

# **Lecture 2: Supervised Learning Concepts**

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

# Today's lecture

Supervised learning setup

Supervised learning concepts

Benchmarking and metrics

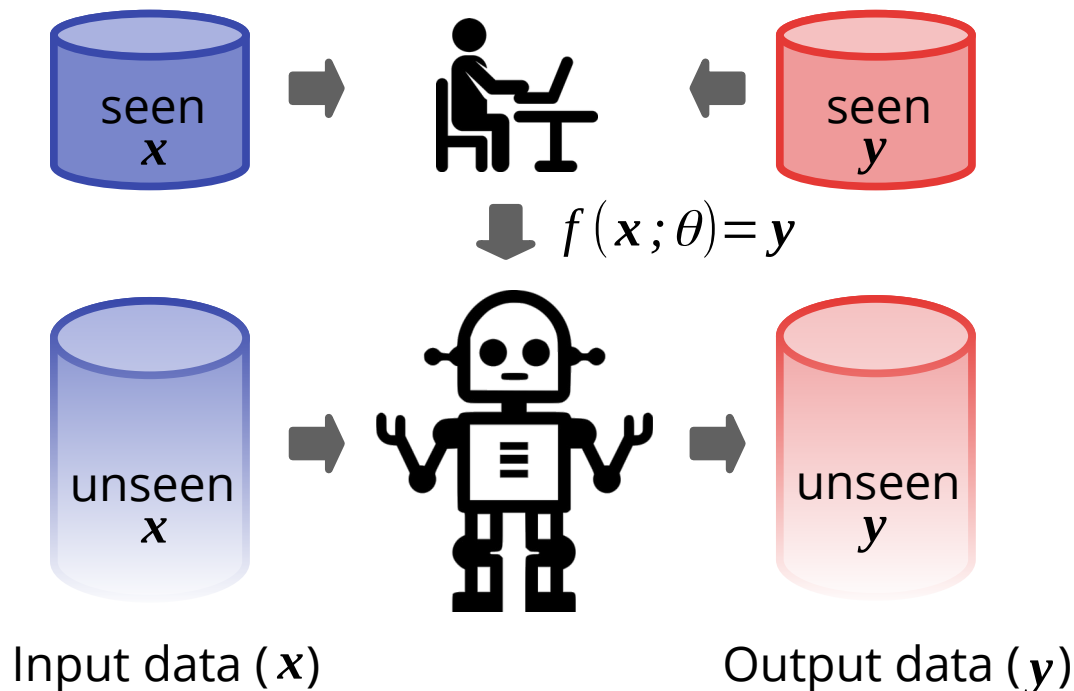
# Supervised Learning setup

## General goal for supervised problems:

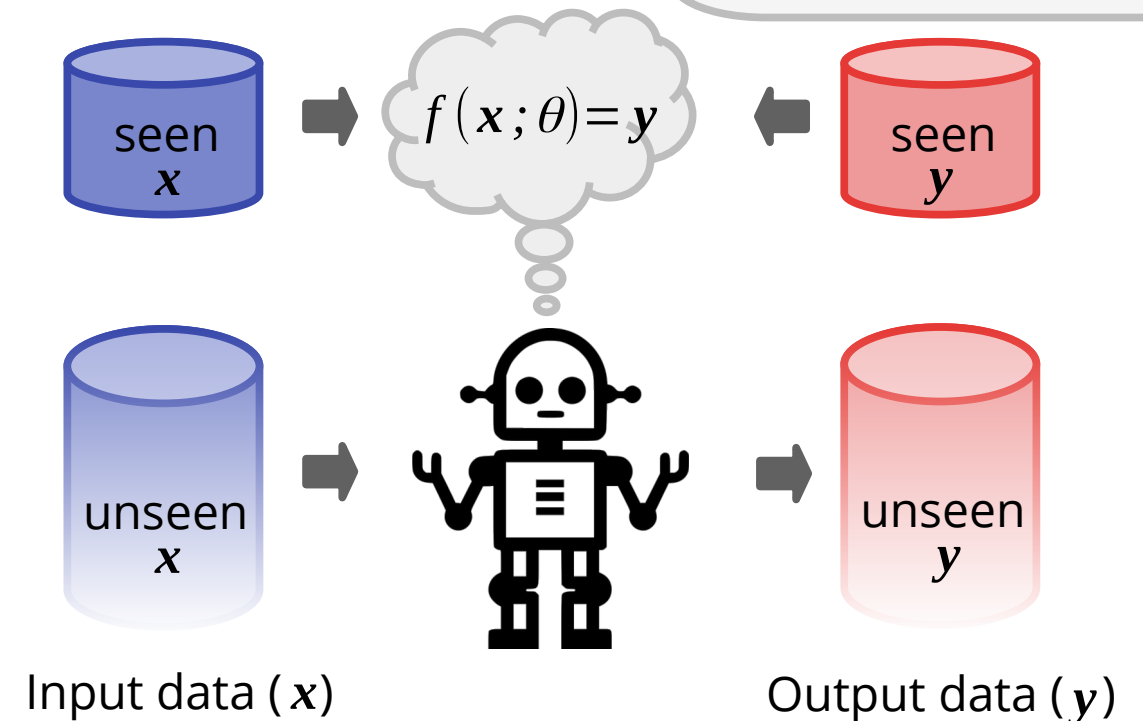
Find a function ("task") that relates input data ( $x$ ) to output data ( $y$ ) with hyperparameters ( $\theta$ )

such that:  $f(x; \theta) = y$

## Traditional (Rule-based) Approach:



## Machine-Learning Approach:



# What tasks can ML learn?

## (Multi-class) Classification:

Mapping input features to discrete classes of a single label

*Example:*

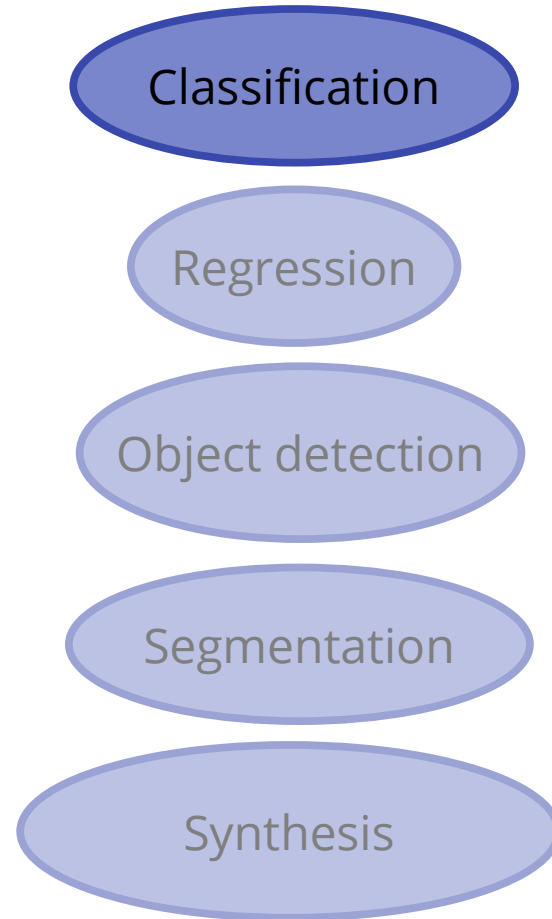
label	<b>Color</b>
classes {	red
	green
	blue

## Binary classification:

Mapping input features to a binary label

*Example:*

label	<b>Status</b>
two classes {	on
	off



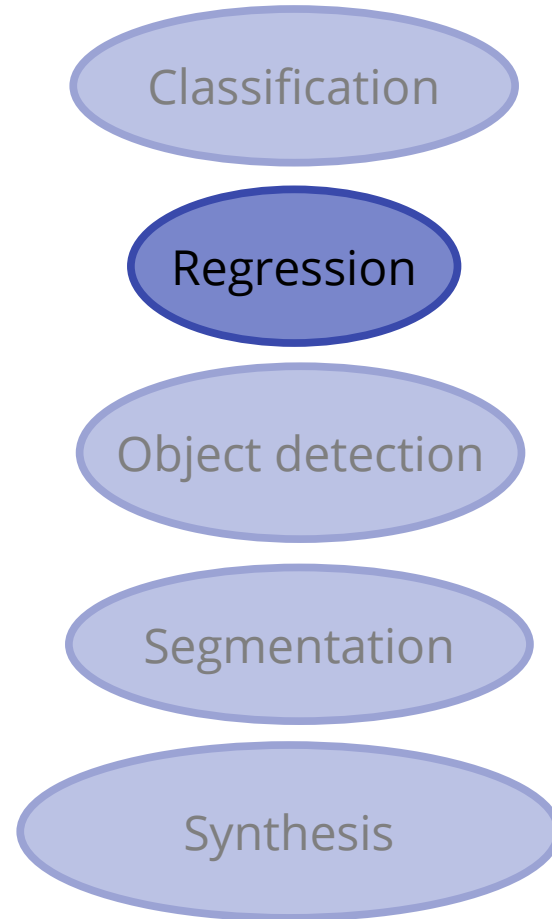
## Multi-label classification:

Mapping input features to discrete classes of multiple labels

*Example:*

labels	<b>Color</b>	<b>Sort</b>	<b>Quality</b>
classes {	red	A	good
	green	B	medium
	blue	C	bad
	...	...	...

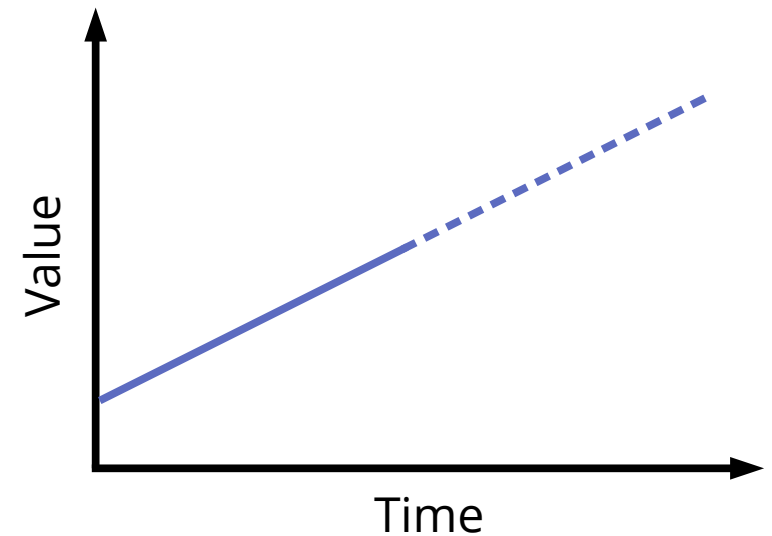
# What tasks can ML learn?



## Regression:

Mapping input features to continuous variable

*Example:*



# What tasks can ML learn?

## Object detection:

Approximately localize features in image data with bounding boxes

*Example:*



Classification

Regression

Object detection

Segmentation

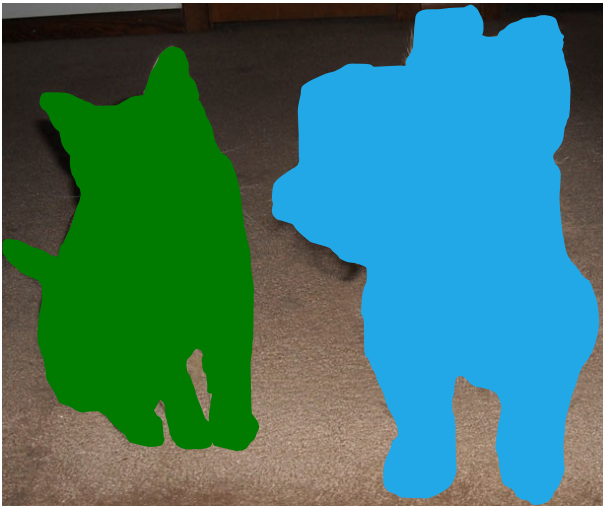
Synthesis

# What tasks can ML learn?

## Semantic segmentation:

Assign class label to each pixel of an image based on what it is showing

*Example:*



Classification

Regression

Object detection

Segmentation

Synthesis

## Instance segmentation:

Assign class label to each pixel of an image based on what it is showing and discriminate different instances of the class

*Example:*





# What tasks can ML learn?

## Synthesis:

Generate new data points based on a learned distribution



StyleGAN2 (Karras et al. 2020)

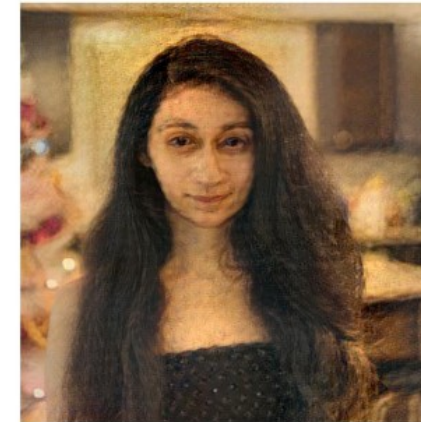
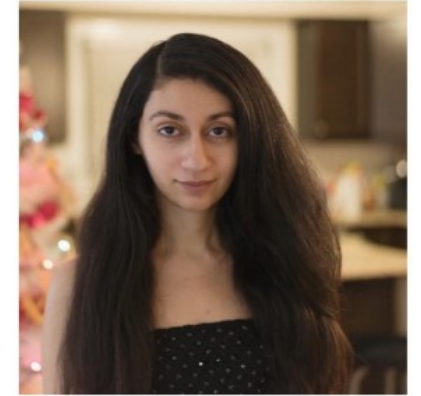
Classification

Regression

Object detection

Segmentation

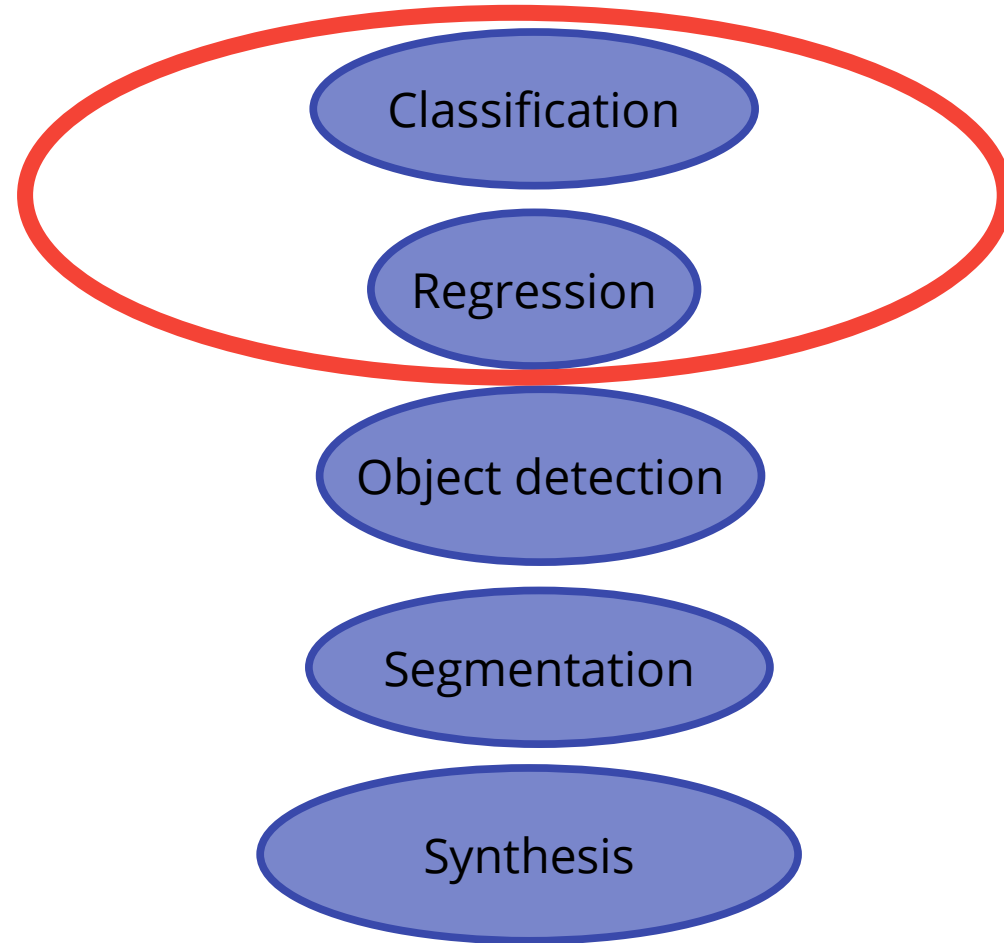
Synthesis



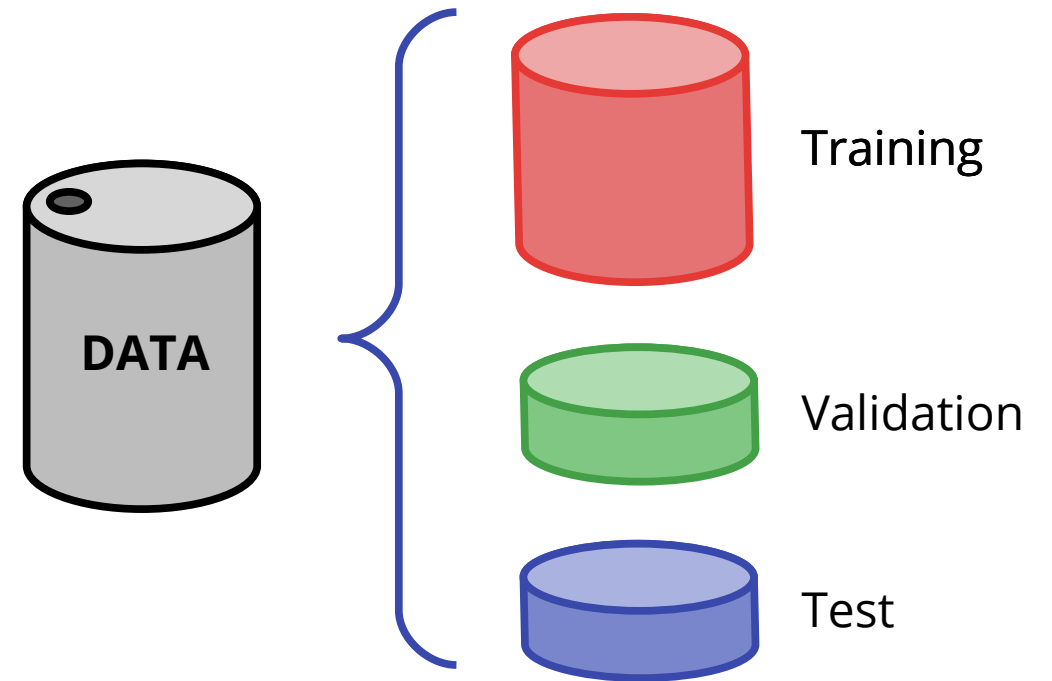
Style Transfer (Gatys et al. 2016)



# What tasks can ML learn?



## Supervised learning concepts

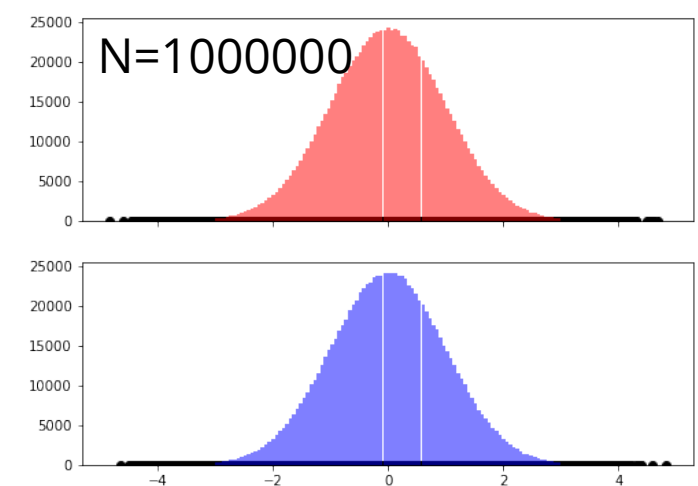
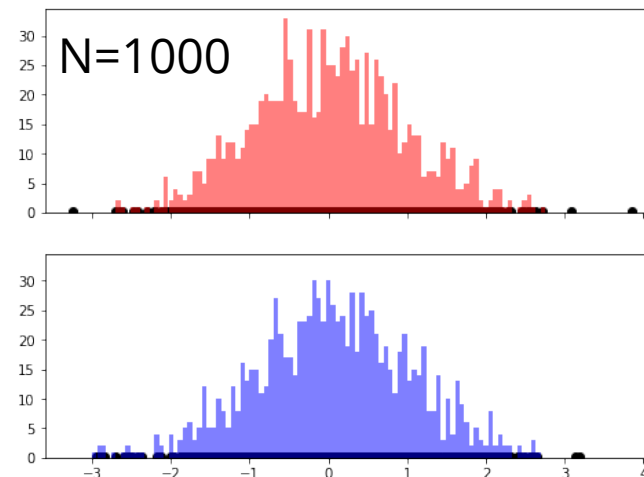
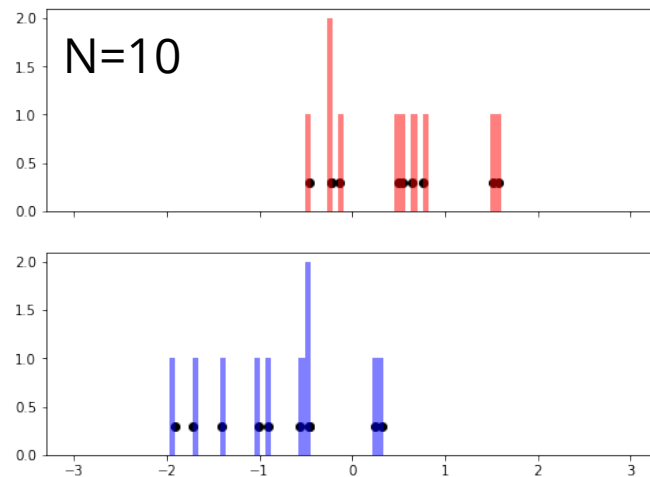


# Independent and identically distributed (iid) data

**iid** is a core concept of ML. When running an ML model on previously unseen data, we implicitly assume that the unseen (new) data and the already seen (training) data are **iid**, i.e., the individual samples in both data sets are *produced by the same data generation process*.

This does not imply that the seen and unseen data sets are identical!

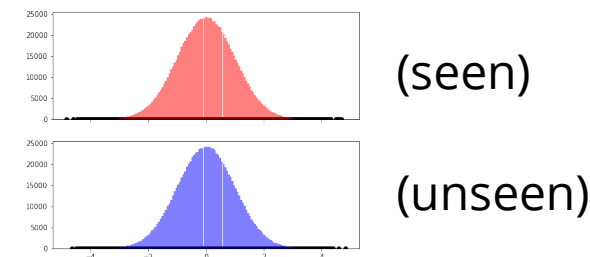
*Example:* sampling from a Normal distribution



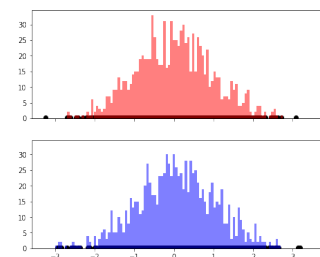
Lesson here: For small sample sizes, data sets that are iid may still differ significantly.

ML models are trained on existing data sets (seen data) and will be evaluated/applied to a new, previously unseen data set. Since **real data sets have a limited extent** (size), these distributions will look different, despite their iid nature.

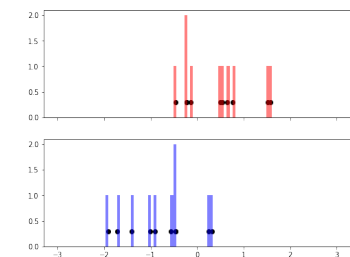
Ideally, the two distributions should be very similar:



But in real life, they tend to look more like this



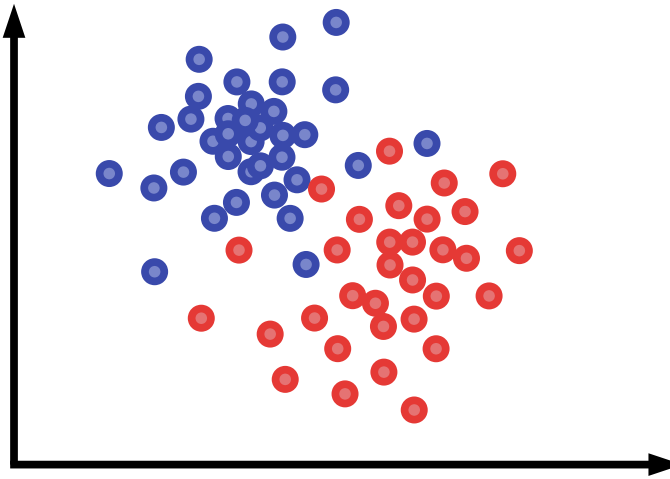
or even this



Successful training on one data set does not imply good performance on unseen data  
 → the model has to **generalize** well by preventing **overfitting**

# Generalization, regularization, overfitting and underfitting

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

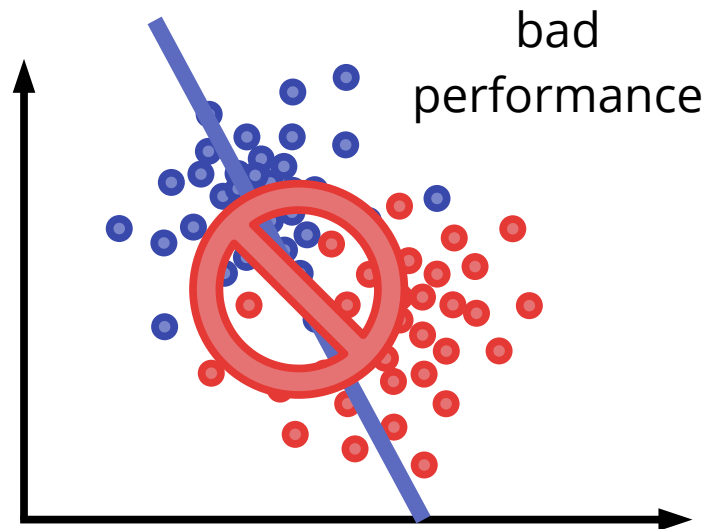


What would be a good decision boundary between the two classes?

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

# Generalization, regularization, overfitting and underfitting

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

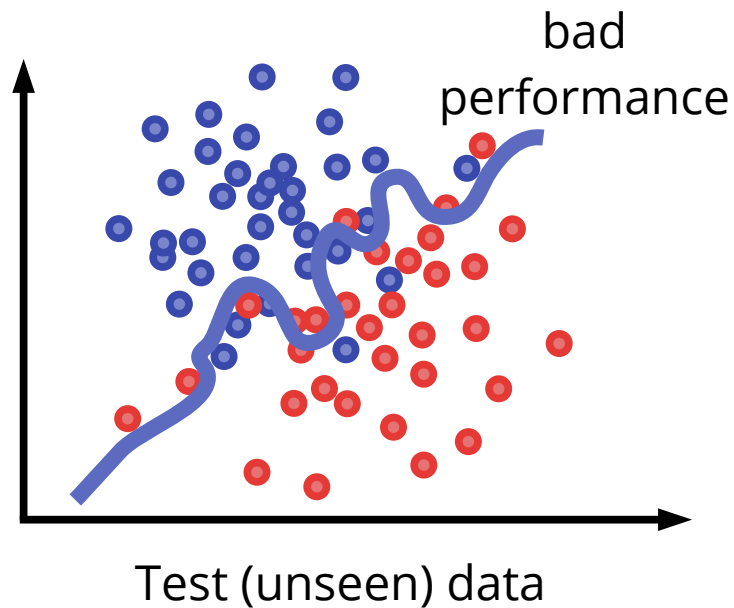


This would not be a good decision boundary as it barely allows to distinguish the two classes.

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

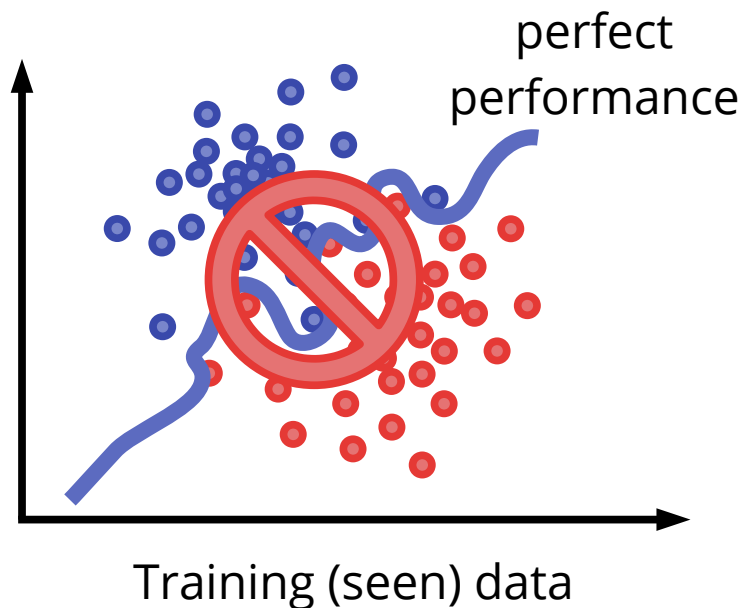
# Generalization, regularization, overfitting and underfitting

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



This model is **overfitting**: it memorizes the structure of the training (seen) data and as a result **generalizes badly** on the overall data distribution.

We can improve its performance through **regularization** methods.



This decision boundary perfectly delineates the two classes in our data set.

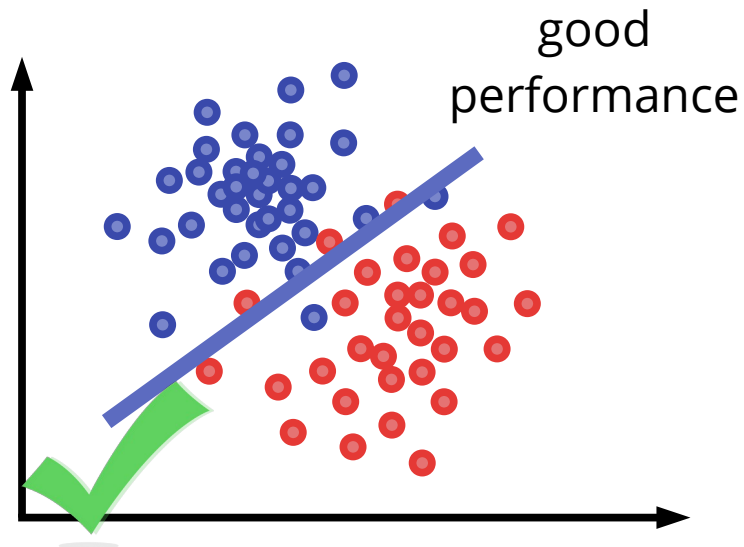
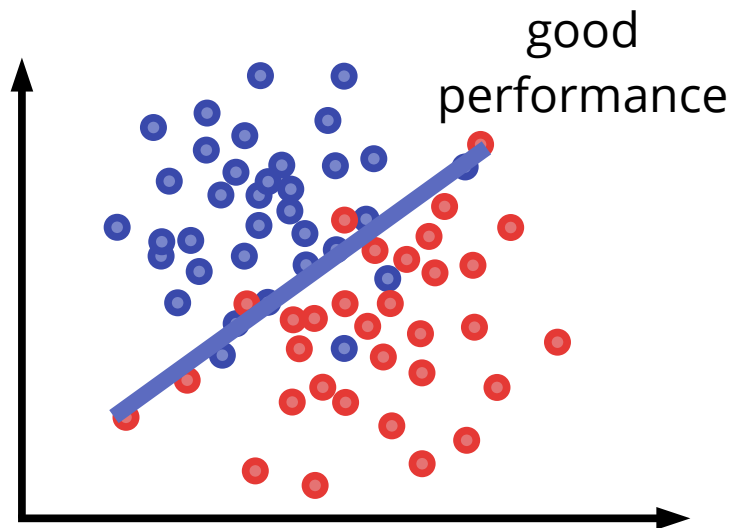
Is this good?

**No**, see what happens if we apply the model to previously unseen data: while it seems to perform perfectly on the seen data, it performs much worse on the unseen data.



# Generalization, regularization, overfitting and underfitting

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



This decision boundary leads to **equally good performance on both data sets**.

The model therefore **generalizes well** on previously unseen data.

This is the desired situation as it provides a realistic view on the expected performance of your model.

How can we check how well the model generalizes?

How can we force the model to generalize?

# Performance metrics

In order to measure how well our model generalizes, we have to define a **performance metric**. A performance metric provides a quantitative assessment of how well our model performs based on:

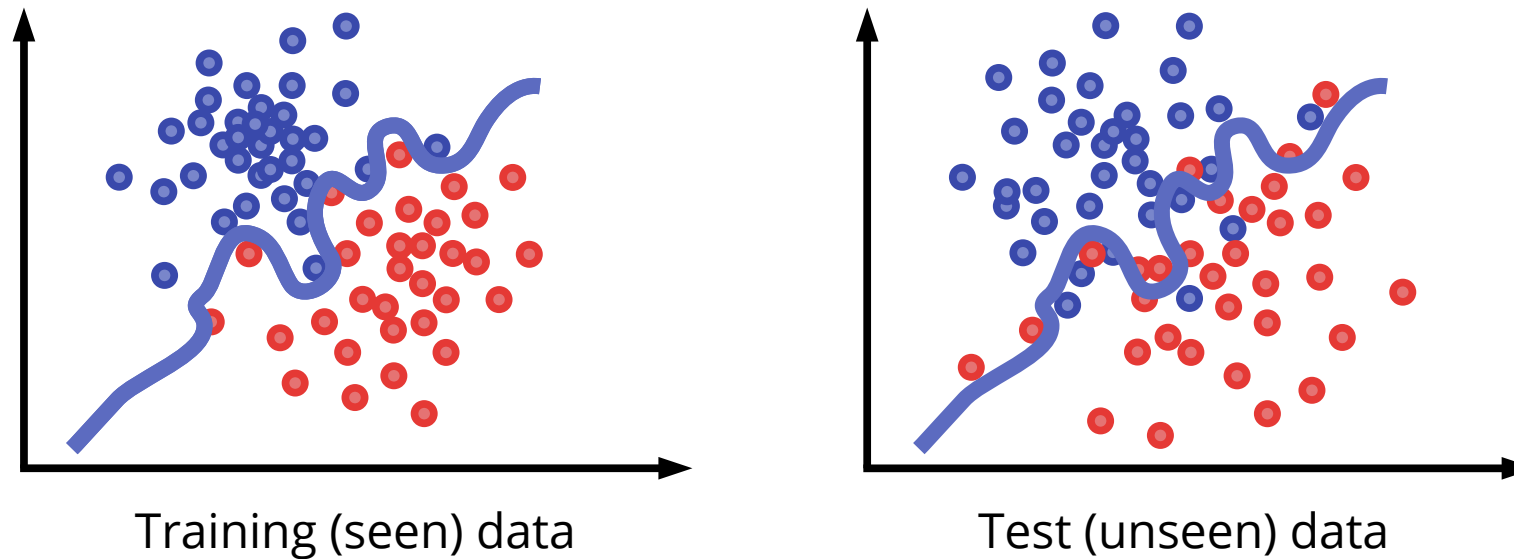
- the machine learning implementation (model type and loss function),
- the dataset,
- the task to be learned.

Performance metrics have to be tailored to the method and task. We will discuss them in detail in the final part of this lecture (Benchmarking and metrics).

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

# Identifying overfitting

Overfitting occurs if the model memorizes patterns specific to the training data instead of learning the general patterns of the overall dataset.



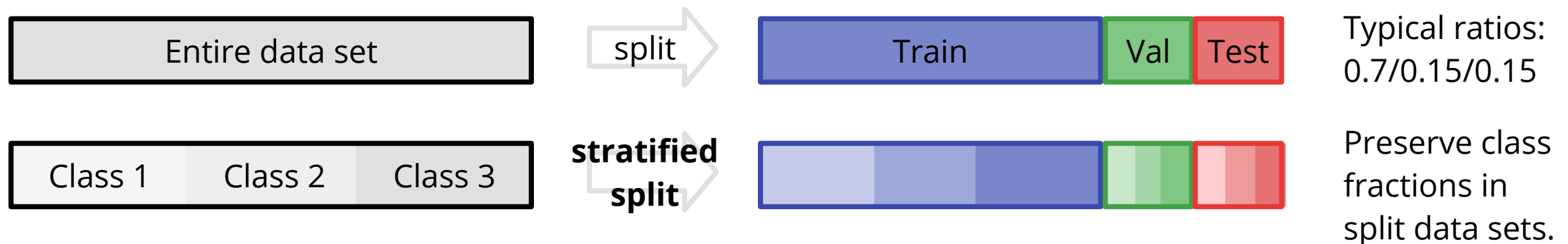
We can identify overfitting by comparing the performance on the seen (training) data and some previously unseen (test) data. But where do we get unseen data from?

# Train/Validation/Test splits

How can we check how well the model generalizes? We synthesize our own unseen data set.

In supervised learning, an existing data set is typically randomly split into three parts:

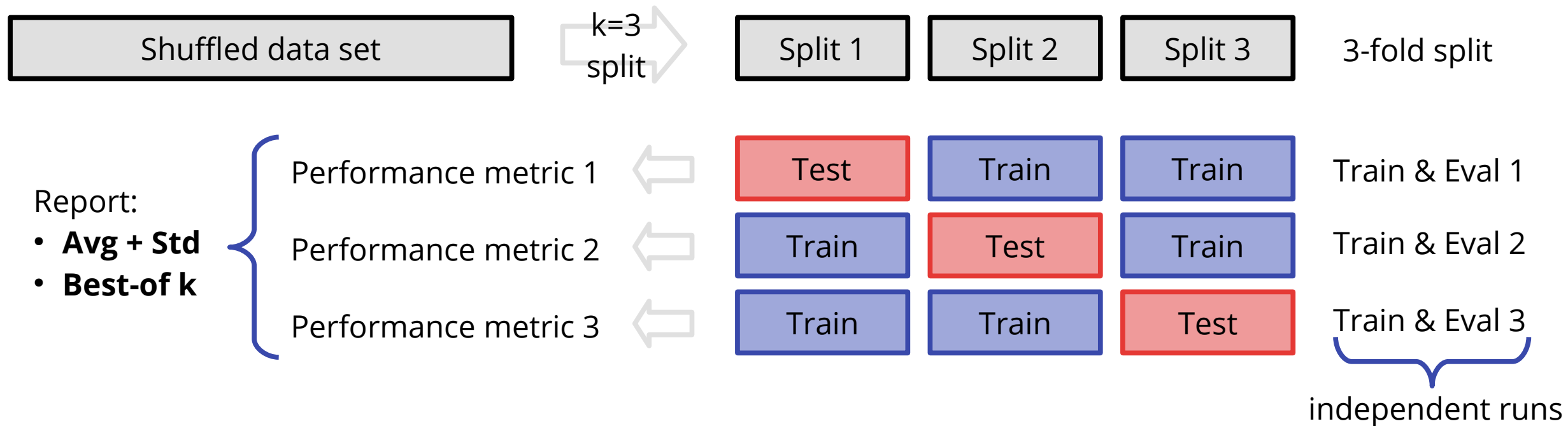
- **Training** data set – the model is trained exclusively on this data set
- **Validation** data set – this data set is used to tune our model's hyperparameter
- **Test** data set – this data set is used to evaluate the model's performance on unseen data



# k-fold cross-validation

Often times the data set available to you is not large enough to perform a meaningful split.

You can “recycle” your data by using cross-validation to get a better estimate of your model performance.



Note: Keep in mind that cross-validation will not improve your model performance; it will simply give you a more reliable estimate of its performance.

# How can we force the model to generalize?

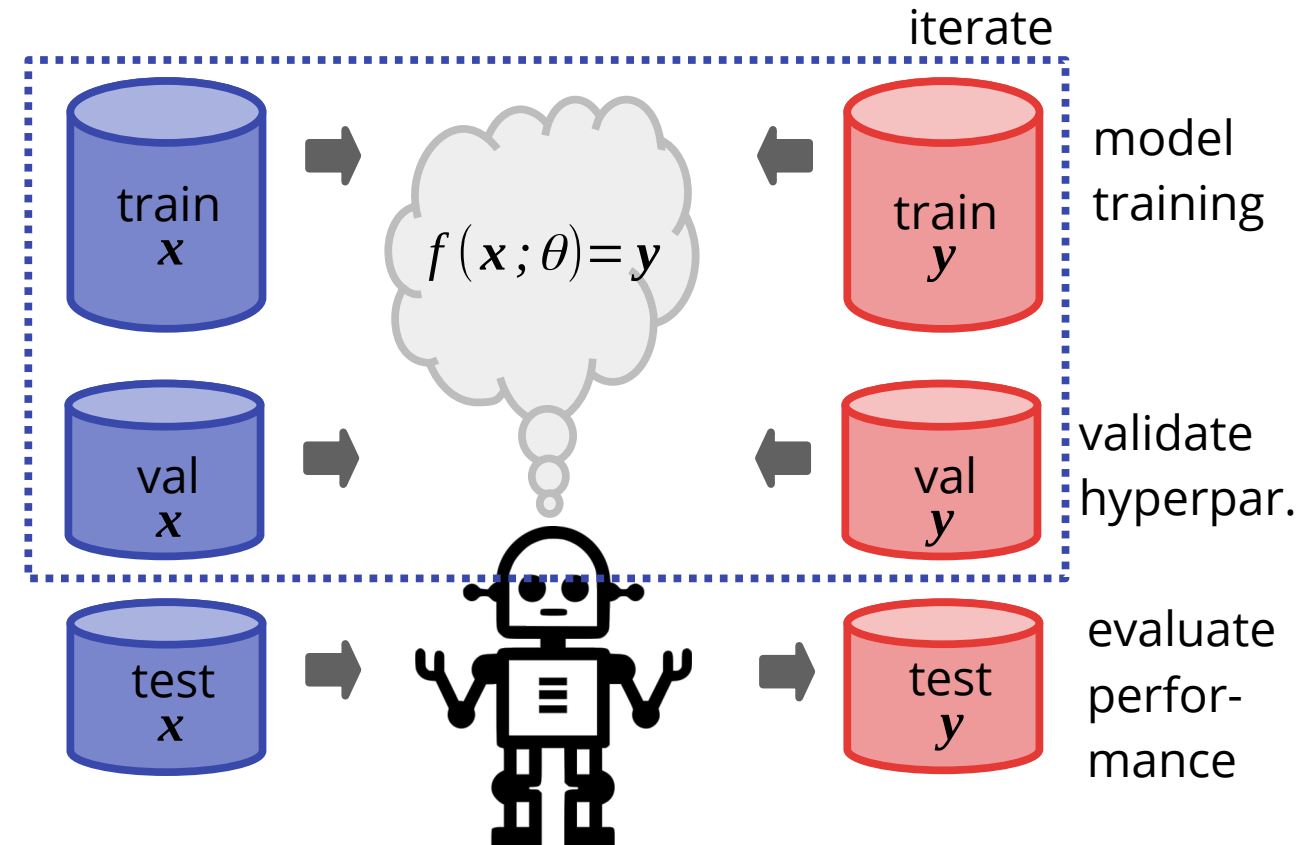
Machine learning relies on **regularization methods** to prevent overfitting. These methods are specific to the model type that is being used and will be discussed in detail with the individual methods in the next lectures.

However, there are some common themes among regularization methods:

- **Limiting model capacity:** achieving regularization by “dumbing down” a model in general (all models)
- **Introducing uncertainty:** systematic penalizing the impact of data on the training process (all models)
- **Dropout:** stochastically ignoring parts of the model to make it more resilient (neural networks)
- **Introducing noise:** adding stochastic noise to the data (all models)
- **Early stopping:** stopping the learning process when learning effects are small (neural networks)
- **Bagging/Ensembling:** training multiple models on the same data, combining their results (all models)

# General supervised learning pipeline

- 1) Feature engineering: raw data → features
- 2) Data scaling
- 3) Data splitting → training, validation, test data
- 4) Define hyperparameters
- 5) Train model on training data for fixed hyperparameters
- 6) Evaluate model on validation data
- 7) Repeat 4) to 6) until performance on validation data maximized
- 8) Evaluate trained model on test data → report test data performance





# **Benchmarking and metrics**



# How do we measure the performance of our model?

**Benchmarking** refers to the process of quantitatively assessing your ML model's performance.

Performance is measured based on pre-defined metrics; a **metric** can be thought of as a measure for how well an ML model performs on a specific task and data set.

*Examples:*

	Which athlete is best?	Which company is successful?	Medical diagnosis
	Based on...	Contributing factors:	What is most important?
metrics	<ul style="list-style-type: none"><li>• speed</li><li>• strength</li><li>• number of victories</li><li>• income</li></ul>	<ul style="list-style-type: none"><li>• revenue</li><li>• overall value</li><li>• number of employees</li><li>• annual CO2 emissions</li></ul>	<ul style="list-style-type: none"><li>• correctness of diagnosis</li><li>• minimizing failures</li><li>• patient's comfort</li><li>• cost</li></ul>

# Regression

## Regression task metrics:

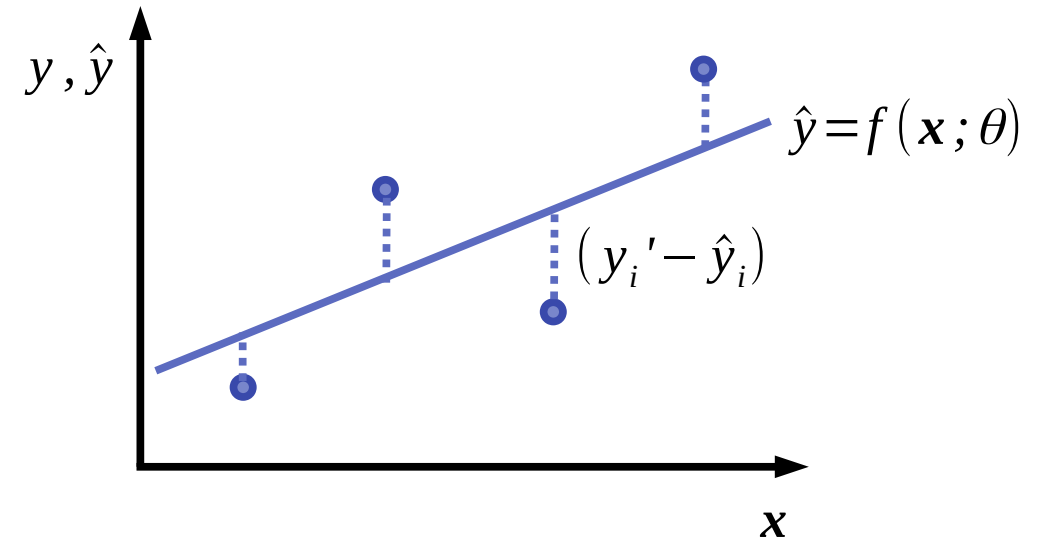
### MAE (Mean Absolute Error)

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

### RMSE (Root Mean Square Error)

$$RMSE = \sqrt{\frac{1}{N} \sum_i^N (y_i' - \hat{y}_i)^2}$$

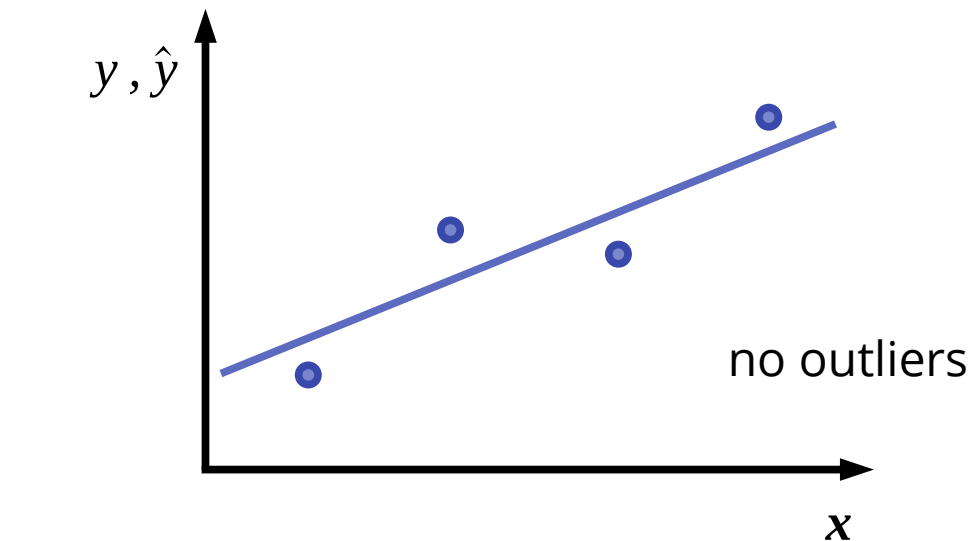
Input data:  $\mathbf{x}_i, i \in \{1 \dots N\}$   
Target ground-truth:  $y_i'$   
Target prediction:  $\hat{y}_i = f(\mathbf{x}_i; \theta)$



Intuition: by how much deviates your model prediction from the ground-truth on average.

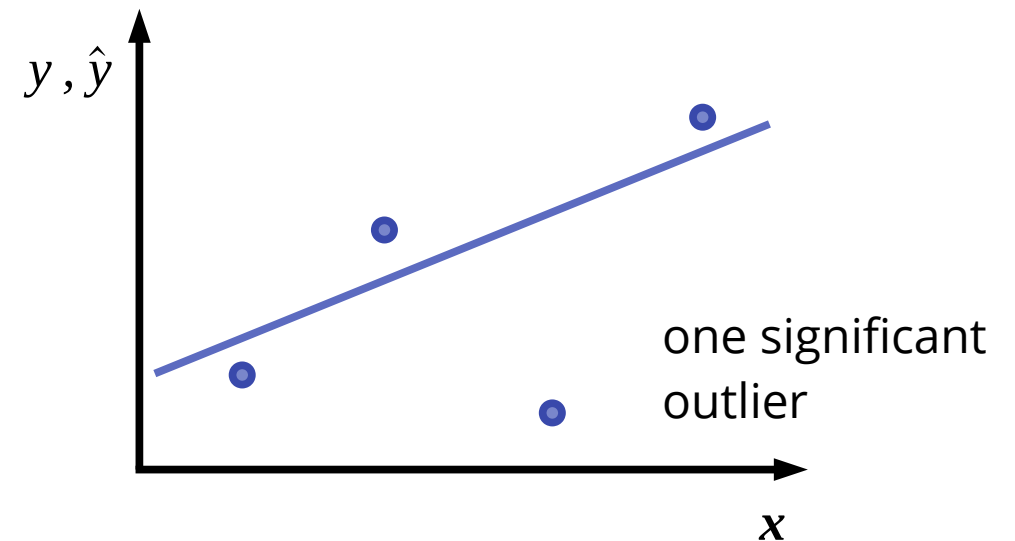
# Comparing regression task metrics

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



$(y_i' - \hat{y}_i):$     -1        1        -1        1

→ MAE = 1; RMSE = 1



$(y_i' - \hat{y}_i):$     -1        1        -10        1

→ **MAE = 3.25; RMSE = 5.07**

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

# Classification

## (Binary) Classification metrics:

**Accuracy** =  $(TP + TN) / (TN + TP + FP + FN)$

*What is the overall fraction of correct (positive and negative) predictions?*

**Precision** =  $TP / (TP + FP)$  (quantifies “correctness”)

*What fraction of our positive predictions is truly positive?*

**Recall** =  $TP / (TP + FN)$  (quantifies “completeness”)

*What fraction of actual positives has been identified?*

Prediction	positive	True positive	False positive
	negative	False negative	True negative
		positive	negative
		Ground-Truth	

# Classification

## (Binary) Classification metrics:

**Accuracy** =  $(TP + TN) / (TN + TP + FP + FN)$

*What is the overall fraction of correct (positive and negative) predictions?*

**Precision** =  $TP / (TP + FP)$  (quantifies “correctness”)

*What fraction of our positive predictions is truly positive?*

**Recall** =  $TP / (TP + FN)$  (quantifies “completeness”)

*What fraction of actual positives has been identified?*

*Example: Is there a dog in the image?*

accuracy = 0.95:

*we correctly identified 95% of all dogs in the images*

precision = 0.95:

*95% of the dogs we predicted are actual dogs*

recall = 0.95:

*we correctly found 95% of the dogs that are in the images*

# Classification

## (Binary) Classification metrics:

**Accuracy** =  $(TP + TN) / (TN + TP + FP + FN)$

Requires somewhat balanced classes

**Precision** =  $TP / (TP + FP)$  (quantifies “correctness”)

Less susceptible to imbalance.

**Recall** =  $TP / (TP + FN)$  (quantifies “completeness”)

Less susceptible to imbalance.

**Class imbalance** is a real issue!

*Example:* Will this asteroid impact Earth?

If our model always predicts *False*, we can easily reach 99.9% accuracy, although the model does nothing useful.

Low precision means that we issue some false alarms – this is something we can deal with.

Low recall means that we miss some asteroids that are about to impact.  
**Recall** is the really important metric here and should be **maximized**.



# Confusion matrix

A common way to visualize the performance of a classification model is to use a confusion matrix:

ground truth	A	0.8	0.2	0.0
	B	0.1	0.9	0.0
	C	0.0	0.3	0.7
		A	B	C
		prediction		

- The confusion matrix provides information on systematic confusion learned by the classifier.
- For a well-trained classifier, the matrix diagonal should have high values; off-diagonal elements should be as low as possible.
- All elements in one row must sum up to unity.
- *How to read the confusion matrix:* 30% of samples from class C were mistaken as samples from class B.

# Object detection/image segmentation



Object detection

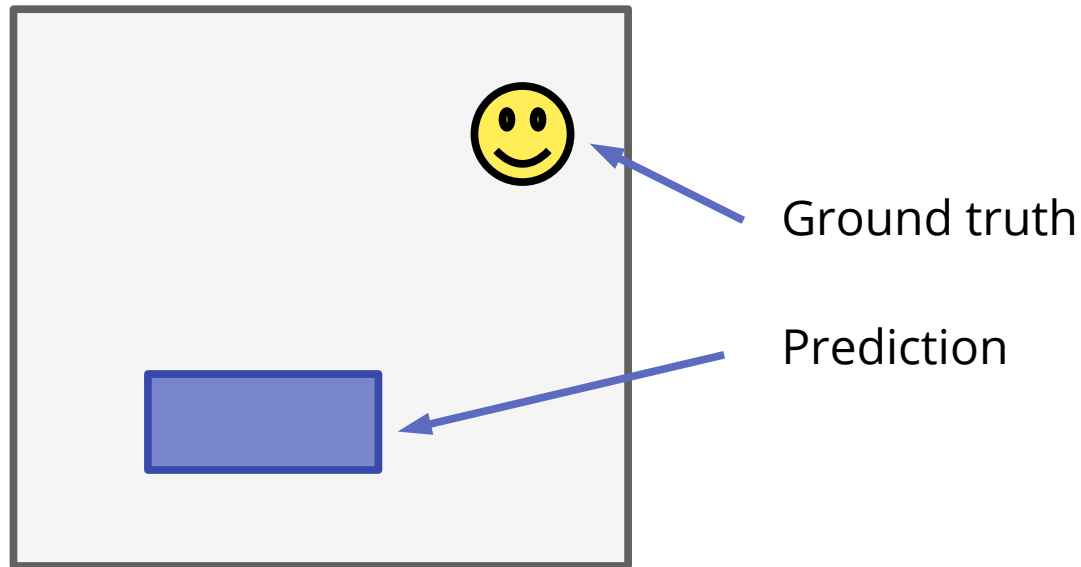


Image segmentation

Would accuracy be a good metric to measure the success of either task?

# Object detection/image segmentation

Using accuracy as a metric:



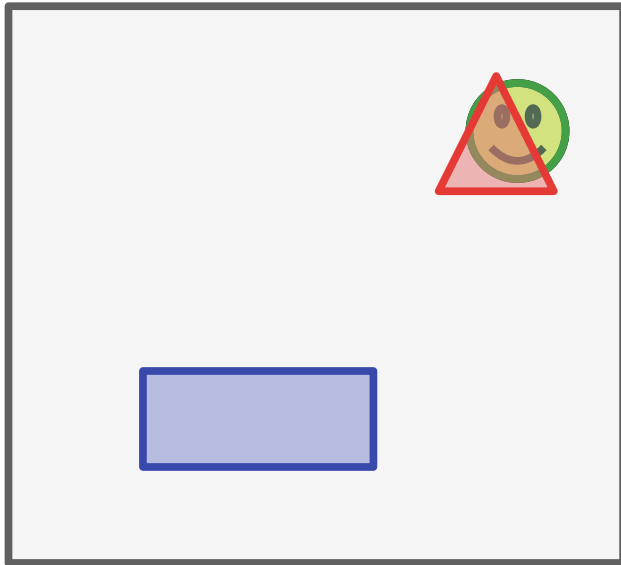
This is obviously a poor prediction.

Nevertheless, ~90% of all pixels in the image have correct predictions ("no smiley").

As a result, the pixel-wise accuracy for this prediction would be ~90%.

Accuracy is a bad metric for object detection and image segmentation tasks.

# Object detection/image segmentation



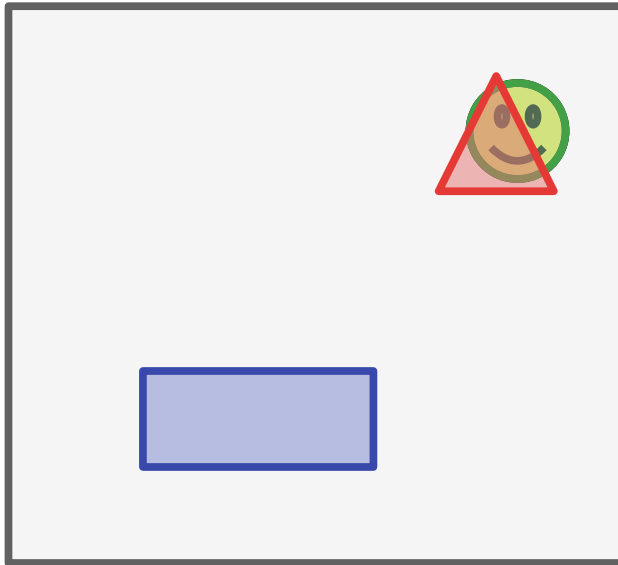
The blue box is a poor prediction and should result in a score of zero.

The green circle is an excellent prediction and should result in a score of one.

The red triangle is a mediocre prediction and should result in a score of 0.5.

Can we define a metric that formulates this schema as an equation?

# Intersection over union metric



$$\text{IoU} = \frac{\text{Intersection}}{\text{Union}} = \frac{A \cap B}{A \cup B}$$

Green circle: intersection = union  $\rightarrow \text{IoU} = 1$

Red triangle: intersection  $\sim 0.5$  \* union  $\rightarrow \text{IoU} \sim 0.5$

Blue box: intersection = 0  $\rightarrow \text{IoU} = 0$

IoU is highly flexible with respect to shape. However, it is undefined if there is a prediction where there is no ground truth. Nevertheless, it is a good metric for object detection and image segmentation.

# How to report metrics?

There are different ways to report metrics:

- **Individual metric:** the metric based on a single model and dataset
- **Best-of- $n$ :** the best result out of  $n$  different model runs (e.g., trained with different seeds or different datasets → cross-validation)
- **Averaging results:** the average metric over  $n$  model runs (e.g., trained with different seeds or different datasets → cross-validation)  
+ standard deviation

 $\alpha$  $\alpha_0 \quad \alpha_1 \quad \alpha_2 \quad \alpha_3$ 

$$\alpha = \sum \alpha_i$$

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

**That's all folks!**