Lecture 3: Supervised Learning

Machine Learning (BBWL)

Michael Mommert, University of St. Gallen

Today’s lecture

Supervised learning setup

Supervised learning concepts

Benchmarking and metrics

Linear models

Nearest Neighbor models

Tree-based models

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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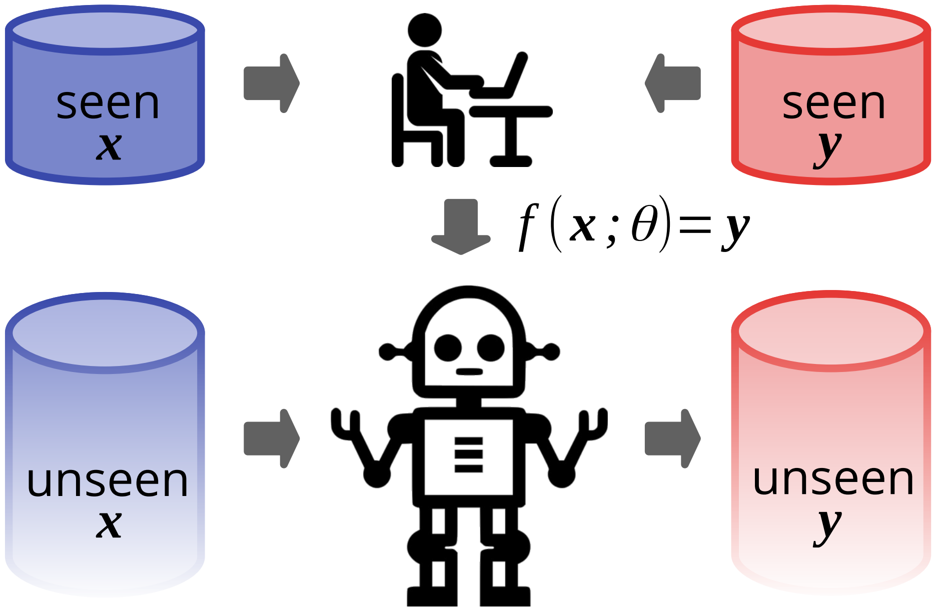

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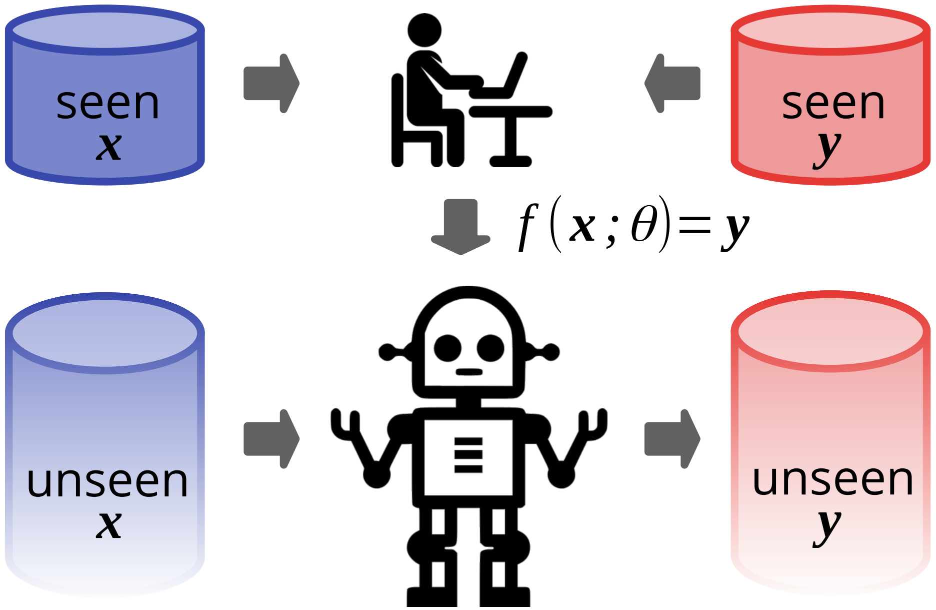

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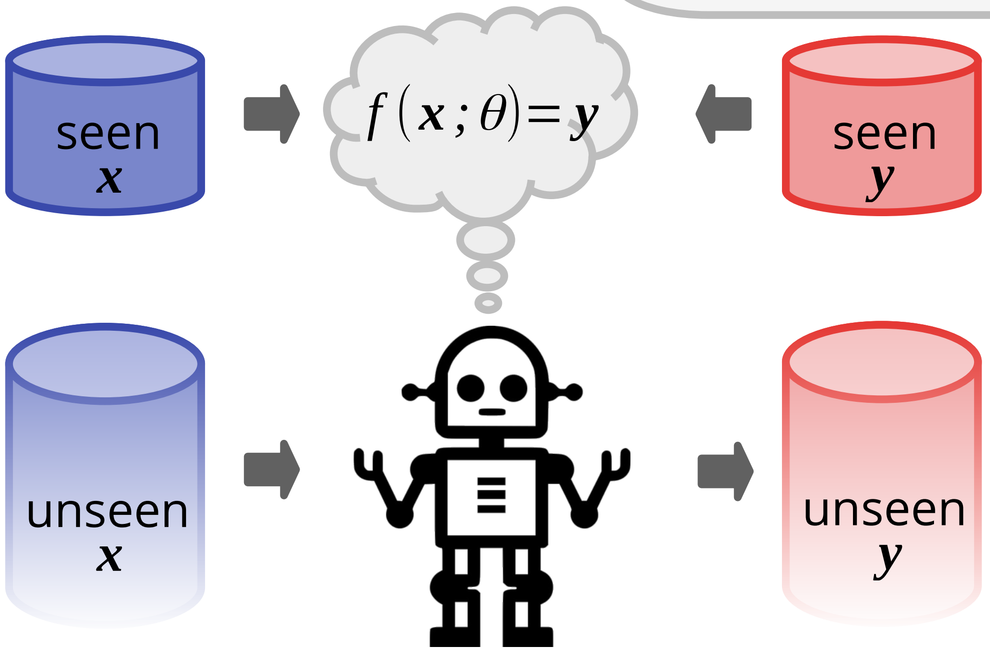
Machine-Learning Approach:



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

What tasks can ML learn?

- Classification
- Regression
- Object detection
- Segmentation
- Anomaly detection
- Synthesis

What tasks can ML learn?

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

Example:

label

classes

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

Example:

label / two classes:

Status
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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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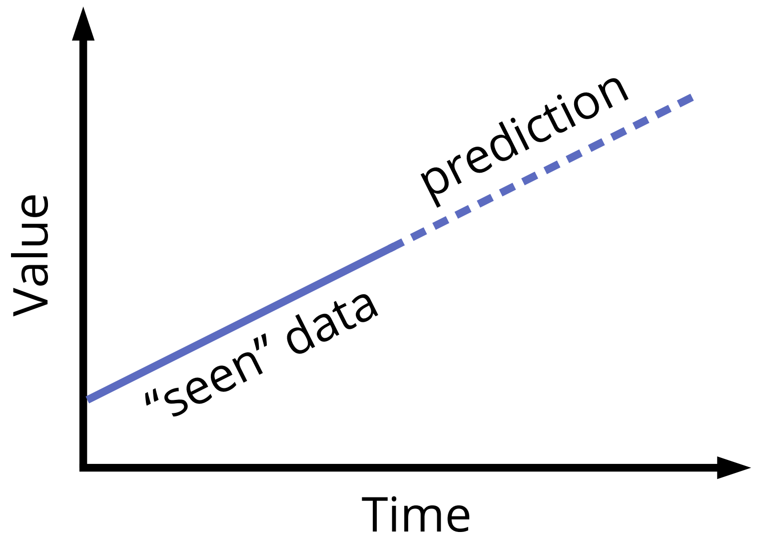
Regression:
Mapping input features to continuous variable

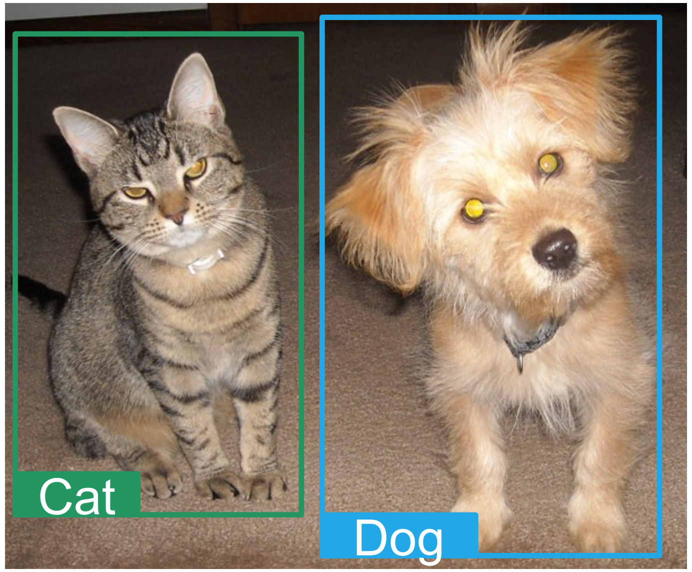
Example:



What tasks can ML learn?

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

Example:



Classification

Regression

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What tasks can ML learn?

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

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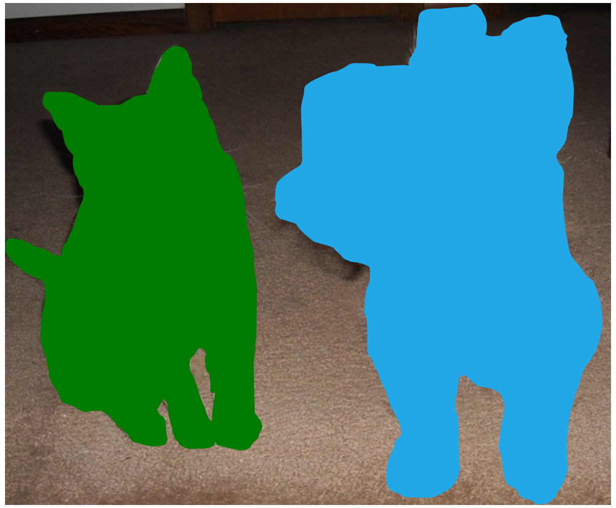

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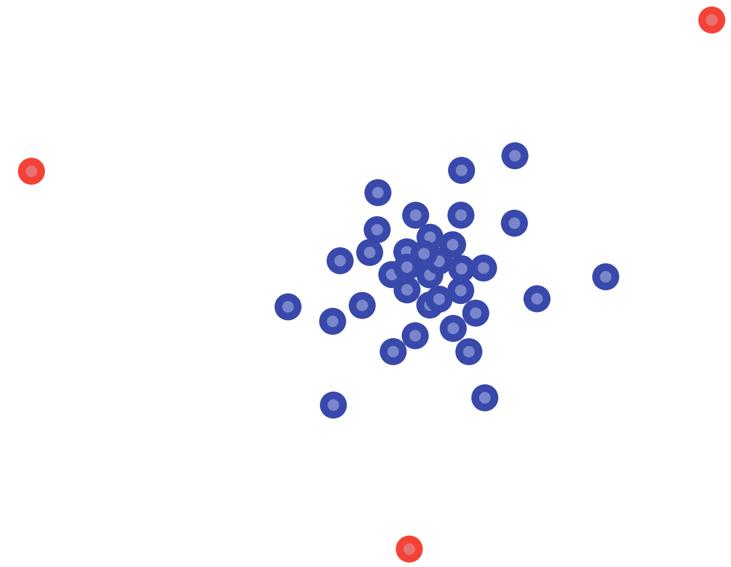
Instance segmentation:
Assign class label to each pixel of an image based on what it is showing and discriminate different instances of the class

Example:

What tasks can ML learn?

Anomaly detection:
Identify anomalous or unusual data points within a data set

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



What tasks can ML learn?

Synthesis:
Generate new data points based on a learned distribution

- Classification
- Regression
- Object detection
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What tasks can ML learn?

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Classification

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Style Transfer (Gatys et al. 2016)

What tasks can ML learn?

Synthesis:
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StyleGAN2 (Karras et al. 2020)

- Classification
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Style Transfer (Gatys et al. 2016)

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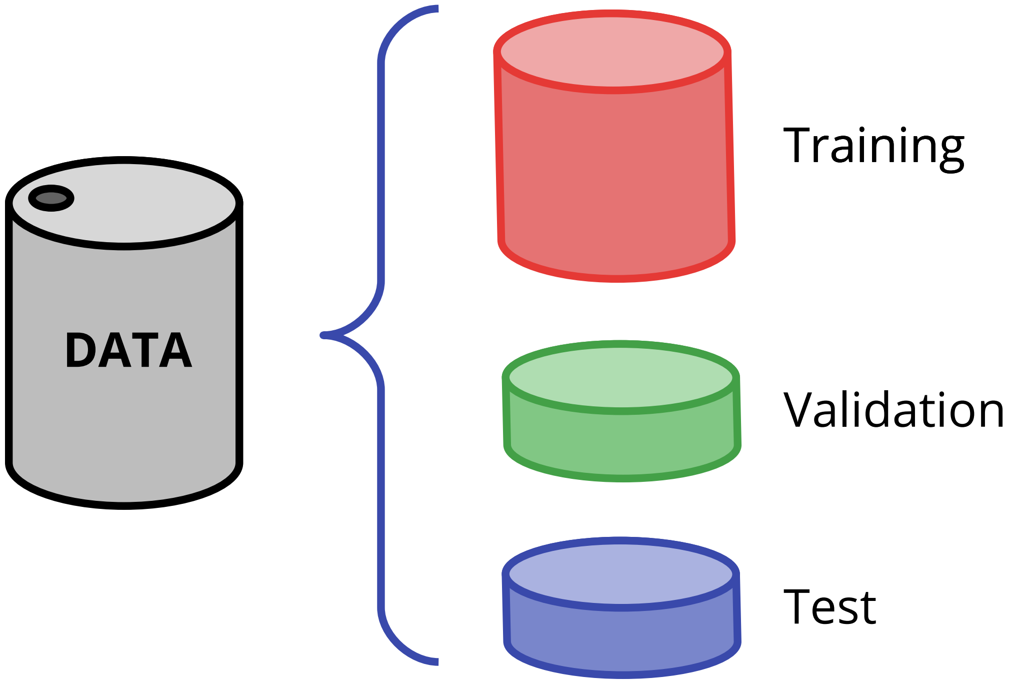
Supervised learning concepts



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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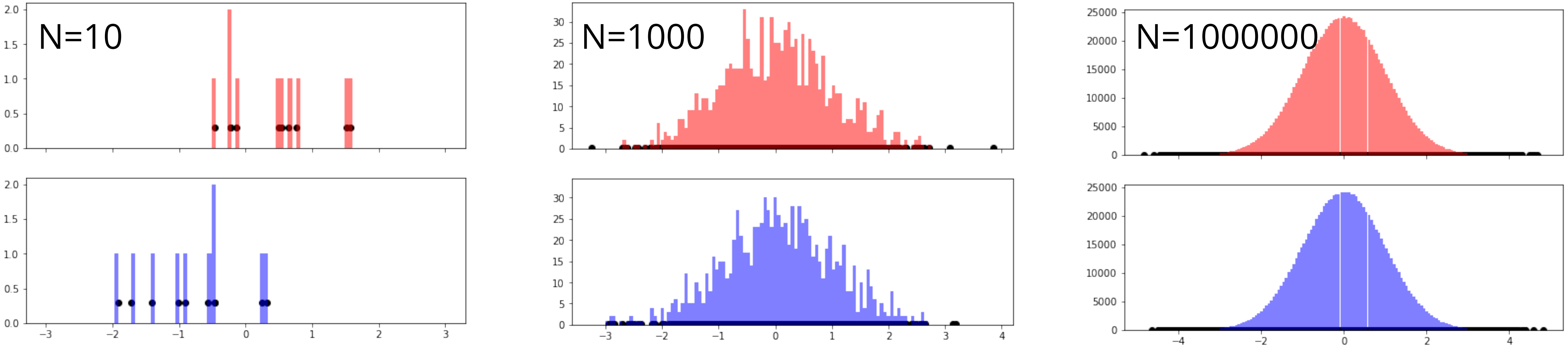

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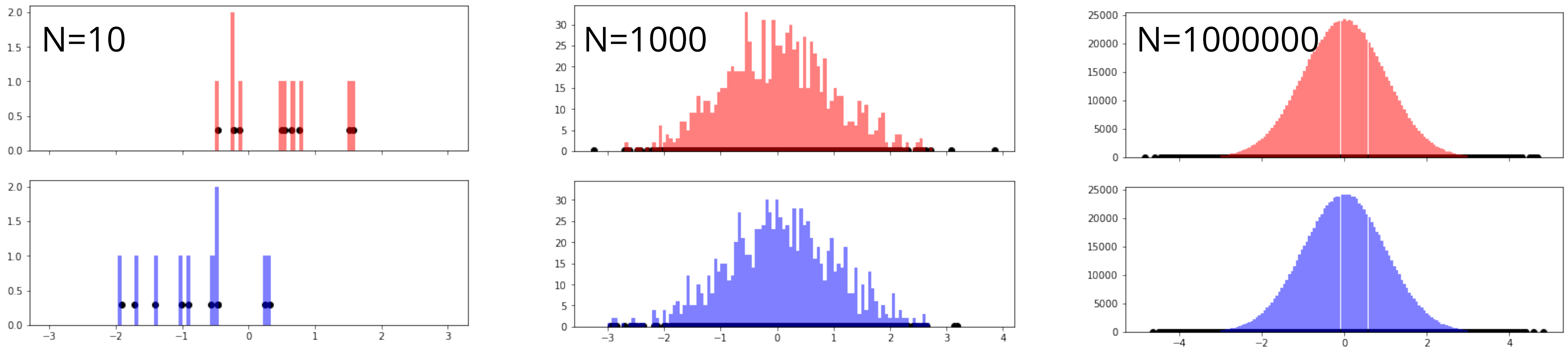
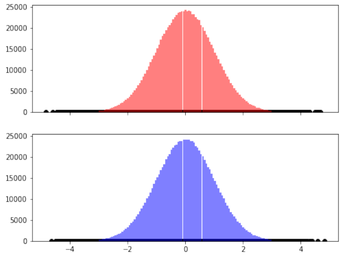


Lesson here: For small sample sizes, data sets that are iid may still differ significantly.

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.

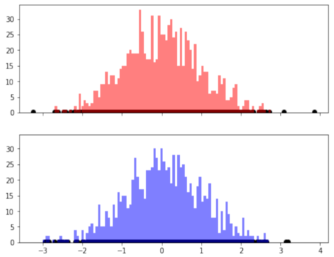
Ideally, the two distributions should be very similar:



(seen)

(unseen)

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



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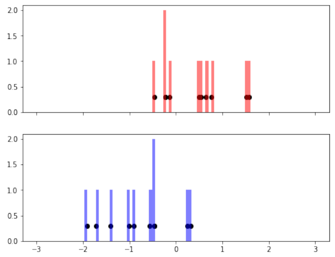

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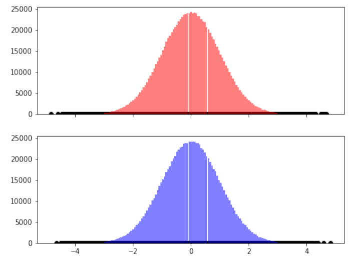

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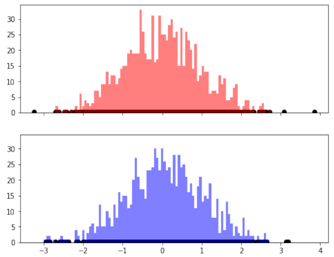

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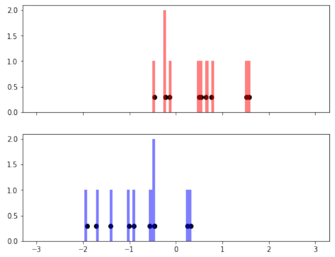
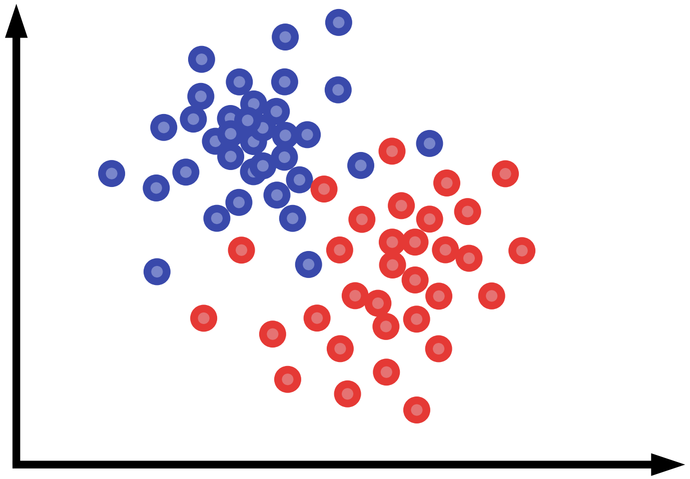


Successful training on one data set does not imply good performance on unseen data
→ the model has to **generalize** well by preventing **overfitting**

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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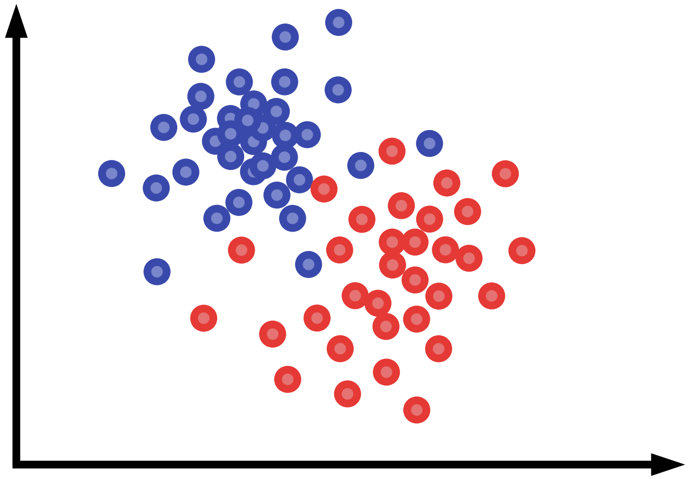

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The **decision boundary** separates the different classes as learned by the trained model.

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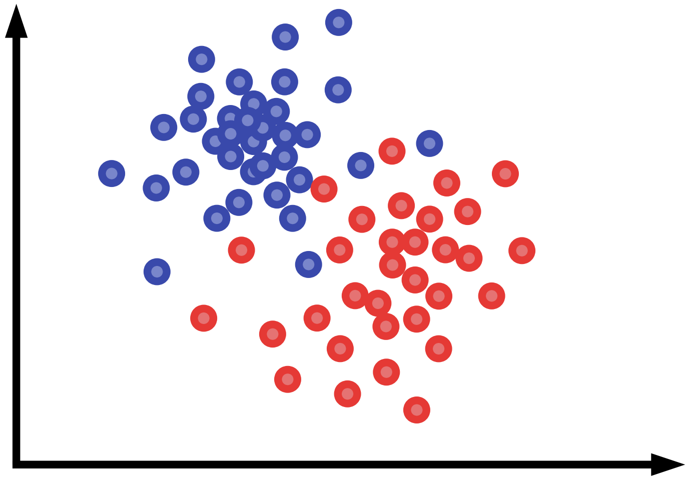

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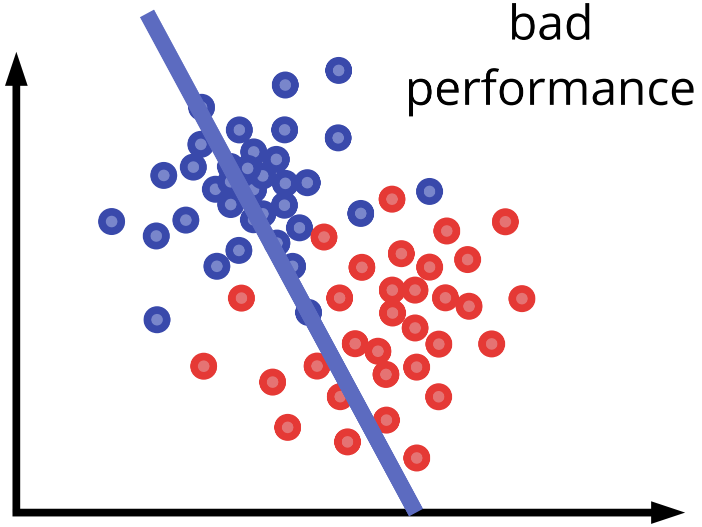

This would not be a good decision boundary as it barely allows to distinguish the two classes.

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

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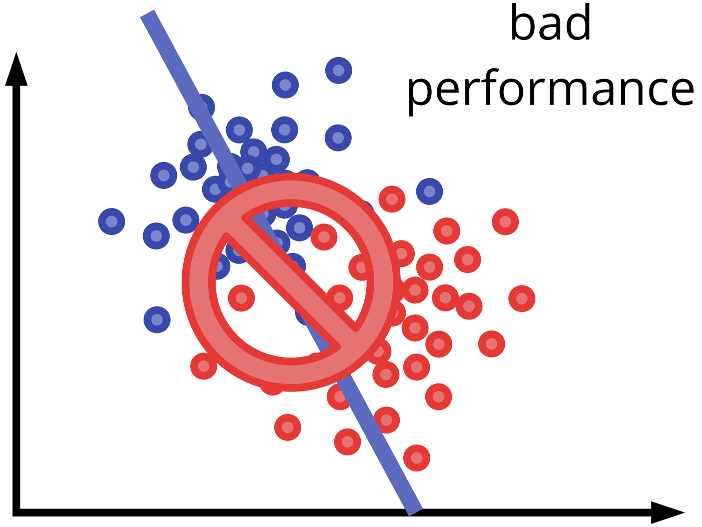

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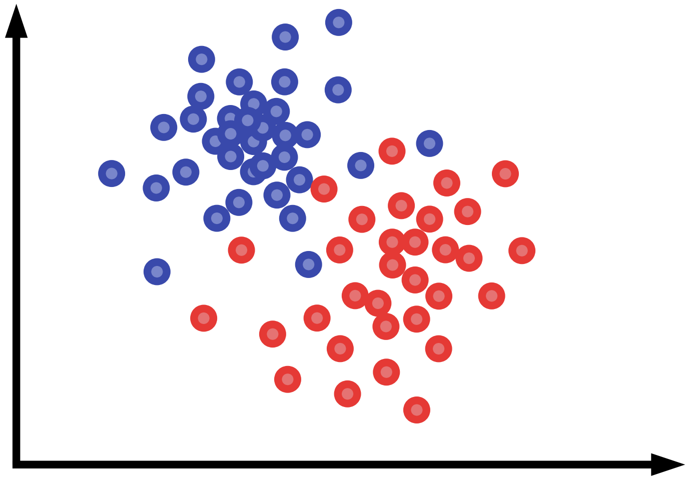

Training (seen) data

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

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

Is this good?

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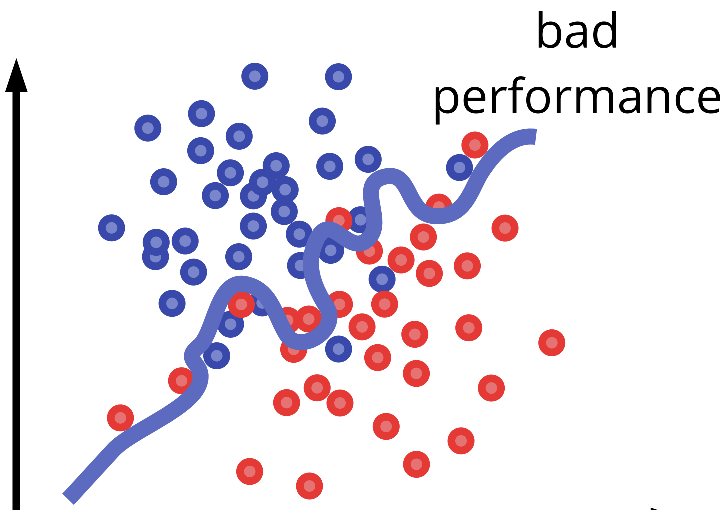
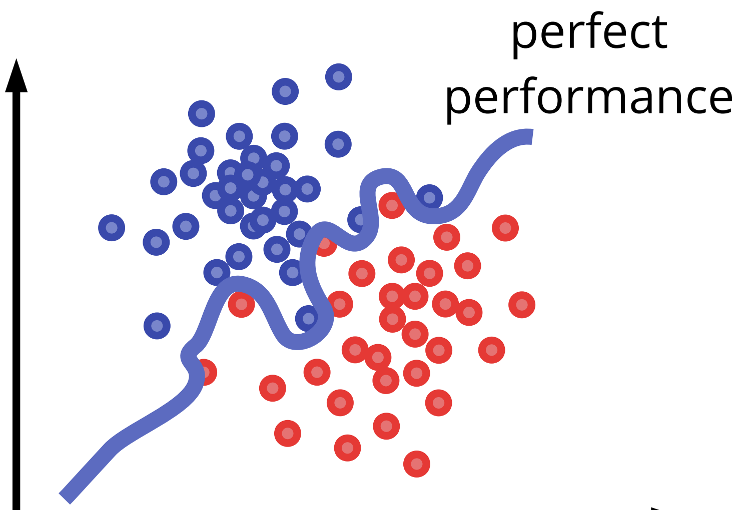


Test (unseen) data



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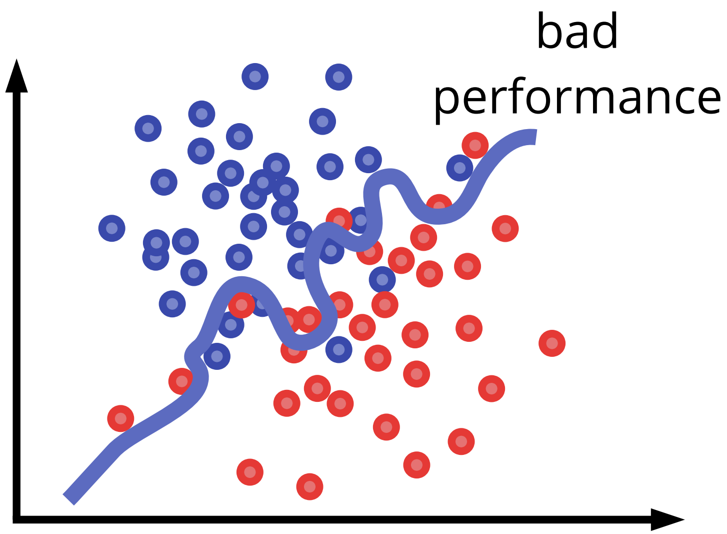

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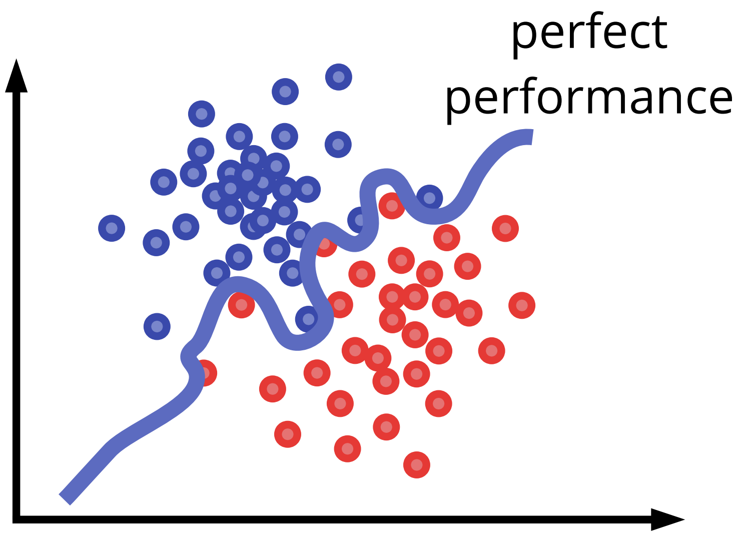

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This model is **overfitting**: it memorizes the structure of the training (seen) data and as a result **generalizes badly** on the overall data distribution.
We can improve its performance through **regularization** methods.

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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.

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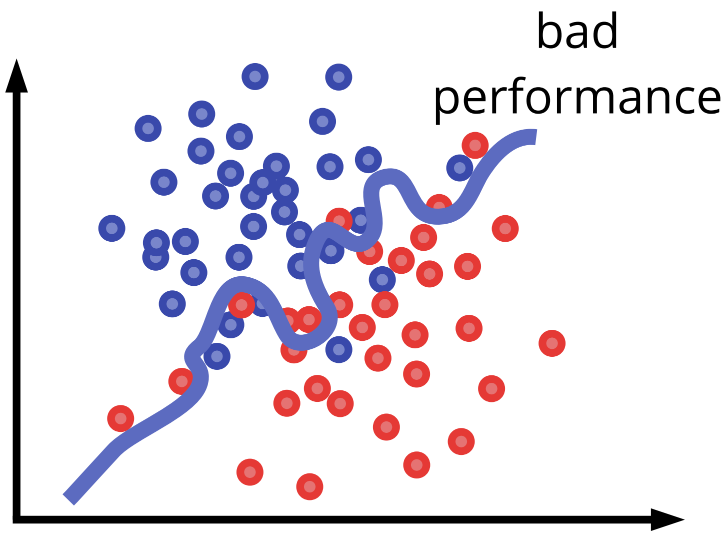

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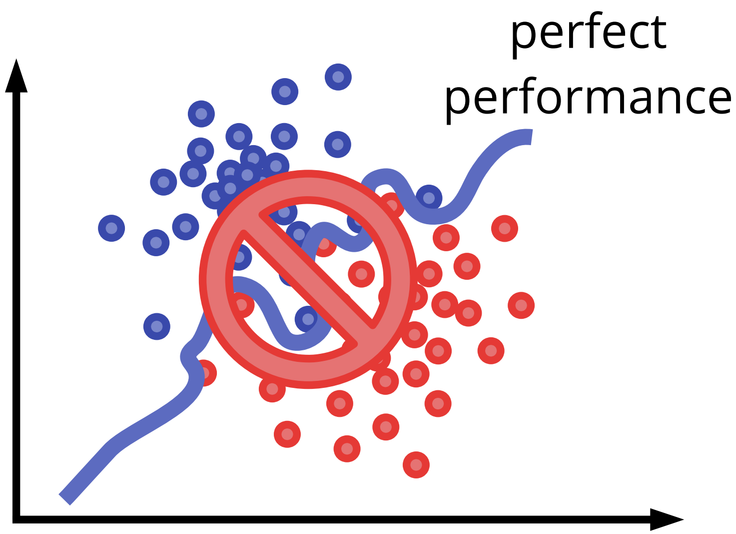

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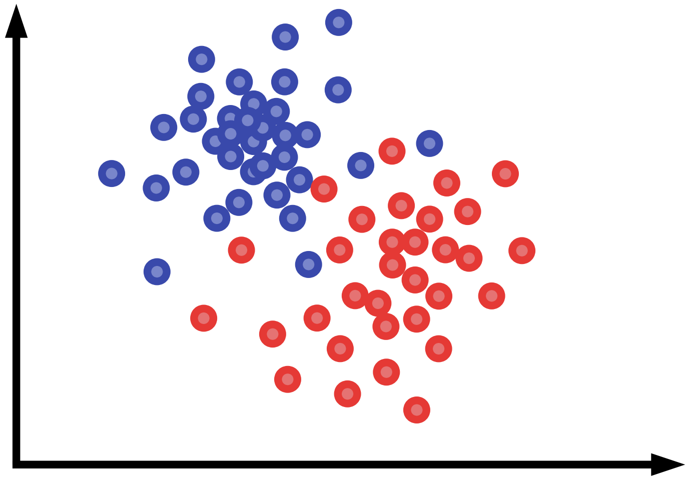

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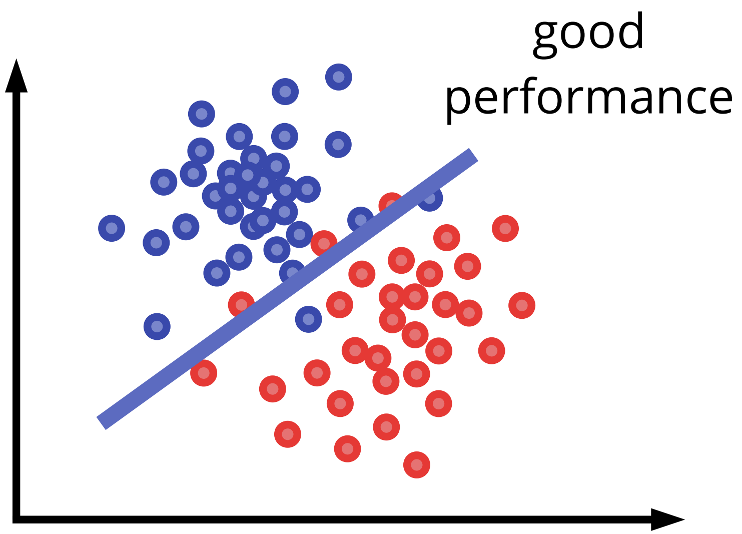

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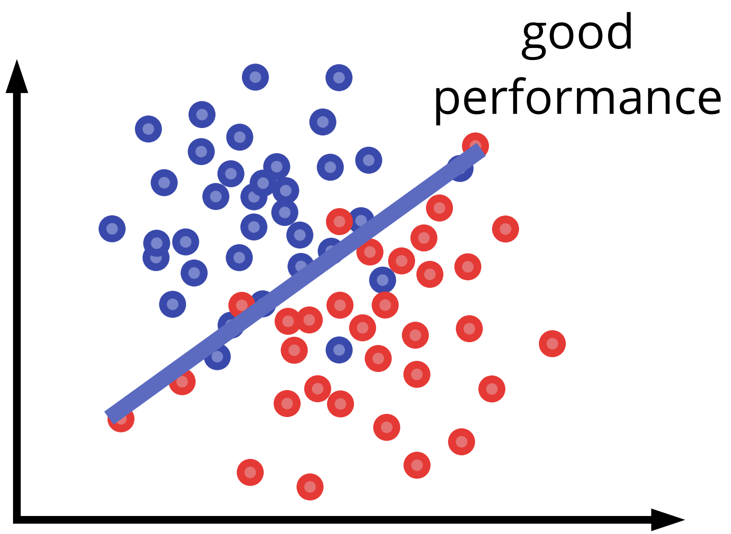

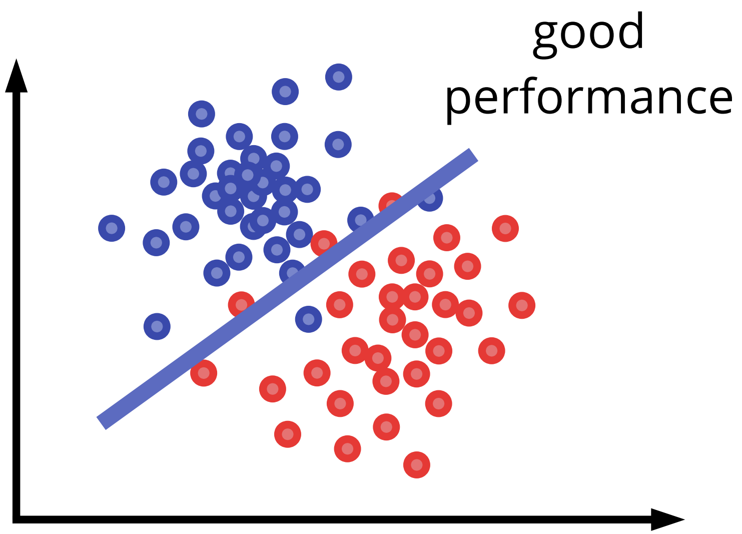

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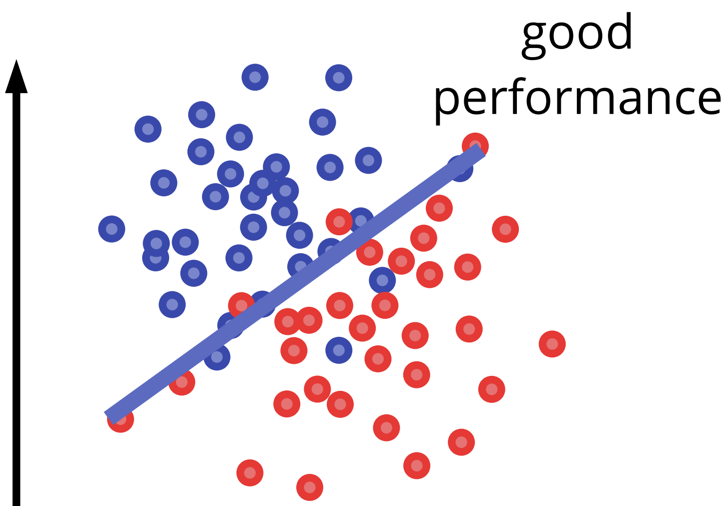

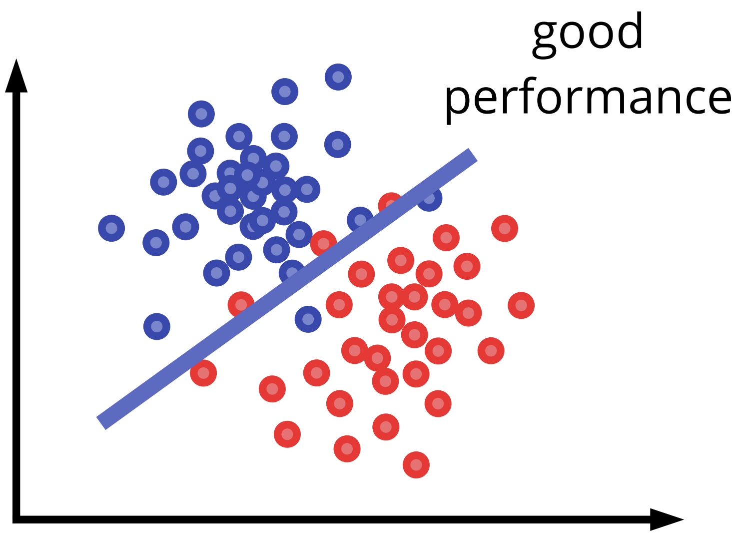

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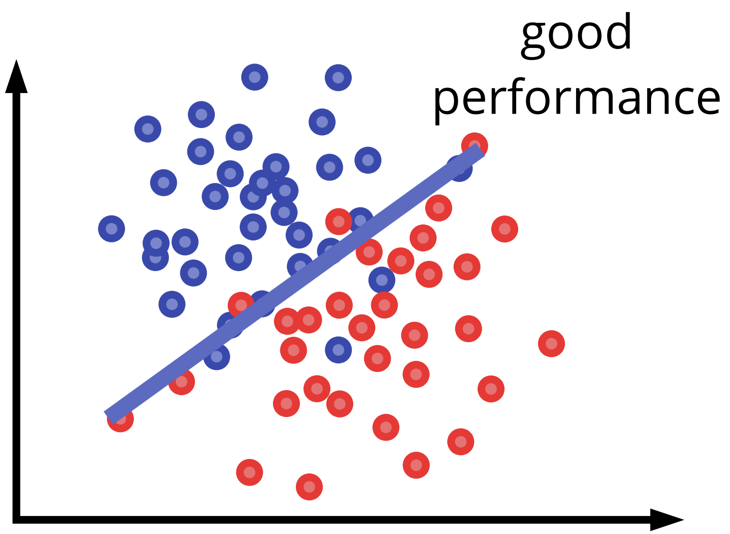

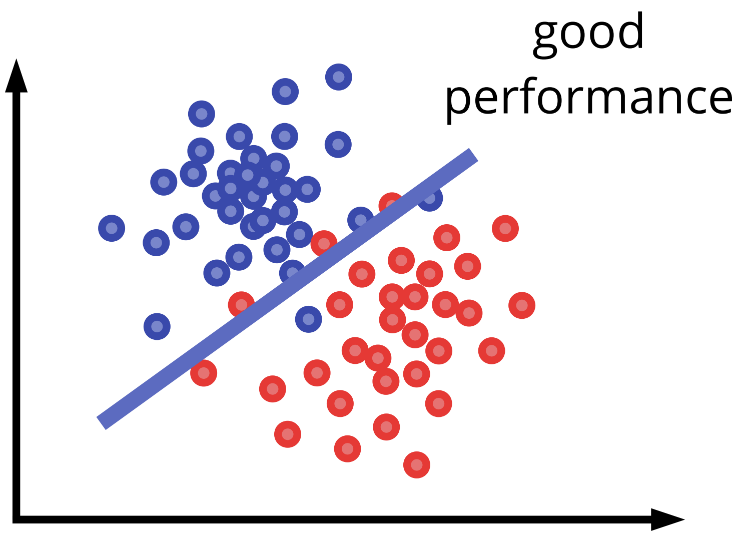

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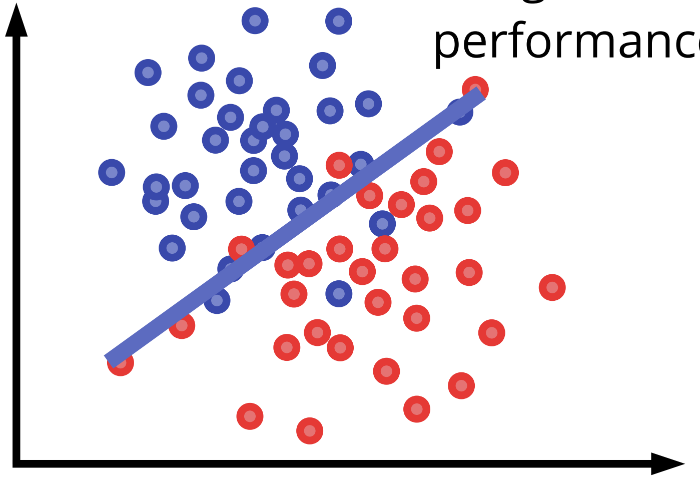

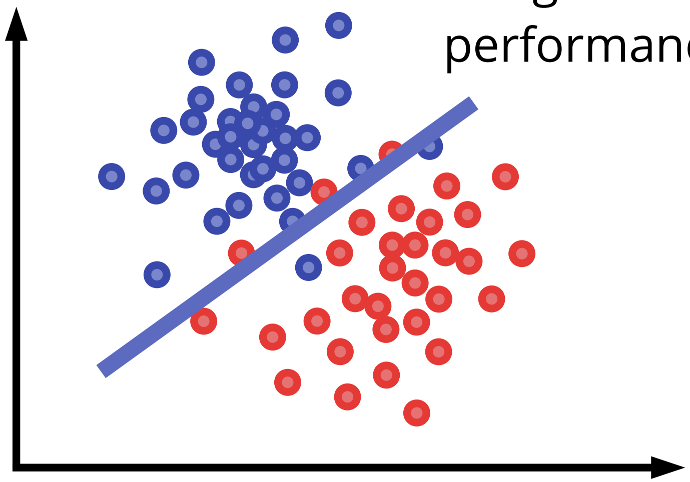

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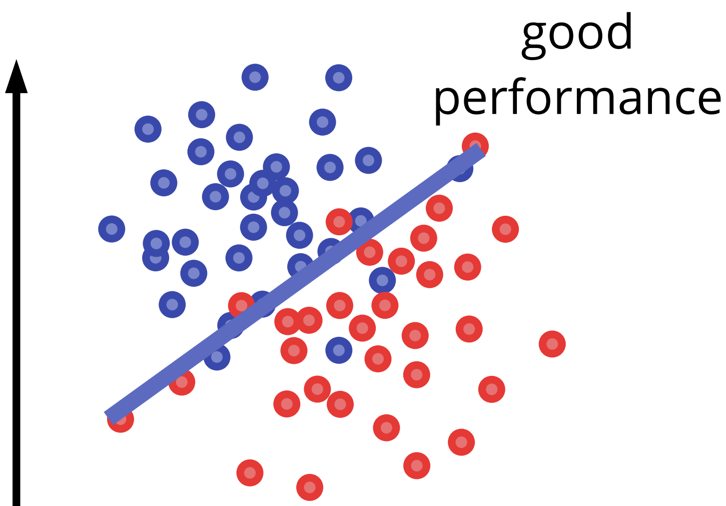

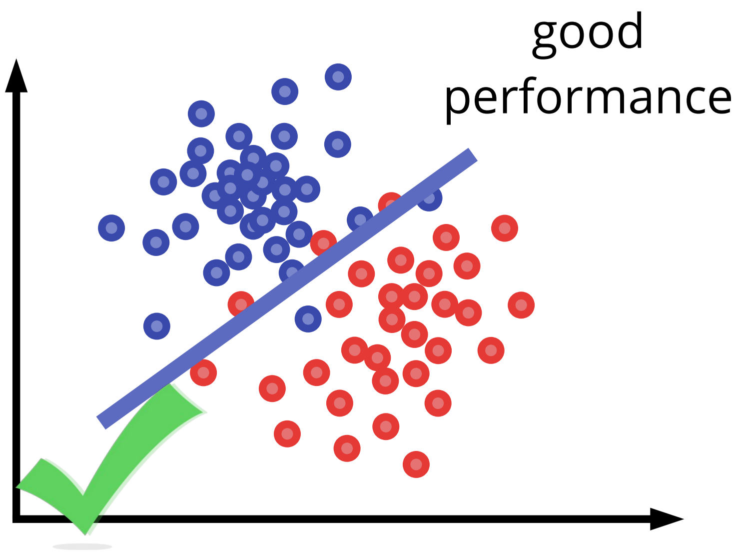

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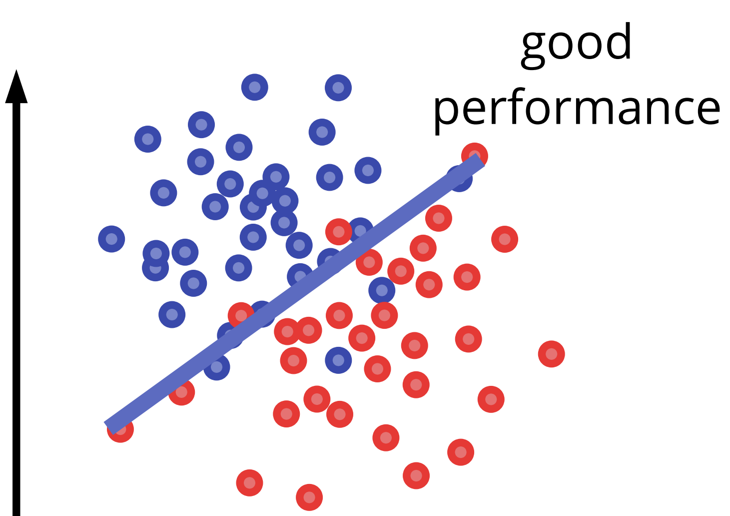

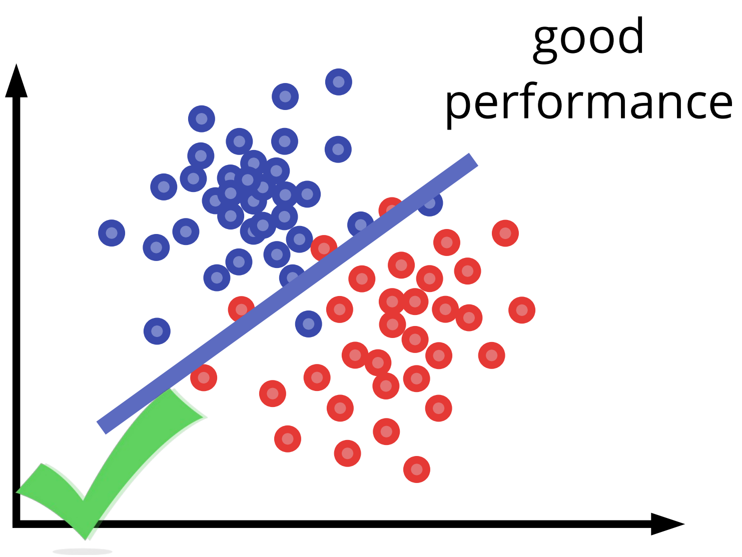

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Train/Validation/Test splits

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Entire data set

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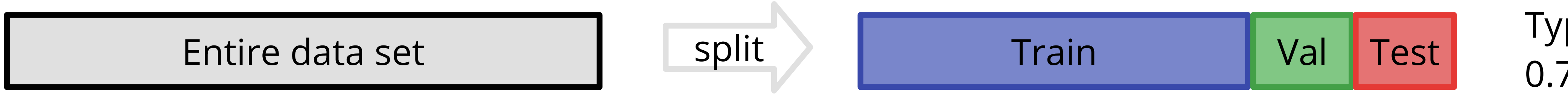

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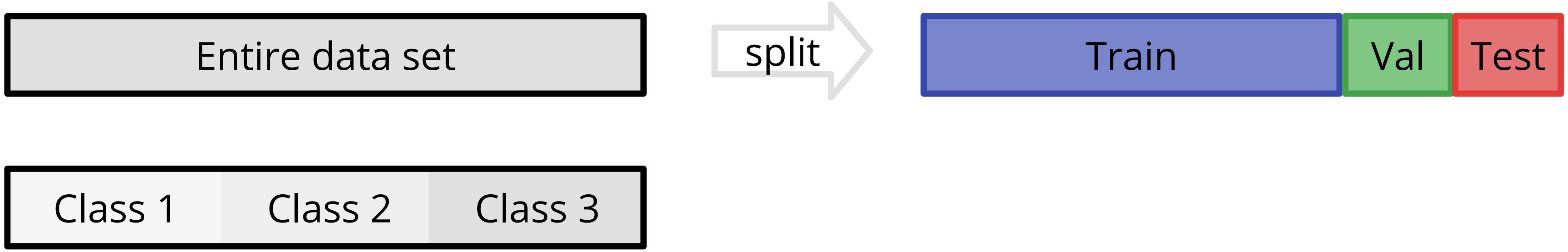

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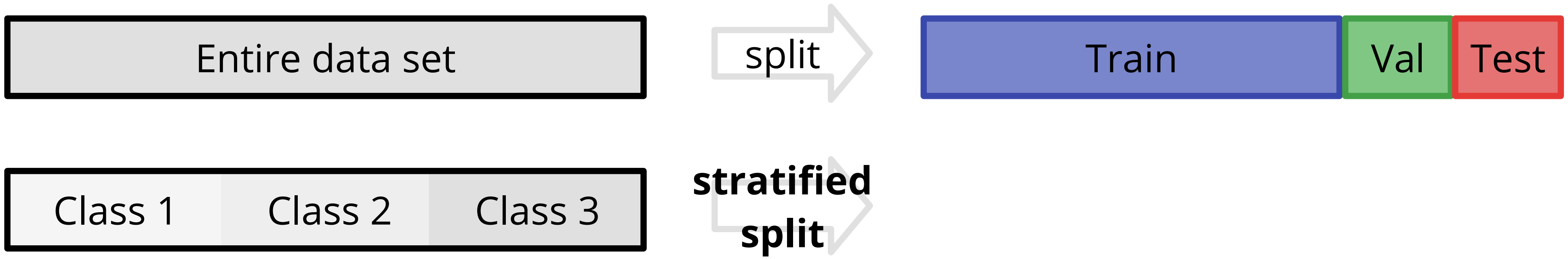

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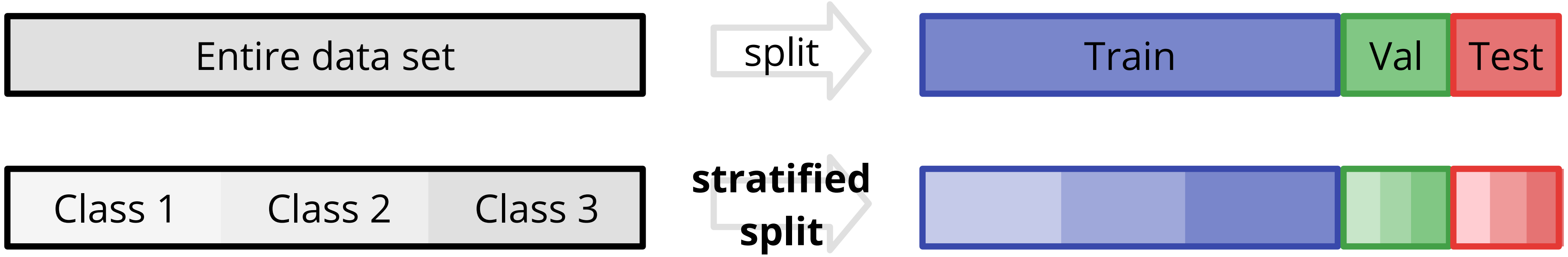

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Preserve class fractions in split data sets.

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.

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k=3
split

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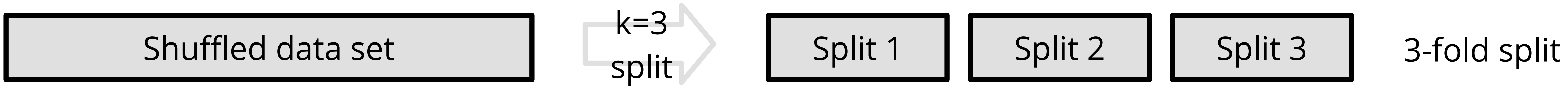

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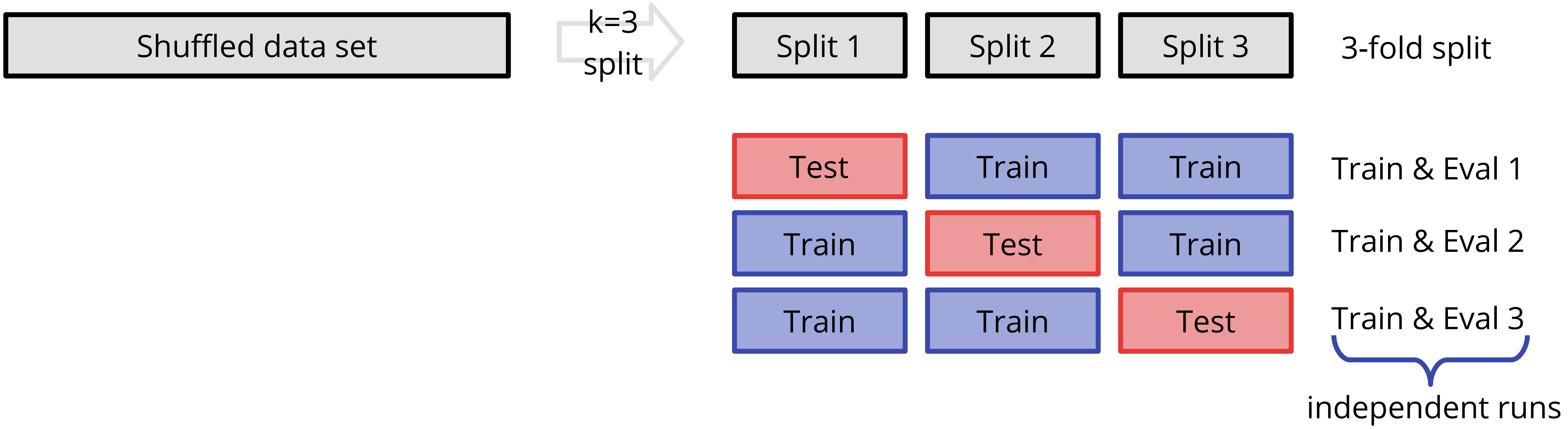

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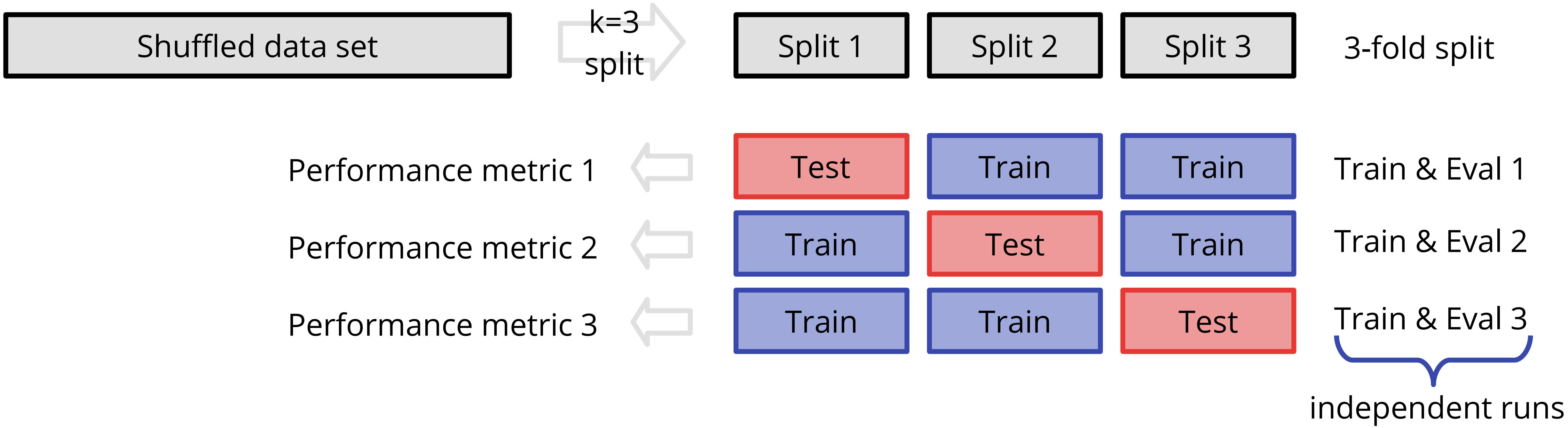

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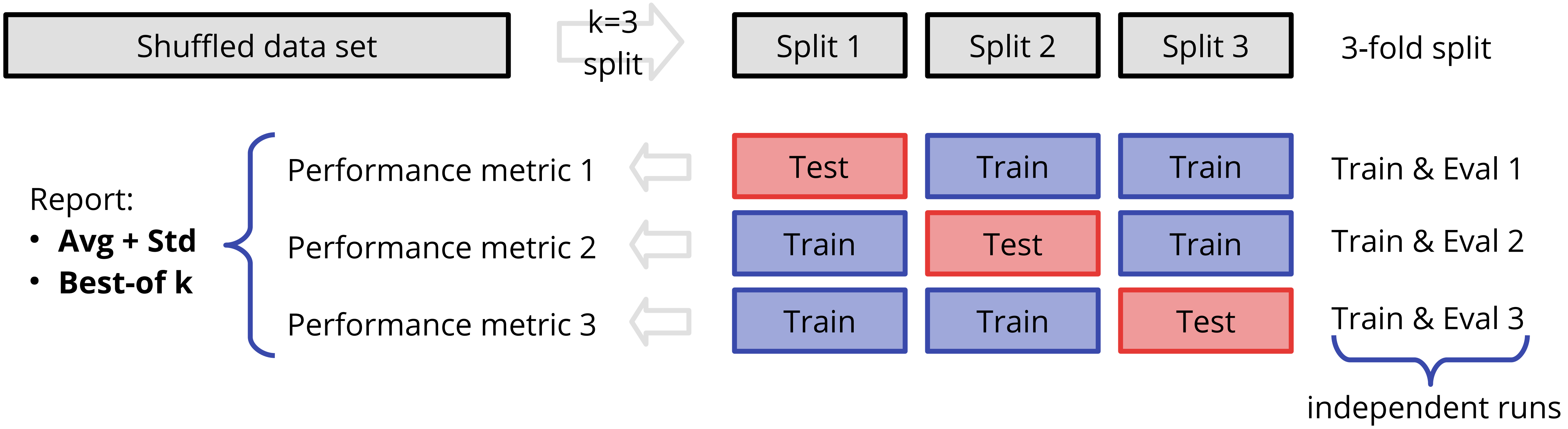

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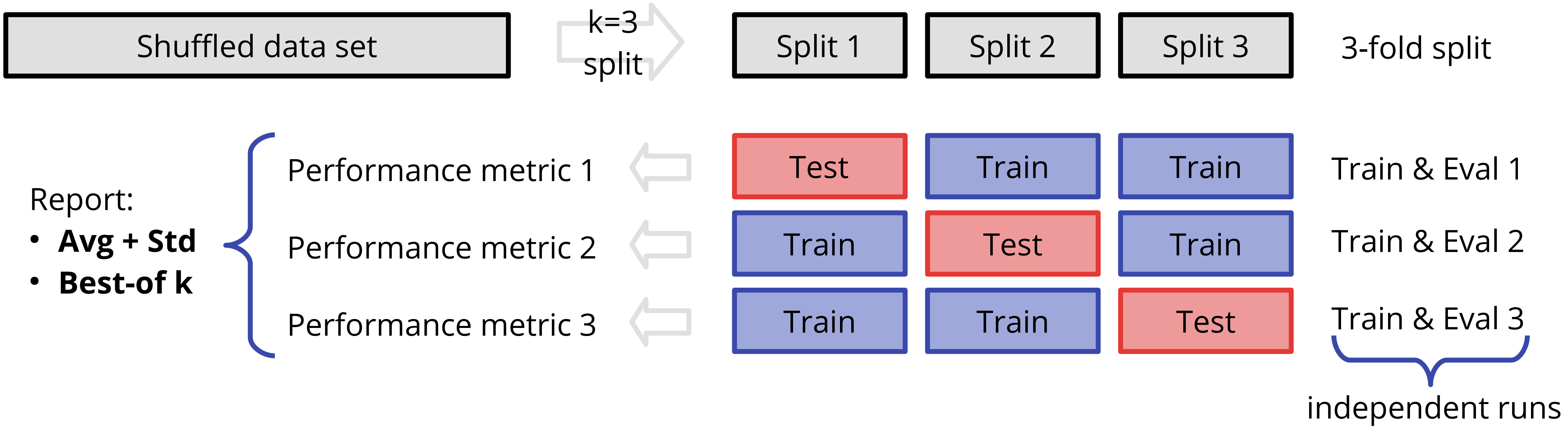
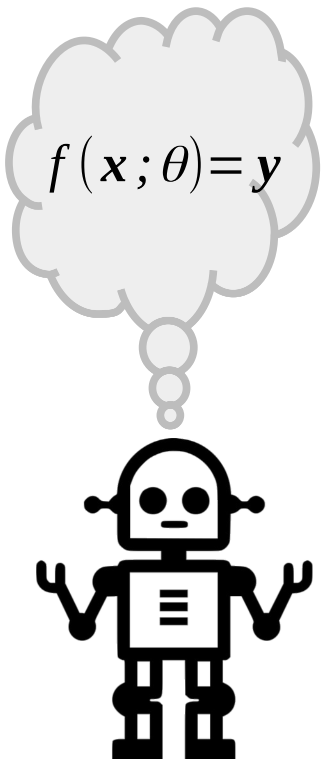


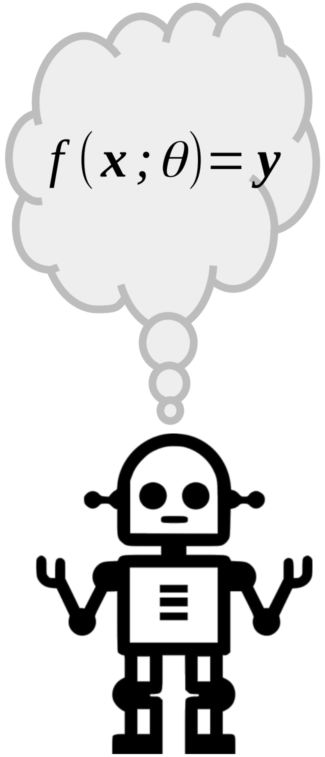
Note: Keep in mind that cross-validation will not improve your model performance;
it will simply give you a more reliable estimate of its performance.

General supervised learning pipeline



General supervised learning pipeline

1) Feature engineering: raw data → features



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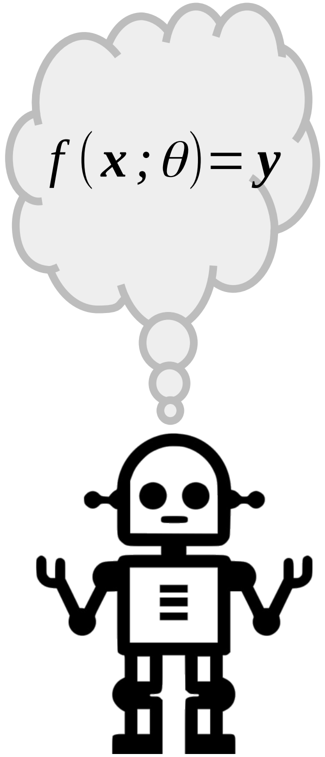

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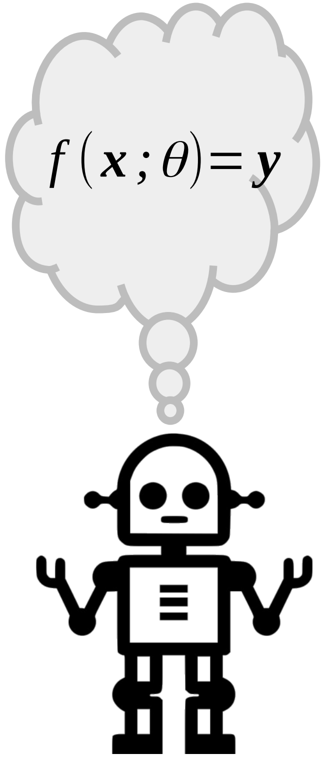
3) Data splitting → training, validation, test data



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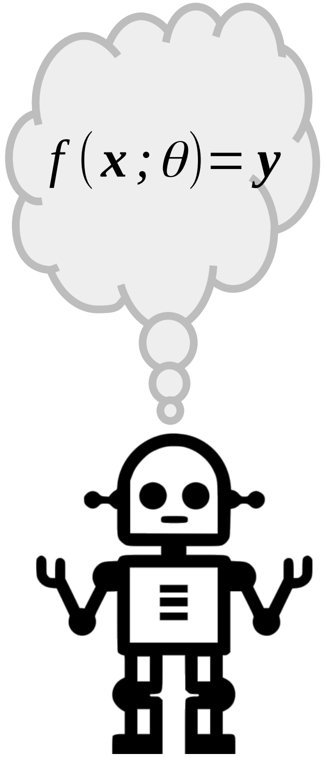

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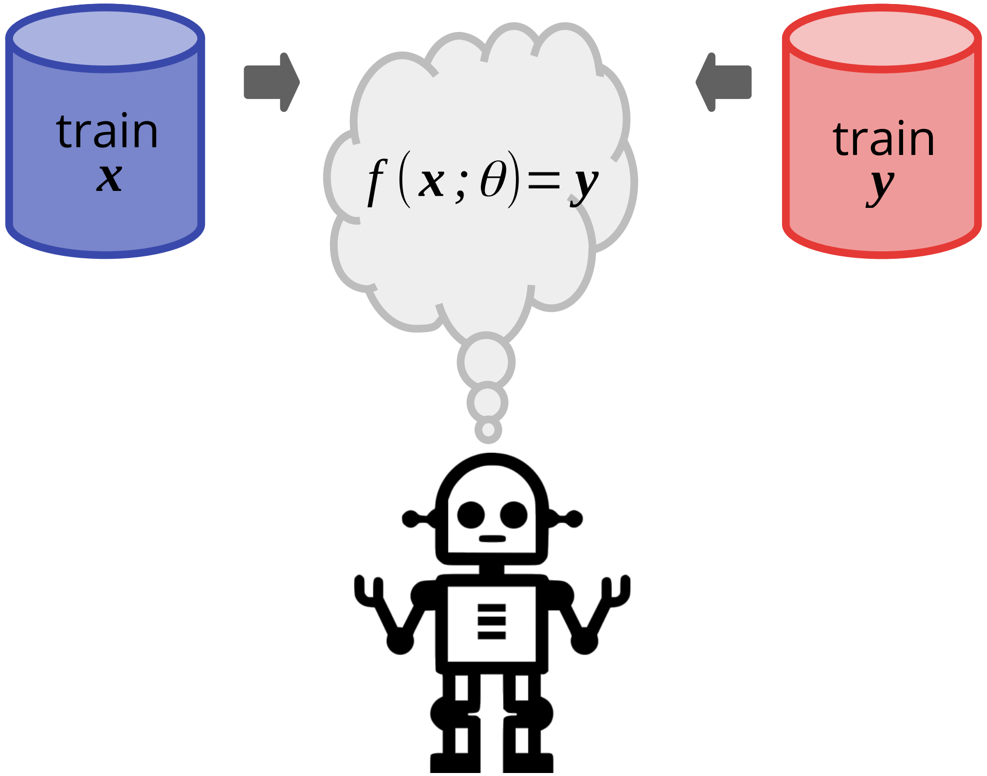

model training

General supervised learning pipeline

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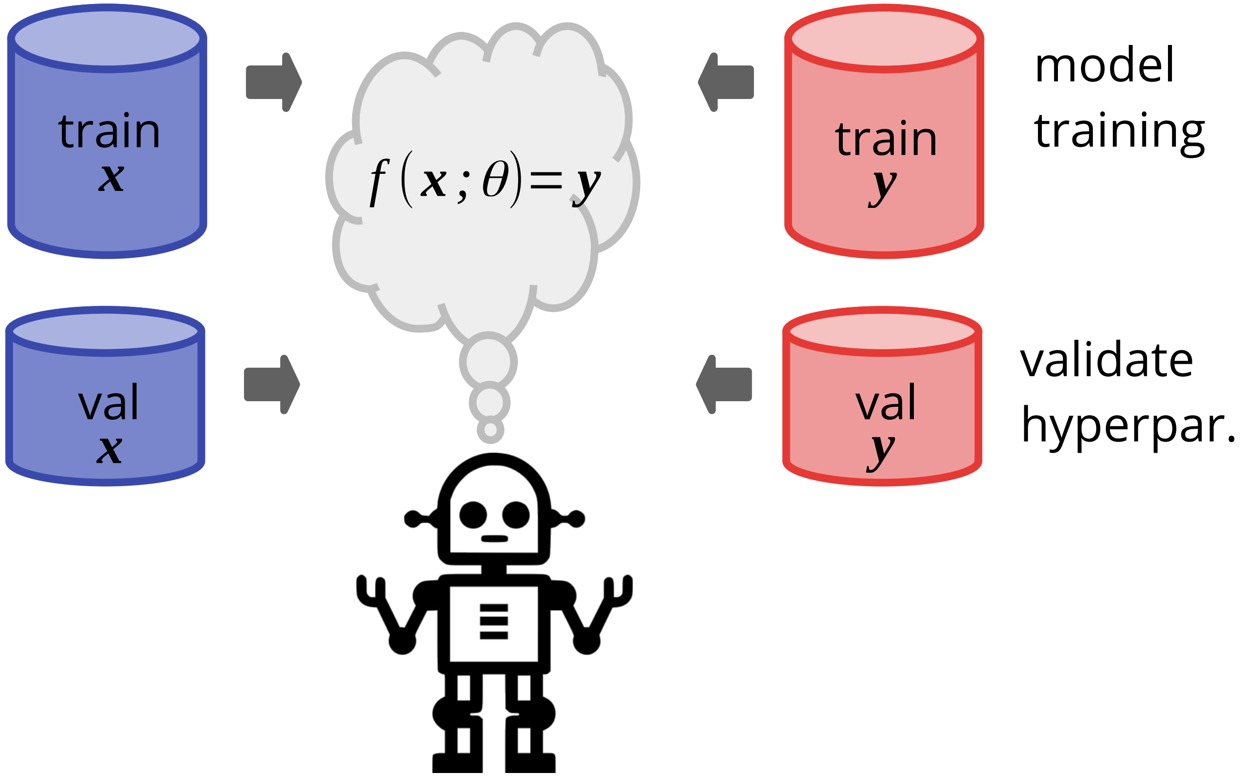

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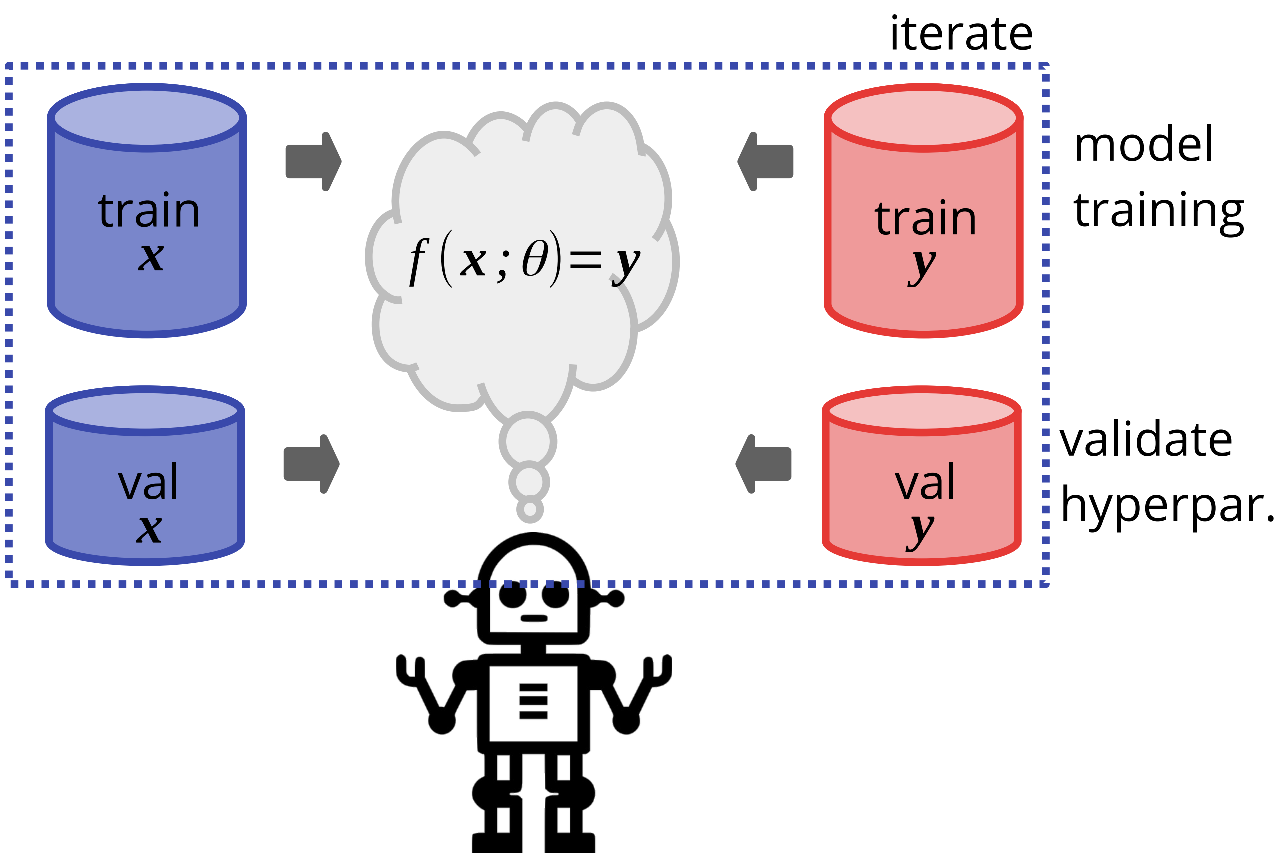

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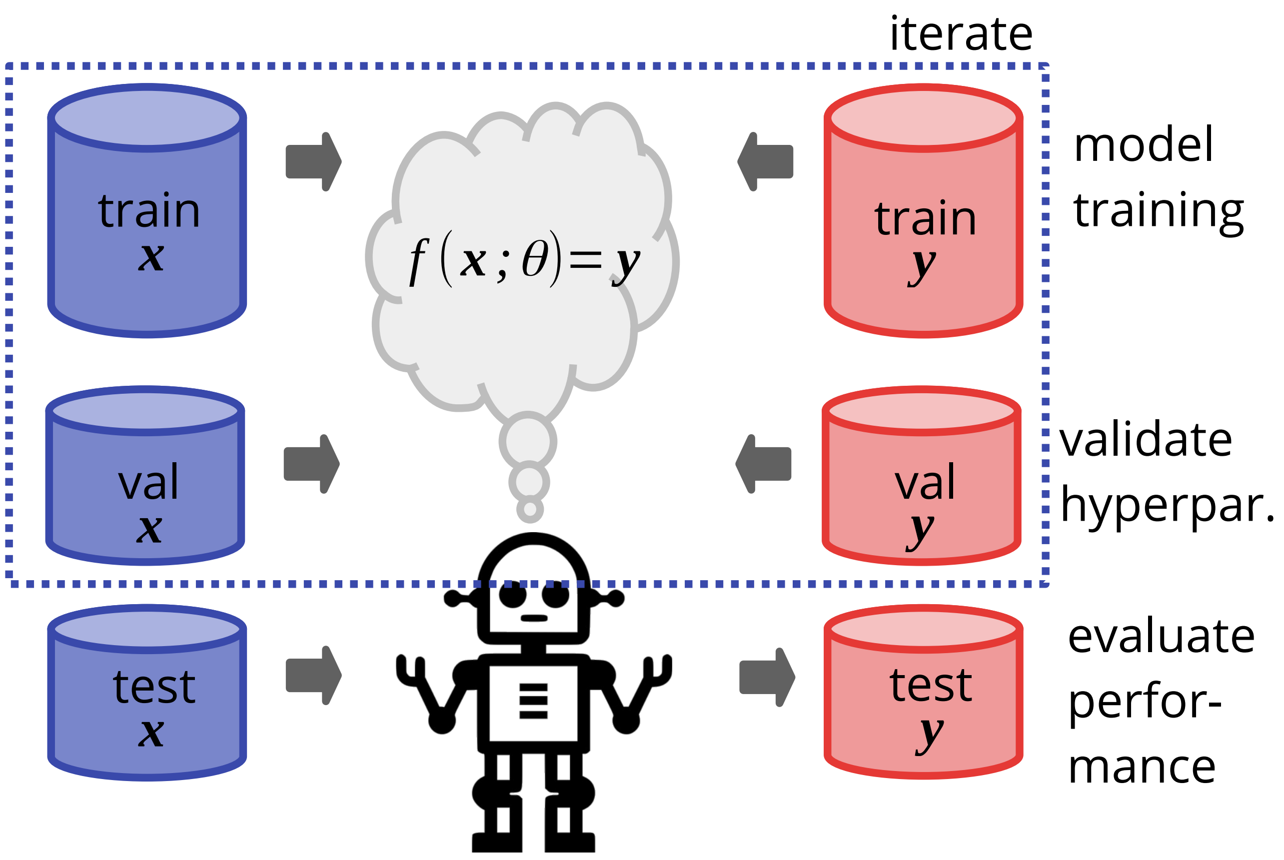
8) Evaluate trained model on test data
   → report test data performance



Benchmarking and metrics

How do we measure the performance of our model?

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:

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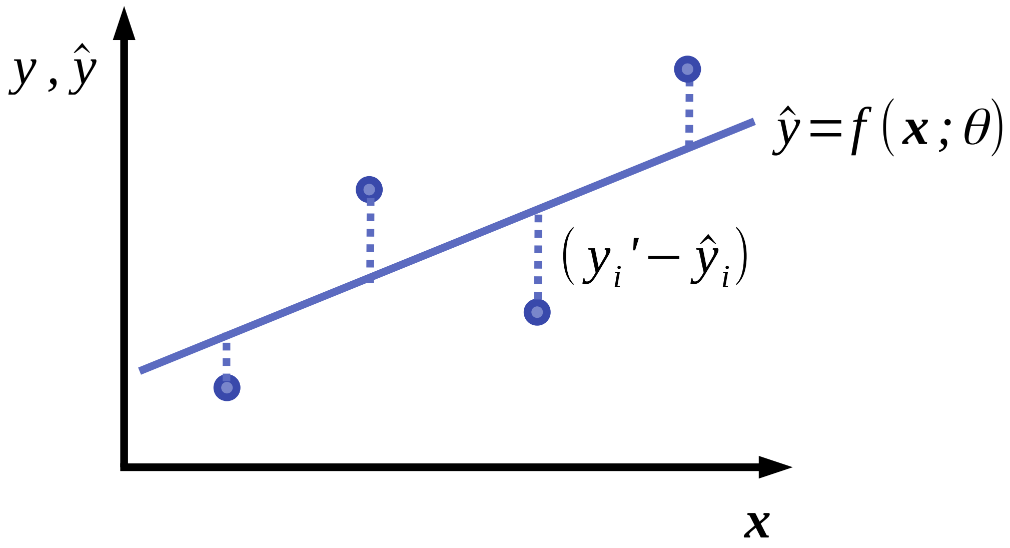
Different ML tasks require different metrics

Regression task:

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



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

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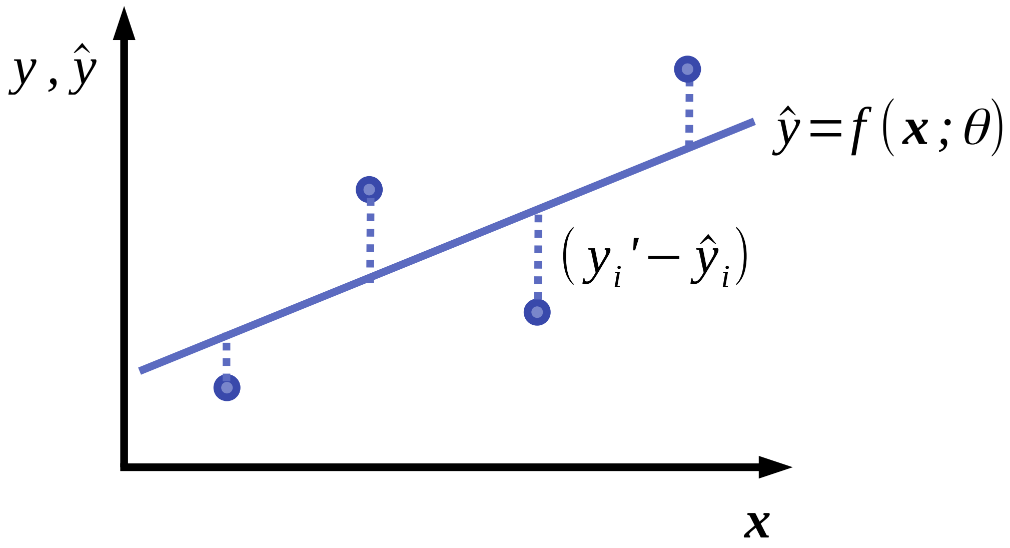

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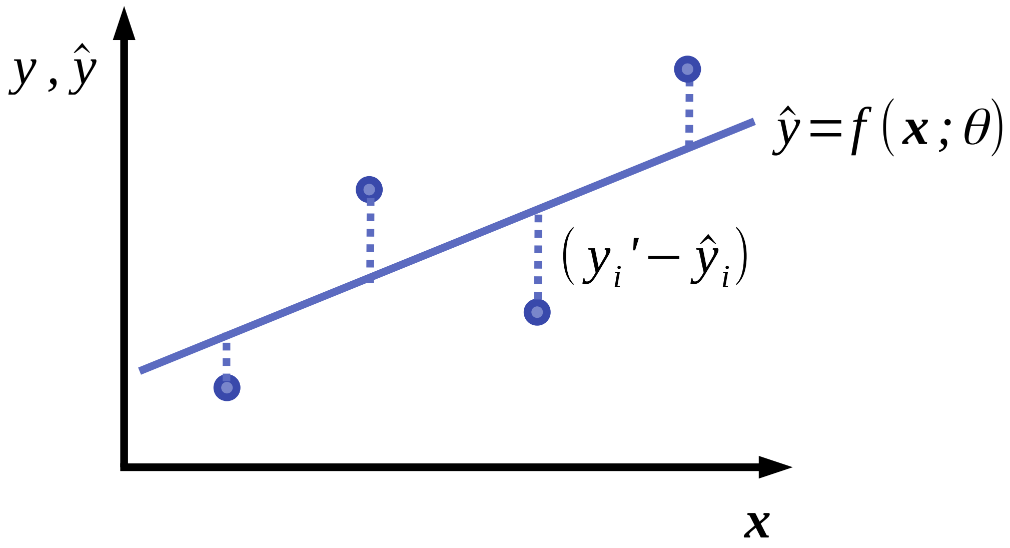

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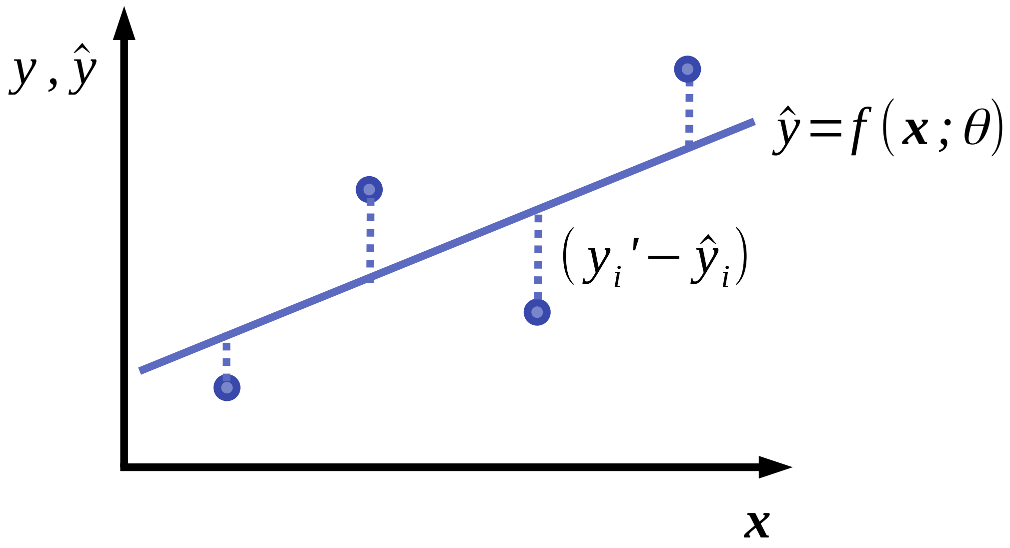

Intuition: by how much deviates your model prediction from the ground-truth on average.

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(Binary) Classification:

		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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Different ML tasks require different metrics

Class imbalance is a real issue!
Example: Will this asteroid impact Earth?

(Binary) Classification:

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

Requires somewhat balanced classes

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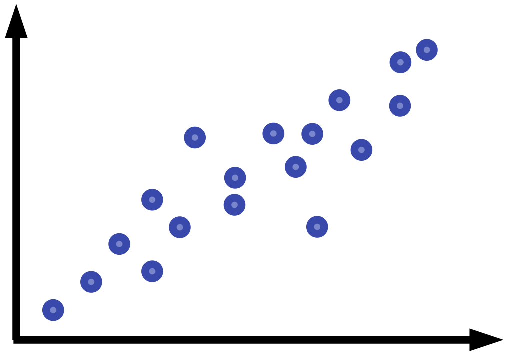
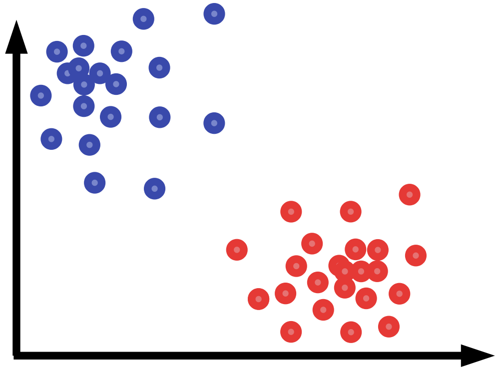
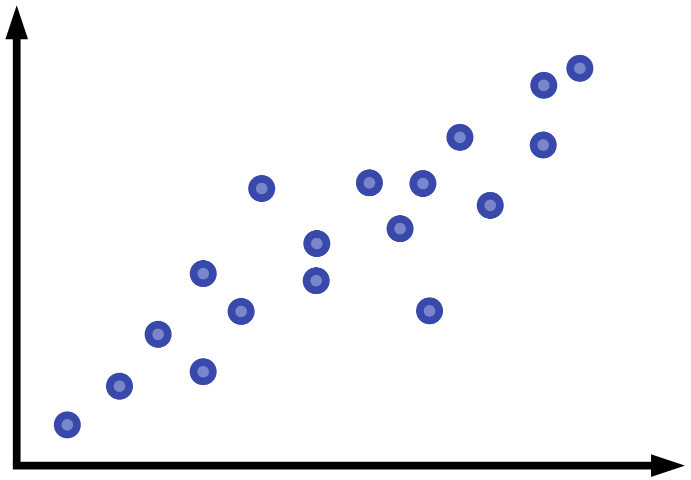
Low recall means that we miss some asteroids that are about to impact, which is not exactly what we want. Therefore, **recall** is the really

Linear models

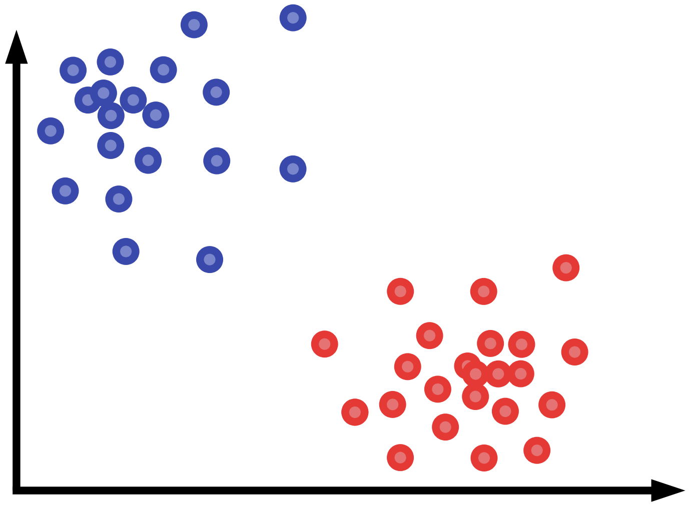




Linear models assume linearity in the underlying data. They are rather simple but convey many of the concepts utilized in other, more complex models.



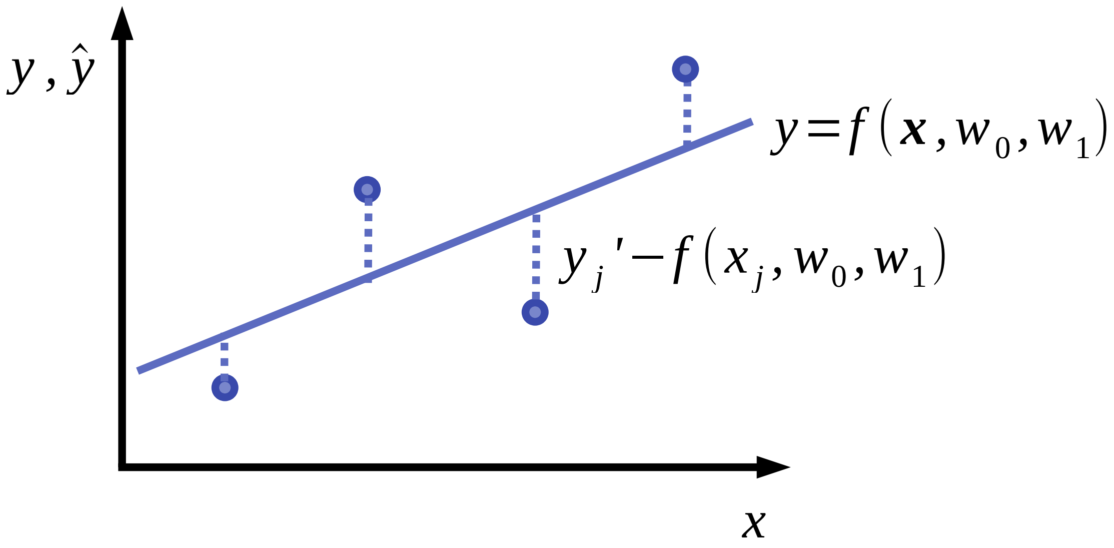
Linear regression



Linear classification

Linear regression (univariate)

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



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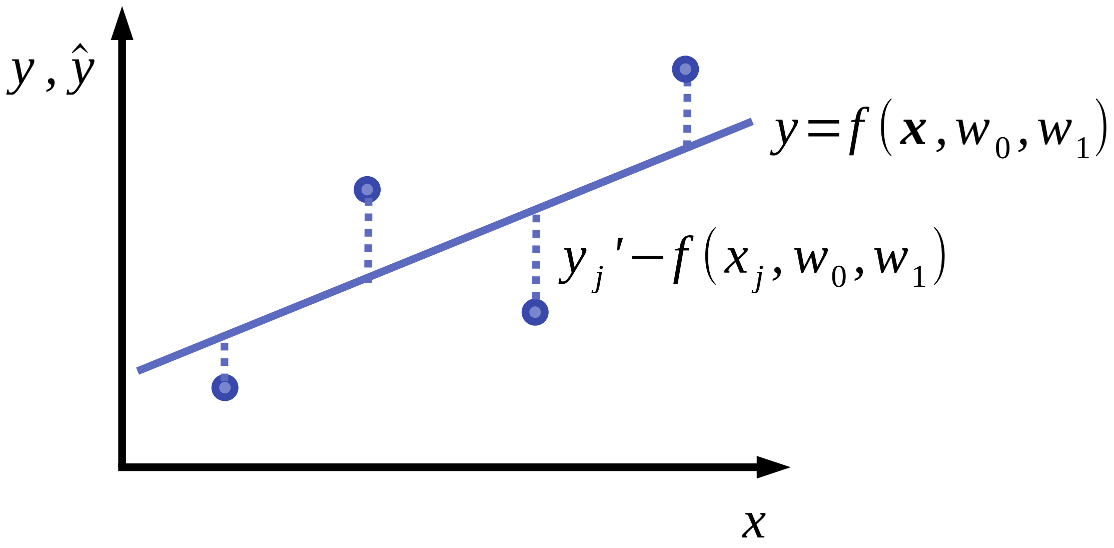
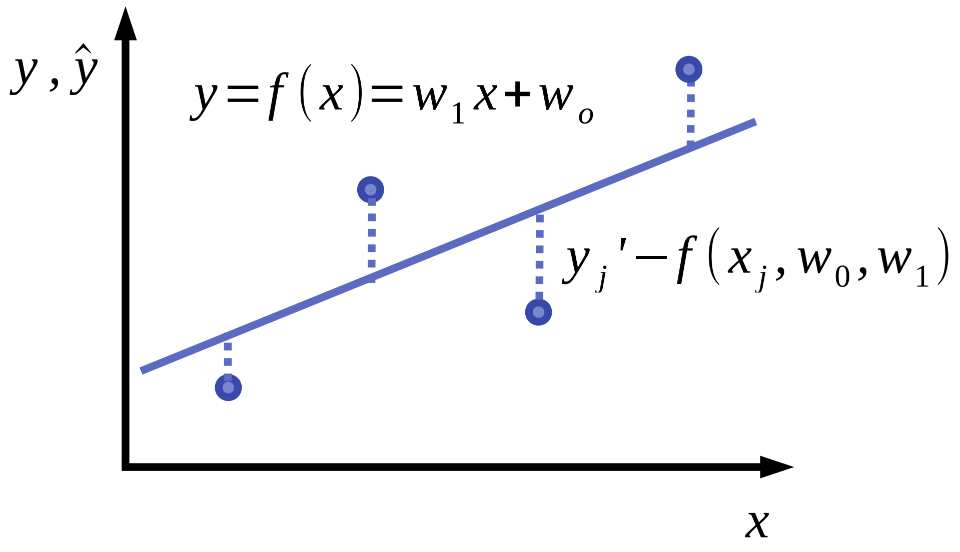


How can we learn w_0 and w_1 from data?

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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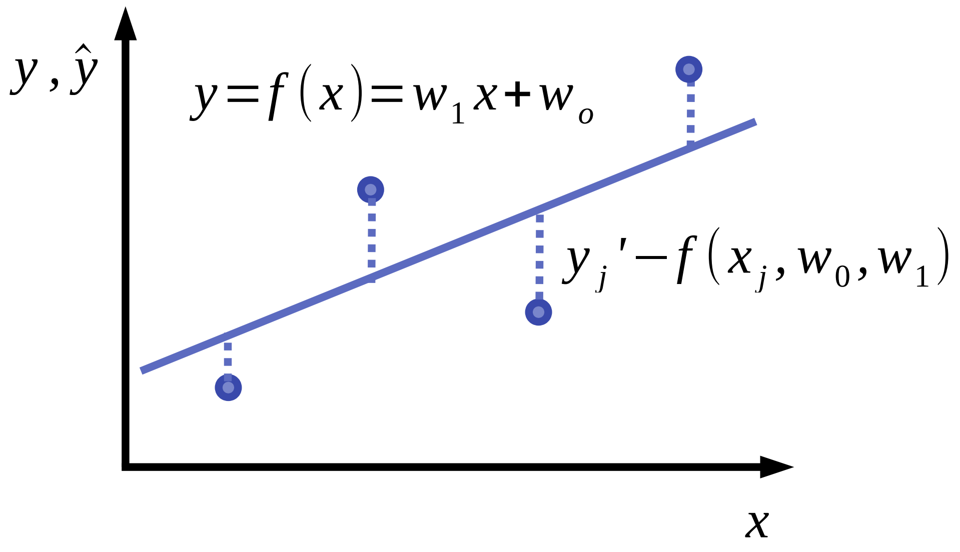

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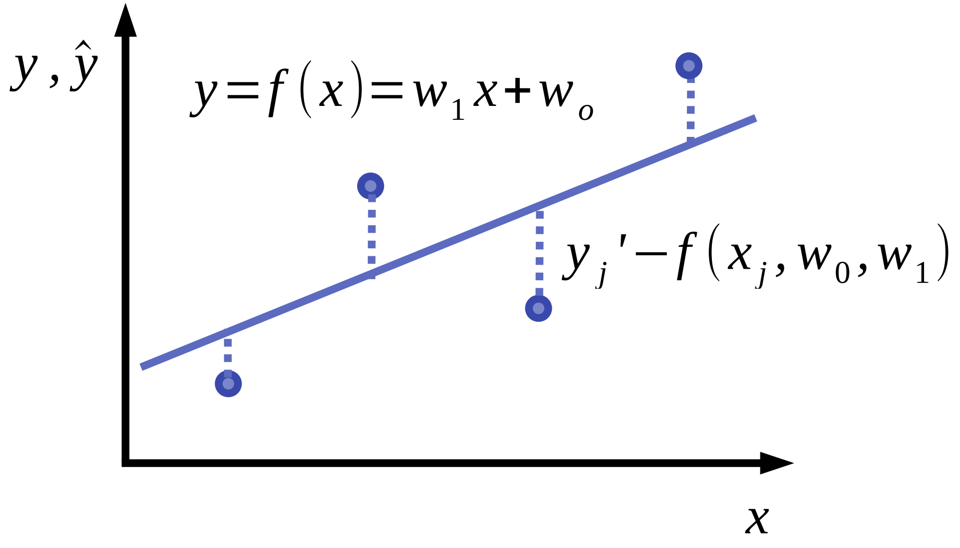

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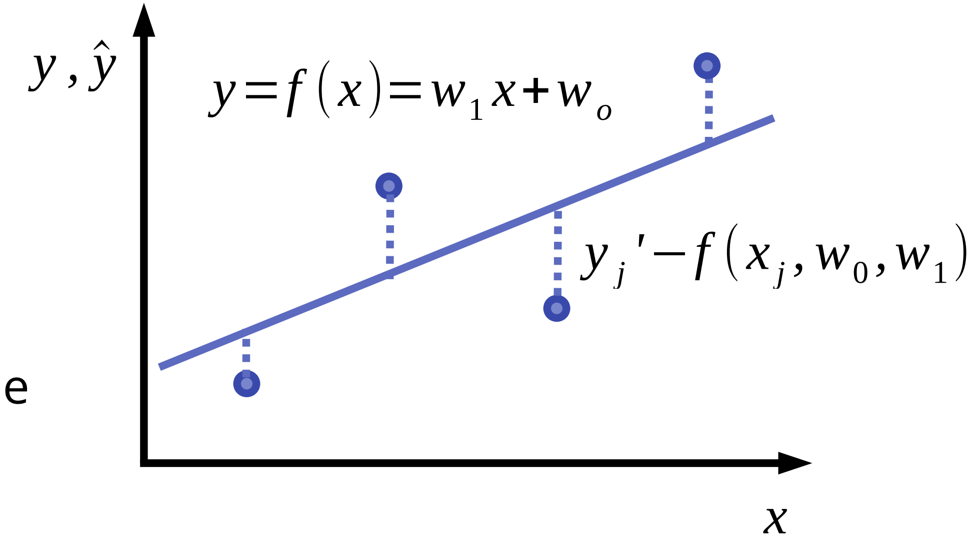

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Linear regression (univariate) – Least squares fitting

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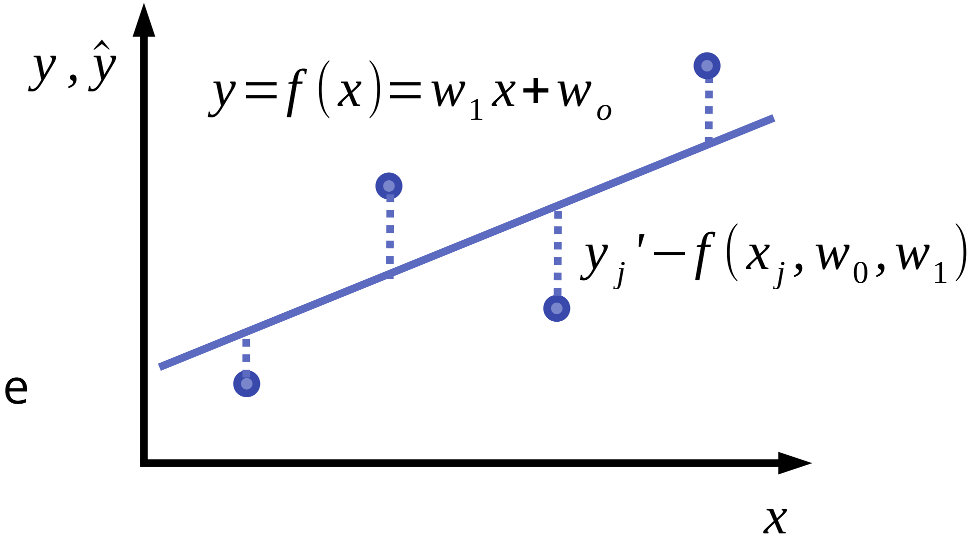

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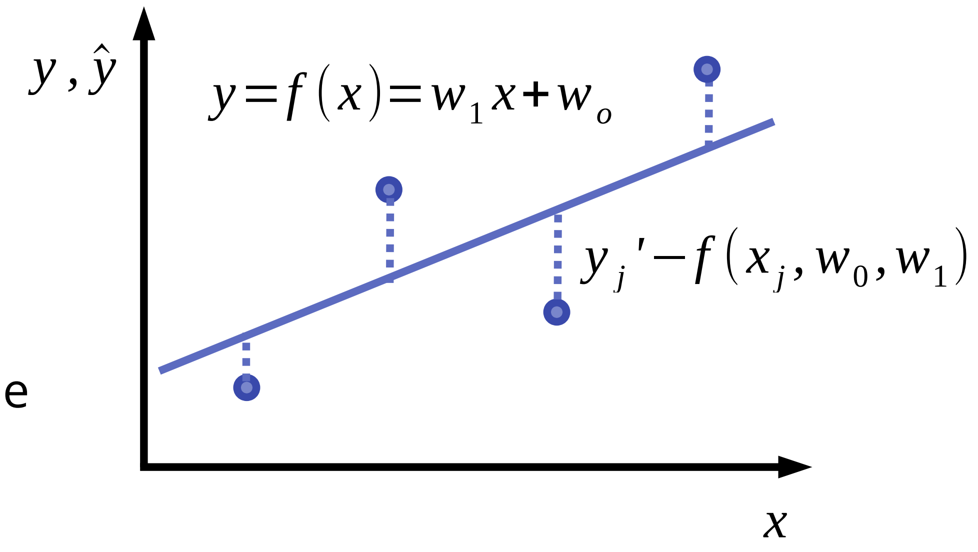

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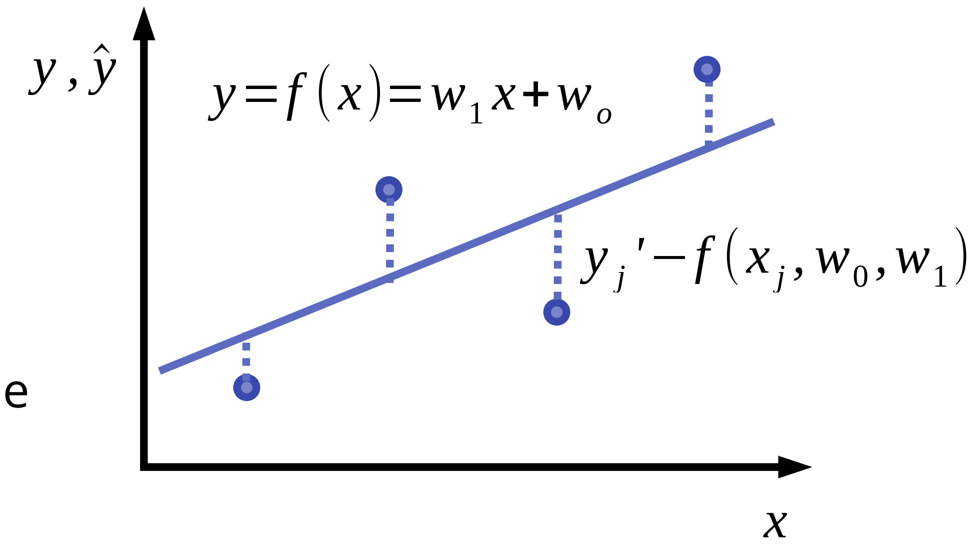

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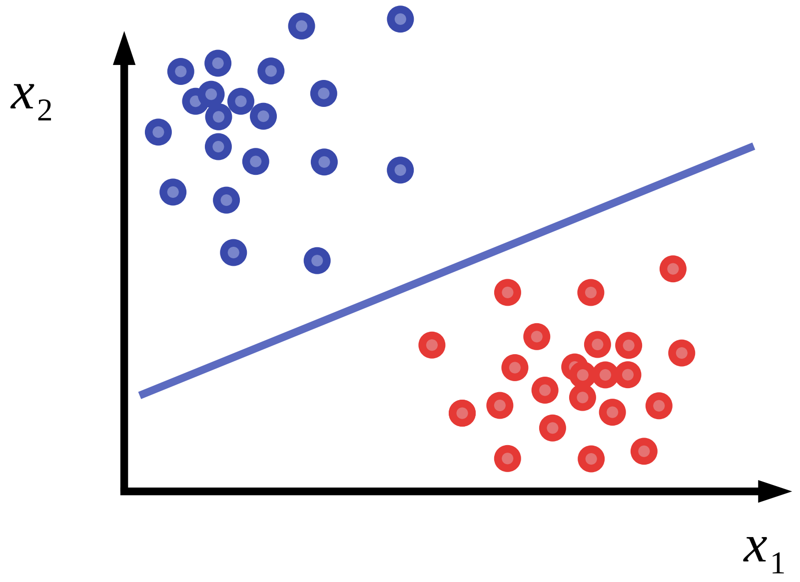
Least-squares + linear model function: the resulting minimum of the Loss function is **global**, i.e., the solution is by default the best-possible solution!

Linear classifier (two-dimensional case)

Linear functions can also be used as a classifier if the data are linearly separable.



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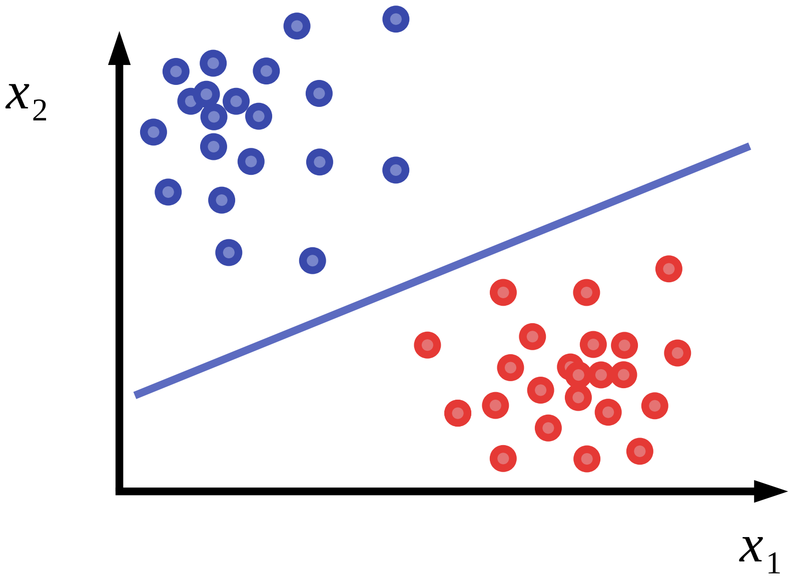

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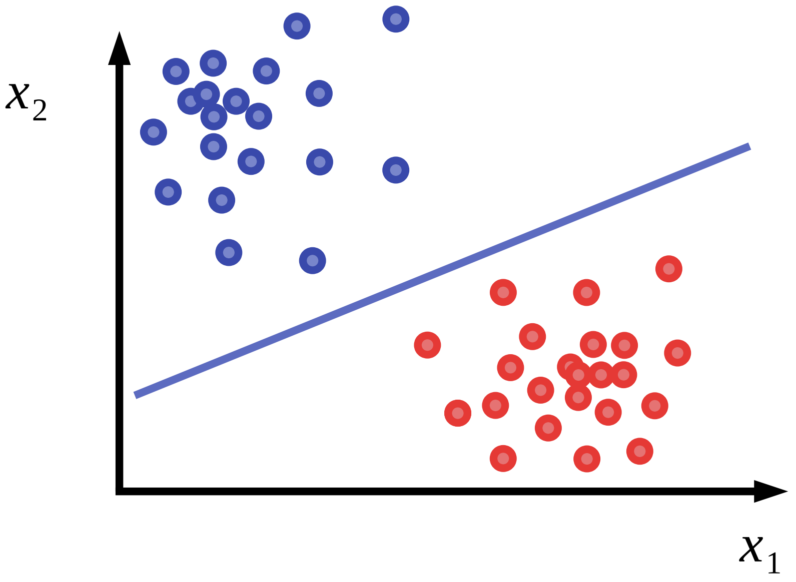

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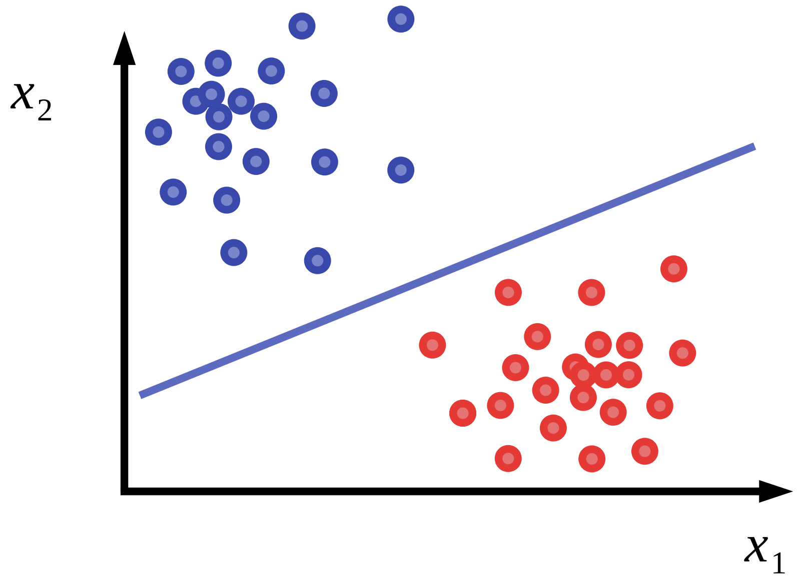

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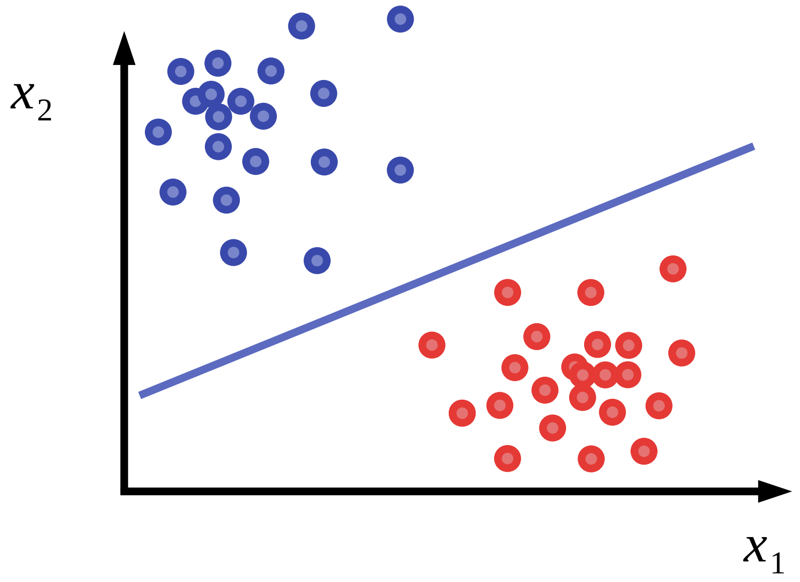
$$\bar{f}(\mathbf{x},\mathbf{w}) = \begin{cases} 1 \text{ if } f(\mathbf{x},\mathbf{w}) \geq 0 \\ 0 \text{ if } f(\mathbf{x},\mathbf{w}) < 0 \end{cases}$$



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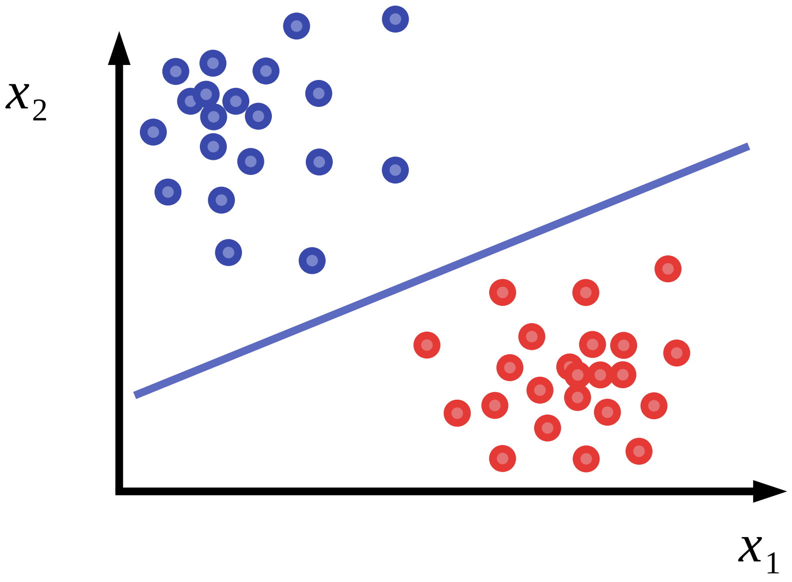
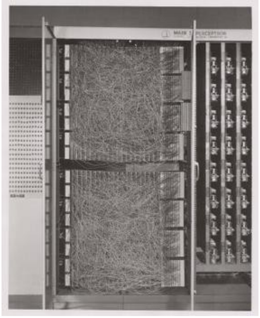


How can we learn $\boldsymbol{w}$ from data?

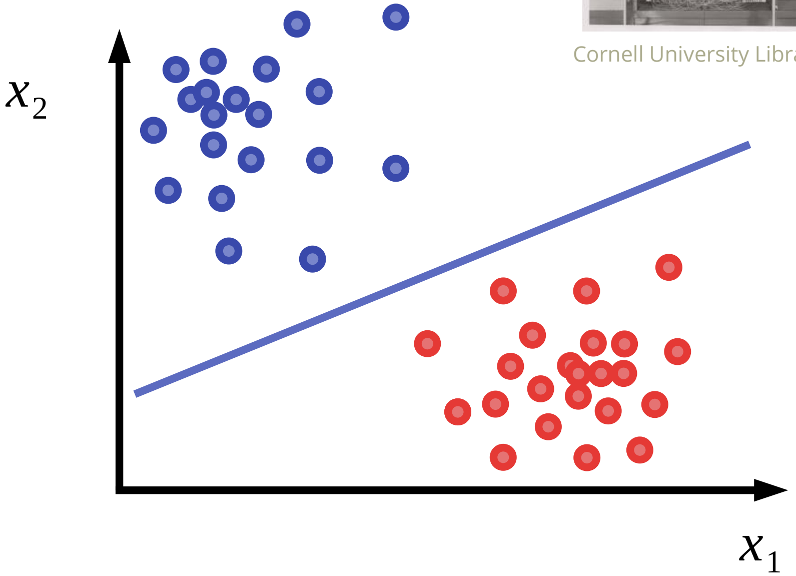
Linear classifier (two-dimensional case) – Perceptron learning rule



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

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

- $\bar{f}(\boldsymbol{x},\boldsymbol{w})=y$, then do nothing.
- $\bar{f}(\boldsymbol{x},\boldsymbol{w})=0$ but $y'=1$, then increase w_i if $x_i \geq 0$, or vice versa.
- $\bar{f}(\boldsymbol{x},\boldsymbol{w})=1$ but $y'=0$, then decrease w_i if $x_i \geq 0$, or vice versa.



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.

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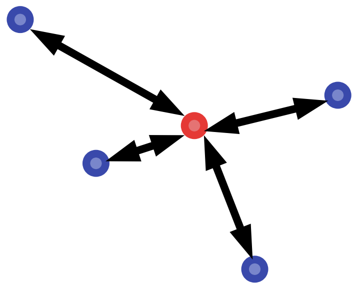
Nearest-Neighbor models



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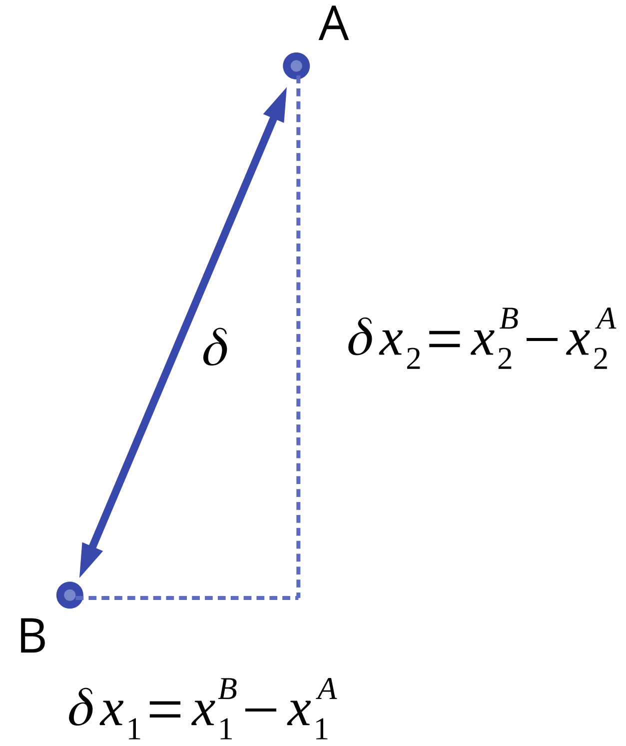

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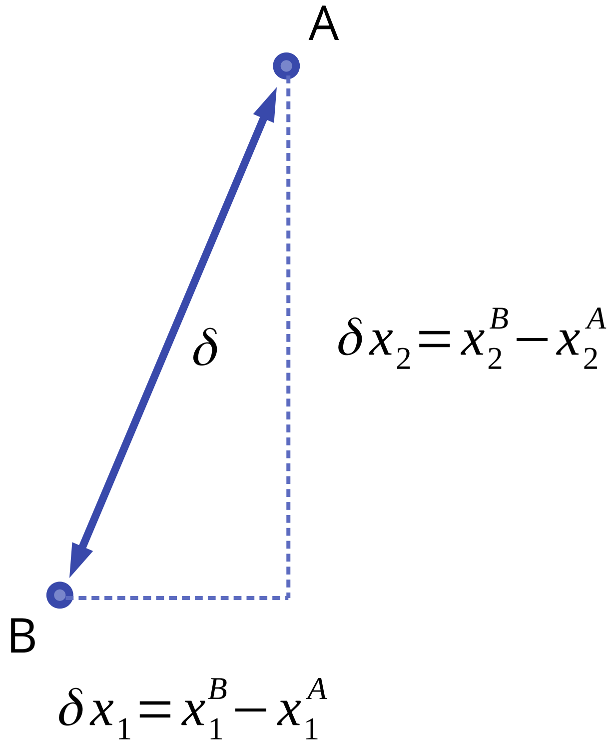

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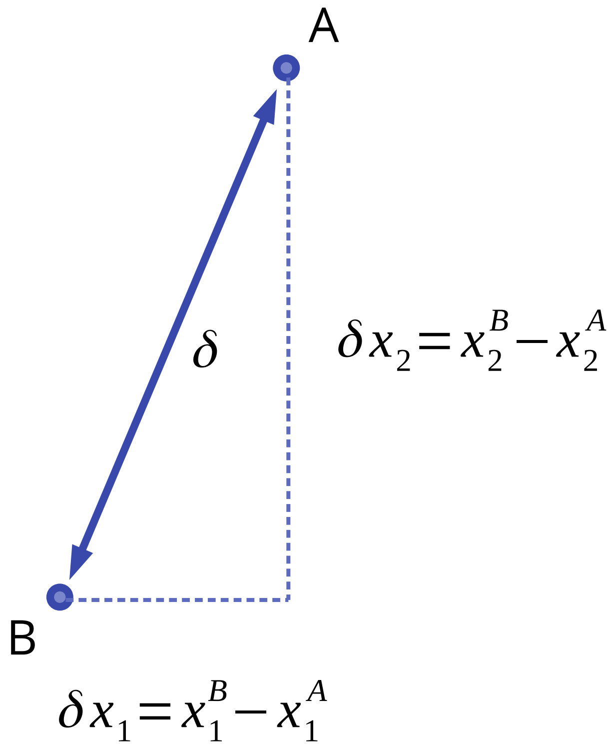
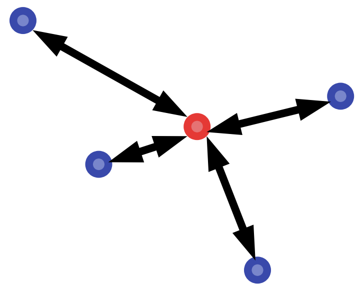


Nearest neighbor methods utilize distances between datapoints for **classification** and **regression** tasks.



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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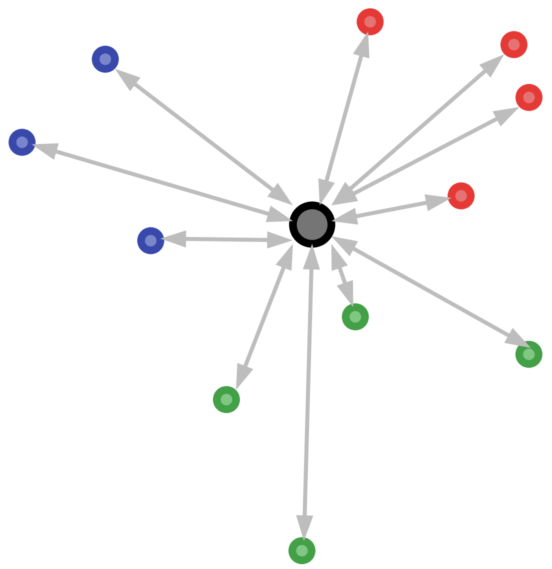

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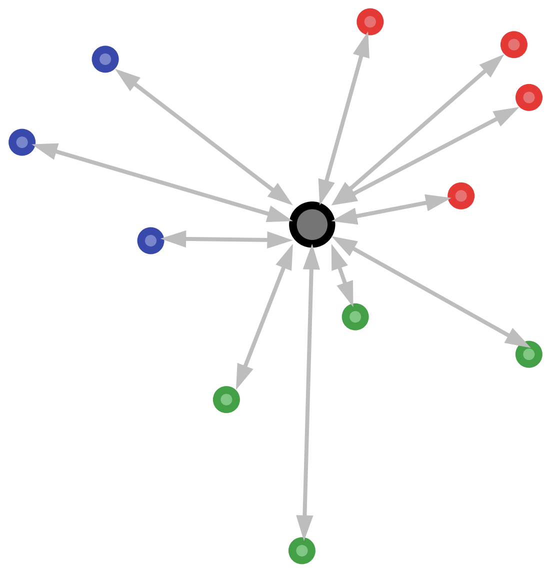

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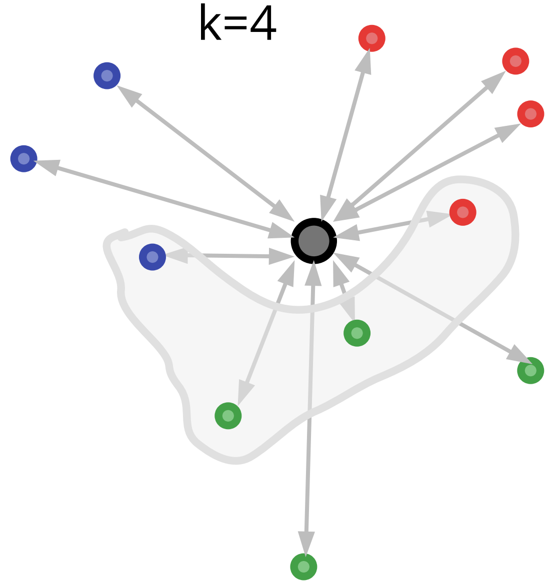

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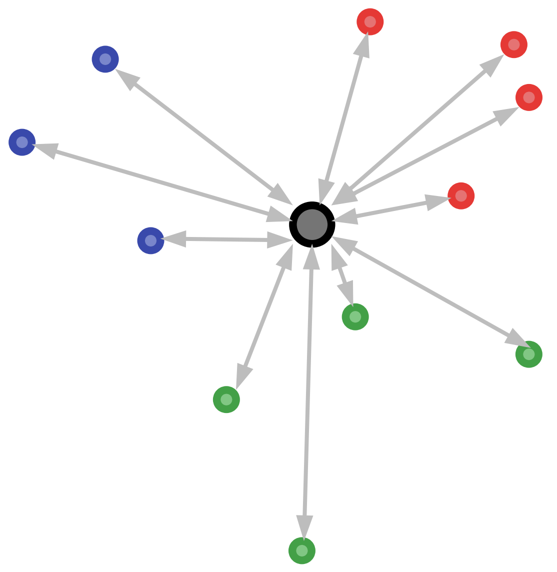

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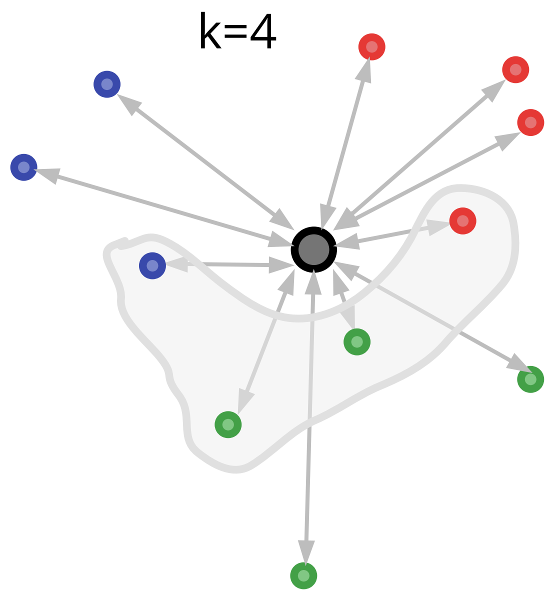

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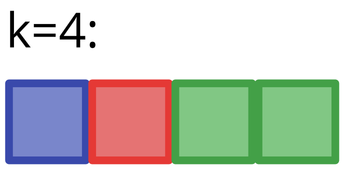

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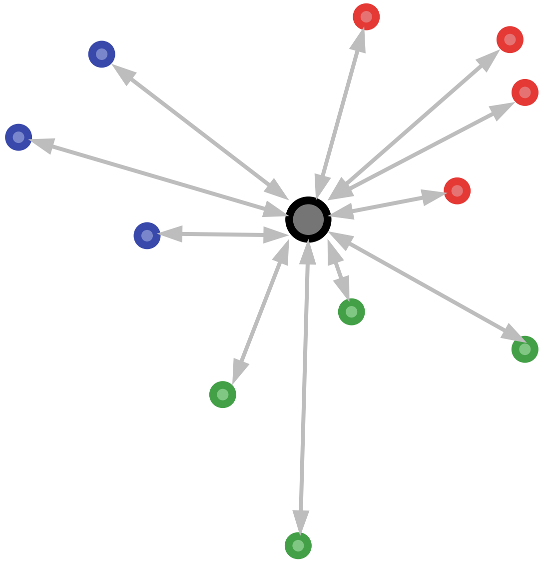

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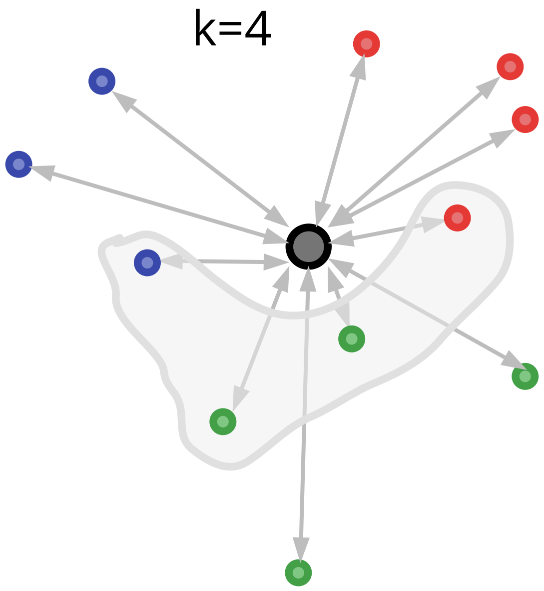

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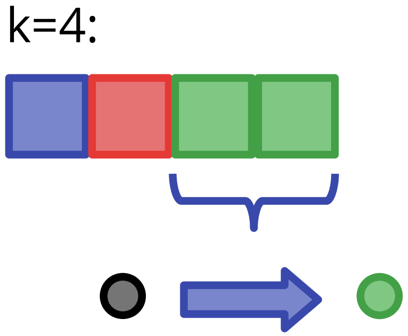
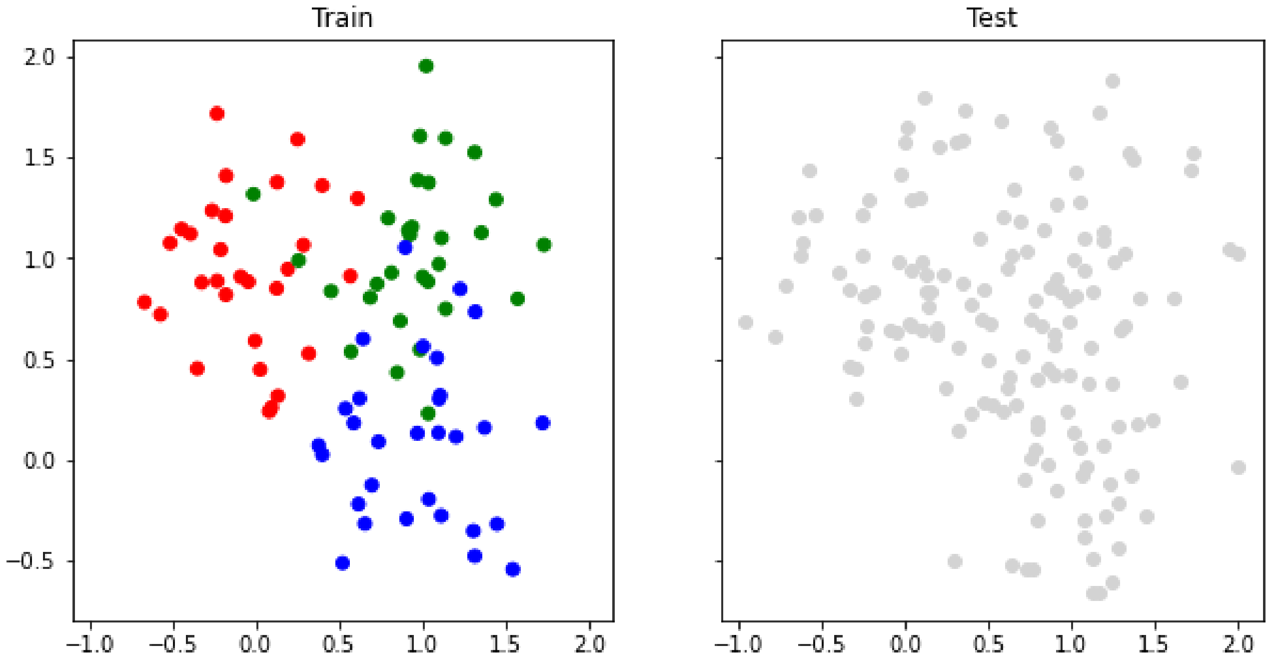


class assignment

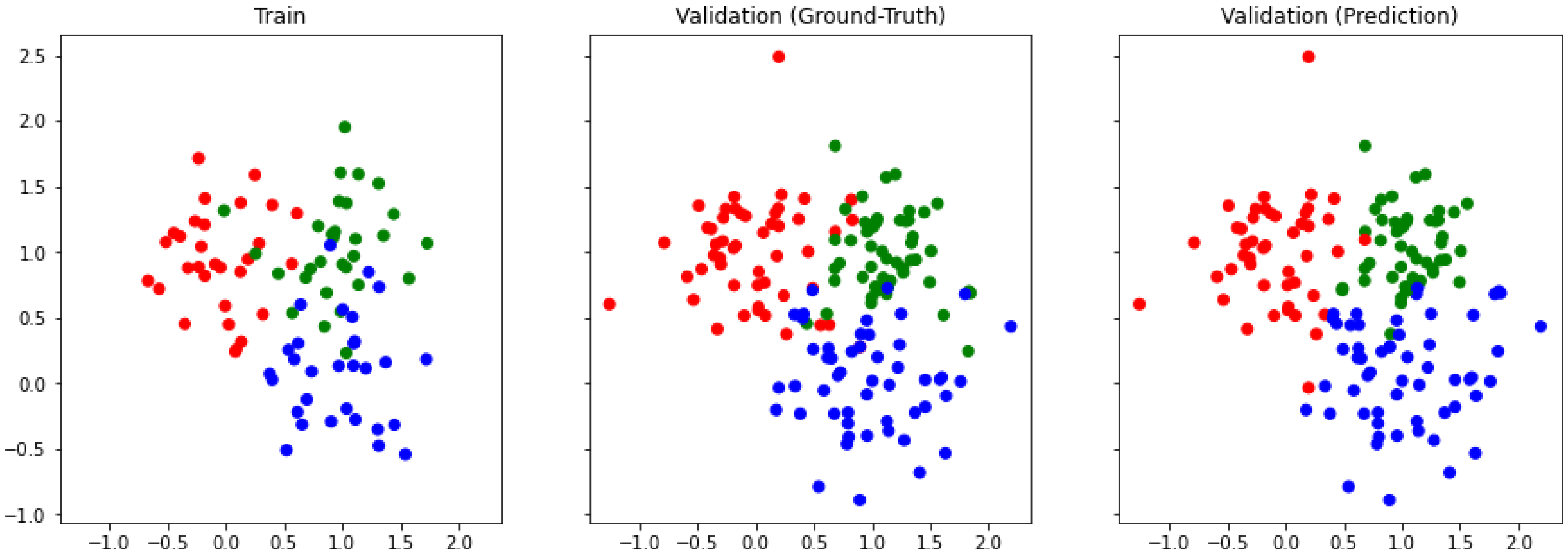
k-nearest neighbor classification - Example



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**!

k-nearest neighbor classification - Example

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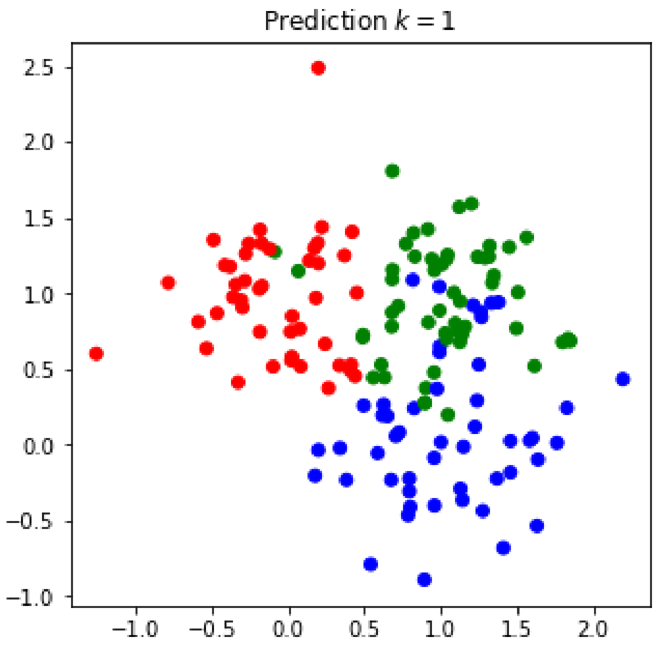

k=1

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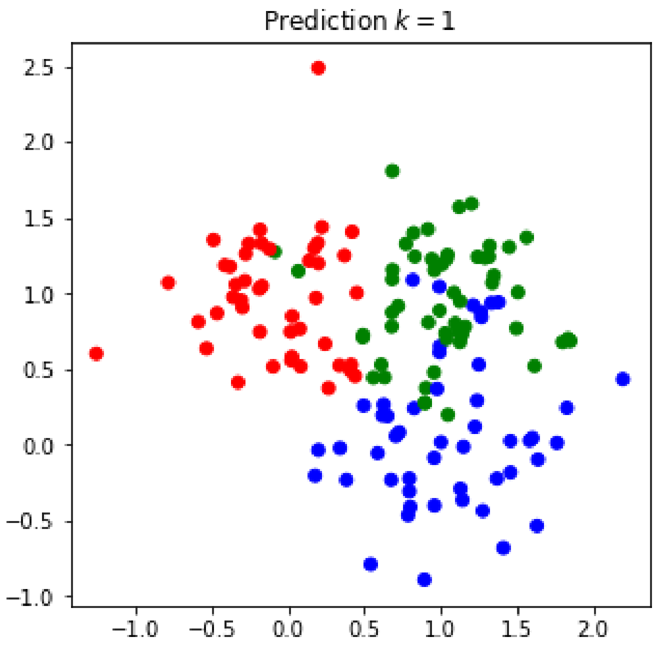

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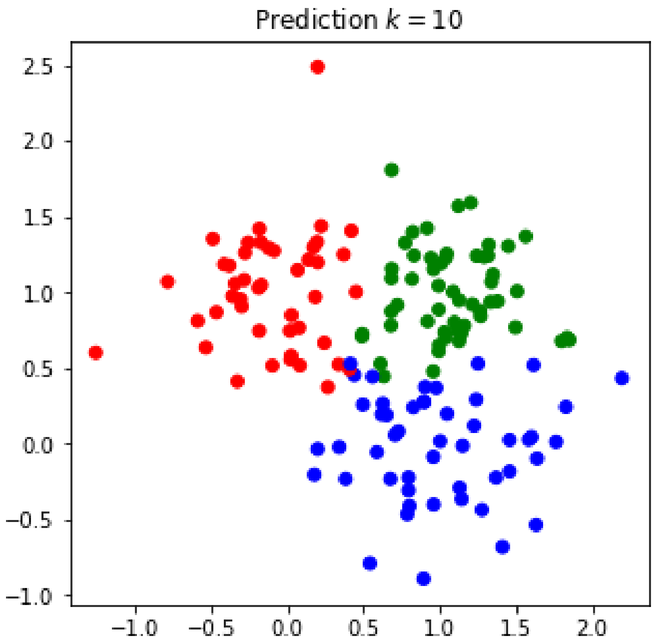

k=10
accuracy$_{val}$=0.893

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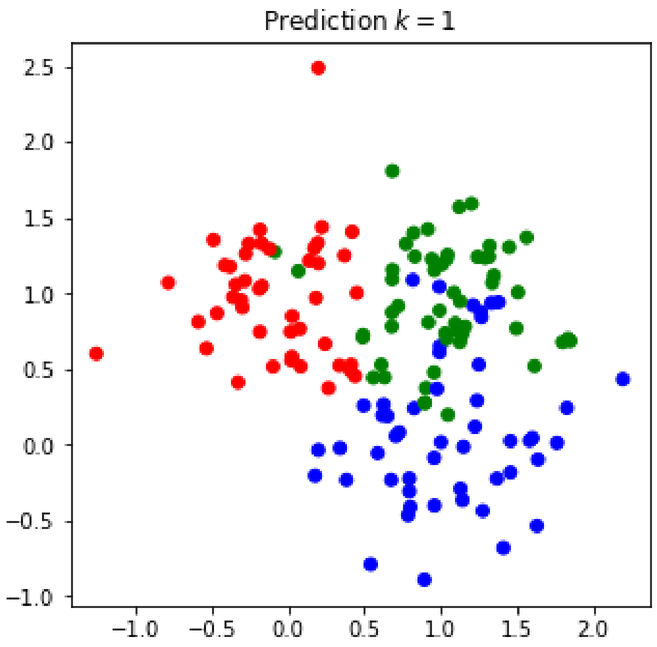

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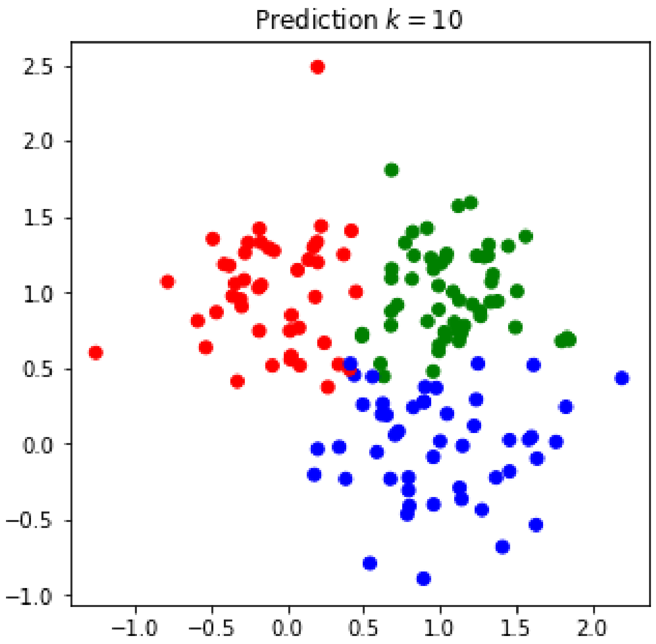

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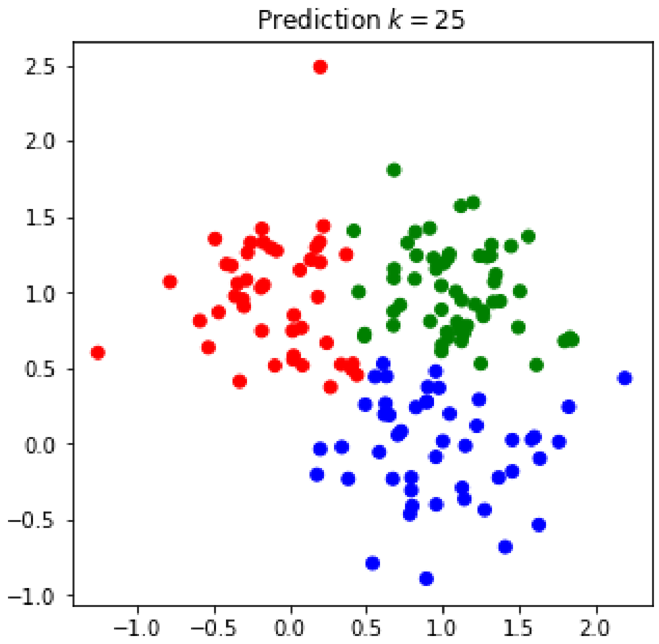

k=25
accuracy$_{\text{val}}$=0.873

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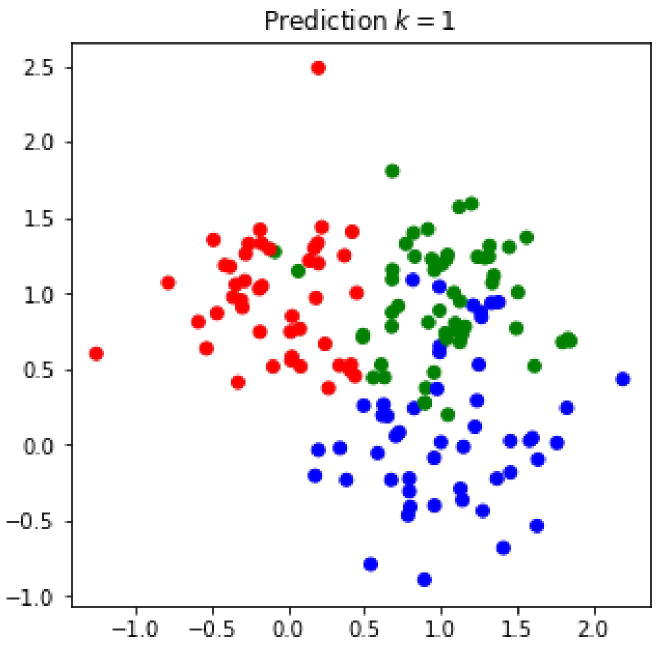

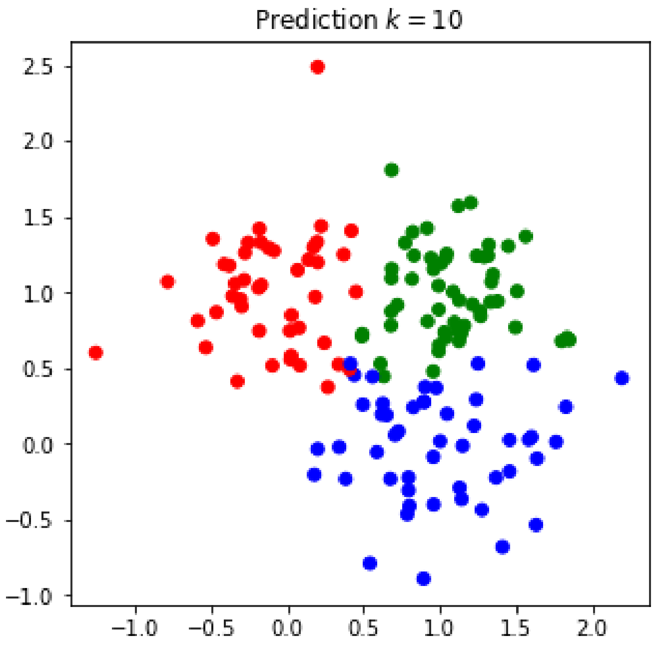

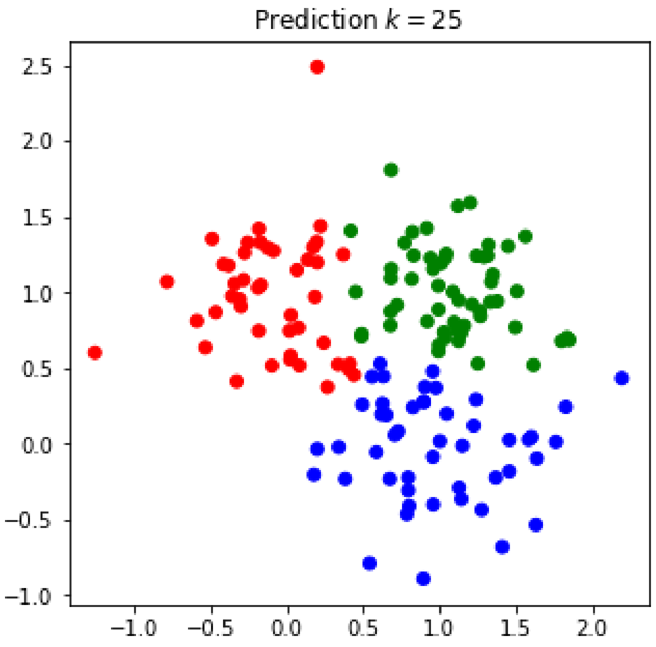

k=1
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Overfitting!

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

accuracy$_{test}$=0.880

Best performance

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Underfitting!

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Number of data points should grow exponentially with data dimensionality.

If parameter space is insufficiently sampled, the model does not have enough data points for training properly.

Bonus Slide: The Curse of Dimensionality

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Example: N=10

d=1

Bonus Slide: The Curse of Dimensionality

Datasets we deal with typically have a limited size, *N*. The number of features in our dataset, *d*, defines the dimensionality of the feature space; the volume of the feature space, *V*, grows exponentially with *d*.

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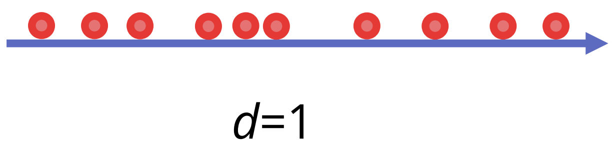

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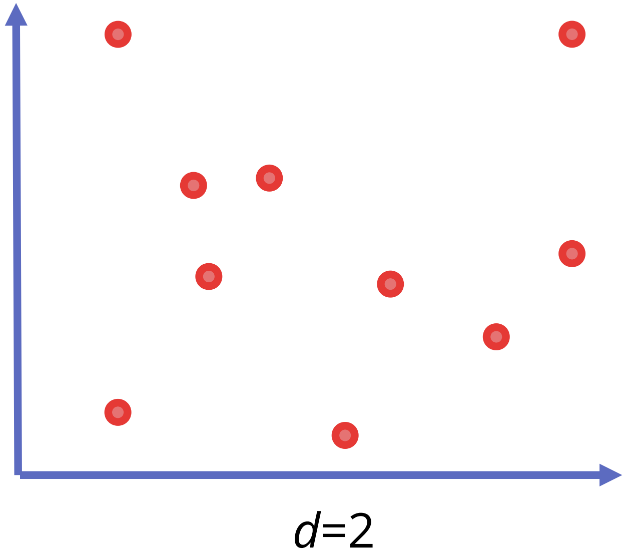

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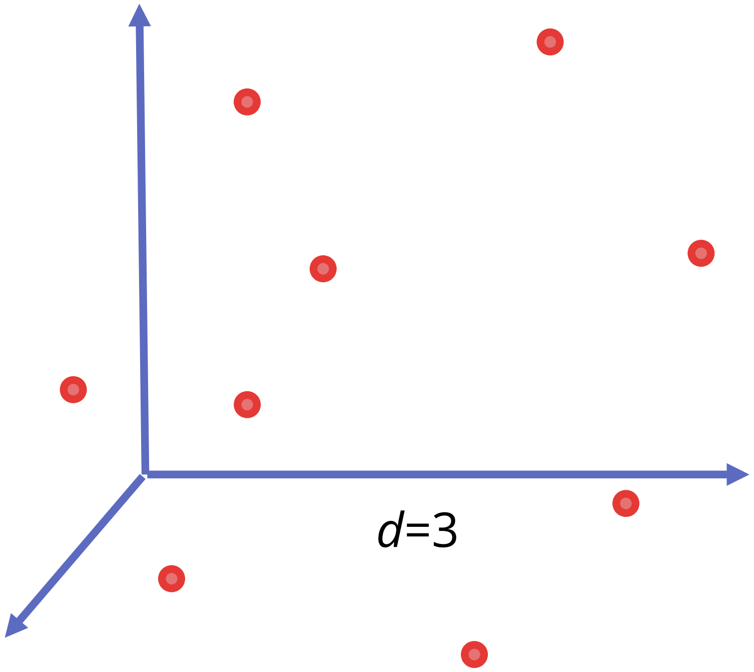

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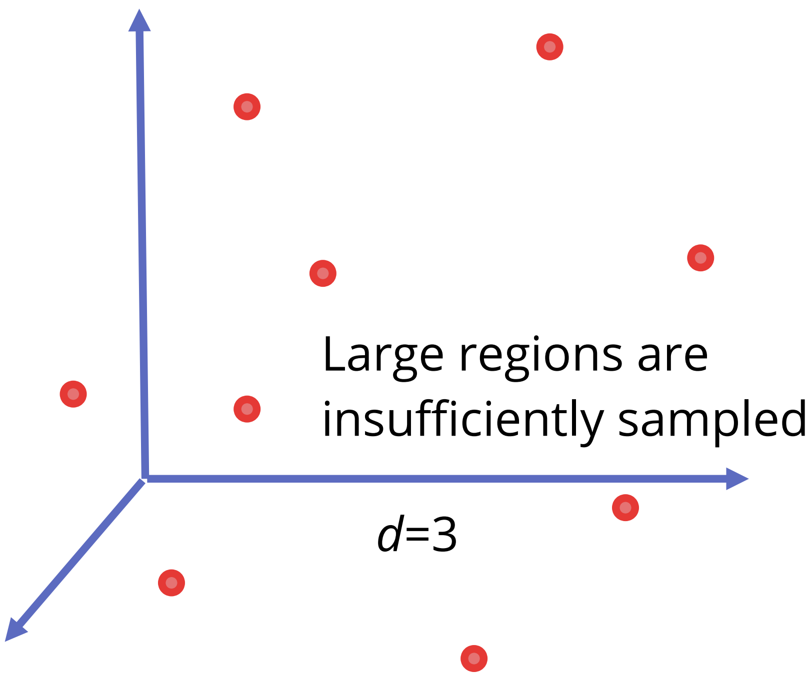

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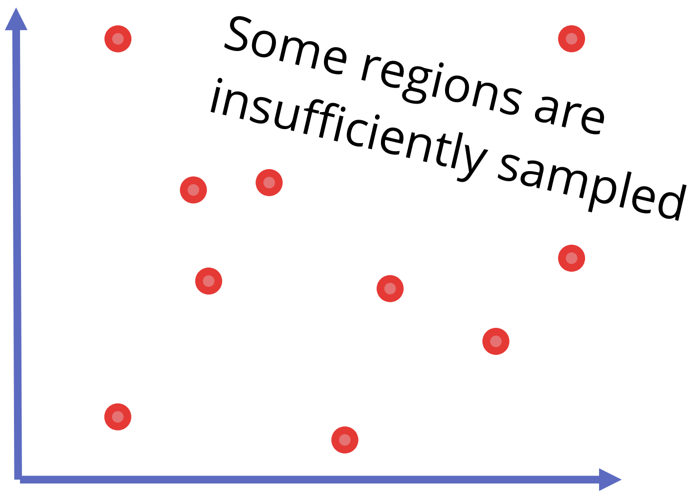

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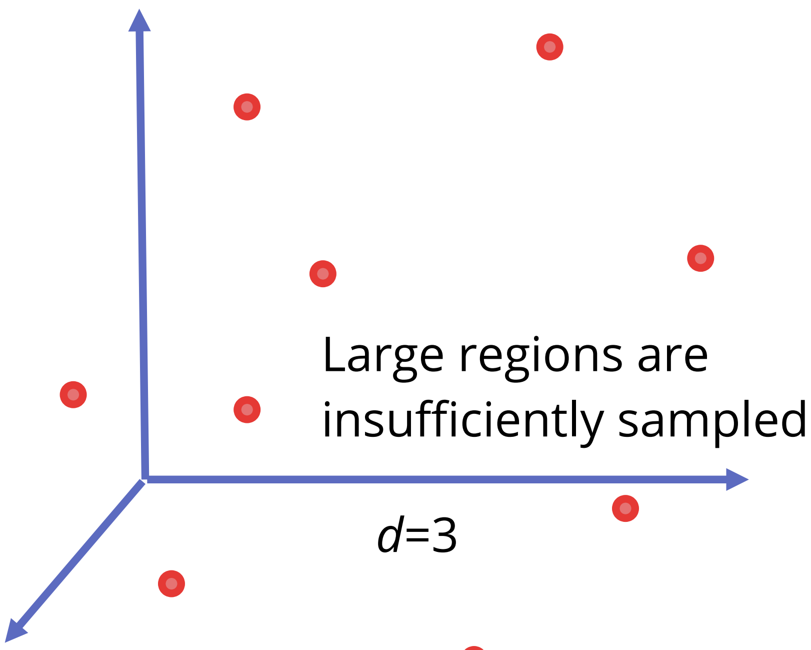
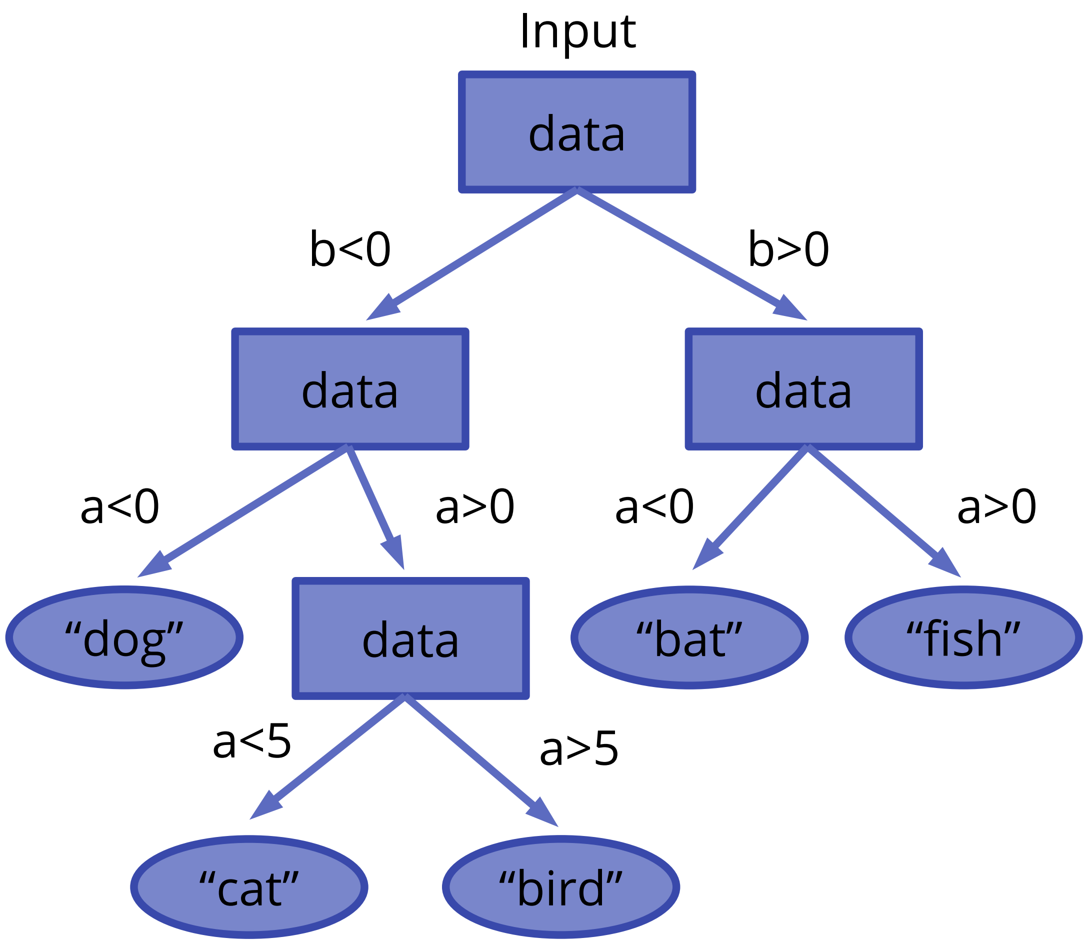


d=3

The higher d, the harder it is for the model to learn.

Tree-based models
(a high-level introduction)



Decision tree classification

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A decision tree is a **rule-based structure** for prediction of scalar output from (potentially) multi-dimensional input data.

Tree properties (hyperparameters):

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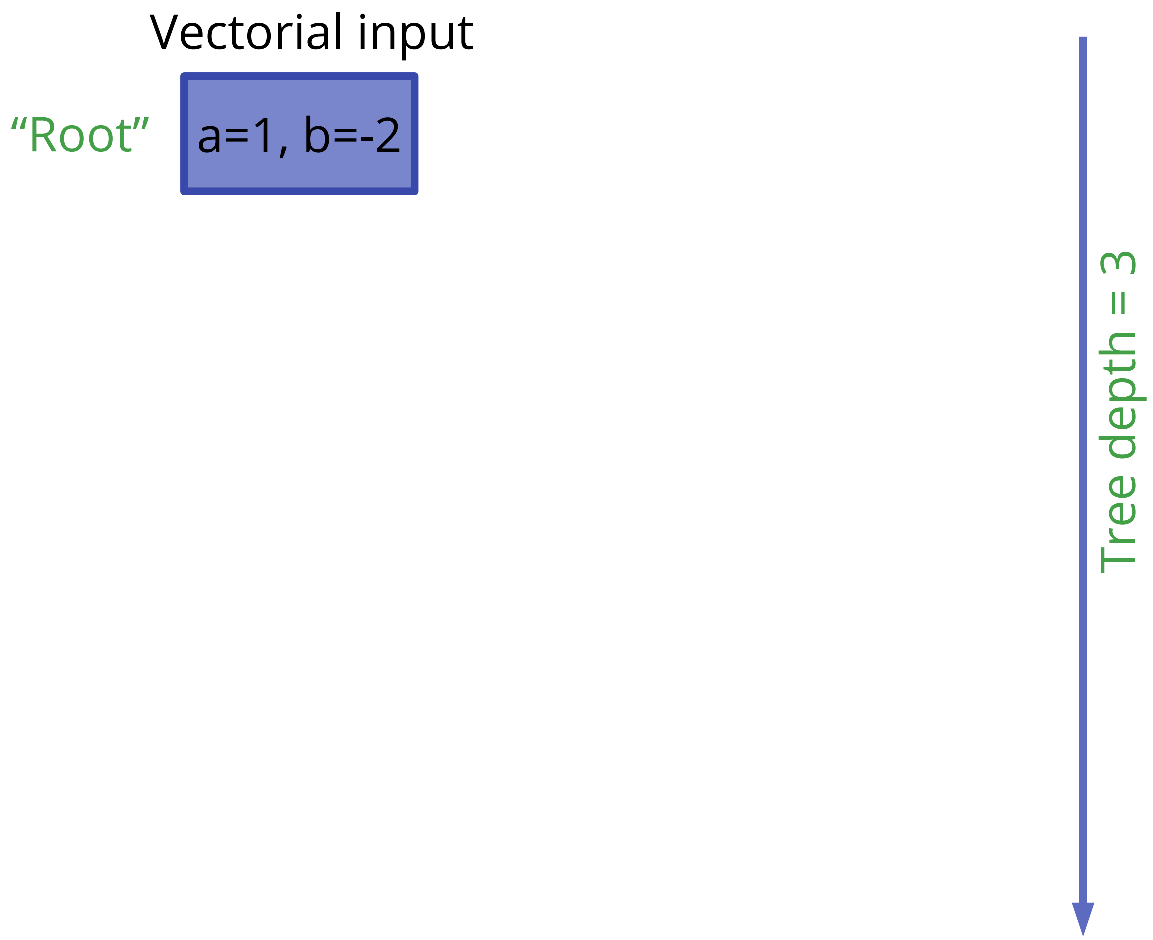

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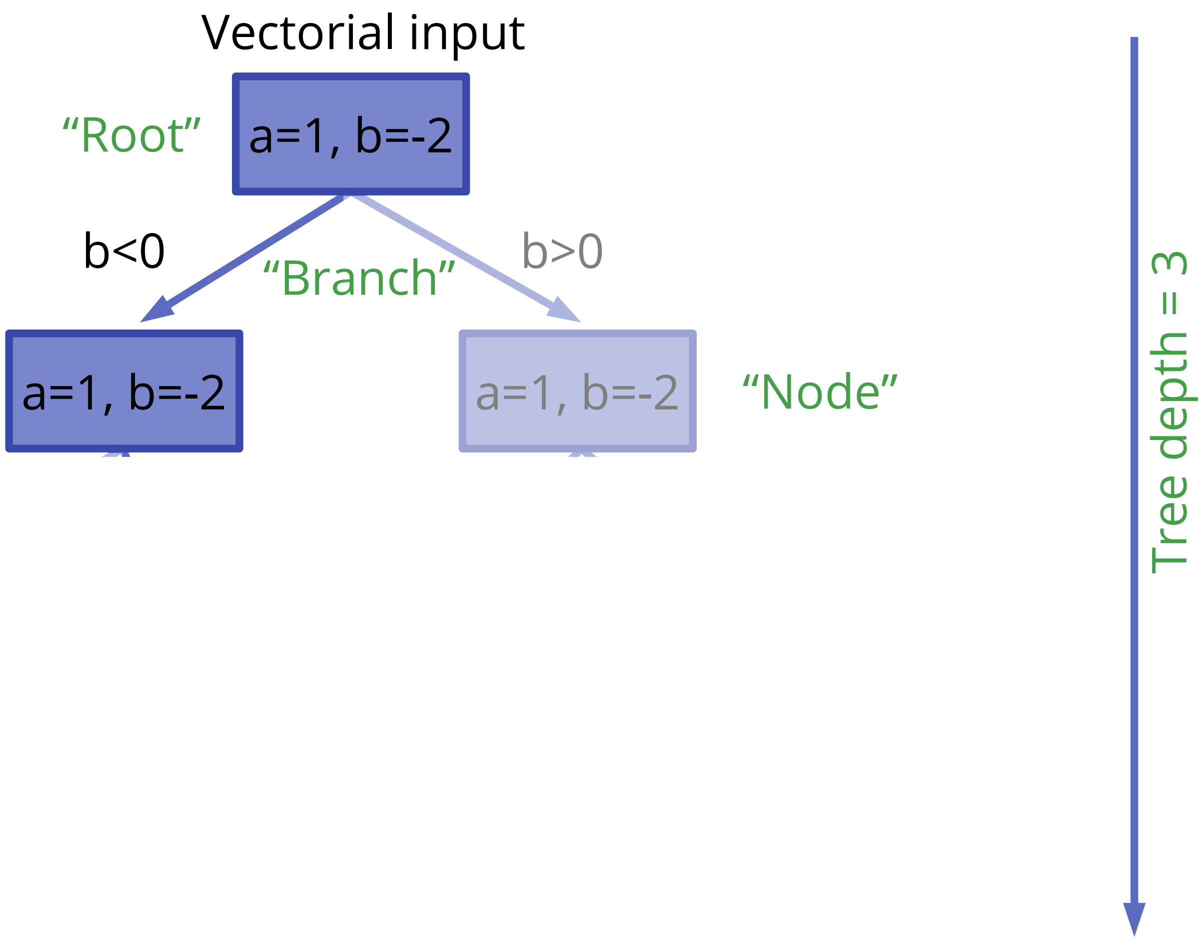

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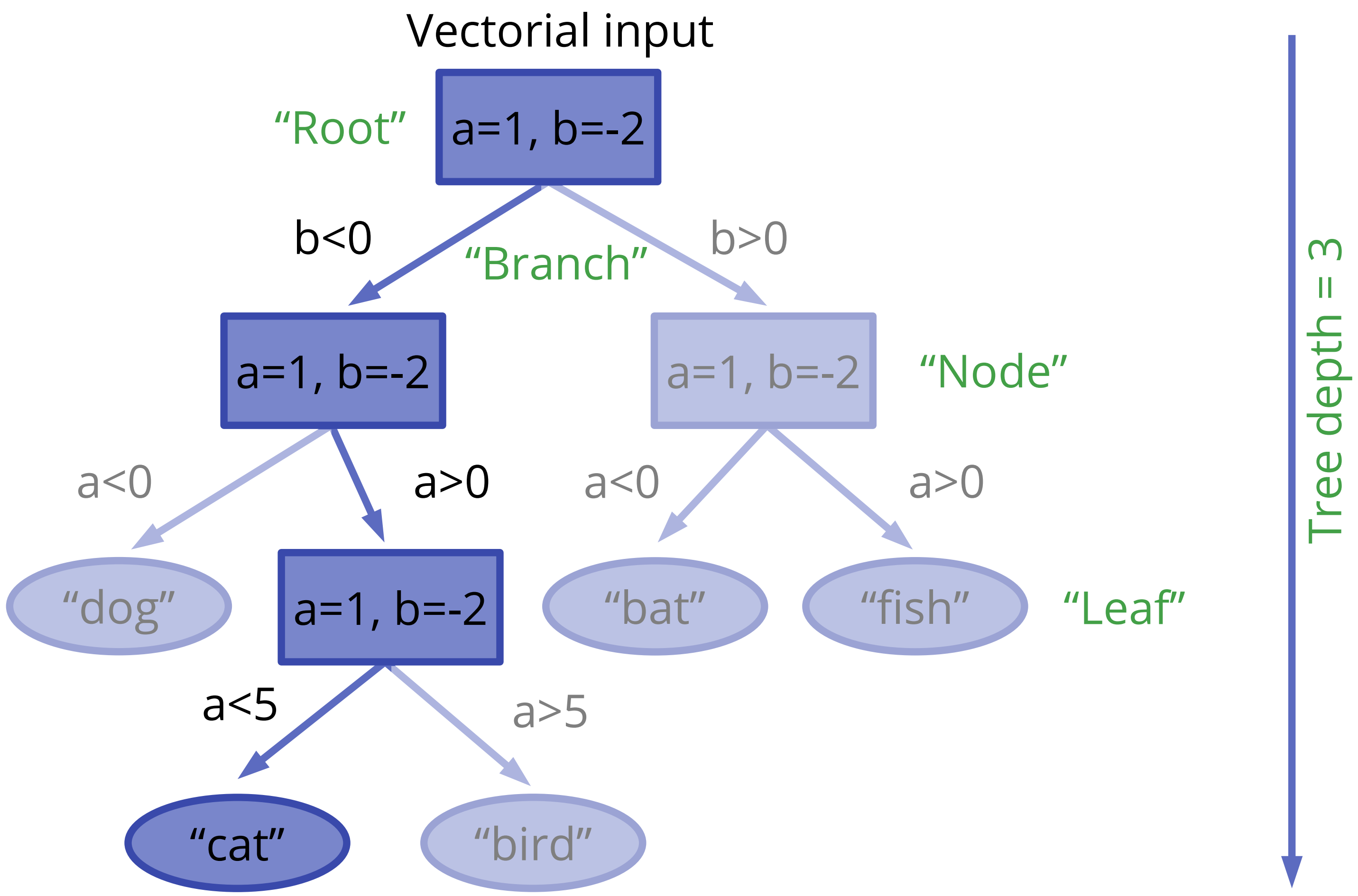

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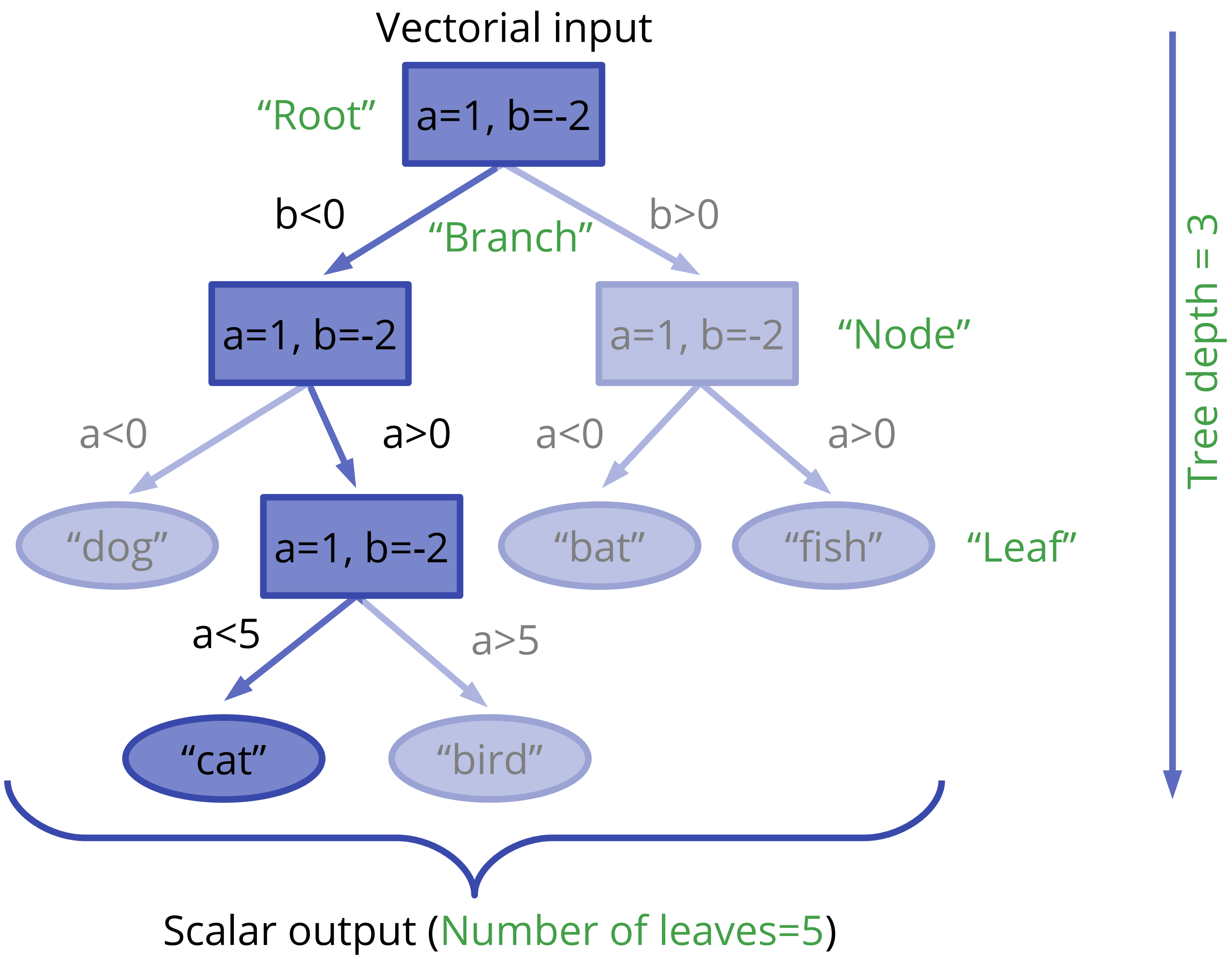

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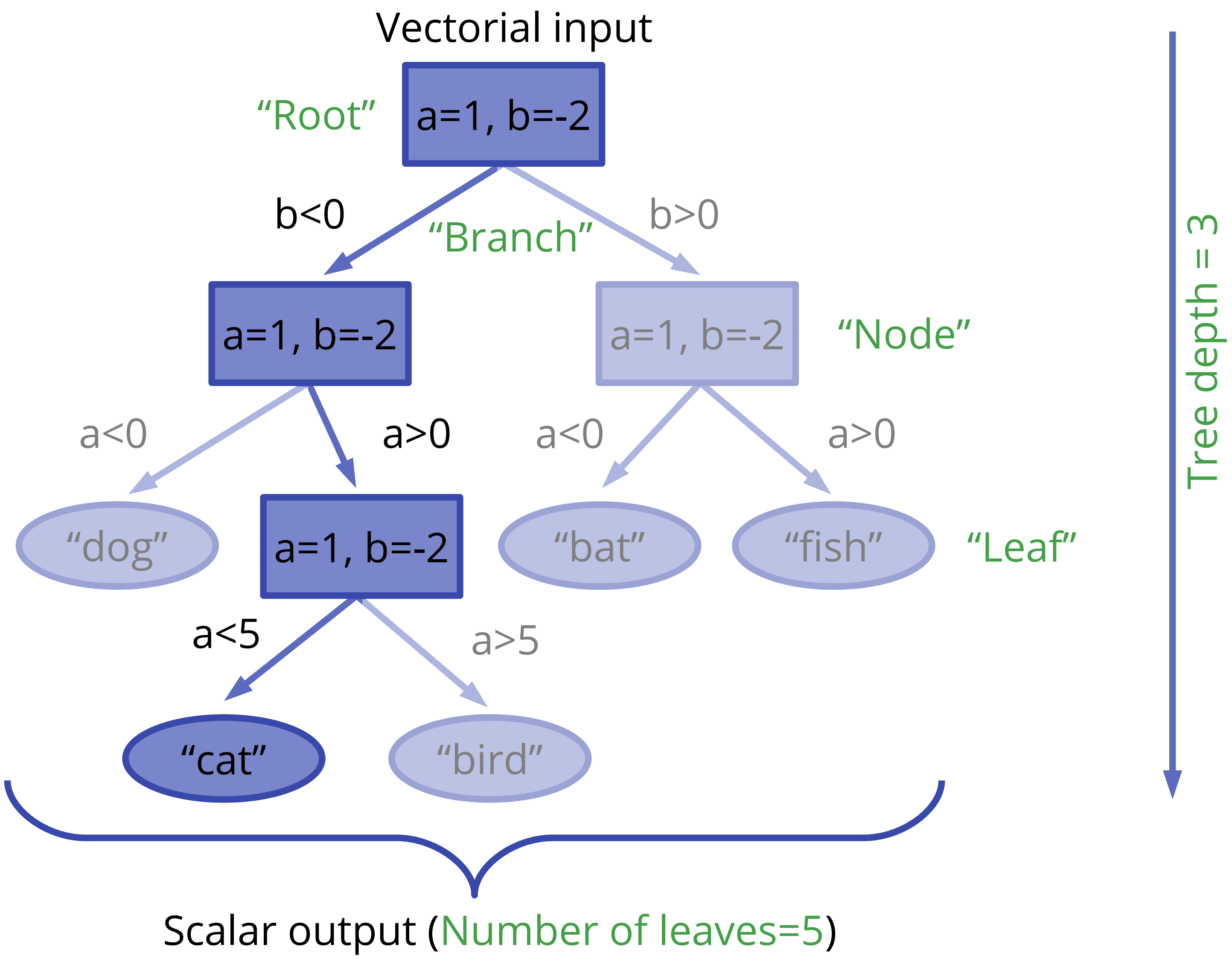
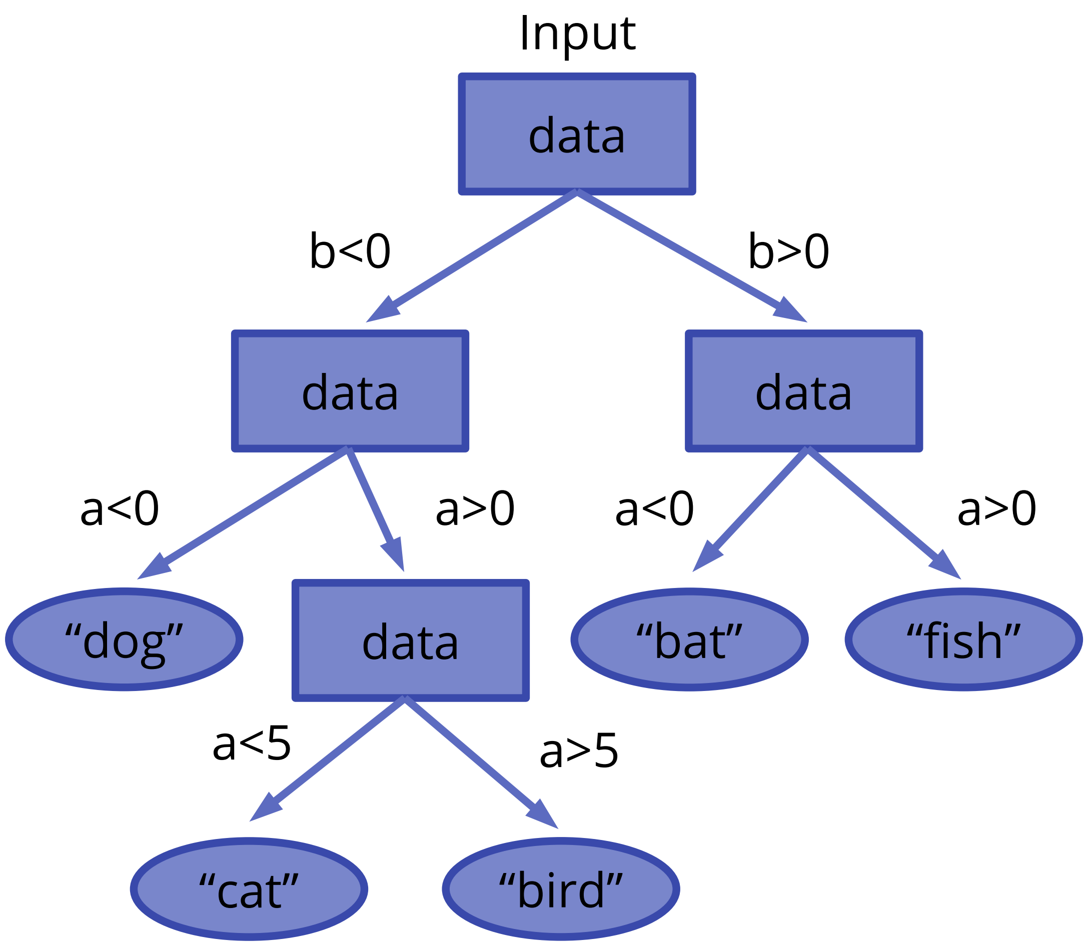
How can the rules stored in the nodes be learned?



Decision tree learning



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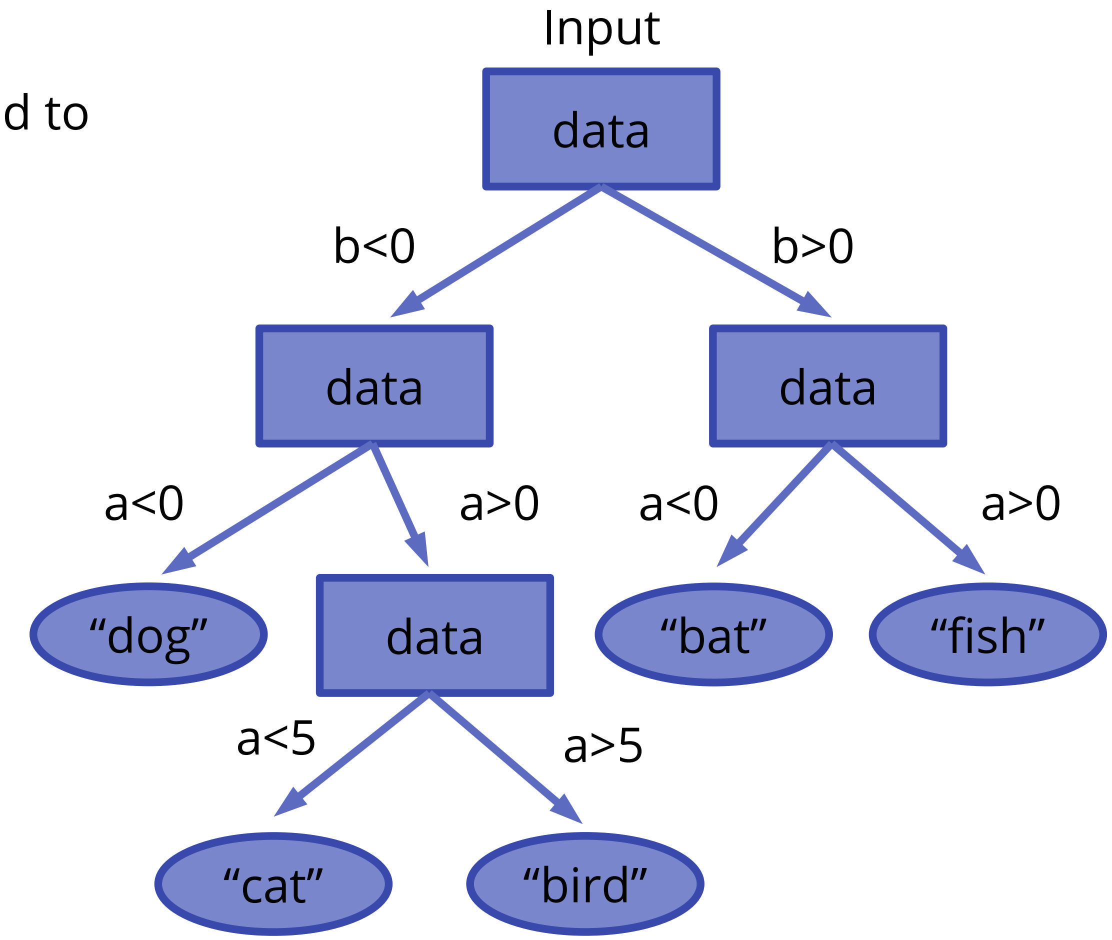
A **greedy divide-and-conquer strategy** is adopted to train decision trees on a training data set in a recursive fashion:



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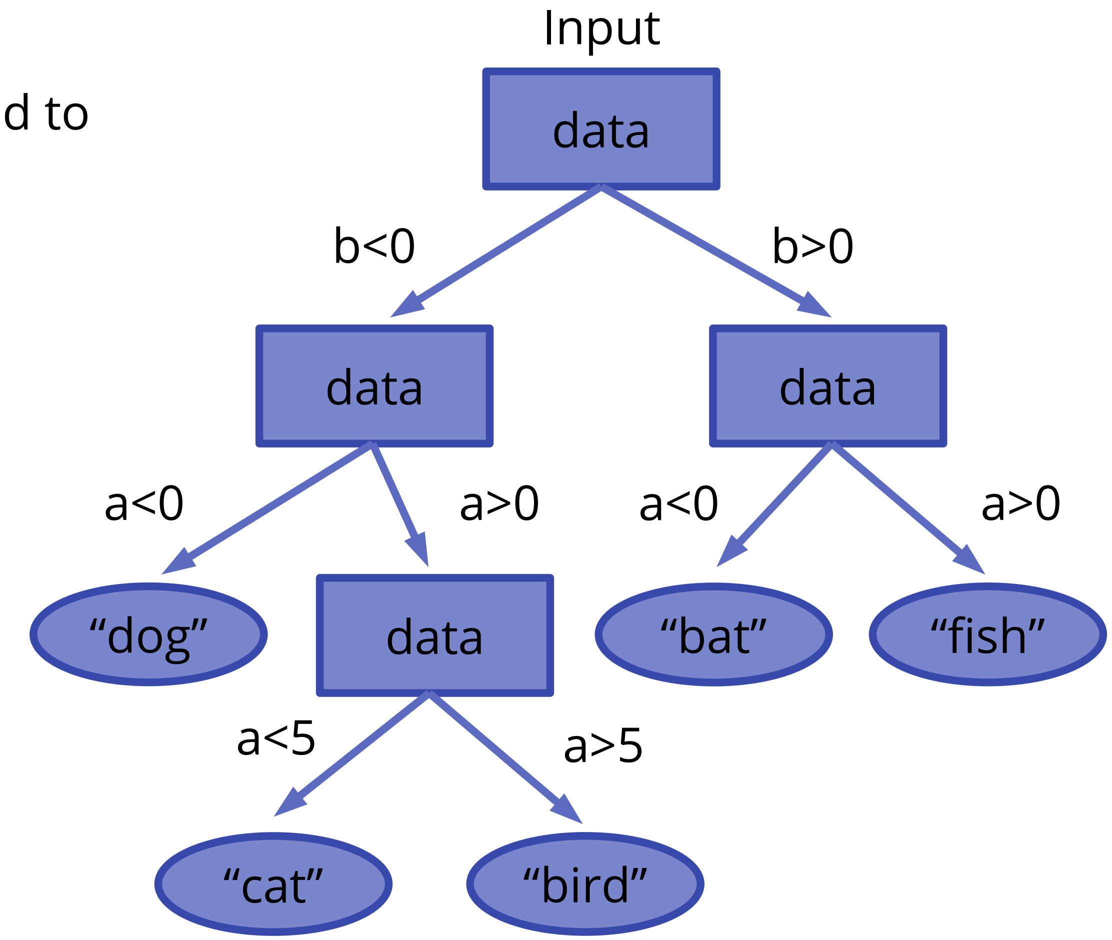

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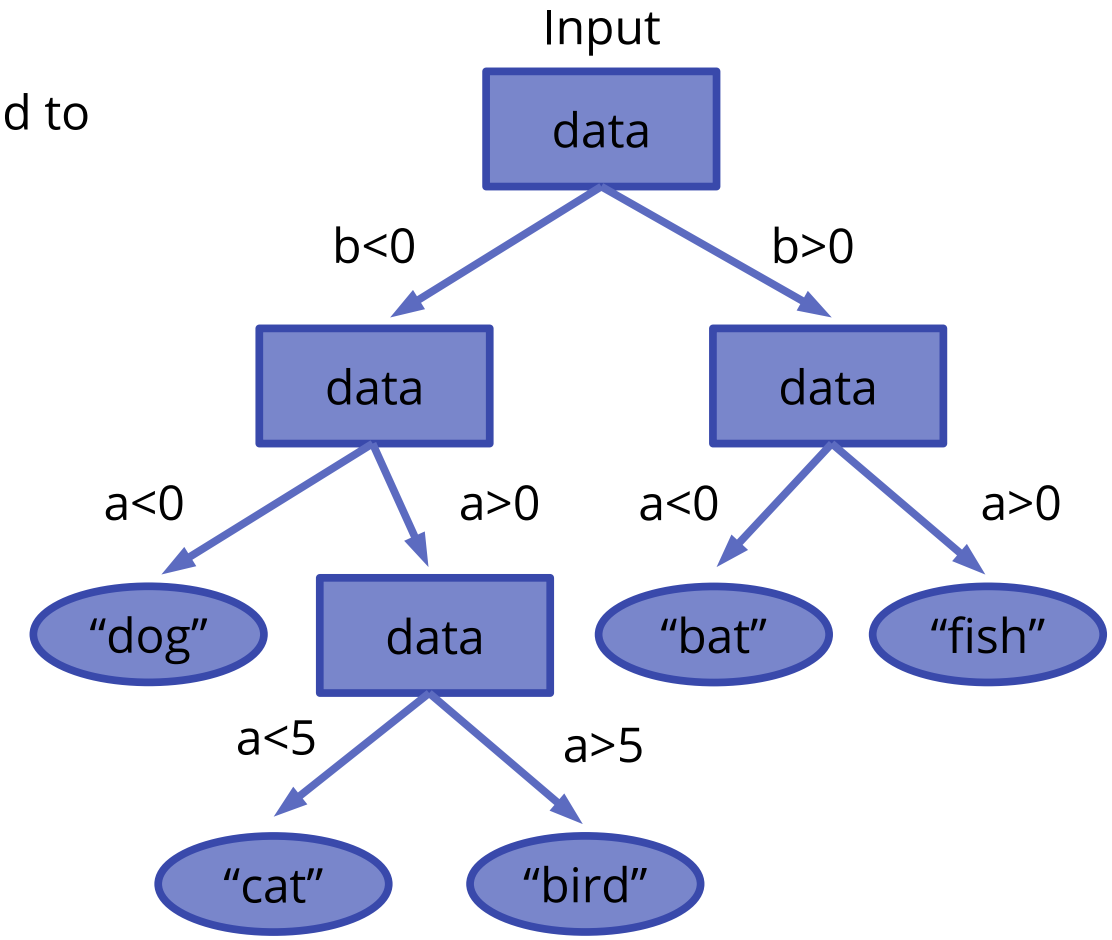

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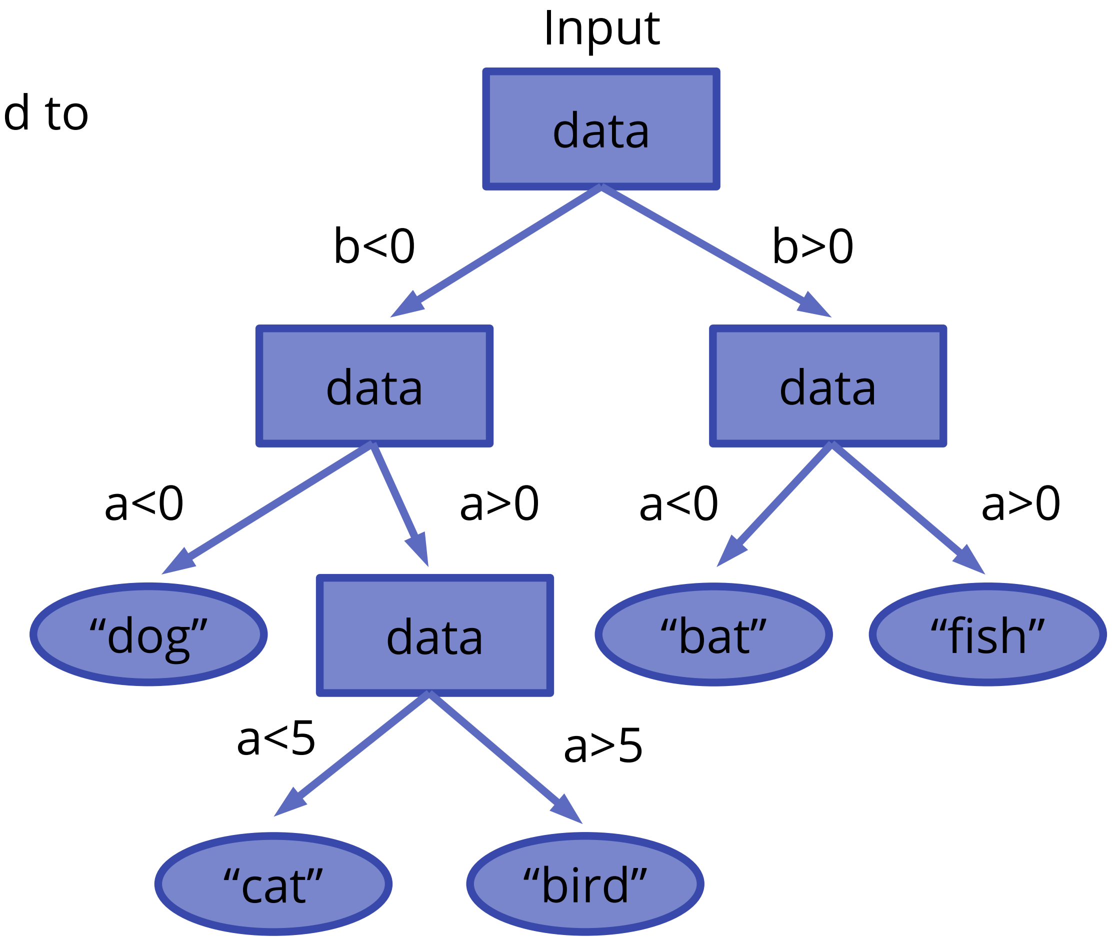

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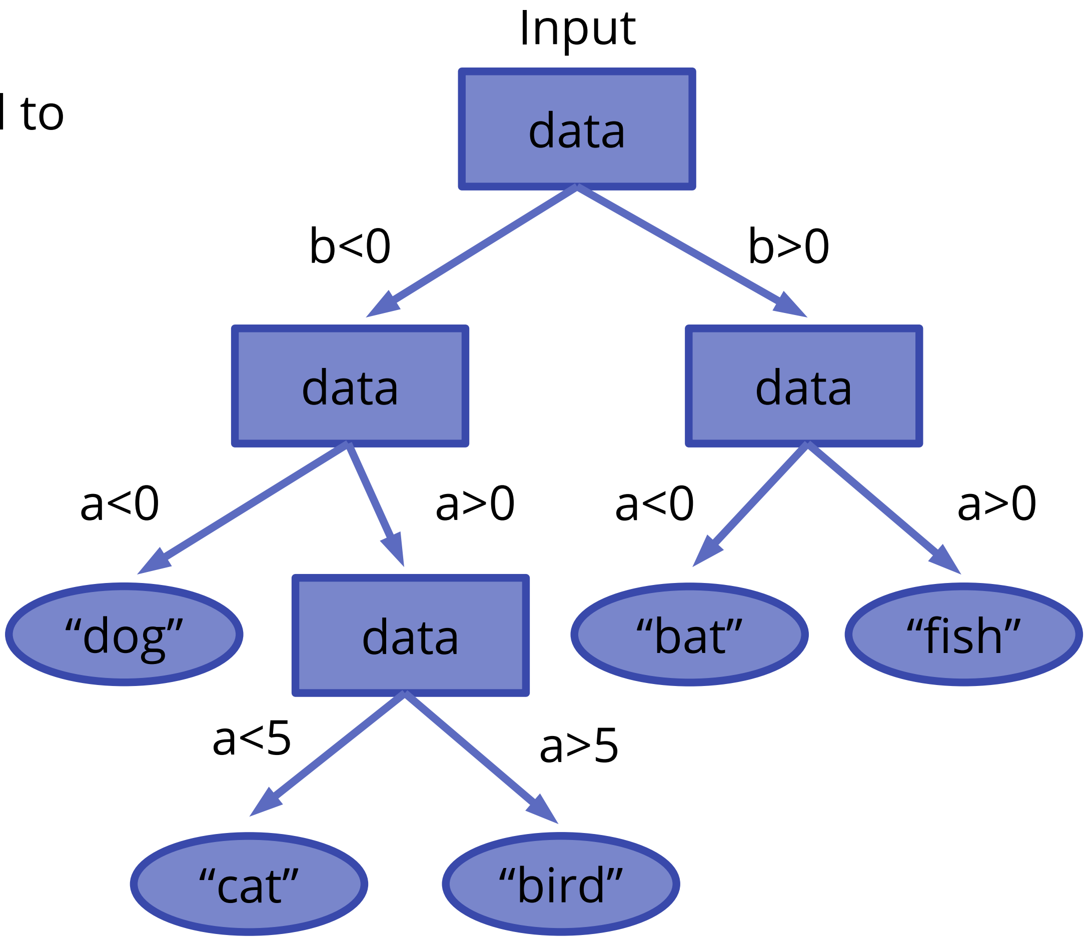

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But what is the “most important feature”?

Generally, it means that feature that makes the most difference to the classification of a single sample.

There different implementation of this definition, e.g., utilizing **information entropy** or other useful measures.

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Trees in a **random forest** are shallower than other decision tree models. The trees therefore act as "**weak learners**" that perform badly by themselves. However, combining a large number of weak learners performs much better than individual trees. The intuition behind is that weak learners "on average" compensate for their individual shortcomings.

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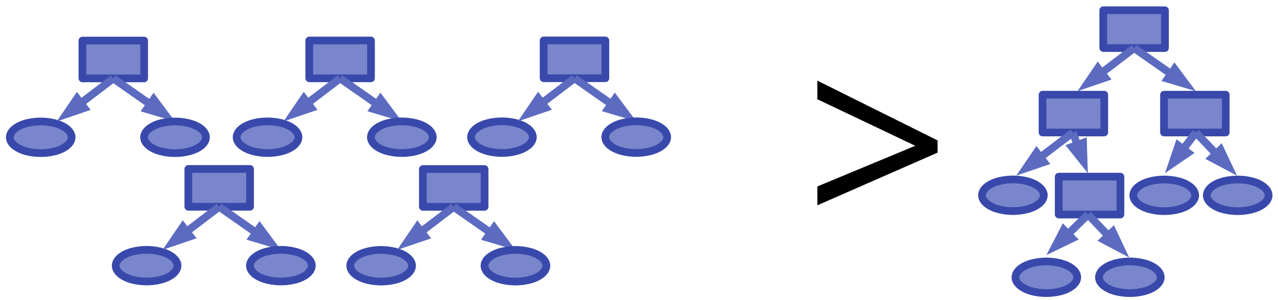

Gradient-boosted tree-based models

Gradient-boosted tree-based models are random forests (decision tree ensembles) that are built successively in such a way that *every newly created tree compensates for the shortcomings of the previous trees*.

The term **gradient-boosting** refers to the fact that new base learners (individual decision trees) are fitted to the model's pseudo-residuals, based on the gradient of the loss of the ensemble:

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$$f(\boldsymbol{x}) = \sum_{m}^{M} \beta_m h(\boldsymbol{x}, \theta_m)$$

Ensemble model with learning rate β_m, base learners $h(\boldsymbol{x}, \theta_m)$ with parameters θ_m.

$$\boldsymbol{r}_m^i = -\left[\frac{\partial L(y^i, f(x^i))}{\partial f(x^i)}\right]_{f=f_{m-1}}$$

Pseudo-residuals to which the next base learner will be fitted; by default, the loss of the updated ensemble will be less or equal to the loss of the current ensemble.

Gradient-boosted tree-based models

Gradient-boosted models are very successful in regression and classification tasks and still represent state-of-the-art in traditional ML.

If you have a classification or regression problem, it is always worth trying out gradient-boosted methods.

Common implementations:

- XGBoost
- LightGBM

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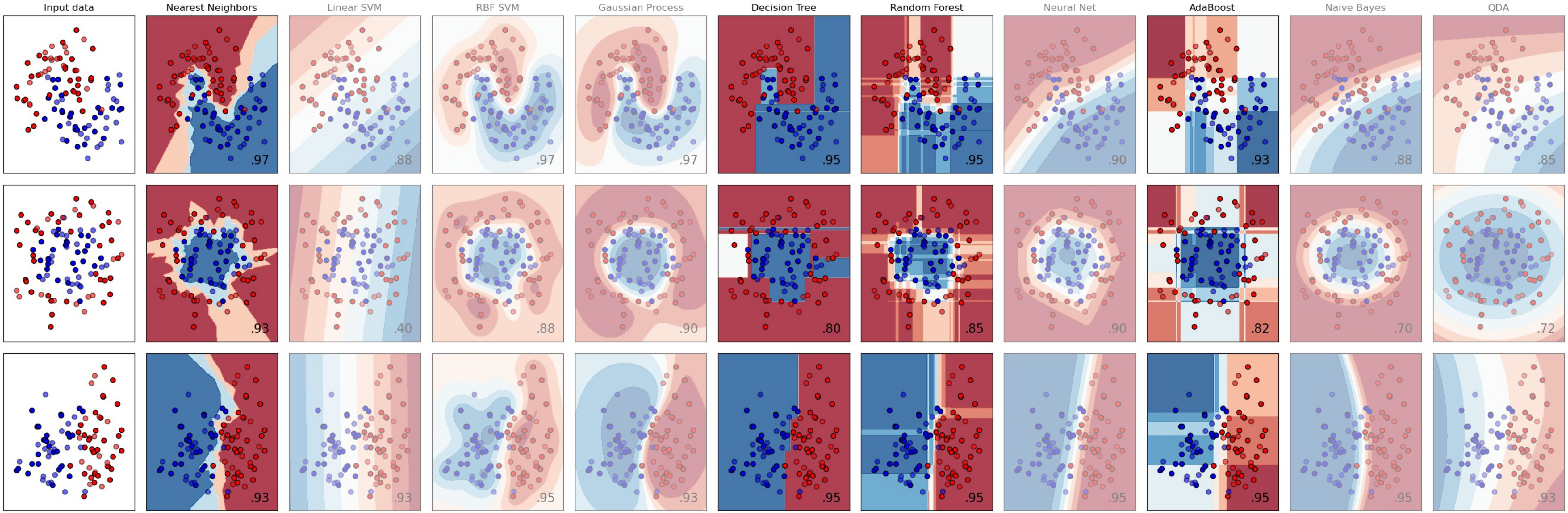
Cons:

- Decision boundaries and regression predictions may be discrete instead of continuous (see next slide)

Supervised learning - summary



(Similar to XGBoost)

Scikit-learn classifier comparison

That’s all folks!

Today's lecture

Supervised learning

Supervised learning setup

Supervised learning concepts

Benchmarking and metrics

Linear models

Nearest Neighbor models

Tree-based models

Next Week:

Lab 1: Supervised learning

Next lecture (20 March)

Unsupervised learning

Unsupervised learning setup

Hierarchical clustering

k-means clustering

Expectation Maximization clustering

DBSCAN

Principal component analysis