Lecture 2: Supervised Learning Concepts

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

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

Today's lecture

Supervised learning setup

Supervised learning concepts

Benchmarking and metrics

Supervised Learning setup

Supervised Learning setup

General goal for supervised problems:
Find a function ("task") that relates input data ($\boldsymbol{x}$) to output data ($\boldsymbol{y}$) with hyperparameters (θ)
such that: $f(\boldsymbol{x};\theta)=\boldsymbol{y}$

A **hyperparameter** is a model parameter that the model not learns.

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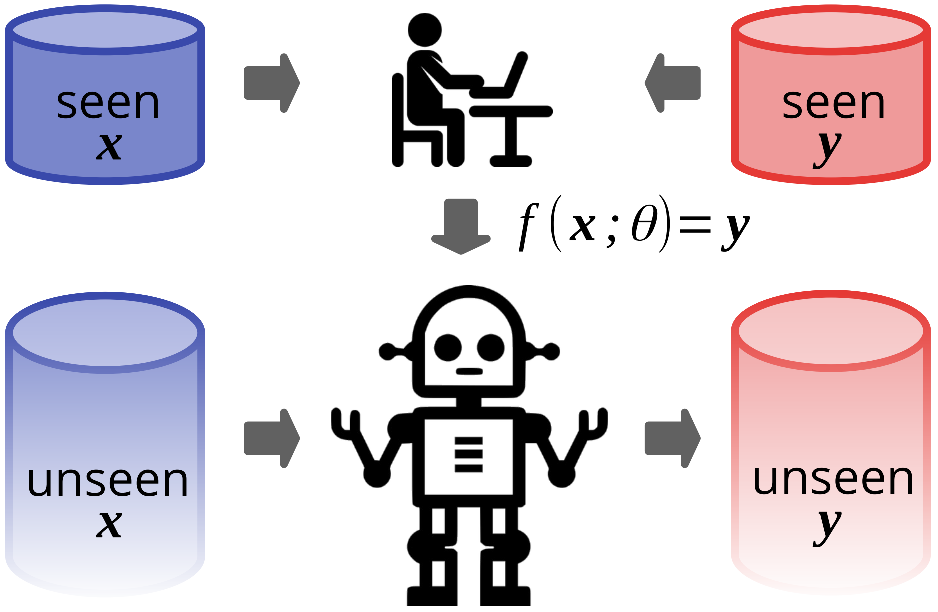
Traditional (Rule-based) Approach:



Input data ($\boldsymbol{x}$) Output data ($\boldsymbol{y}$)

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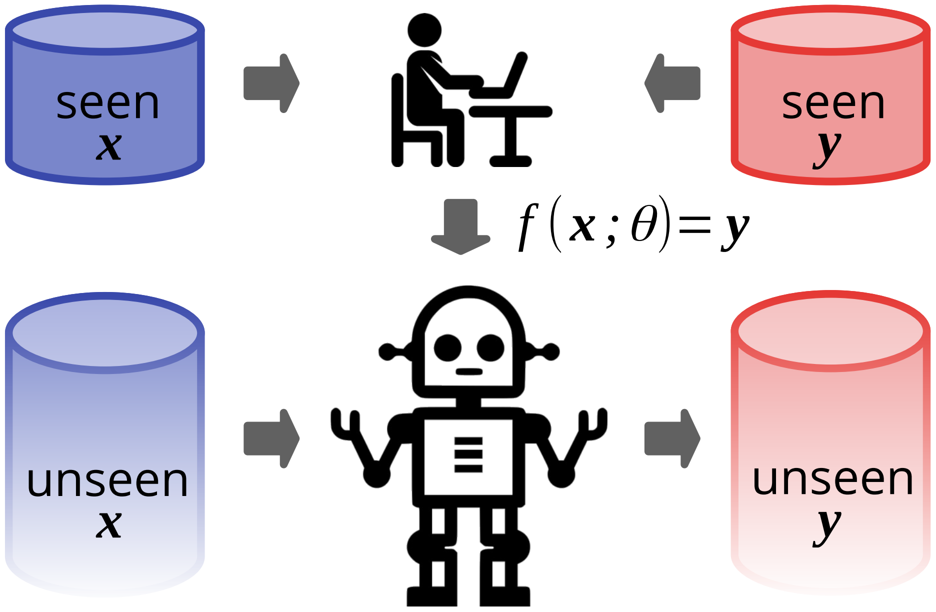
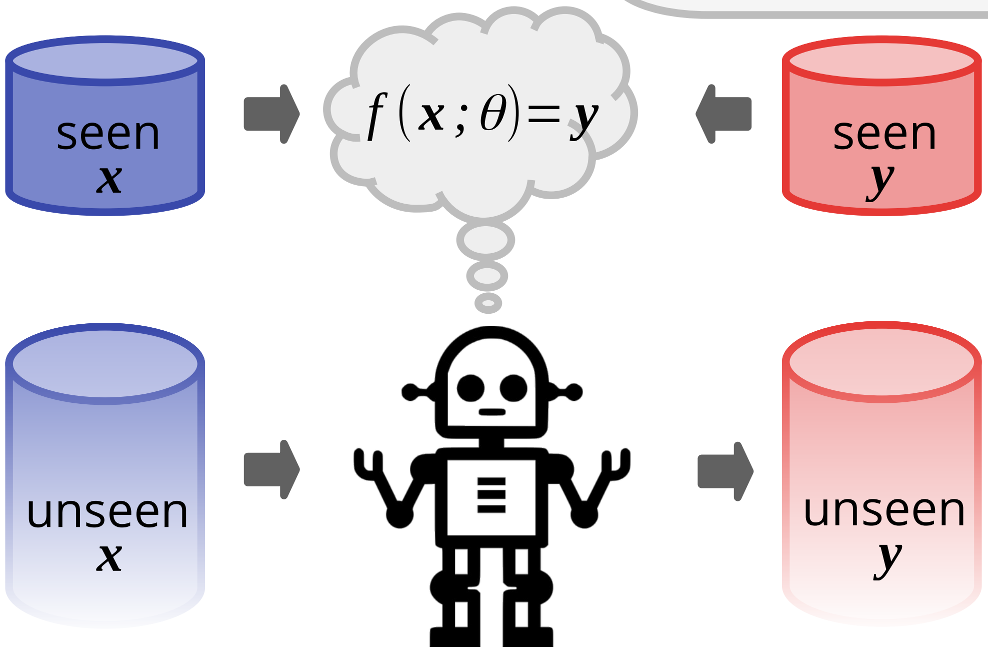


Input data ($\boldsymbol{x}$) Output data ($\boldsymbol{y}$)

Machine-Learning Approach:



Input data ($\boldsymbol{x}$) Output data ($\boldsymbol{y}$)

What tasks can ML learn?

- Classification
- Regression
- Object detection
- Segmentation
- Synthesis

What tasks can ML learn?

(Multi-class) Classification:
Mapping input features to discrete classes of a single label

Example:

label

Color
red
green
blue

classes

Classification

Regression

Object detection

Segmentation

Synthesis

What tasks can ML learn?

(Multi-class) Classification:
Mapping input features to discrete classes of a single label

Example:

label / classes

Color
red
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Binary classification:
Mapping input features to a binary label

Example:

label / two classes

Status
on
off

- **Classification**
- Regression
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What tasks can ML learn?

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label / two classes

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Classification

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Multi-label classification:
Mapping input features to discrete classes of multiple labels

Example:

labels / classes

Color	Sort	Quality
red	A	good
green	B	medium
blue	C	bad
…	…	…

What tasks can ML learn?

Classification

Regression

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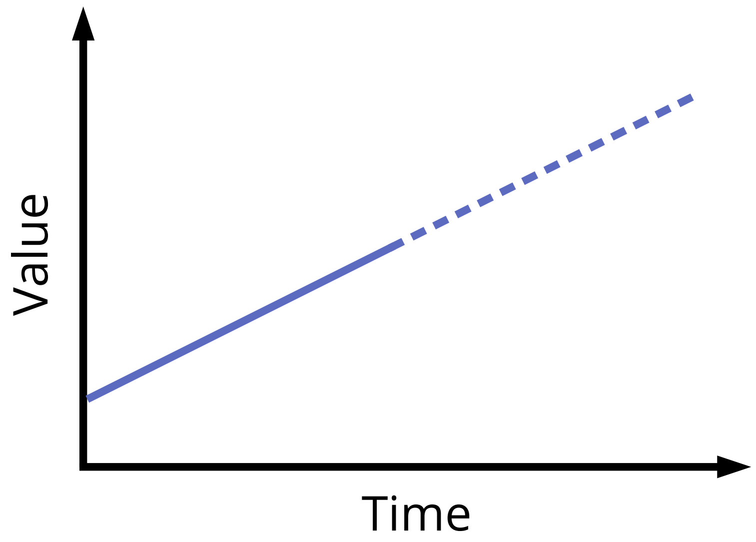
Regression:
Mapping input features to continuous variable

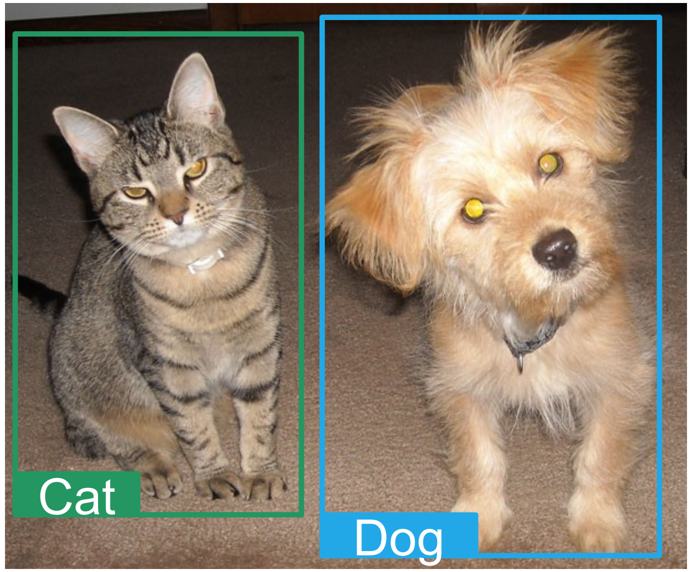
Example:

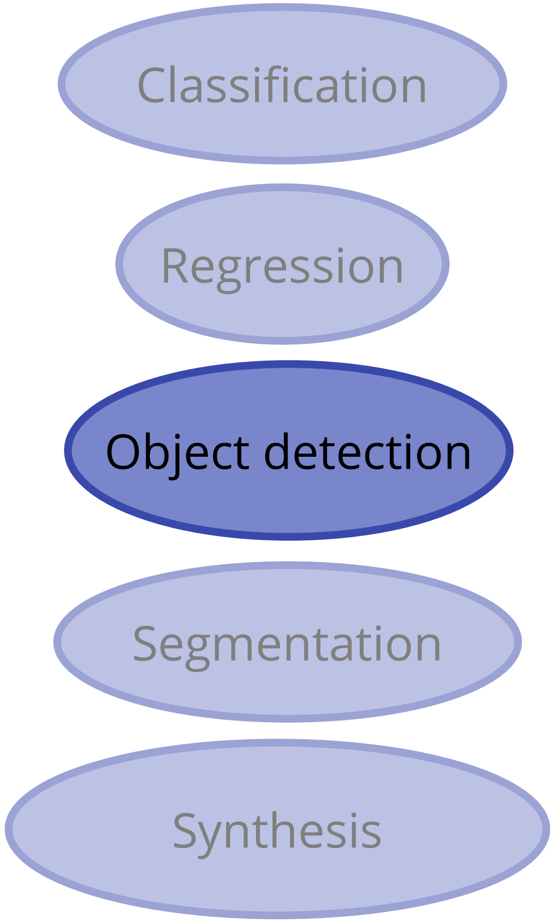


What tasks can ML learn?

Object detection:
Approximately localize features in image data with bounding boxes

Example:

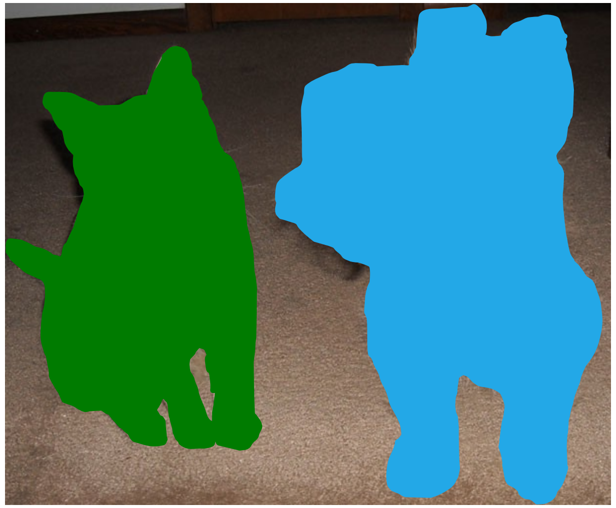




What tasks can ML learn?

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

Example:



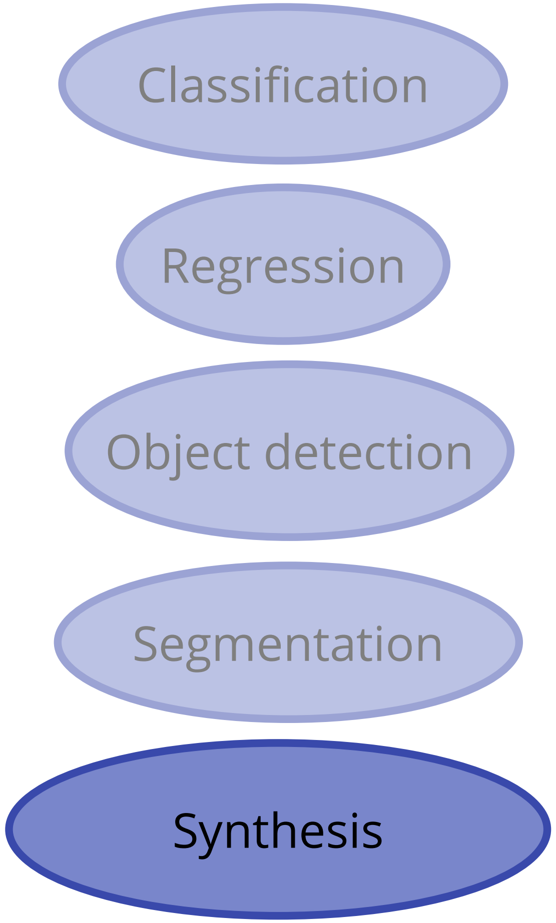
- Classification
- Regression
- Object detection
- **Segmentation**
- Synthesis

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



What tasks can ML learn?

Synthesis:
Generate new data points based on a learned distribution

- Classification
- Regression
- Object detection
- Segmentation
- **Synthesis**

Style Transfer (Gatys et al. 2016)

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?

Classification

Regression

Object detection

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What tasks can ML learn?

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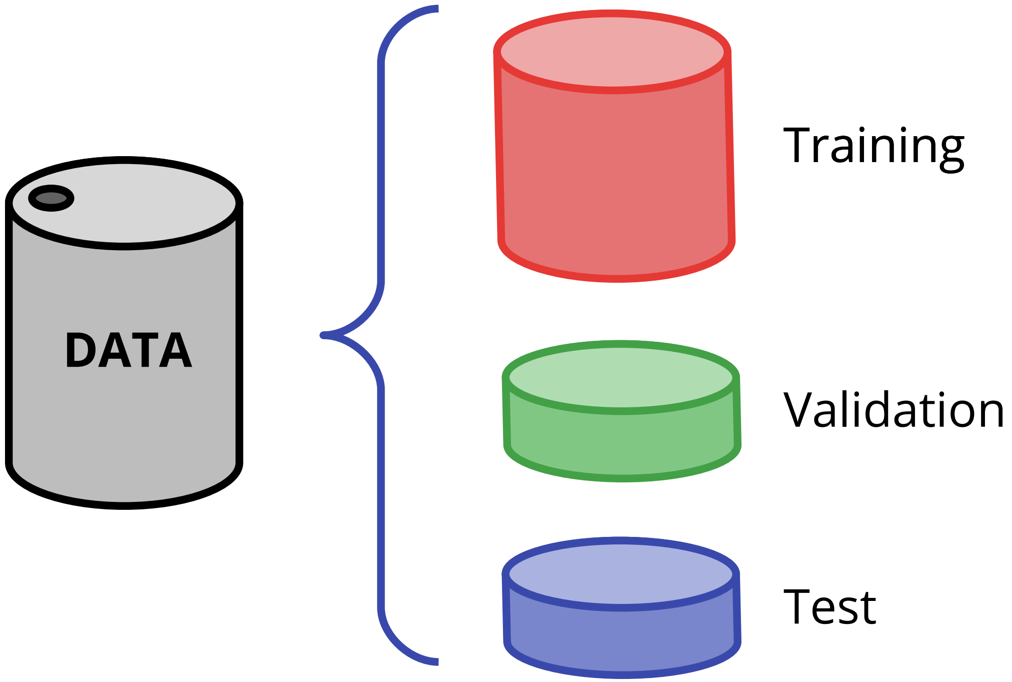
Supervised learning concepts



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 indiviual 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

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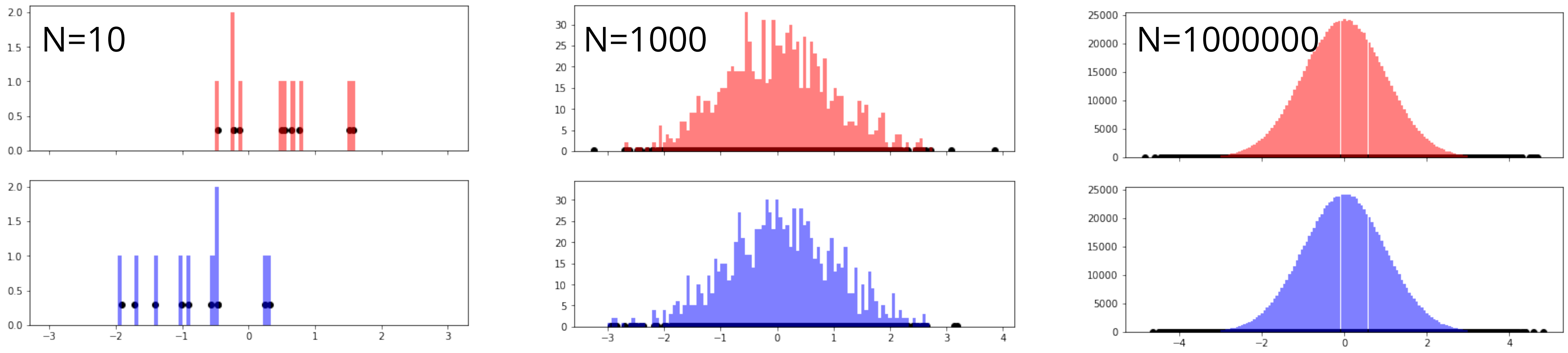

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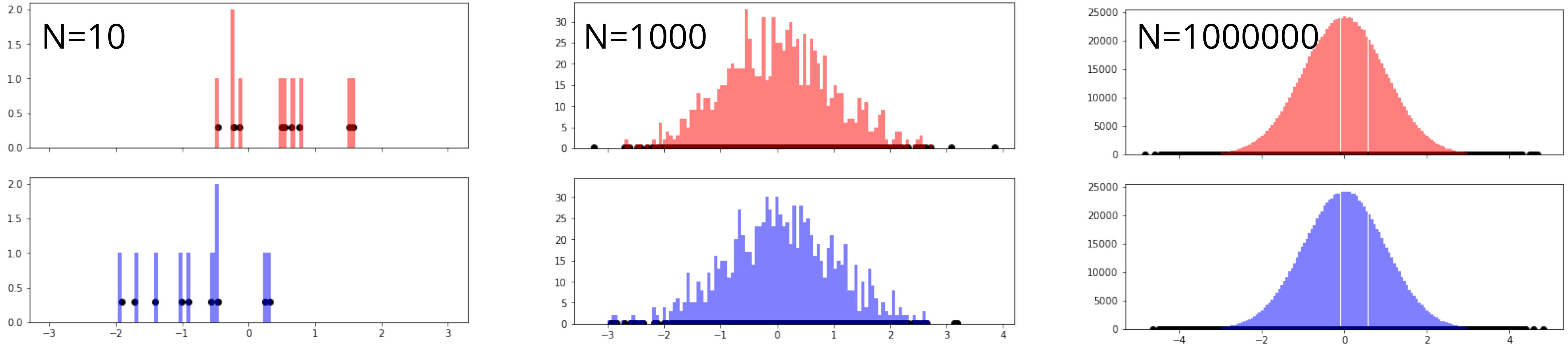
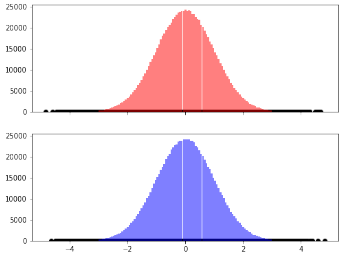


Lesson here: For small sample sizes, data sets that are iid may still differ significantly.

Real data sets

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.

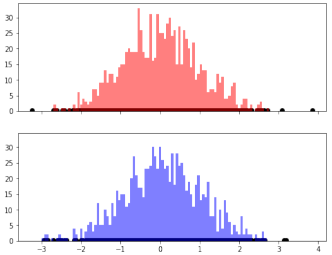
Ideally, the two distributions should be very similar:



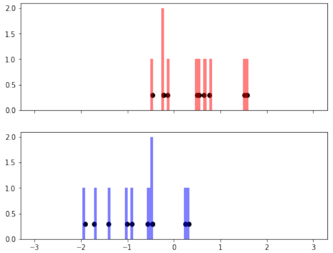
(seen)

(unseen)

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



or even this



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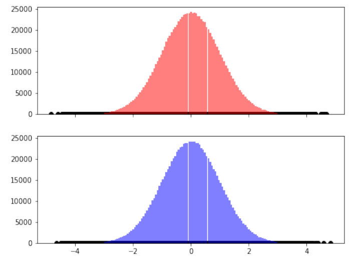

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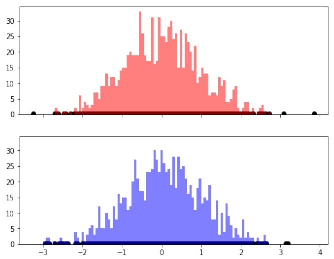

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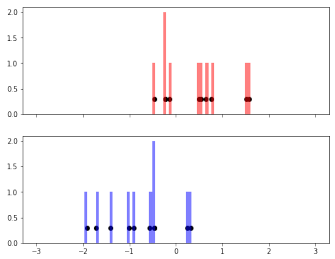
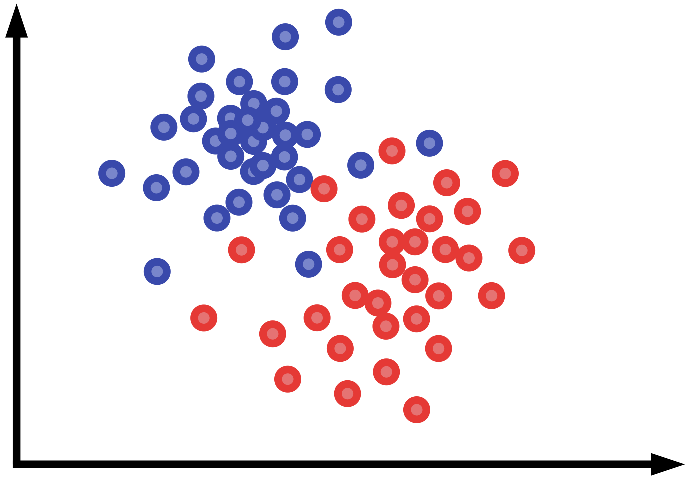


Successful training on one data set does not imply good performance on unseen data
→ the model has to **generalize** well by preventing **overfitting**

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?

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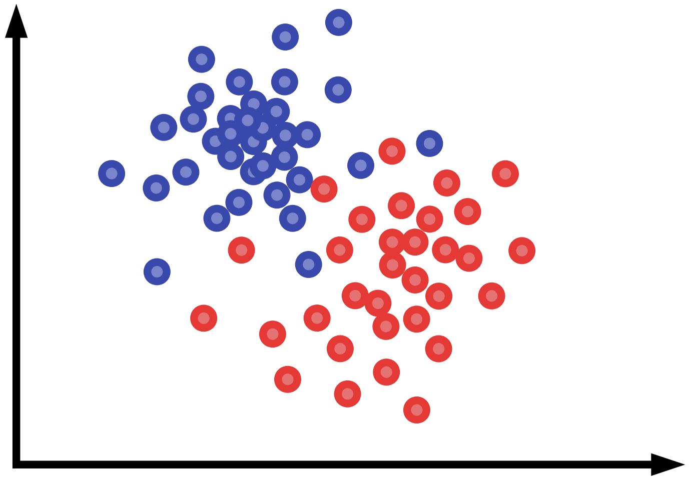

What would be a good decision boundary between the two classes?

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

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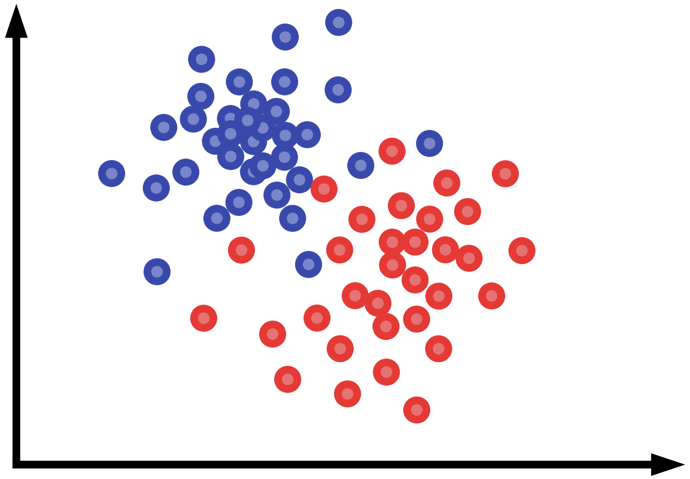

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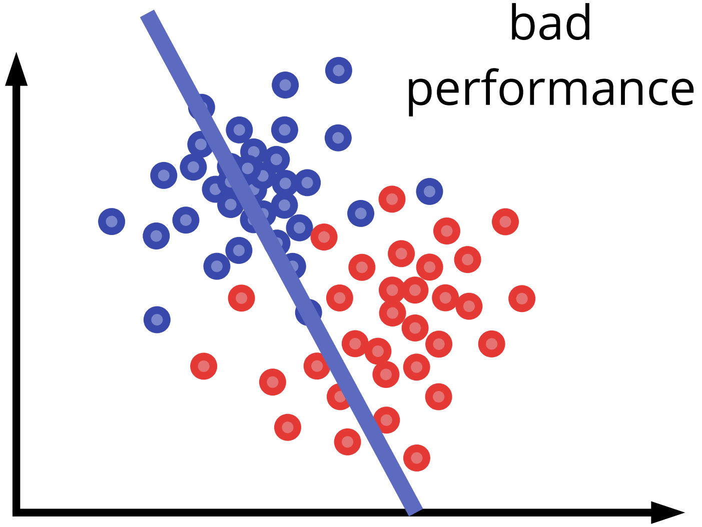

This would not be a good decision boundary as it barely allows to distinguish the two classes.

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

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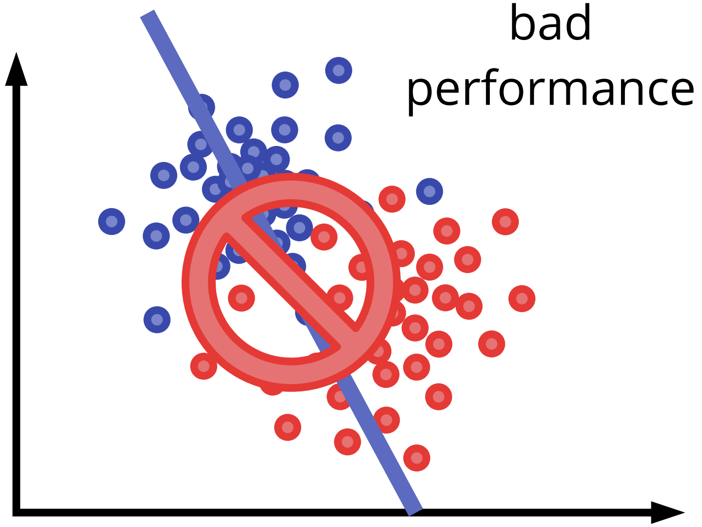

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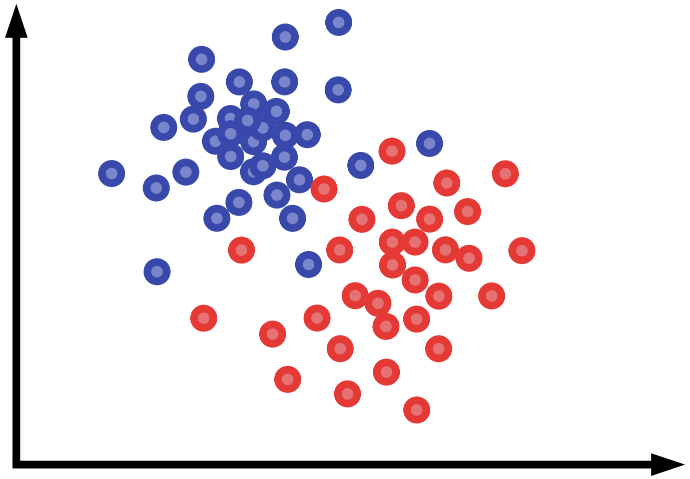

Training (seen) data

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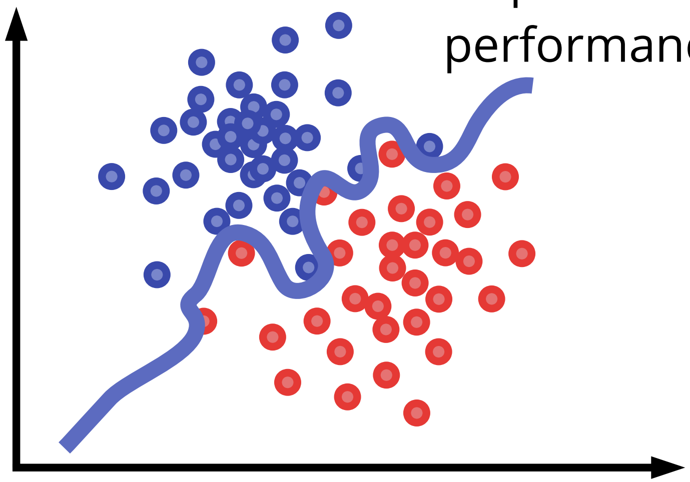

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Is this good?

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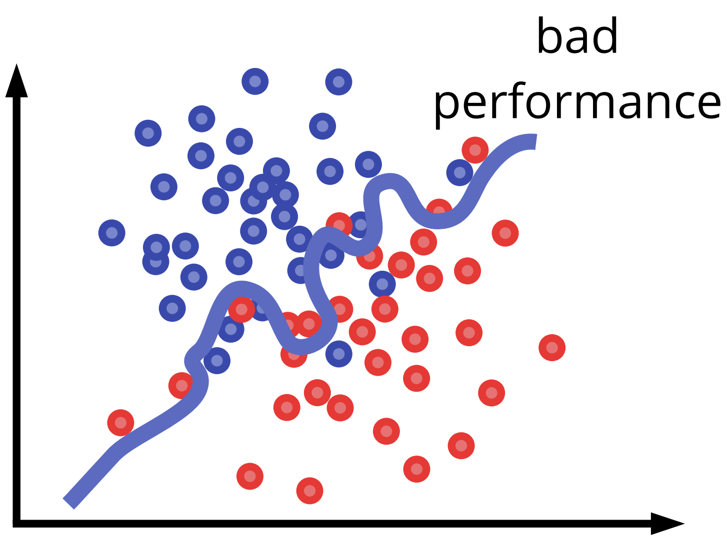
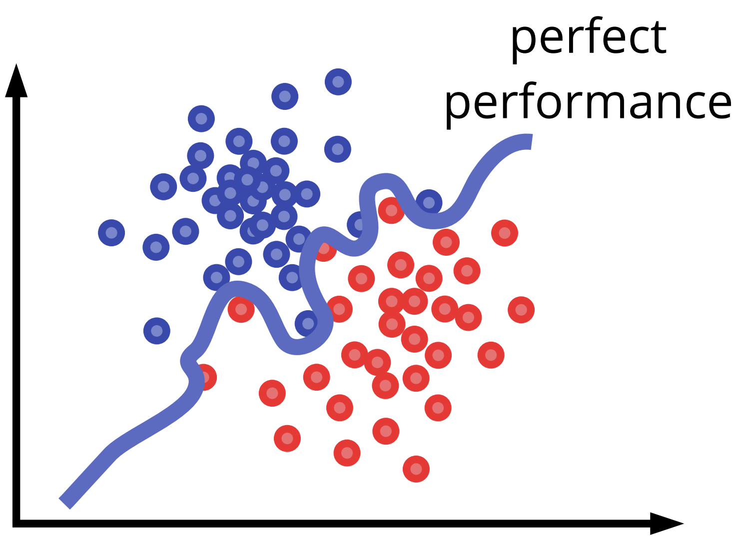


Test (unseen) data



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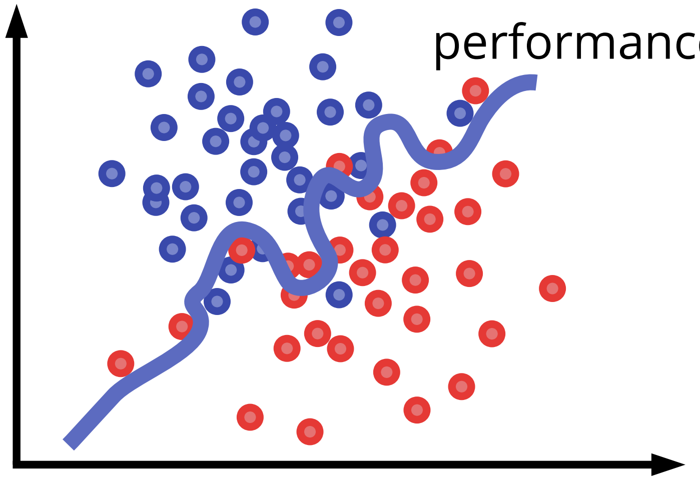

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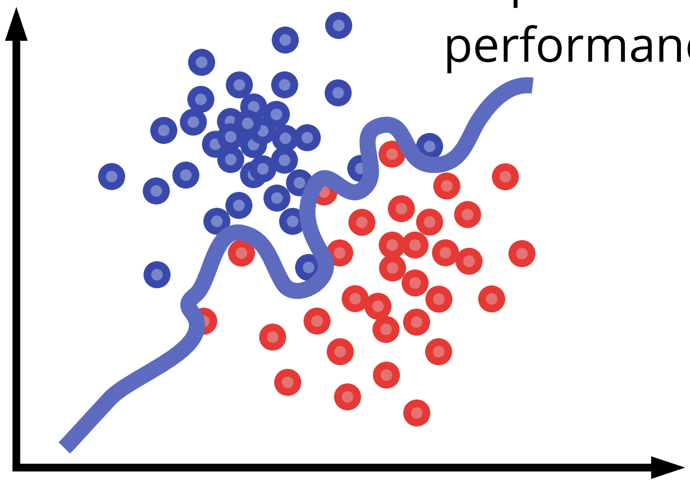

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We can improve its performance through **regularization** methods.

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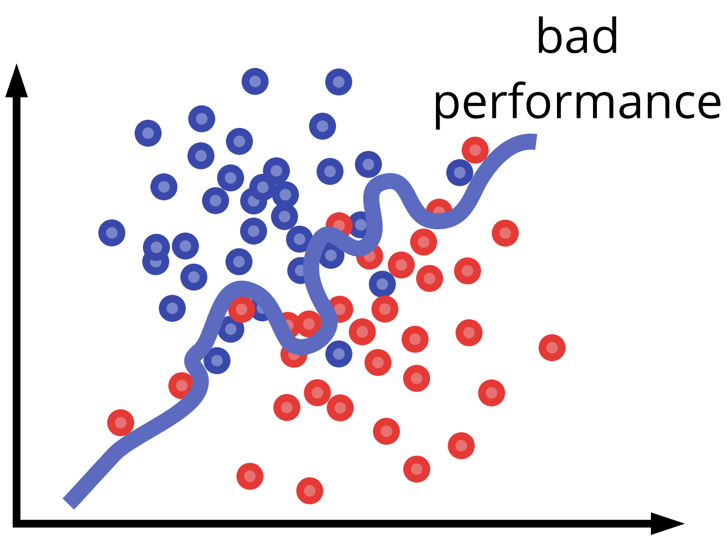

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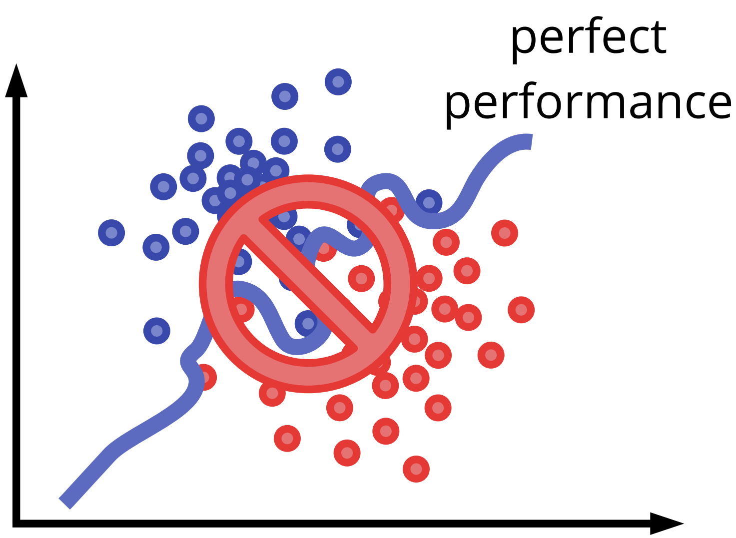

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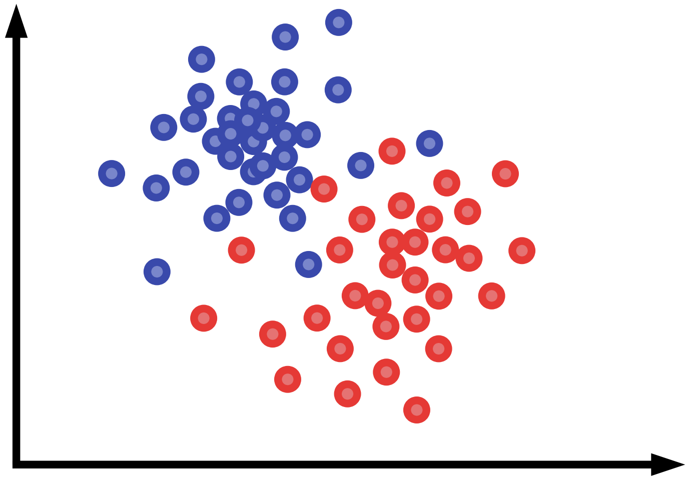

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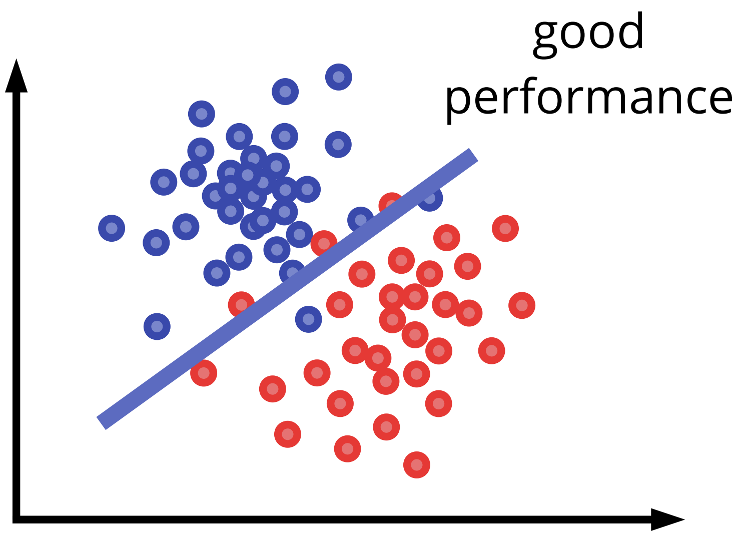
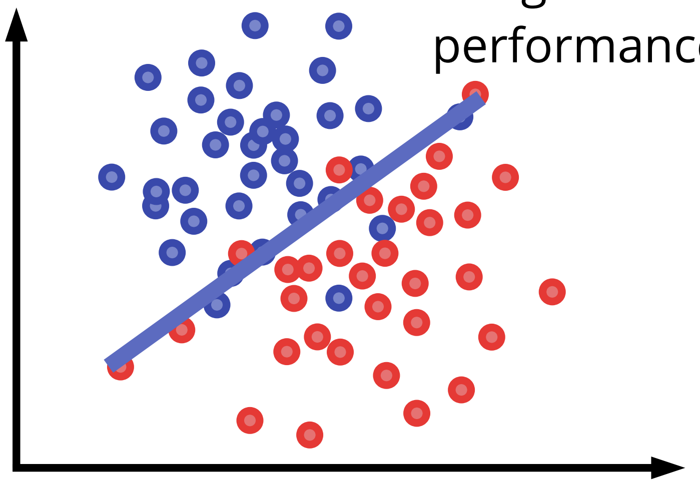


Generalization, regularization, overfitting and underfitting

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

good performance



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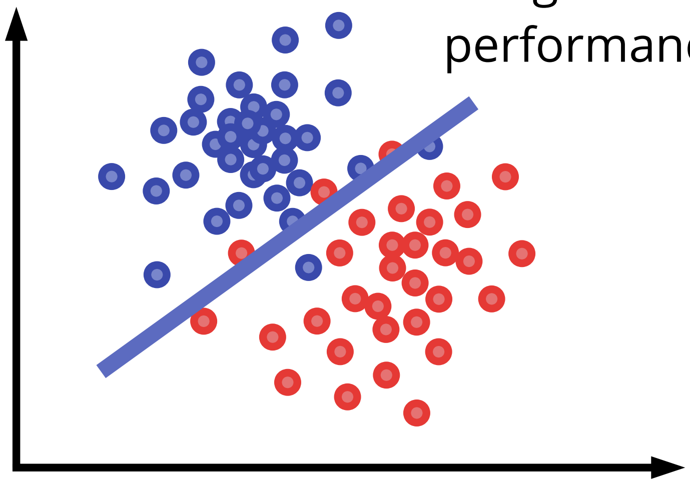

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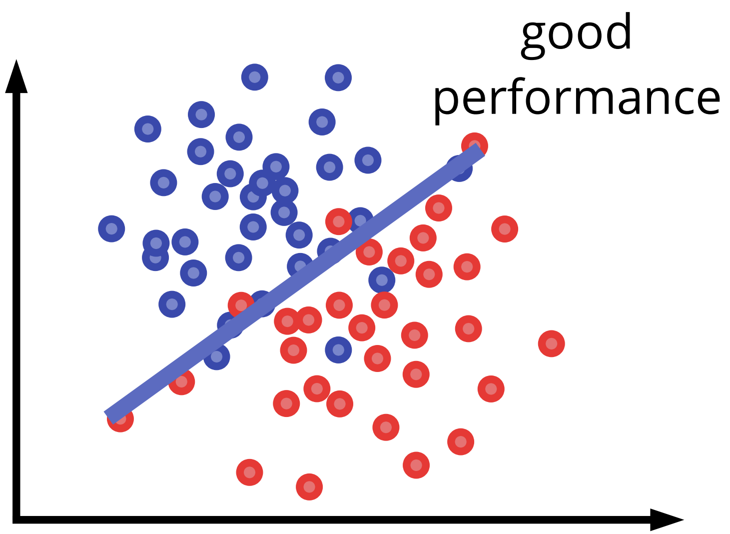

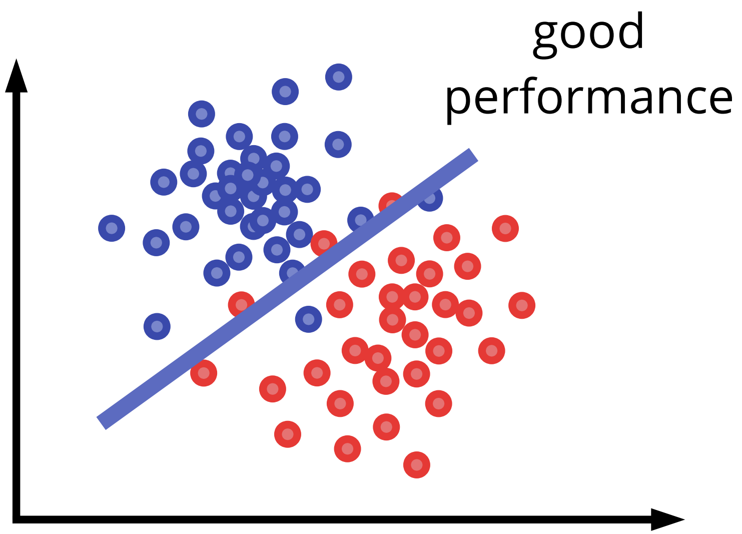

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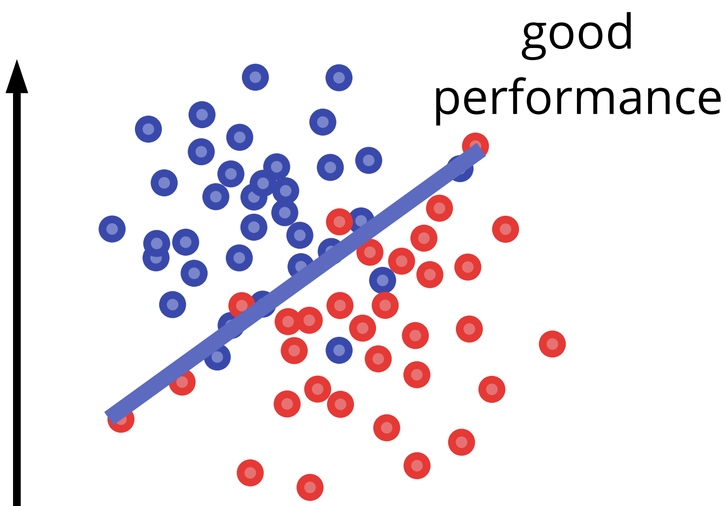

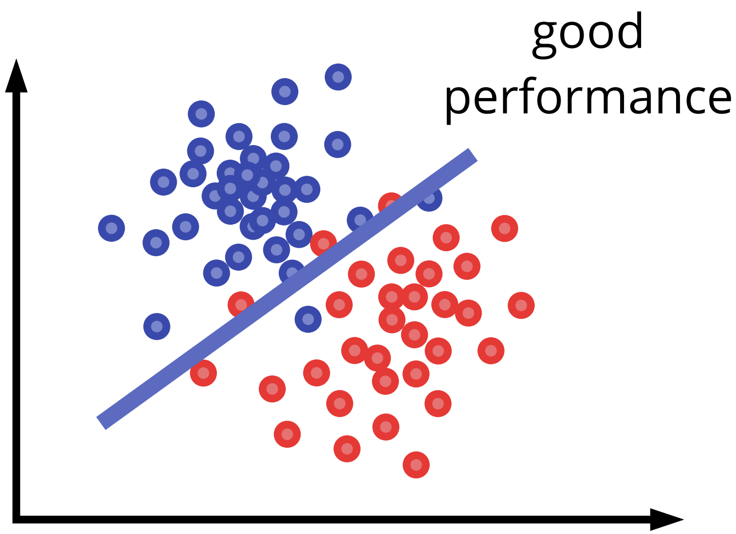

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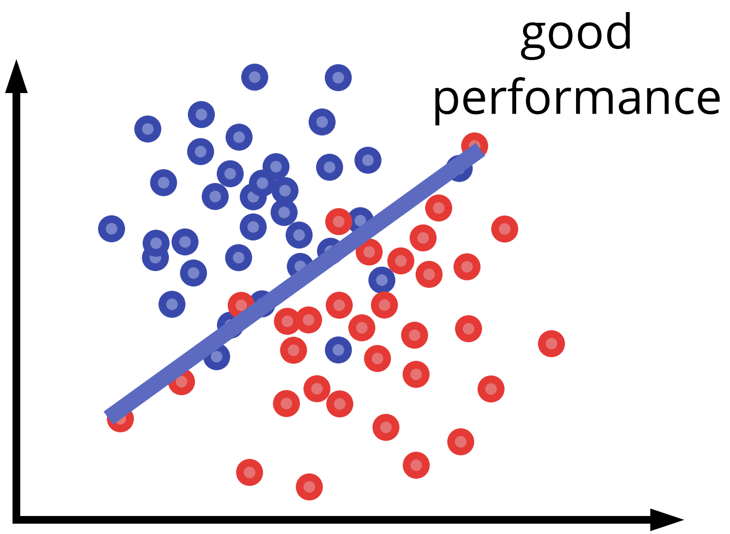

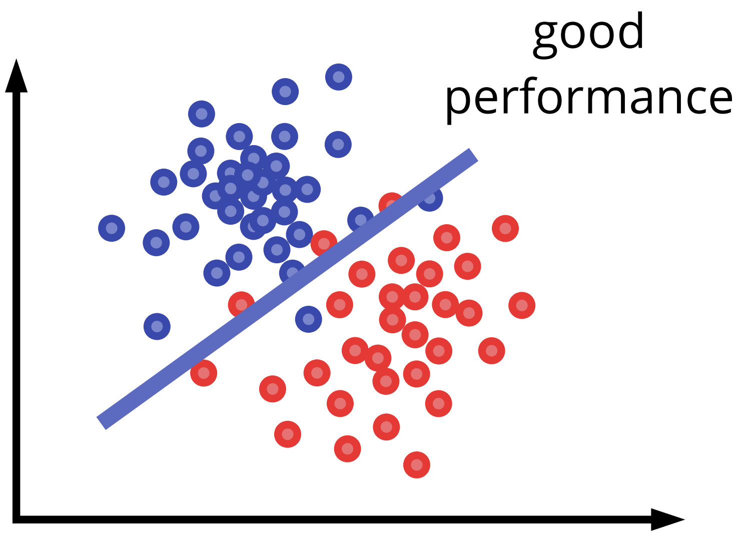

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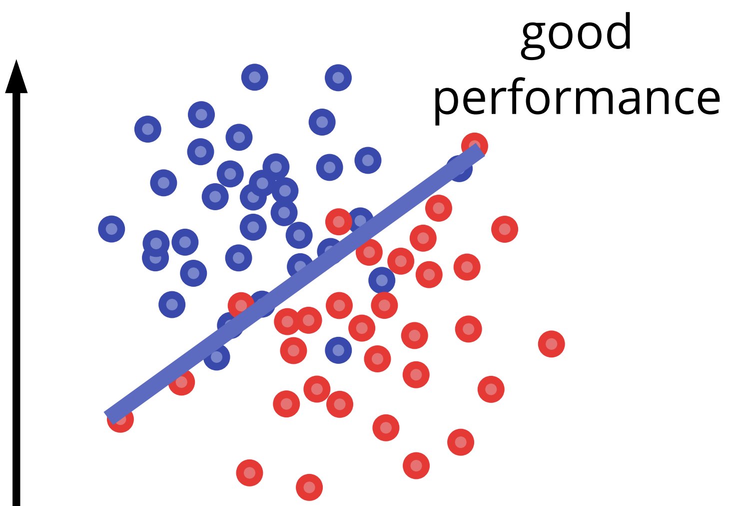

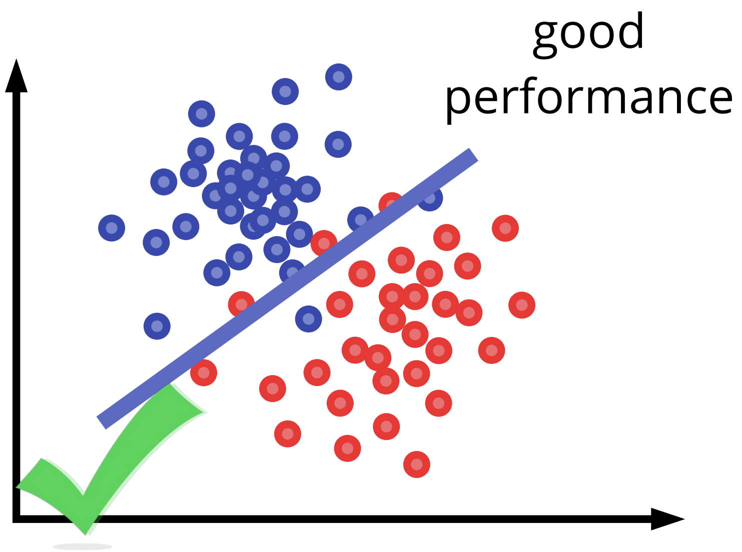

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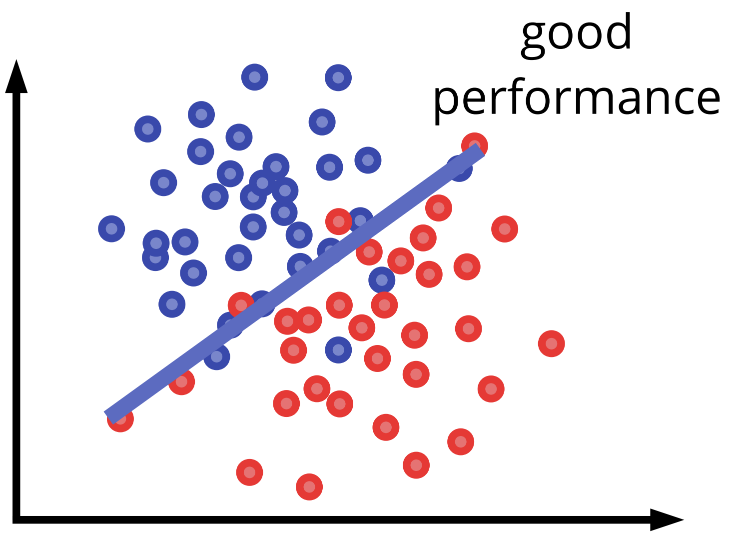

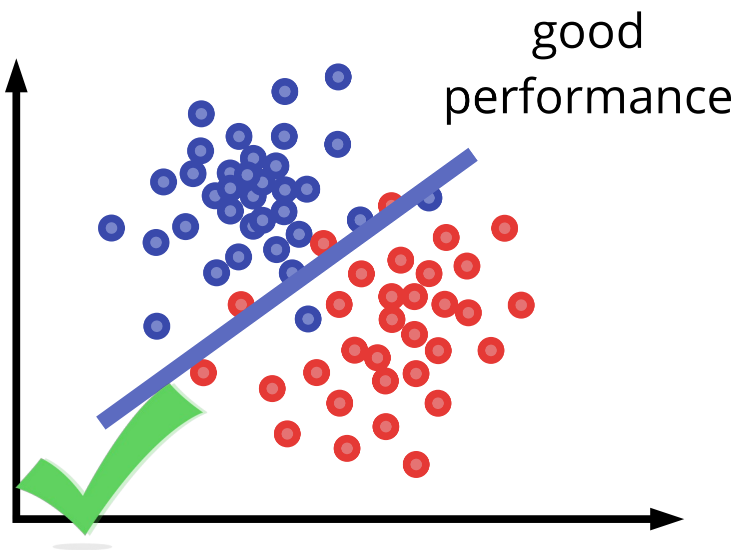

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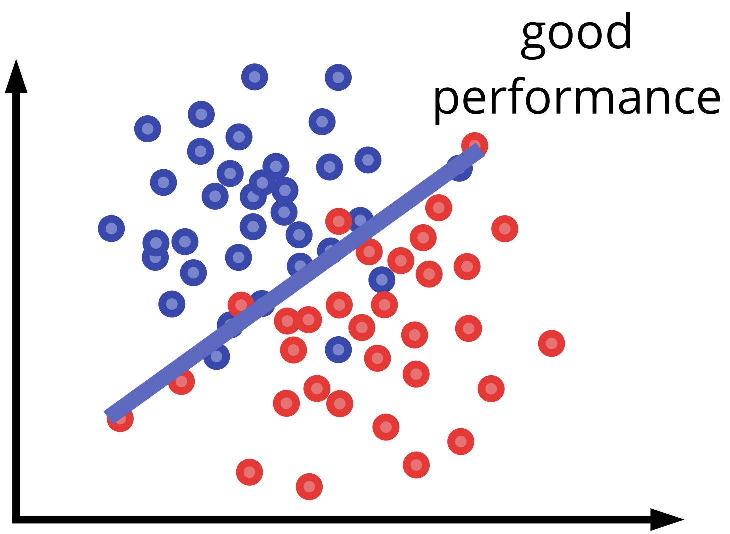

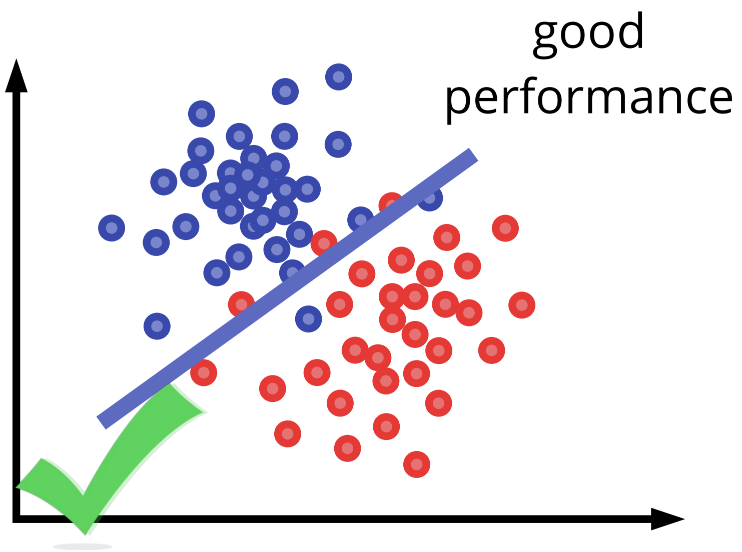

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How can we check how well the model generalizes?

How can we force the model to generalize?

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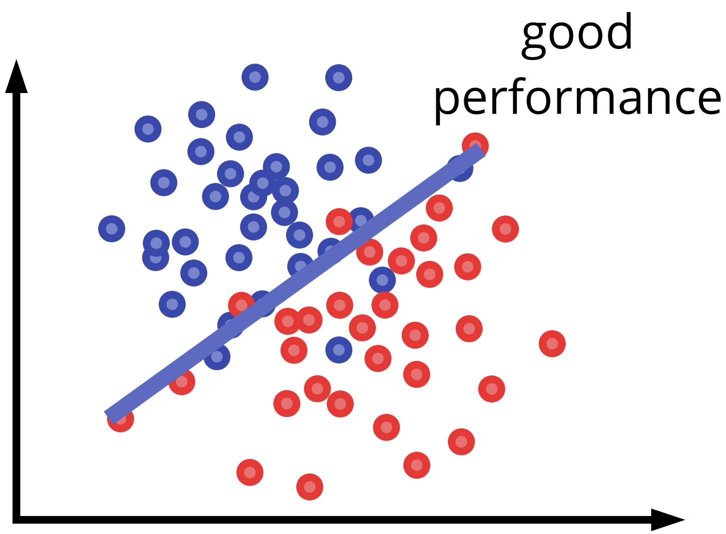

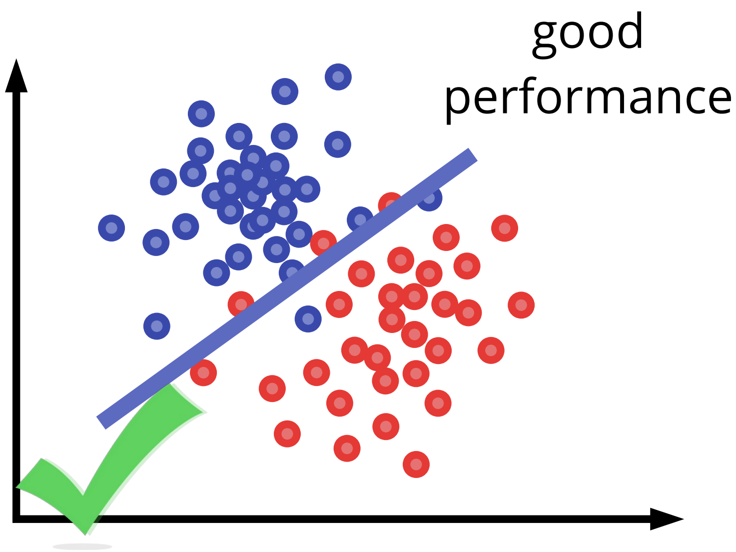

This decision boundary leads to **equally good performance on both data sets**.

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

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

Identifying overfitting

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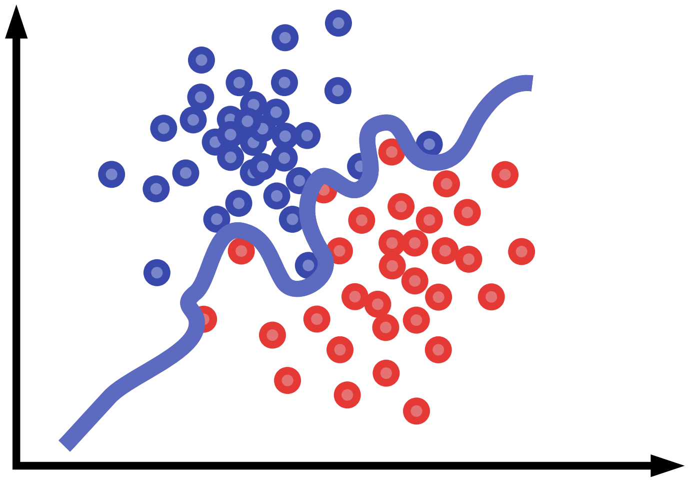

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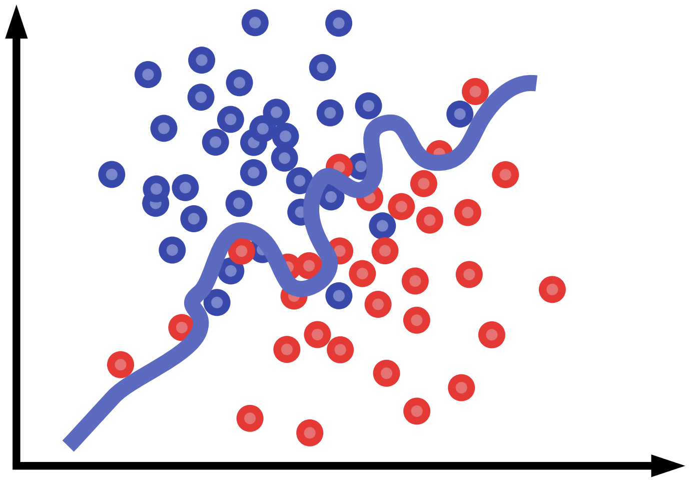

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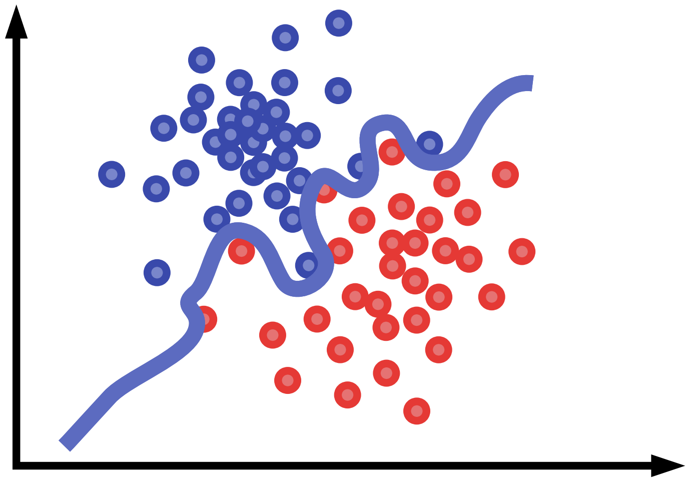

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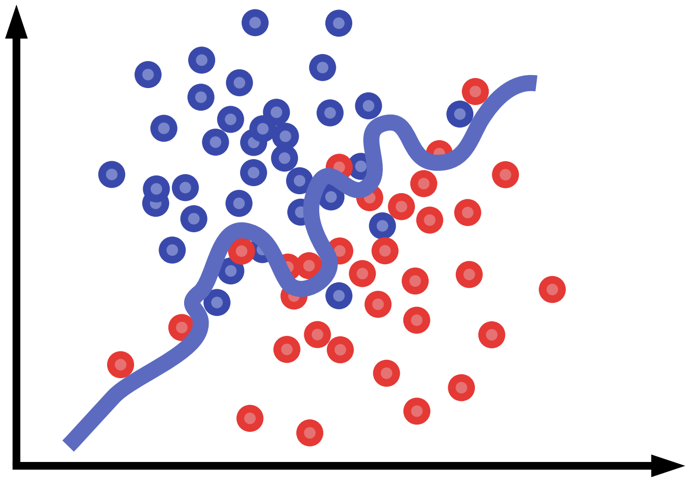

Test (unseen) data

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.

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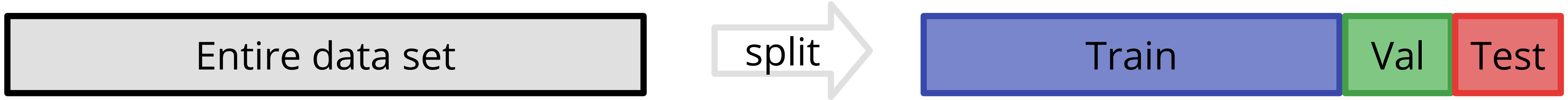

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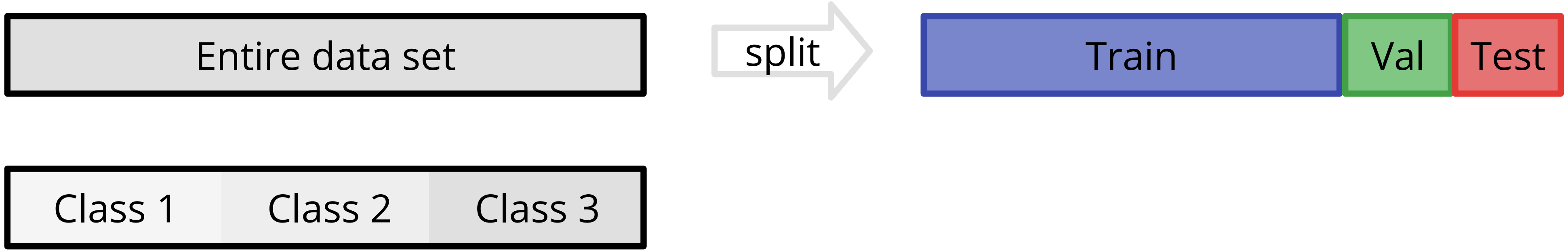

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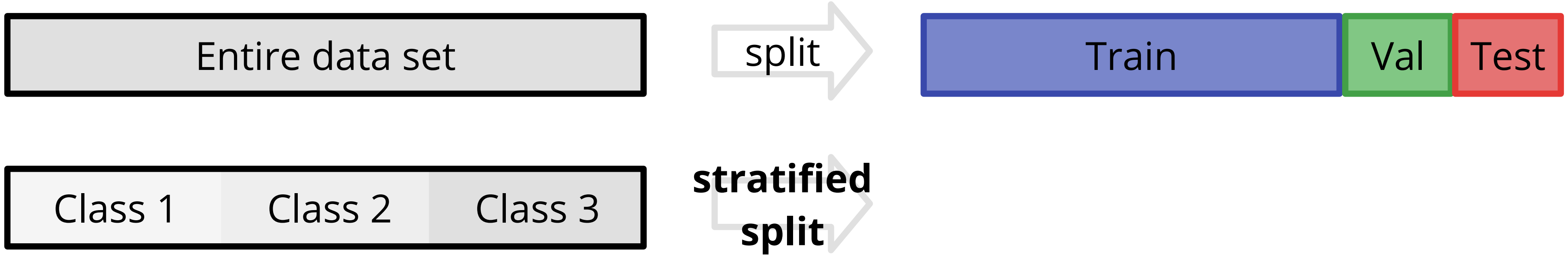

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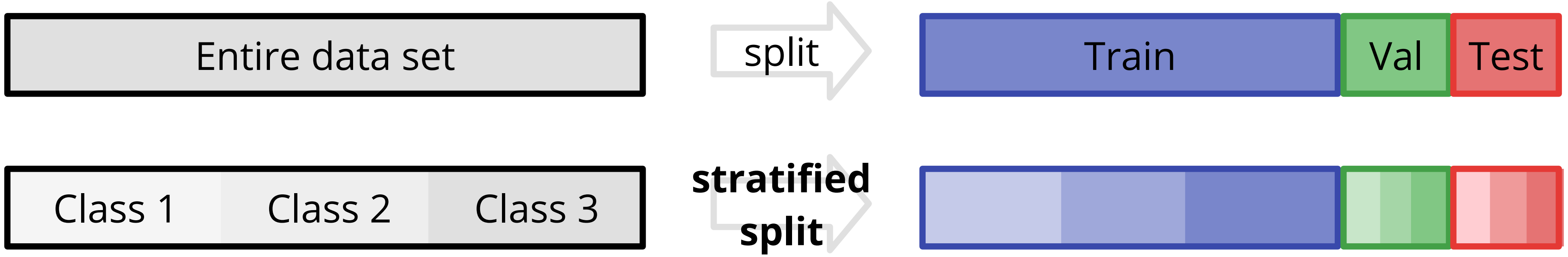

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Preserve class fractions in split data sets.

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Shuffled data set → k=3 split → Split 1 | Split 2 | Split 3 — 3-fold split

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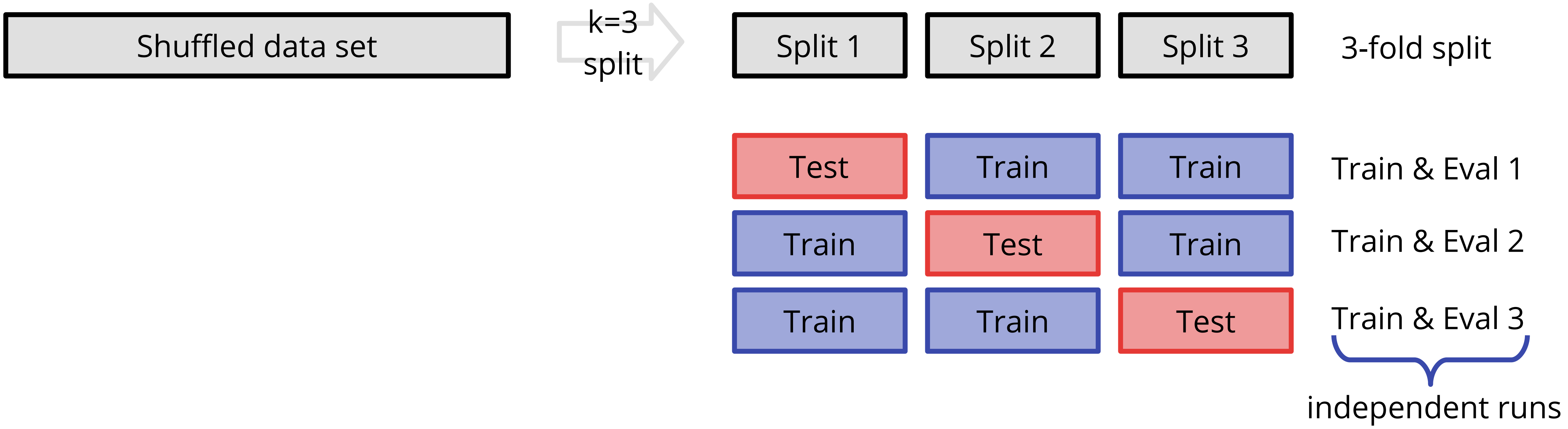

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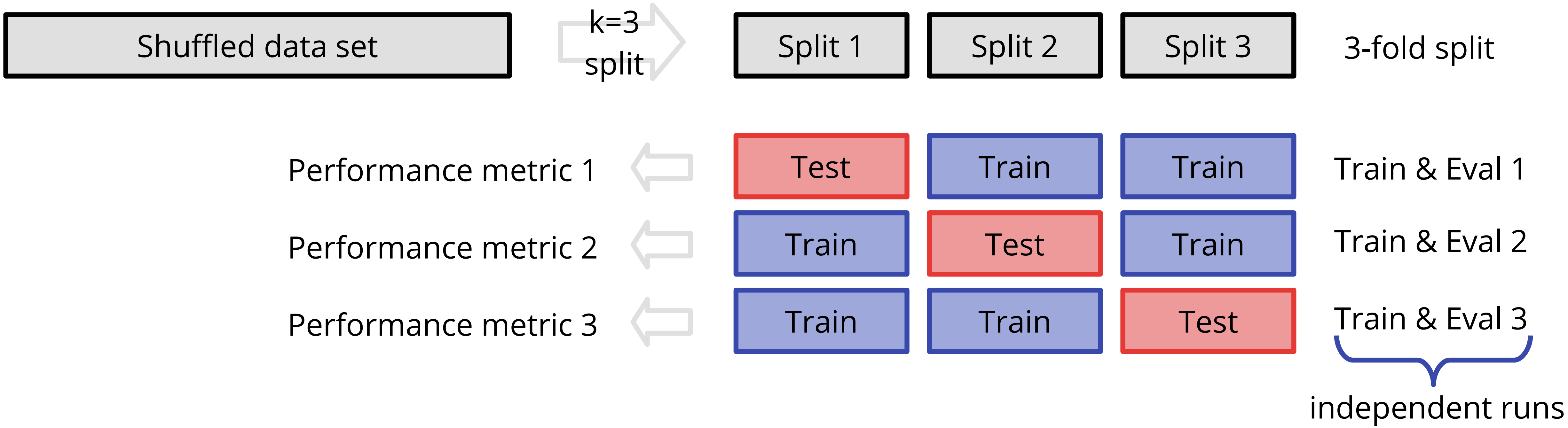

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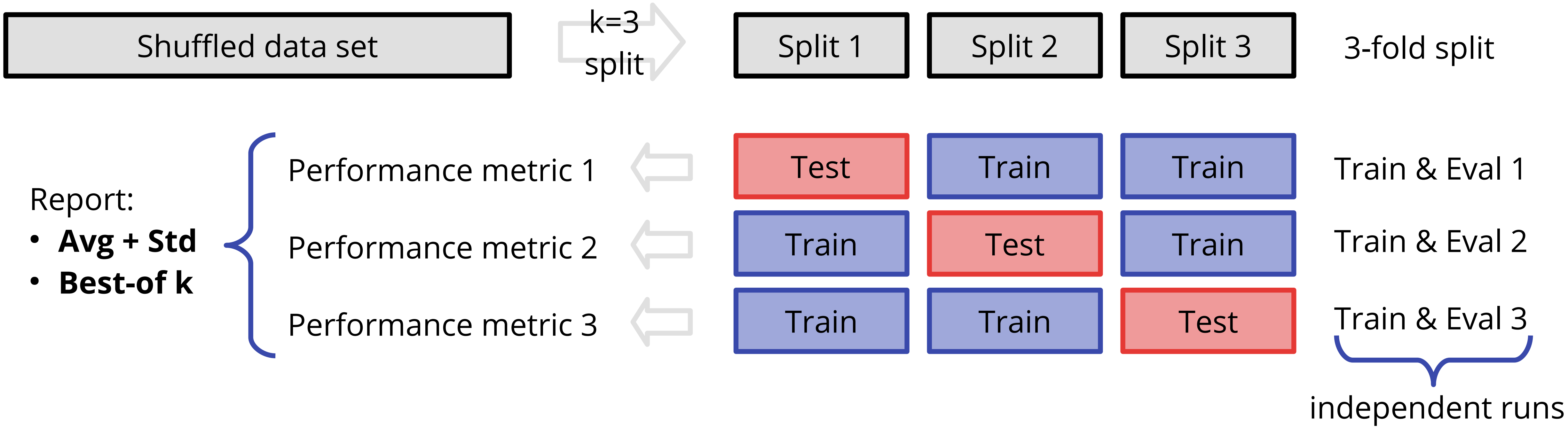

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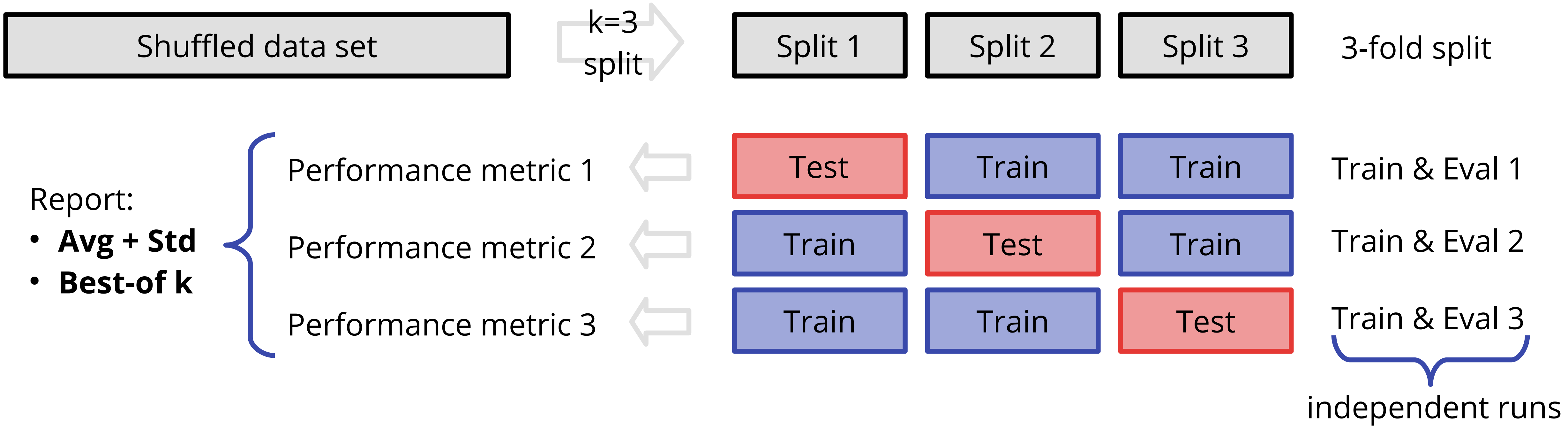

Note: Keep in mind that cross-validation will not improve your model performance;
it will simply give you a more reliable estimate of its performance.

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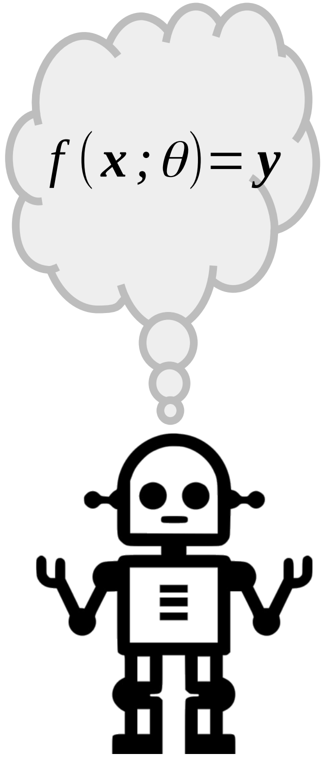
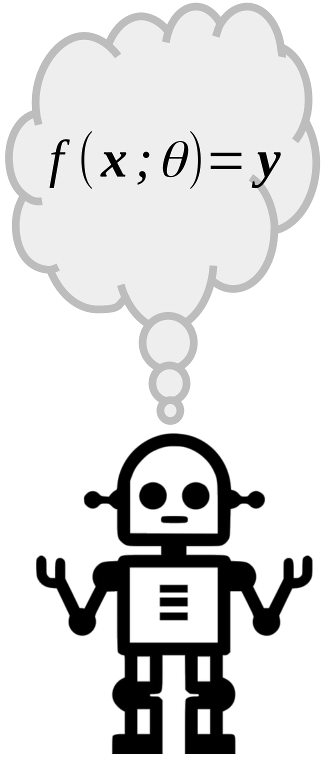
- **Bagging/Ensembling**: training multiple models on the same data, combining their results (all models)

General supervised learning pipeline



General supervised learning pipeline

1) Feature engineering: raw data → features



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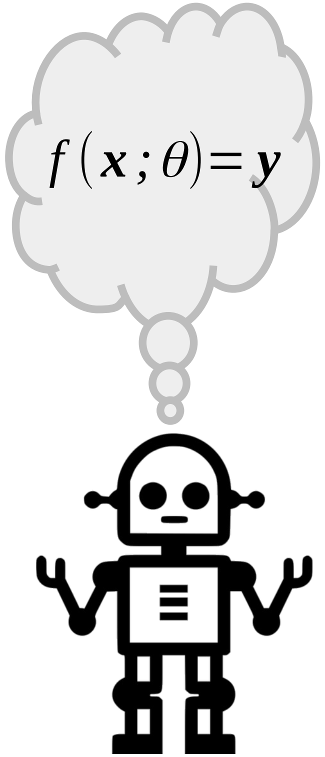

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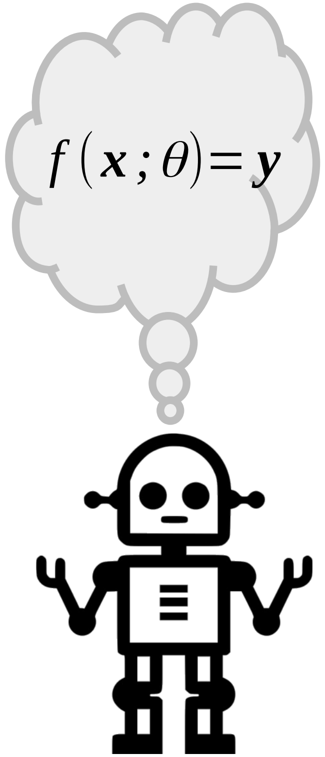
3) Data splitting → training, validation, test data



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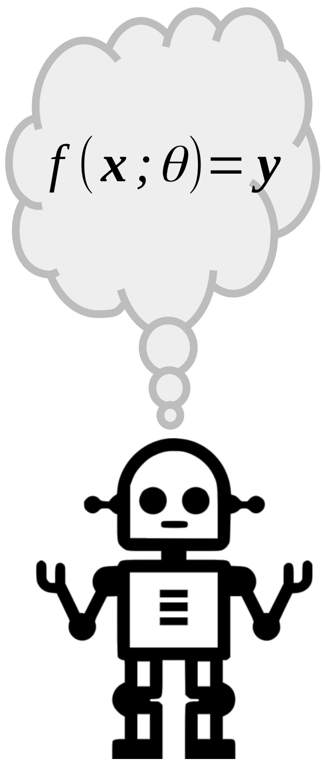

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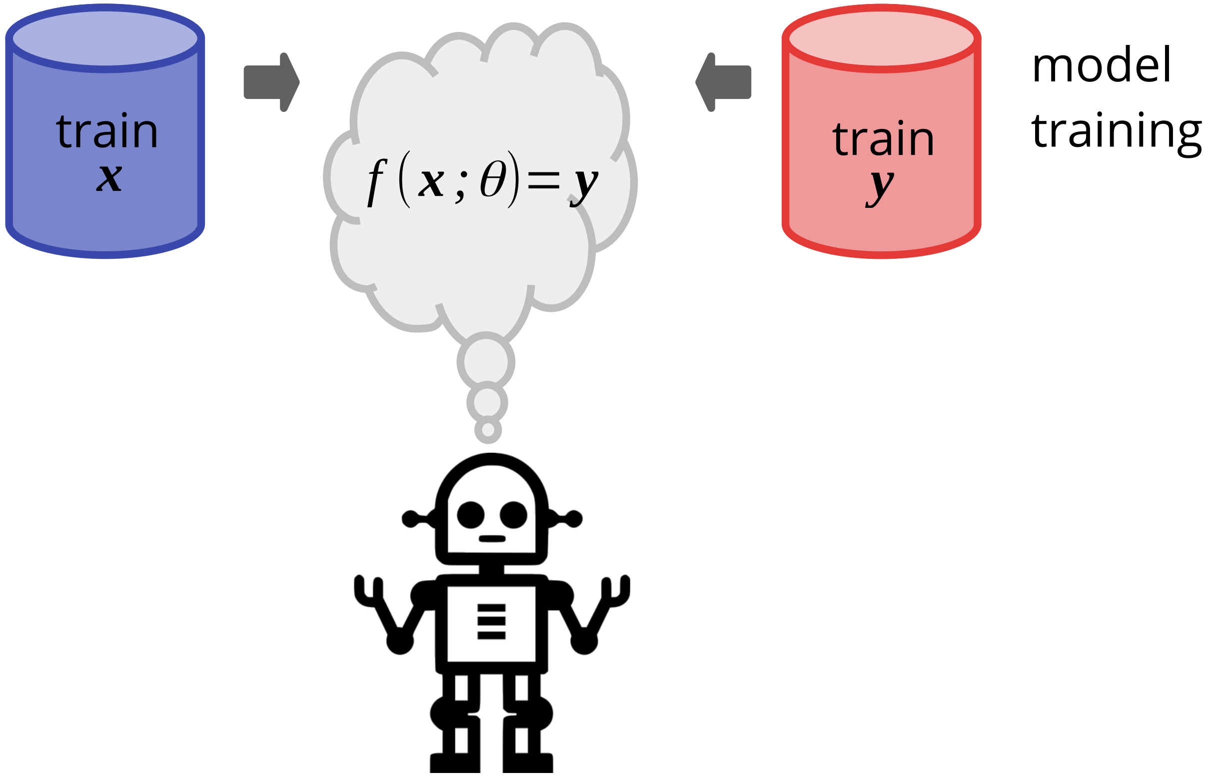

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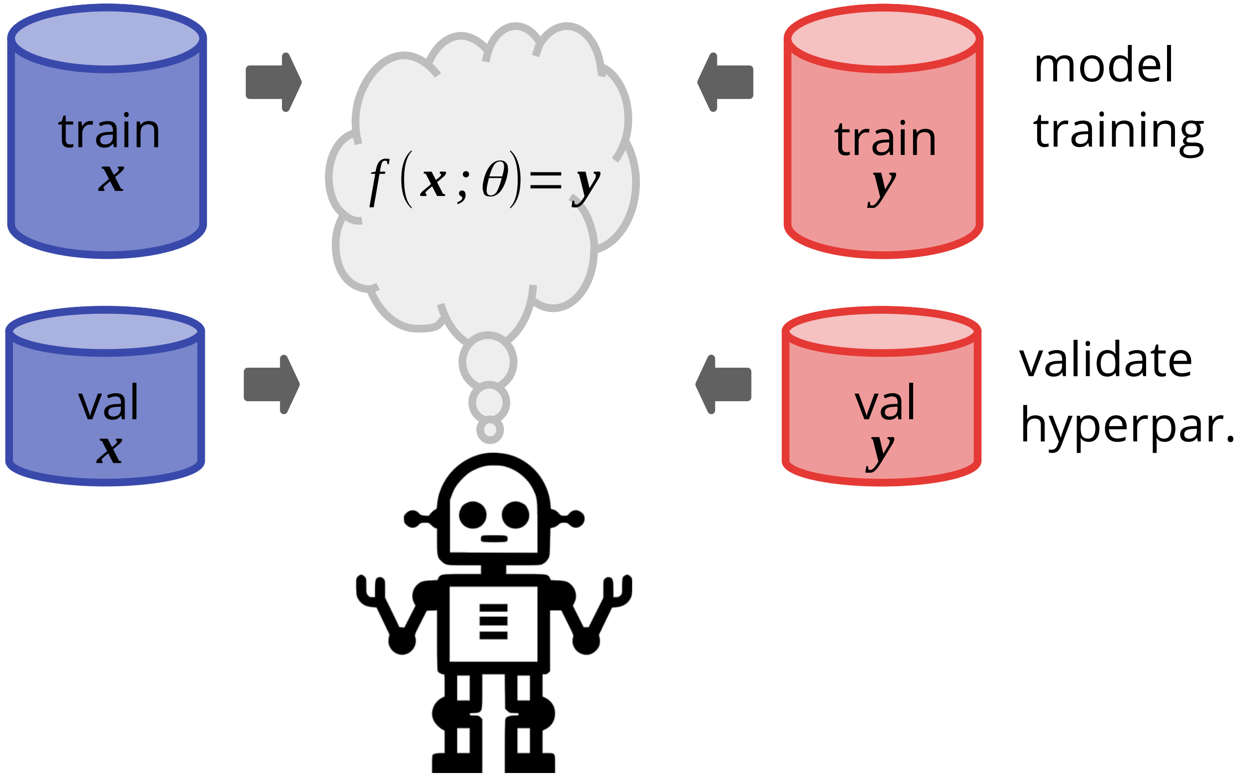
6) Evaluate model on validation data



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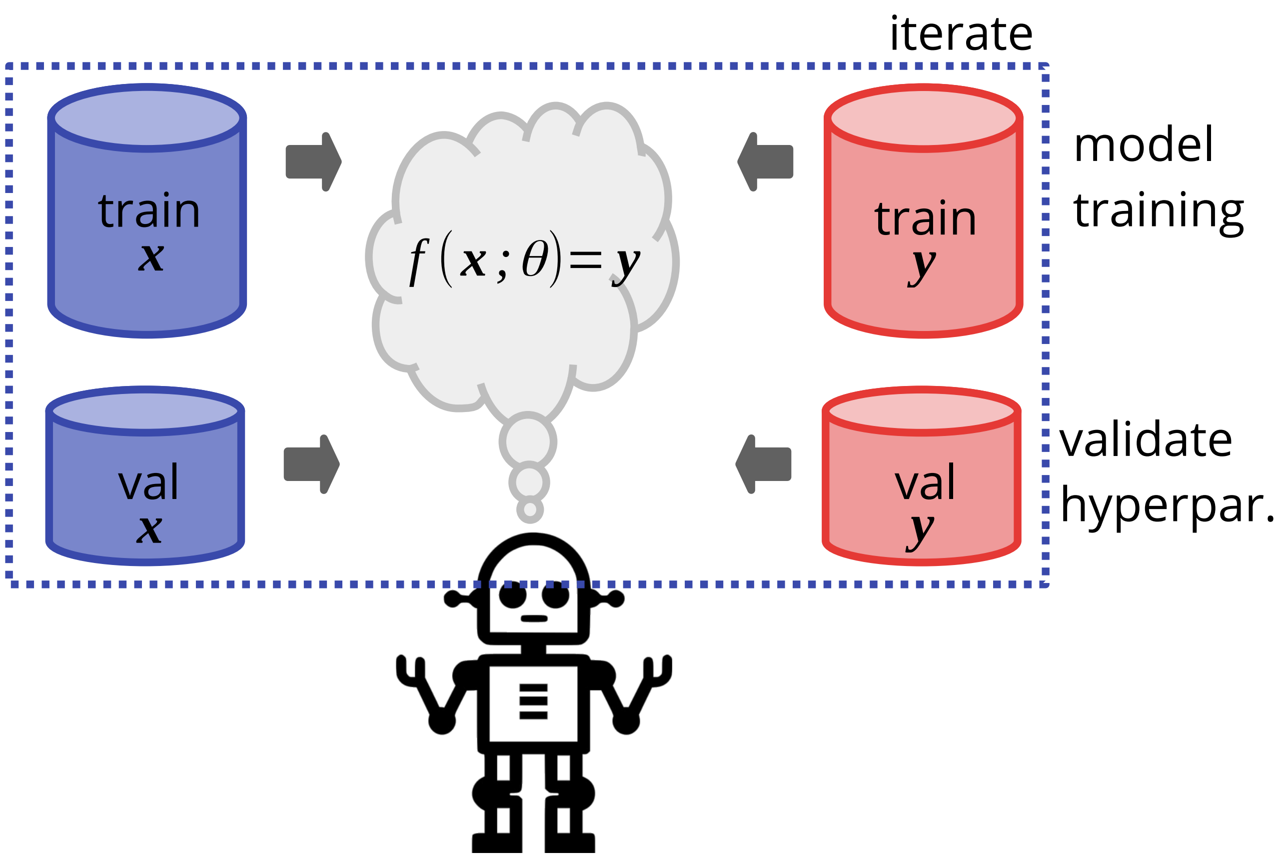

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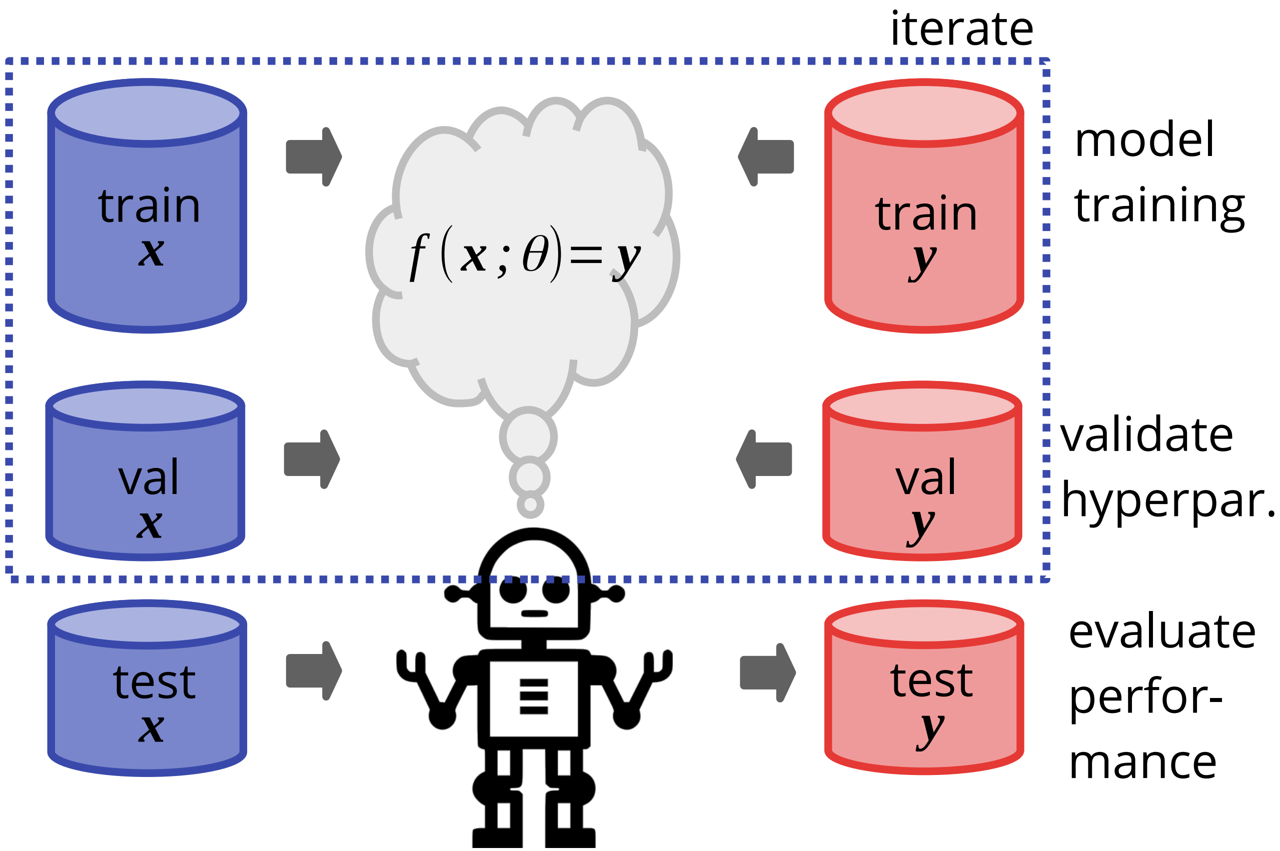
8) Evaluate trained model on test data → report test data performance



Benchmarking and metrics

How do we measure the performance of our model?

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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.

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What is most important?
- correctness of diagnosis
- minimizing failures
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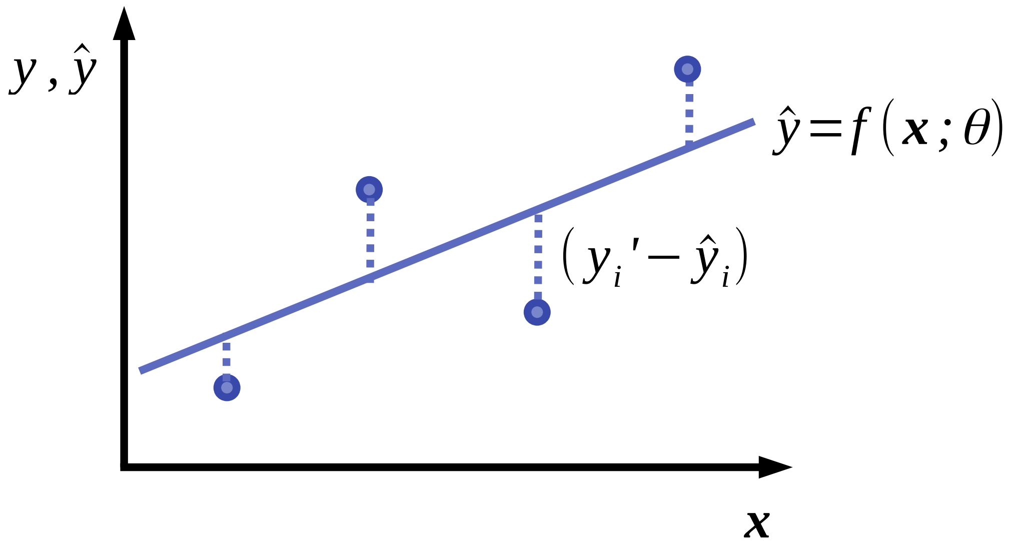
metrics	• speed • strength • number of victories • income	• revenue • overall value • number of employees • annual CO2 emissions	• correctness of diagnosis • minimizing failures • patient's comfort • cost

Regression task metrics:

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



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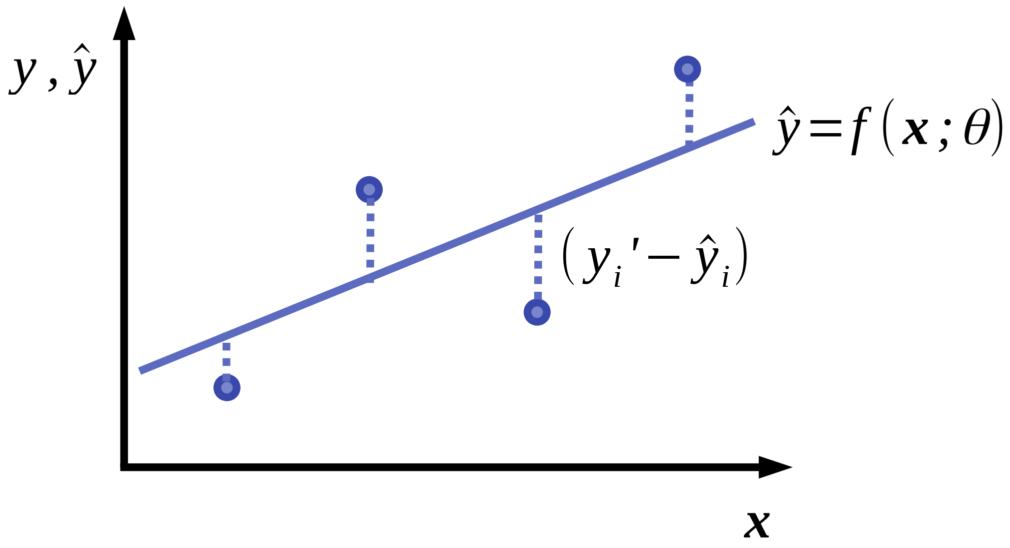

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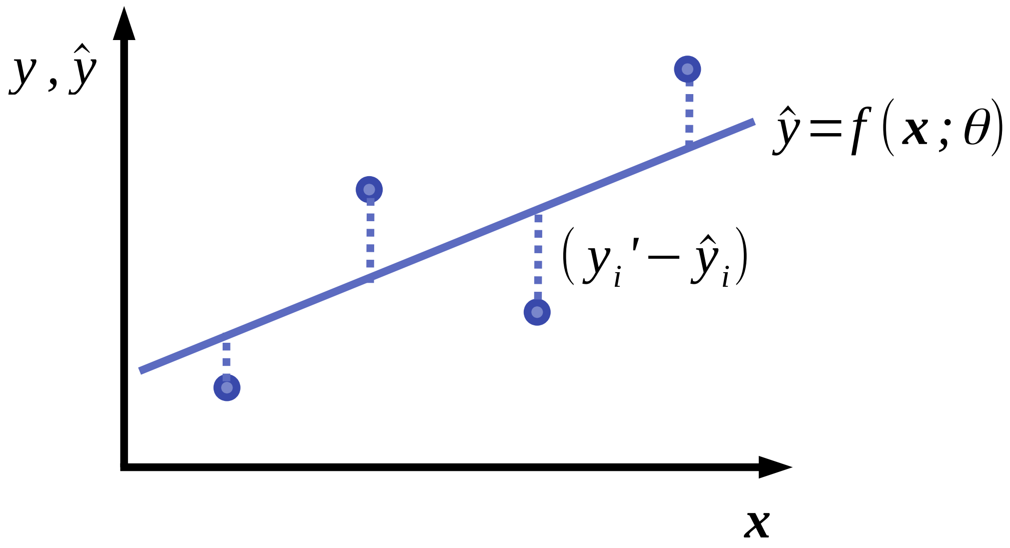

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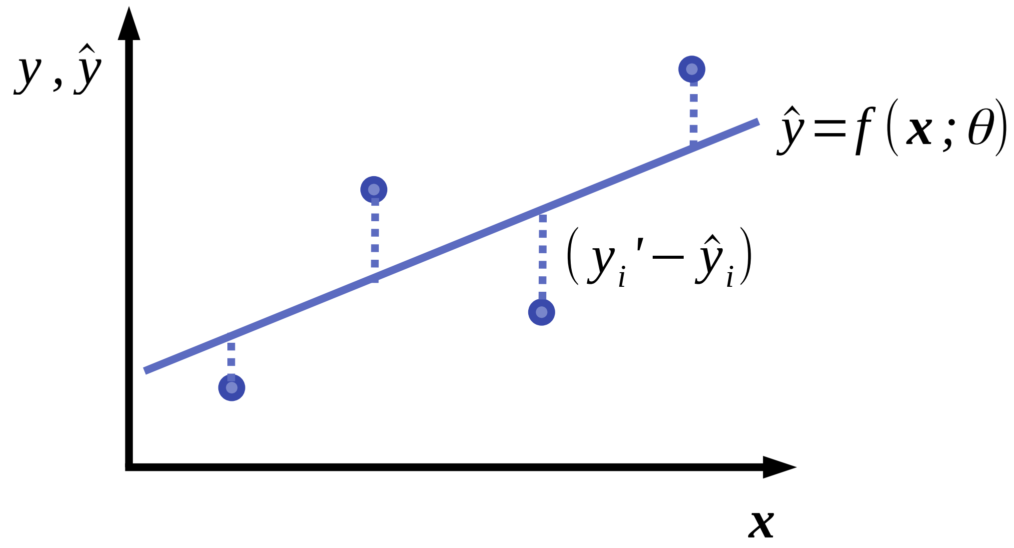

Intuition: by how much deviates your model prediction from the ground-truth on average.

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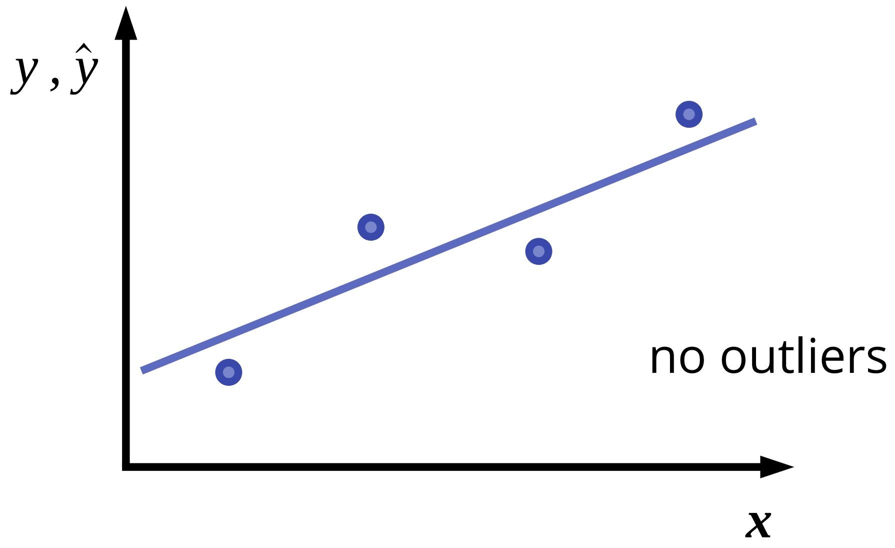

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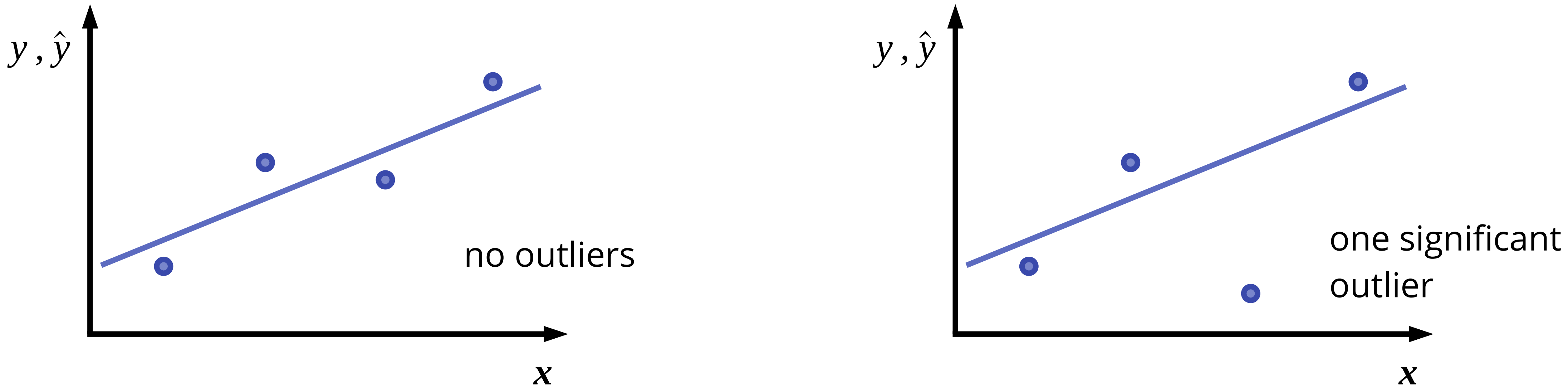

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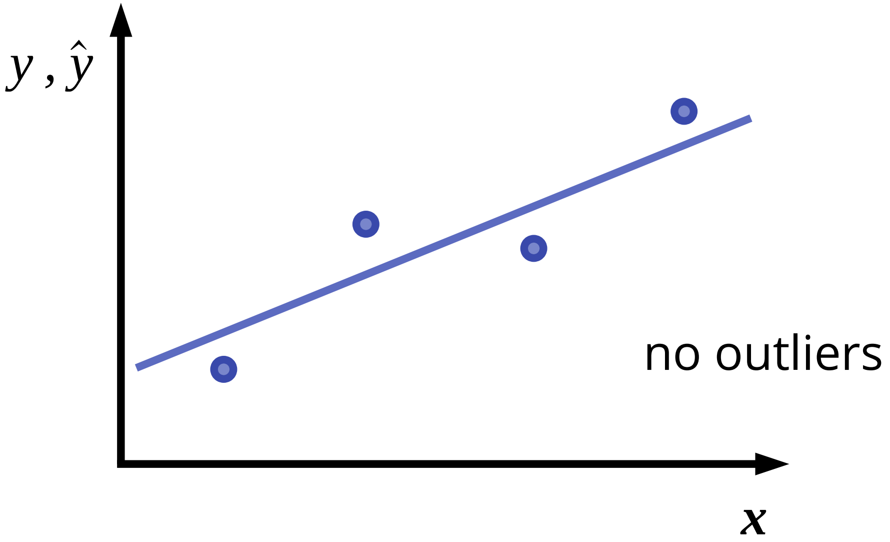
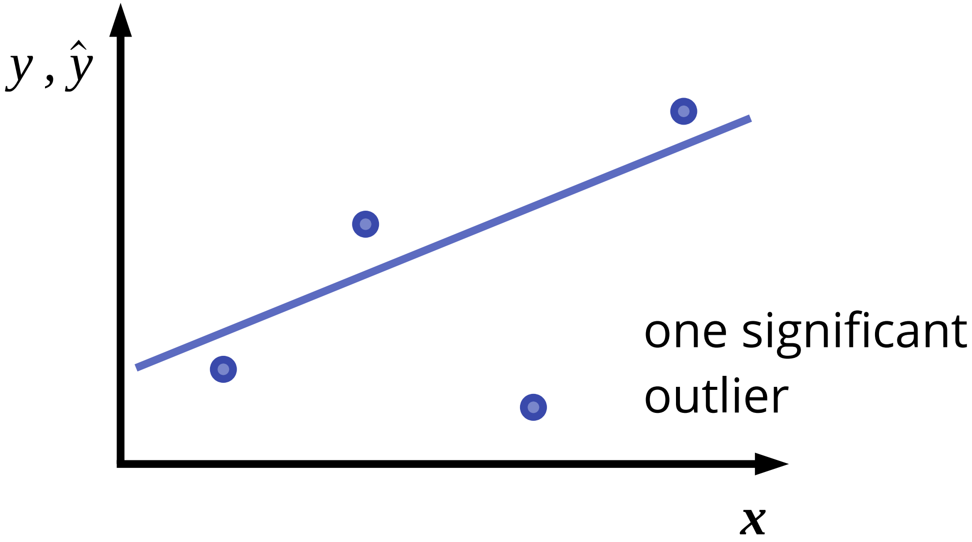
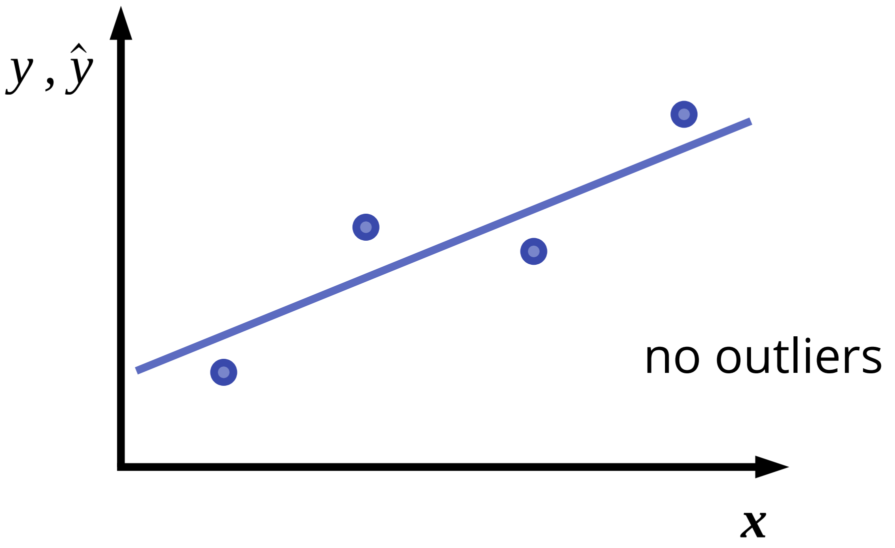


$(y_i' - \hat{y}_i)$: -1 1 -1 1



Comparing regression task metrics

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



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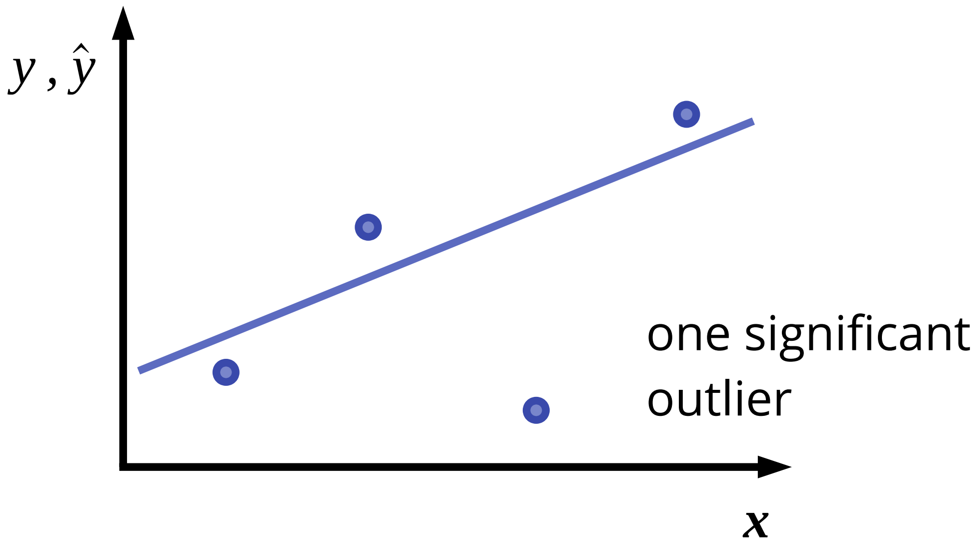

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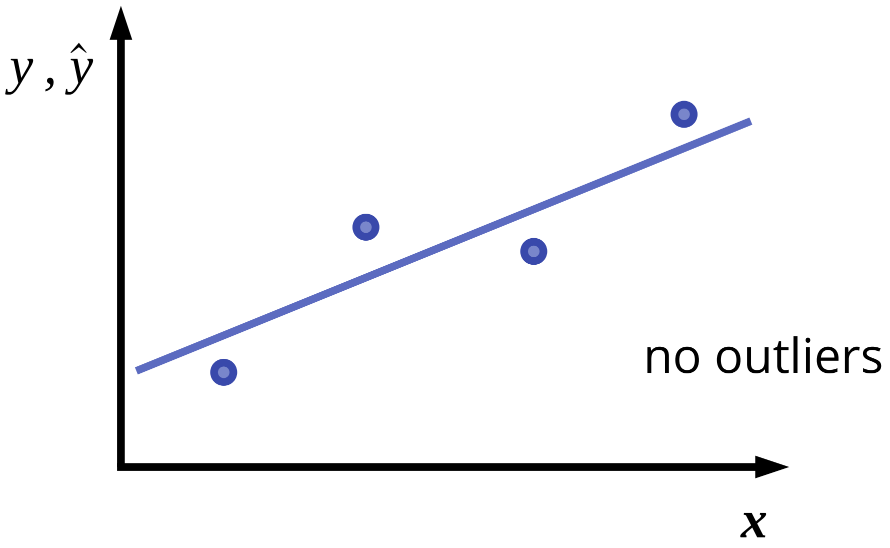

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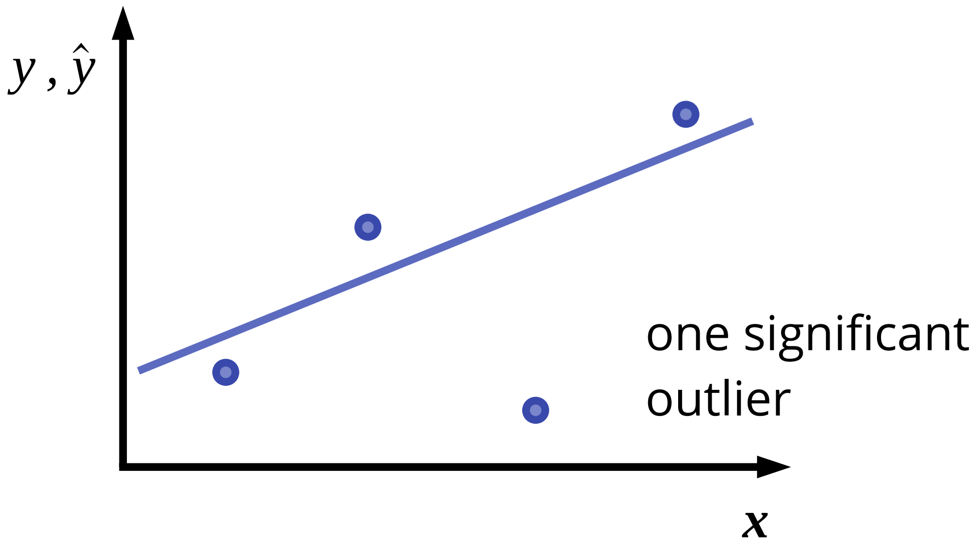

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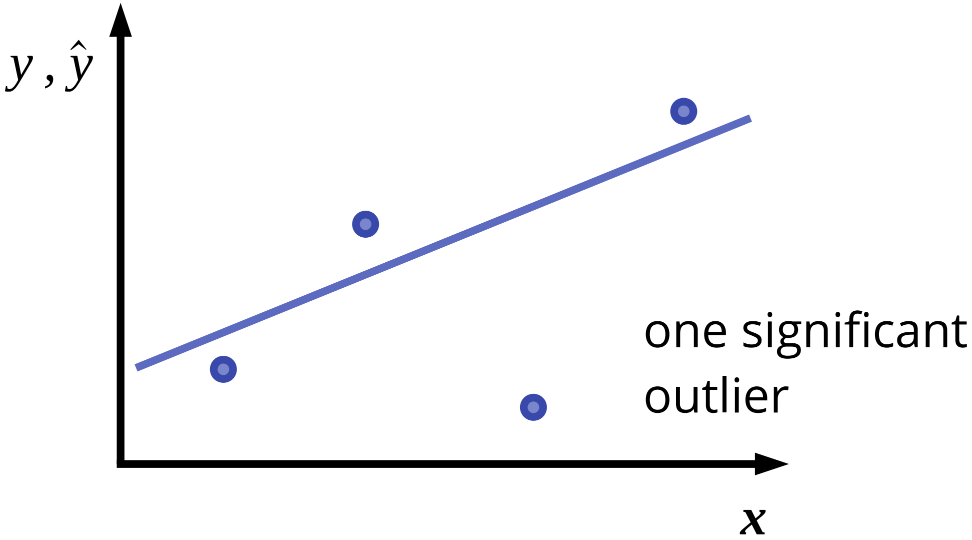

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→ MAE = 3.25; RMSE = 5.07

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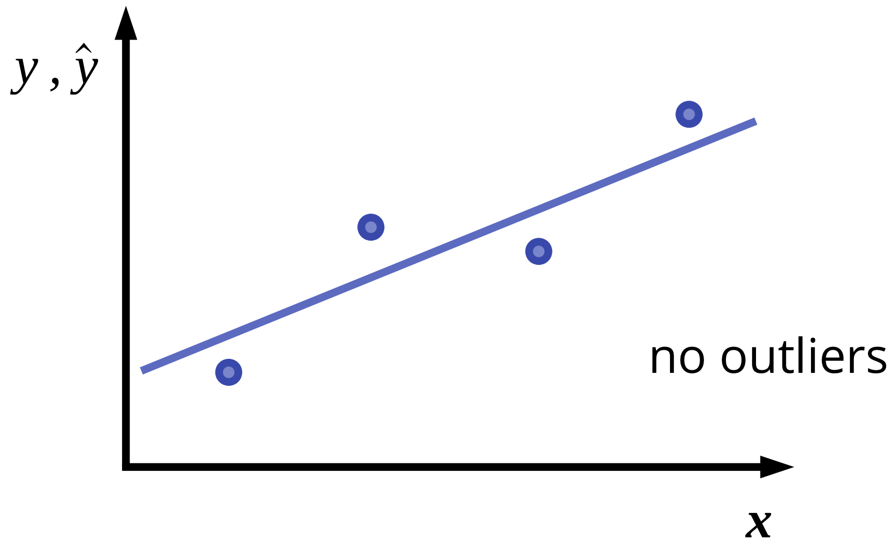

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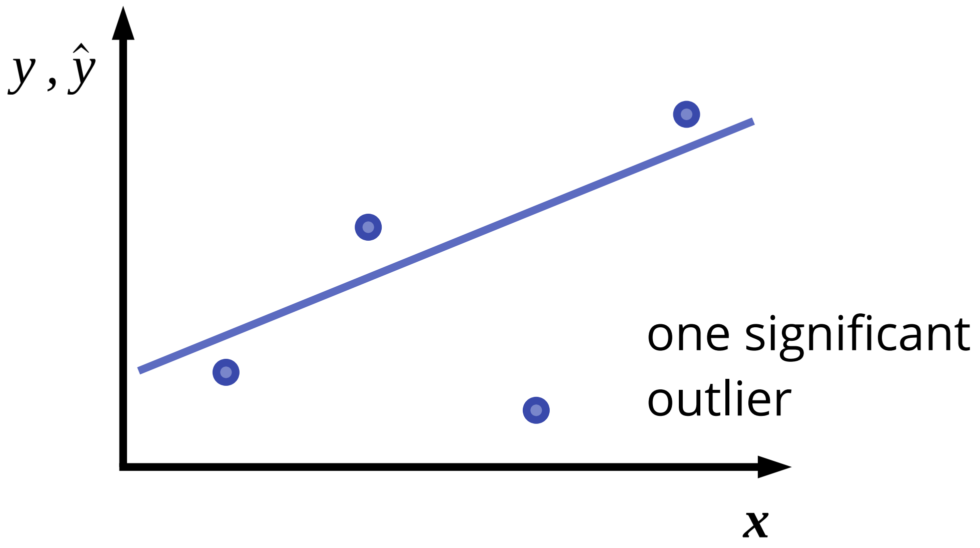

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→ **MAE = 3.25; RMSE = 5.07**

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

Classification

(Binary) Classification metrics:

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

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Accuracy = (TP + TN) / (TN + TP + FP + FN)
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Class imbalance is a real issue!

Example: Will this asteroid impact Earth?

(Binary) Classification metrics:

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

Requires somewhat balanced classes

Precision = TP / (TP + FP) (quantifies “correctness”)
Less susceptible to imbalance.

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

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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**.

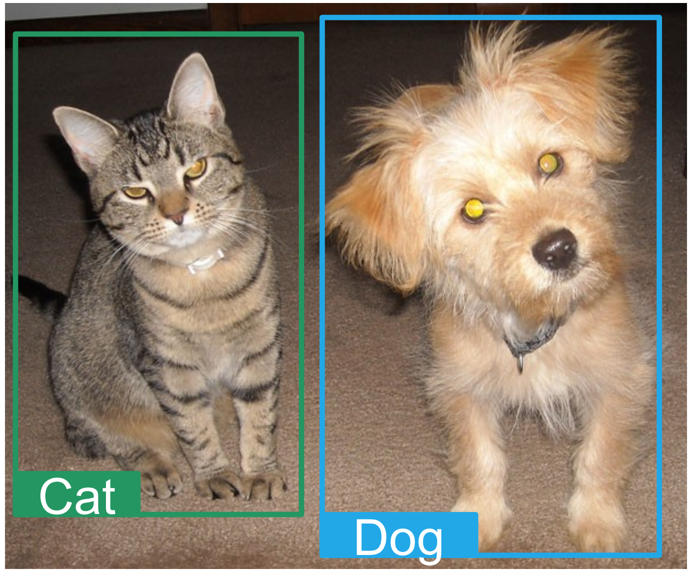
Confusion matrix

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

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

- 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

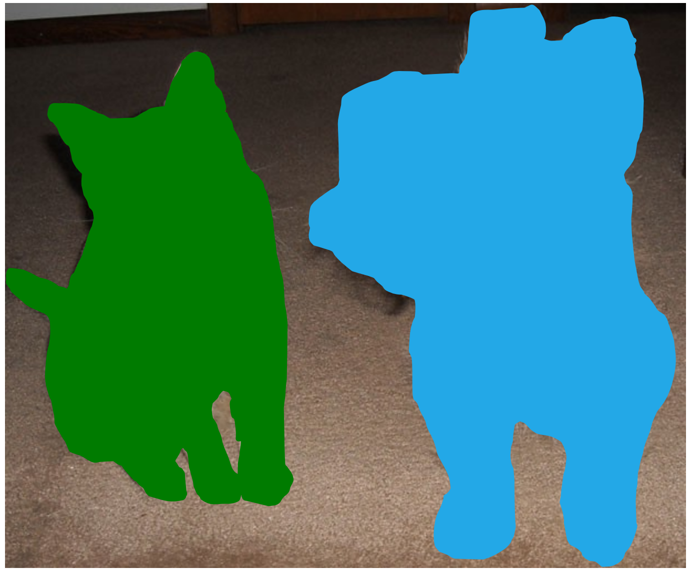


Image segmentation

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

Object detection/image segmentation

Using accuracy as a metric:

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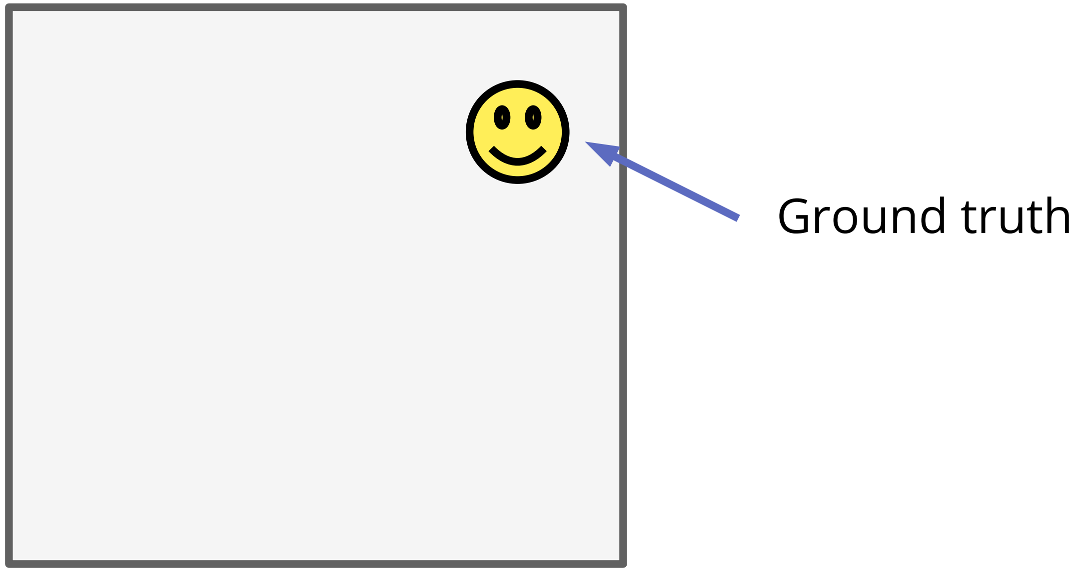

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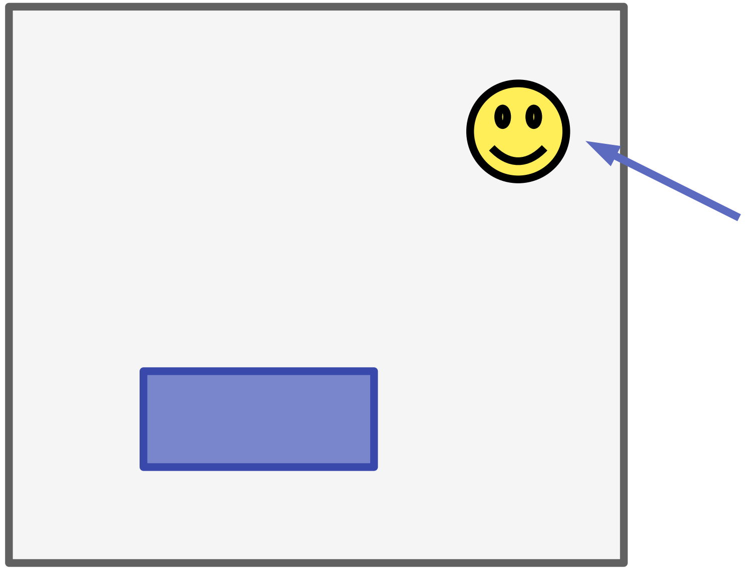
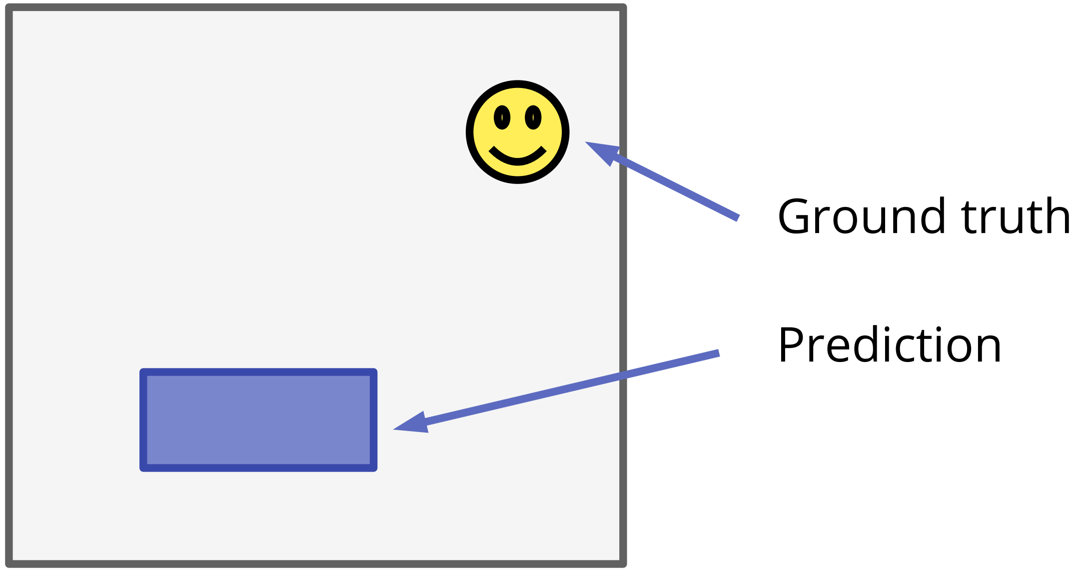


Ground truth

Object detection/image segmentation

Using accuracy as a metric:



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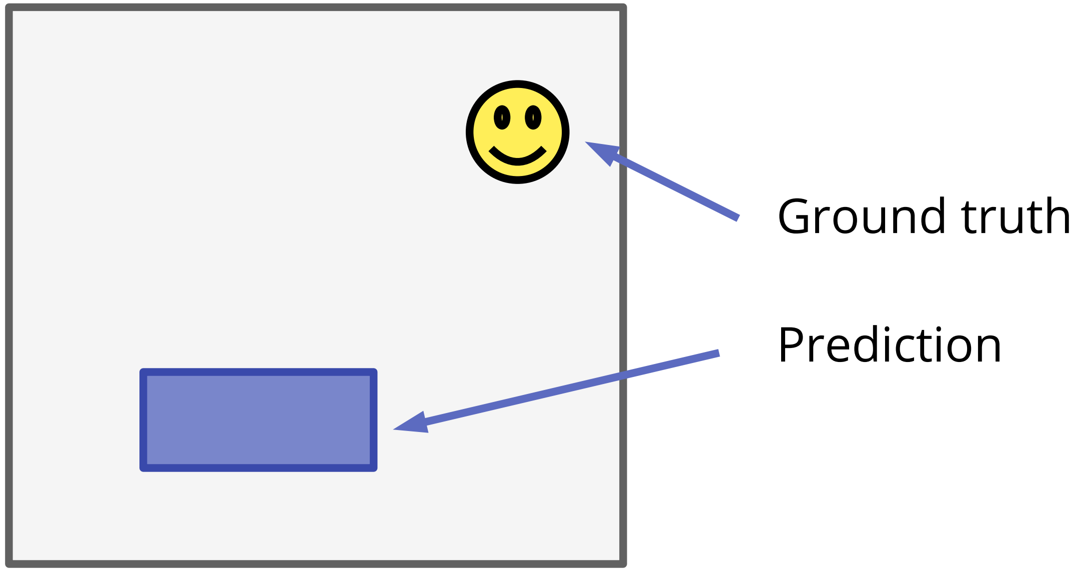

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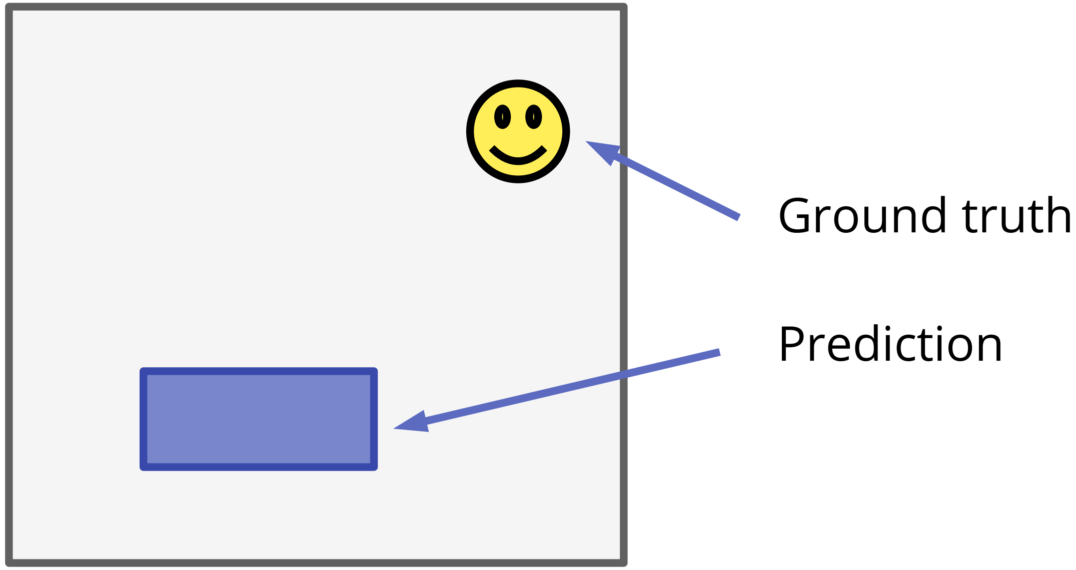

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Nevertheless, ~90% of all pixels in the image have correct predictions (“no smiley”).

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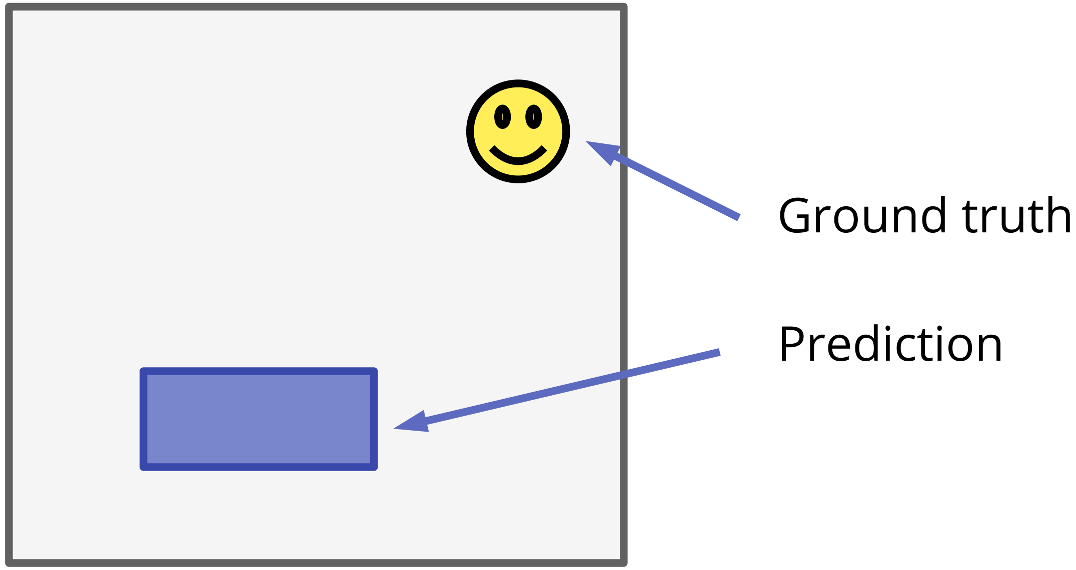

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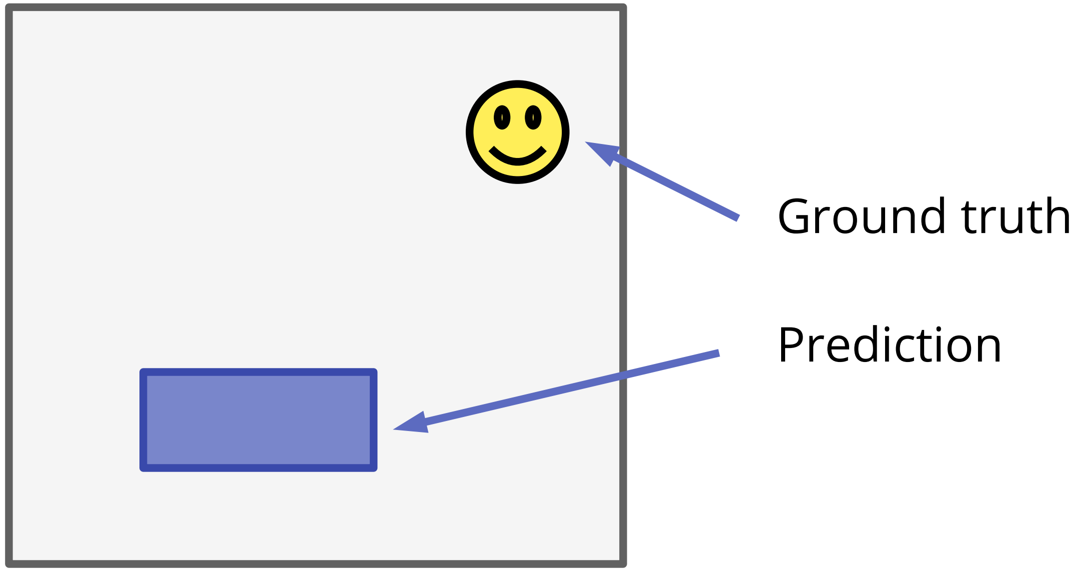

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Accuracy is a bad metric for object detection and image segmentation tasks.

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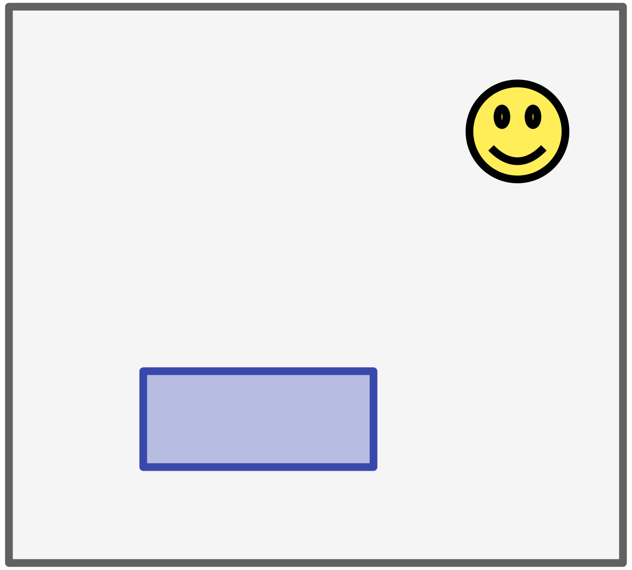

The blue box is a poor prediction and should result in a score of zero.

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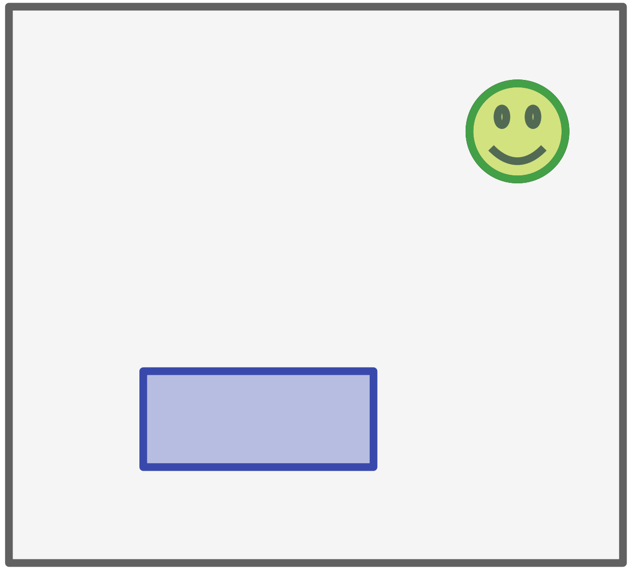

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The green circle is an excellent prediction and should result in a score of one.

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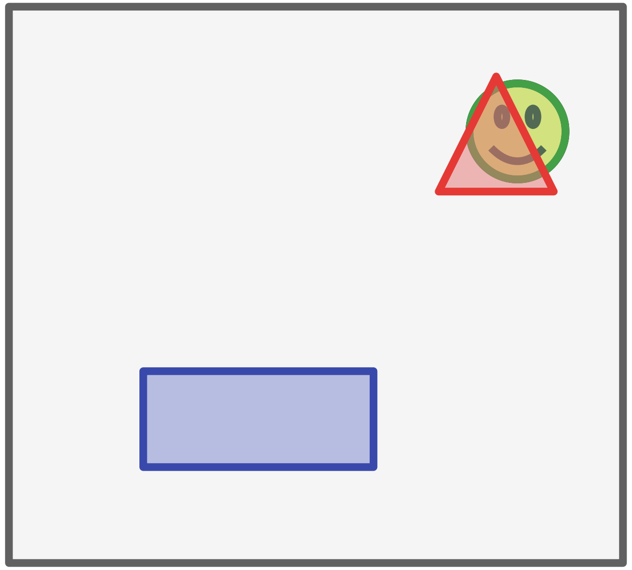

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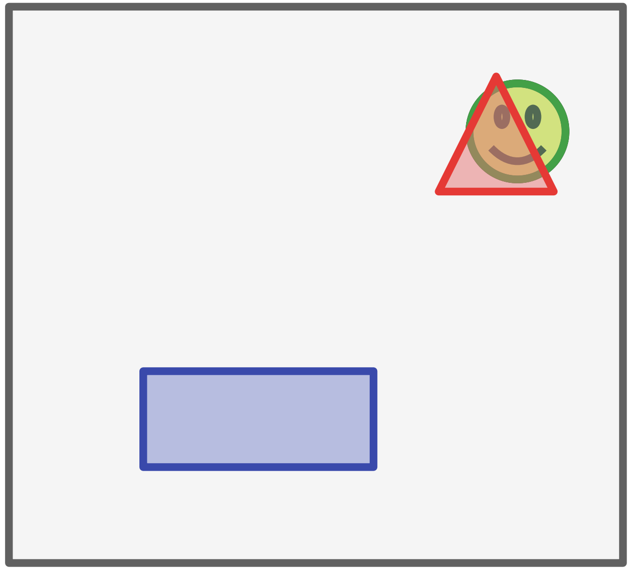

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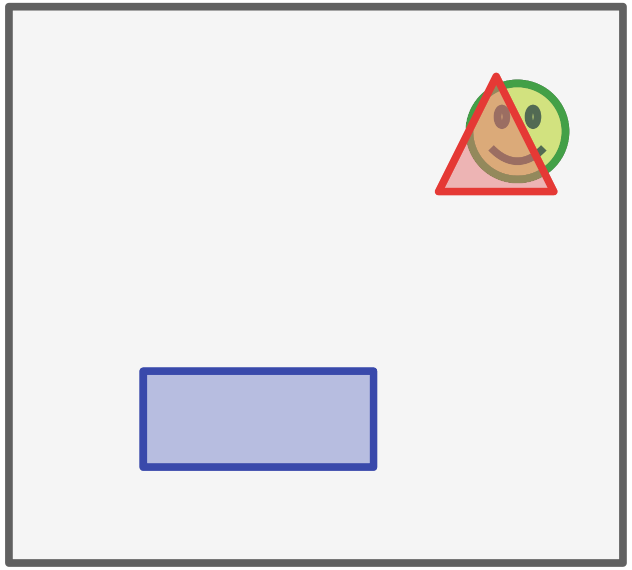
Can we define a metric that formulates this schema as an equation?

Intersection over union metric



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

Green circle: intersection = union → IoU = 1

Red triangle: intersection ~ 0.5 * union → IoU ~ 0.5

Blue box: intersection = 0 → IoU = 0

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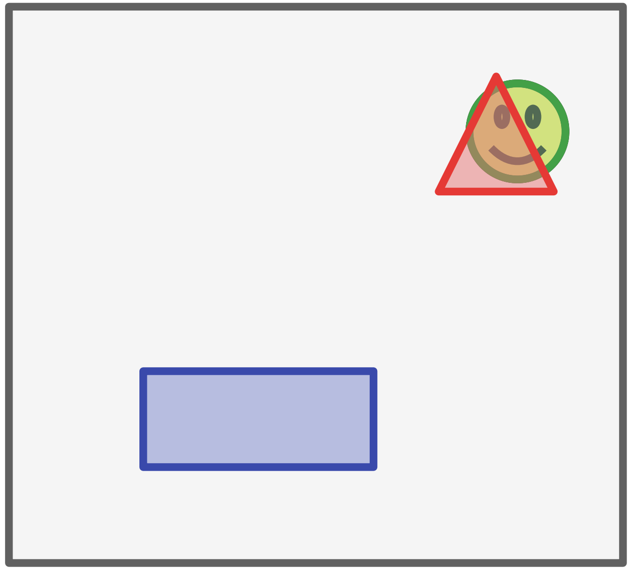

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IoU is highly flexible with respect to shape. However, it is undefined if there is a prediction where there is no ground truth. Nevertheless, it is a good metric for object detection and image segmentation.

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

That's all folks!