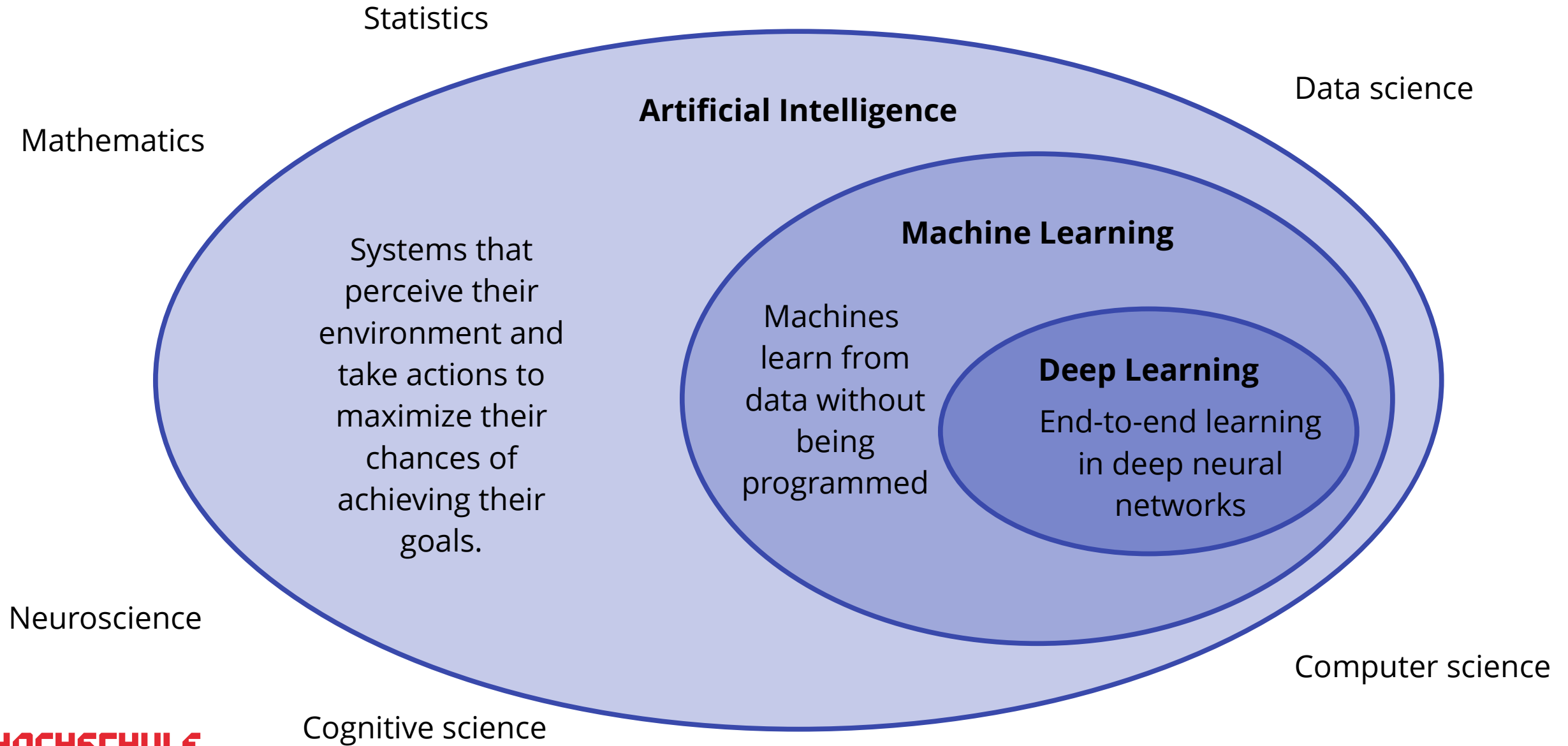
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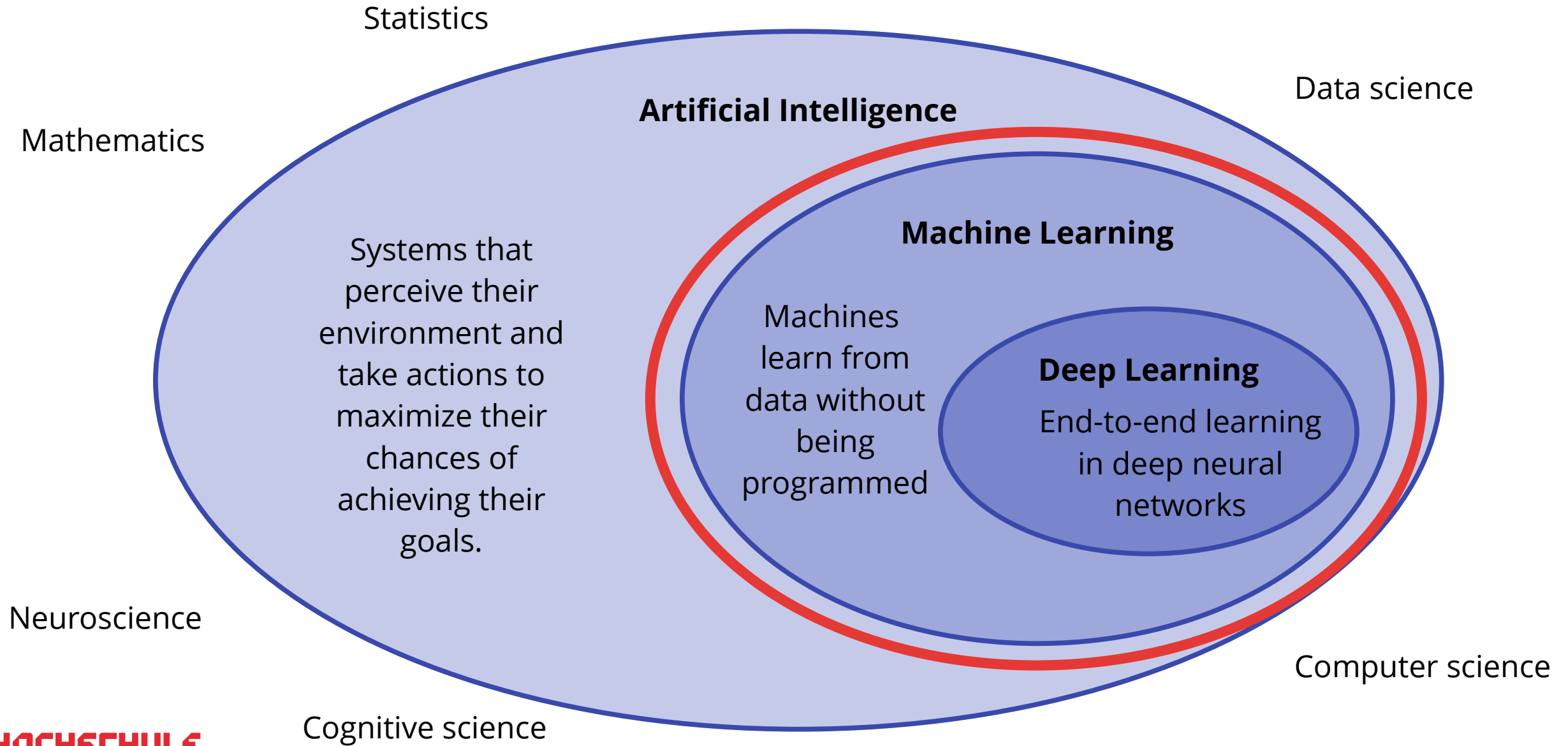
Mapping terminology



Mapping terminology



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:

- **Supervised learning**

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

- **Unsupervised learning**

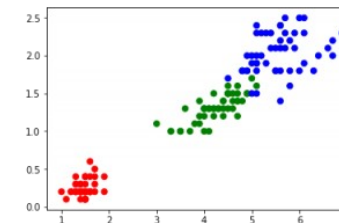
Find structure within a data set.

- **Reinforcement learning**

Learn a task in a dynamic and responsive environment.



Iris Versicolor



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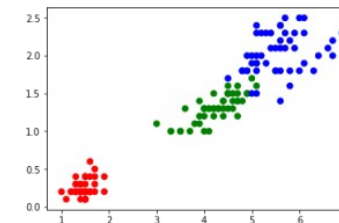
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Learn a task in a dynamic and responsive environment.



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Supervised Machine Learning

Supervised Machine Learning

General goal for supervised problems:

Find a function (“task”) that relates input data ($\mathbf{x}$) to output data ($\mathbf{y}$) such that: $f(\mathbf{x}) = \mathbf{y}$

This function has to be “trained” before it can be applied to previously unseen data (“inference”).

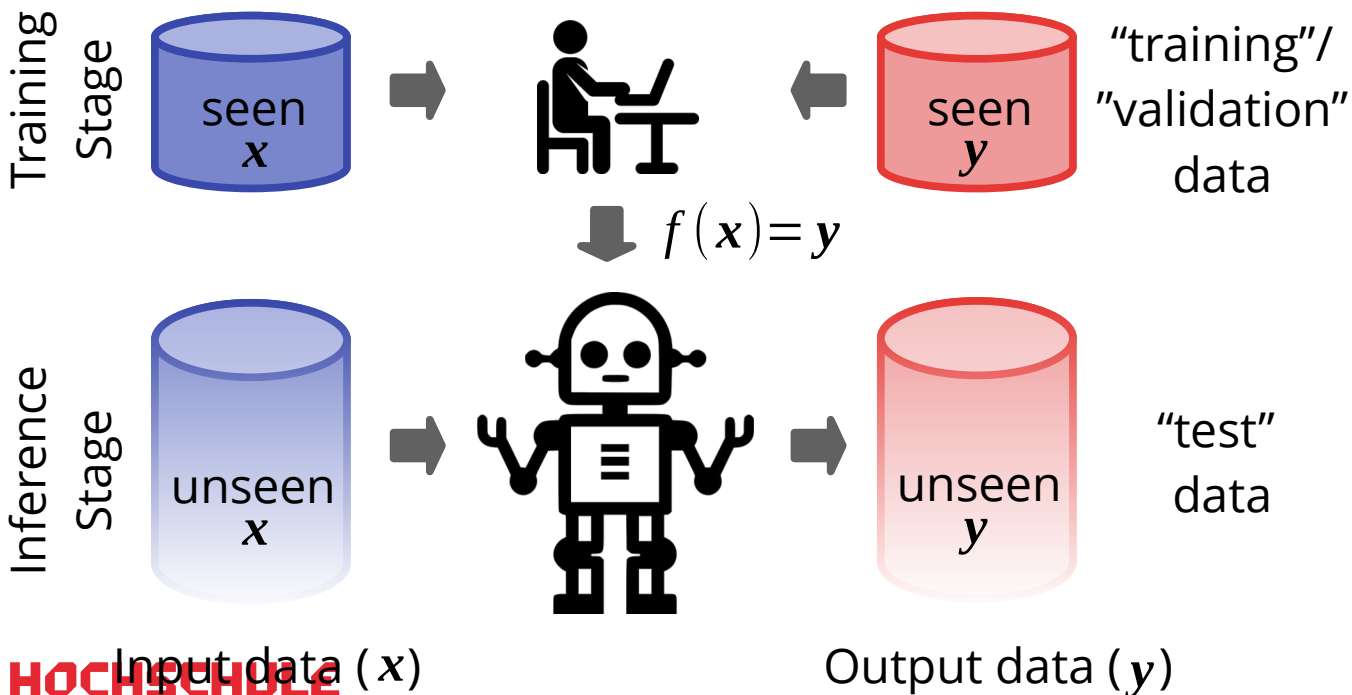
Supervised Machine Learning

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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Traditional (Rule-based) Approach:



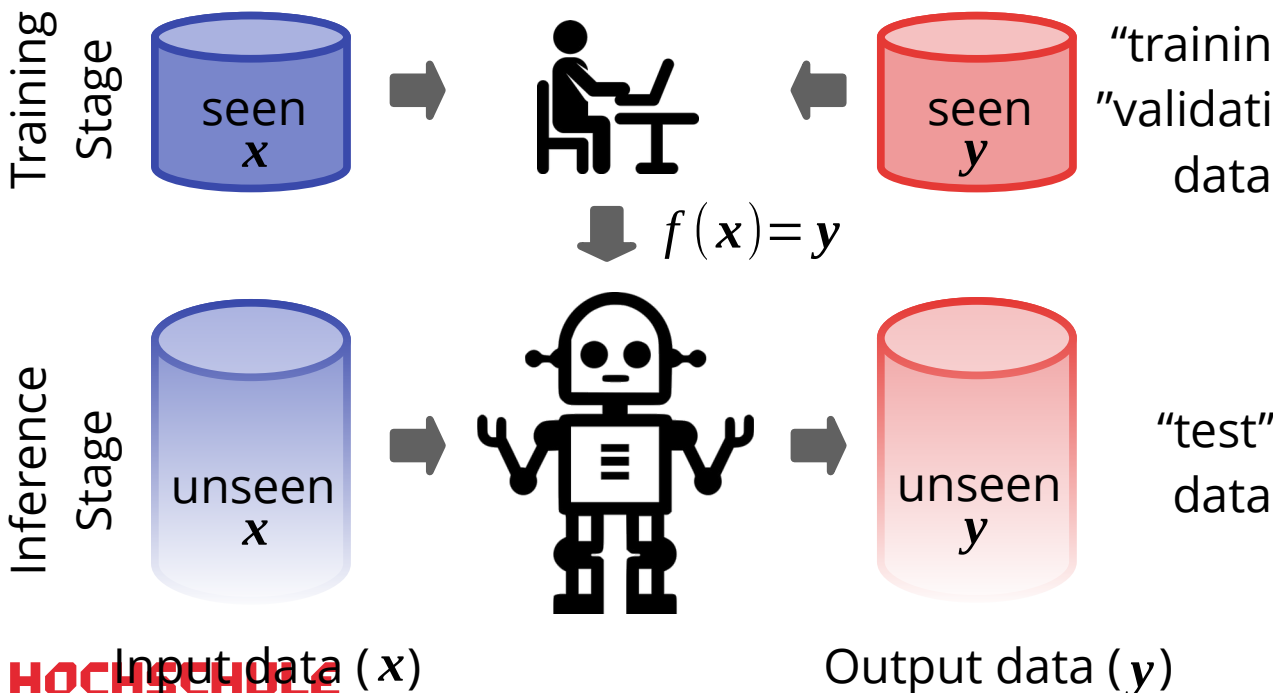
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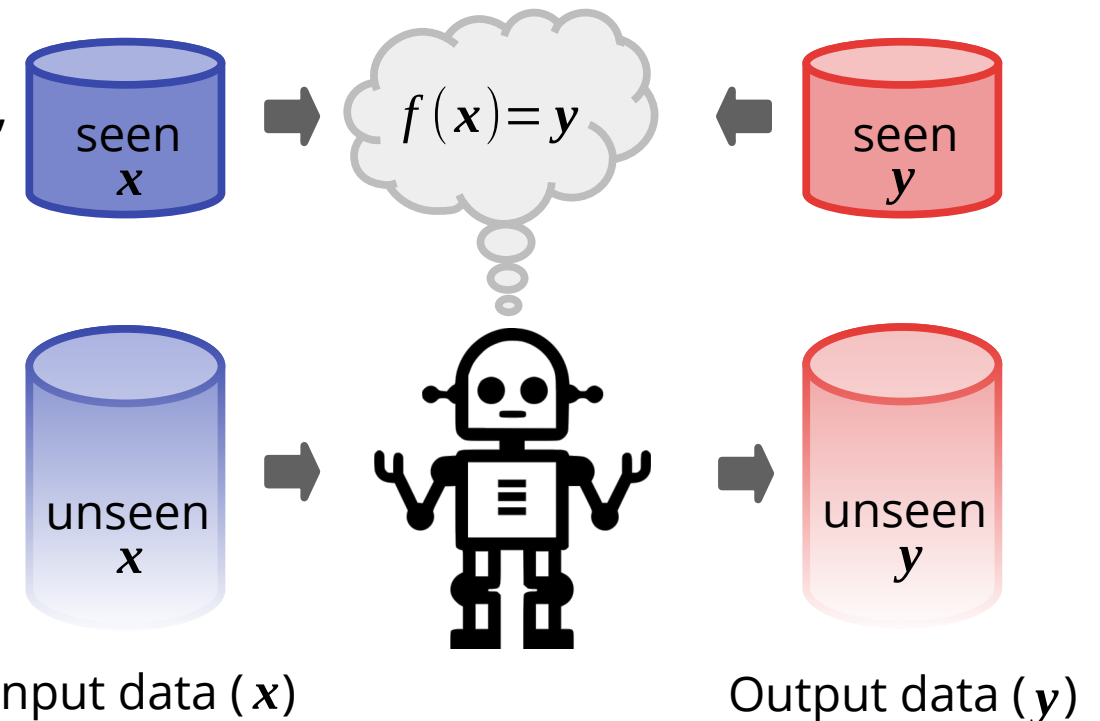
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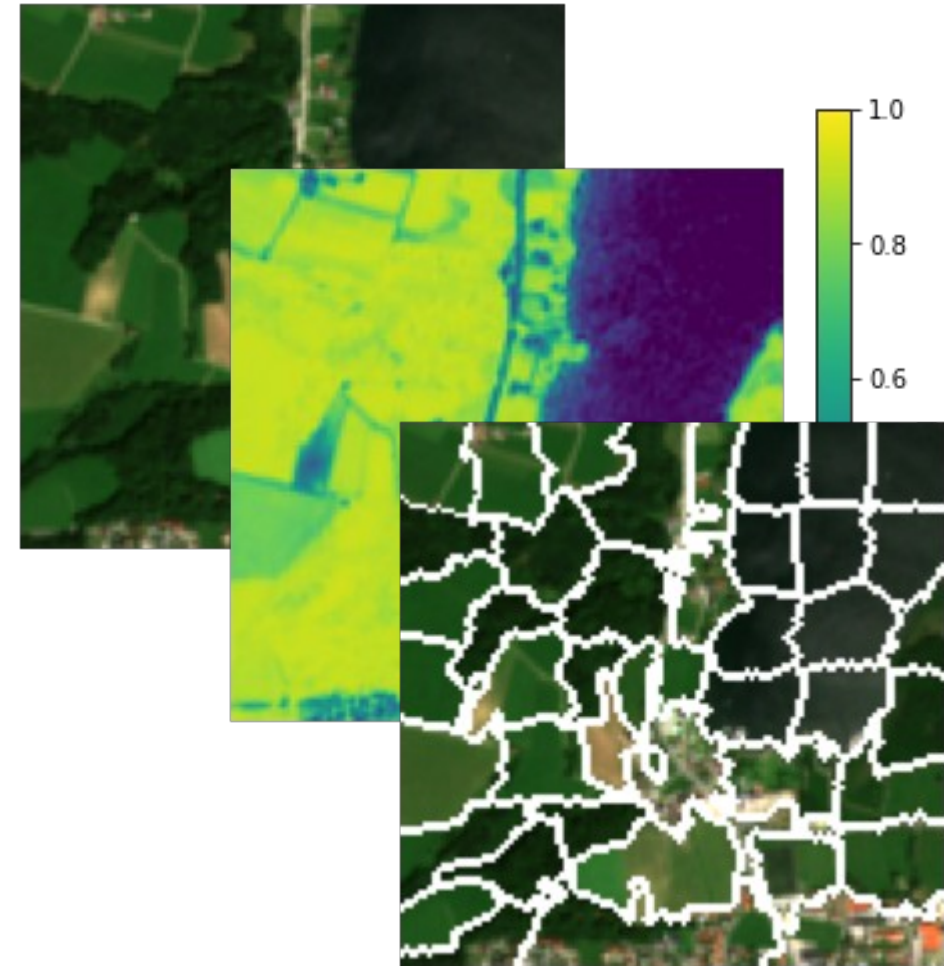
Traditional (Rule-based) Approach:



Machine-Learning Approach:



Data and Features



Data for Machine Learning

A wide range of data modalities exists.

Data for Machine Learning

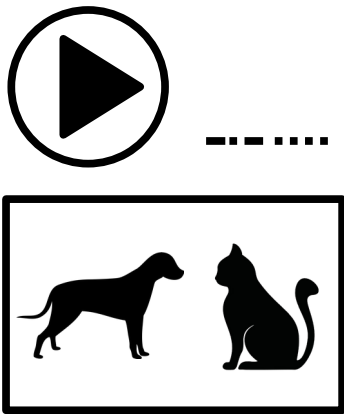
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Not all data modalities can be readily used in Machine Learning models: most models require **numerical features** (quantitative data, see next slide) as input. This means that suitable and meaningful features have to be extracted from the data modality.

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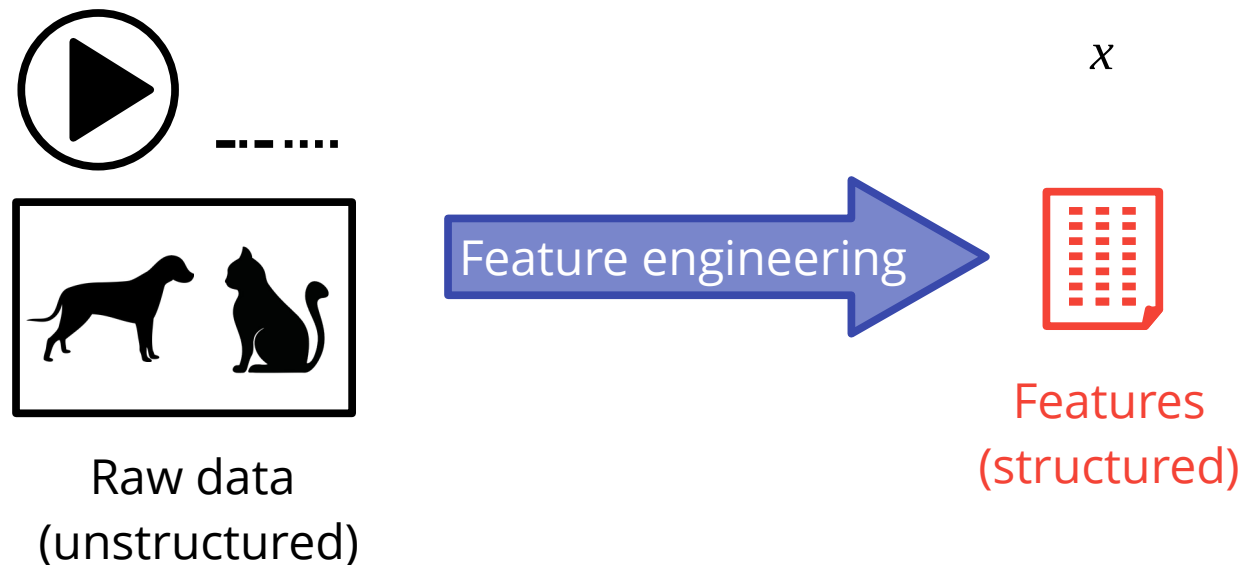


Raw data
(unstructured)

Data for Machine Learning

A wide range of data modalities exists.

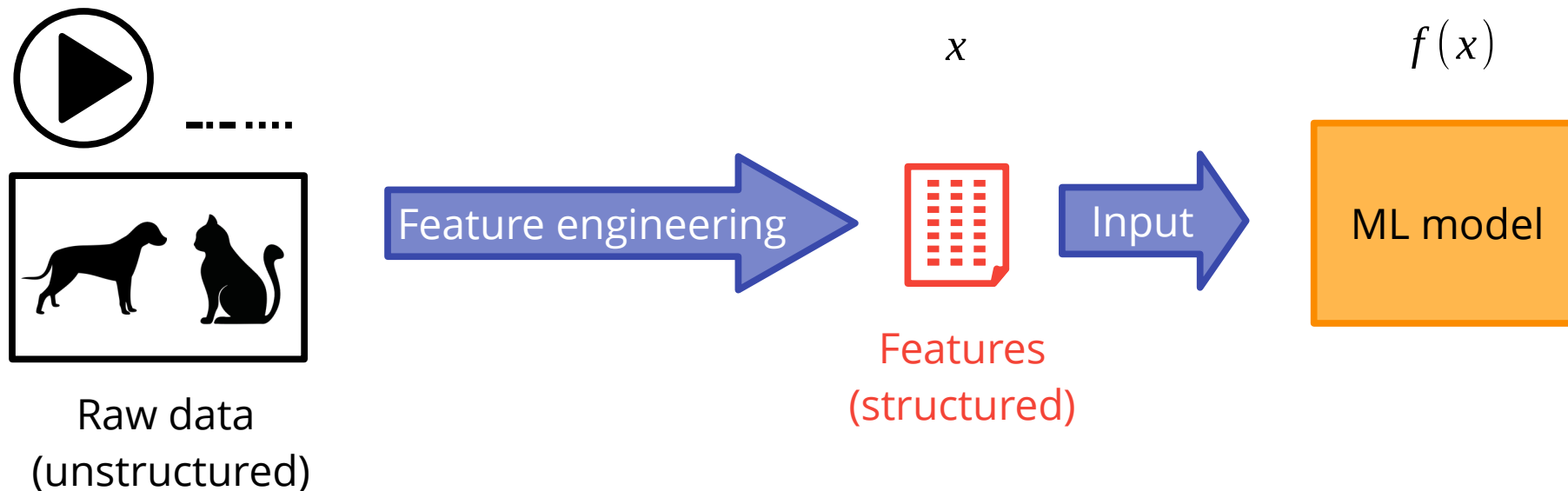
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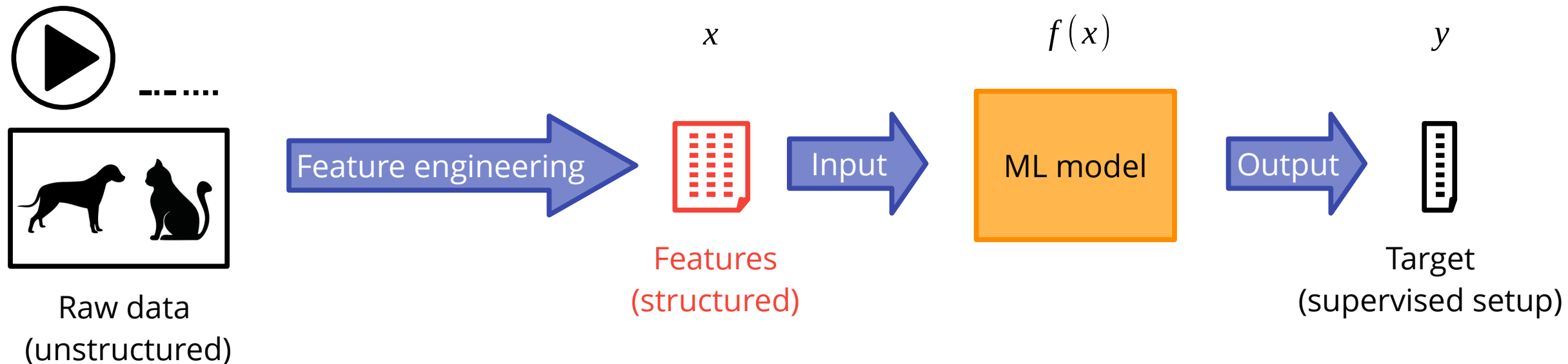
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Structured vs unstructured data

Structured vs unstructured data

Structured data

Preprocessed and formatted data that is easily queryable.

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Quantitative data



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Unstructured data

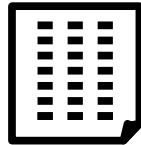
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Qualitative data

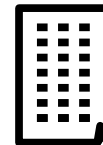
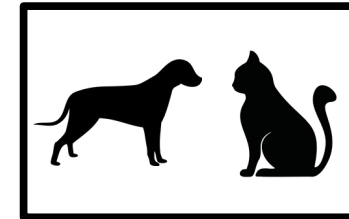


Image data



Video data



Textual data



Data stream

.....

Audio data



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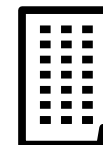
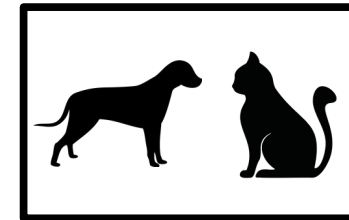


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Data complexity



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Only continuous/
discrete numbers:
"features"

Each sample
represented as a
feature vector

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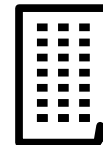
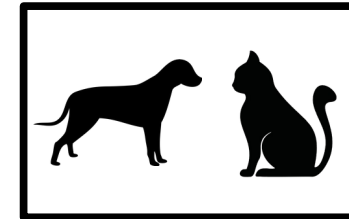


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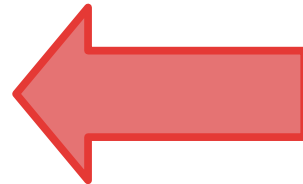
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Processing unstructured
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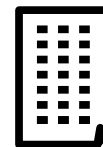
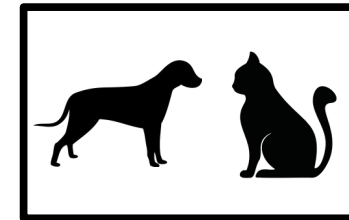


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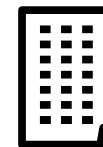
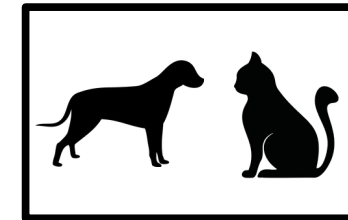


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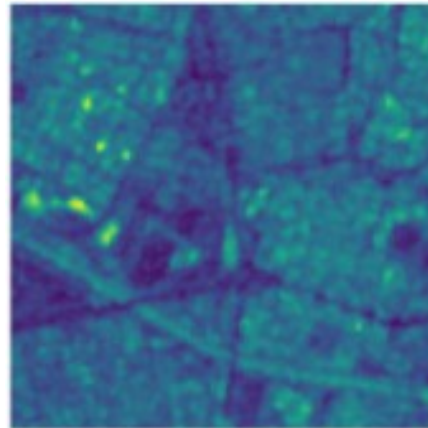


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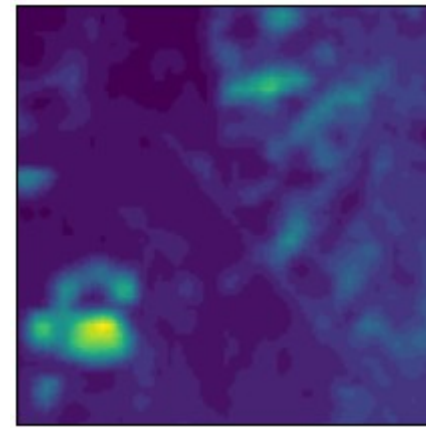
Images or **image-like data representations** are very common as model input. Image-like data are rasterized (projected to a regular); rasterization happens at the time of acquisition (e.g., as part of the imaging process) or synthetically (e.g., by projecting GIS polygons on a grid).



Multispectral Imaging
(e.g., Sentinel-2)



SAR Polarization
(e.g., Sentinel-1)



Digital Elevation Model
(e.g., GTOPO30)



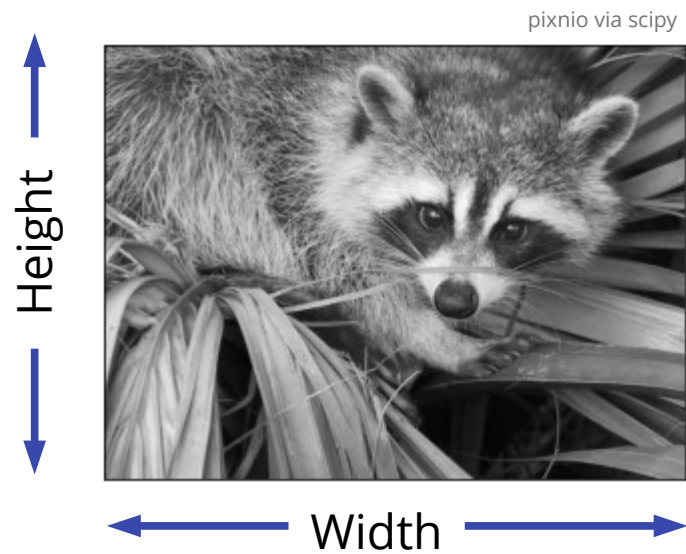
Land Use/Land Cover
(e.g., ESAWorldcover)

How are images represented?

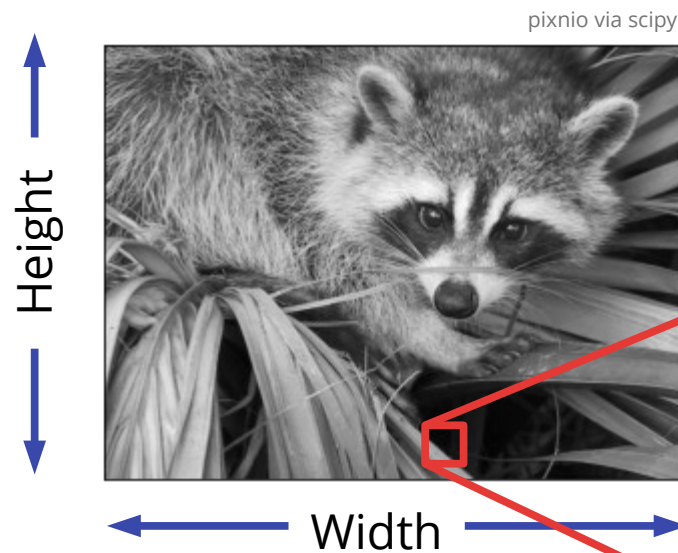
pixnio via scipy



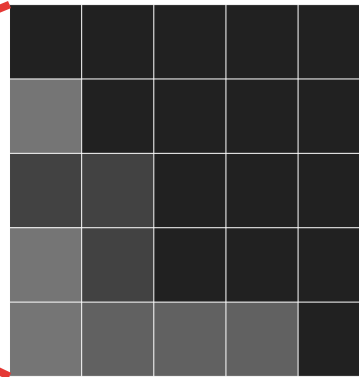
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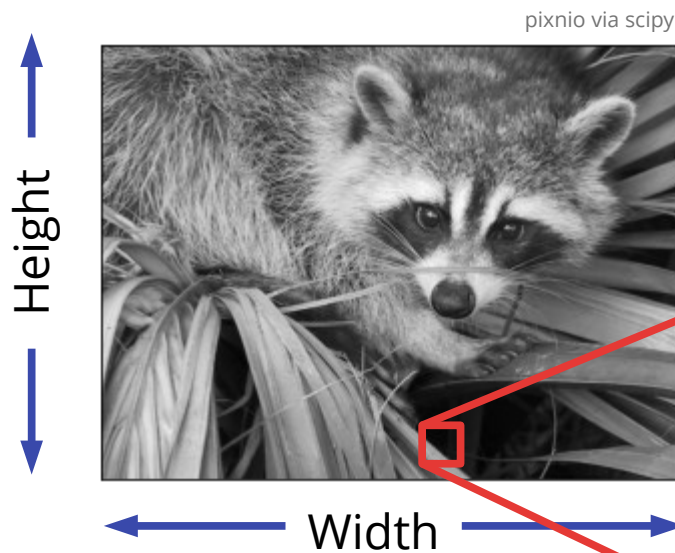
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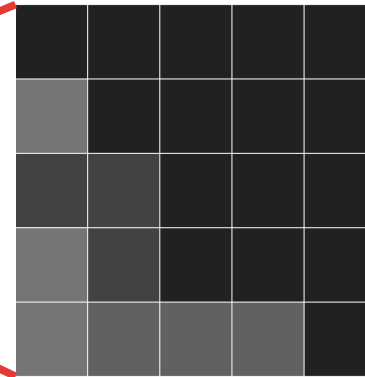
Images consist of quadratic “Picture elements”, **pixels**. An image of height H and width W contains $H \times W$ pixels.



How are images represented?



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In a **greyscale** image, the brightness of each pixel is represented by a single value $[0, 1]$ (8-bit encoding: $[0, 256]$): 0 refers to a black pixel and the max value to a white pixel.

0	0	0	0	0
0.3	0	0	0	0
0.1	0.1	0	0	0
0.3	0.1	0	0	0
0.3	0.2	0.2	0.2	0

Remote sensing data may use a higher dynamic range: e.g., Sentinel-2 MSI: 16bit ($[0, 65536]$)

How are images represented?

Greyscale



pixnio via scipy



```
✓ [7] image.shape  
0s  
"2-d" (600, 400)
```

How are images represented?

Greyscale



pixnio via scipy

Color (RGB)



=



✓ [7] image.shape
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"2-d" (600, 400)

✓ [5] image.shape
0s
"3-d" (600, 400, 3)

Color images typically consist of **three channels** (RGB), each of which is a grayscale image in itself.

More on color spaces later in this course...

How are images represented?

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pixnio via scipy

Color (RGB)



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"3-d" (600, 400, 3)
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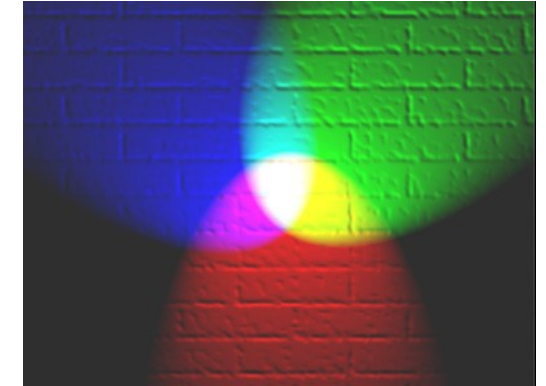


=



Why RGB?

Every color can be synthesized through additive mixing of red, green and blue.



Bb3cxv @ wikipedia

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Feature engineering – image data

How can we feed image data into ML models?

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Each pixel is represented by its channel-wise values.

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[86, 183, 106, ...]

Number of bands: C

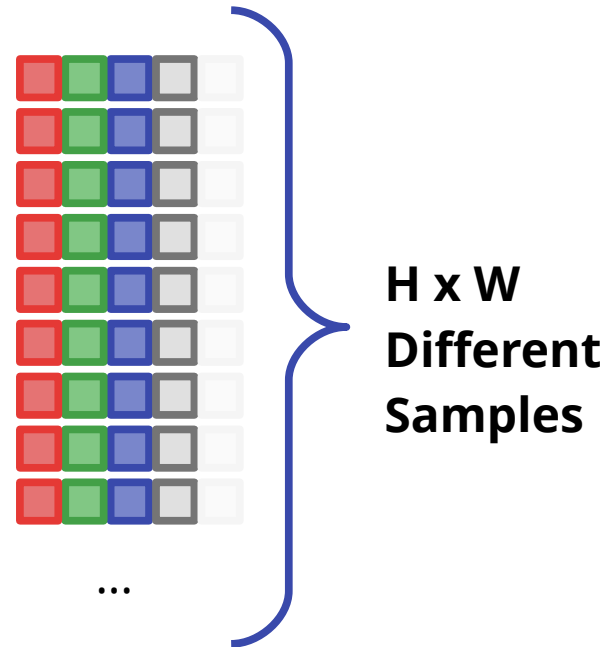
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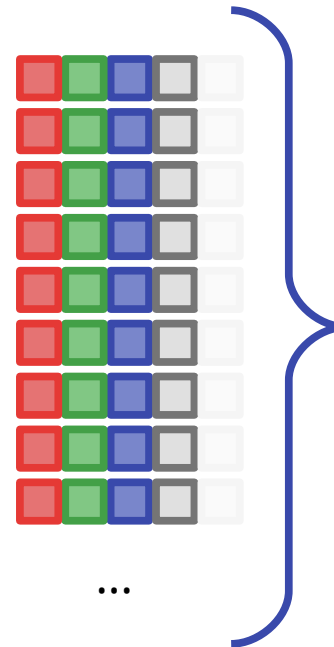
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[86, 183, 106, ...]

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**H x W
Different
Samples**

**C different
Features**

Each pixel is represented by its channel-wise values.

Very common in remote sensing applications (e.g., multiband, hyperspectral data).

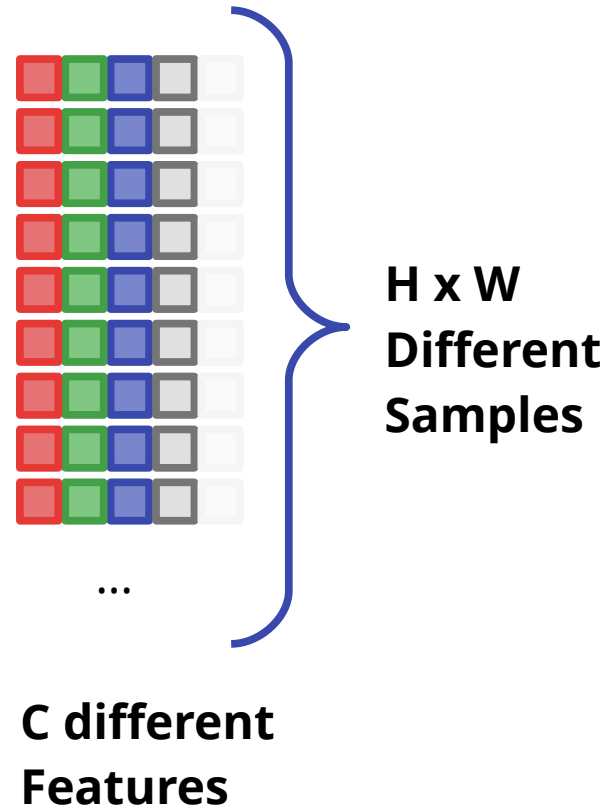
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[86, 183, 106, ...]

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Each pixel is represented by its channel-wise values.

Very common in remote sensing applications (e.g., multiband, hyperspectral data).

Downside: each pixel is treated separately (neighborhood is ignored).

Feature engineering – image data

An **object-based image analysis approach** finds “objects” in the image data. Objects are image areas that share common properties, such as spectral properties, size, shape or texture. Unsupervised methods such as SLIC find such objects (“superpixels”) using a segmentation approach.

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Other features:

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Other features:

- Edges

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Other features:

- Edges
- Lines
- Keypoints (SIFT)

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.

Remote Sensing-related Example: **Land-use/land-cover classification**

R	G	B	NIR	NDVI
0.12	0.16	0.83	0.21	0.03
0.23	0.18	0.76	0.18	0.07
0.51	0.73	0.48	0.81	0.93
0.43	0.76	0.27	0.76	0.83
0.73	0.68	0.61	0.23	0.01
...	...	...	...	...

LULC Class
water
water
forest
forest
built-up
...

(This is a multi-class classification problem)

Final data set nomenclature

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Remote Sensing-related Example: **Land-use/land-cover classification**

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

R	G	B	NIR	NDVI	LULC Class
0.12	0.16	0.83	0.21	0.03	water
0.23	0.18	0.76	0.18	0.07	water
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Samples/Instances = Image Pixels	R	G	B	NIR	NDVI	LULC Class
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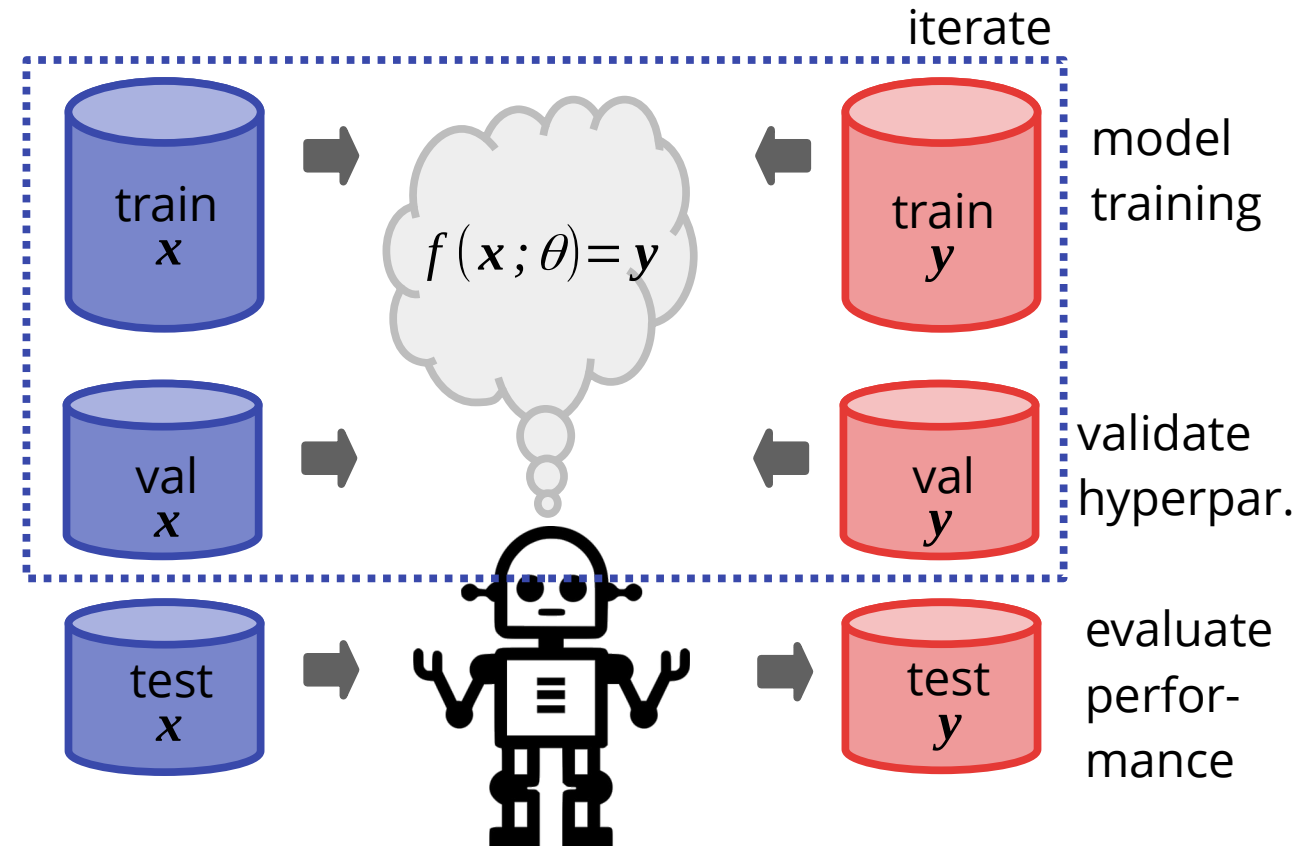
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Samples/Instances = Image Pixels	R	G	B	NIR	NDVI	LULC Class	
	0.12	0.16	0.83	0.21	0.03	water	} classes of label "LULC Class"
	0.23	0.18	0.76	0.18	0.07	water	
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	...	...	...	...	...	...	

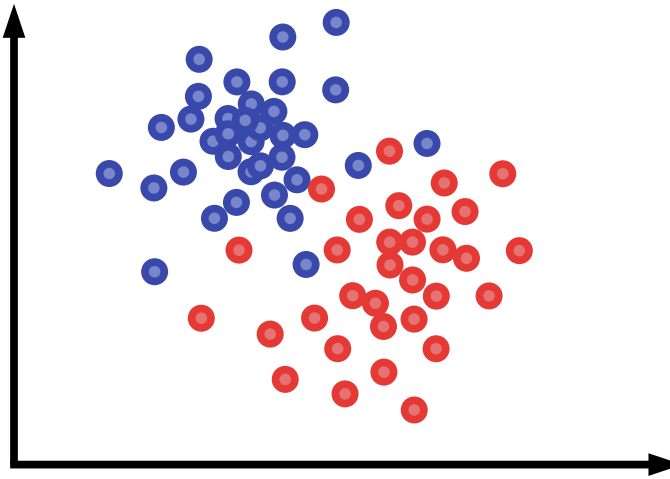
(This is a multi-class classification problem)

Model Training



Generalization, regularization, overfitting and underfitting

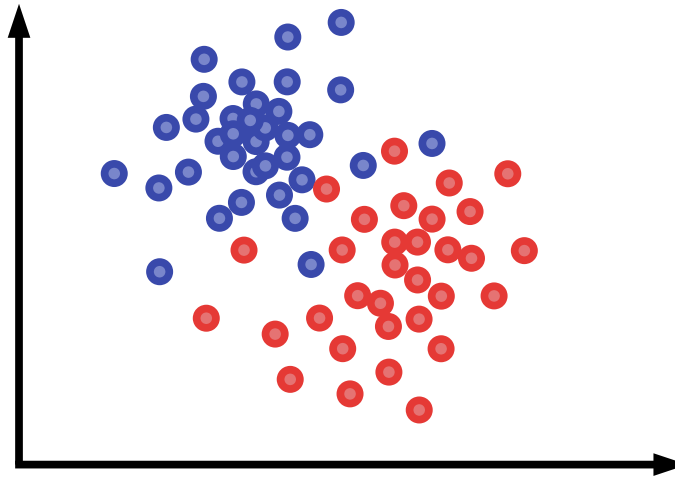
Consider the following data set on which we train a ML model to classify two distinct class:



What would be a good decision boundary between the two classes?

Generalization, regularization, overfitting and underfitting

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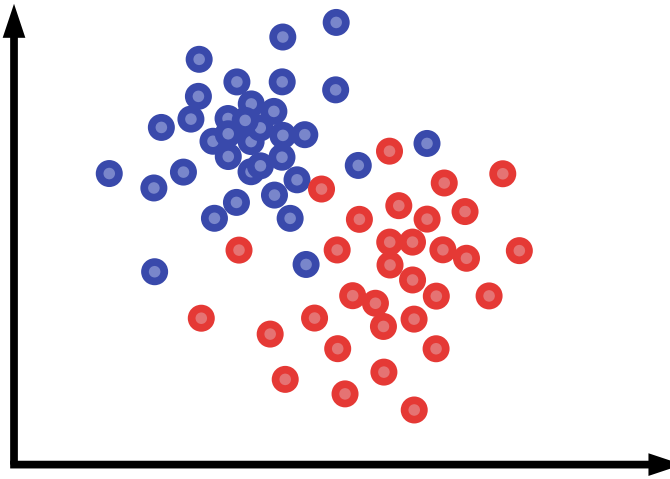


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The **decision boundary** separates the different classes as learned by the trained model.

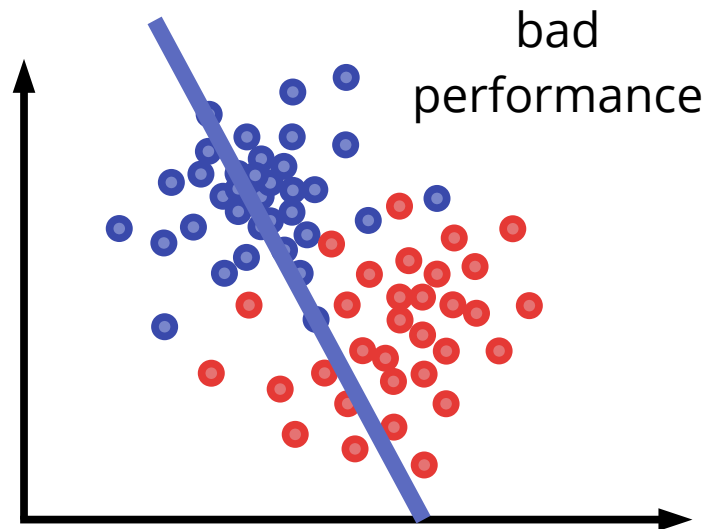
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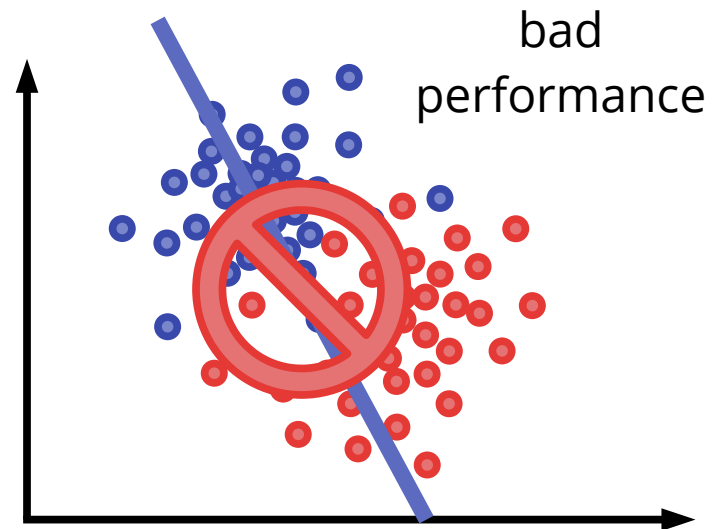


This would not be a good decision boundary as it barely allows to distinguish the two classes.

This model clearly **underfits** the data and leads to **poor performance**.

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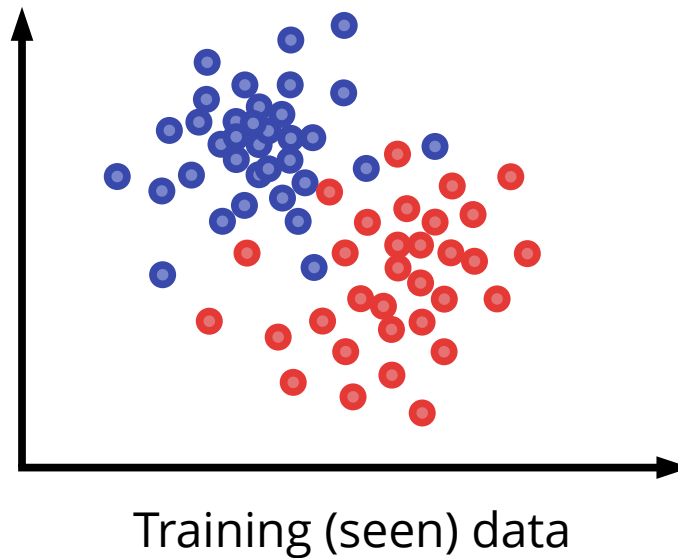


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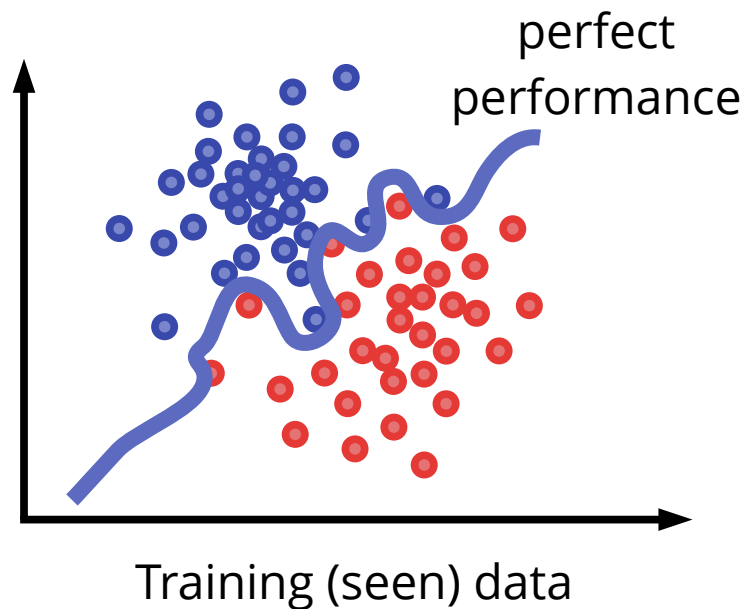
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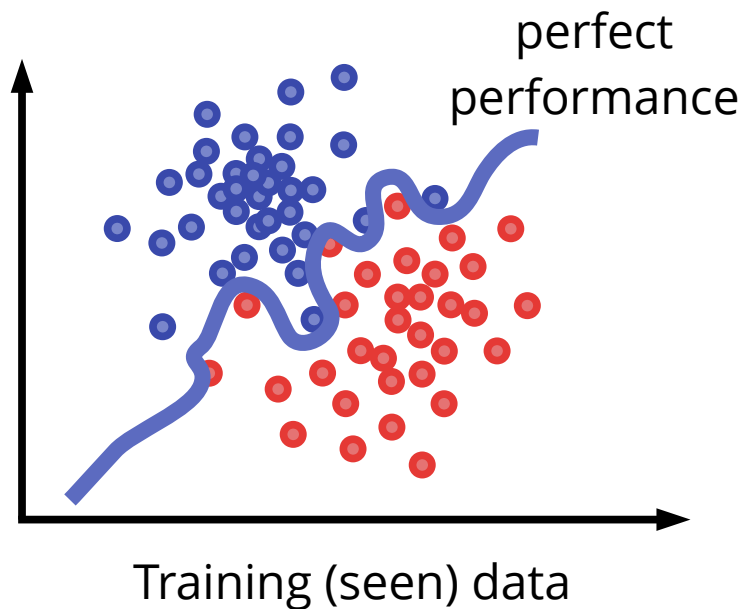
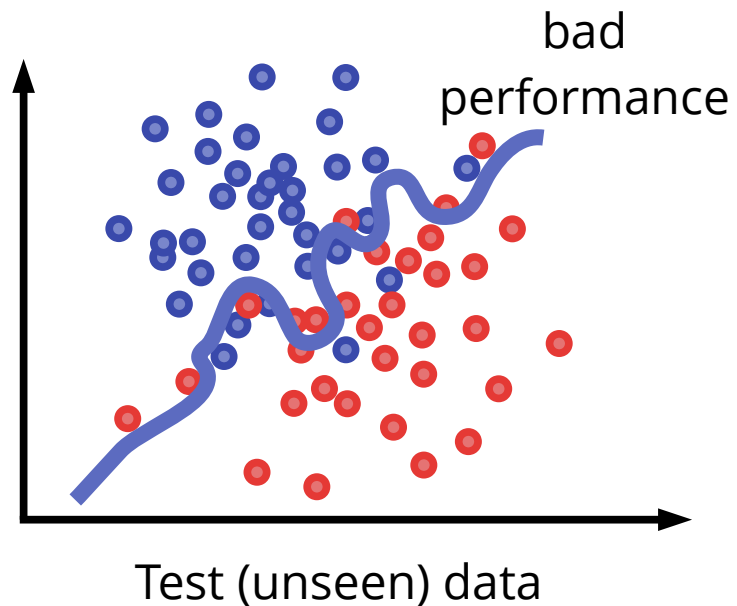


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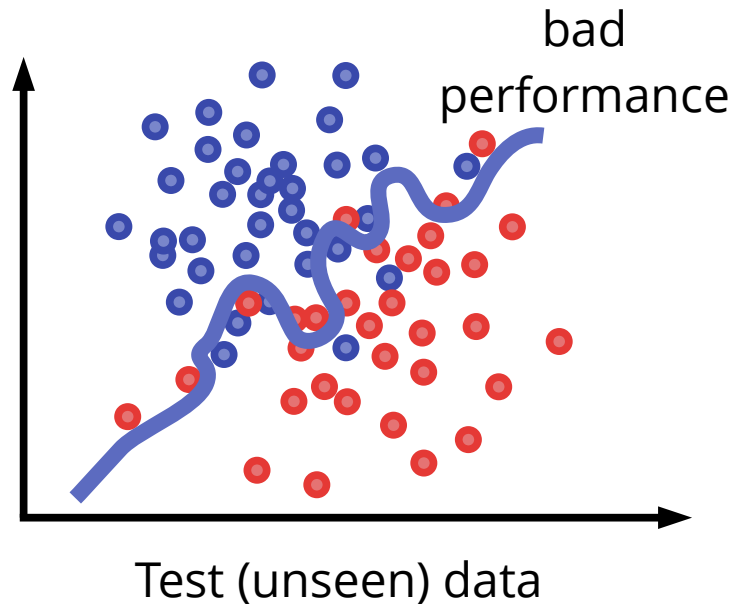
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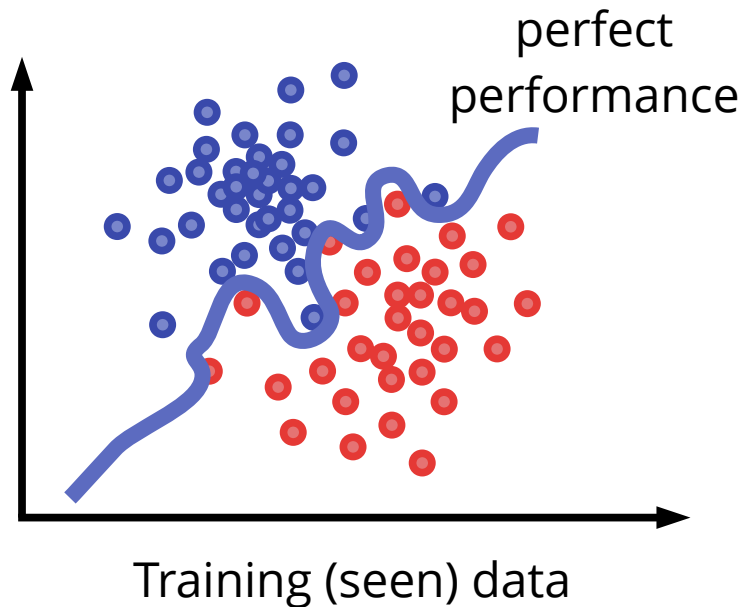
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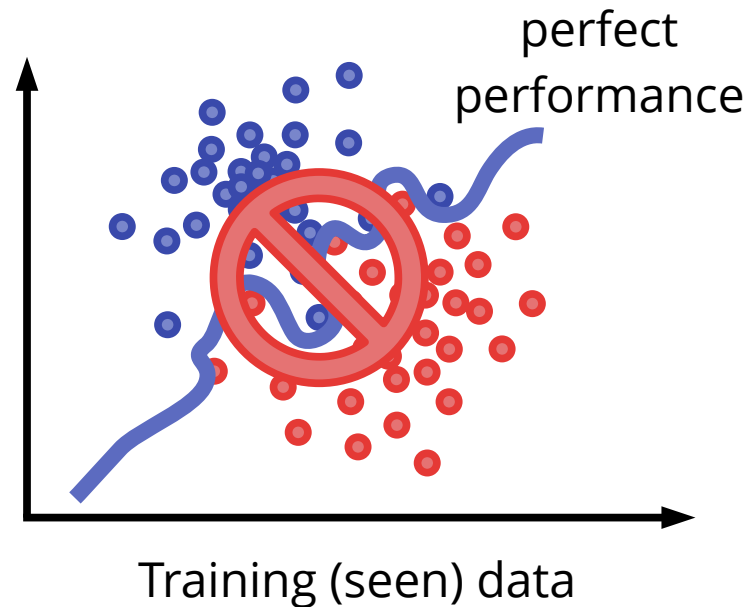
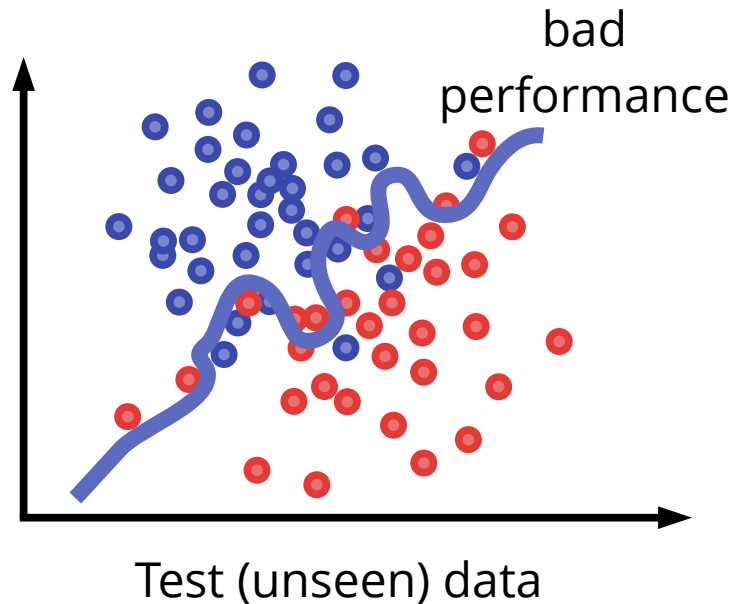
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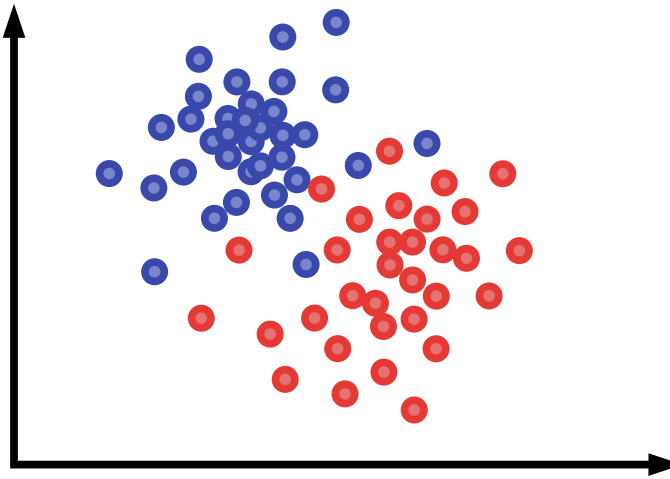
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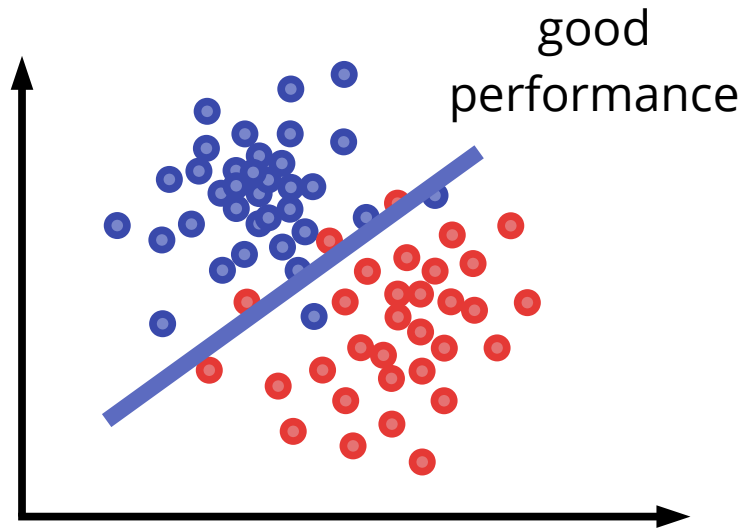
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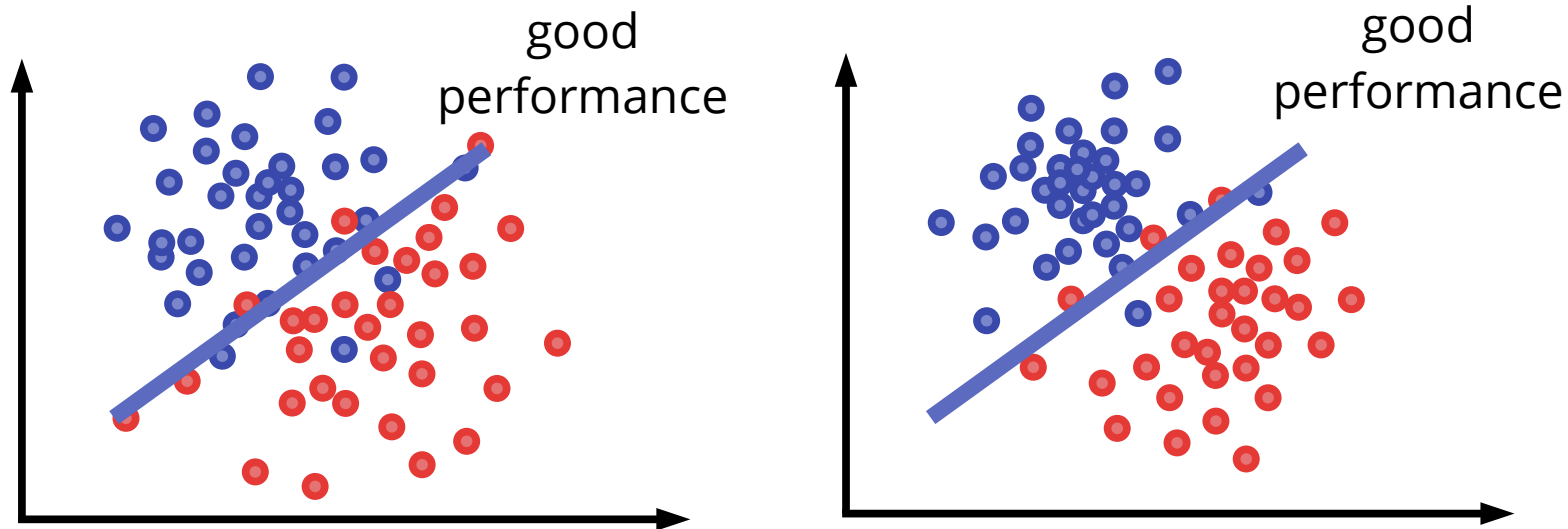
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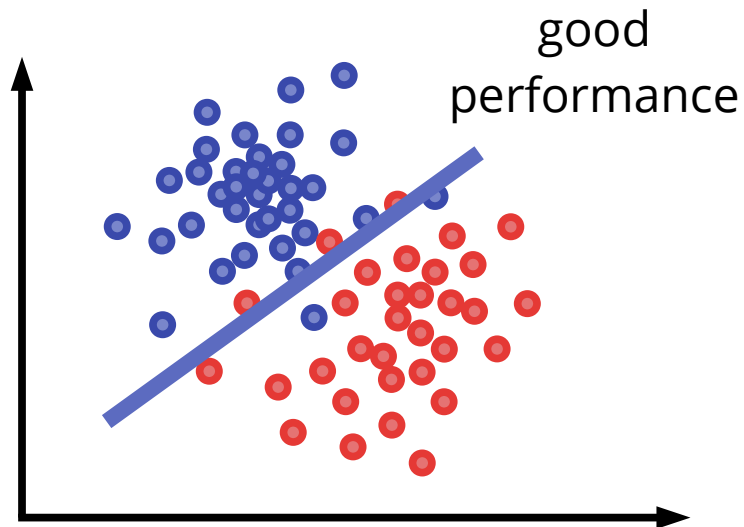
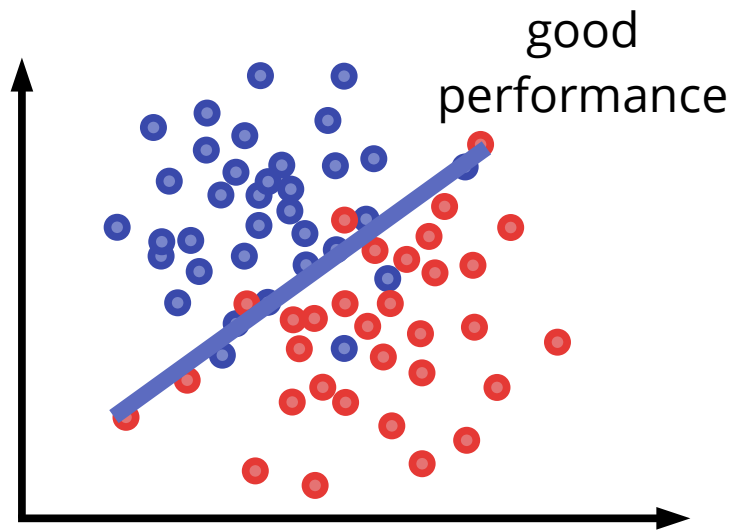
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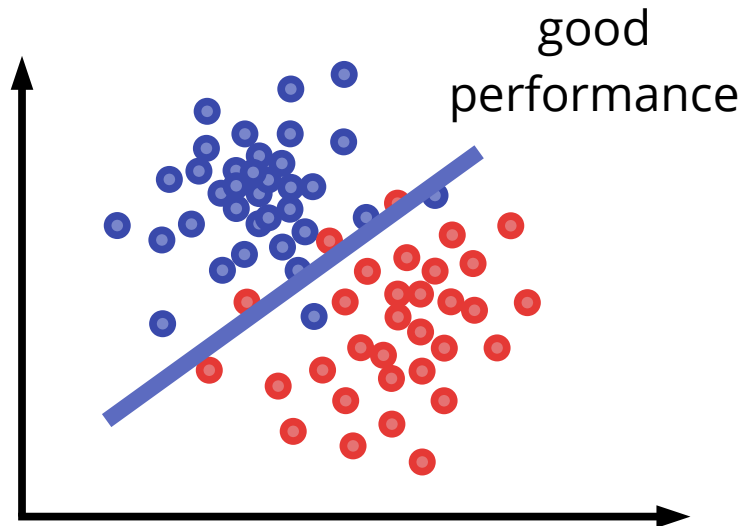
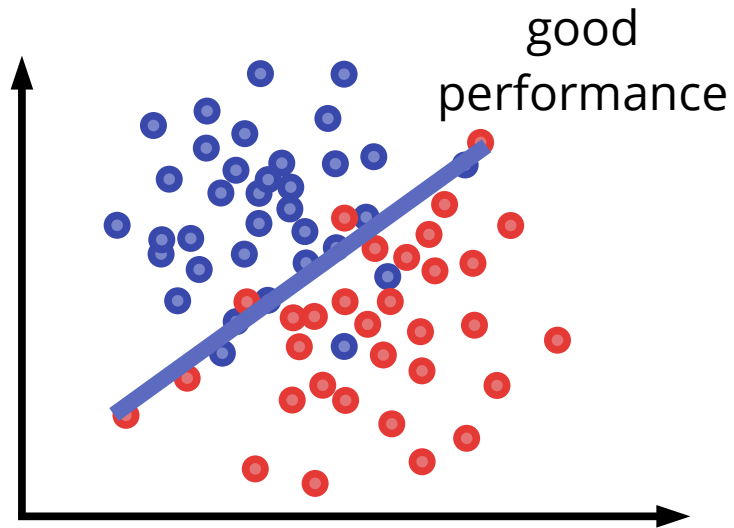
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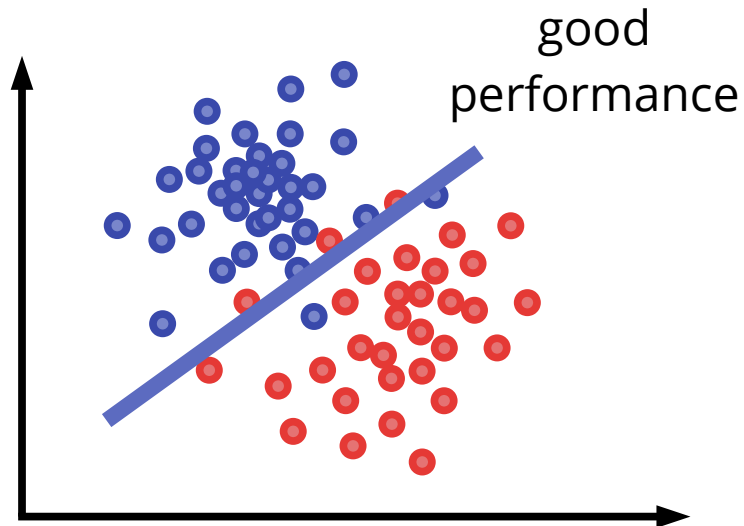
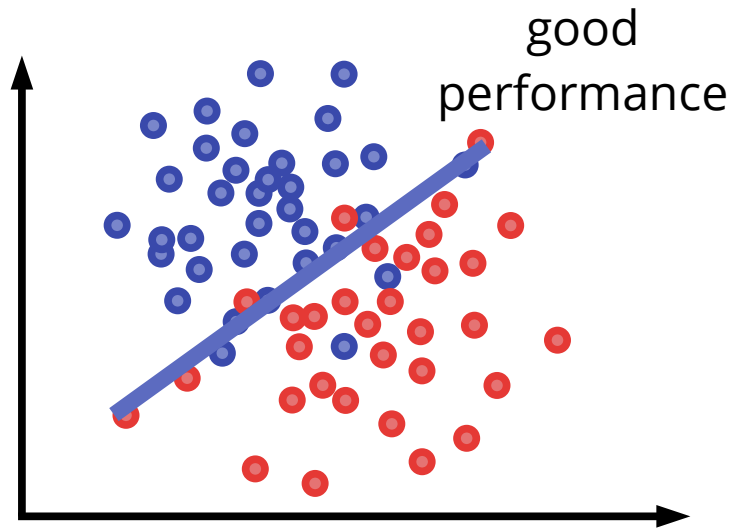


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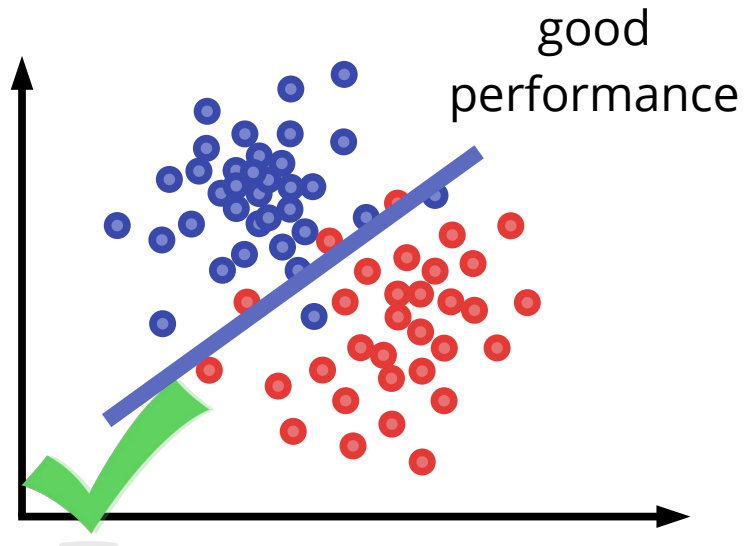
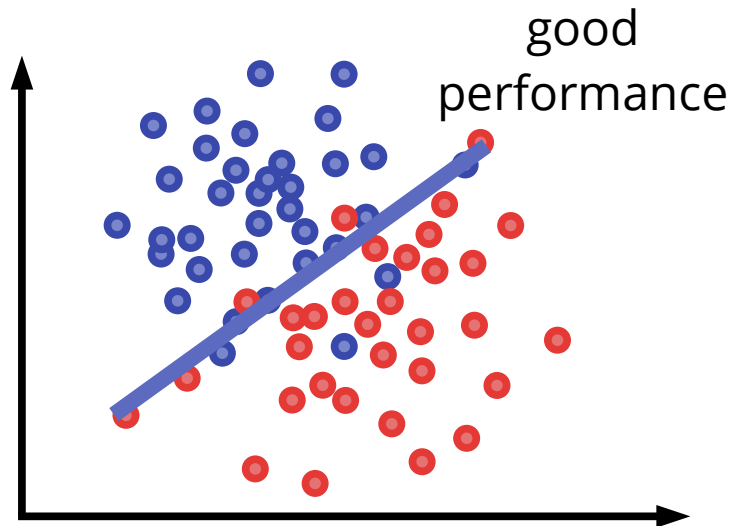
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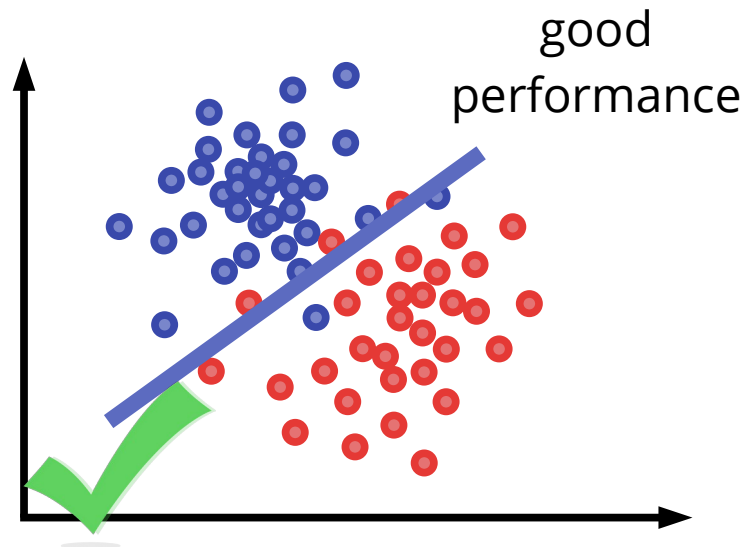
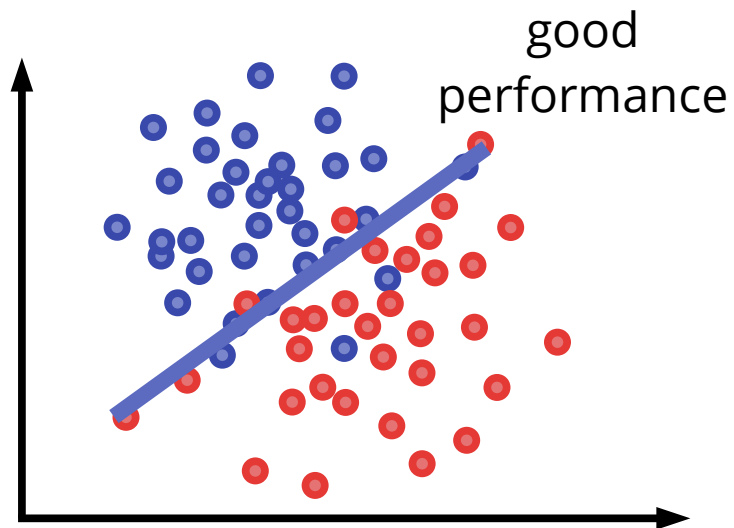
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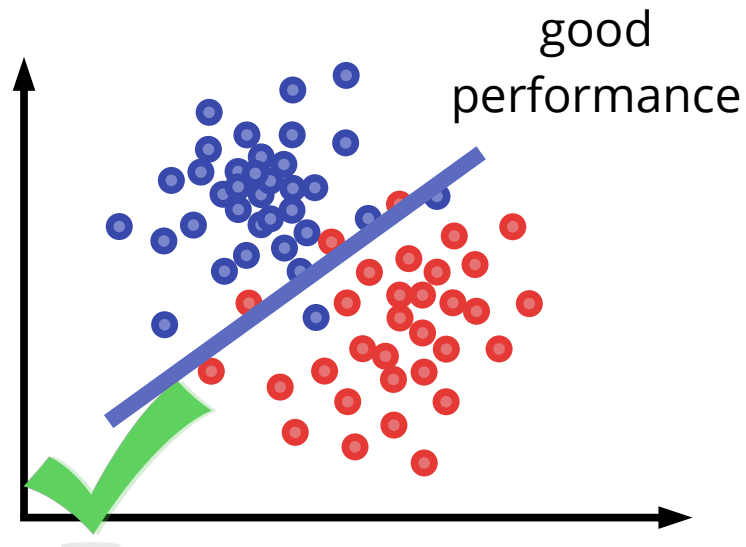
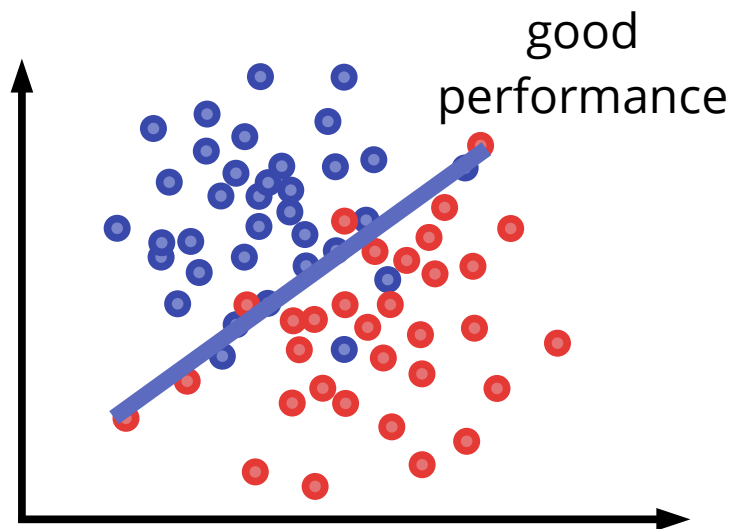
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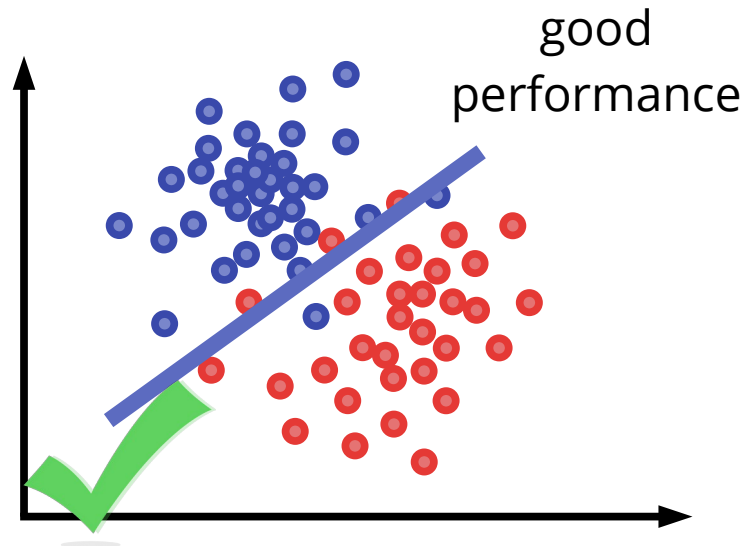
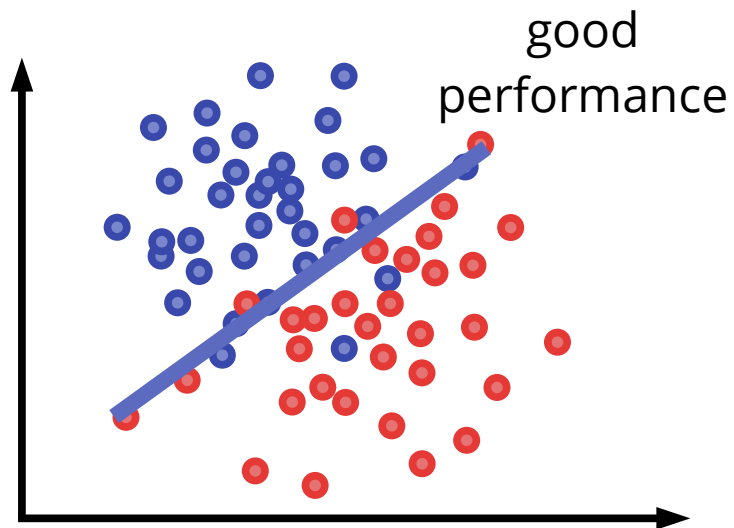
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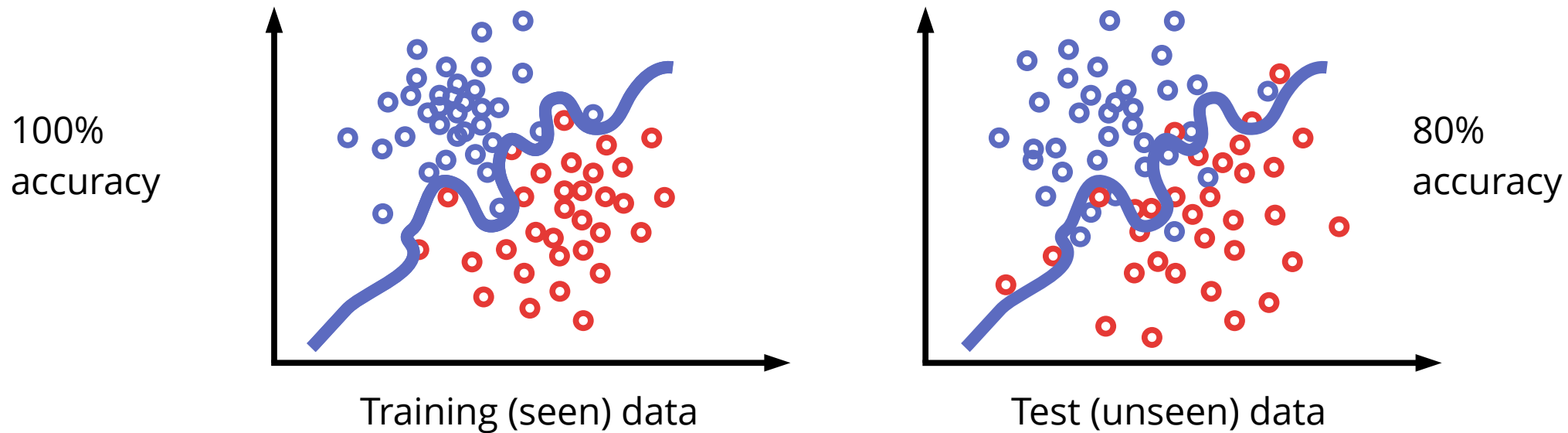
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Assuming that we have such a performance metric implemented, how can we identify overfitting?

Identifying overfitting

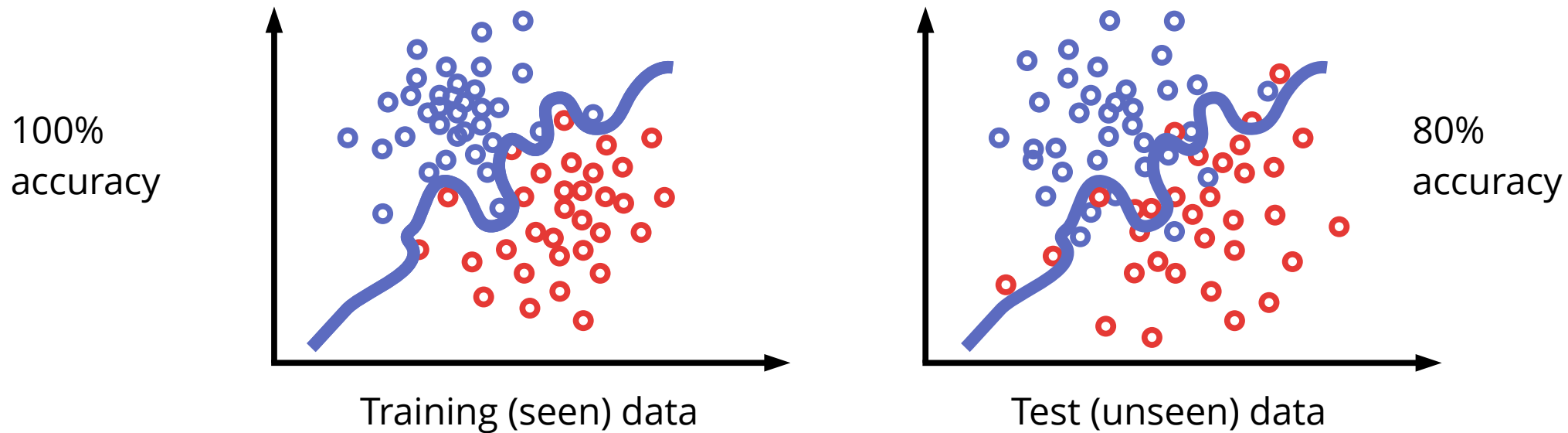
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We can identify overfitting by comparing the performance on the seen (training) data and some previously unseen (test) data. But **where do we get unseen data from?**

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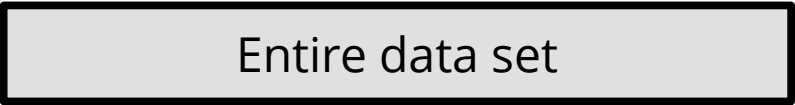
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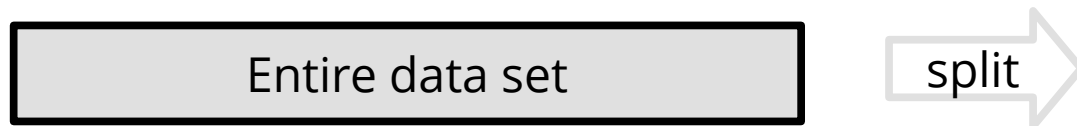
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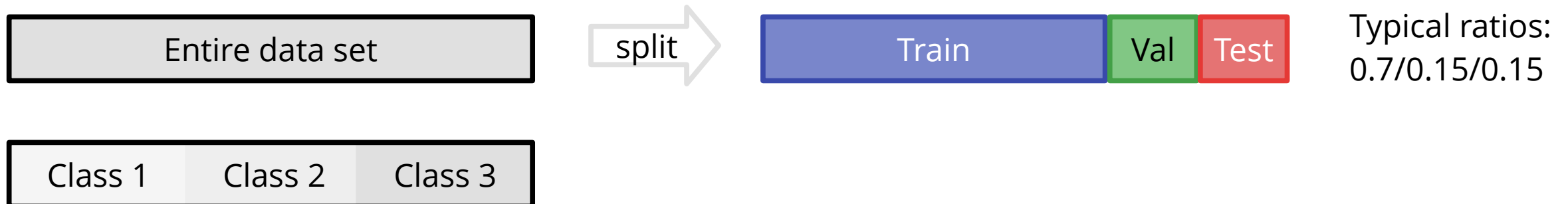
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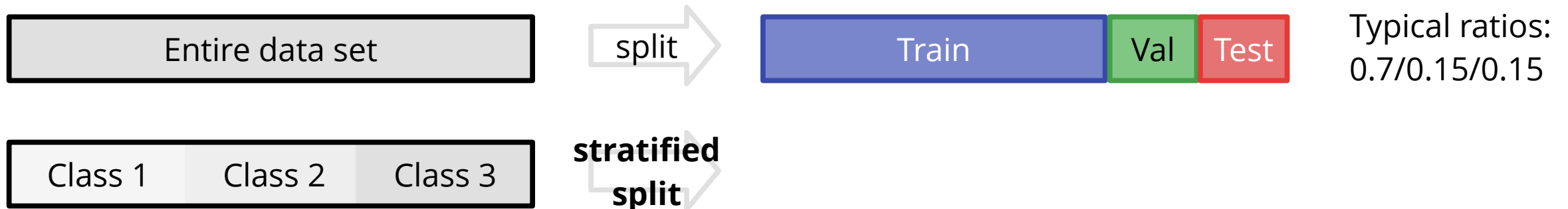
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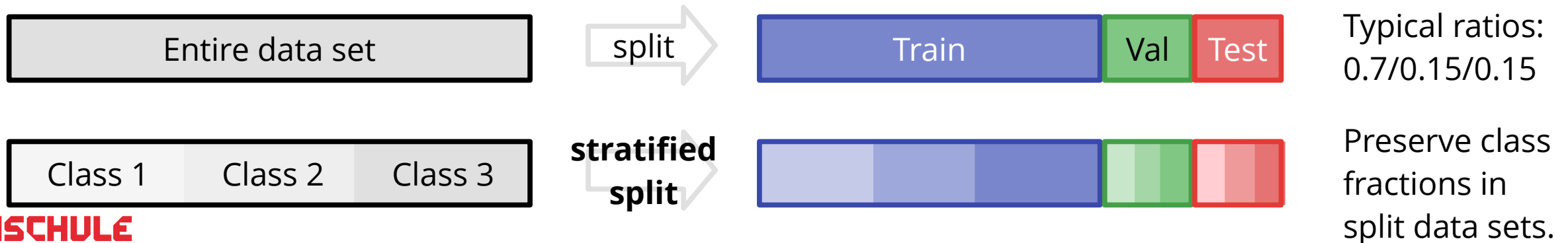
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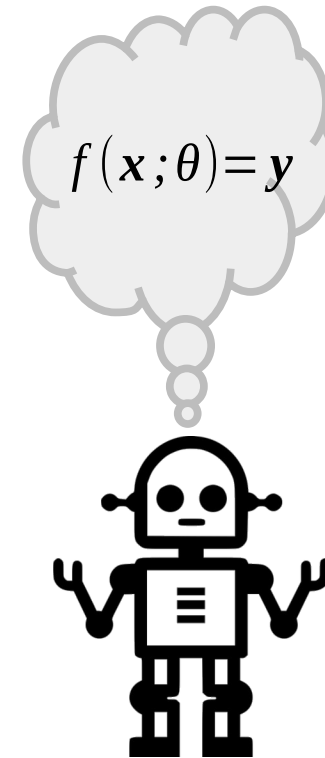
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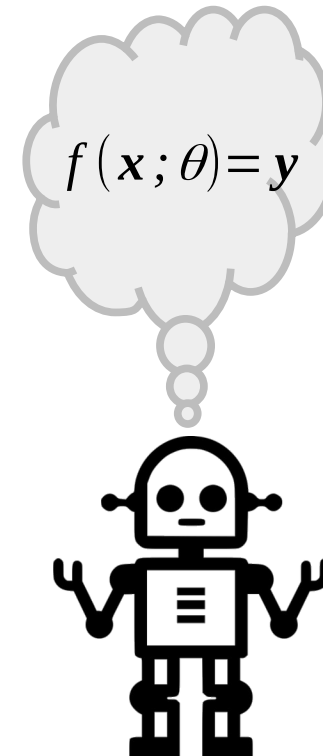


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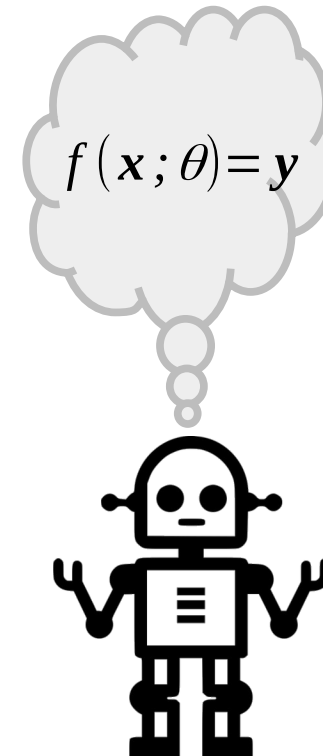
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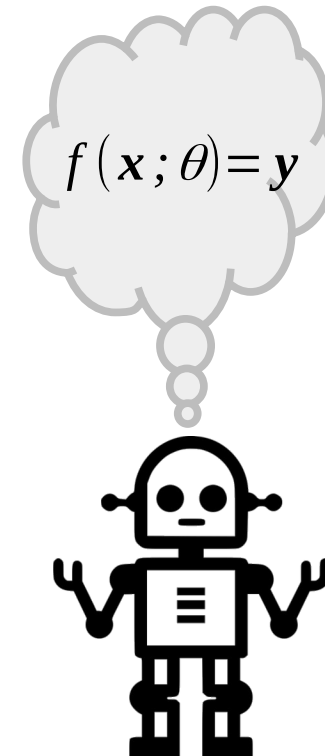
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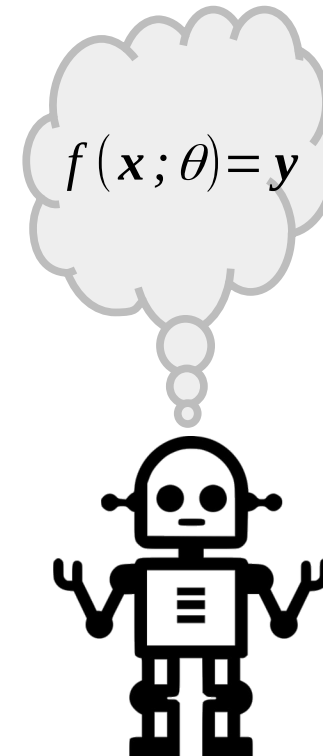
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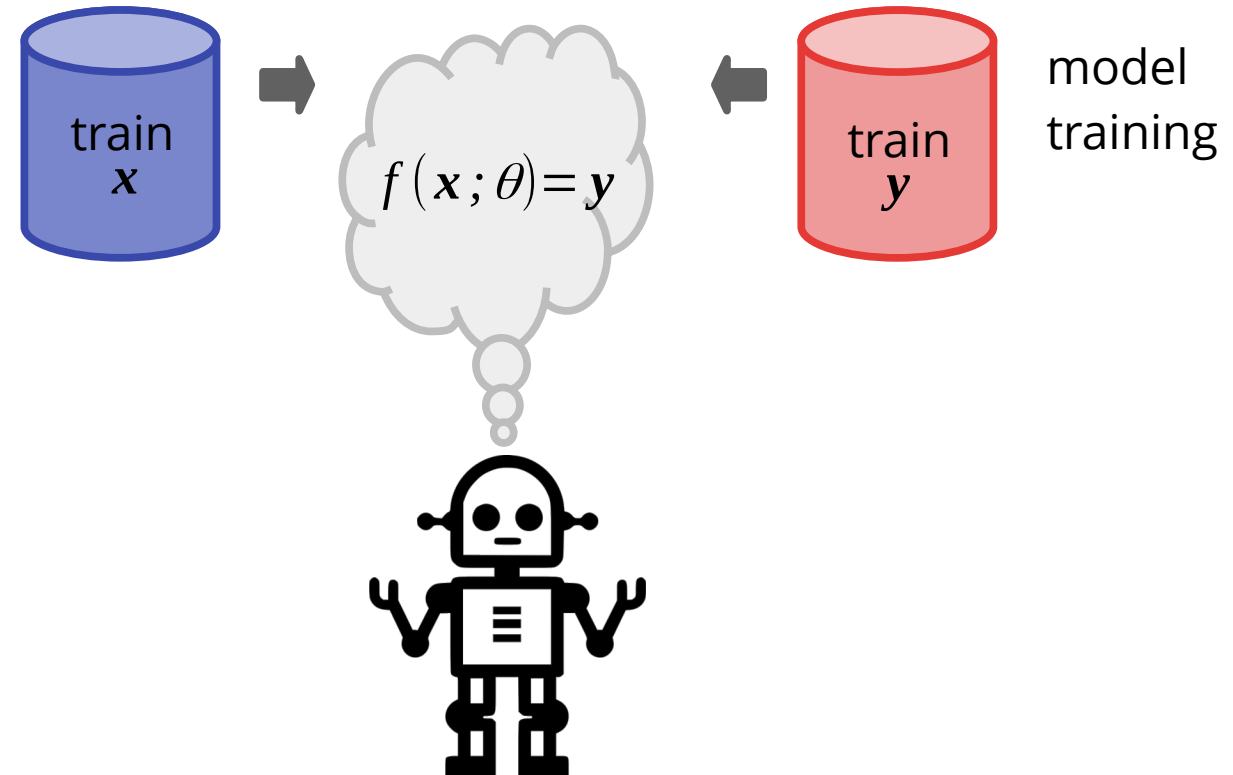
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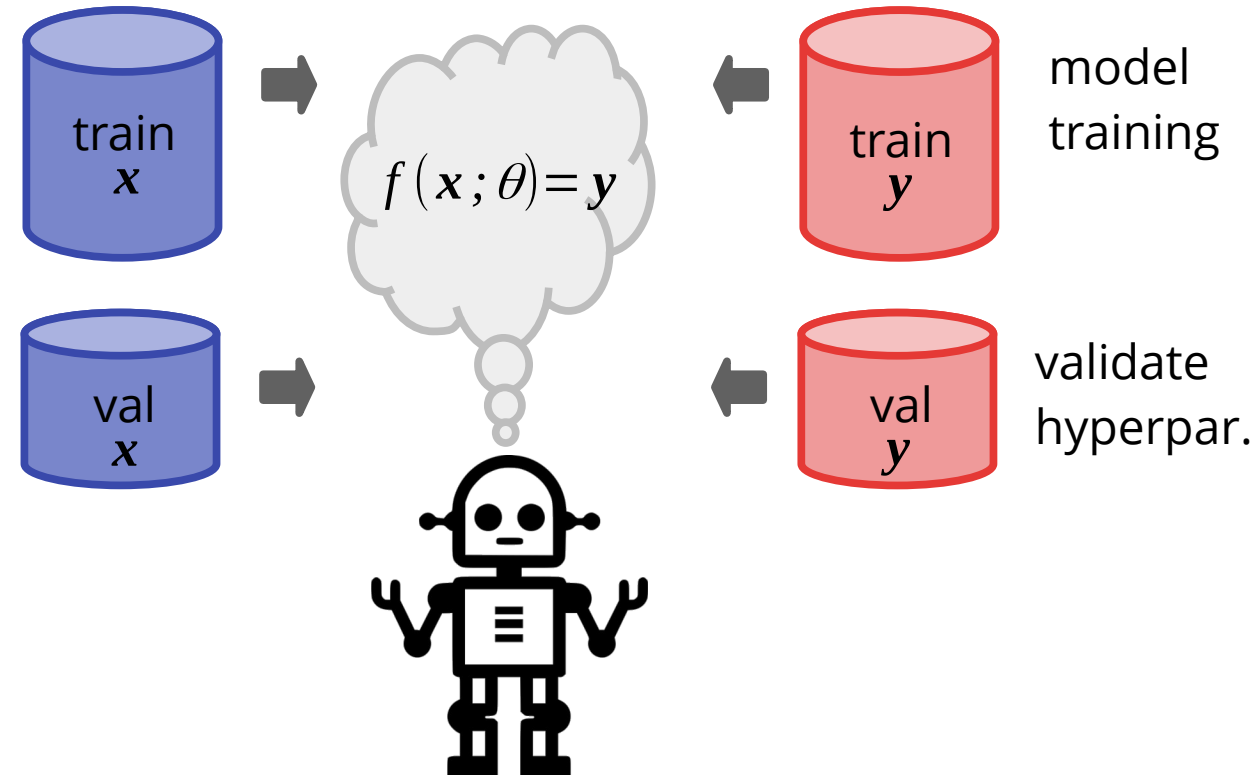
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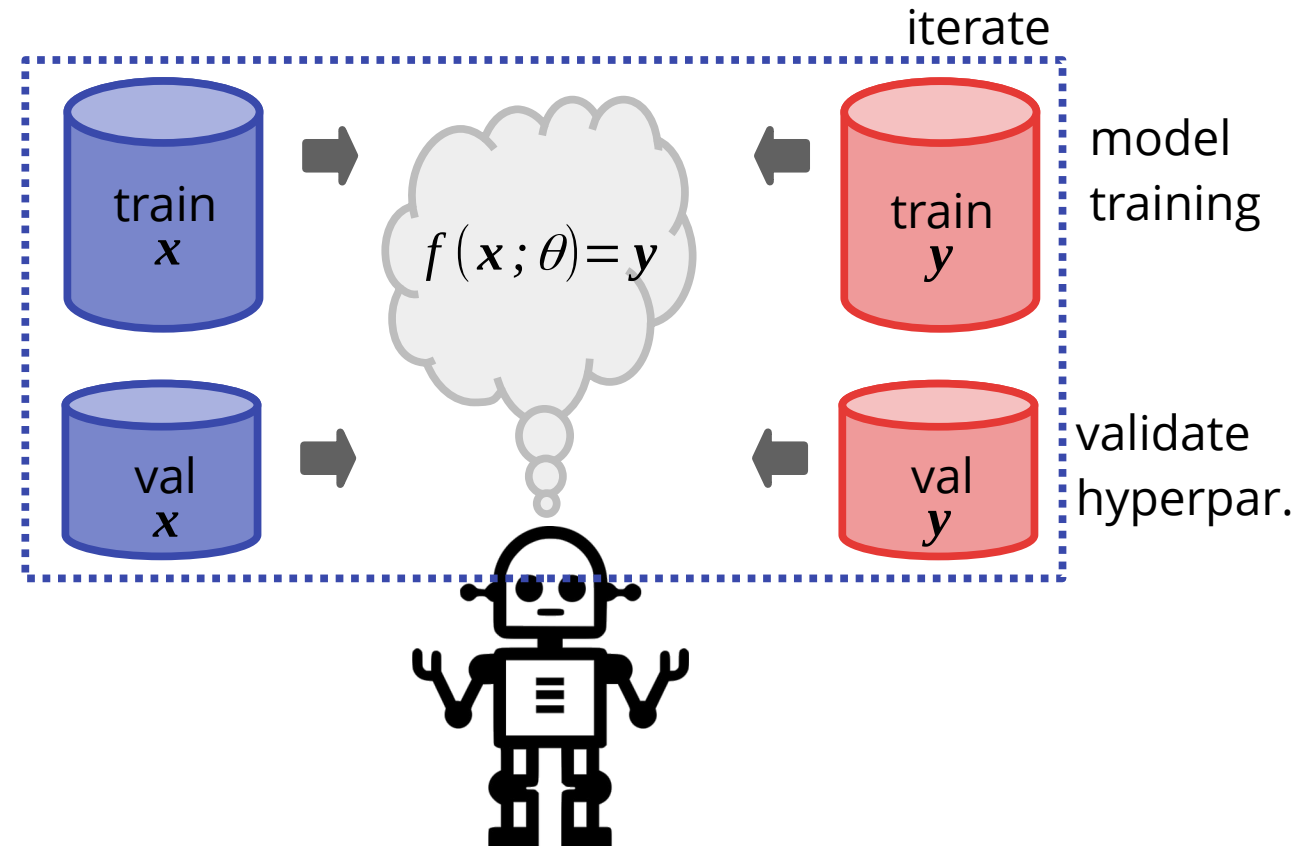
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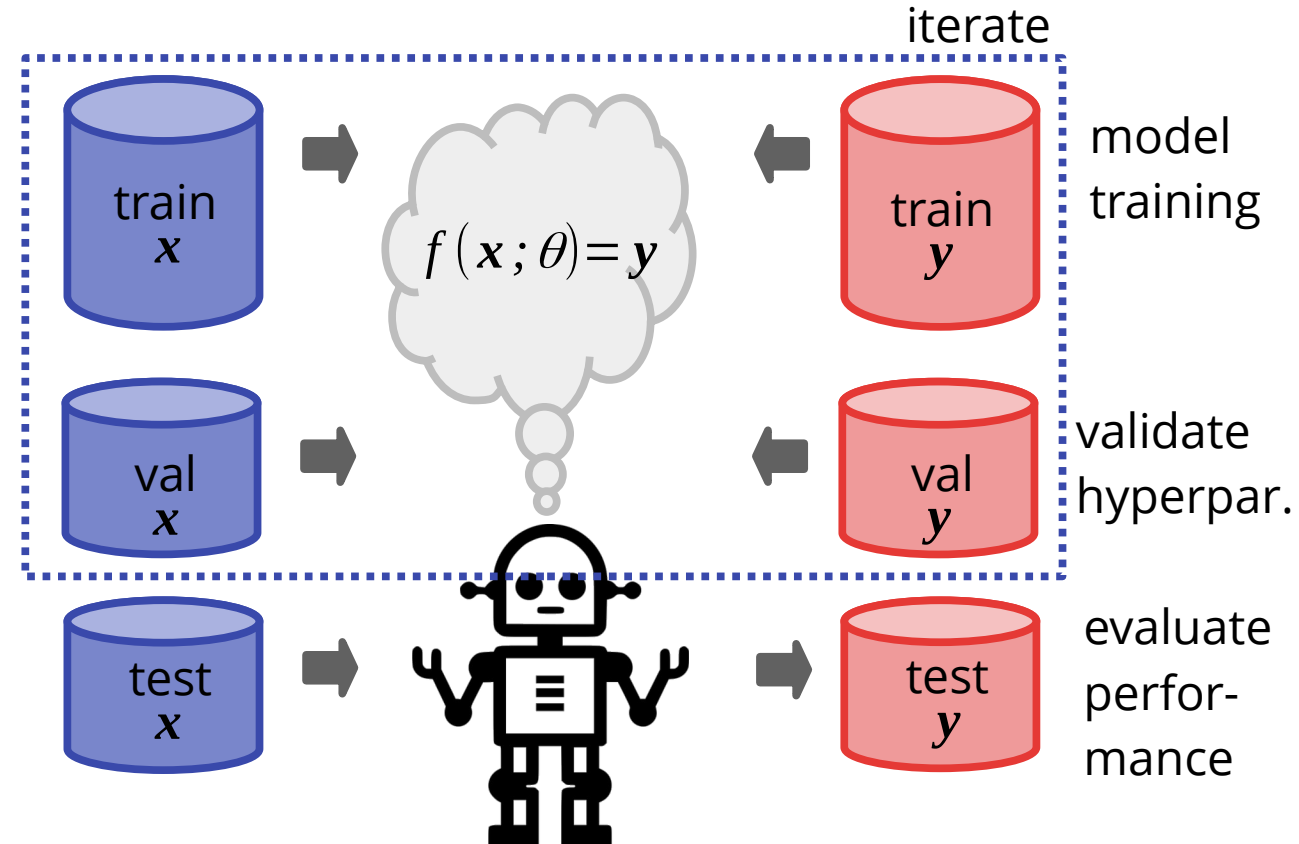
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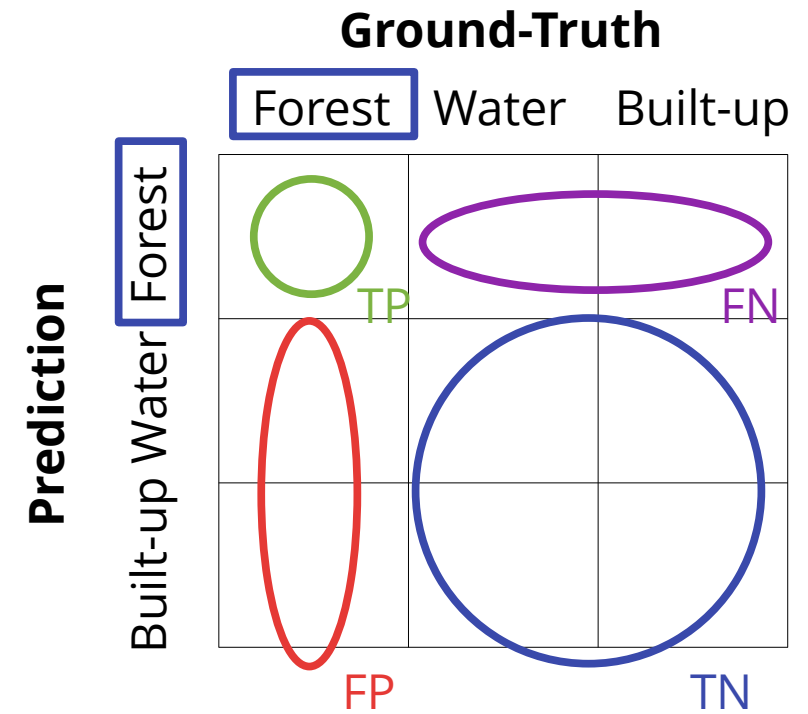


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- 7) Repeat 4) to 6) until performance on validation data maximized
- 8) Evaluate trained model on test data
→ report test data performance



Model Evaluation



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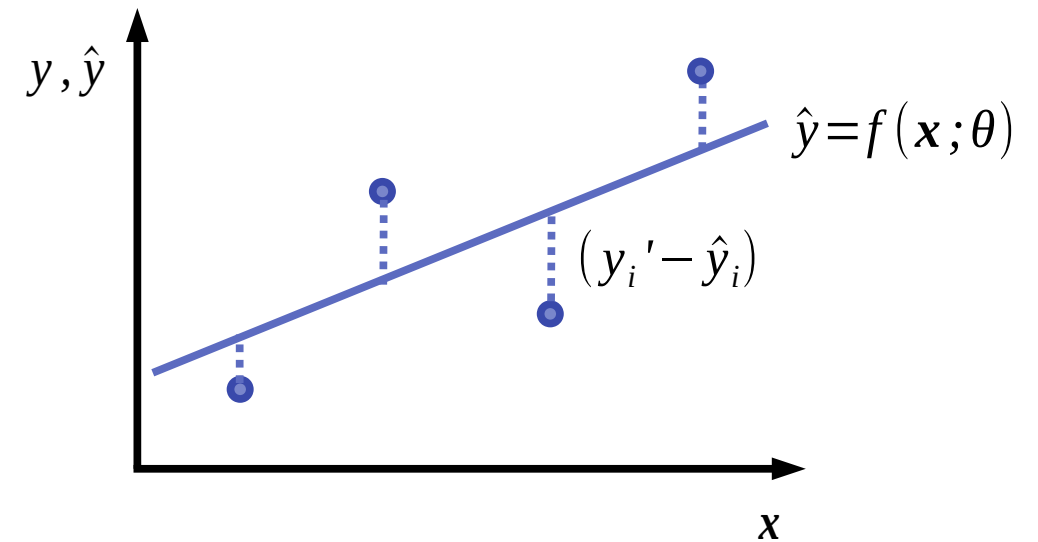
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Only if both conditions are met, the reported results mirror the performance of the model on previously unseen data.

Regression

Regression task metrics:

Input data: $\mathbf{x}_i, i \in \{1 \dots N\}$
Target ground-truth: y_i'
Target prediction: $\hat{y}_i = f(\mathbf{x}_i; \theta)$



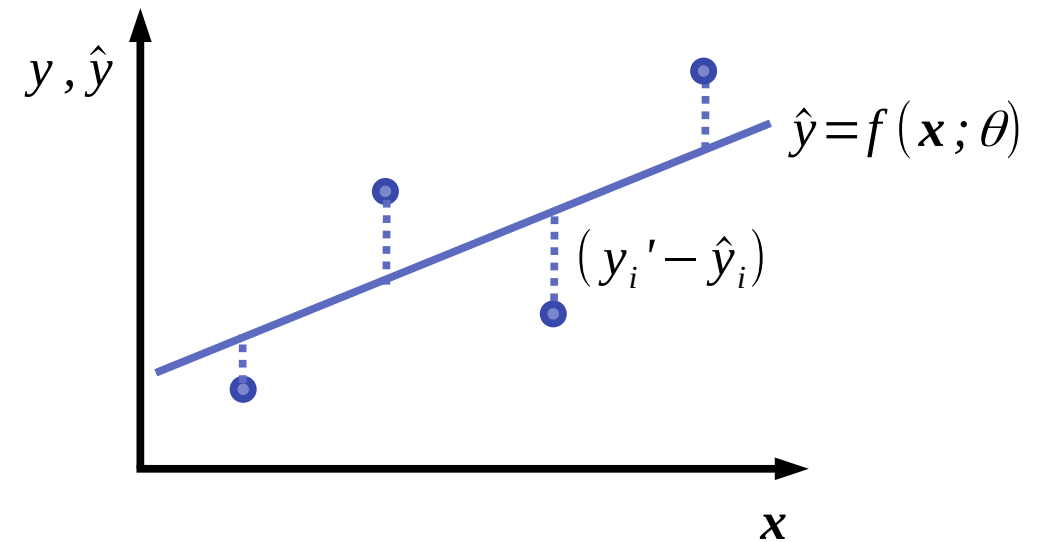
Regression

Regression task metrics:

MAE (Mean Absolute Error)

$$MAE = \frac{1}{N} \sum_i^N |y_i' - \hat{y}_i|$$

Input data: $\mathbf{x}_i, i \in \{1 \dots N\}$
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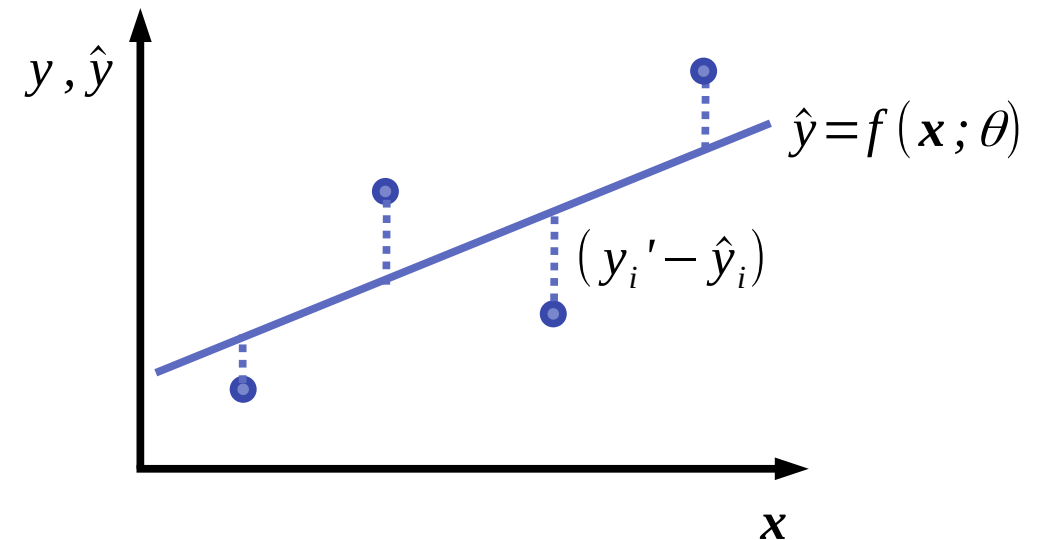
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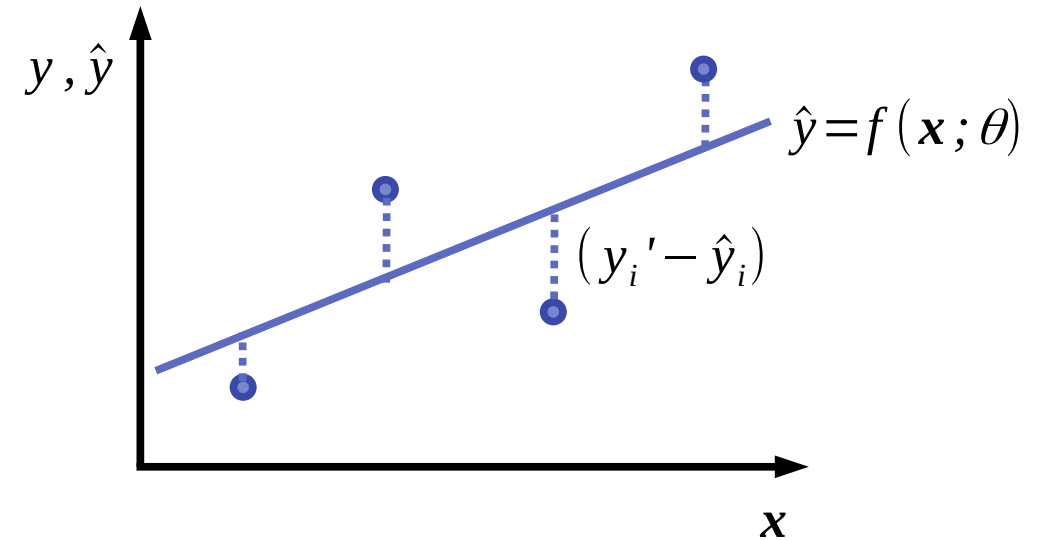
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Intuition: by how much deviates your model prediction from the ground-truth on average.

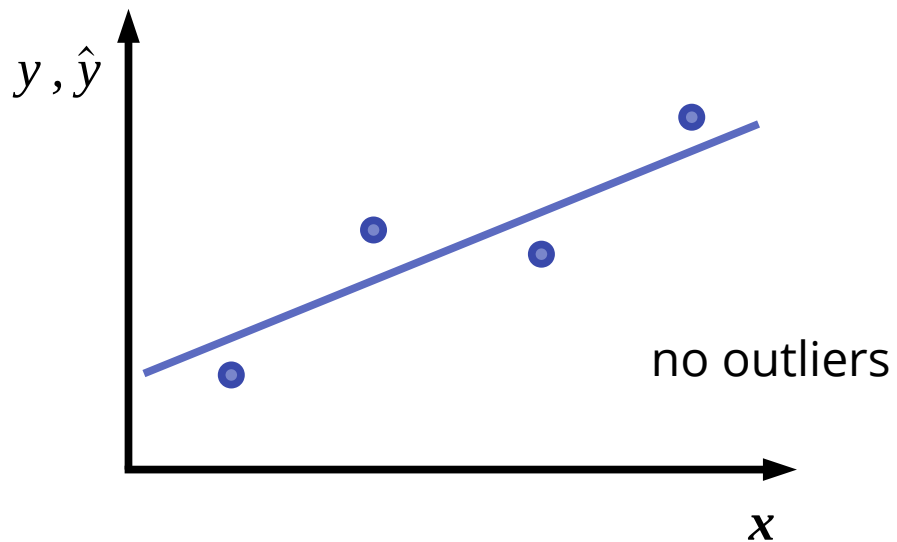
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We compare both MAE and RMSE for two different (and tiny) datasets:

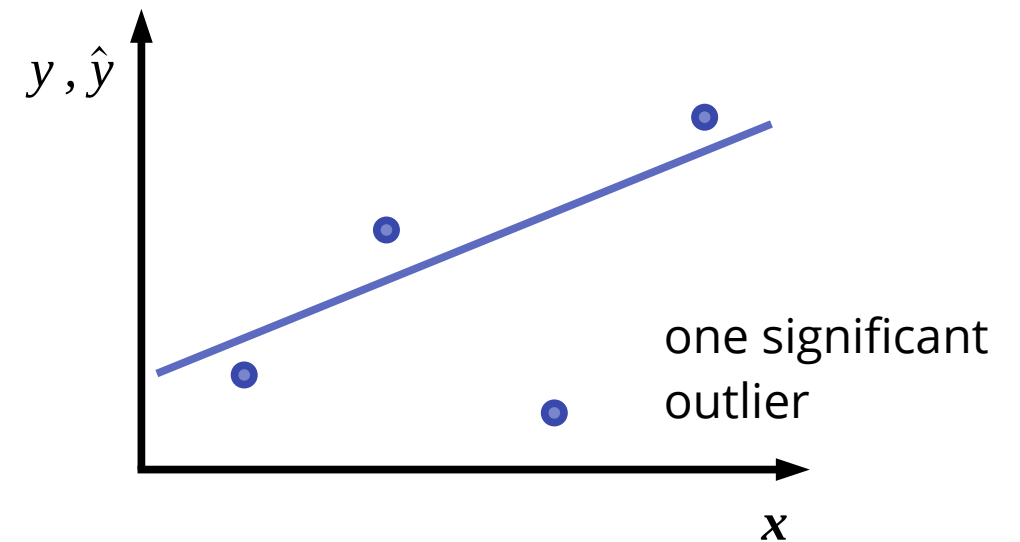
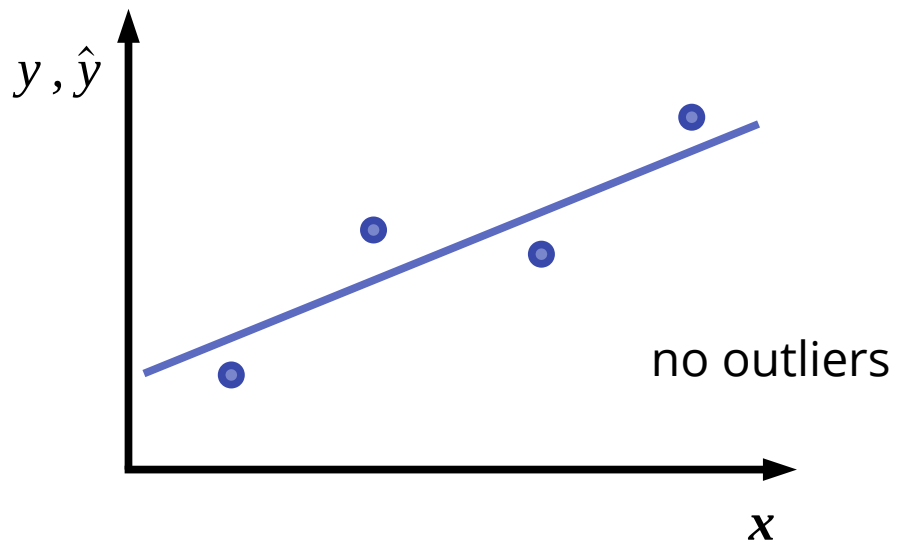
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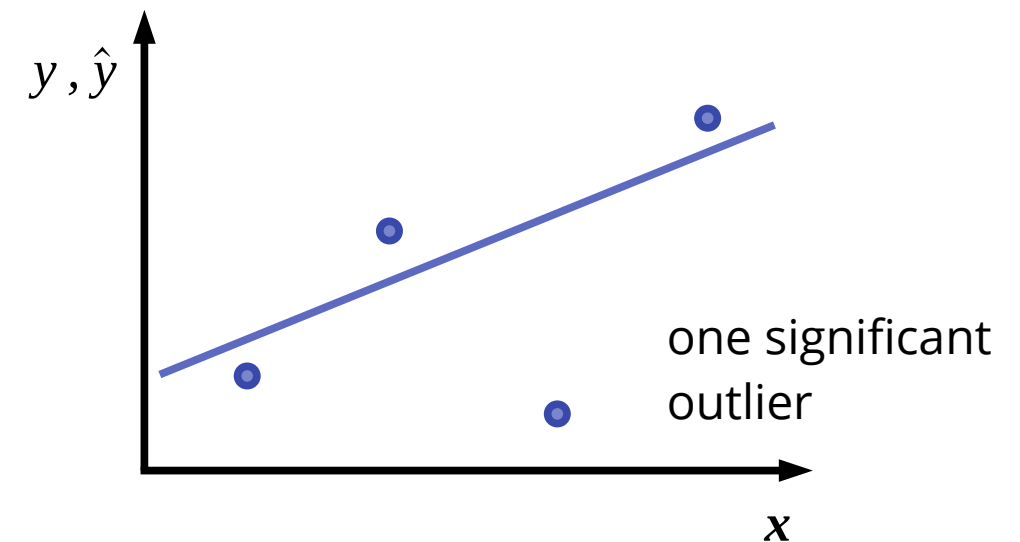
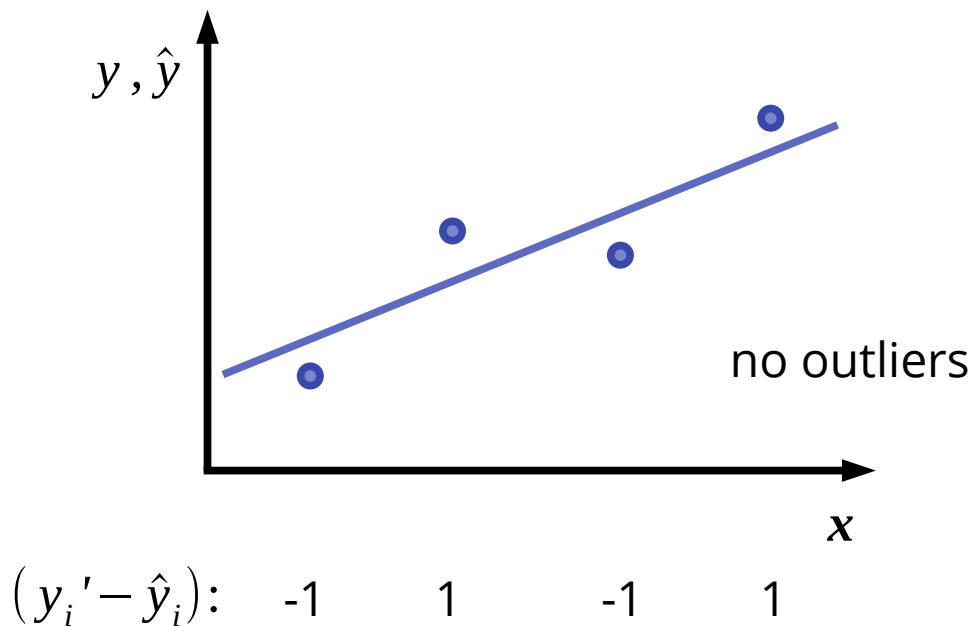
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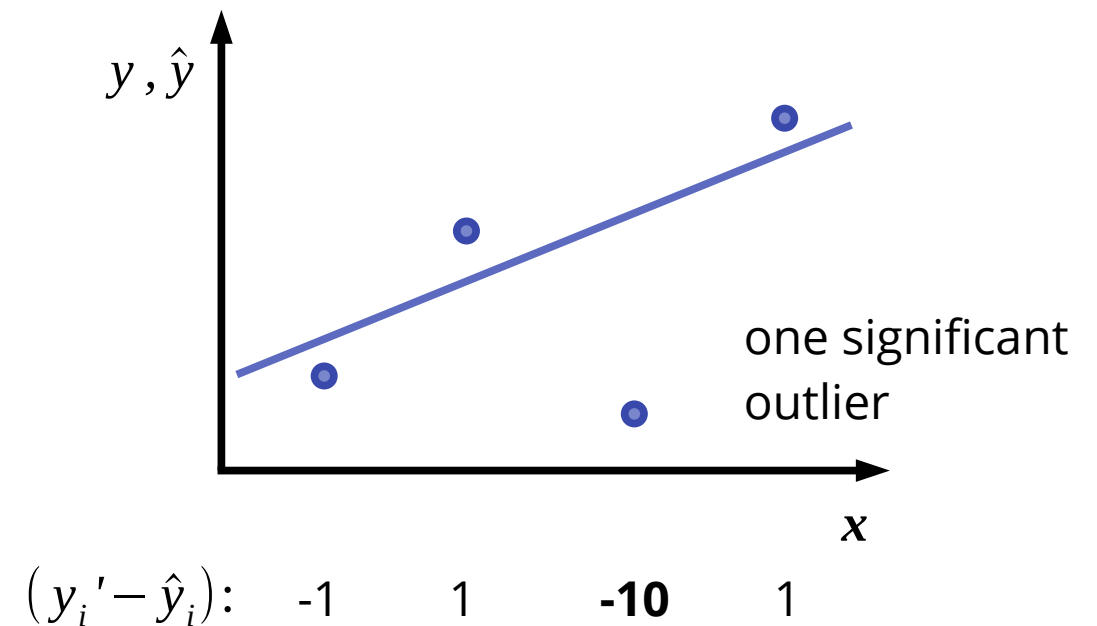
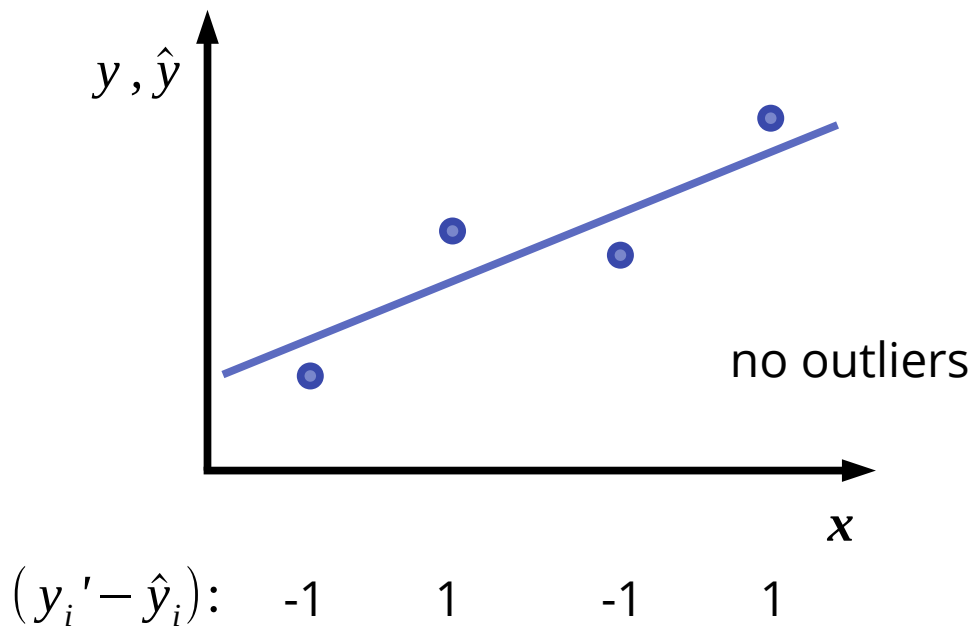
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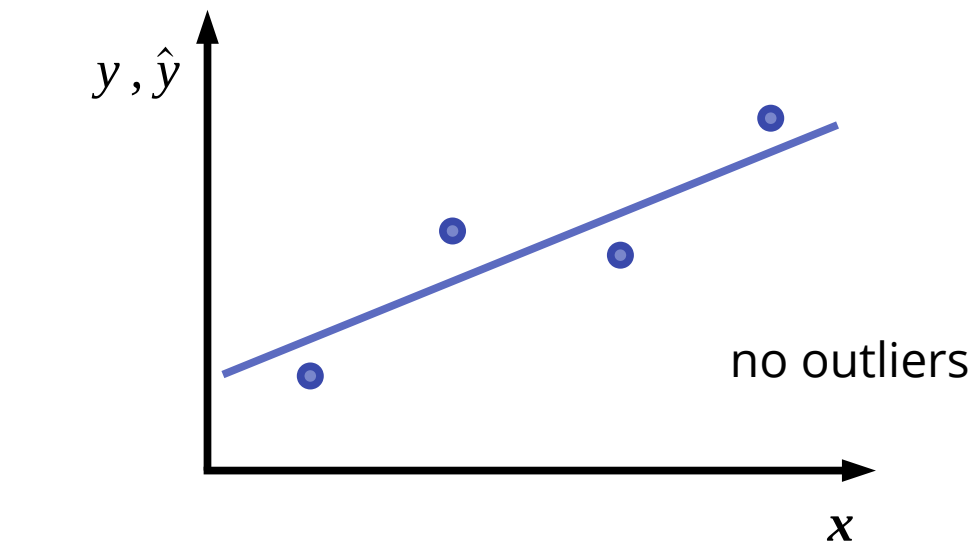
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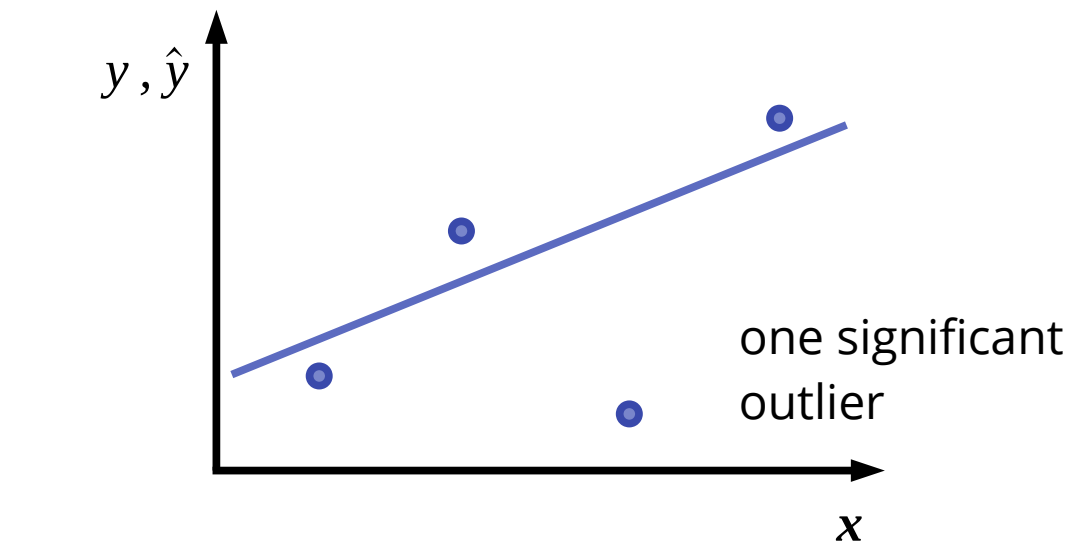
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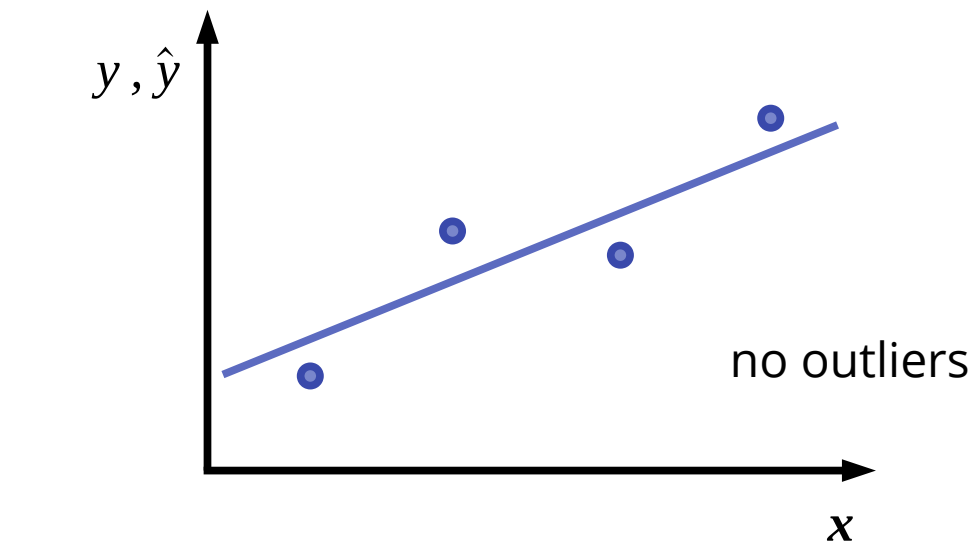
→ MAE = 1; RMSE = 1



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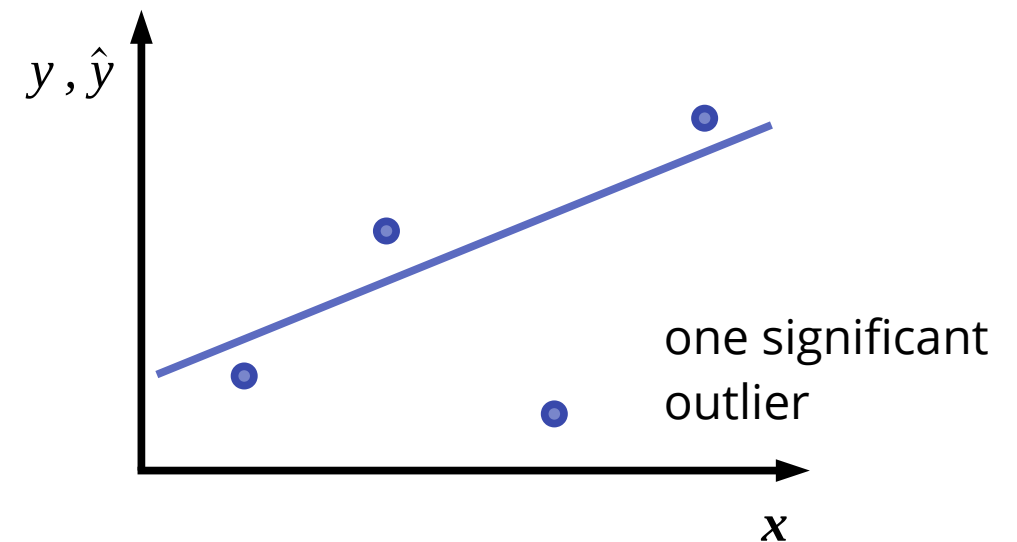
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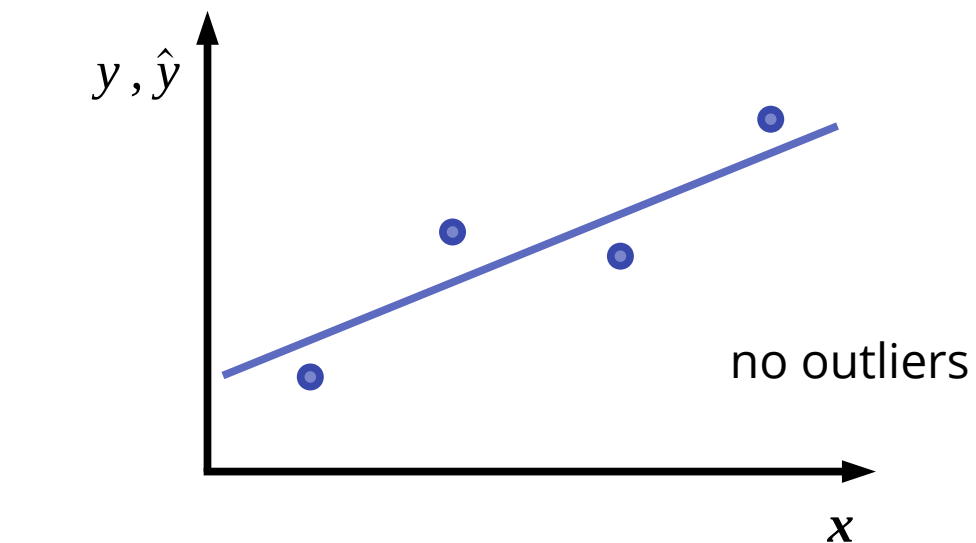


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→ **MAE = 3.25; RMSE = 5.07**

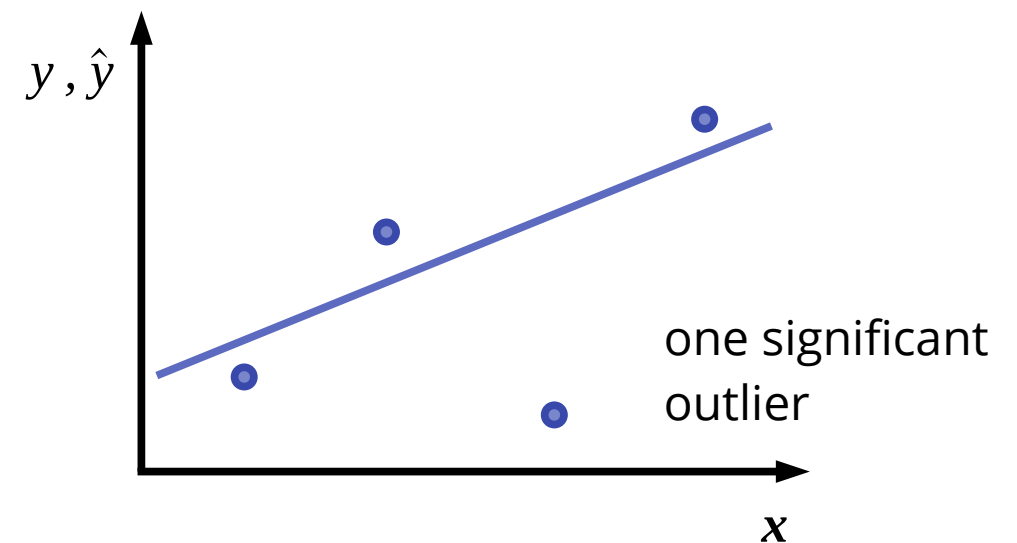
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RMSE is more sensitive to outliers. It depends on your model and problem if this is beneficial, or not.

Binary classification metrics

In a **binary classification** problem, we can simply compare our predictions with the ground-truth, which allows us readily to define a number of different classification metrics:

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we correctly identified 95% of all pixels as either correctly forest or correctly non-forest

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we correctly identified 95% of the forest pixels in the entire image

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The best choice depends on the specific problem and use case.

Confusion matrix

A common way to visualize the performance of a classification model in a multi-class scenario and to find systematic problems, is to use a confusion matrix:

		Ground-Truth		
		Forest	Water	Built-up
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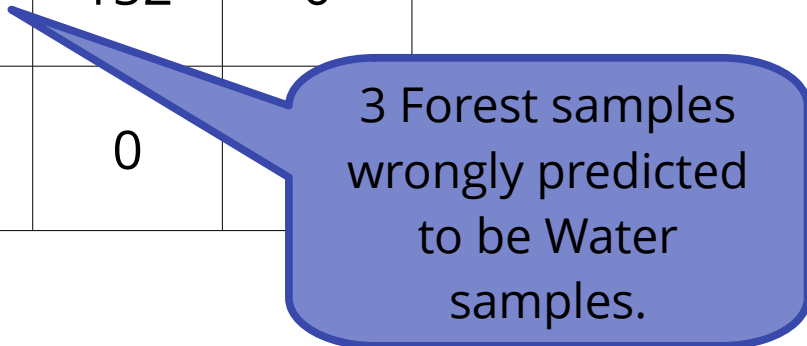
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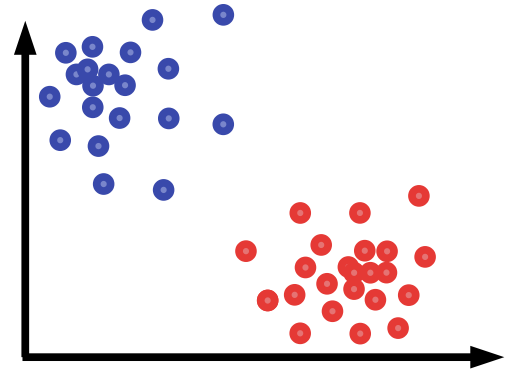
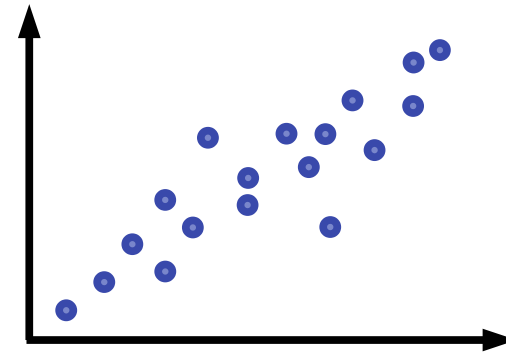
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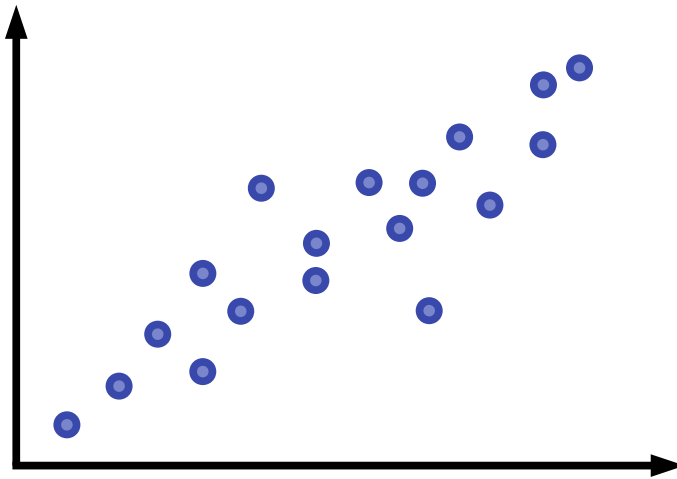
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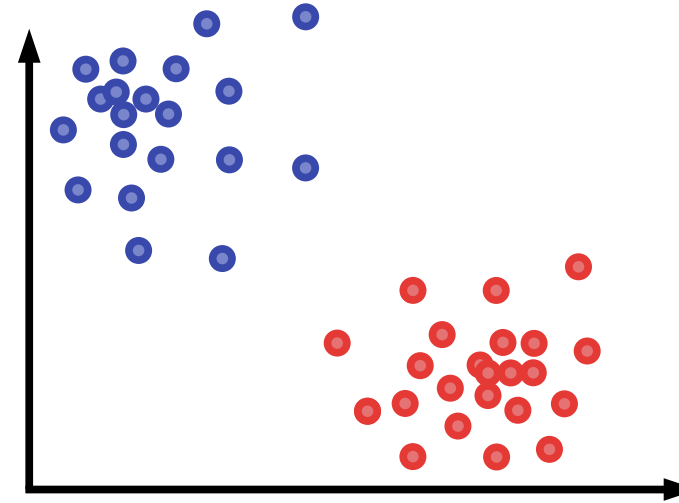
Linear models



Linear models assume **linearity** in the underlying data. They are rather simple but convey many of the concepts utilized in other, more complex models.



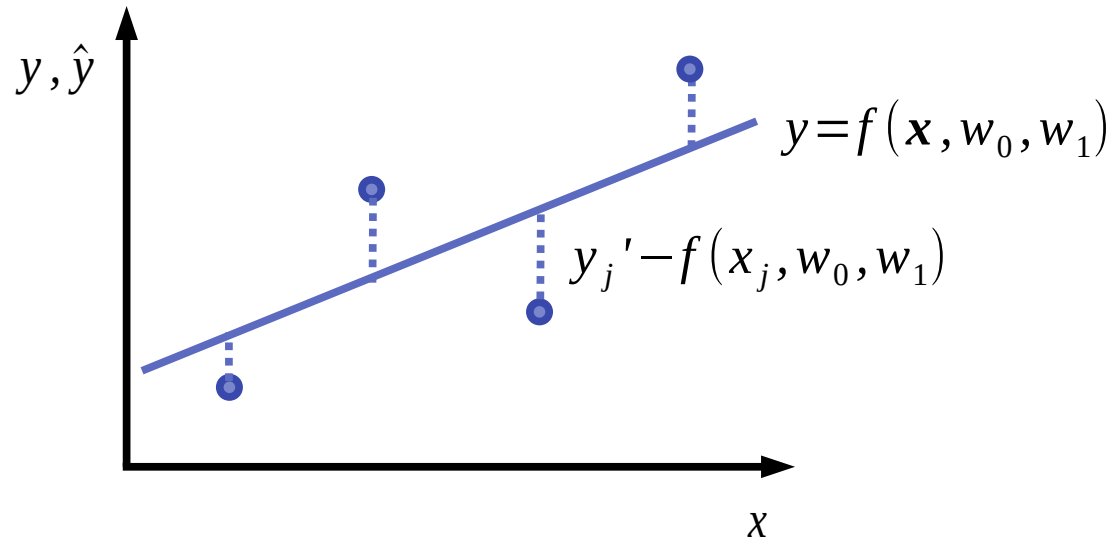
Linear regression



Linear classification

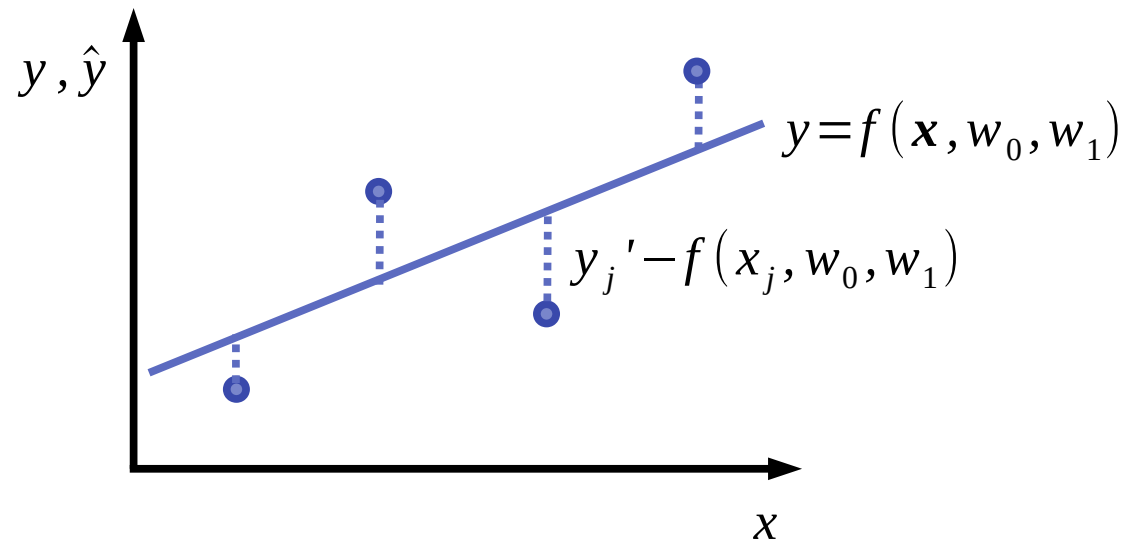
Linear regression (univariate)

Find weights w_0 and w_1 so that the linear function $f(x) = w_1 x + w_0$ with input x and output y best fits the data containing ground-truth values y' .



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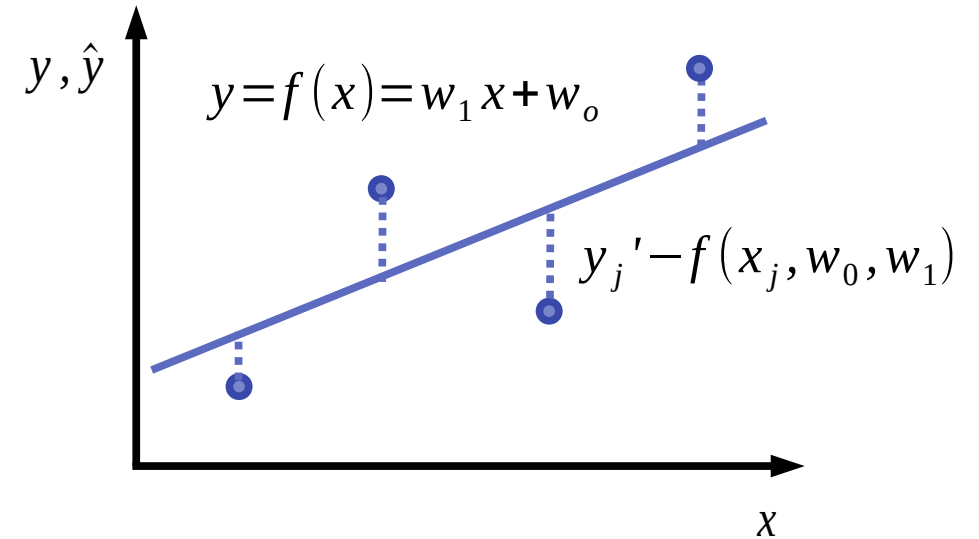


How can we learn w_0 and w_1 from data?

Linear regression (univariate) – Least squares fitting

Idea: minimize squared errors of prediction with respect to ground truth for each data point:

for data point j : $[y_j' - f(x_j, w_0, w_1)]^2$

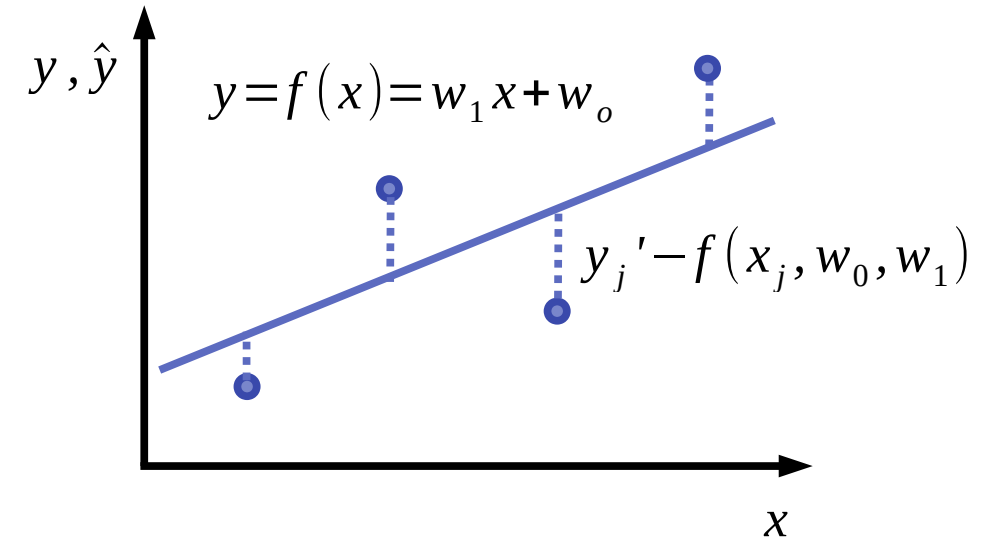


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We define a **Loss** (or Objective) function that is the sum of the squared errors over all data points:



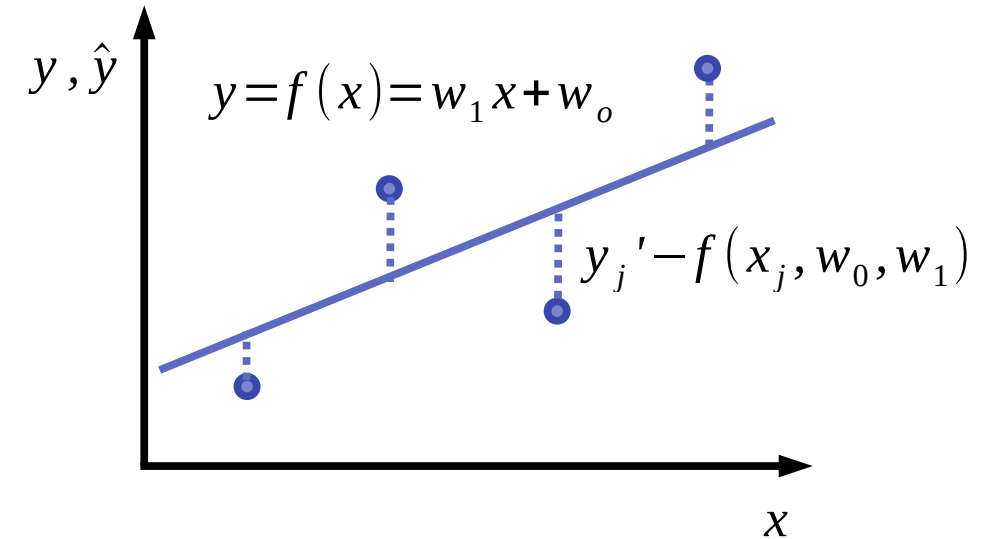
Linear regression (univariate) – Least squares fitting

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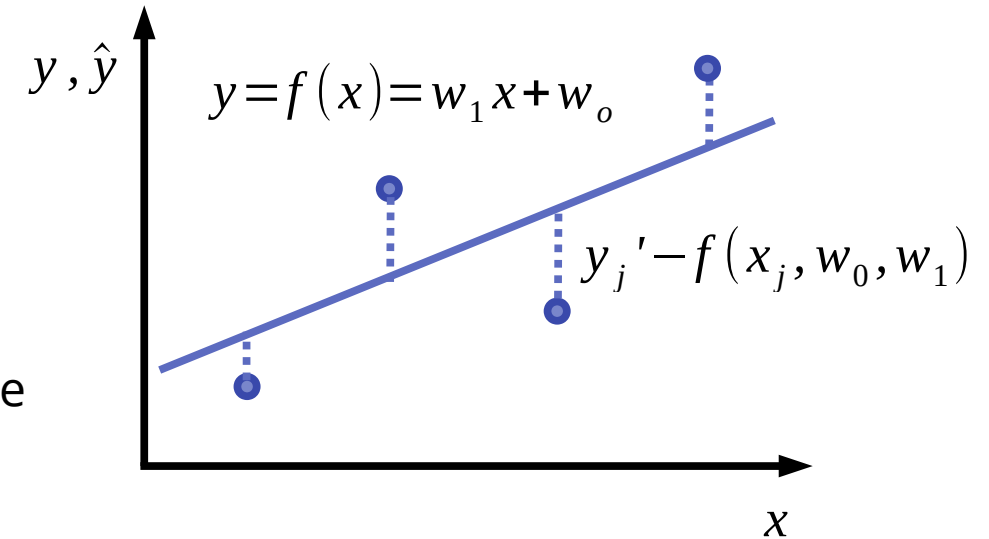
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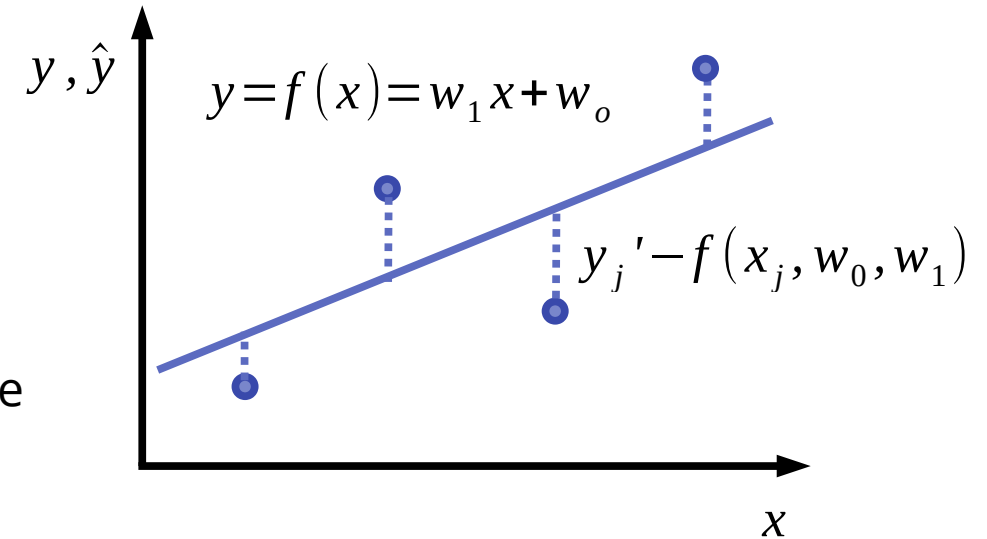
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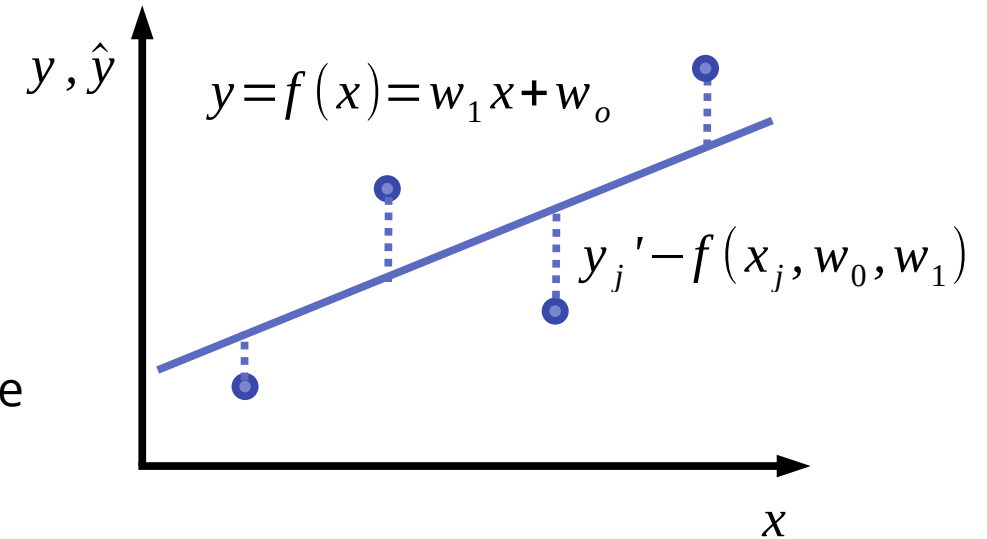
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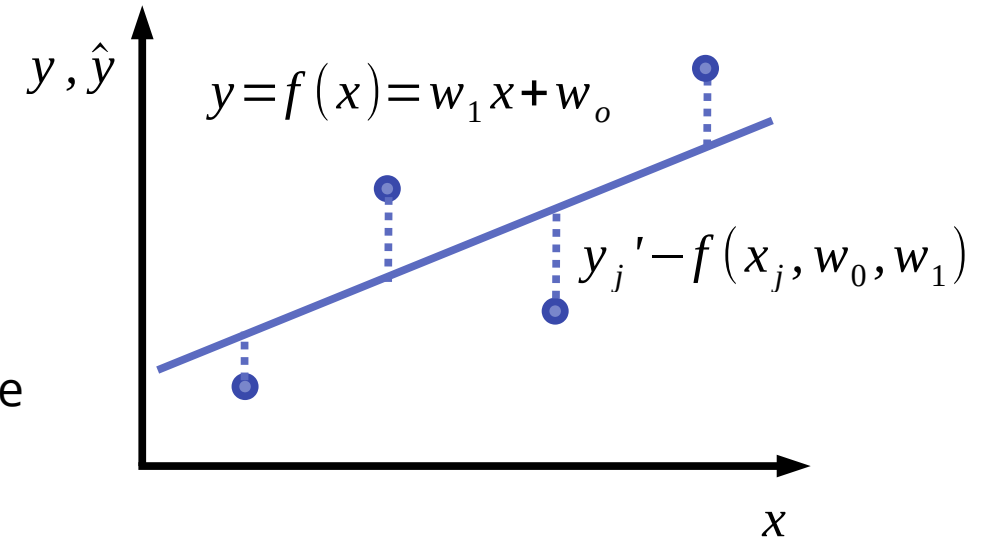
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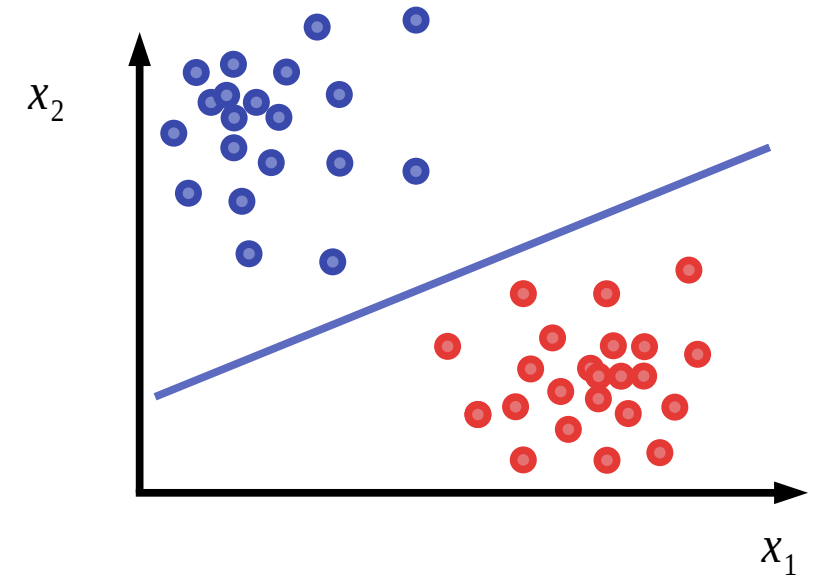
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Least-squares + linear model function: the resulting minimum of the Loss function is **global**, i.e., the “learns” immediately the best-possible solution!

Linear classifier (two-dimensional case)

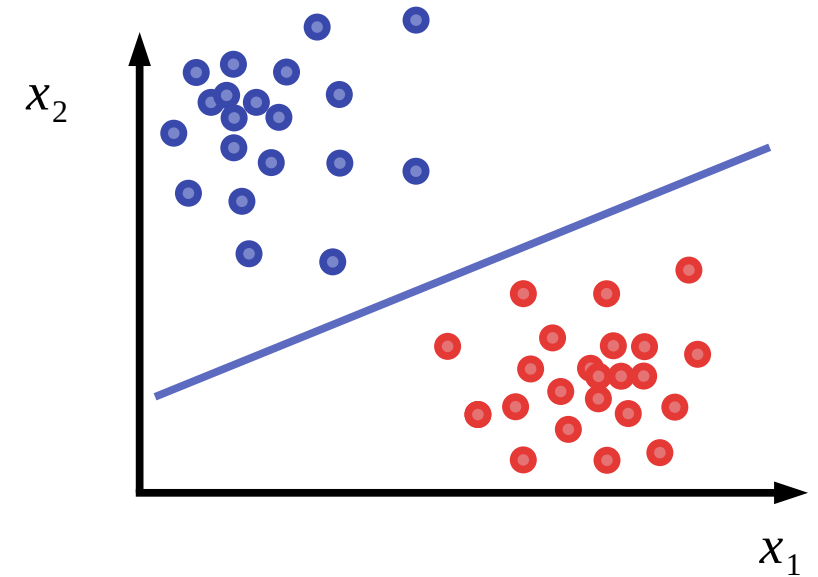
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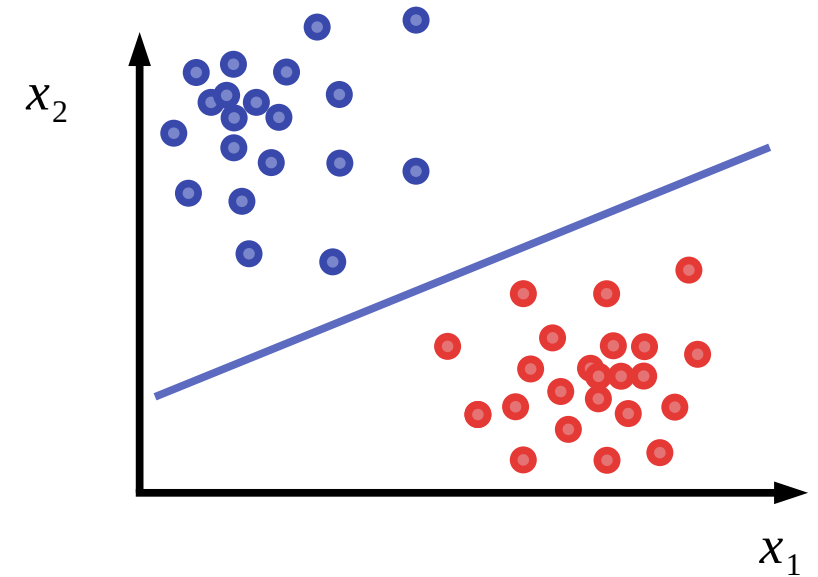


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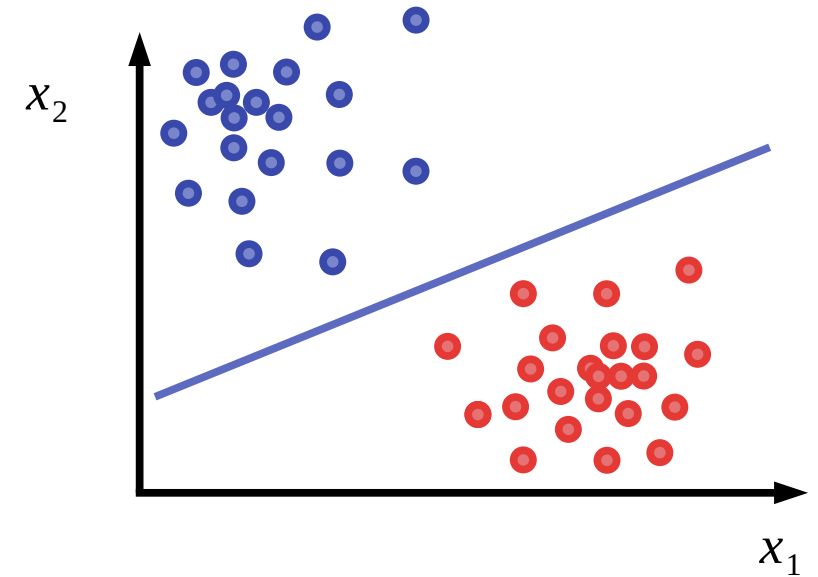
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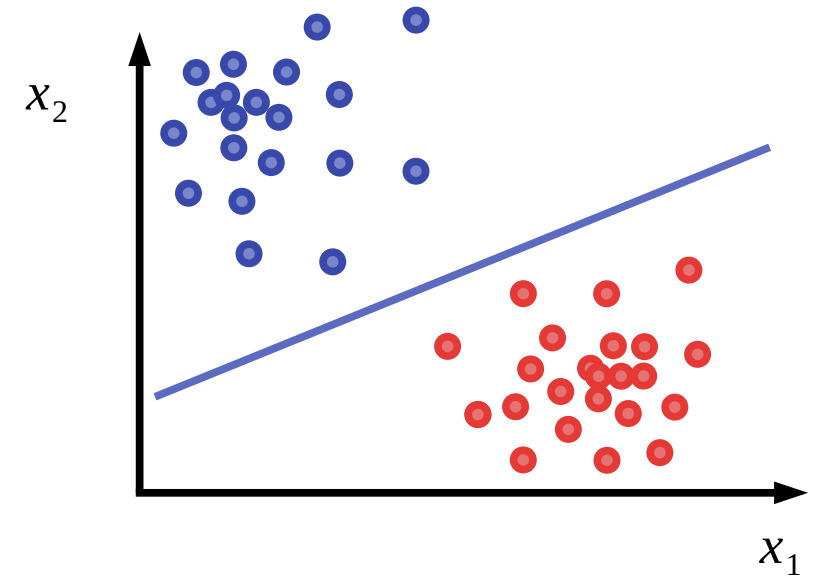
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We can define class assignments through a threshold function:

$$\bar{f}(\mathbf{x}, \mathbf{w}) = \begin{cases} 1 & \text{if } f(\mathbf{x}, \mathbf{w}) \geq 0 \\ 0 & \text{if } f(\mathbf{x}, \mathbf{w}) < 0 \end{cases}$$



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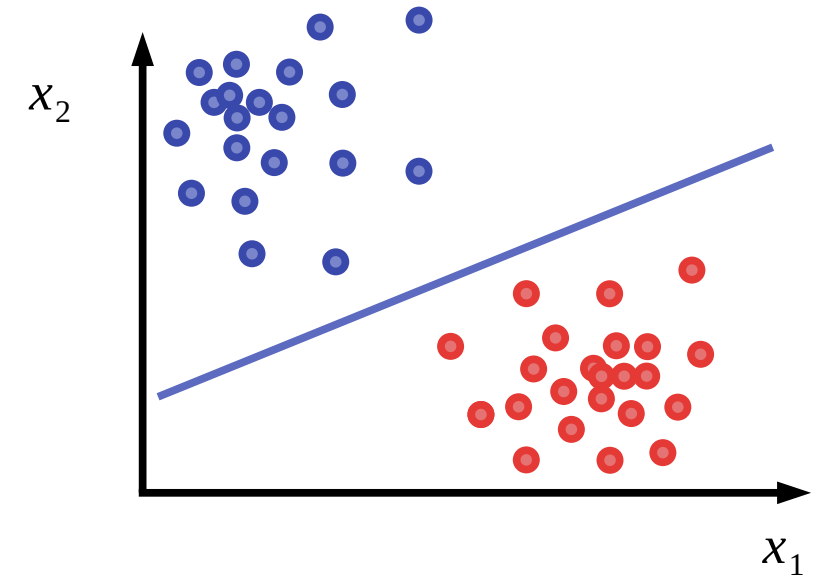
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How can we learn $\mathbf{w}$ from data?

Linear classifier (two-dimensional case) – Perceptron learning rule

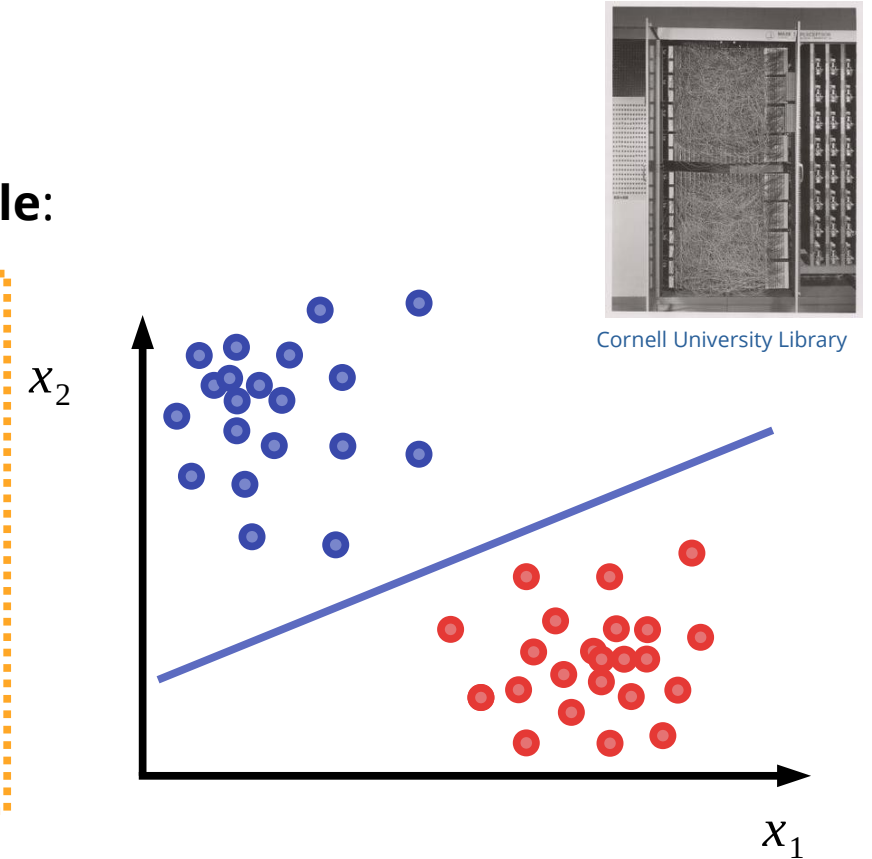
We define the following algorithm as the **Perceptron learning rule**:

We consider each data point, consisting of $\mathbf{x}$ and ground-truth label y' and check whether the prediction from $\bar{f}(\mathbf{x}, \mathbf{w})$ is correct, or not. If...

$\bar{f}(\mathbf{x}, \mathbf{w}) = y$, then do nothing.

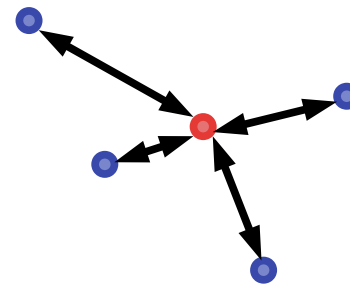
$\bar{f}(\mathbf{x}, \mathbf{w}) = 0$ but $y' = 1$, then increase w_i if $x_i \geq 0$, or vice versa.

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Weights are adjusted by a step size that is called the **learning rate**. By iteratively running this algorithm over your training data multiple times, the weights can be learned so that the model performs properly. A solution is “learned” iteratively here.

Nearest-Neighbor models



Nearest neighbor models

Nearest neighbor models are **non-parametric** and simply rely on **distances** between data points.

Nearest neighbor models

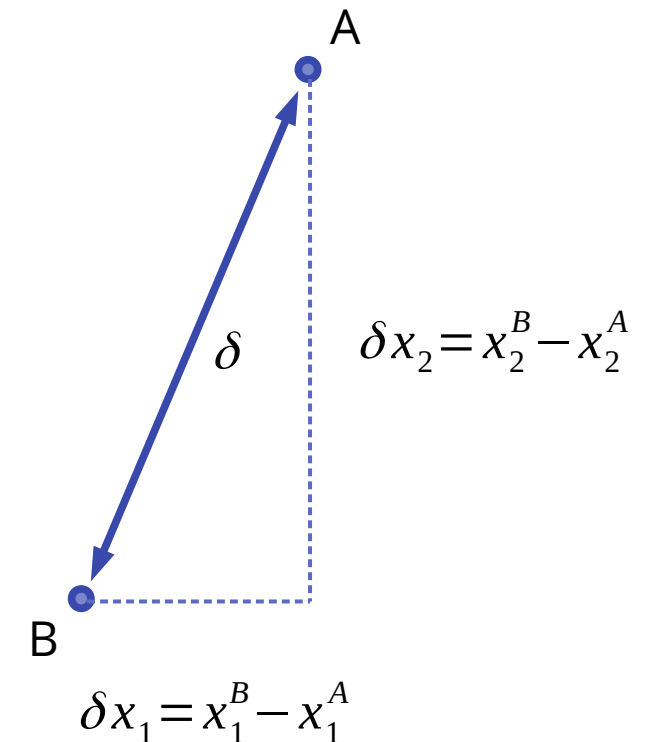
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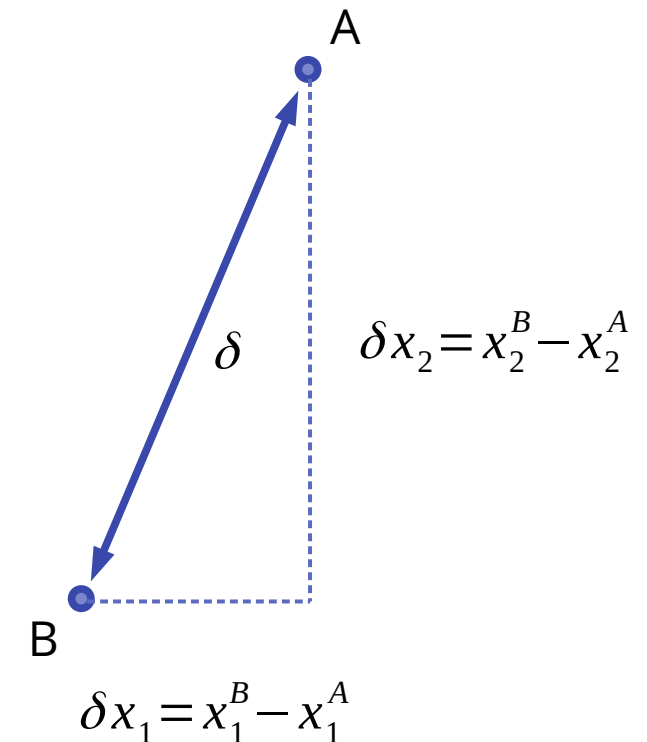


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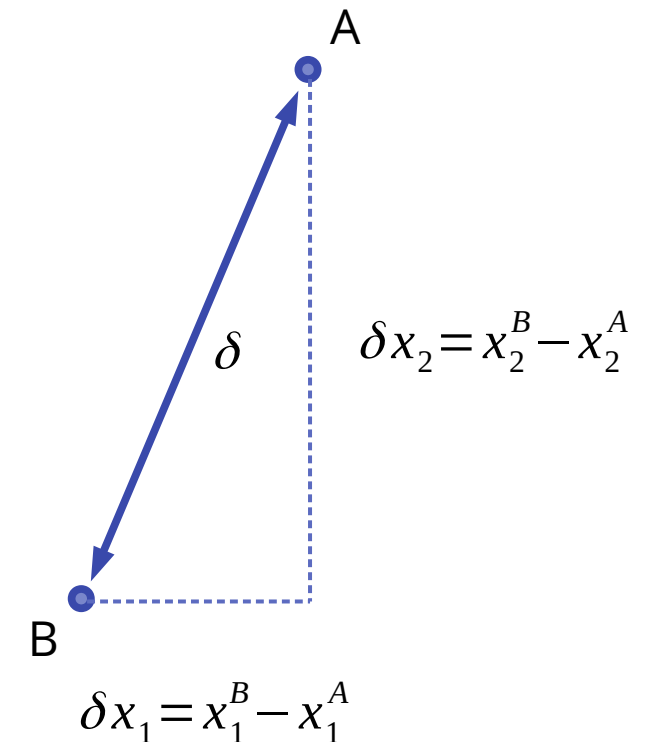
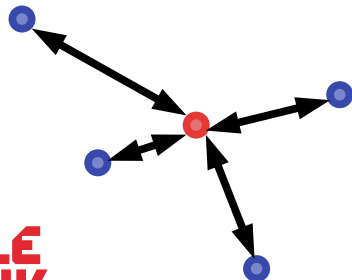
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Nearest neighbor methods utilize distances between datapoints for **classification** and **regression** tasks.



***k*-nearest neighbor classification**

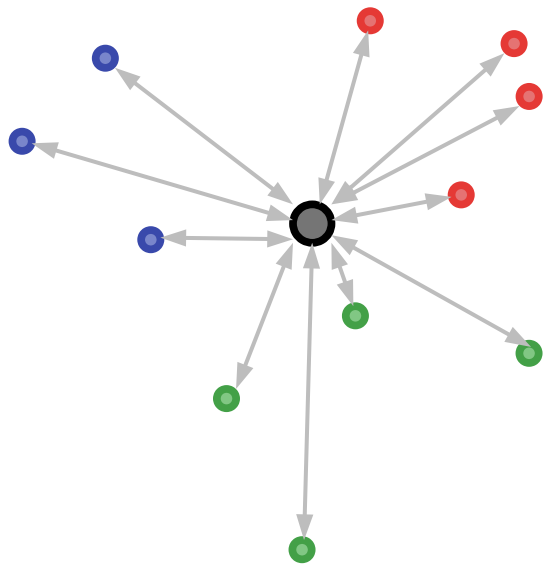
k-nearest neighbor (knn) classifiers predict class affiliation of an unseen data point based on **majority voting** of its ***k* nearest neighbors** in a seen data set with ground-truth labels.

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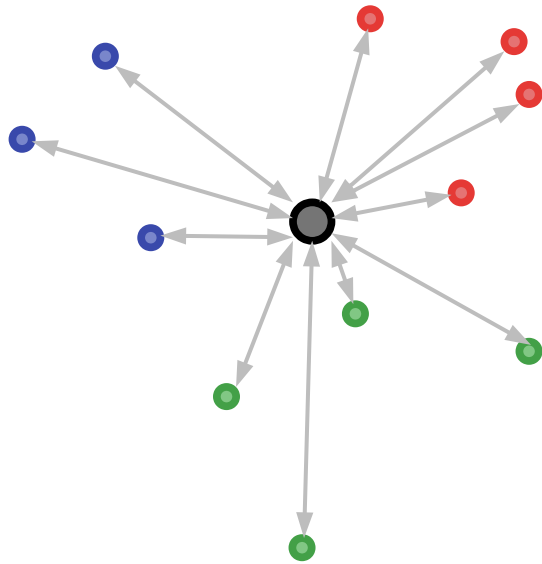


compute distances

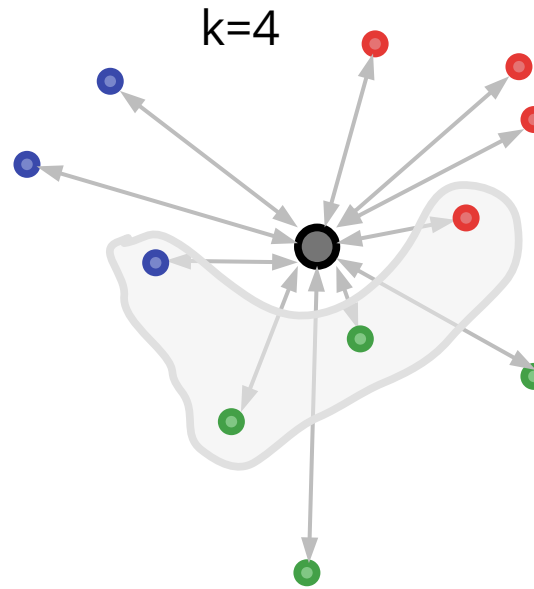
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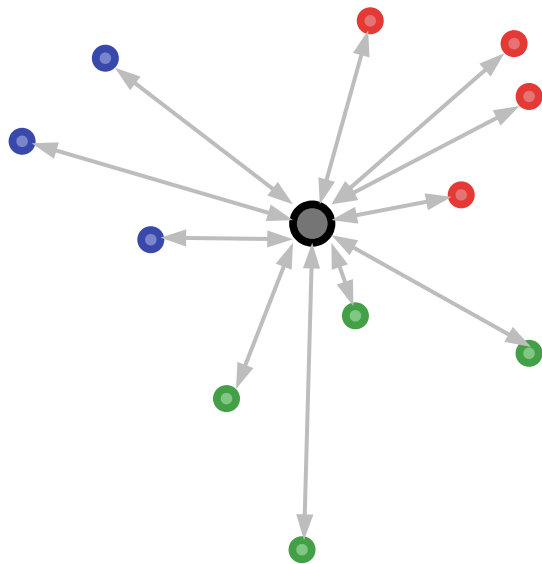


identify *k* nearest neighbors

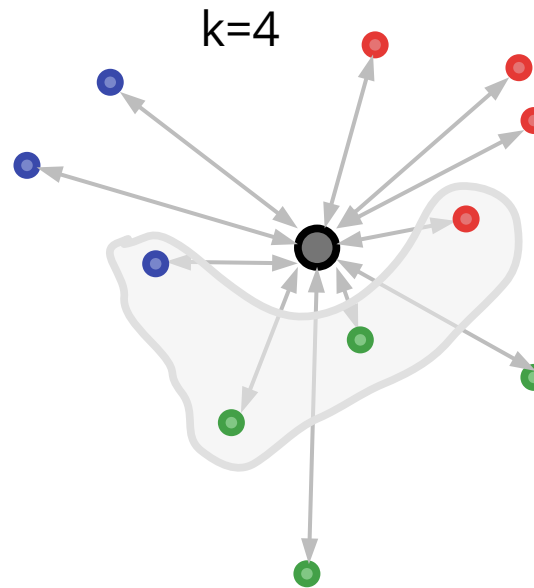
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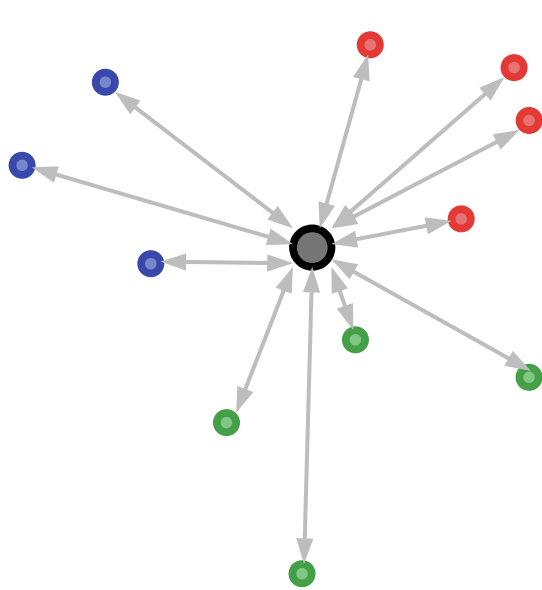
k=4:



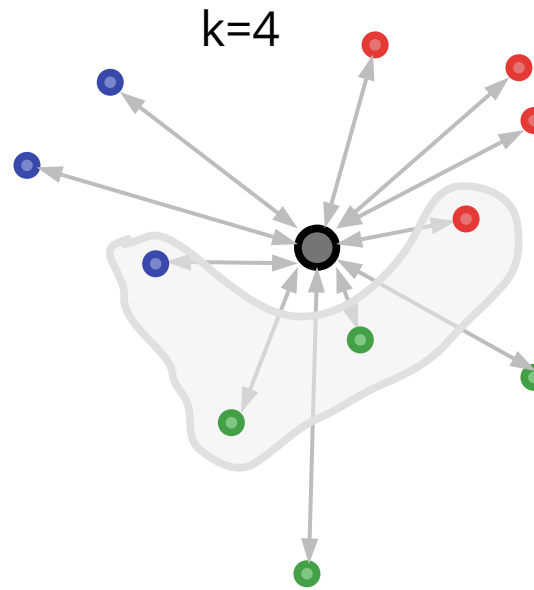
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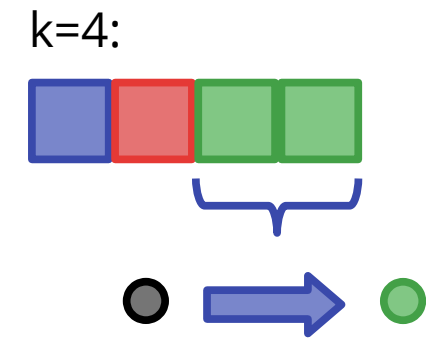
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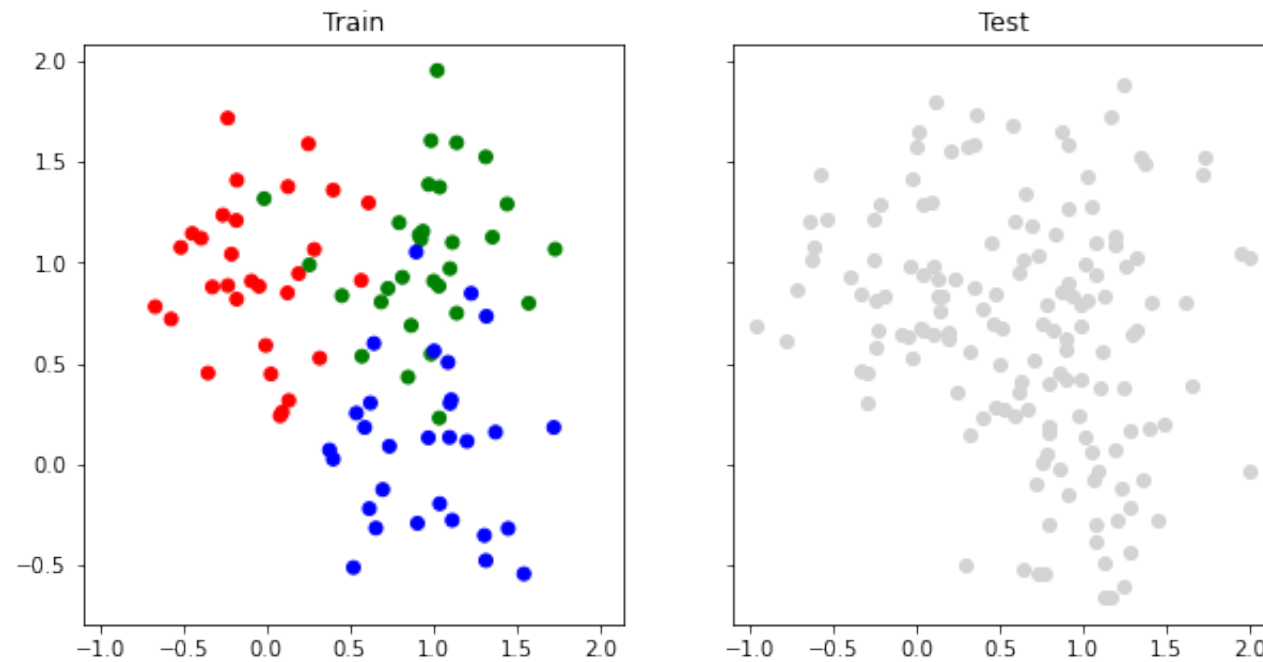


identify k nearest neighbors



class assignment

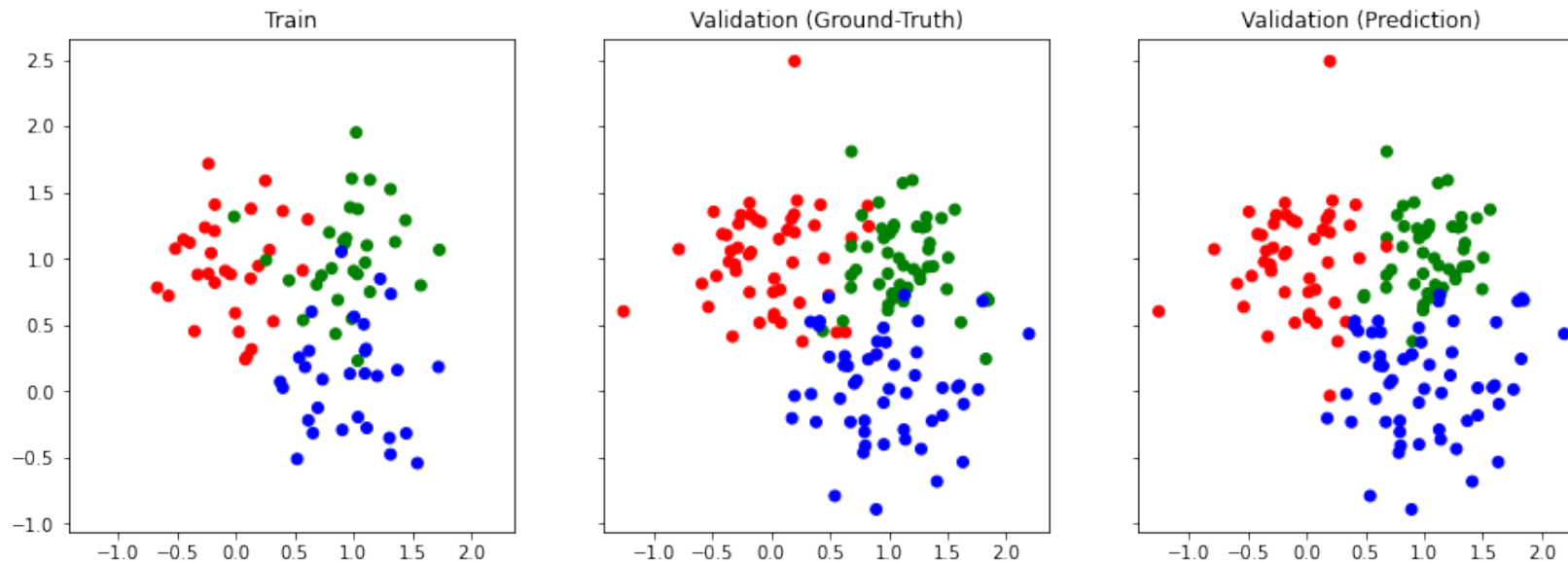
k-nearest neighbor classification - Example



3 overlapping clusters

How well can knn classify
our test data set?

k-nearest neighbor classification - Example

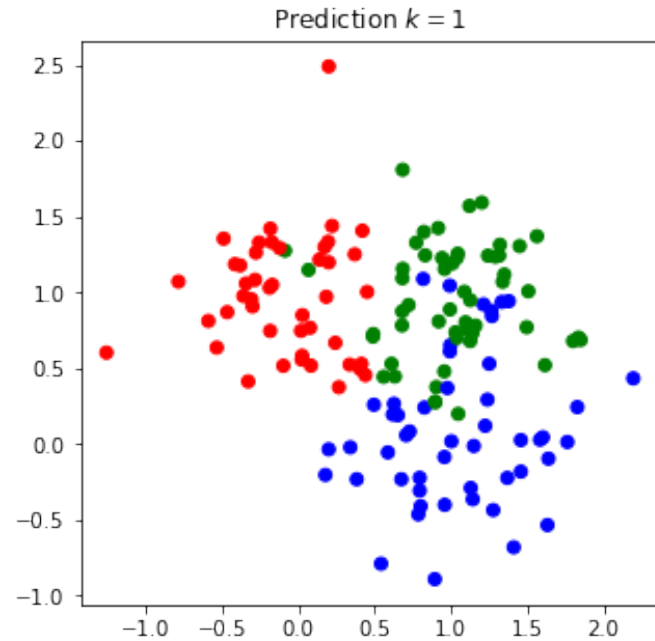


k=5: accuracy=0.867

Hyperparameter k has an impact on how well the model generalizes to unseen data: perform a **hyperparameter search**!

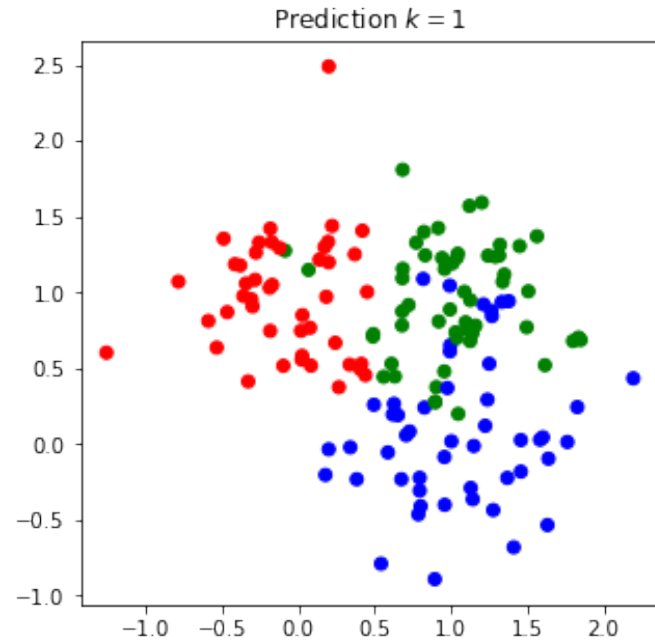
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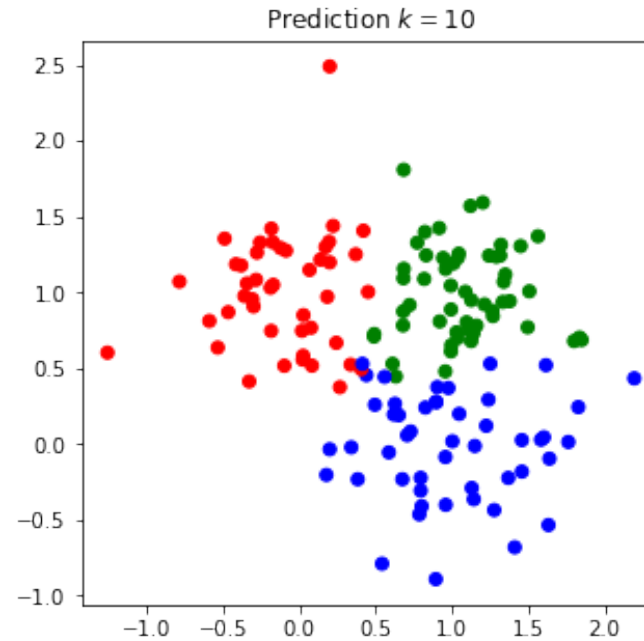


$k=1$
 $\text{accuracy}_{\text{val}}=0.800$

k-nearest neighbor classification - Example

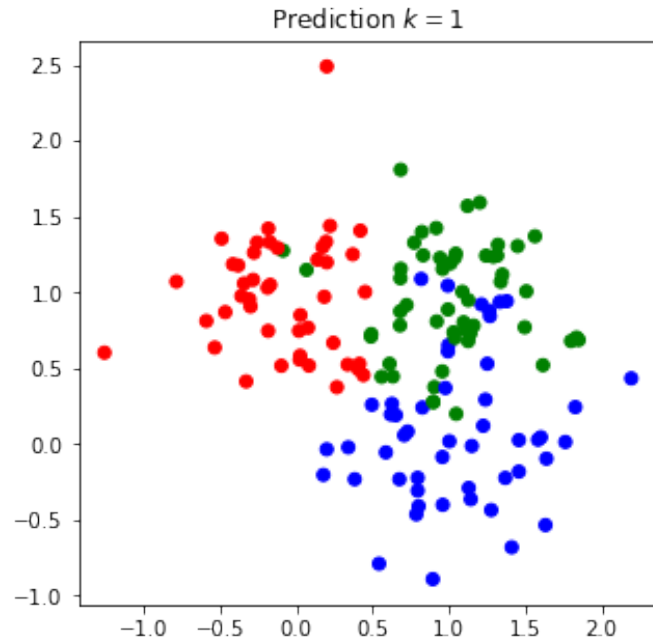


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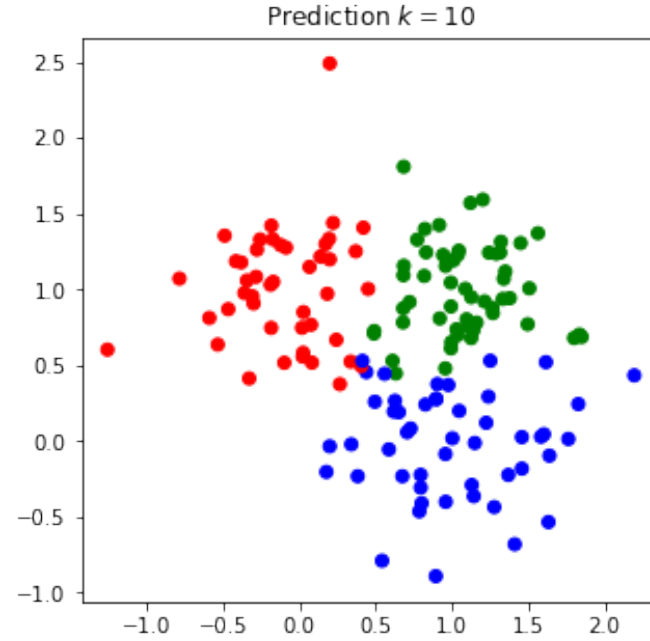


$k=10$
 $\text{accuracy}_{\text{val}}=0.893$

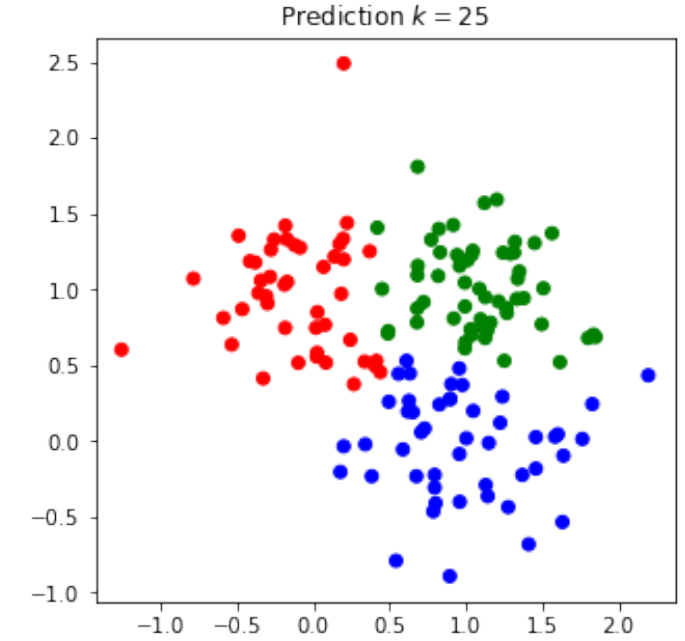
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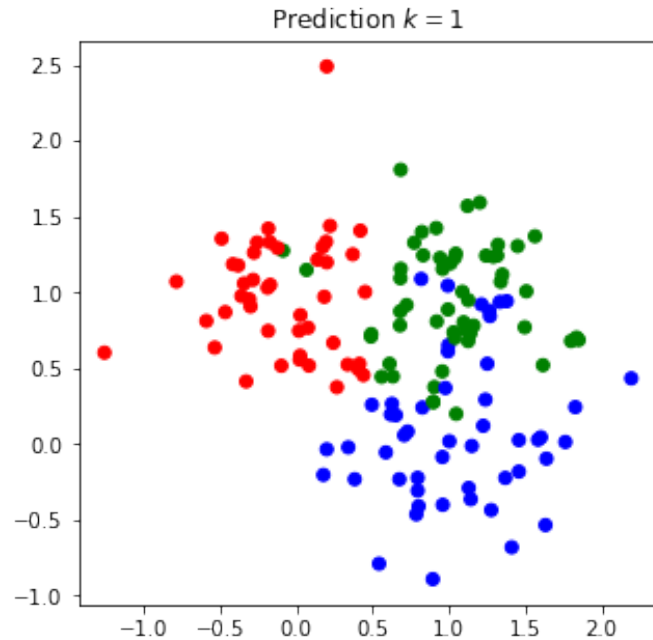


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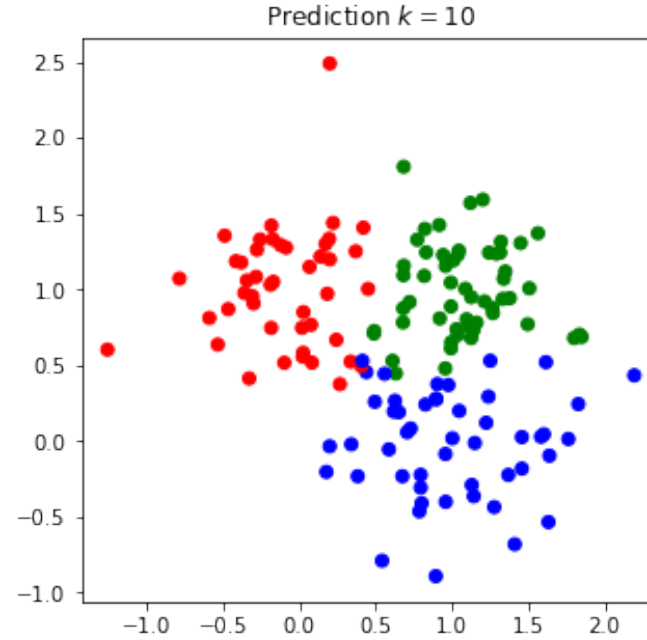
$k=25$
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k-nearest neighbor classification - Example



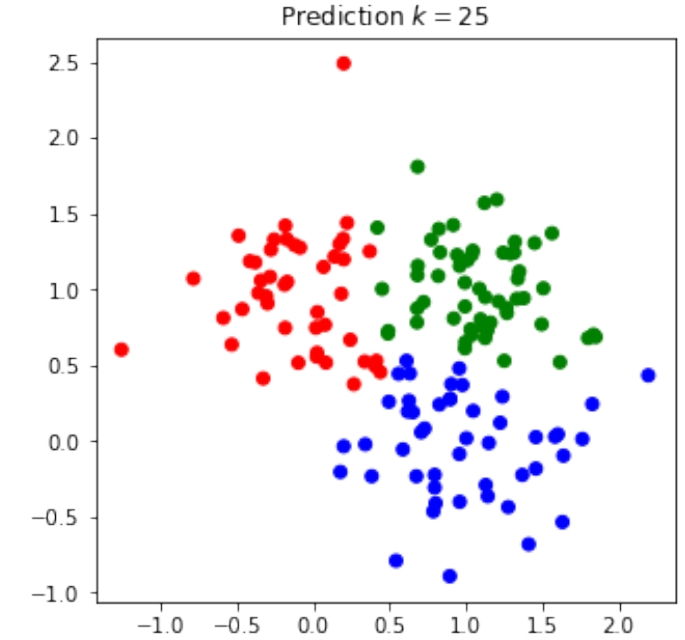
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Overfitting!



$k=10$
 $\text{accuracy}_{\text{val}}=0.893$
 $\text{accuracy}_{\text{test}}=0.880$

Best performance

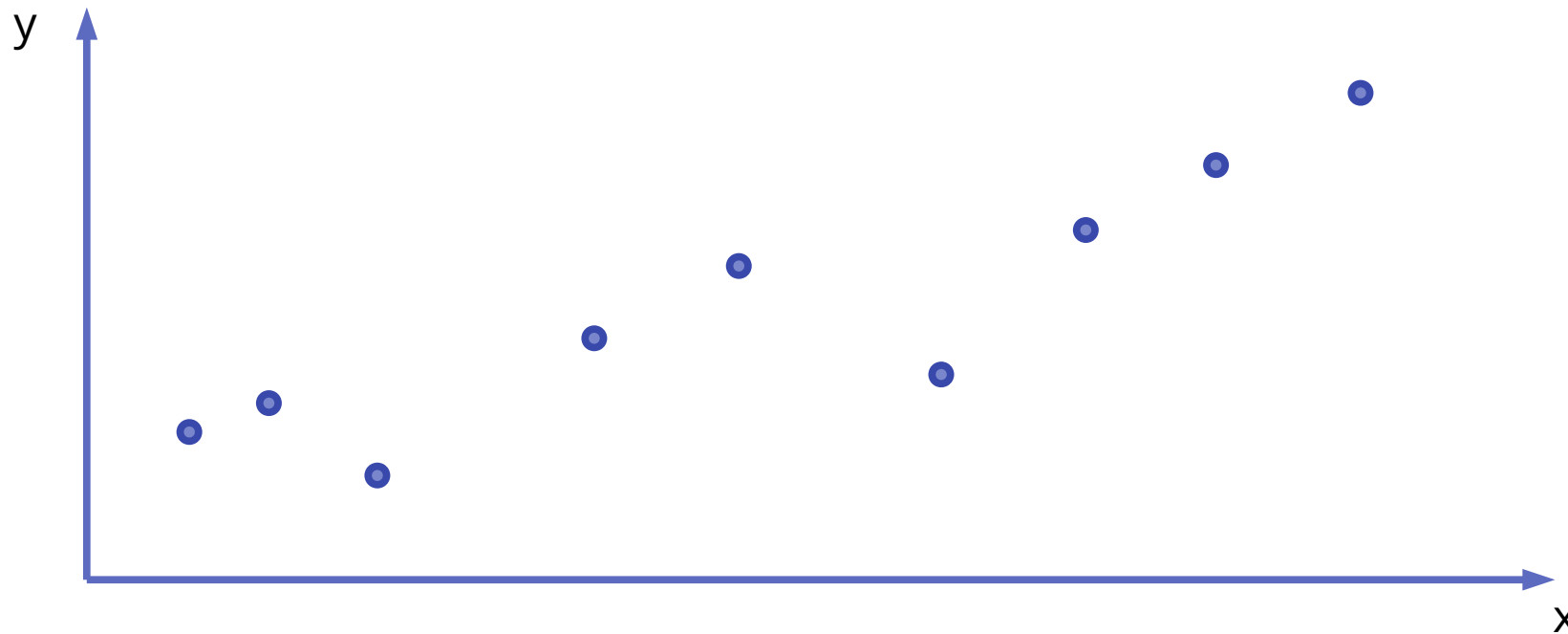


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Underfitting!

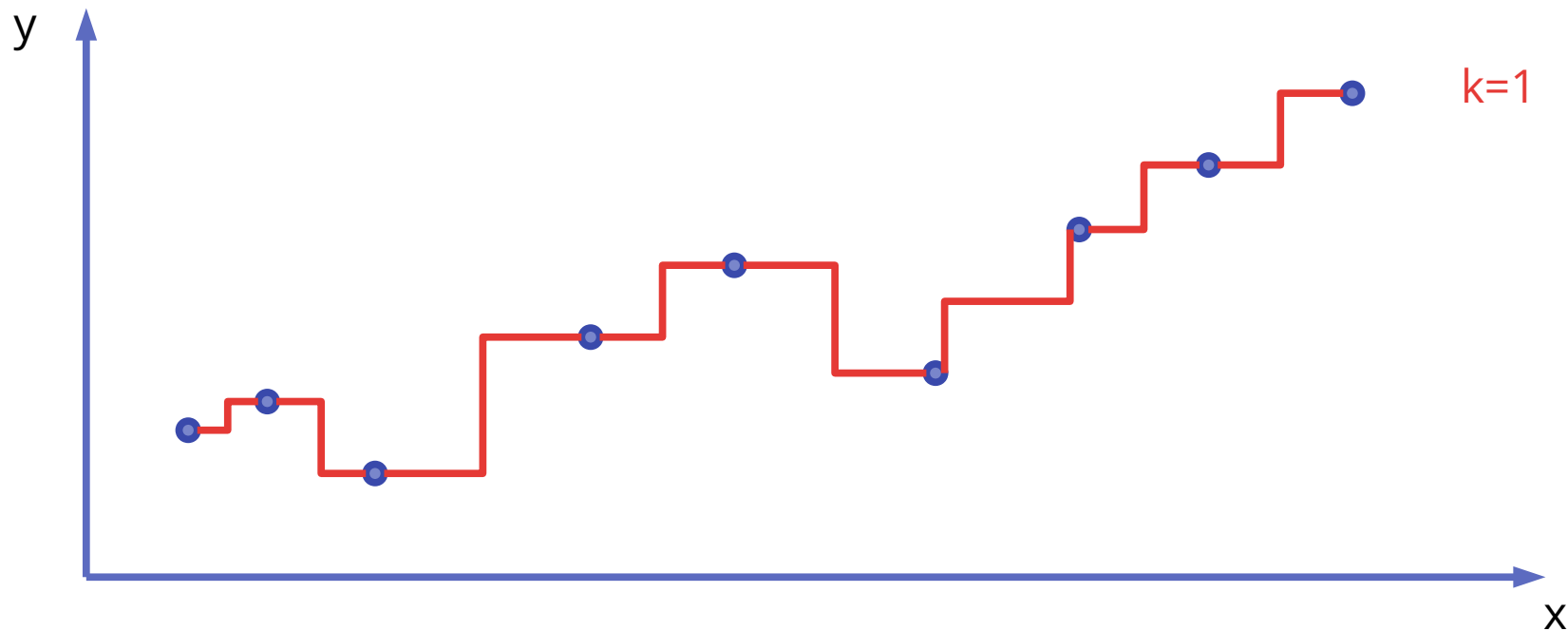
k-nearest neighbor regression

Nearest neighbor methods can also be implemented as regressors that are able to **interpolate** between and **smoothen** available data.



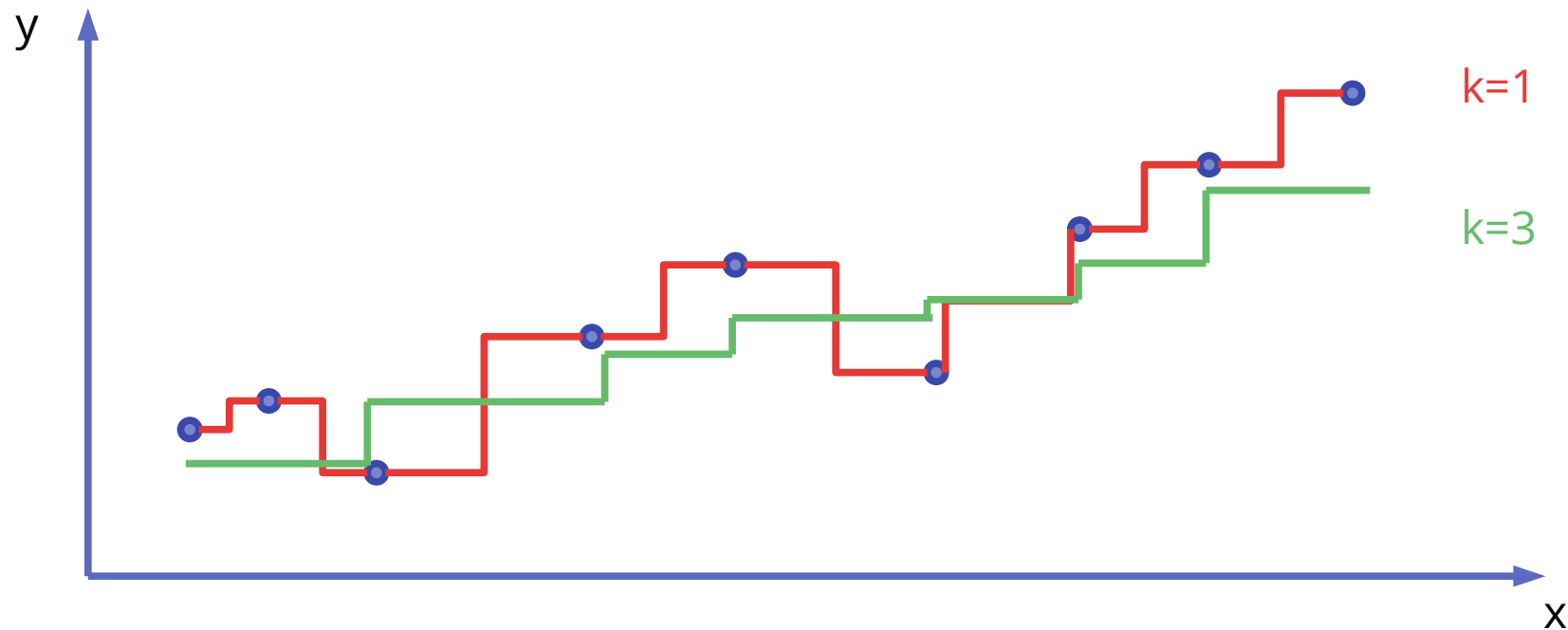
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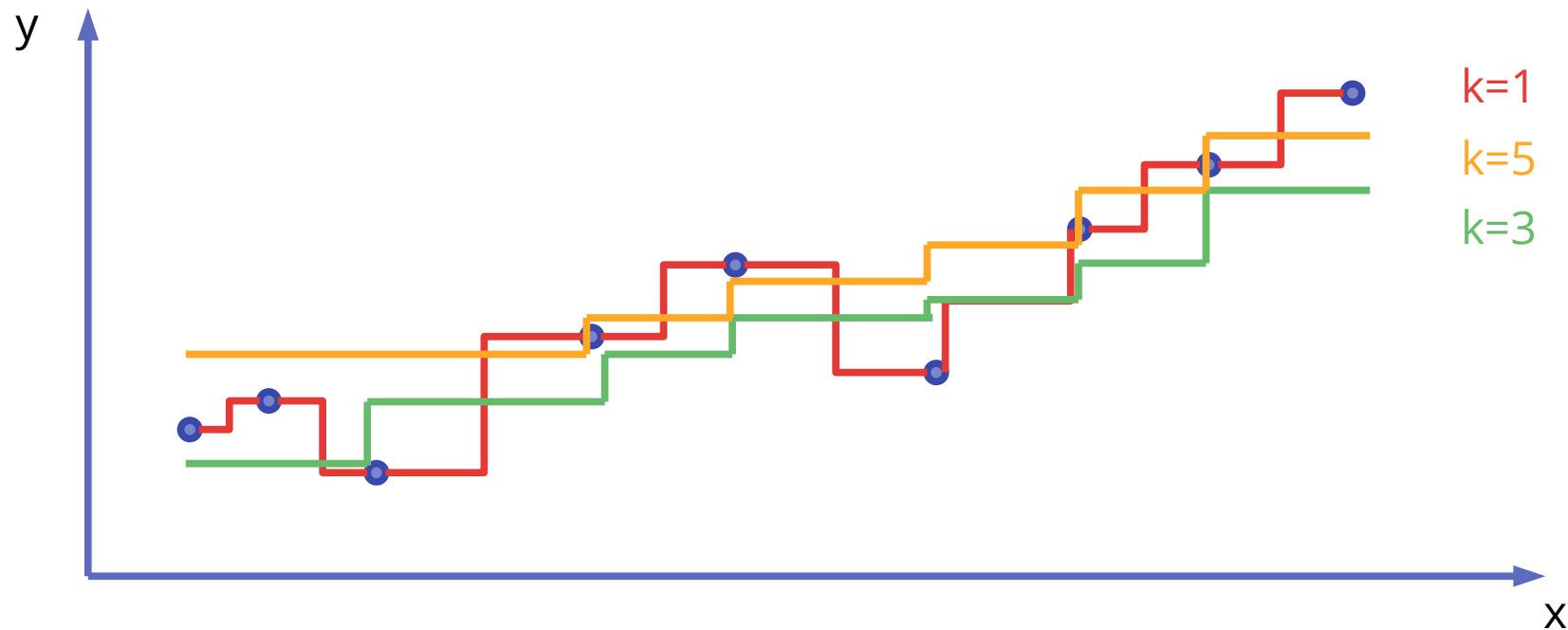
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That's all folks!