Supervised Learning

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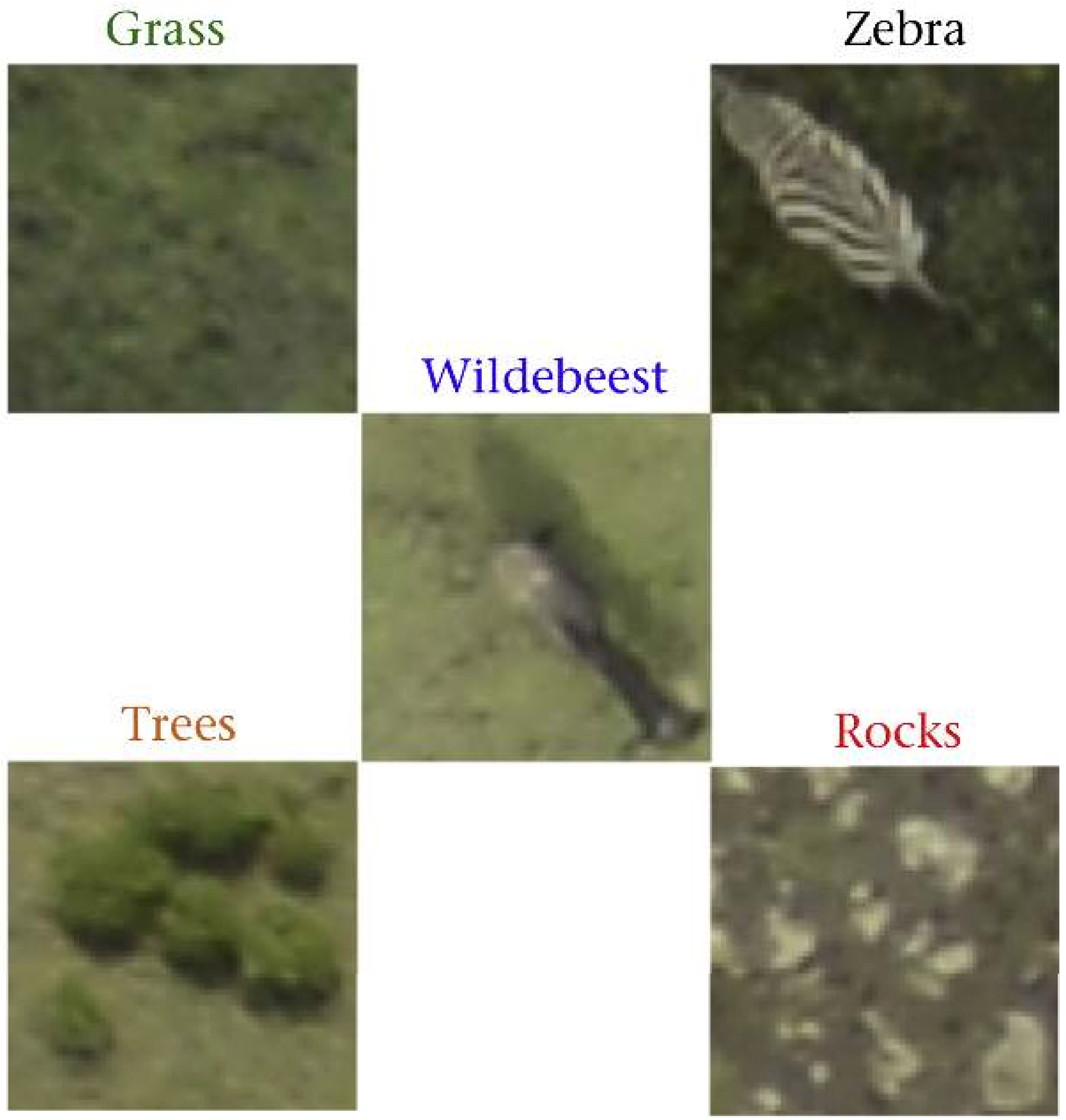
@TWlyY29

Supervised Machine Learning



https://exeter-data-analytics.github.io/MachineLearning/supervised-learning-1.html

Supervised Machine Learning

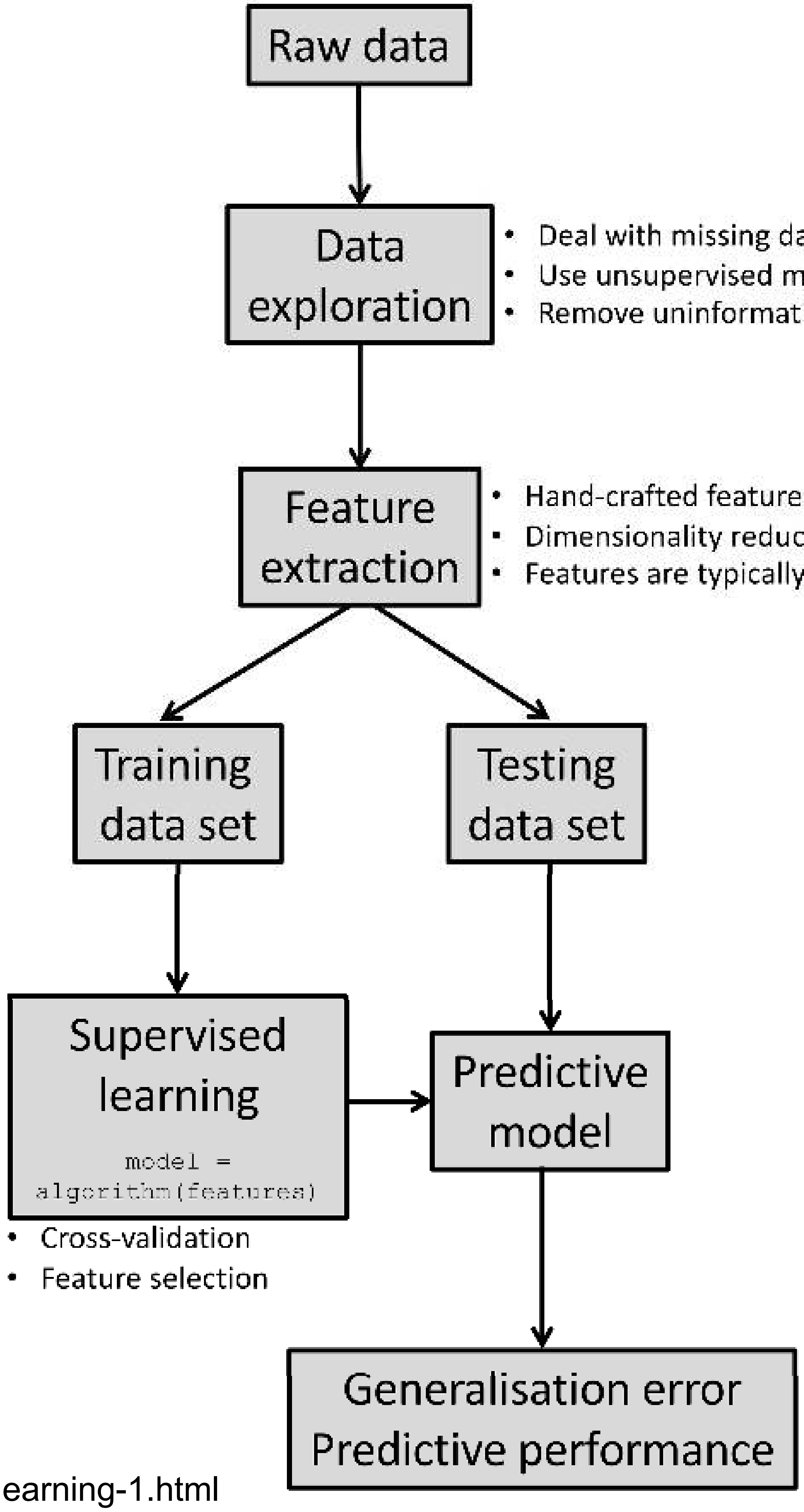
Objective:
learn the *class label* y for each value of x, the *feature vector* consisting of multiple *features* (categorical or numerical)

Result:
A function $f(x) = y$ that best predicts y for each value of x

If y is

- a real number, a regression model is learned
- a Boolean value (true/false, +1/-1), we speak of *binary classification*
- a nominal value of some finite set, it is a *multiclass classification*

Supervised Machine Learning: Bird View



Raw data

Data exploration
- Deal with missing data (ignore/impute)
- Use unsupervised methods to accentuate the data's structure
- Remove uninformative variables (crude filtering)

Feature extraction
- Hand-crafted features
- Dimensionality reduction techniques
- Features are typically normalized/standardized

Training data set

Testing data set

Supervised learning

```
model =
algorithm(features)
```

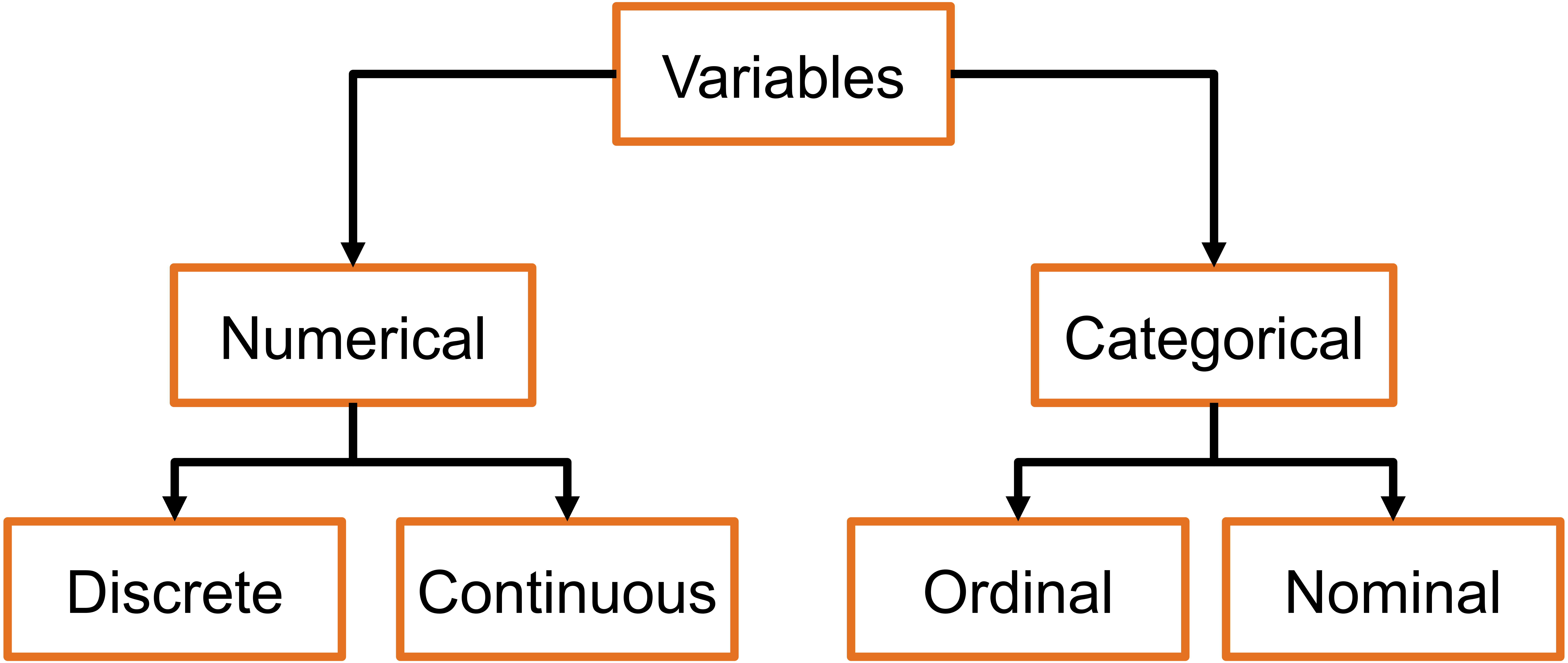
- Cross-validation
- Feature selection

Predictive model

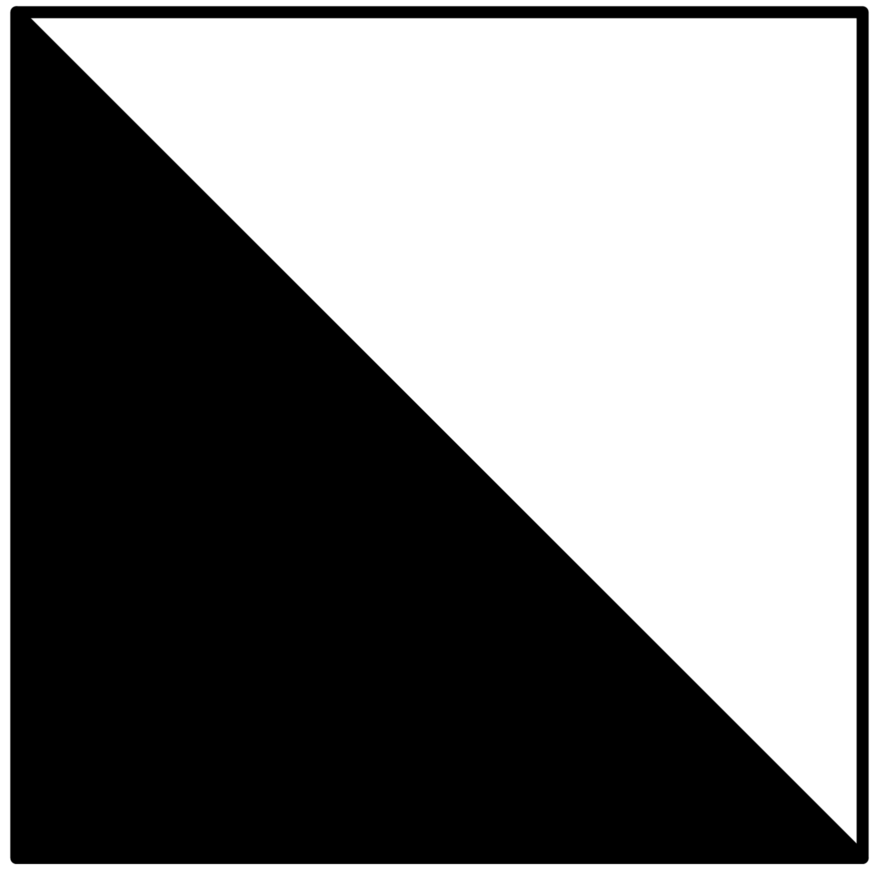
Generalisation error
Predictive performance

https://exeter-data-analytics.github.io/MachineLearning/supervised-learning-1.html

Hello Data


Variables
Numerical
Categorical
Discrete
Continuous
Ordinal
Nominal

Discrete vs. Continuous



Dichotomous data:

Data points can only take up 2 values

Discrete data:

Data points can only take up values from a set of possible values.

Either finite or infinite but countable

Continuous data:

Data points can be measured to an arbitrary level of exactness

Scales

Nominal

Values divide space of possible values into different segments

No order between segments

Example: gender, nationality

Ordinal

Allows for rank order – data can be sorted

No relative degree or relative difference between groups

Example: school grades

Interval

Order and difference between groups is defined

No natural „zero“ & ratio between points is undefined

Example: temperature in Celsius

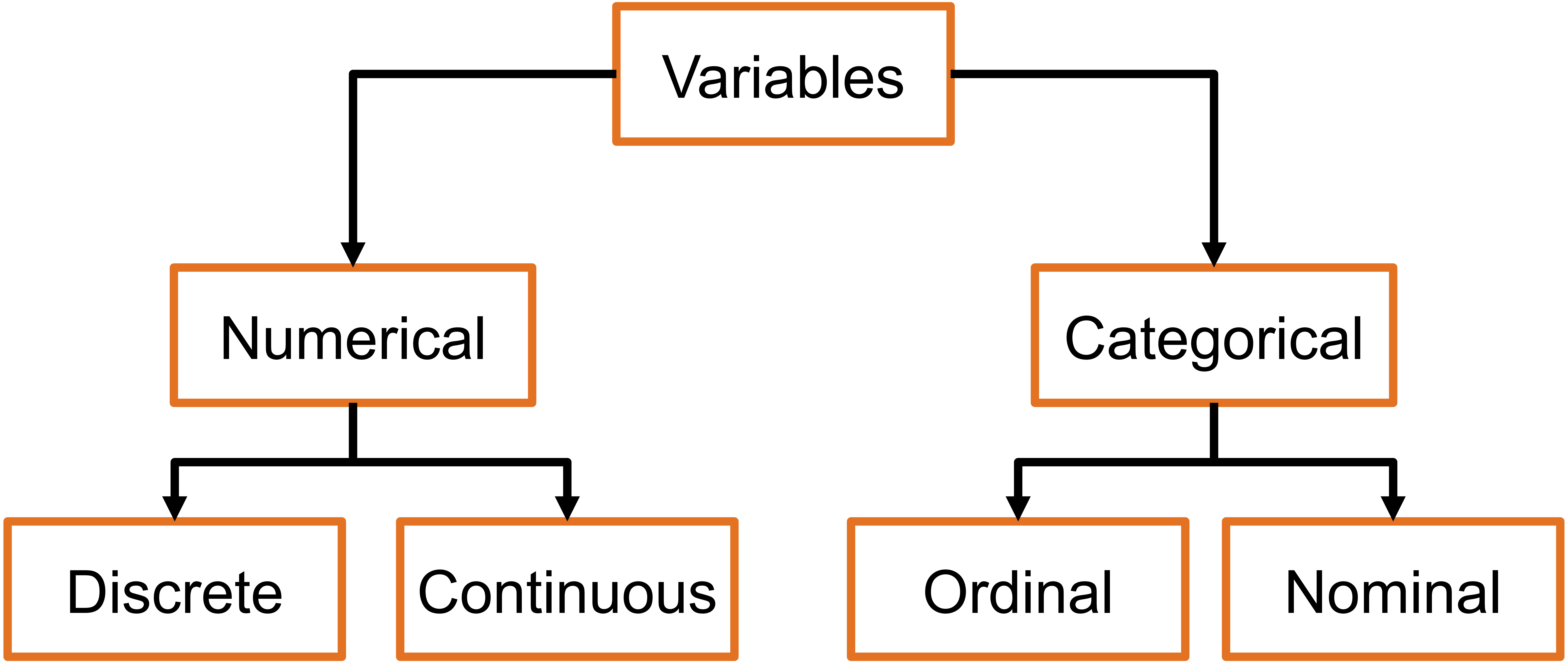
Ratio

Meaningful zero, i.e. unique and non-arbitrary

Example: temperature in Kelvin, age, weight, height

S. S. Stevens: On the Theory of Scales of Measurement. In: Science. 1946, 103, S. 677–680.

Hello Data



Variables

Numerical

Categorical

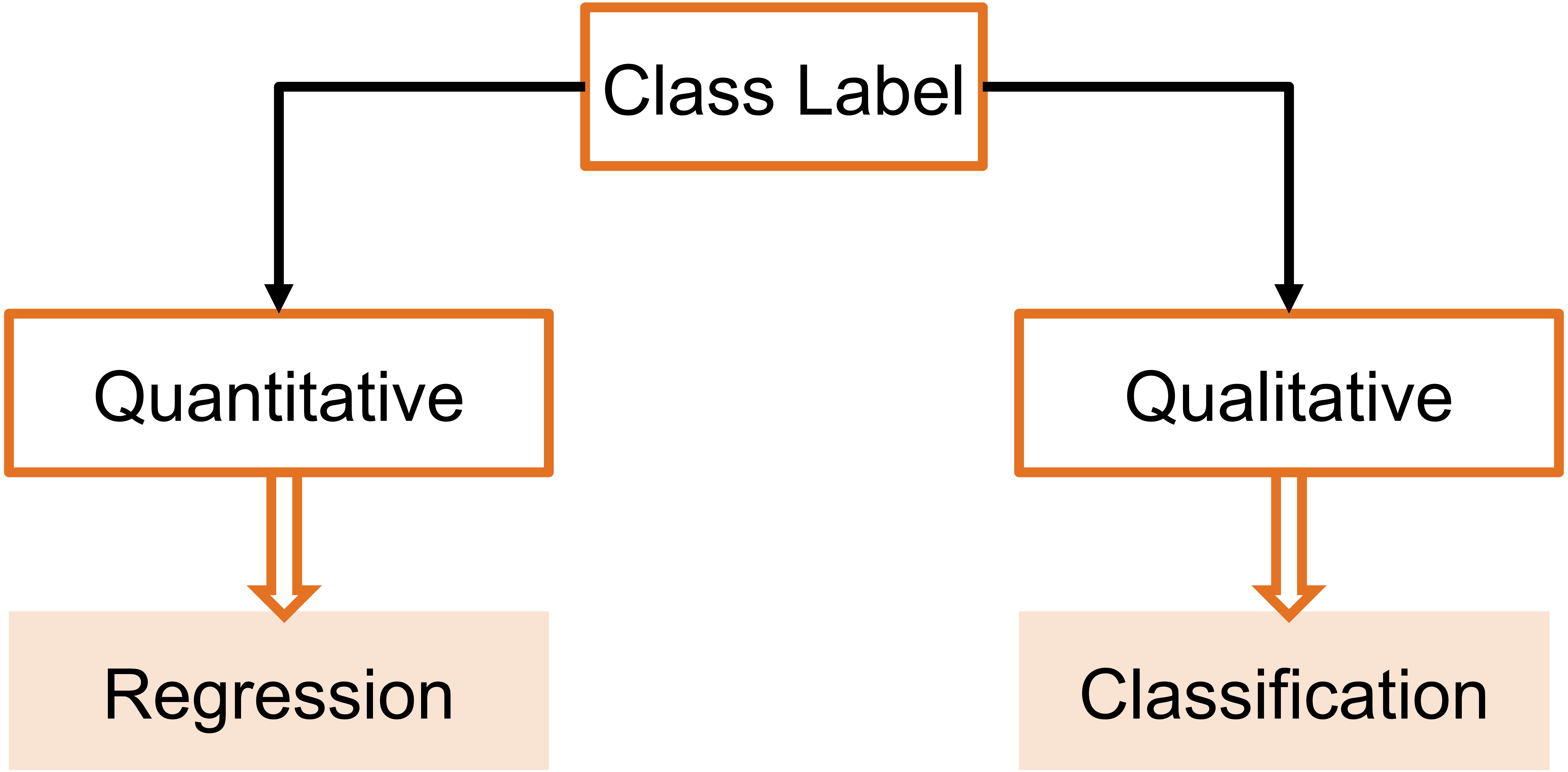
Discrete

Continuous

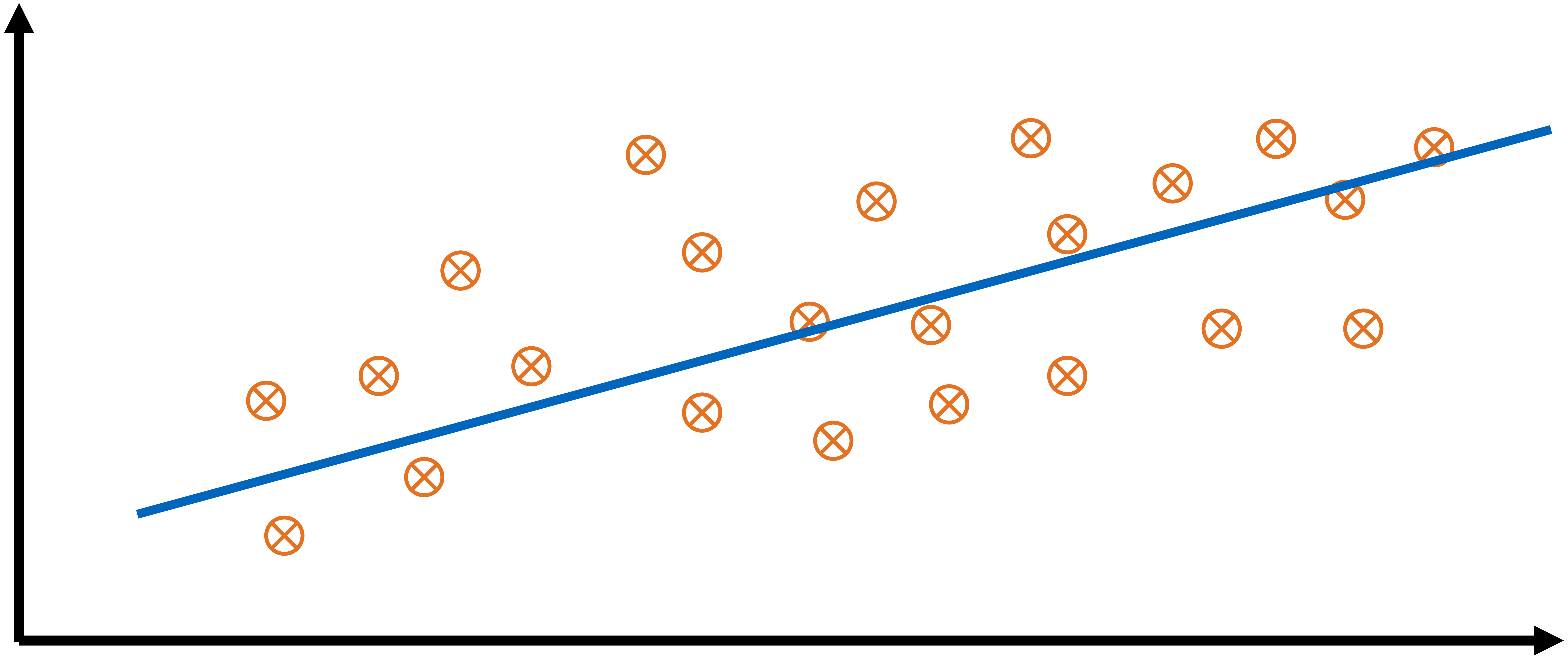
Ordinal

Nominal

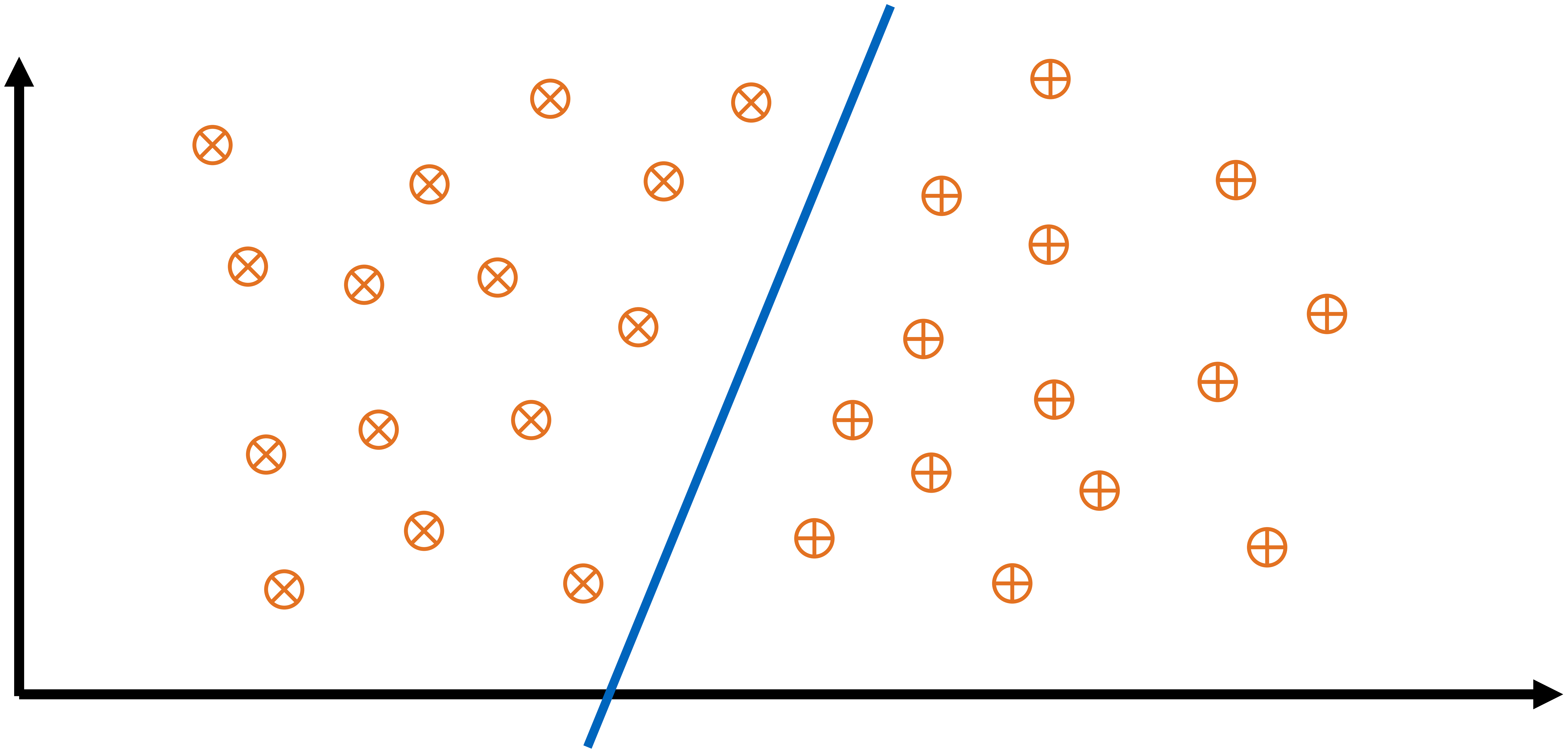
Nature of the Class Label



Regression



Classification



Supervised Machine Learning…in other words

Supervised Machine Learning aims at forecasting class labels for measured data

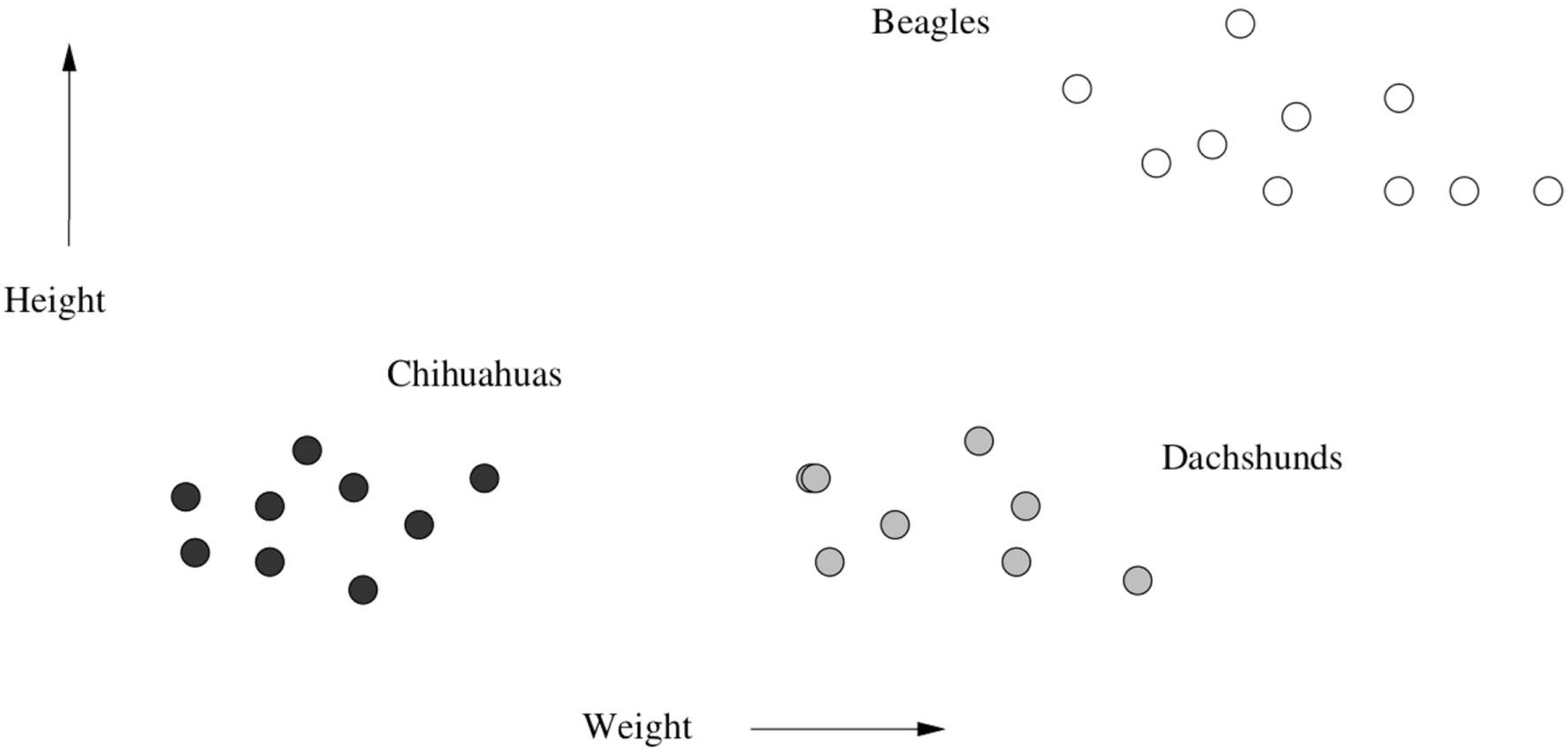
Correct class labels are known for training data

Training means to search for a good function mapping measured artifacts to known class labels

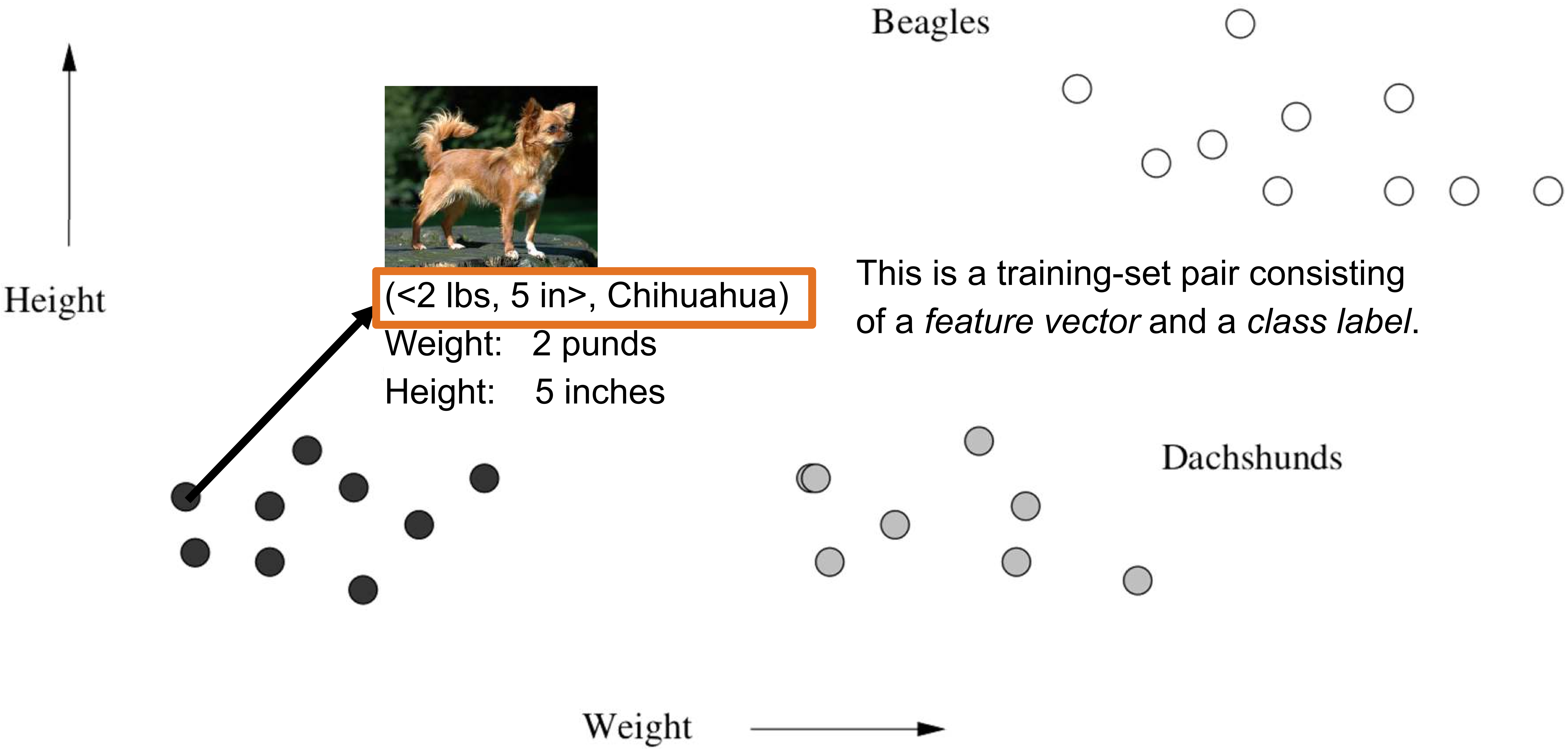
What you need:

- Classificator
- Measured data
- Class labels

An Example



An Example



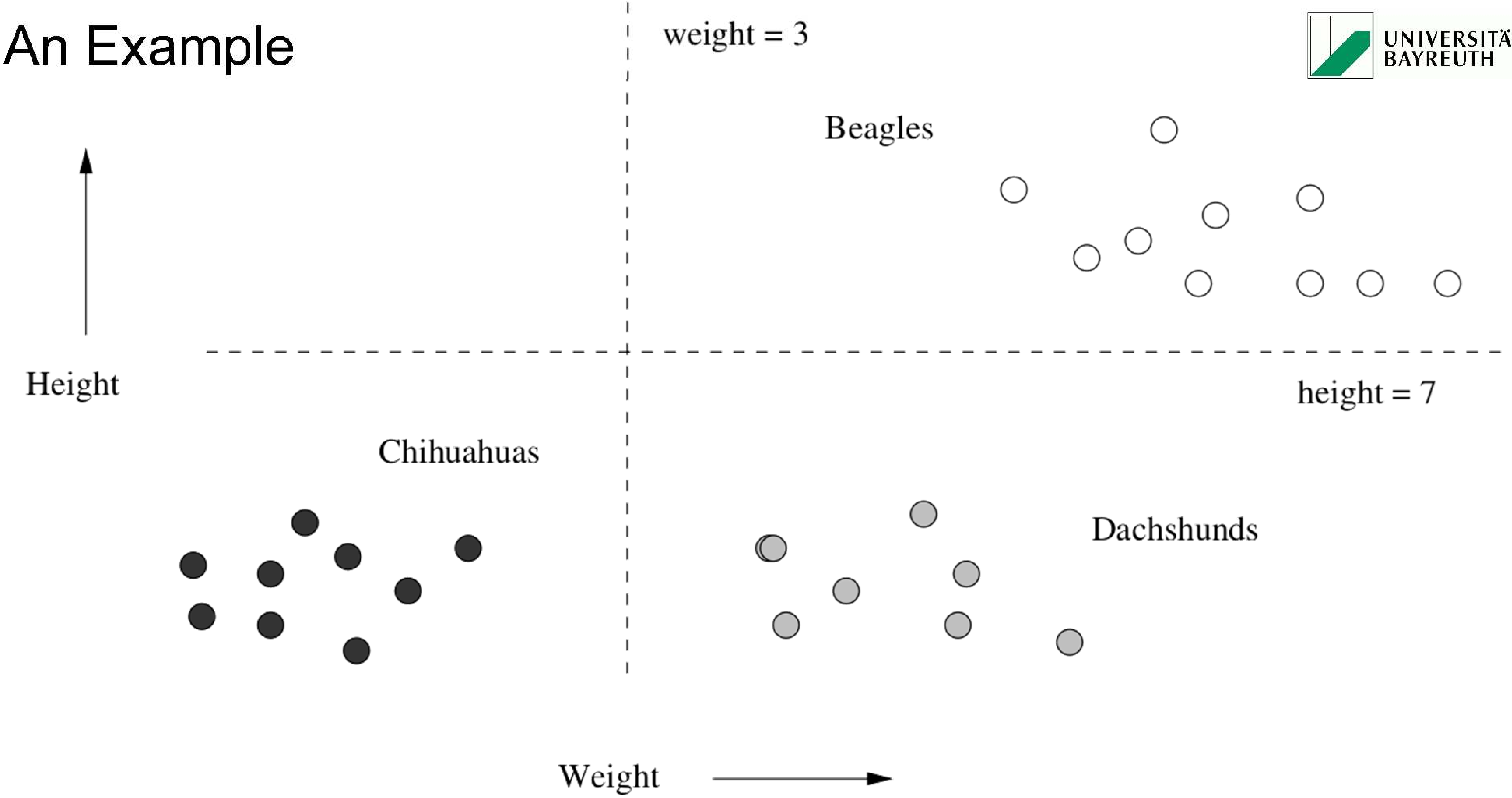
(<2 lbs, 5 in>, Chihuahua)

Weight: 2 punds

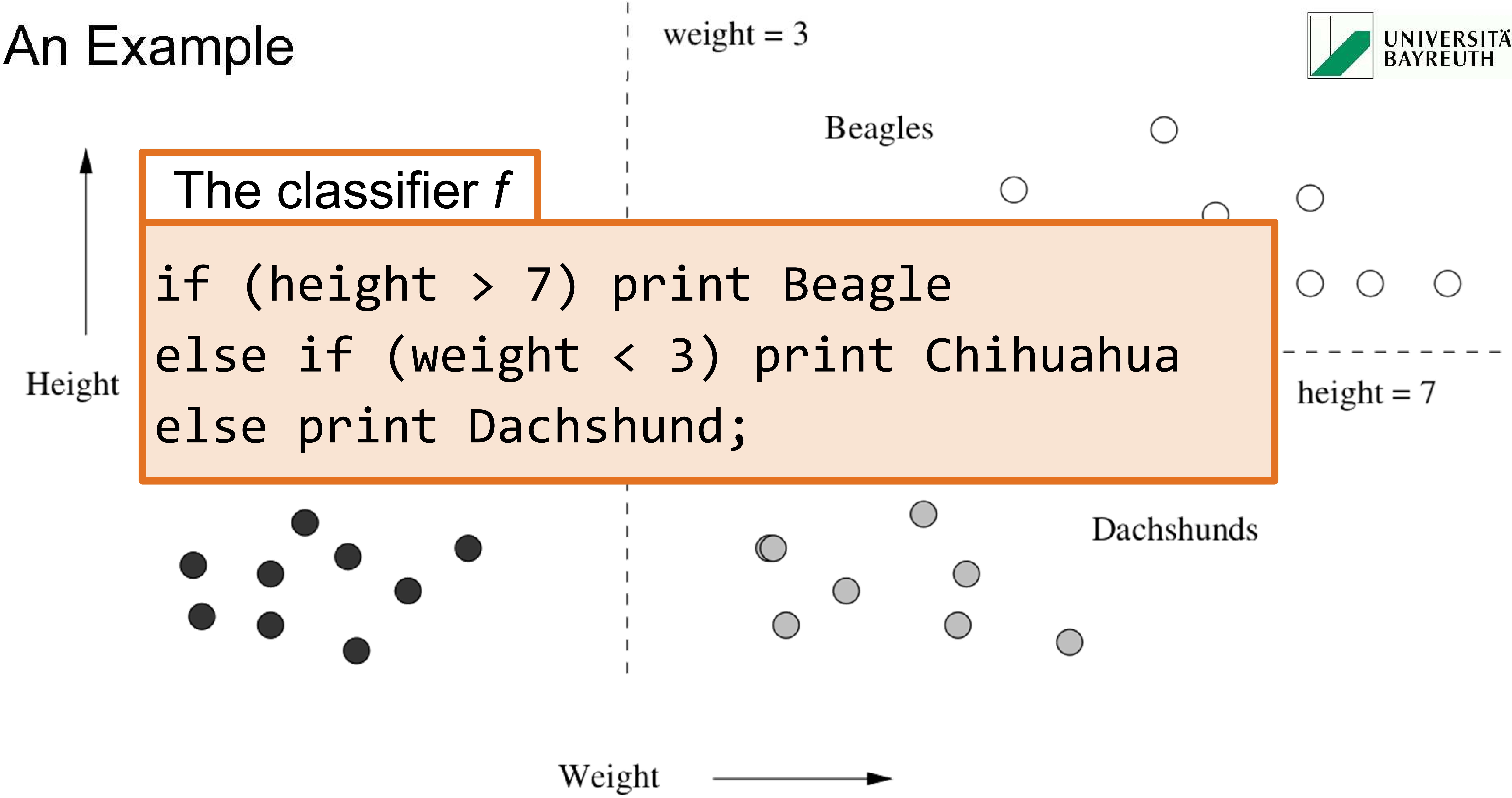
Height: 5 inches

This is a training-set pair consisting of a *feature vector* and a *class label*.

An Example


weight = 3
Beagles
Height
height = 7
Chihuahuas
Dachshunds
Weight

An Example



The classifier *f*

```
if (height > 7) print Beagle
else if (weight < 3) print Chihuahua
else print Dachshund;
```

Relation to Clustering

Classification:

- Class label is discrete
- Enough training data for *each class*

Regression:

- Target variable is numeric

Clusters could be used to identify new classes

Clustering:

- no class label / target variable
- no training – input data without pre-defined classes
- produces partitioning of data

Major Classes of Classifiers

- Decision trees

  Suitable for binary and multiclass classification with a limited number of features
- Perceptrons

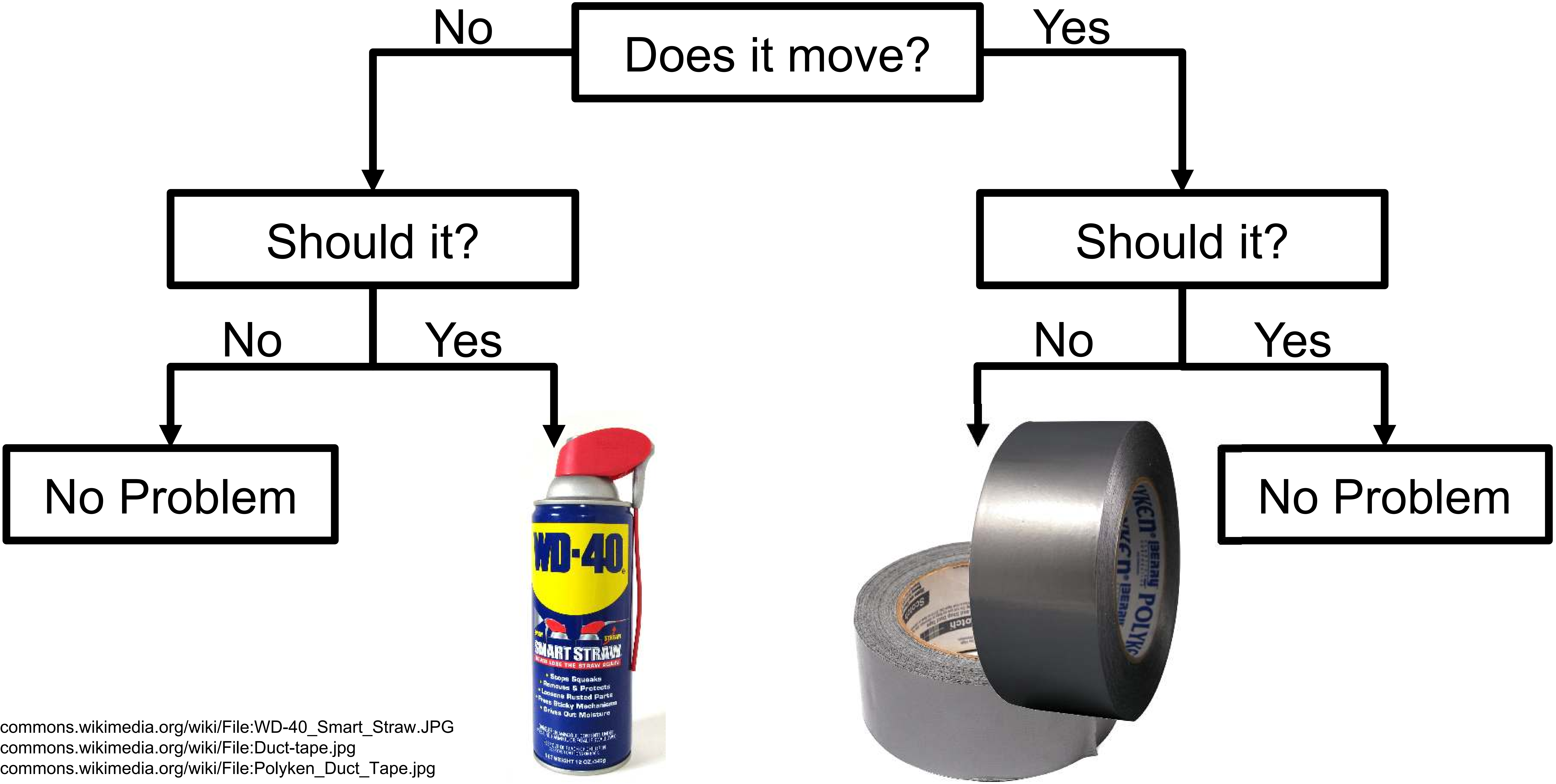
  Applies weights to components of vectors. Output +1 if sum exceeds a threshold, otherwise -1.
- Neural networks

  Acyclic networks of perceptrons
- Instance-based learning

  Compares instances of data to the entire training set. Example: k-nearest neighbor.
- Support-vector machines

  Maps training examples to points in space so as to maximise the gap between categories

Decision Trees



Does it move?

No

Yes

Should it?

Should it?

No

Yes

No

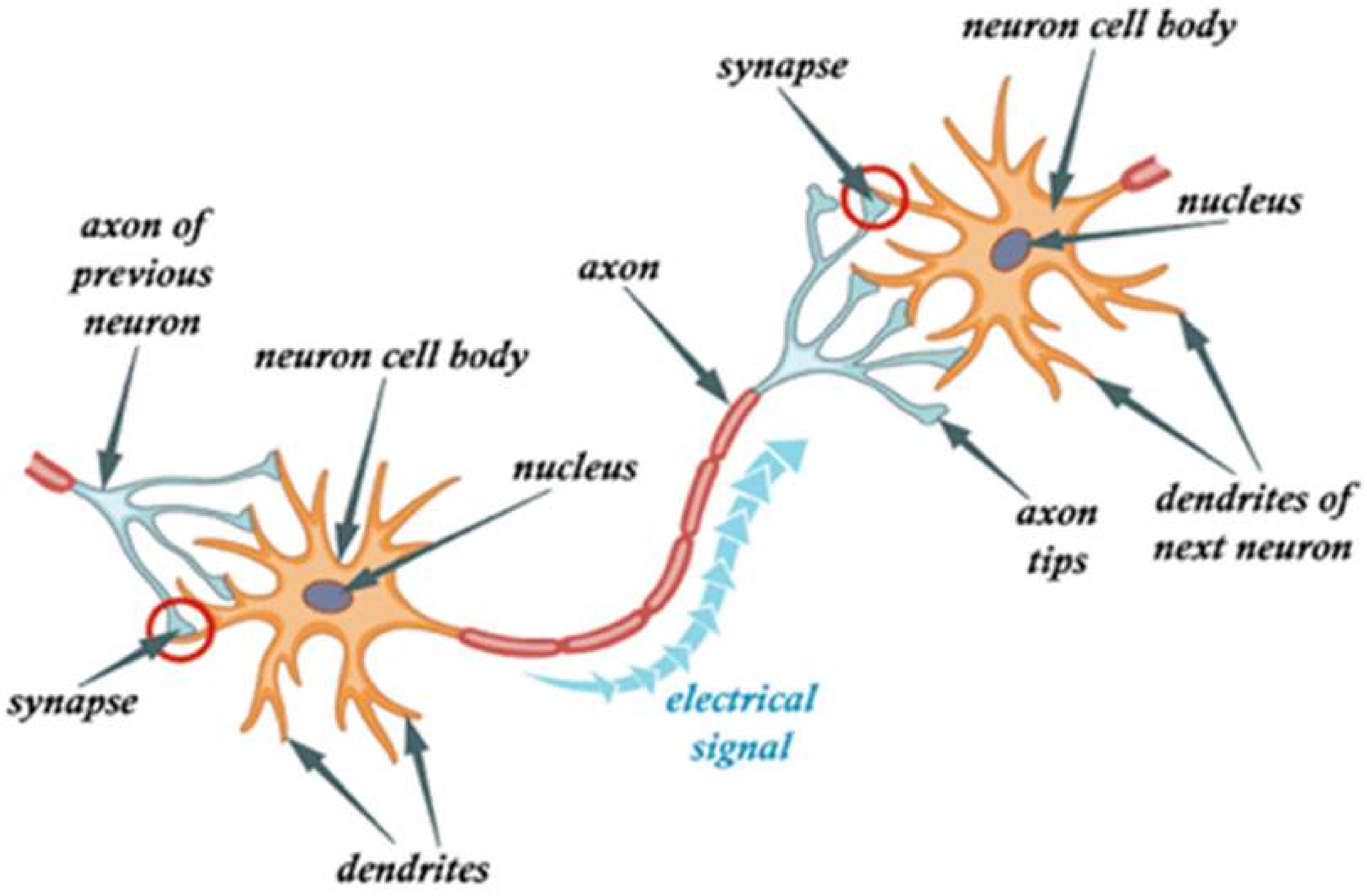
Yes

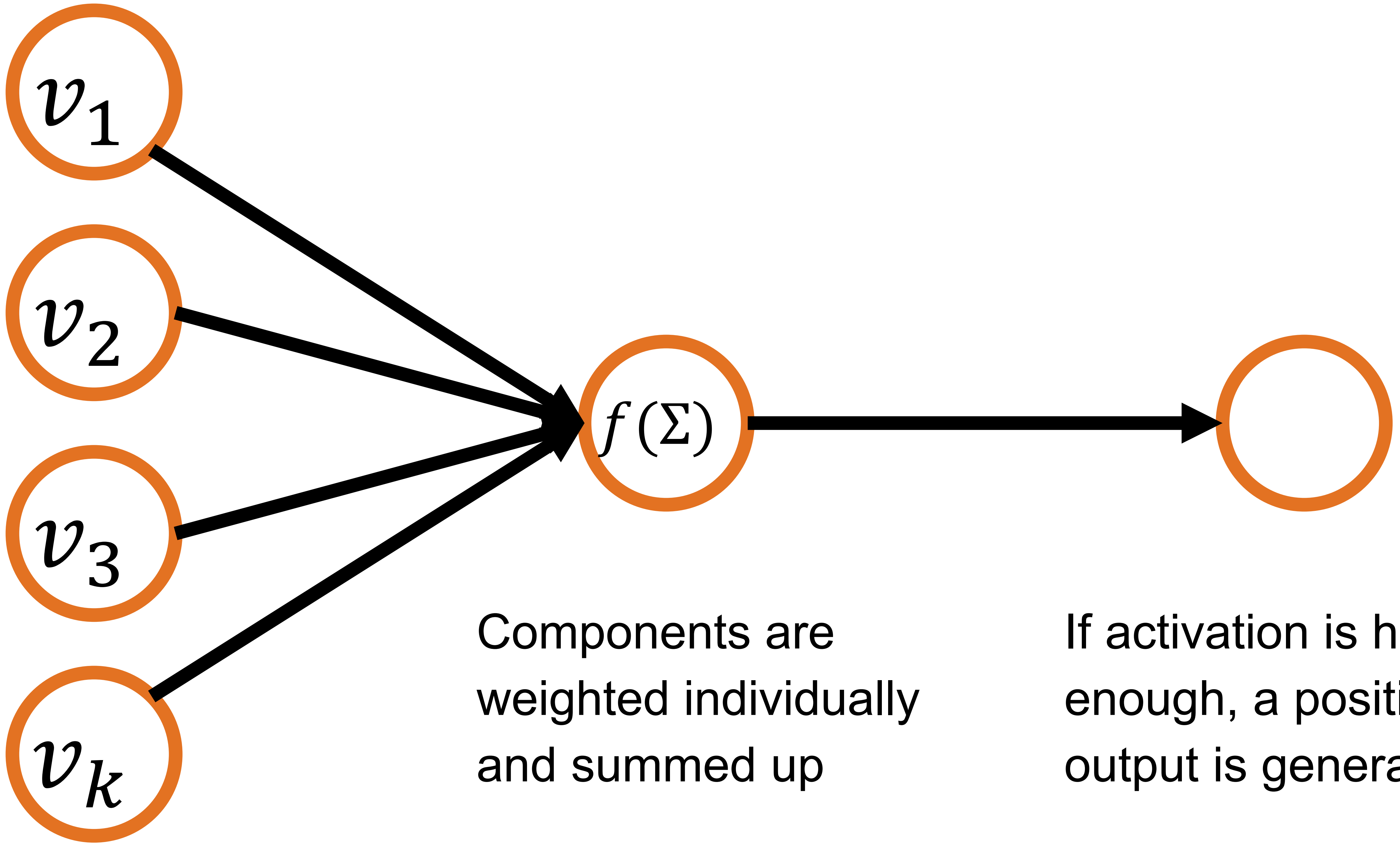
No Problem

No Problem

https://commons.wikimedia.org/wiki/File:WD-40_Smart_Straw.JPG
https://commons.wikimedia.org/wiki/File:Duct-tape.jpg
https://commons.wikimedia.org/wiki/File:Polyken_Duct_Tape.jpg

Perceptrons





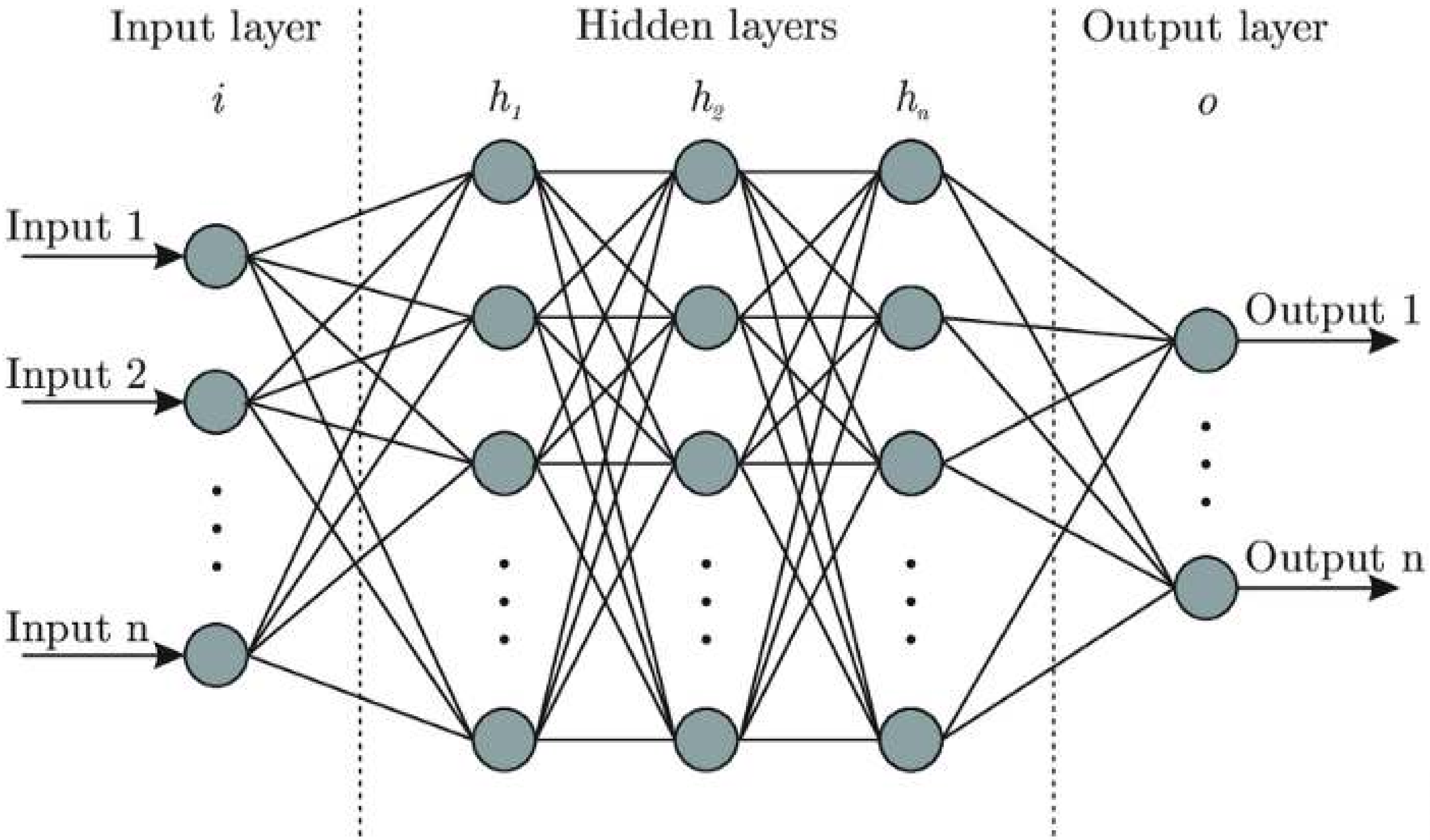
Components are weighted individually and summed up

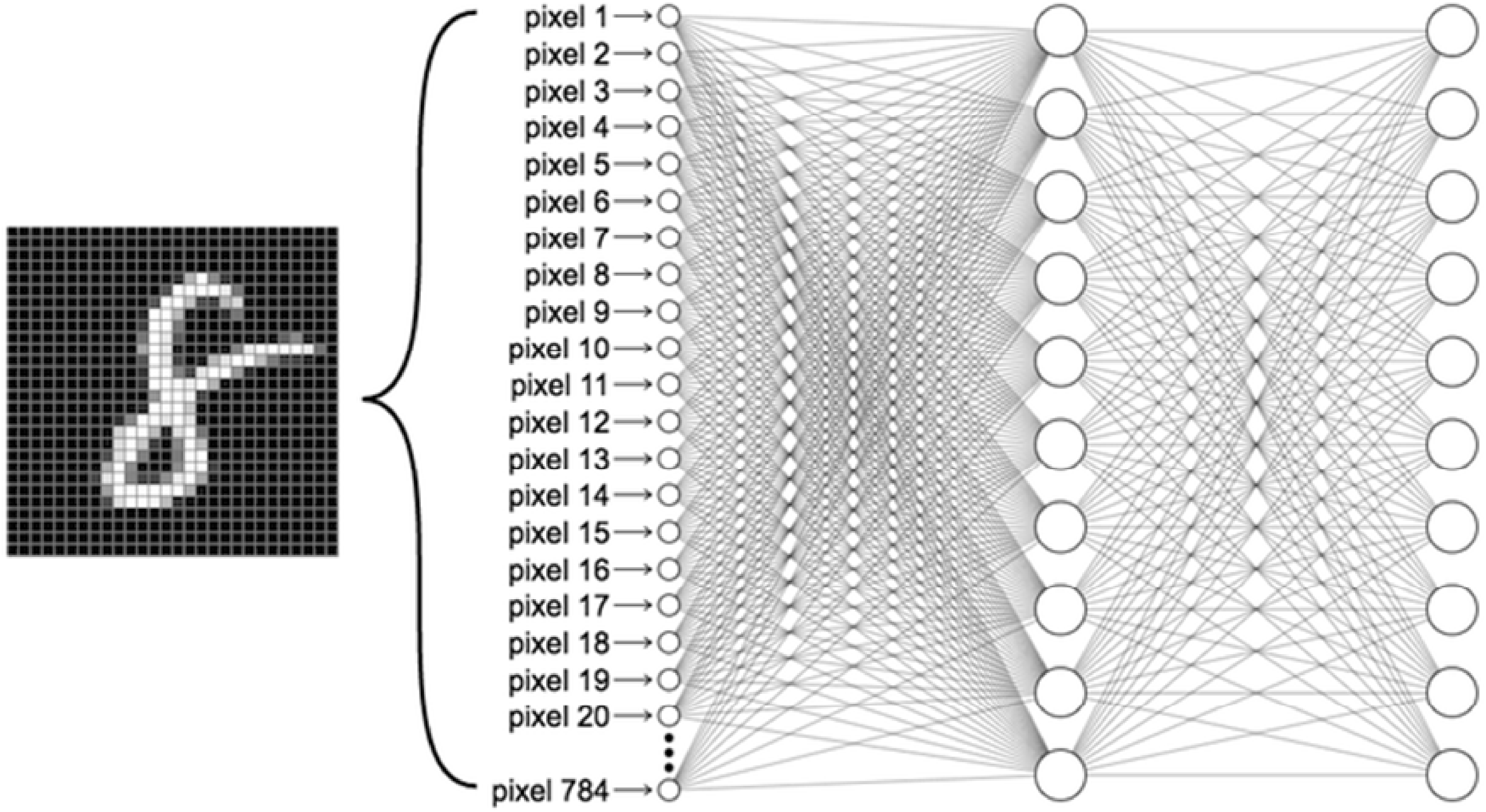
If activation is high enough, a positive output is generated

Components of instances

https://www.deeplearningtrack.com/single-post/2017/07/09/Introduction-to-NEURAL-NETWORKS-Advantages-and-Applications

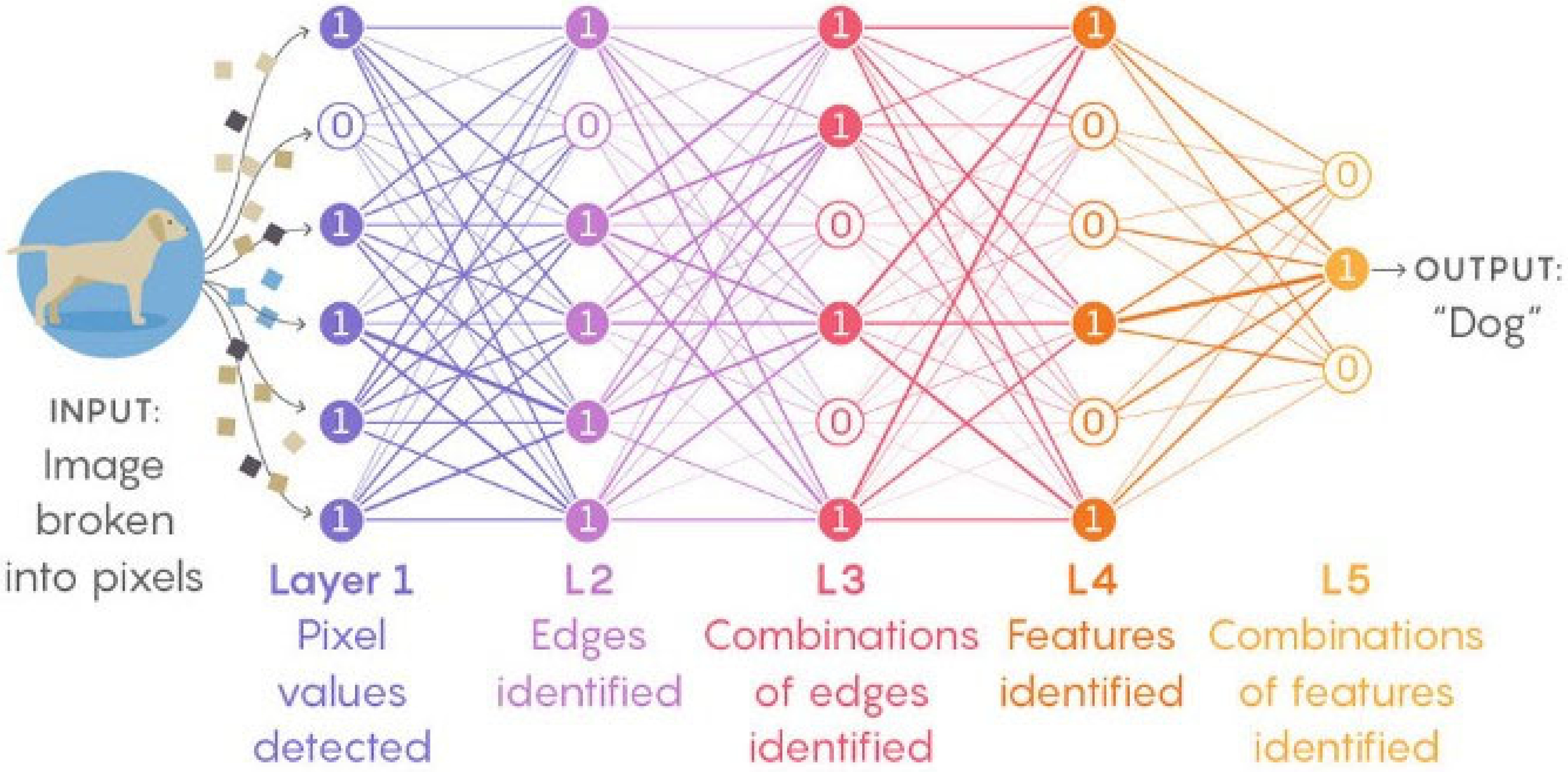
Neural Networks





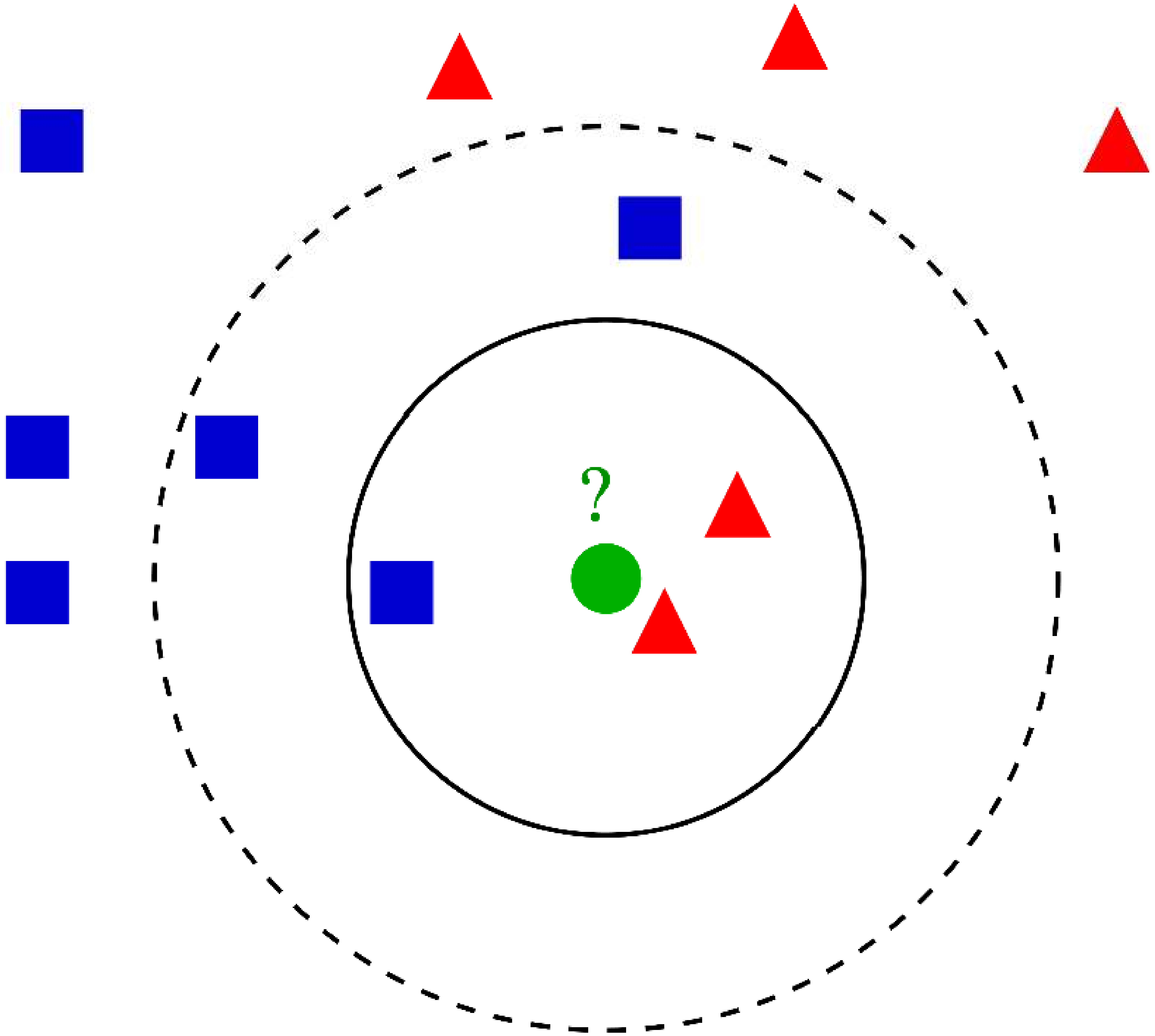
https://towardsdatascience.com/designing-your-neural-networks-a5e4617027ed

Neural Networks



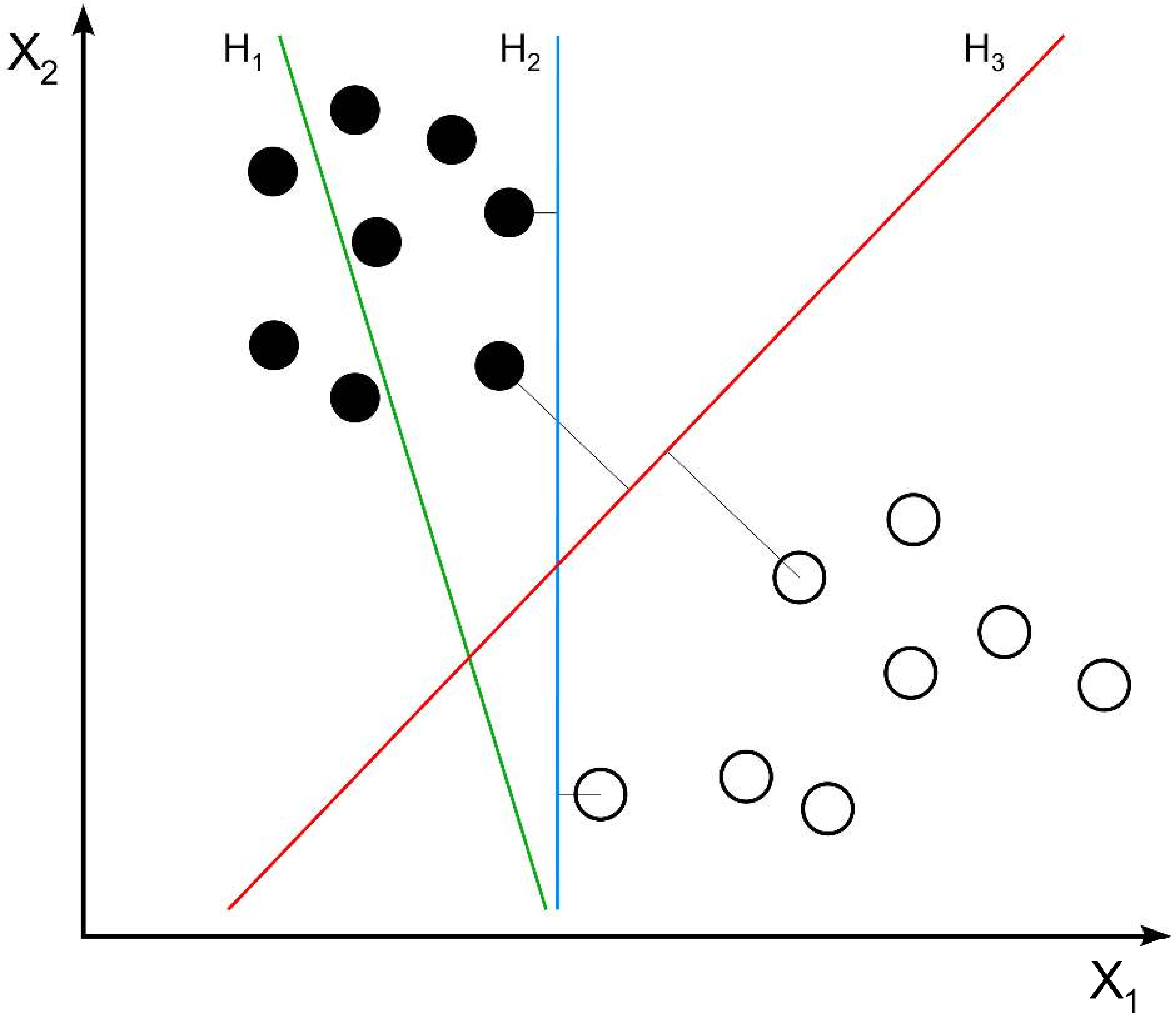
https://towardsdatascience.com/designing-your-neural-networks-a5e4617027ed

k-Nearest Neighbors



https://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm

Support Vector Machines



https://en.wikipedia.org/wiki/Support-vector_machine

Some Classification Algorithms Compared

Input data
Nearest Neighbors
Linear SVM
RBF SVM
Gaussian Process
Decision Tree
Random Forest
Neural Net
AdaBoost
Naive Bayes
QDA
.97
.88
.97
.97
.95
.95
.90
.93
.88
.85
.93
.40
.88
.90
.80
.85
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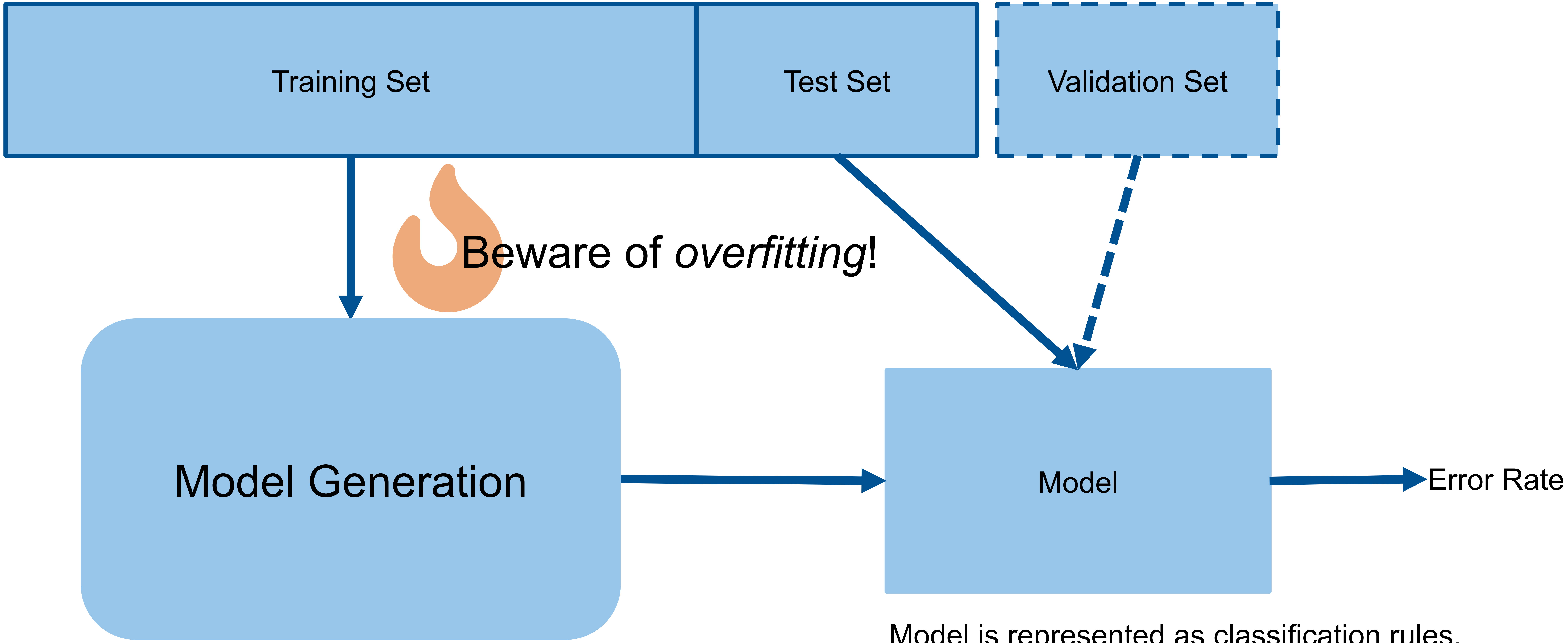
https://scikit-learn.org/stable/auto_examples/classification/plot_classifier_comparison.html

Supervised Learning: Training and Testing

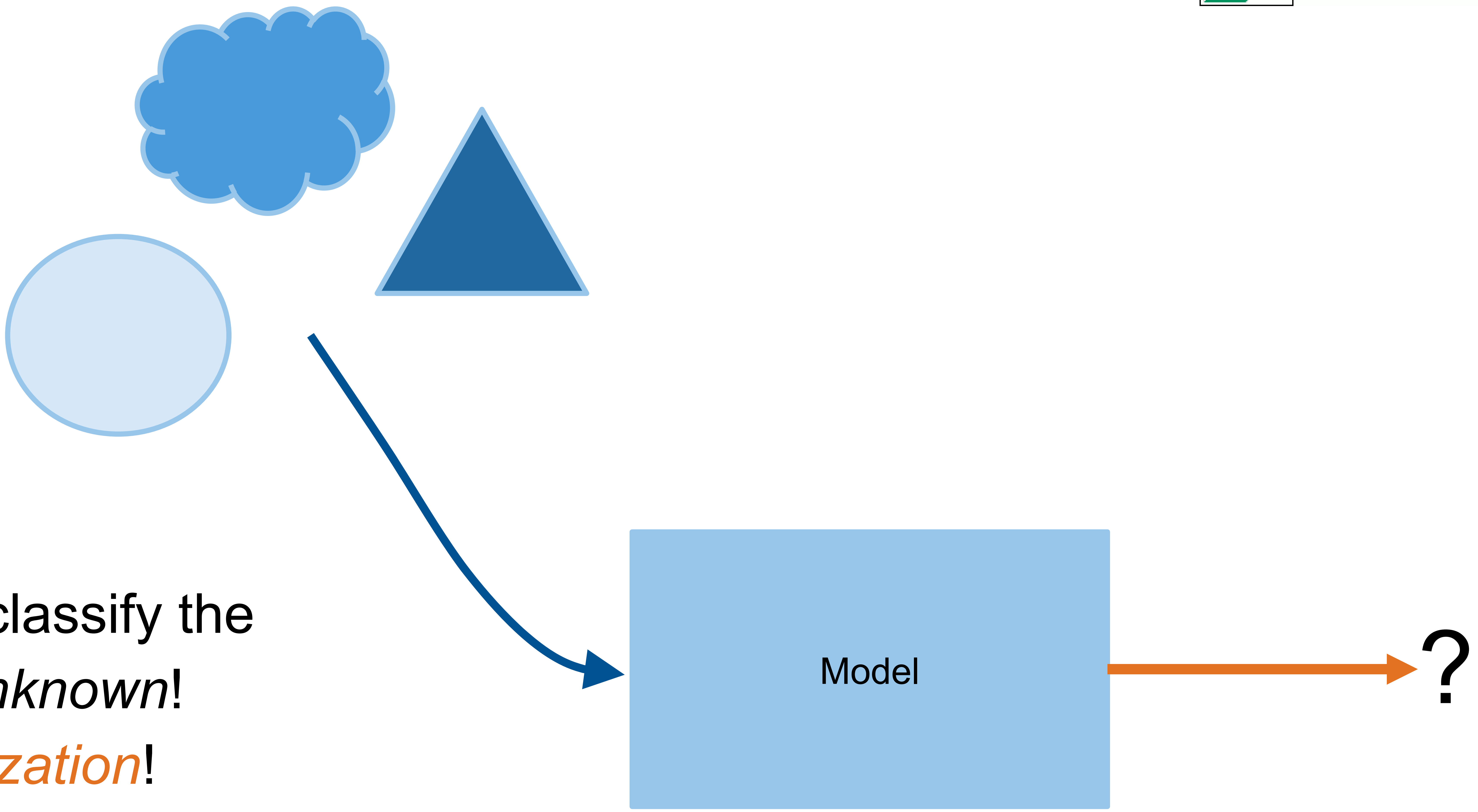


Beware of *overfitting*!

Model is represented as classification rules, decision trees, or mathematical formulas

Leskovec, J., Rajaraman, A. and Ullman, J.D., 2020. *Mining of massive data sets*. Cambridge university press.

What the Model is for



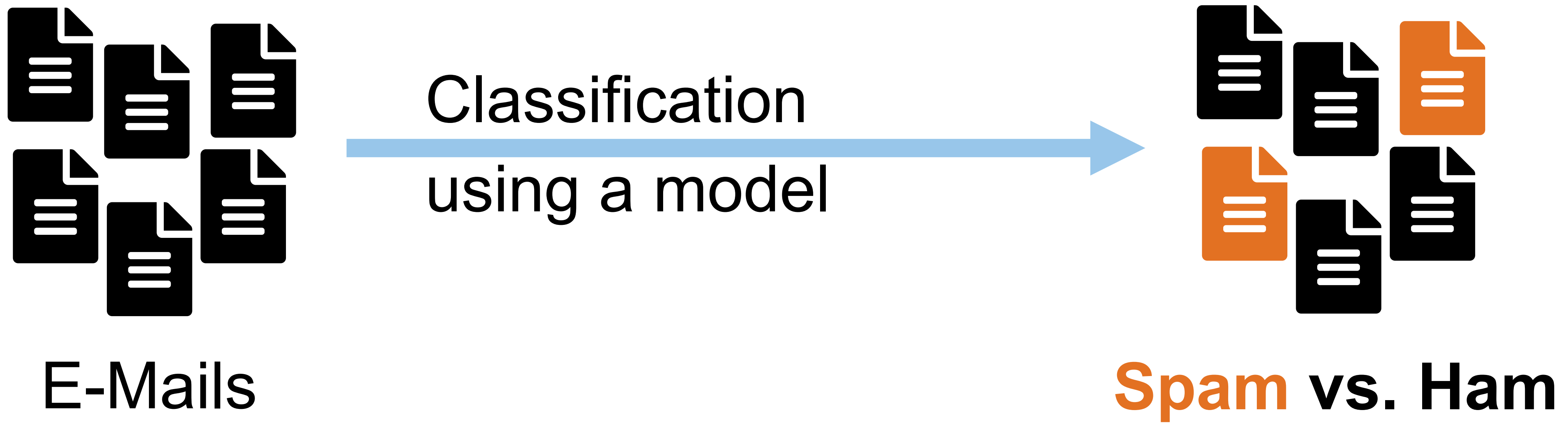
The model is used to classify the data whose class is *unknown*!

Its purpose is *generalization*!

How to Design a Model: Feature Selection

Formulate characteristics that help distinguishing between classes.

For spam-detection: find words or combinations of words that indicate a mail being spam.



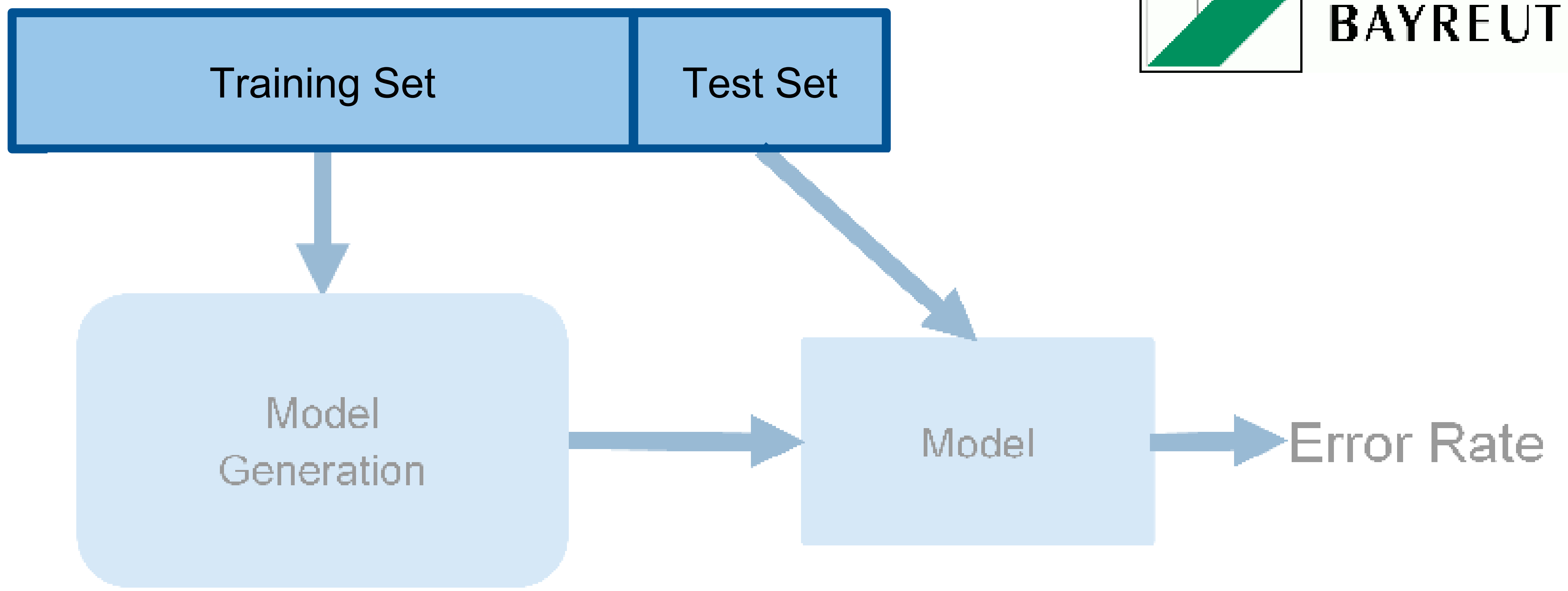
Spam: Wholesale Fashion Watches -57% today. Designer watches for cheap ...
Spam: You can buy ViagraFr$1.85 All Medications at unbeatable prices! ...
Spam: WE CAN TREAT ANYTHING YOU SUFFER FROM JUST TRUST US ...
Spam: Sta.rt earn*ing the salary yo,u d-eserve by o'btaining the prope,r crede'ntials!

Ham: The practical significance of hypertree width in identifying more ...
Ham: Abstract: We will motivate the problem of social identity clustering: ...
Ham: Good to see you my friend. Hey Peter, It was good to hear from you. ...
Ham: PDS implies convexity of the resulting optimization problem (Kernel Ridge ...

Curse of Dimensionality:

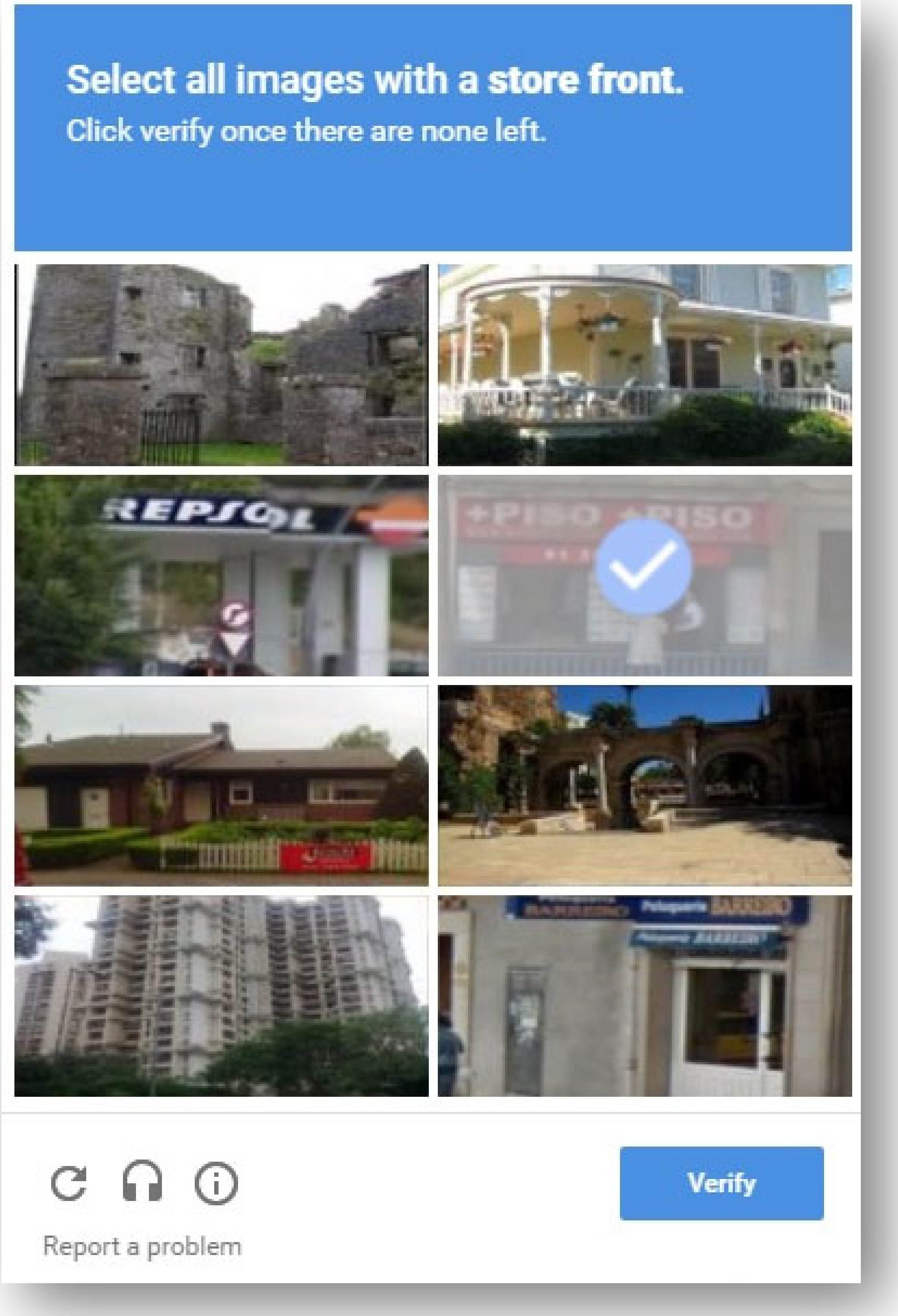
Including more features will improve classification *conceptually* but will render computation increasingly difficult.

/kæp.tʃə/ or Creating a Training Set



Label Data Manually?

Often time consuming and costly process for large training sets

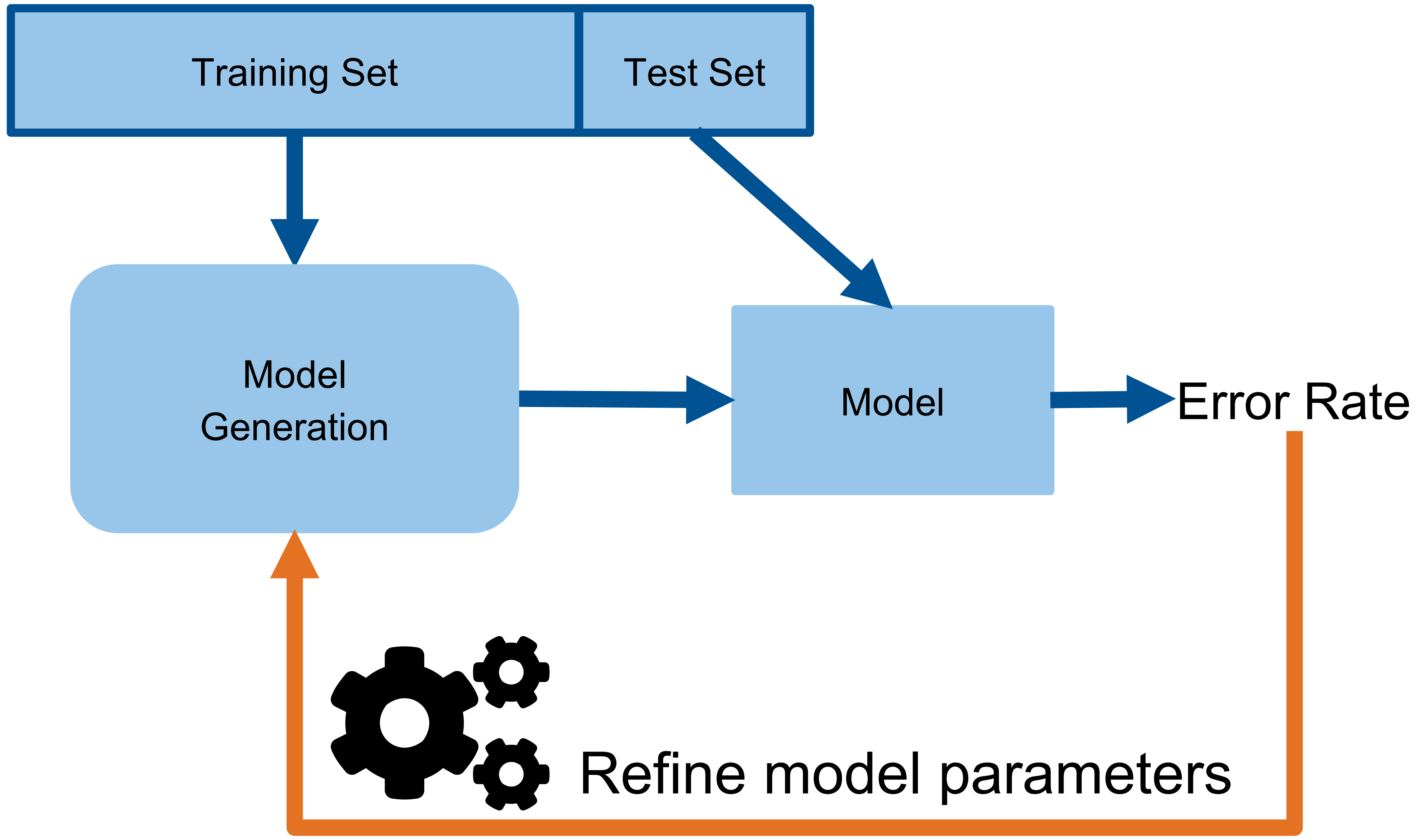

Select all images with a store front.
Click verify once there are none left.

Active learning:

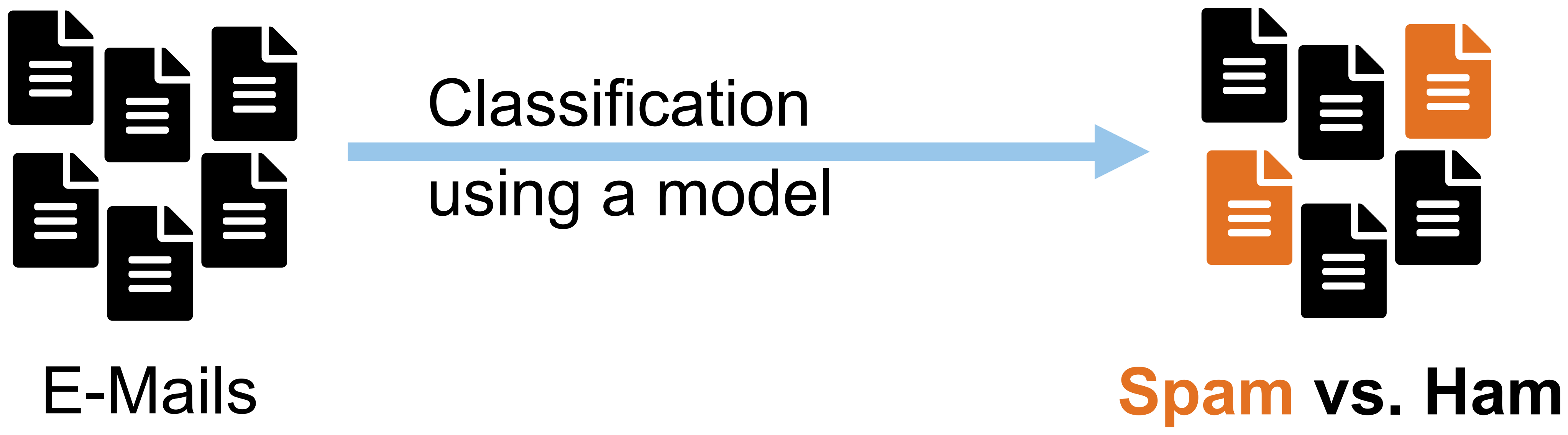
kick start a classifier only with some training examples, but leave it primarily with unclassified data, which it must classify. If the classifier is unsure of the classification (e.g., the newly arrived example is very close to the boundary), then the classifier can ask for ground truth at some significant cost

How to Choose a Model

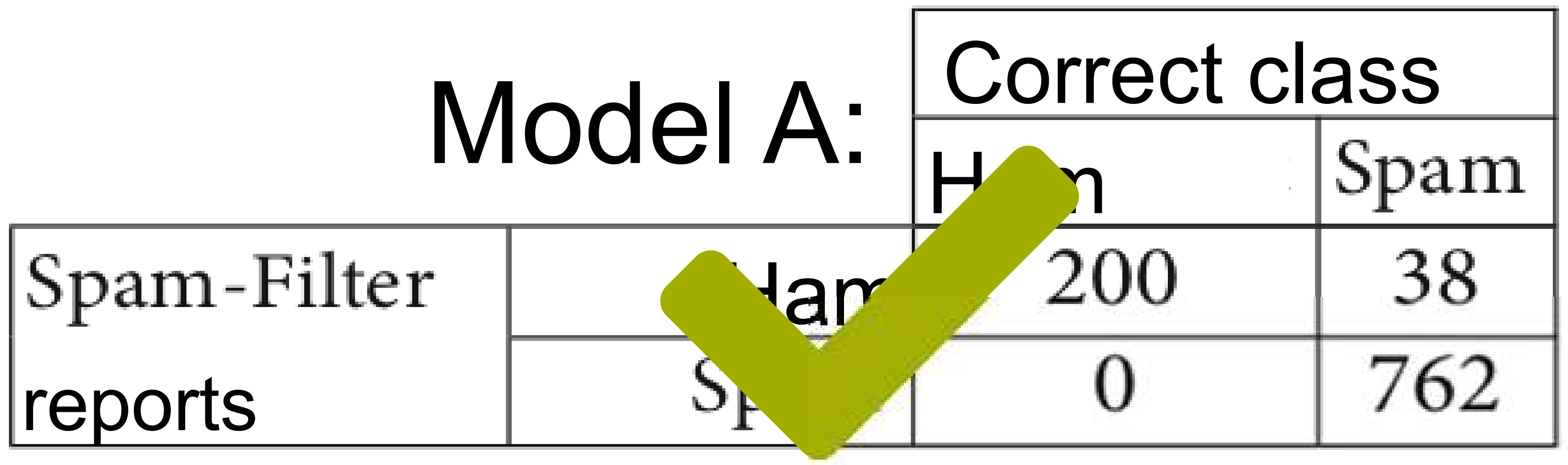
Minimize error rate



Maximize *utility*

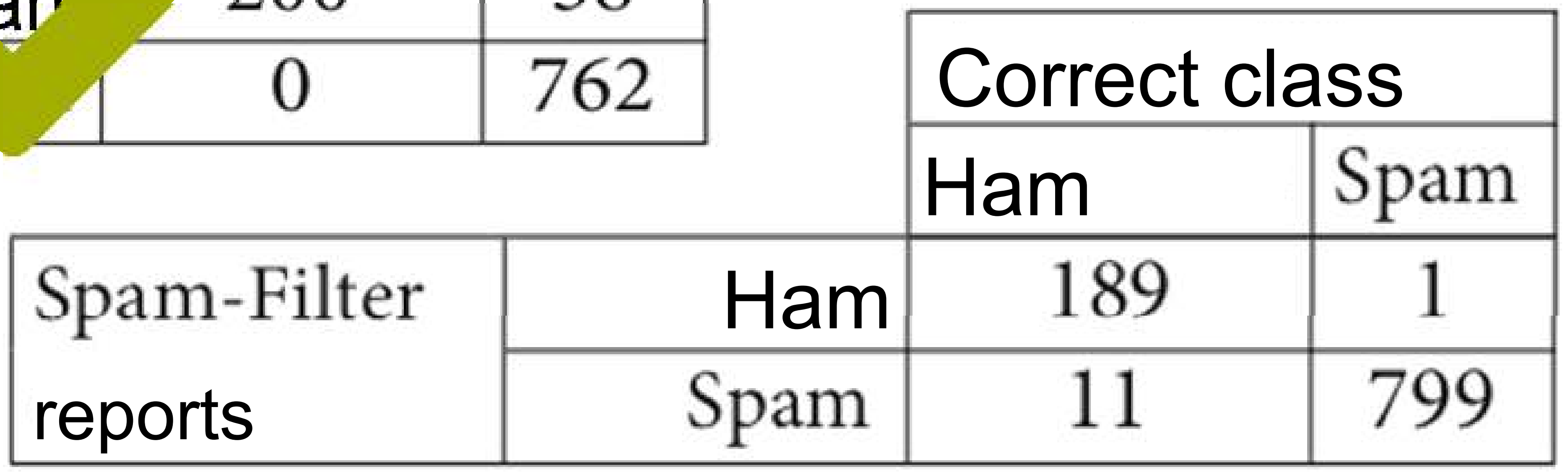


Model A: ✓



		Correct class	
		Ham	Spam
Spam-Filter reports	Ham	200	38
	Spam	0	762

Model B:



		Correct class	
		Ham	Spam
Spam-Filter reports	Ham	189	1
	Spam	11	799

Beware of Overfitting

Two types of classification errors:

1. Training error – misclassification on training data
2. Generalization error – expected error on *unseen* data

Overfitting:

Good results on training data (low training error) and
bad results with test/validation data (high generalization error)

Error significantly *underestimated* – severe problem in application scenarios

Detecting overfitting:

Evaluation of training with *new* data – NOT using training data!

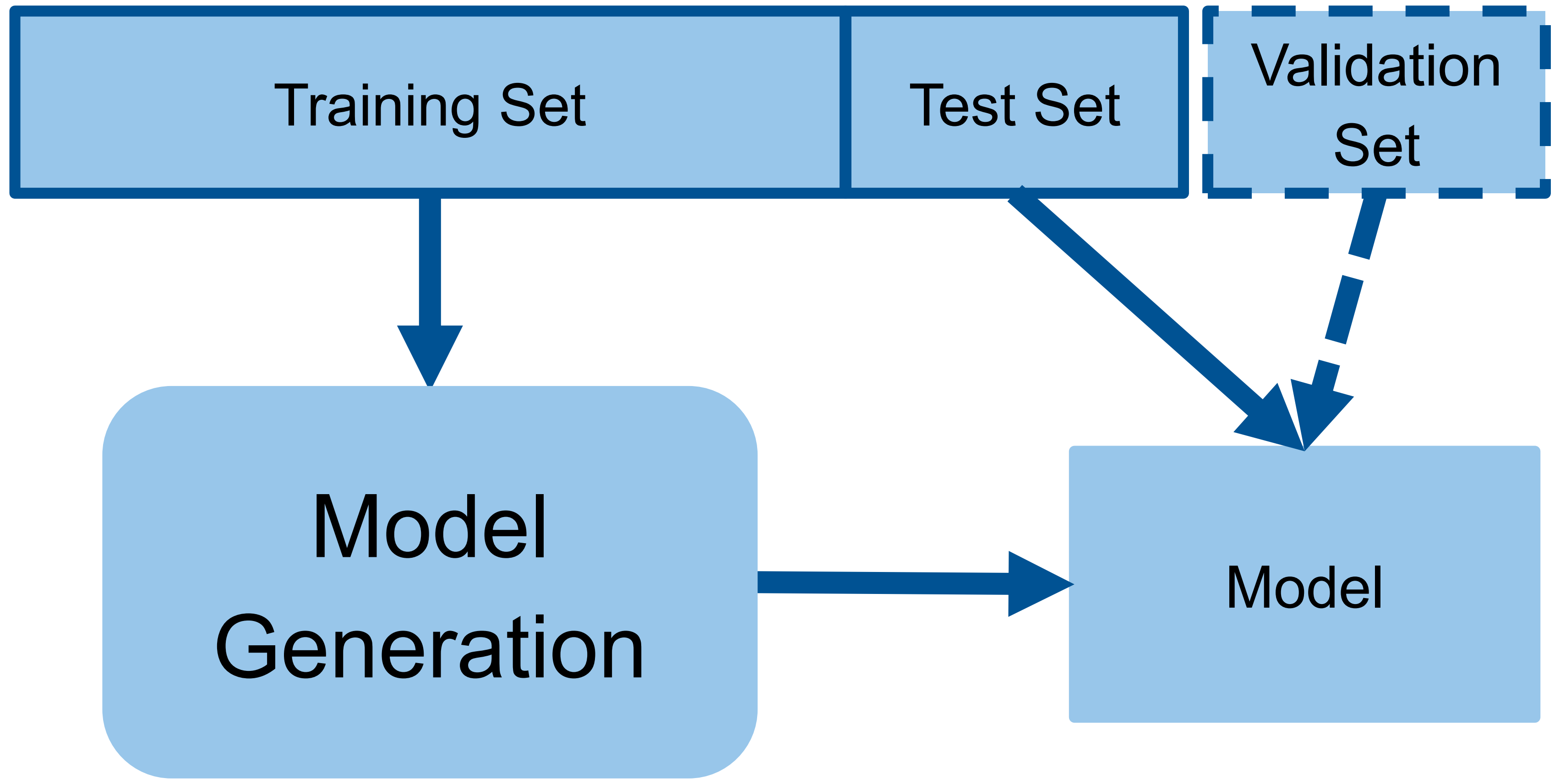
Training Test Split

Split training data *at least* in training and testing (Popular splits: 2:1 / 90:10)

Recommended: Split data in training, testing *and validation*
Splits: 80:10:10

Choose best classificator *only* on training and test data
Estimate accuracy & tune parameters of model

Keep validation-data *secret*! Use that only *once* to estimate the generalization power of the model!



Terminology of test and validation data is often mixed up.

What if…

Prepare data

Chose classificator

Train it

Test it

Validate it

Results do not look good

Repeat

What‘s the problem?

Repeated testing leads to overfitting

Once the validation data is used, do not go back to improve classification!

Cross-Validation

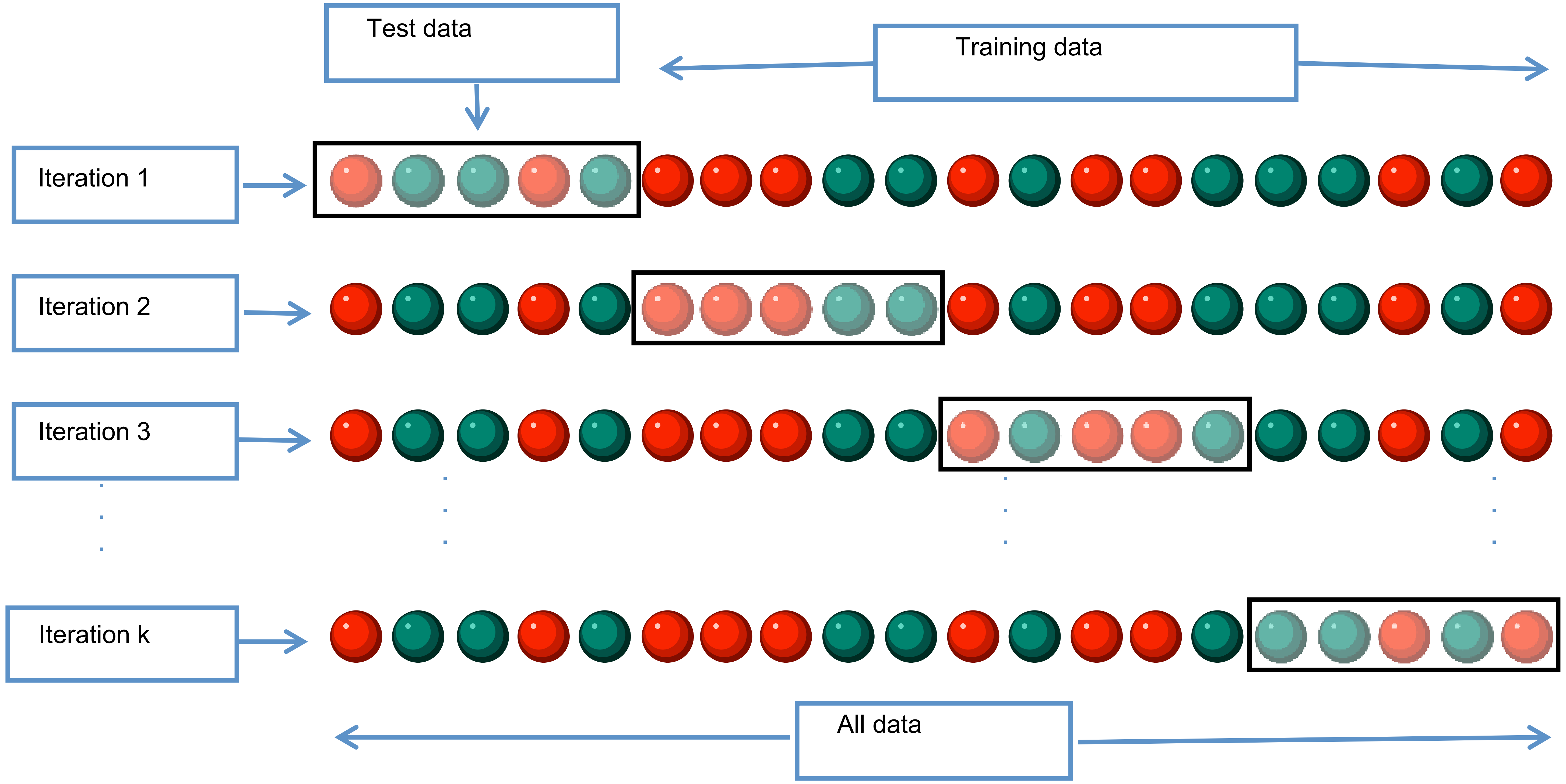
Cross-validation is a technique to help choosing classificator and optimal parameters

Partition data in *k* non-overlapping parts of equal size

During *i*th iteration, use data in partition D_i for validation, all other data as training data

Quality of classificator:

mean over all *k* iterations



https://en.wikipedia.org/wiki/File:K-fold_cross_validation_EN.svg

Exhaustive Cross-Validation

Cross-validation methods which learn and test on all possible combinations to divide the original sample into training and test set.

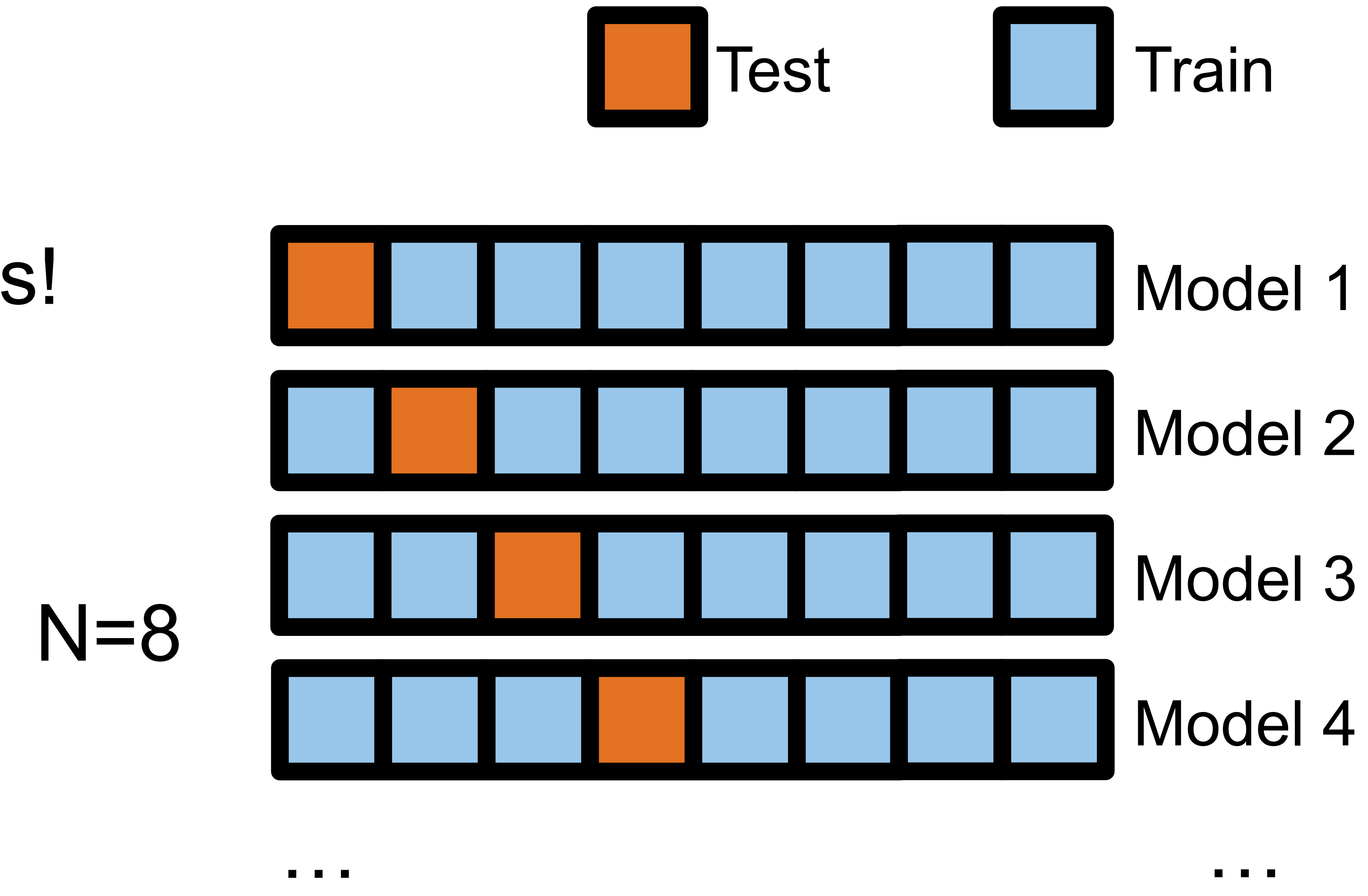
Leave-p-out cross-validation:

Use p observations as the test set and the remaining observations as training set.

Leave-one-out cross-validation:

Leave-p-out cross validation with p=1

Means finding one classificator for each instance – N classificators!



Imbalanced data

Imbalance:
Number of samples of different classes are diverging significantly.

Often, collecting samples of a certain class is difficult because these are rare events.

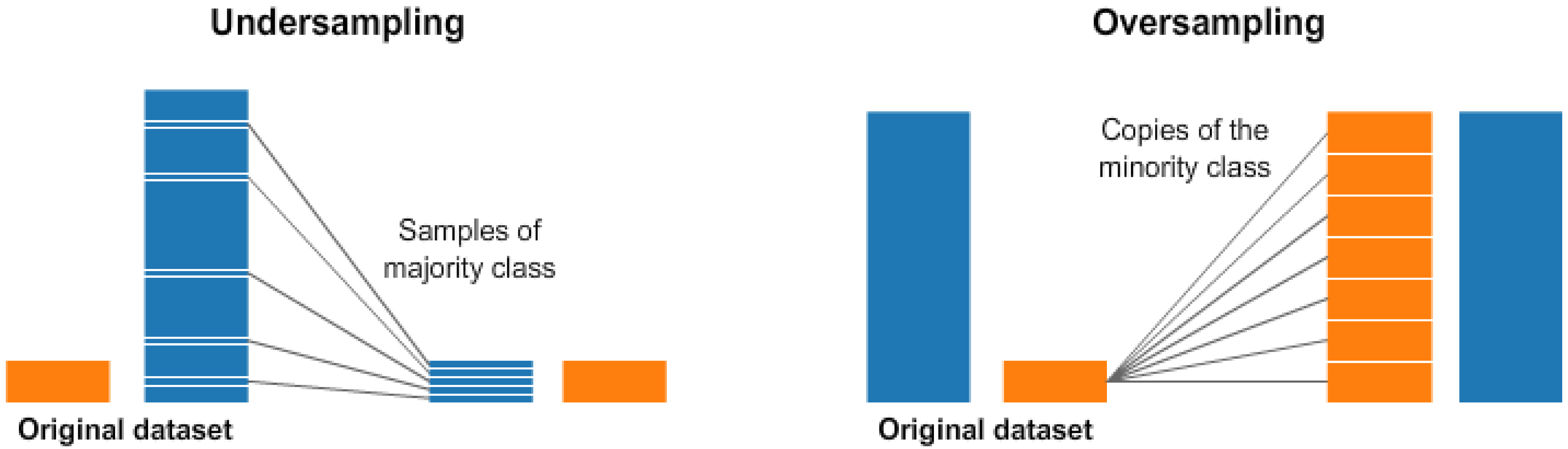
Consequences of building models using imbalanced data:

- Bias
  Classifiers are more sensitive to detecting the majority class
- Optimization metrics
  Metrics like accuracy may not report true performance

Has implications for sampling for cross validation!

Resampling

Balancing classes by removing samples from the majority class (under-sampling) and/or adding more examples from the minority class (over-sampling)



Various strategies, e.g. under-sampling by generating cluster-cendroids, over-sampling by synthesizing elements (SMOTE), …

https://www.kaggle.com/rafjaa/resampling-strategies-for-imbalanced-datasets

Overfitting can occur on subtle ways

- Evaluation and task are adapted to solution
- Preprocessing of data tells something about solution
- Unbalanced data
- Little variety of data
- New observations
- Insufficient data

No Free Lunch Theorem

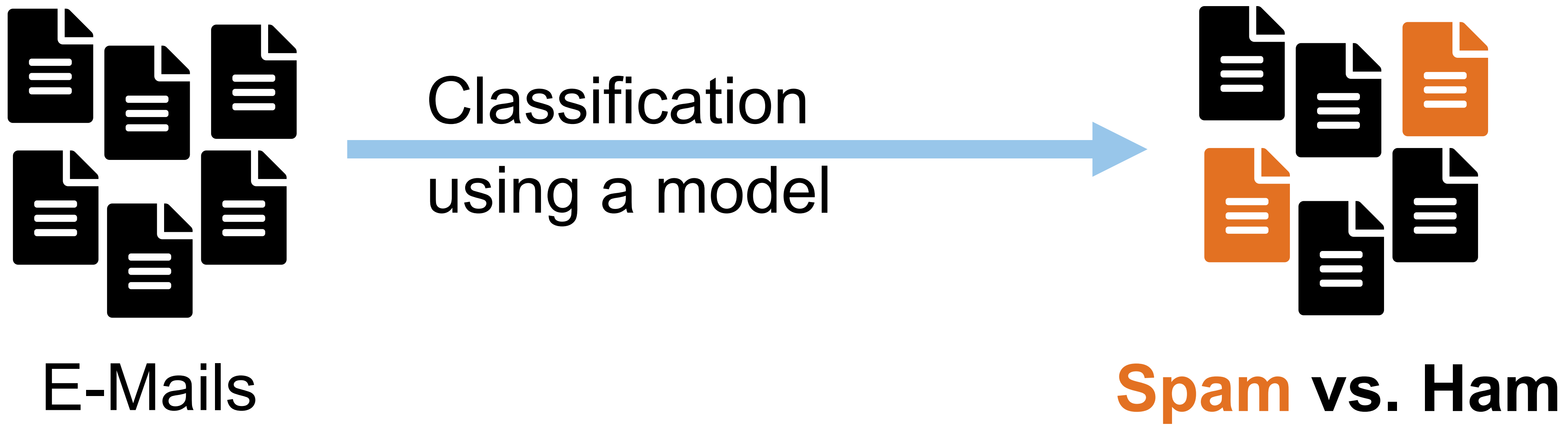
Choosing an appropriate algorithm requires making *assumptions*

With no assumptions, there will be no universal algorithm „better“ than random choice

> […] what an algorithm gains in performance on one class of problems is necessarily offset by its performance on the remaining problems;

Wolpert, David H., and William G. Macready. "No free lunch theorems for optimization." IEEE transactions on evolutionary computation 1.1 (1997): 67-82.

Good Classifications: The Confusion Matrix



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		Ham	Spam
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	Spam	0	762

Model B:

		Correct class	
		Ham	Spam
Spam-Filter reports	Ham	189	1
	Spam	11	799

		Correct	
		Positive (P)	Negative (N)
Predicted	Positive	True Positive	False Positive
	Negative	False Negative	True Negative

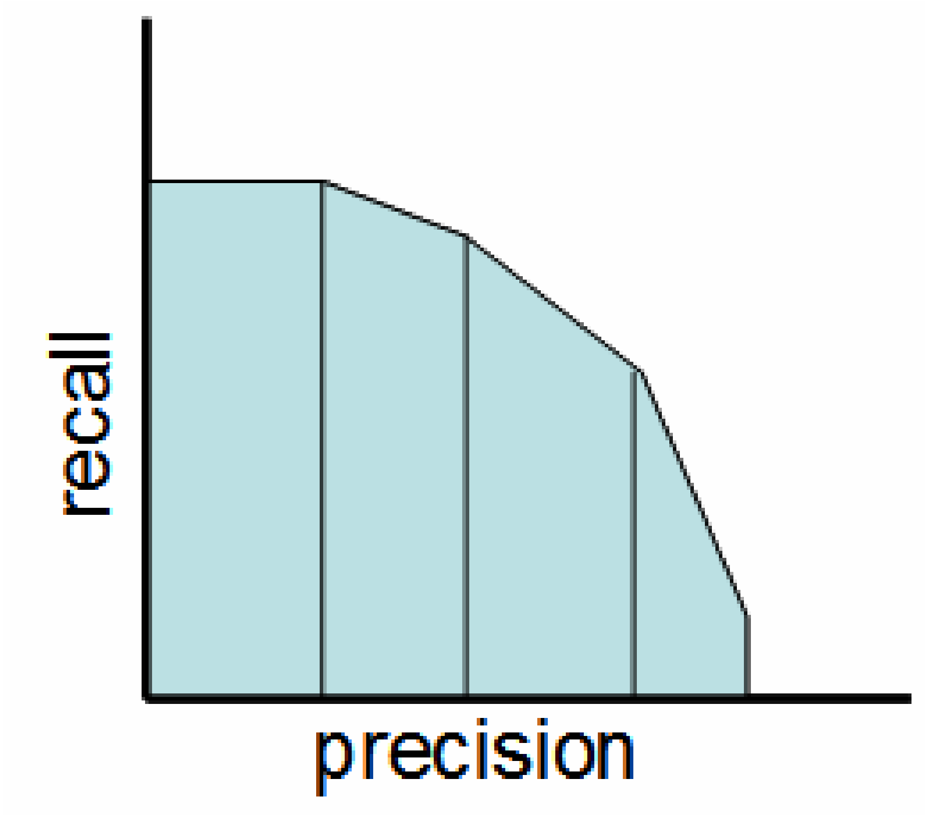
Measuring Goodness

- **Precision**: Proportion of predicted positives that are truly positive
  good choice when we need to be very sure of prediction

$$\frac{TP}{TP + FP}$$

- **Recall**: Proportion of actual positives that are correctly classified
  good choice when as many positives as possible should be captured

$$\frac{TP}{TP + FN}$$



https://towardsdatascience.com/the-5-classification-evaluation-metrics-you-must-know-aa97784ff226

		Correct	
		Positive (P)	Negative (N)
Predicted	Positive	True Positive	False Positive
	Negative	False Negative	True Negative

Measuring Goodness

- **Accuracy**: Proportion of true results among total number of cases
  good choice when classes are balanced

$$\frac{TP + TN}{TP + FP + FN + FN}$$

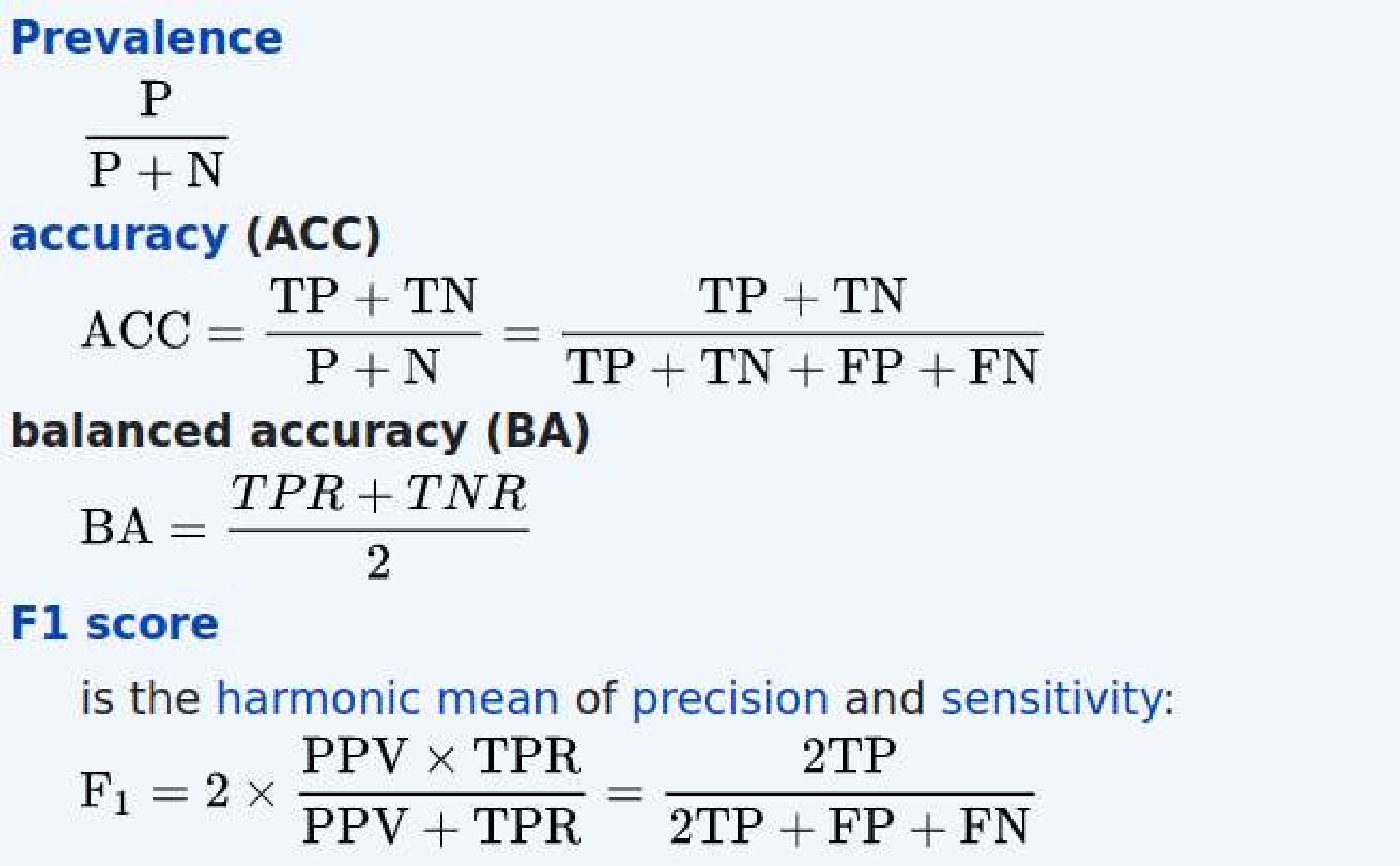
- $\boldsymbol{F_1}$ **Score**: harmonic mean between precision & recall – a number between 0 and 1
  good choice when we want a model with both good precision and recall

$$2 * \frac{precision\ * recall}{precision + recall}$$

Important variant F_β allows to apply a custom weight to precision & recall

		Correct	
		Positive (P)	Negative (N)
Predicted	Positive	True Positive	False Positive
	Negative	False Negative	True Negative

Measuring Goodness & more



Prevalence

$$\frac{\mathrm{P}}{\mathrm{P+N}}$$

accuracy (ACC)

$$\mathrm{ACC} = \frac{\mathrm{TP+TN}}{\mathrm{P+N}} = \frac{\mathrm{TP+TN}}{\mathrm{TP+TN+FP+FN}}$$

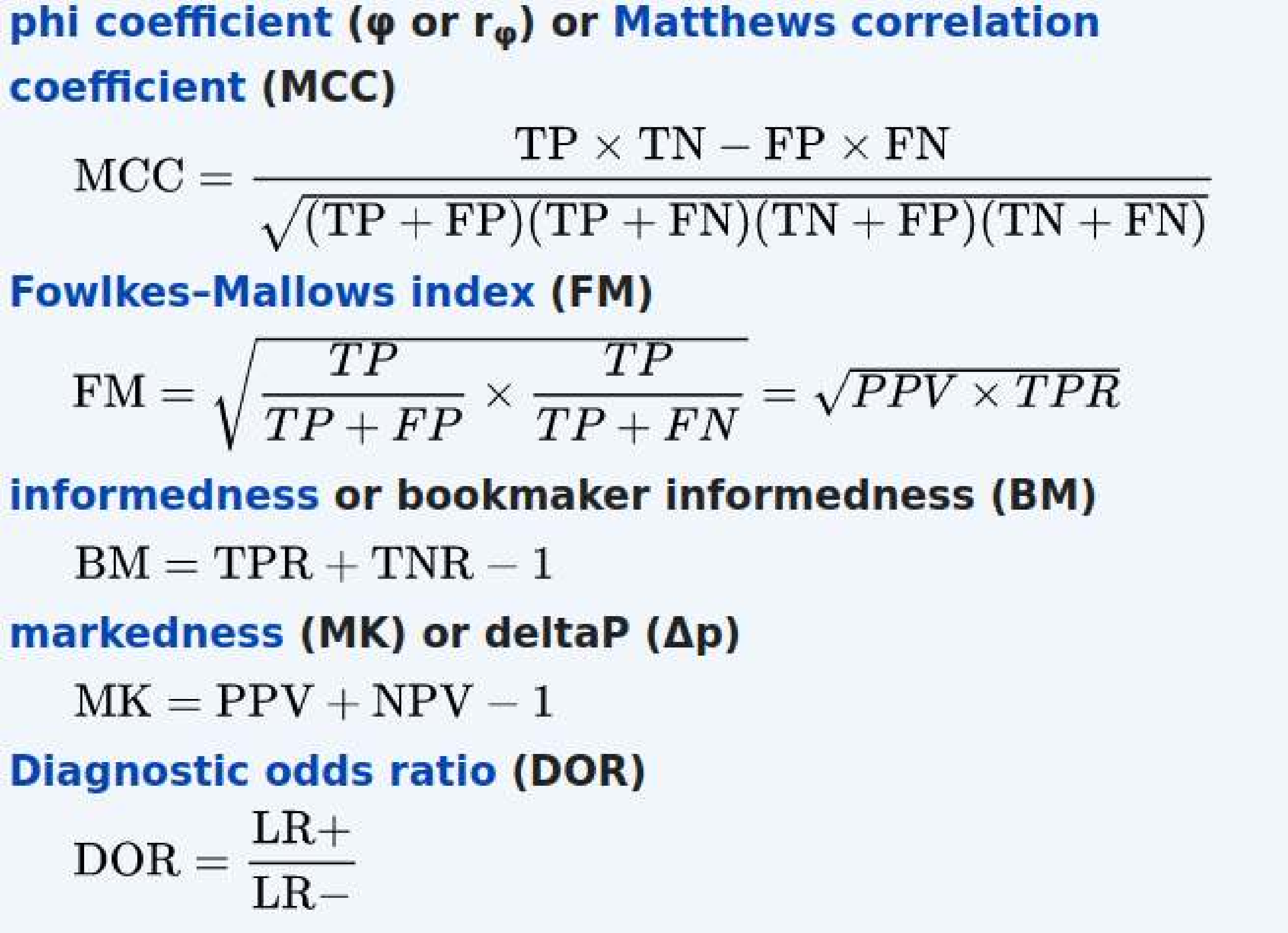
balanced accuracy (BA)

$$\mathrm{BA} = \frac{TPR+TNR}{2}$$

F1 score

is the harmonic mean of precision and sensitivity:

$$\mathrm{F}_1 = 2 \times \frac{\mathrm{PPV \times TPR}}{\mathrm{PPV + TPR}} = \frac{\mathrm{2TP}}{\mathrm{2TP+FP+FN}}$$



phi coefficient (φ or r_φ) or Matthews correlation coefficient (MCC)

$$\mathrm{MCC} = \frac{\mathrm{TP \times TN - FP \times FN}}{\sqrt{\mathrm{(TP+FP)(TP+FN)(TN+FP)(TN+FN)}}}$$

Fowlkes-Mallows index (FM)

$$\mathrm{FM} = \sqrt{\frac{TP}{TP+FP} \times \frac{TP}{TP+FN}} = \sqrt{PPV \times TPR}$$

informedness or bookmaker informedness (BM)

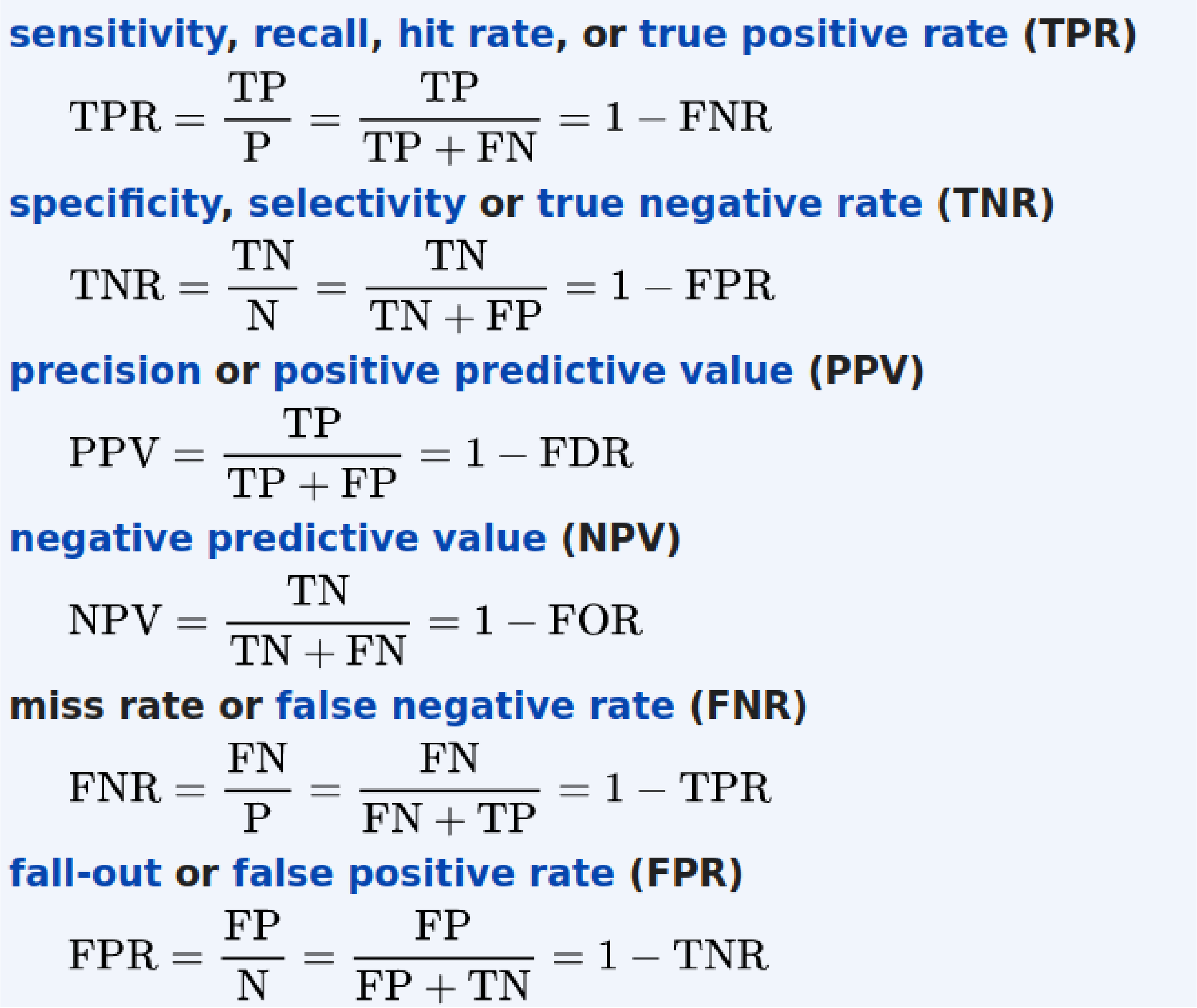
$$\mathrm{BM = TPR + TNR - 1}$$

markedness (MK) or deltaP (Δp)

$$\mathrm{MK = PPV + NPV - 1}$$

Diagnostic odds ratio (DOR)

$$\mathrm{DOR} = \frac{\mathrm{LR+}}{\mathrm{LR-}}$$



sensitivity, recall, hit rate, or true positive rate (TPR)

$$\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{P}} = \frac{\mathrm{TP}}{\mathrm{TP+FN}} = 1 - \mathrm{FNR}$$

specificity, selectivity or true negative rate (TNR)

$$\mathrm{TNR} = \frac{\mathrm{TN}}{\mathrm{N}} = \frac{\mathrm{TN}}{\mathrm{TN+FP}} = 1 - \mathrm{FPR}$$

precision or positive predictive value (PPV)

$$\mathrm{PPV} = \frac{\mathrm{TP}}{\mathrm{TP+FP}} = 1 - \mathrm{FDR}$$

negative predictive value (NPV)

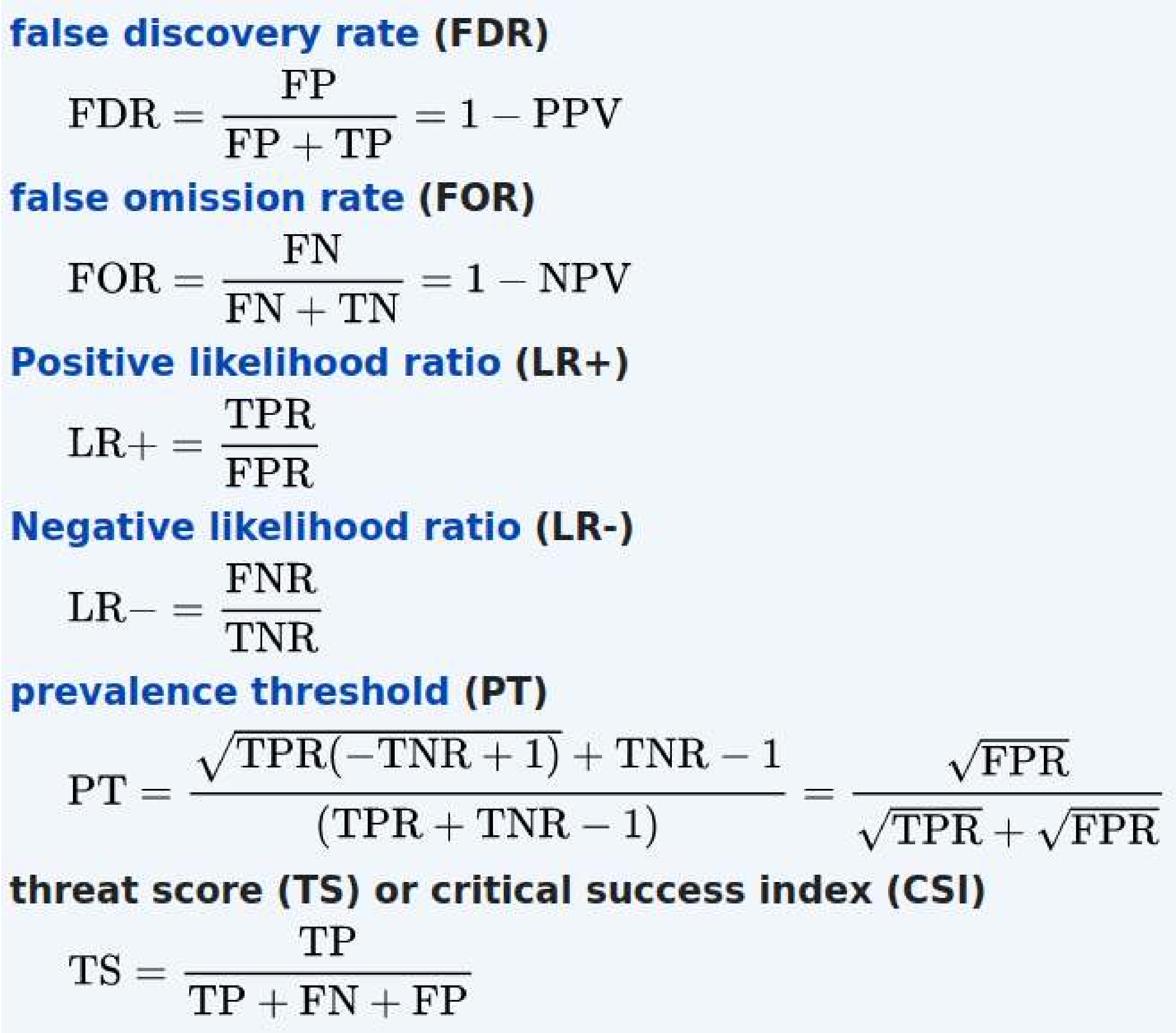
$$\mathrm{NPV} = \frac{\mathrm{TN}}{\mathrm{TN+FN}} = 1 - \mathrm{FOR}$$

miss rate or false negative rate (FNR)

$$\mathrm{FNR} = \frac{\mathrm{FN}}{\mathrm{P}} = \frac{\mathrm{FN}}{\mathrm{FN+TP}} = 1 - \mathrm{TPR}$$

fall-out or false positive rate (FPR)

$$\mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{N}} = \frac{\mathrm{FP}}{\mathrm{FP+TN}} = 1 - \mathrm{TNR}$$



false discovery rate (FDR)

$$\mathrm{FDR} = \frac{\mathrm{FP}}{\mathrm{FP+TP}} = 1 - \mathrm{PPV}$$

false omission rate (FOR)

$$\mathrm{FOR} = \frac{\mathrm{FN}}{\mathrm{FN+TN}} = 1 - \mathrm{NPV}$$

Positive likelihood ratio (LR+)

$$\mathrm{LR+} = \frac{\mathrm{TPR}}{\mathrm{FPR}}$$

Negative likelihood ratio (LR-)

$$\mathrm{LR-} = \frac{\mathrm{FNR}}{\mathrm{TNR}}$$

prevalence threshold (PT)

$$\mathrm{PT} = \frac{\sqrt{\mathrm{TPR(-TNR+1)}} + \mathrm{TNR} - 1}{\mathrm{(TPR+TNR-1)}} = \frac{\sqrt{\mathrm{FPR}}}{\sqrt{\mathrm{TPR}} + \sqrt{\mathrm{FPR}}}$$

threat score (TS) or critical success index (CSI)

$$\mathrm{TS} = \frac{\mathrm{TP}}{\mathrm{TP+FN+FP}}$$

		Correct	
		Positive (P)	Negative (N)
Predicted	Positive	True Positive	False Positive
	Negative	False Negative	True Negative

https://en.wikipedia.org/wiki/Receiver_operating_characteristic

Interpretability

Large project set out to evaluate ML application to problems in healthcare

Scenario: predicting pneumonia risk

Goal: predict probabilty of death for patients with pneumonia

The most accurate model of the study was a multitask neural net.

Outperformed other models by wide margin but was still dropped. Why?

One rule-based system learned the rule „patient has asthma ➔ lower risk“

Reflected a true pattern in training data

The best model was the least intelligible one – was deemed to risky

No way of checking the features that were picked up

Cooper, Gregory F., et al. "An evaluation of machine-learning methods for predicting pneumonia mortality." Artificial intelligence in medicine 9.2 (1997): 107-138.
Caruana, Rich, et al. "Intelligible models for healthcare: Predicting pneumonia risk and hospital 30-day readmission." Proceedings of the 21th ACM SIGKDD. 2015.

Goals of Interpretable Models

- Trust: Identify and mitigate *bias*

  Recognizing bias in a black-box algorithm is *very* hard
- Causality: Account for context

  Helps you understand how the factors included in the model led to the prediction
- Informativeness: Extract knowledge

  Helps you determine if patterns that appear to be present in the model are really there.

  Rather learning from the model than evaluating it (compared to identifying bias)
- Transferability: Generalize

  Models are trained on carefully collected datasets to solve narrowly defined problems. Interpretable models should help you determine if and how they can be generalized
- Fair and Ethical Decision-Making

  algorithmic decision-making mediates more and more of our interactions. Need a way to make sure that decisions conform to ethical standards

Lipton, Zachary C. "The Mythos of Model Interpretability: In machine learning, the concept of interpretability is both important and slippery." Queue 16.3 (2018): 31-57.
https://shapeofdata.wordpress.com/2016/11/17/goals-of-interpretability/

Properties of Interpretable Models

1. Transparency
   - Simulatability

     Transparency at the level of the entire model
   - Decomposability / Intelligibility

     Transparency at the level of the individual components, e.g. parameters
   - Algorithmic Transparency

     Transparency at the level of the training algorithm

Lipton, Zachary C. "The Mythos of Model Interpretability: In machine learning, the concept of interpretability is both important and slippery." Queue 16.3 (2018): 31-57.

Properties of Interpretable Models

2. Post-hoc Interpretability
   - Text Explanations
   - Visualization
   - Local Explanations
   - Explanation by Example

Lipton, Zachary C. "The Mythos of Model Interpretability: In machine learning, the concept of interpretability is both important and slippery." Queue 16.3 (2018): 31-57.

Ensemble Models

Inspectable models ease debugging problems in data collection, feature engineering, etc

Ensemble models provide ways to restrict features to separate models that otherwise would interact in unintended ways

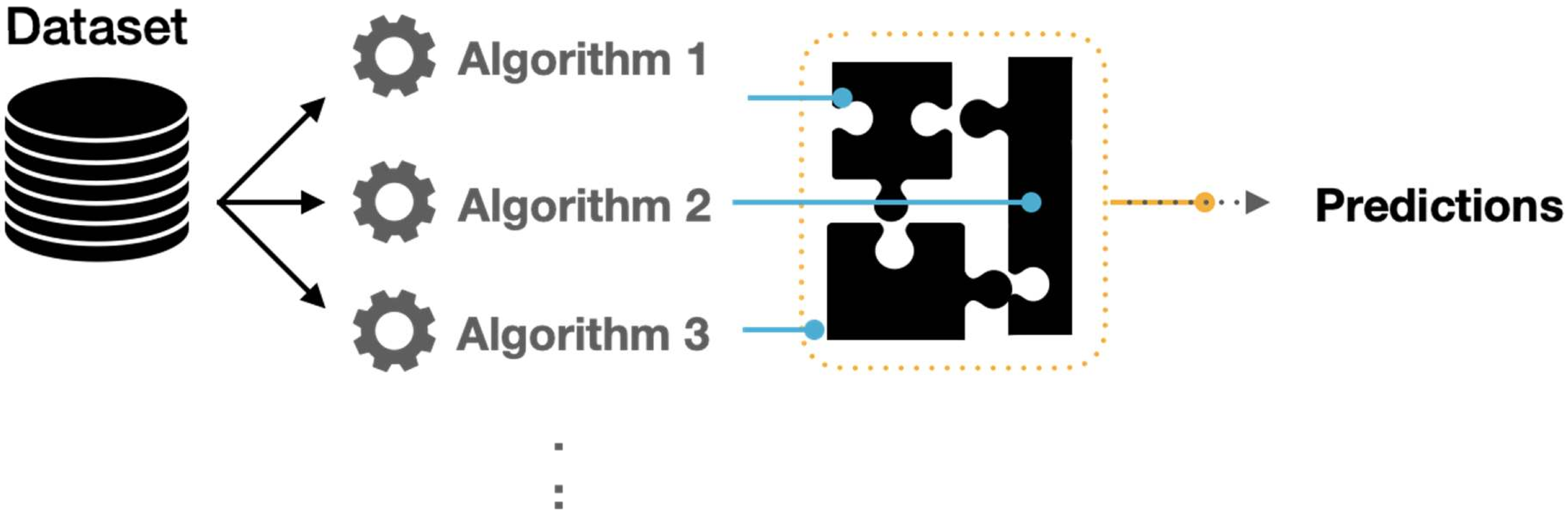
Helps overcoming

- high variance: single estimators are very sensitive to inputs to the learned features
- low accuracy: single models/algorithms might not be good enough
- features noise and bias: single estimators might rely heavily on one or few features

Various ways to combine models

Ensemble Models

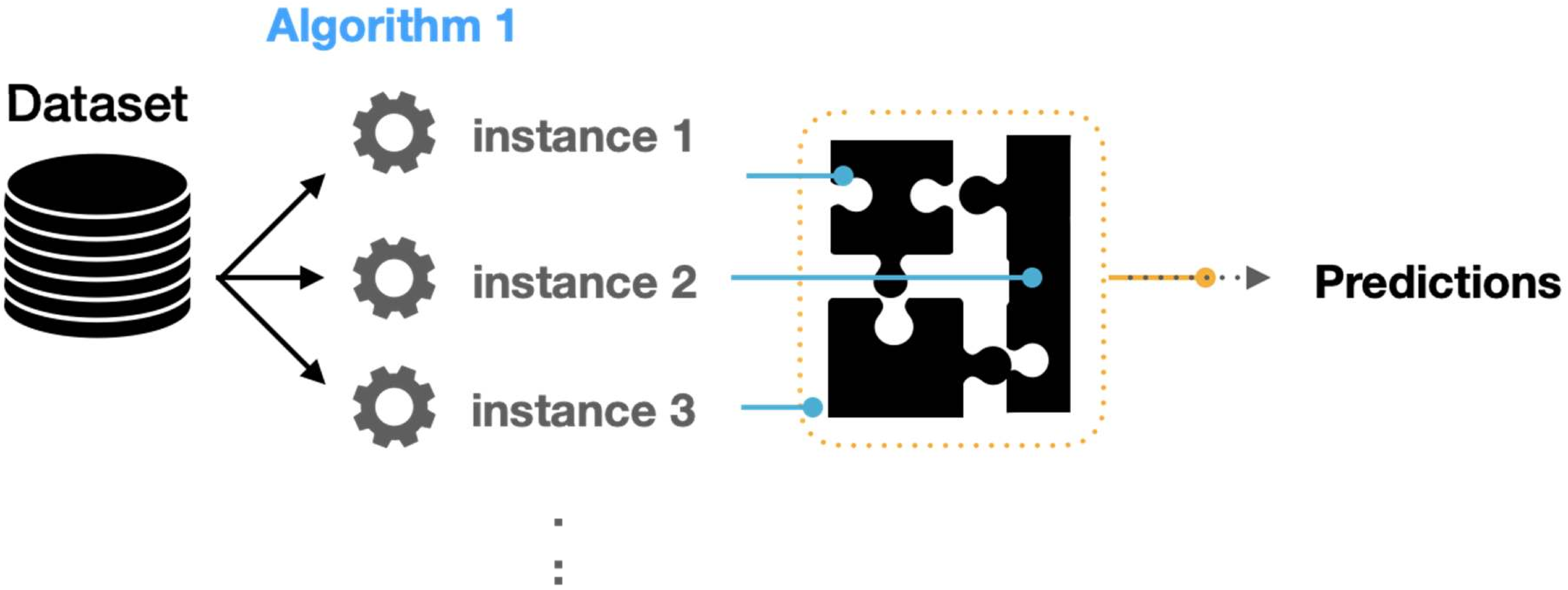
Using multiple algorithms to diversify model predictions



https://towardsdatascience.com/ensemble-models-5a62d4f4cb0c

Ensemble Models

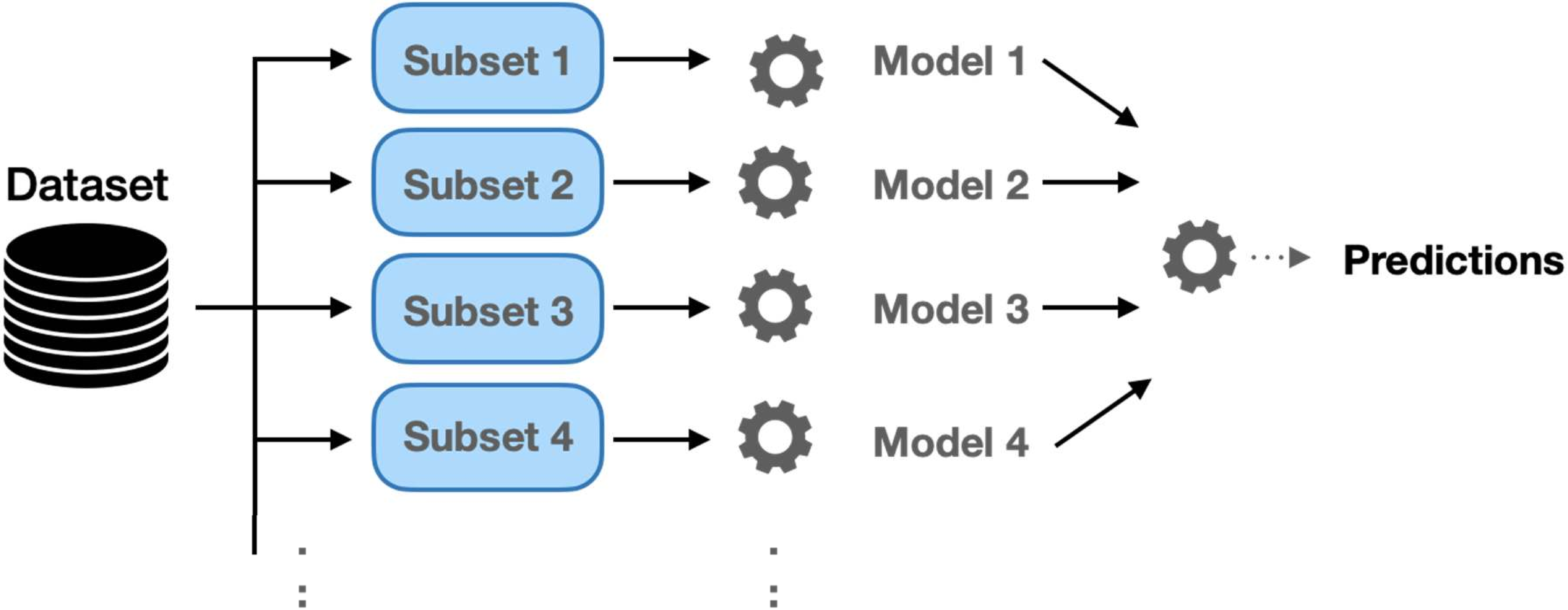
Using multiple weak instances of the same algorithm



https://towardsdatascience.com/ensemble-models-5a62d4f4cb0c

Ensemble Models: Bagging & Bootstrapping

Combine predictions from multiple models

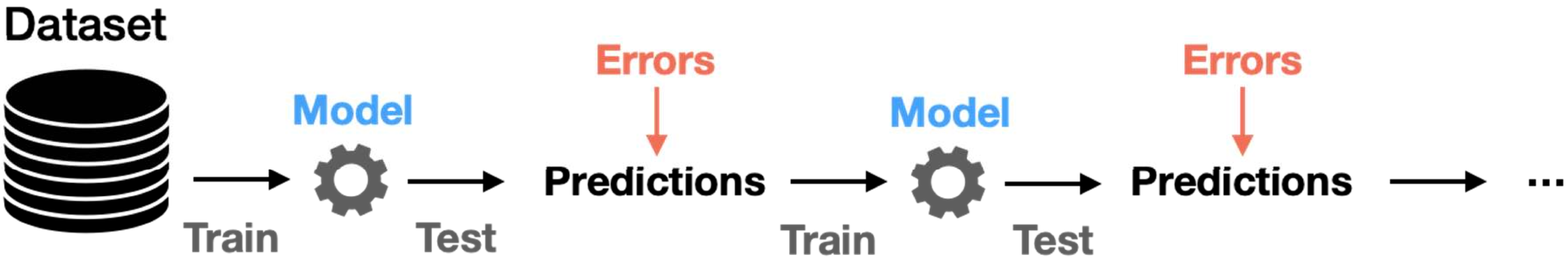


https://towardsdatascience.com/ensemble-models-5a62d4f4cb0c

Ensemble Models: Boosting

Ensemble of algorithms that builds models on top of several weak learners

Here: Sequental Adaptive Boosting (AdaBoost)



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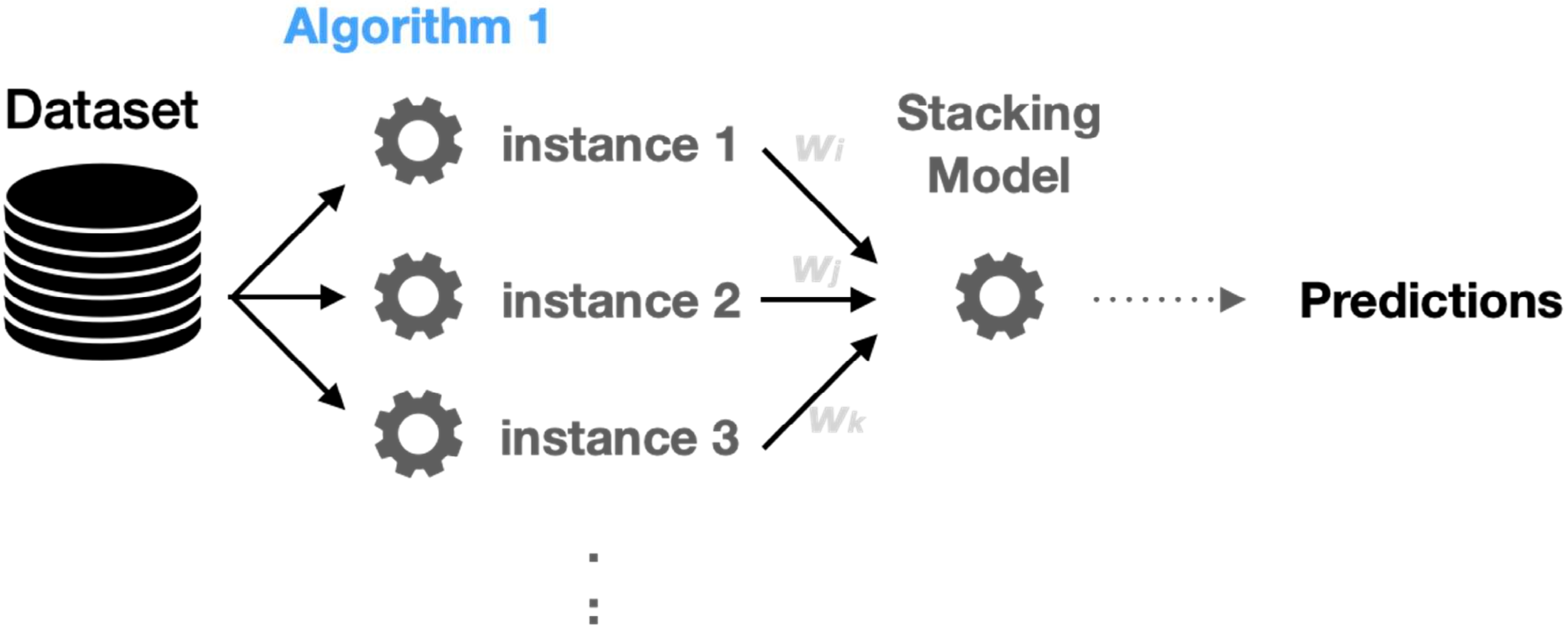
Ensemble Models: Stacking

Stacking intermediate predictions to make a final prediction



https://towardsdatascience.com/ensemble-models-5a62d4f4cb0c

How to select a model?

- Quality of predictions

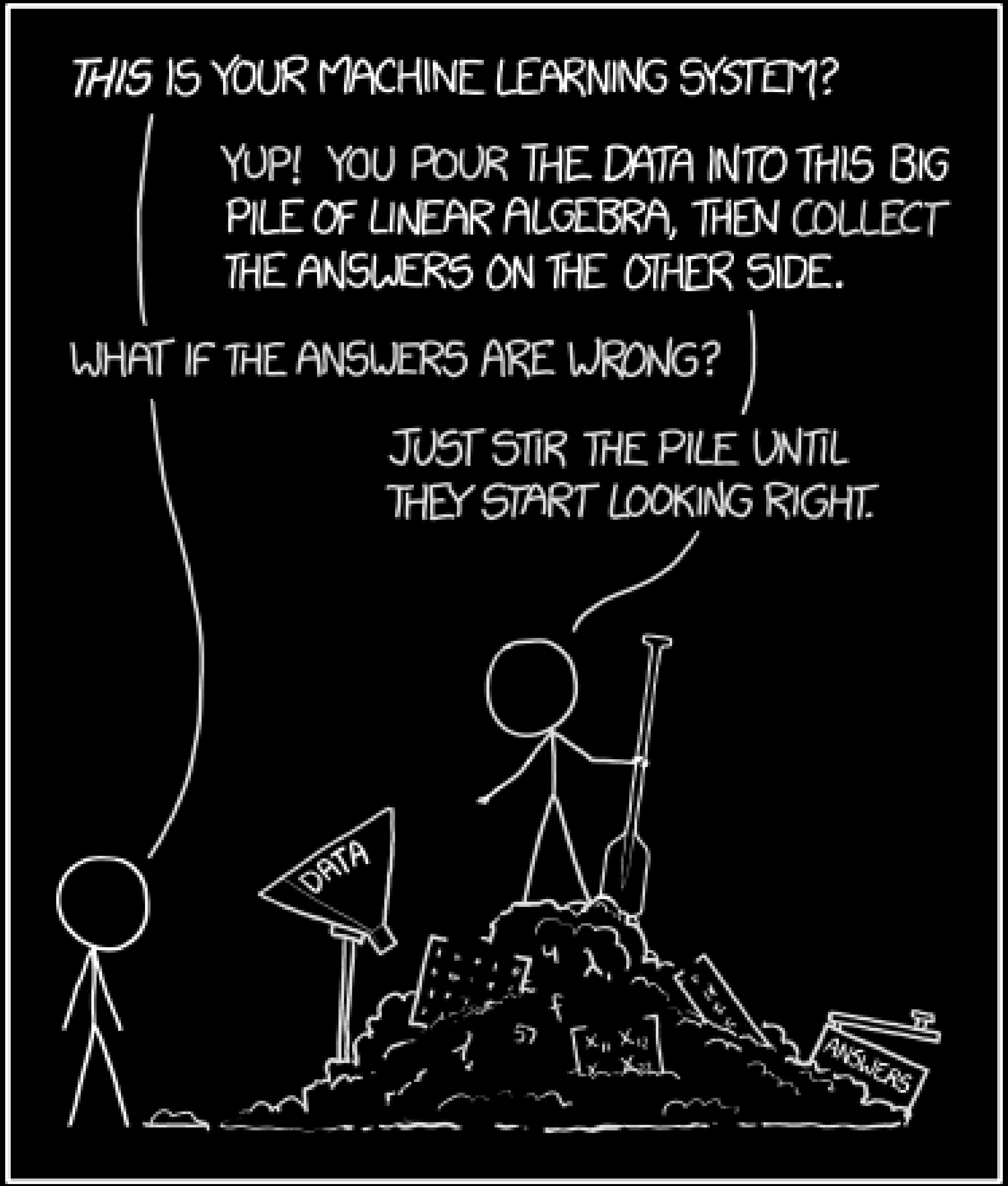
  i.e. performance in terms of a quality metric
- Speed

  i.e. training time, prediction time
- Robustness

  i.e. handling noise or missing values and still classify correctly
- Scalability

  i.e. computational efficiency
- Interpretability

  subjective means
- Other


THIS IS YOUR MACHINE LEARNING SYSTEM?
YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.
WHAT IF THE ANSWERS ARE WRONG?
JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.
DATA
ANSWERS

https://xkcd.com/1838/

Thanks.

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