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# Multimedia Retrieval

## Chapter 1: Performance Evaluation

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## 1.1 Introduction

- In this course, we consider a number of retrieval models, feature extraction algorithms, and search algorithms. At some point, we need to understand the performance of an approach to determine what is the better retrieval method. Often, there is no absolute answer what is the best method; instead the performance of a method varies from application to application:
  - Vector space retrieval was proven to outperform Boolean retrieval (similarly: probabilistic retrieval). Nevertheless, web search engine such as AltaVista (used vector space retrieval) and Inktomi (probabilistic retrieval) could not compete with Google (Boolean retrieval)
  - When searching for similar images (still photos), it is well accepted that color is more important than texture, and texture is more important than shape. In medical imagery, however, the contrary is true: color is often meaningless (X-ray, MRI, CT, ...), texture often plays an important role to detect the type of tissue, but shape is of highest importance (e.g., skin cancer).
  - Machine learning with Deep Neuronal Networks outperforms most other classification methods, but AI comes with high computational costs. Is the additional effort worth the better performance, or is “simpler & faster” just good enough, e.g., plain old web search or meta data search?
- We note that the performance of an approach depends on
  - the collection,
  - the type of queries / learning scenarios,
  - the information needs of users,
  - … and some non-functional constraints (e.g., costs, time, storage)

  With other words: for each retrieval and learning task, a new evaluation is required to determine the best approach. Generalization do work to a certain degree, but not always.

- Evaluation of <u>retrieval systems</u> differentiates between two types:
  - Boolean approaches that return an (unordered) set of documents, and
  - retrieval methods that return a ranking of documents ordered by their relevance for the current information need (i.e., how well it matches the query)

  An important criteria of the evaluation is the so-called relevancy ordering, i.e., the information whether and how well a document matches the query. We may use a simple black & white view: the document is “relevant” or “not relevant”. Or, we can employ a more sophisticated approach with pair-wise assessment of documents with regard to their relevance to the query. For example, the preference pair $(A <_p B)$ denotes that “$B$ is more useful/relevant than $A$”. A retrieval system works well (or as expected), if it ranks $B$ before $A$, and does similarly for any other given pair of preference.

  Defining a sound benchmark is the first step of an evaluation. A benchmark consists of a collection, query types, and relevance assessments. There are a number of benchmarks available for different retrieval areas. In the following, we shortly consider the benchmark provided by INEX.

- Evaluation of <u>learning methods</u> depend on the desired task and output. Assessment of
  - binary classification is very similar to Boolean retrieval (precision, recall)
  - multi-class classification uses so-called confusion matrices to understand for which combinations of classes the algorithm performs good/bad
  - classification with scores and thresholds requires us to determine good thresholds and a metric to compare different methods (given different thresholds)
  - classification with probability distributions is often based on entropy (log-loss)
  - regression tasks (fitting real valued output data) uses mean squared error (MSE)
  - deep learning uses various methods to define what “good” means

# 1.2 Defining a Benchmark for Retrieval

- So what makes a good benchmark? First of all, we need a sound collection that provides a diverse set of different documents matching the retrieval scenario. We also need queries (many of them) covering various aspects of the retrieval task. And, we need an assessment of all documents against all queries. Finally, we need an evaluation method to capture the essence of “what is good”
  - **Challenge 1**: non trivial queries that can result in different results for the methods under investigation. Queries that are easily answered by all methods do not add much differentiation.
  - **Challenge 2**: finding the “correct” answers for the queries given. For instance, if you evaluate web search engine, how do you know what should be the best answer to a query?

- Here is an example form the past: INEX started in 2002 to provide a yearly competition among research groups focusing on XML Retrieval (similar to TREC from the classical area). To define the challenge, the following steps were taken (see next pages for details):
  - Selection of an appropriate collection
  - Definition of queries
  - Relevance assessments for each query over the collection
  - Evaluation method (see Section 1.3ff)

- We use INEX here only for illustration how to setup a good benchmark; XML retrieval itself is no longer playing an important role these days

- The collection for the competition in 2002 consisted of 12’107 Articles of IEEE journals between 1995 and 2001 (about 500 MB).

```
<article>
  <fm>
    <ti>IEEE Transactions on ...<ti>
    <atl>Construction of ...</atl>
    <au>
      <fnm>John</fnm><snm>Smith</snm>
      <aff>University of ...</aff>
    </au>
    <au>...</au>
  </fm>
  <bdy>
    <sec>
      <st>Introduction</st>
      <p>...</p>  ...
    </sec>
    <sec>
      <st>...</st>  ...
      <ss1>...</ss1>
      <ss1>...</ss1>  ...
    </sec>  ...
  </bdy>
    <bm>
      <bib>
      <bb>
      <au>...</au><ti>...</ti>
      ...
      </bb>
      ...
      </bib>
    </bm>
</article>
```

- **Challenge 1:** There were two types of queries: "Content-and-structure" (CAS) queries, and "Content-only" (CO) queries. An example for a CO-Query was (about 30 such queries were defined):

```
<INEX-Topic topic-id="45" query-type="CO" ct-no="056">
   <Title>
     <cw>augmented reality and medicine</cw>
   </Title>
   <Description>
     How virtual (or augmented) reality can contribute to improve the medical and
     surgical practice. and
   </Description>
   <Narrative>
     In order to be considered relevant, a document/component must include
     considerations about applications of computer graphics and especially
     augmented (or virtual) reality to medecine (including surgery).
   </Narrative>
   <Keywords>
     augmented virtual reality medicine surgery improve computer assisted aided
     image
   </Keywords>
</INEX-Topic>
```

- **Challenge 1:** An example of a CAS-Query is given below (about 30 such queries existed):

```
<INEX-Topic topic-id="09" query-type="CAS" ct-no="048">
  <Title>
      <te>article</te>
      <cw>nonmonotonic reasoning</cw> <ce>bdy/sec</ce>
      <cw>1999 2000</cw> <ce>hdr//yr</ce>
      <cw>-calendar</cw> <ce>tig/atl</ce>
      <cw>belief revision</cw>
  </Title>
  <Description>
      Retrieve all articles from the years 1999-2000 that deal with works on
      nonmonotonic reasoning. Do not retrieve articles that are calendar/calls for
      papers.
  </Description>
  <Narrative>
      Retrieve all articles from the years 1999-2000 that deal with works on
      nonmonotonic reasoning. Do not retrieve articles that are calendar/calls for
      papers.
  </Narrative>
  <Keywords>
      nonmonotonic reasoning belief revision
  </Keywords>
</INEX-Topic>
```

- **Challenge 2:** How do we get the relevance assessments? Do we really have to assess each of the 12’107 articles against each of these 60 queries? Such an approach seems not very practical…
- A better approach is the following one: rather than absolute performance, relative performance ordering of the methods under investigation is sufficient. Assume each retrieval method returns a set of documents but misses one but the same relevant answer. It would have been good to find that relevant document as well, but, clearly, that missed answer does not change the relative ordering of the methods under investigation.
- We conclude from this observation, that the performance ordering of the methods only depend on the set of documents returned by any of the methods (the union of all results). This massively simplifies the approach as the methods typically have huge overlaps in their answers and the union set remains relatively small.
- To avoid any bias in the relevance assessment towards one or the other method, each participant has to assess the results for a subset of the queries. In summary, the approach taken by INEX was:
  - The INEX coordinator selects a collection, defines the queries (sometimes submitted by the participants), and sets an evaluation metric (usually precision/recall graphs)
  - The participants evaluate all queries with their retrieval method, and submit the result lists to the INEX coordinator
  - The INEX coordinator then asks each participant to assess a subset of the queries against the union of returned answers from methods in the competition (typically this is well below a 500 documents)
  - The assessment results are collected by the INEX coordinator who then computes the performance value for each participant

# 1.3 Boolean Retrieval

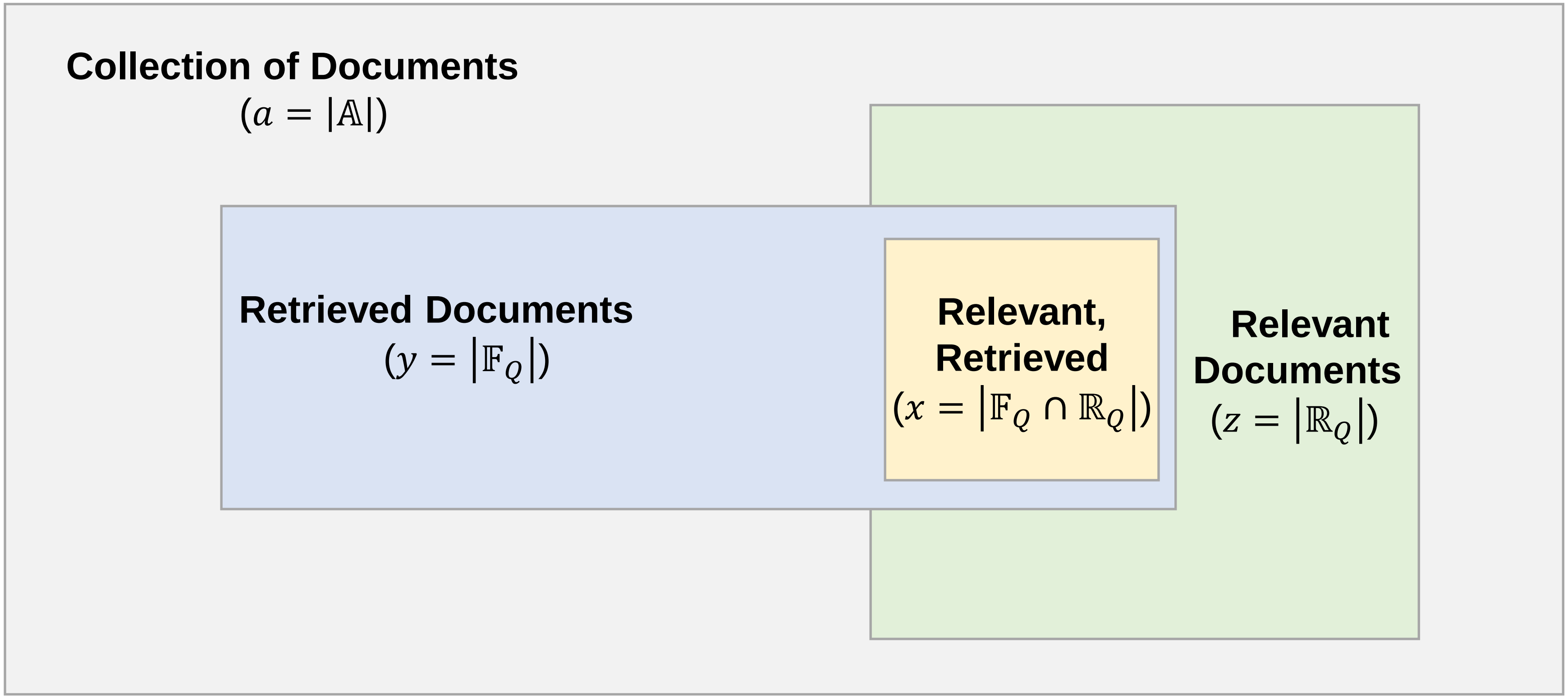
- Boolean retrieval returns a set of documents without order. In other words, the retrieval method does not distinguish between "highly relevant" and “maybe relevant"
- **Precision** and **recall** are the most important measures used for the evaluation of algorithms. Precision denotes how many of the answers are relevant from a user's perspective. Recall describes the percentage of retrieved and relevant answers over all relevant documents in the collection. A further measure, **fallout**, is used to describe a system's ability to discard non-relevant documents from the users (false hits).
- Notations:

| | |
|---|---|
| $\mathbb{A}$ | Set of all documents |
| $\mathbb{R}_Q$ | Set of relevant documents for a query $Q$ in the collection $\mathbb{A}$ |
| $\mathbb{F}_Q$ | Set of documents retrieved by a system for query $Q$ |

- Then, precision $p$, recall $r$ and fallout $f$ are defined as follows:

$$p = \frac{\left|\mathbb{F}_Q \cap \mathbb{R}_Q\right|}{\left|\mathbb{F}_Q\right|} \qquad r = \frac{\left|\mathbb{F}_Q \cap \mathbb{R}_Q\right|}{\left|\mathbb{R}_Q\right|} \qquad f = \frac{\left|\mathbb{F}_Q \setminus \mathbb{R}_Q\right|}{\left|\mathbb{A} \setminus \mathbb{R}_Q\right|}$$

- Visualization



**Collection of Documents**
$(a = |\mathbb{A}|)$

**Retrieved Documents**
$(y = |\mathbb{F}_Q|)$

**Relevant, Retrieved**
$(x = |\mathbb{F}_Q \cap \mathbb{R}_Q|)$

**Relevant Documents**
$(z = |\mathbb{R}_Q|)$

Precision: $p = \frac{x}{y}$ Recall: $r = \frac{x}{z}$ Fallout: $f = \frac{y - x}{a - z}$

- Next to precision, recall and fallout, literature mentions a few other measures. We will see more definitions when we consider the performance of machine learning tasks.
  - **Total Recall:** (how many relevant documents are in the collection?)

    $$g = \frac{|\mathbb{R}_Q|}{|\mathbb{A}|}$$

    It follows that:

    $$f \cdot p \cdot (1 - g) = r \cdot g \cdot (1 - p)$$

  - **F-Measure:** Combines Precision and Recall to a single value. The parameter $\beta$ determines how more important Recall over Precision shall be. With $\beta = 0$ only Precision counts; with $\beta = \infty$ only Recall counts.

    $$F_\beta = \frac{(\beta^2 + 1) \cdot p \cdot r}{\beta^2 \cdot p + r}$$

    The larger the F-Measure, the better an algorithm or system works. A typical value is $\beta = 1$**.** Having a single measure instead of two values simplifies comparisons; $\beta$ is pushing either precision (need some relevant documents) or recall (need all relevant documents).

- Usually, we are not just using a single experiment to assess the performance of methods. Rather, we run a series of queries and then compute an "average" precision and recall. Let $N$ be the number of queries, and for each query $Q_i$, we obtain a set $\mathbb{F}_i$ (retrieved documents for query $Q_i$) and a set $\mathbb{R}_i$ (relevant documents for query $Q_i$). For each query, we can compute the precision-recall pair $(p_i, r_i)$. To obtain an average value, two method exist:
  - **Macro Evaluation**: $p$ and $r$ are given as average value over $p_i$ and $r_i$ , respectively:

$$p = \frac{1}{N}\sum_{i=1}^{N} p_i = \frac{1}{N}\sum_{i=1}^{N}\frac{|\mathbb{F}_i \cap \mathbb{R}_i|}{|\mathbb{F}_i|} \qquad r = \frac{1}{N}\sum_{i=1}^{N} r_i = \frac{1}{N}\sum_{i=1}^{N}\frac{|\mathbb{F}_i \cap \mathbb{R}_i|}{|\mathbb{R}_i|}$$

  - **Micro Evaluation**: summing up numerators and denominators leads to:

$$p = \frac{\sum_{i=1}^{N}|\mathbb{F}_i \cap \mathbb{R}_i|}{\sum_{i=1}^{N}|\mathbb{F}_i|} \qquad r = \frac{\sum_{i=1}^{N}|\mathbb{F}_i \cap \mathbb{R}_i|}{\sum_{i=1}^{N}|\mathbb{R}_i|}$$

The micro evaluation is more stable if the sets $\mathbb{F}_i$ and $\mathbb{R}_i$ vary significantly in size.

# 1.4 Retrieval with Ordering

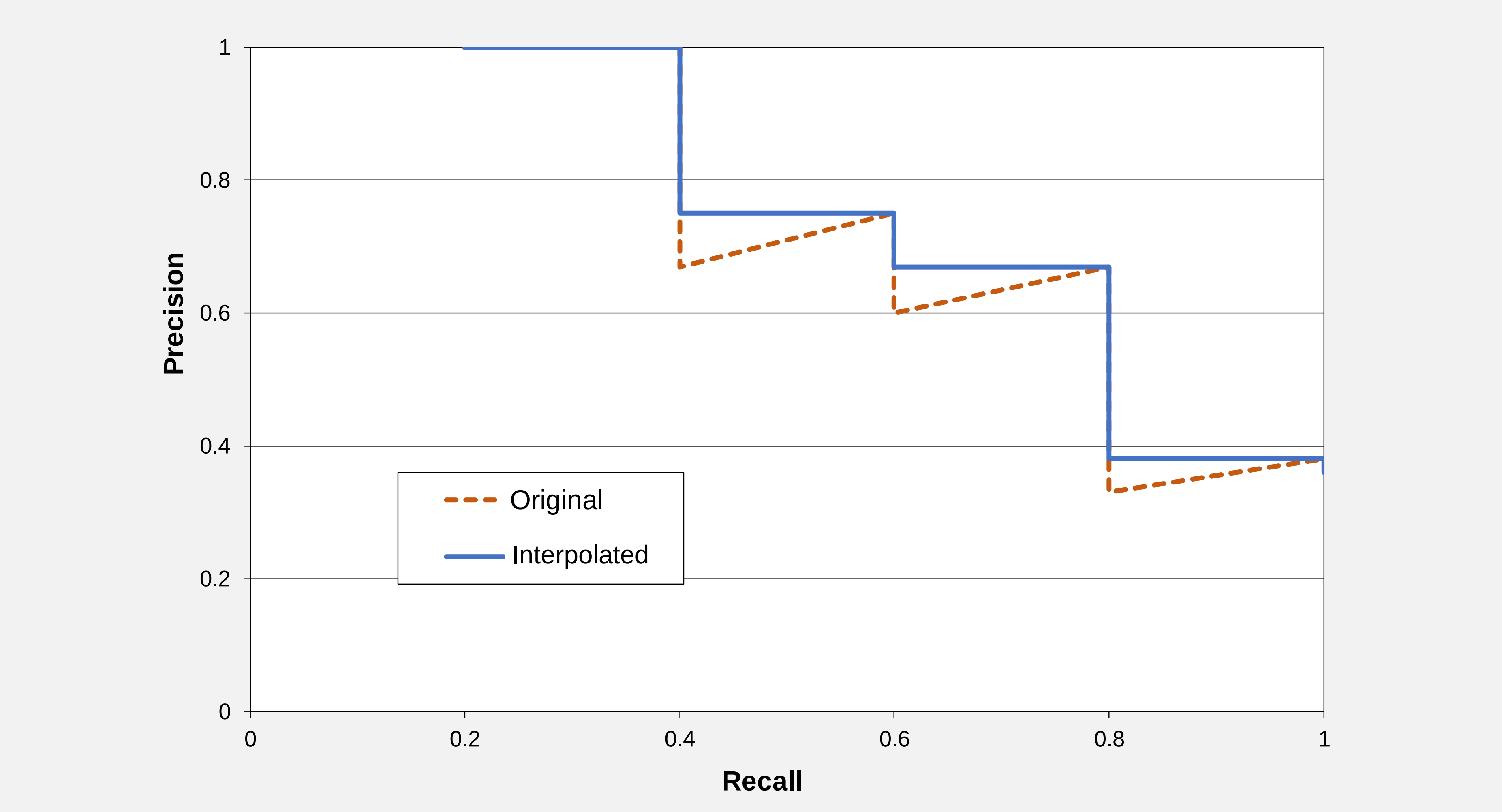
- Most retrieval methods return a ranked list, and we want to take the ranking somehow into account. Intuitively, a method that has a lot of relevant documents at the top of the list is perceived better than a method that shows the relevant document only later in the list.
- The precision-recall curve addresses this as follows: at each rank position, the precision and recall up to this point is computed. These precision-recall pairs are then depicted in a two dimensional plot. Let’s look at an example: assume that the collection has 5 relevant documents for a query $Q$ and a retrieval system produces the following ranked list:

| $rank$ | docID | relevance | $p_i$ | $r_i$ |
|---|---|---|---|---|
| 1 | 588 | x | 1.00 | 0.20 |
| 2 | 589 | x | 1.00 | 0.40 |
| 3 | 576 |  | 0.67 | 0.40 |
| 4 | 590 | x | 0.75 | 0.60 |
| 5 | 986 |  | 0.60 | 0.60 |
| 6 | 592 | x | 0.67 | 0.80 |
| 7 | 984 |  | 0.57 | 0.80 |
| 8 | 988 |  | 0.50 | 0.80 |
| 9 | 578 |  | 0.44 | 0.80 |
| 10 | 985 |  | 0.40 | 0.80 |
| 11 | 103 |  | 0.36 | 0.80 |
| 12 | 591 |  | 0.33 | 0.80 |
| 13 | 772 | x | 0.38 | 1.00 |
| 14 | 990 |  | 0.36 | 1.00 |

P-R pair for the first 4 documents: we observe 3 relevant documents, hence $p = 3/4$, and we have seen 3 of 5 relevant documents, hence, $r = 3/5$.

generally: we compute $p$ and $r$ for the first $\boldsymbol{rank}$ documents in the result

- We now can draw the P-R pairs of the example in a 2-dimensional plot. Notice that recall values only increase while precision values increase whenever a new relevant document is in the list, and decrease otherwise. To smooth the P-R curve, we often interpolate the values to obtain a step curve as depicted below in blue.



- Interpretation of P-R-Curve:
  - Close to $(r = 0, p = 1)$: most retrieved documents are relevant but not all relevant documents were found. This case is optimal for queries where one is just interested in a correct answer; for example: *"is this mushroom poisonous"*
  - Close to $(r = 1, p = 0)$: all relevant documents were retrieved but lots of the retrieved document are non-relevant. High recall is important for queries like *"is there a patent"*
  - $p = 1$ is usually difficult to achieve; $r = 1$ is simple—just return all documents
- To simplify comparison and ranking, we want to obtain a single value out of the many precision-recall pairs. Intuitively, we want to favor high precision and recall values. But given the observations above, high recall values are only seldom required. More frequently, we may want to favor a high precision with a reasonable recall. Thus, there are different ways to summarize pairs:
  - **System Efficiency:** prefers an ideal system that returns all relevant and only relevant documents. That is, we prefer both high precision and high recall values. In the precision-recall plot, if the curve of a method $A$ lies closer to the point $(r = 1, p = 1)$ than the curve of a method $B$, then we consider $A$ to outperform $B$. Let $d$ be the minimal distance of the precision-recall pairs to $(r = 1, p = 1)$. The system efficiency $\mathrm{E}$ is then given as:

$$E = 1 - \frac{d}{\sqrt{2}}$$

  - **R-Precision:** if we favor precision over recall, the R-Precision is a good alternative. It denotes the precision of a method after having retrieved a given percentage of all relevant documents:

$$RP = \max_{p,r} \begin{cases} 0 & if\ r < r_{threshold} \\ p & if\ r \geq r_{threshold} \end{cases}$$

  - An other method to summarize the pairs is to compute the **Area Under the Curve** (AUC, we will see this later again for the ROC curve). Like with the system efficiency, an ideal system that only returns relevant documents and all of them will obtain the maximum value of 1. The method prefers high precision values across all recall values.
- As with Boolean retrieval, we conduct a benchmark with many experiments and obtain several sets of precision-recall curves. How do we "average" these different sets of pairs to obtain a meaningful average curve? Again, different methods exist depending on the objective of the benchmark:
  - Compute the average precision and recall values over all queries for the first 5, 10, 15, 20, …, results and use these average values for the precision-recall curve. The method is simple but sensitive to outliers.
  - Alternatively, determine the precision over all queries for fixed recall values (see R-Precision) and average these precision values to obtain P-R pairs for the fixed recall values. This method correspond to the approach of "averaging" the curves by drawing a vertical line and determine the mean precisions along the intersections of the vertical line with the precision-recall curves. The method is more robust to outliers and provides an intuitive meaning to what "average" is.

# 1.5 Machine Learning Basics

- The Machine Learning Problem

> A computer program is said to learn from experience $E$ with respect to some class of tasks $T$ and performance measure $P$ if its performance at tasks in $T$, as measured by $P$, improves with experience $E$   [Mitchell 1997]

- There is a wide variety of machine learning problems as a combination of what the task is, what experience is provided and how performance is measured. Subsequently, we look at each individual component independently to categorize the different flavors of machine learning.
- Often, real-life examples employ a set of different approaches and combine them to achieve the overall objective of the problem. For instance, in credit card fraud, the first component is to learn fraudulent transaction based on past transactions and investigations. This knowledge is used to predict fraud in real-time for new transaction. A second component segments transactions to identify outliers or anomalies that may lead to new types of fraud that have not been identified/learned yet. While the first component is an example for supervised learning where the algorithms get labeled data to learn from, the second component is unsupervised, i.e., we don’t know what we are looking for and the algorithm must identify the patterns without any human interaction or feedback.
- Other examples include cascading several methods: for instance, a first step reduces dimensionality and eliminates outliers (unsupervised learning), a second step learns that mapping of reduced features to a set of labels (supervised learning).
- Modern approaches in Deep Learning build excessively deep sequences with neuronal networks to apply multiple different approaches to extents that require vast amounts of compute power to train and then to use the network.

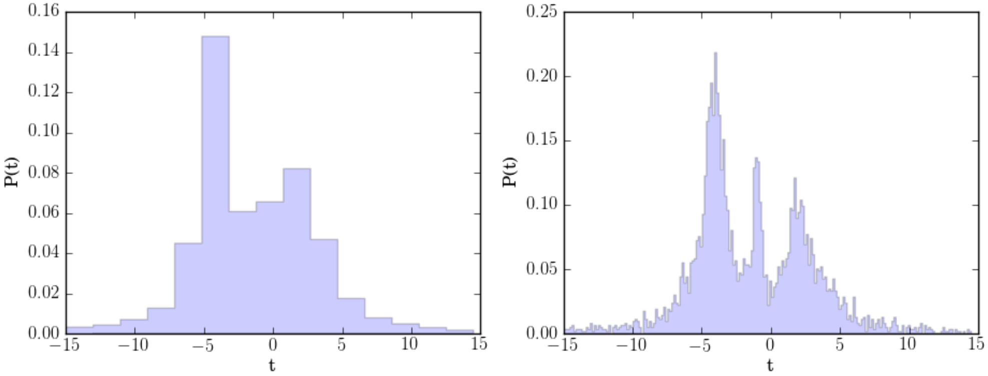
# 1.5.1 Tasks

- With task, we do not mean the learning process itself. Rather the ability that the machine is supposed to perform. For instance, if we want a car to drive autonomously, then driving is the task. Often, machine learning tasks involve a set of input features that the system needs to process into a “correct” set of output features.
- **Classification** is the task of mapping the input features to a set of $K$ categories. Typically this means to find a function $f$ that maps a $M$-dimensional vector $\boldsymbol{x}$ to a category represented by a numeric value $y$, i.e., $y = f(\boldsymbol{x})$ with $f\colon \mathbb{R}^M \rightarrow \{1, \ldots, K\}$. A variant of the classification task requires a probability distribution $P(y)$ over all classes $y$ with $P(y) = 1$ denoting the class $y$ is certain and $P(y) = 0$ denoting the class $y$ is impossible, i.e., $P(y) = f(\boldsymbol{x})$ with $f\colon \mathbb{R}^M \rightarrow [0,1]^K$
  - Applications include object recognition in images, text categorization, spam filtering, handwriting and speech recognition, credit scoring, pattern recognition, and many more

| Sample | fixed acidity | volatile acidity | citric acid | pH | alcohol | quality |
|---|---|---|---|---|---|---|
| #1 | 8.5 | 0.28 | 0.56 | 3.3 | 10.5 | 7 |
| #2 | 8.1 | 0.56 | 0.28 | 3.11 | 9.3 | 5 |
| #3 | 7.4 | 0.59 | 0.08 | 3.38 | 9 | 4 |
| #4 | 7.9 | 0.32 | 0.51 | 3.04 | 9.2 | 6 |
| #5 | 8.9 | 0.22 | 0.48 | 3.39 | 9.4 | 6 |

- **Classification with missing input** is similar to classification with the exception that some input values can be missing. Instead of a single function $f$, a set of functions is needed to map different subsets of inputs to a category $y$ (or distribution $P(y)$), potentially $2^M$ functions. A better way is to learn the probability distributions over all relevant features and to marginalize out the missing ones. All tasks have a generalization with missing inputs.

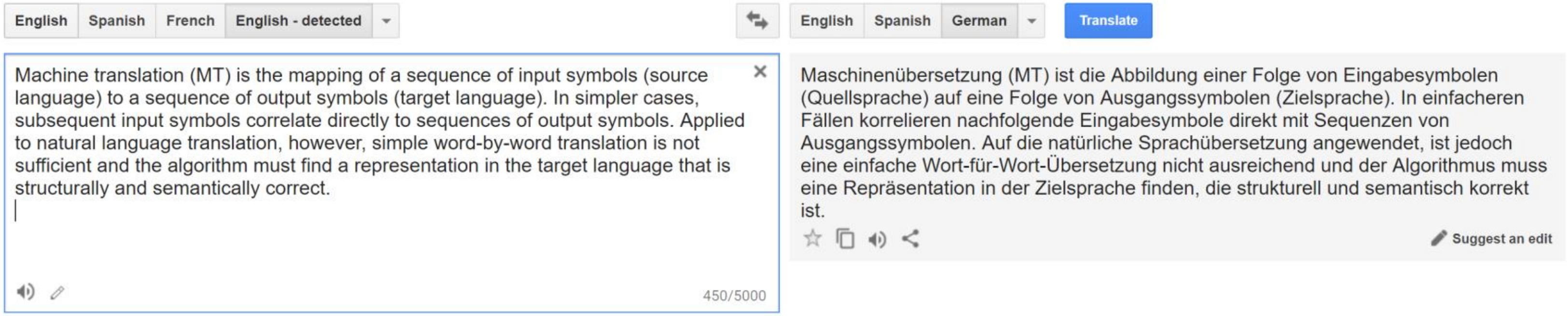
- **Regression** is the task of predicting a numerical value given the input features. The learning algorithm must find a function $f$ that maps an $M$-dimensional vector $\boldsymbol{x}$ to a numeric value, i.e. $f: \mathbb{R}^M \rightarrow \mathbb{R}$. The difference to classification is the output: instead of a category, a real number is required. Also, regression does not deliver distribution functions over all possible values.
  - Applications: predictions / extrapolations to the future, statistical analysis, algorithmic trading, expected claim (insurance), risk assessment (financial), cost restrictions, budgeting, data mining, pricing (and impact on sales), correlation analysis
- **Clustering** divides a set of inputs into groups. Unlike in classification, the groups (and the number of groups) are not known beforehand and the machine learning algorithm must find them. As the output is not known at training time, this type of task is called “unsupervised” while the ones before are “supervised” (we told the machine in the examples before what outputs we expect).
  - Applications: human genetic clustering, market segmentation (groups of customers), social network analysis (communities), image segmentation, anomaly detection, crime analysis
- **Density estimation (probability mass function estimation)** is the construction of an estimate of an underlying, unknown probability density function given the input features. In the most simple case, the algorithm must learn a function $p$: $\mathbb{R}^M \rightarrow \mathbb{R}$ where $p(x)$ is interpreted as a probability density function (if $\boldsymbol{x}$ is discrete p is called probability mass function). The most basic form is shown in the example on the right with histogram based density estimation using two different numbers of bins.
  - Applications: age at death for countries, modelling of complex patterns, feature extraction, simplification of models



- **Imputation of missing values** requires an algorithm to replace (estimate / guess) missing data with substituted values. For a new example $\boldsymbol{x} \in \mathbb{R}^M$ with some missing $x_j$, the algorithm must provide a prediction for the missing values.
  - Applications: incomplete sensing data, demographics (incomplete data over person), medical analysis (incomplete or expensive test data), restoration of signal (after data loss)
- **Synthesis and sampling** is a type of task where the machine learning algorithm must generate new examples that are similar to the training data. In video games, for example, large portions of the immersive landscape are generated automatically instead of by hand. This also requires some sort of variance in the output to break "dull" patterns that are easily recognized as artificial landscape (see example on the right side). Other examples include speech synthesis where a written text is emitted as an audio waveform for the spoken version of the text. The challenge for the algorithm is the lack of a "correct answer" and the necessity to include large quantities of variation in the output.

- **Anomaly detection** requires the algorithm to flag unusual, incorrect, or atypical events or data points. The output can be a simple $\{0,1\}$ flag (1 indicating an anomaly) or a probability for an anomaly. Supervised anomaly detection needs a training set with labels "normal (0)" and "abnormal (1)". Unsupervised anomaly detection requires the algorithm to describe the normal behavior (e.g., using density estimation) and then to detect outliers automatically.
  - Applications: credit card fraud, intrusion detection (cyber security), outliers to improve statistics, change detection, system health monitoring, event detection, fault detection

- **Machine translation (MT)** is the mapping of a sequence of input symbols (source language) to a sequence of output symbols (target language). In simpler cases, subsequent input symbols correlate directly to sequences of output symbols. Applied to natural language translation, however, simple word-by-word translation is not sufficient and the algorithm must find a representation in the target language that is structurally and semantically correct.
  - Google Translate

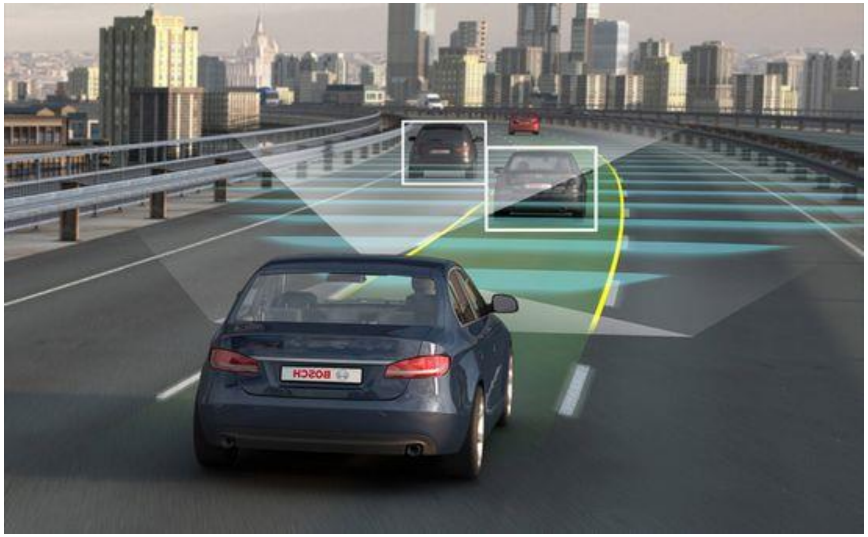


Machine translation (MT) is the mapping of a sequence of input symbols (source language) to a sequence of output symbols (target language). In simpler cases, subsequent input symbols correlate directly to sequences of output symbols. Applied to natural language translation, however, simple word-by-word translation is not sufficient and the algorithm must find a representation in the target language that is structurally and semantically correct.

Maschinenübersetzung (MT) ist die Abbildung einer Folge von Eingabesymbolen (Quellsprache) auf eine Folge von Ausgangssymbolen (Zielsprache). In einfacheren Fällen korrelieren nachfolgende Eingabesymbole direkt mit Sequenzen von Ausgangssymbolen. Auf die natürliche Sprachübersetzung angewendet, ist jedoch eine einfache Wort-für-Wort-Übersetzung nicht ausreichend und der Algorithmus muss eine Repräsentation in der Zielsprache finden, die strukturell und semantisch korrekt ist.

- **Transcription** asks a machine learning algorithm to observe a unstructured representation of the data and to transcribe it into a discrete (often textual) form. The most widely known versions are optical character recognition (OCR) and speech recognition.
- **Dimensionality Reduction** simplifies the input vectors to a lower-dimensional space. In many cases, the output is interpreted as topics or concepts that are key to disseminate the input vectors as good as possible (topic modelling). This allows the machine to more easily find documents that cover similar topics, i.e., instead of considering hundred thousands of different terms (words), only a few topics are considered. Dimensionality reduction is often used to reduce the amount of input data but to keep as much of the core information as possible.
  - Application: data mining, latent semantic analysis, principal component analysis, statistical analysis, data reduction/compression

- **Reasoning** is the process of generating conclusions from knowledge using logical techniques such as deduction and induction. Knowledge-based systems have been used over the past 30 years including expert-system written in prolog. Facts and rules were used to prove (or disprove) a new statement within a closed world. Newer approaches use machine learning to prove theorems or constraint solvers. Cognitive reasoning and cognitive AI have recently boosted performance of chat bots and speech recognition.
- **Autonomous Robots** work with reinforcement learning, i.e., it is not possible to provide samples that connect input signals with correct or expected output signals. Rather, robots need to adjust their behavior based on incentives and penalties provided by the environment. The rise of autonomous driving has created an entire new set of challenges on reinforcement learning: machine ethics. While this sounds like science fiction, there are many scenarios where robots must make decisions that programmers cannot foresee or hard code. As an example, if the car is inevitably hitting an animal or a person on the street, should the machine try a risky evasive maneuver and endangering its passengers or accept the potential death of the animal or person on the street?
  - While the field is relatively young, recent progress was accelerated by deep learning techniques. Tesla states that its autopilot is 10 times safer than the average driver.
  - Laws for and acceptance of robots in society are in its infancy. People are worried about safety, privacy, and car hacking
  - Further obstacles are insurance issues (who pays for a mistake of a robot)

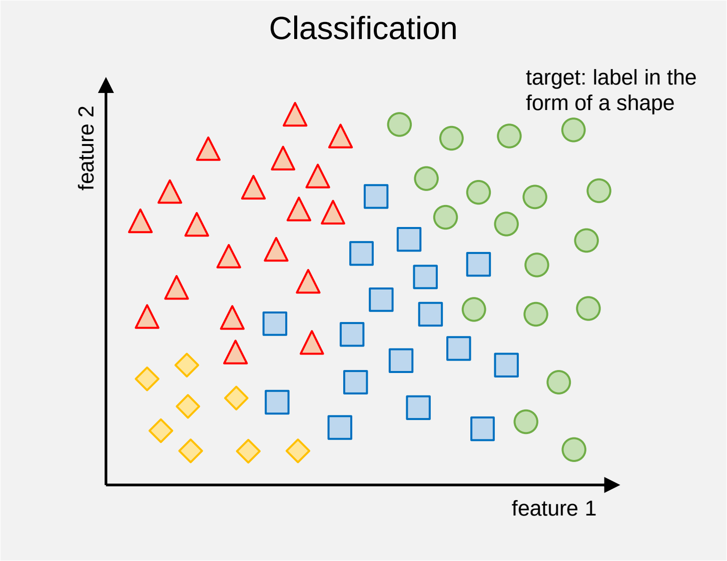


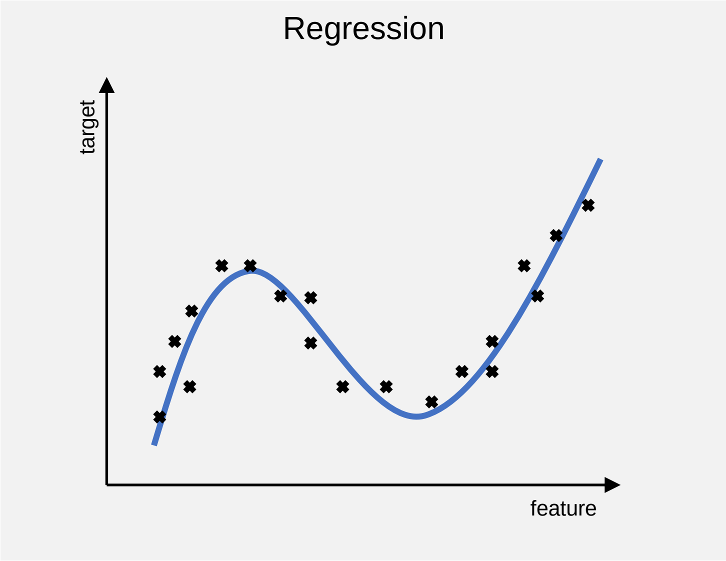
## 1.5.2 Performance

- To evaluate (and improve) a machine learning algorithm, we need to provide a quantitative measure for the “accuracy” of carrying out the task $T$. We will look deeper into these methods later in this chapter following this machine learning introduction. A short summary:
  - **Binary classification** (0-1 decisions) uses a **confusion matrix** to assess the performance, and provides numeric summary values to optimize for a desired optimum for the task. Typical measures include precision, accuracy and so on.
  - **Multi-class classification** (one out of a set of classes) requires a generalized **confusion matrix** resulting in a table with pair-wise “confusion”. Accuracy still works fine; in addition, we can summarize performance of a single class against all other classes.
  - **Binary classification with scores and thresholds** is a simple extension of the confusion matrix. With increasing threshold values, we obtain a method to optimize the threshold (adjustment of a hyper-parameter), and the Receiver Operating Characteristic Curve (ROC Curve). The area under the ROC curve is a simple method to assess performance.
  - **Multi-class Classification with Probabilities** measures the performance based on the probabilities of the class labels of an object. Typically, this is based on cross-entropy with the log-loss measure being a simpler version of it.
  - With **Regression** tasks, we measure the performance as the **mean squared error (MSE)** between the actual values and the predicted ones.
  - As we will see, machine learning algorithms not only use these measures to evaluate performance but also employ them to find an optimal set of parameters to minimize the error/loss function. In addition, it can also be used to control so-called hyper-parameters (→ learning process).

## 1.5.3 Experience

- **Supervised Learning** algorithms observe a data set with features and a target for each instance of the data set. The goal is to learn a general rule that maps features to targets and that can be applied to predict the outcome of newly presented data items. The term “supervised” originates from the view that the target is provided by an instructor or teacher. As an example, classification tasks presents for each example, described as a set of feature, a target in the form of a label (or set of labels). The “teacher” instructs the algorithm how the sets of features are correctly mapped to labels and the algorithm should learn the mapping rule.



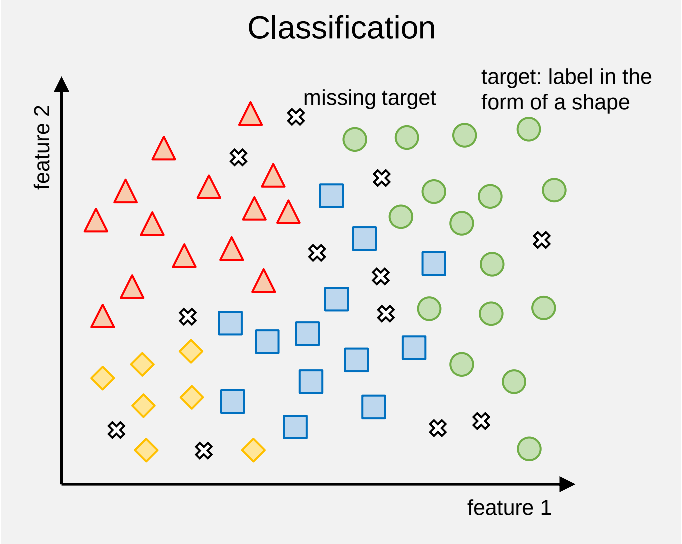


  - The teacher also provides an error measure that allows the machine learning algorithm to assess accuracy during training sessions
  - Even though targets are given, the algorithm must be able to deal with noise in the output values due to human errors (wrong labelling) or sensor errors (defects, distortion)

- **Semi-Supervised Learning** is a special case of supervised learning. The algorithm is presented with features and targets, however, some features or targets are missing (incomplete observation) in the training data. Depending on the task, the algorithm must either complete the missing features or predict targets for newly presented data sets.
  - **Missing targets:** The training set consists of complete features but some objects do not have targets (or labels). Incomplete targets often result if the labeling process is expensive or labour intensive. Consider a data set for credit card fraud detection with billions of transactions. Naturally, credit card firms investigate only a small subset of "suspicious" transactions and label them based on the outcome of an investigation ("fraud", "no fraud"). The vast amount is not labeled. To learn from such data sets, algorithms make one of the following assumptions:

    1) Smoothness: points in close proximity share the same label, i.e., the distribution function is continuous
    2) Cluster: data tends to form clusters and all objects in the same cluster share the same label
    3) Manifold: often, features are high-dimensional but there are only a few labels. Hence, the data is more likely to lie on a low dimensional manifold

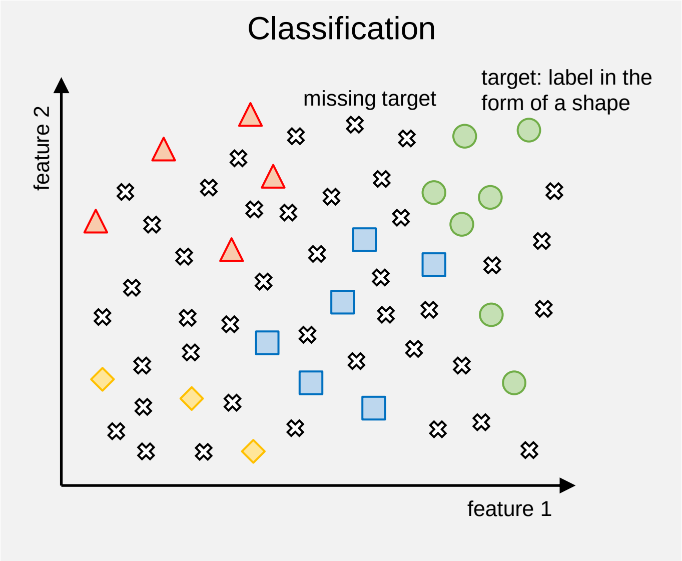
    Semi-supervised learning takes ideas both from supervised learning and from unsupervised learning.



    - **Induction:** if only a few labels are missing, a good strategy is to learn the distribution from the labeled data items with a supervised learning method. We can then go back and predict the missing labels. However, this does not work well if lots of objects have no label as the training set is not sufficient to capture the true distribution of labels. Evidently, such training ignores most of the data (information loss).

- **Transduction:** to consider all data points, transductive algorithms identify clusters in the data set and apply the same label to all objects in the cluster. A simple approach is the partitioning transduction:
  1. Start with a single cluster with all objects
  2. While a cluster has two objects with different labels Partition the cluster to resolve the conflict
  3. For all clusters: assign the same label to all objects in the cluster

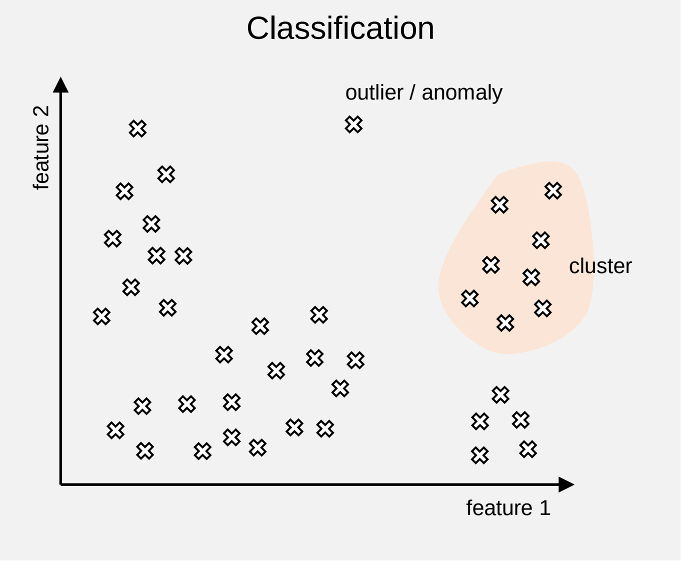
  There are other variants to develop the clusters.



– **Missing features:** The training set has complete targets, but some objects lack some of the features. For newly presented data, potentially with missing features, the algorithm must predict the target. A good example is disease prediction where the target (“healthy”, “has disease”) must be predicted from a set of test results. Laboratory tests are expensive and naturally not all features (test results) are available. Prediction of missing features depends on the AI method:

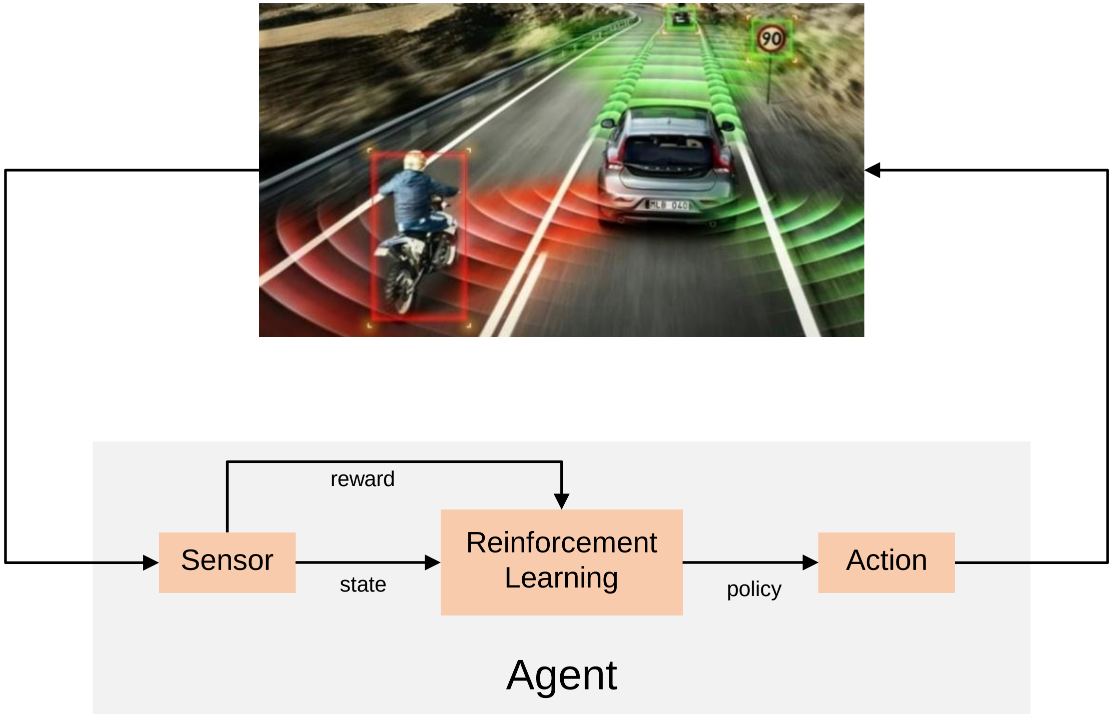
- Naïve Bayes (more details later in the deck) is a simple technique for building classifiers based on conditional probabilities. Let there be $K$ classes $C_k$ and $M$ features $x_i$. The best class $k^*$ is then given by $k^* = \underset{k}{\operatorname{argmax}} P(C_k) \prod_i P(x_i|C_k)$. The probabilities $P(C_k)$ and $P(x_i|C_k)$ are learned from the training data (ignoring missing features $x_i$). To predict the class for a new object with missing features, we simply ignore them in the Naïve Bayes optimization.
- If we have learned the distribution function over all features, we can simply “integrate” or “average” over the missing features, i.e., we assume that the missing features follow the distribution of the training set and we approximate them with an expected value.

- **Unsupervised Learning** algorithms observe a data set without targets and infer a function that captures the inherent structure and/or distribution of the data. In other words, we want to identify interesting facts in the data and derive new knowledge about its structure. In contrast to supervised learning, there is no instructor or teacher that provides targets or assess the performance of the outcome. The algorithm must learn without any guidance.



  - Clustering: the most common task for unsupervised learning is to identify groups of objects that “belong” together (with regard to a distance function). The number of clusters is often not known and must be learned too.
  - Outlier/Anomaly detection: the algorithm must learn the “normal” behavior through any means and identify outliers that significantly differ from the other objects. Note that the training data may also contain outliers.
  - Density function: describe the data set through an “appropriate” density function. A simple method is a Gaussian approximation and learning its mean value and variance from the data. More complex methods choose from a set of different distribution functions and optimize to the “best fit”
  - Dimensionality reduction: high-dimensional features often disguise an inherently much simpler characteristic of the data. Principle component analysis extracts “core concepts” along principal directions in the feature space that provide a simpler (but still accurate) view on the data.
  - Self-organizing maps (SOM): a SOM produces a discrete (often 2-dimensional) presentation of the data in a mesh of nodes, thereby mapping high-dimensional data to a low-dimensional view. It uses a competitive learning approach.

- **Reinforcement learning** evaluates possible actions in an environment so as to maximize the cumulative award. The problem is very general and broad and studied in various fields such as game theory, control theory, operations research, simulations, and genetic algorithms. Reinforcement learning is different to supervised learning as correct input/output correlations are not known. The focus is on finding a balance between exploration (of unknown situations) and exploitation (of current knowledge).
  - A reinforcement agent typically interacts with its environment in discrete time steps. At each time *t*, the machine observes the environment including potential rewards. It then chooses and action from the set of available actions and performs it against the environment receiving rewards for the transition. The objective is to maximize the cumulative rewards.



reward

Sensor

state

Reinforcement Learning

policy

Action

Agent

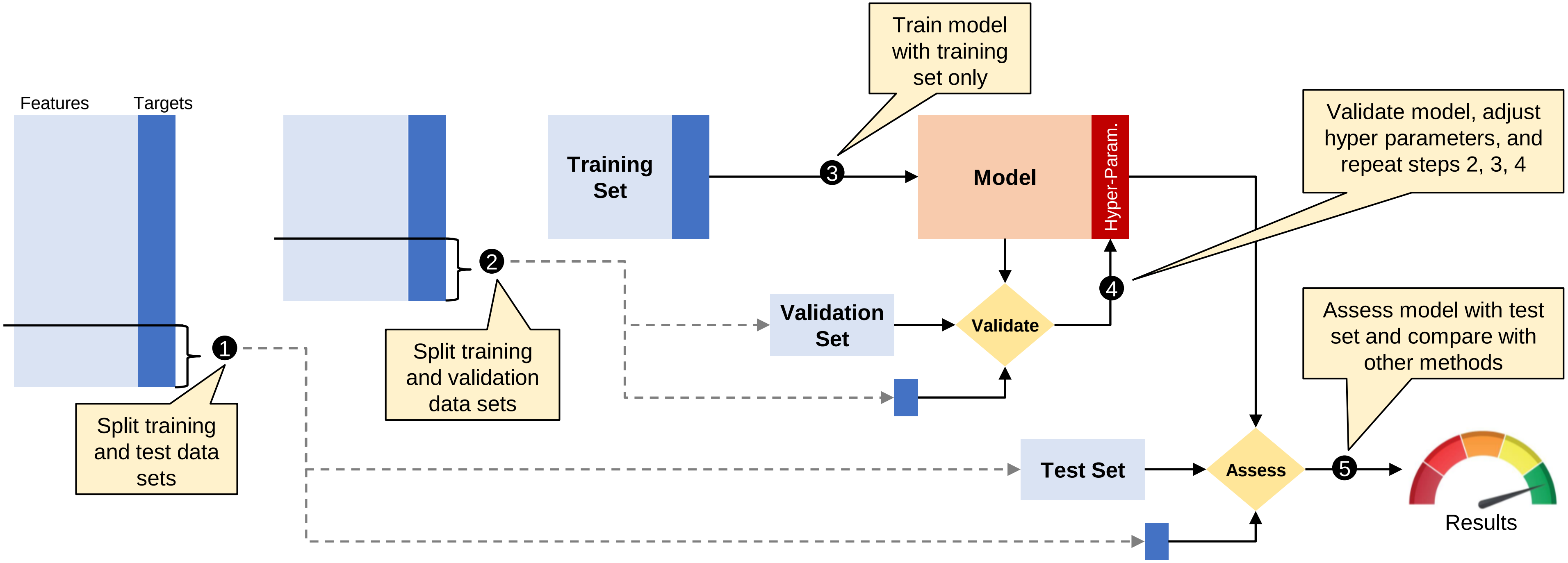
- A policy is a series of actions. Instead of optimizing for individual actions, reinforcement learning algorithms define policies and choose the best policy for immediate and cumulative rewards. Exploration is the process of developing (or composing) new policies, while exploitation is the application of the best known policy. Exploration can lead to algorithms that are no longer understood by the human developers. AlphaGo, Google's Go program that has beaten the world champion is a good example: it is not clear how the computer decided and what the winning strategy is; we (humans) can also not improve our gameplay based on the algorithm
- Reinforcement learning is an efficient approach if the environment behaves non-deterministic or even chaotic due to incomplete or erroneous observations. It is the only viable option if we lack an accurate error (or success) measure. Driving autonomously in a city is a good example for the chaotic and non-deterministic nature of such tasks. Though it is possible to describe broadly what success means ("arrive safely at the target within $n$ minutes"), it is not possible to provide accurate measures for every point in time (as they are mostly unknown at the time of learning)

# 1.6 The Learning Process

- Machine learning algorithm learn from data. It is critical that we feed the “right” data into this process for the task that we want it to solve. “Right” is not only referring to good data quality, complete data, but also the extraction of meaningful features. A number of challenges arises in this context:
  - Feature selection, i.e., ability to capture essential information to learn a task
  - Data cleansing, i.e., ability to remove the negative impact of outliers or of noise
  - Normalization, i.e., ability to address correlation between features and to normalize scales
  - Curse of dimensionality, i.e., inability to learn underlying structure due to sparse data space
  - Overfitting, i.e., inability to generalize well from training data to new data sets
  - Underfitting, i.e., inability of the algorithm to capture the true essence of the data structure

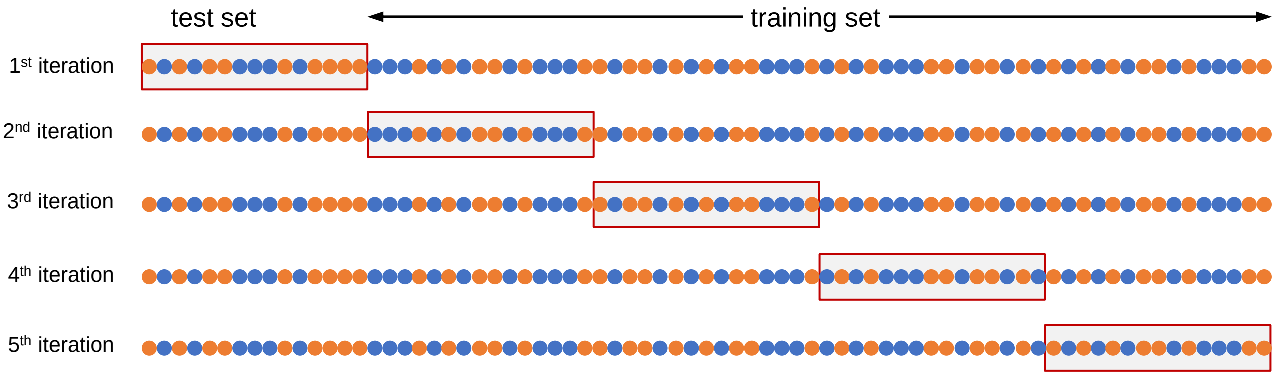
- Data preparation is a 3-step approach which we do not further discuss in this section. With the term “data” we always include features and targets (if they are available)
  1) Select Data
  2) Preprocess Data
  3) Transform Data

- We need to pay attention how we divide the data sets into training sets, validations sets, and test sets. The latter aspects is essential to adjust hyper-parameter of the algorithm including capacity and to measure its ability to correctly generalize. In the following, we focus on the overall learning process and address the above overfitting and underfitting issues.


Features
Targets
1
Split training and test data sets
2
Split training and validation data sets
Training Set
3
Train model with training set only
Model
Hyper-Param.
Validate model, adjust hyper parameters, and repeat steps 2, 3, 4
Validation Set
Validate
4
Assess model with test set and compare with other methods
Test Set
Assess
5
Results

- To understand how well a machine learning algorithms can generalize to new data sets, it is essential that training sets and test sets are distinct. Otherwise, we can construct a memorizing algorithm that simply stores all features and targets. Assessments of such an algorithm will produce the best possible results, but the algorithm will perform poorly on new data.
- Most algorithms have models with so-called hyper parameters that drive their inherent **capacity** or structure. For example, we can vary the degree of a polynomial regression model to adjust to a larger variety of functions. In a neural network, the capacity is provided by the number of neurons and connections. In a nutshell, models with small capacity struggle to fit the training data and to capture its distribution; models with high capacity tend to overfit the training data and poorly generalize to new data sets. The usage of validation sets (again, distinct from the training sets) allows algorithms to optimize their hyper-parameters.

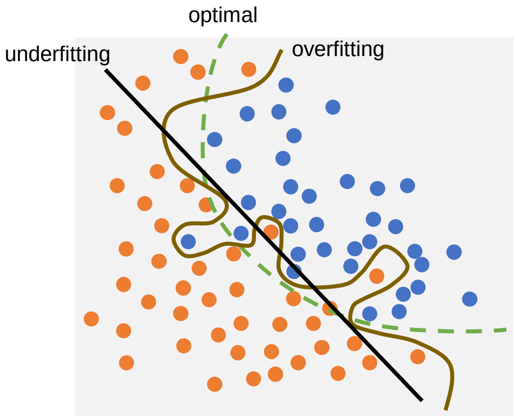
- To drive the learning process, we partition the original data set (and its targets) into a training set (70-80% of data) and test set (20-30% of data). If the model has need to optimize some hyper-parameters, we further partition the data to obtain the validation set (20-30% of data):
  - The **training set** is used for learning, i.e., to fit the parameters/weights minimizing training error
  - The **validation set** is used to tune hyperparameters (models, capacity) to prevent underfitting and overfitting issues. Validation data is not used for training and also not used for final testing
  - The **test set** is used to assess the performance, i.e., the ability of the model to generalize
- Ideally, the three data sets are large enough to represent the true distribution equally well. If the data set is too small, however, validation and testing lack statistical certainty on average errors making it difficult to assess and compare performance. **Cross-validation** uses rotation schemes an multiple iterations to improve the accuracy of validation and testing.
  - **k-fold cross validation** partitions the original data set into $k$ equal sized subsamples. In each iteration, one subsample denotes the test set, and the remaining $k$-$1$ subsample form the training set. The $k$ results are averaged to produce a single value. $k$=$10$ is a typical value. The same approach can be used for the validation set.

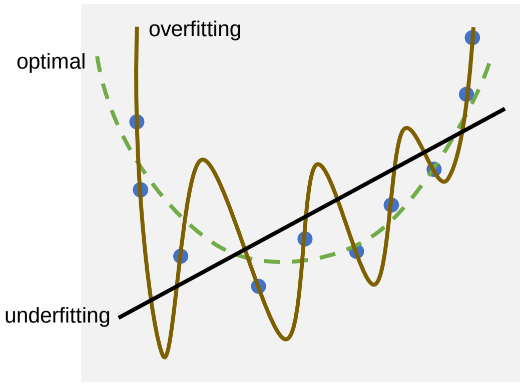


The same applies for the validation set

- What is the right complexity and the right capacity of a model to explain observed facts sufficiently?
  - Too simple: “if the sun is out, it is warm”
  - Too complex: “if the sun is out and it is a summer month and you are on the north side or it is a winter month and you are on the south side or you are equatorial or you are in a dessert and it is not an ice dessert and it is not cloudy or raining or snowing and there is not a strong wind and there is not a sun eclipse and there is not a volcano eruption and you are not in the water or in a cave or in the shadows or in a house with air conditioning or in a car with air conditioning or in a freezer … then it is warm”
- Our brain is excellent in finding the right level of abstraction despite the limitations of a simple model
  - Example: “birds can fly” (but wait, not all birds can fly)
    - we use a simple model to generalize (80-95%) and then deal with exceptions separately
  - Example: “describe what makes a chair a chair”
    - write down 3-5 attributes that describe how a chair must look like
    - compare with some examples from the web → no definition is good enough
    - look at counter examples: sofa, bank, anything else you can sit on
  - Example: “horse” → much narrower in terms of what is accepted to match the concept of a horse (e.g., donkey, zebra, giraffe and other hoofed animals do not count as horses)
  - Example: “dog” → wide variety of forms that count as dogs yet we recognize them immediately (different ratios of body lengths, colors, face features, tail, hair)
  - Example: “sketches of people”, comics and face features that make a person recognizable (cartoon, caricature of real people)
  - Example: “throw a basketball from 20m distance such that it lands in the target circle” (a lot of physics and math in combination with the right speed and force of contraction of many muscles)

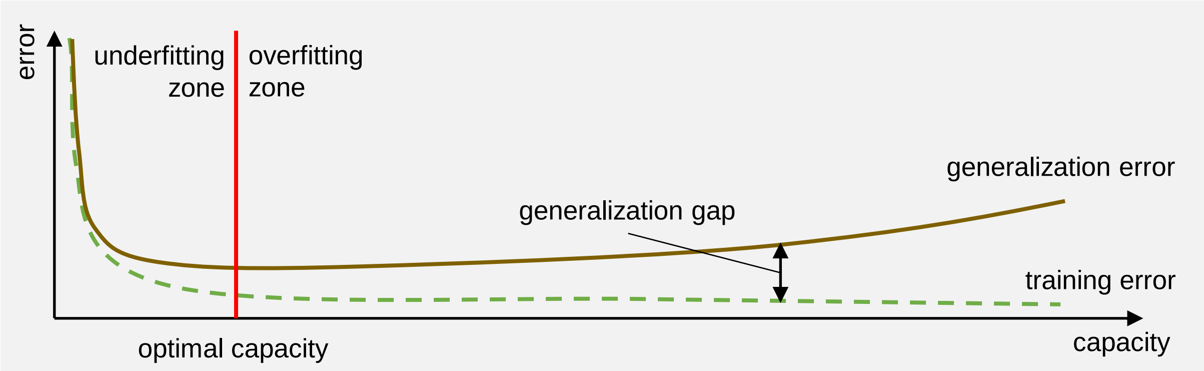
- **Overfitting** and **underfitting** are common problems in machine learning. Overfitting occurs when the model is excessively complex to match the training data as accurately as possible. Often, such a model has too many parameters relative to the number of training items. But even worse, the model is likely to overreact to minor changes leading to poor predictive performance (see figure on the right hand side as an example). Underfitting, on the other side, occurs when the model cannot capture the underlying trend of data and over-simplifies the distribution. For instance, fitting a linear model to a non-linear data distribution will result in a high training error and poor predictive performance.





  - As illustrated above, we can observe that overfitting is the result of optimizing for the training data with too many parameters. Typically, an overfitting model shows small errors indicating its ability to adapt nicely to the training data, but it can not predict new data points well enough.
  - Underfitting, on the other side, shows both large errors on the training data and poor prediction performance for new data points; it obviously cannot capture the true essence of the distribution.
  - We can control overfitting and underfitting by altering the **capacity of the model**. Optimal capacity is reached if the model exhibits small errors on both the training set and the validation set. To work best, training set and validation set must be distinct; but we can run several iterations to adjust the capacity with different partitioning of training and validation set.

- When altering the capacity of the model, **Occam's razor** provides an intuitive heuristic. The principle was first stated by William of Ockham (c. 1287-1347) and has been made more precise over time, most notably in the 20th century for statistical learning. The principle states:
  - Numquam ponenda est pluralitas sine necessitate [Plurality must never be posited without necessity]
  - In a more modern language, the principle states that among competing hypothesis that explain observations equally well, one should choose the "simplest" one
  - Indeed, simpler models are better able to generalize but we must choose a sufficiently complex model to achieve low training error. Typically, training error decreases gradually as capacity increases. The generalization error, however, has a U-shaped curve as a function of capacity:



- The **bias-variance tradeoff** (or **dilemma**) is the problem of simultaneously minimizing two sources of errors that prevent models to generalize well beyond their training data
  - The bias is the test error of a model causing it to miss relevant relations in the data (underfitting)
  - The variance is the error from sensitivity to small changes in the input. High variance can cause the model to adopt to noise in the training data rather than to the data (overfitting)

  The **bias-variance decomposition** is a way to analyze the expected generalization error. It uses the sum of the bias, variance, and irreducible error (noise) in the problem.

# 1.7 Perfomance of Machine Learning

- In machine learning, the performance measure is not only used for final evaluations. Some methods also require performance metrics to validate some of the hyper-parameters of the model. This validation is used to prevent under-fitting and over-fitting to the training data and essentially alters the internal structure in a pre-defined way. For example, using polynomial regression, the degree of polynoms is such a hyper-parameter.
- In addition, some methods like neural networks and regression use the performance metric as an error or loss function that needs to be optimized (find parameters/weights of the model that minimize the error). In some cases, we can use different metrics to train, validate, and test the system to optimize different aspects of the model

- To evaluate (and improve) a machine learning algorithm, we need to provide a quantitative measure for the "accuracy" of carrying out the task $T$. Different types of measures exists:

- **Binary classification** (0-1 decisions) uses a **confusion matrix** to assess the performance, and provides numeric summary values to optimize for a desired optimum for the task

| | | Actual Condition (as observed) | | | |
|---|---|---|---|---|---|
| | Population | Positive ($P$) | Negative ($N$) | | |
| Predicted Condition (as computed) | “Yes” | **True Positive** ($TP$) | **False Positive** ($FP$) | Positive Predictive Value ($PPV$), Precision | False Discovery Rate ($FDR$) |
| | “No” | **False Negative** ($FN$) | **True Negative** ($TN$) | False Omission Rate ($FOR$) | Negative Predictive Value ($NPV$) |
| | | True Positive Rate ($TPR$), Sensitivity, Recall, Hit Rate | False Positive Rate ($FPR$), Fall-Out | Accuracy ($ACC$) | |
| | | False Negative Rate ($FNR$), Miss Rate | True Negative Rate ($TNR$), Specificity | | Error Rate ($ERR$), Misclassification Rate |

$$TPR = \frac{TP}{P}$$

$$TNR = \frac{TN}{N}$$

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

$$NPV = \frac{TN}{TN + FN}$$

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

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

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

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

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

$$ERR = \frac{FP + FN}{P + N} = 1 - ACC$$

- Example: Cancer test

| | | Actual Condition (as observed) | | |
|---|---|---|---|---|
| | Population ($2030$) | Positive ($P=30$) | Negative ($N=2000$) | |
| Predicted Condition (as computed) | “Yes” ($200$) | **True Positive** ($TP=20$) | **False Positive** ($FP=180$) | $PPV = \frac{20}{200} = 10\%$ |
| | “No” ($1830$) | **False Negative** ($FN=10$) | **True Negative** ($TN=1820$) | $NPV = \frac{1820}{1830} = 99.5\%$ |
| | | $TPR = \frac{20}{30} = 67\%$ | $TNR = \frac{1820}{2000} = 91\%$ | $ACC = \frac{1840}{2030} = 90.6\%$ |

precision

recall

- Is this a good test for cancer?
  - We note that the false discovery rate ($1 - PPV = 90\%$) is very high, i.e., a lot of tests are positive but the patient does not have cancer. Hence, there is little confidence in positive outcomes and further tests are required.
  - We further note that the false omission rate ($1 - NPV = 0.5\%$) is very low, i.e., a negative test result is almost always a true negative case. This is an important element of the diagnosis of exclusion, especially if the above test is very cheap to conduct. The high true negative rate ($TNR = 91\%$) indicates that the elimination is in 91% successful.
- Using $NPV$ as a driving performance metric is very common in cases where most of the population is considered negative.
- Accuracy ($ACC$) is not a reliable metric: assume an “oracle” that always predicts “No”. This oracle yields an accuracy of $\frac{0+2000}{2030} = 98.5\%$ and, hence, beats the predictions in the above example. On the other side, $PPV = 0\%$, $NPV = 98.5\%$, $TPR = 0\%$ and $TNR = 100\%$ clearly indicate the limitations of this oracle.

- **Multi-class classification** (one out of a set of classes) requires a generalized **confusion matrix** resulting in a table such as the example below with people recognition in images:

| | | Actual Class | | |
|---|---|---|---|---|
| | Population (*100*) | Woman (*20*) | Man (*20*) | *Child (60)* |
| Recognized Class | Woman (*19*) | *13* | *4* | *2* |
| | Man (*18*) | *2* | *15* | *1* |
| | Child (*63*) | *5* | *1* | *57* |

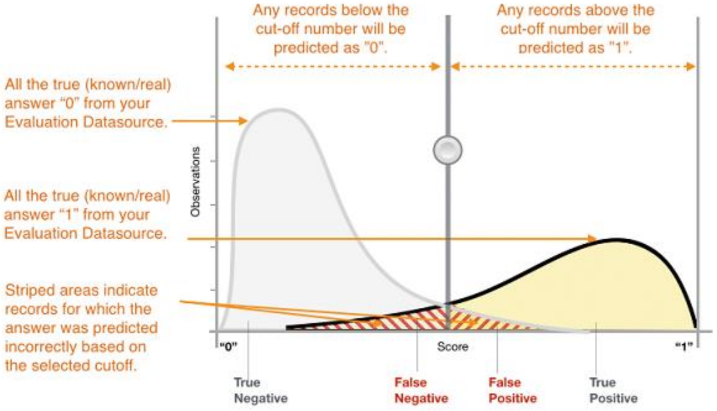
  - The confusion matrix allows to easily spot correct classifications (on the diagonal) and prediction errors (outside the diagonal). The table also depicts the cases for which the algorithm struggles to distinguish classes. In the example above, the algorithm recognized
    - 13  out of 20 women correctly, but 2 were wrongly classified as man and 5 as children
    - 19 women in total but only 68% (13) were actually women
    - 57 out of 60 children correctly, and children were more often confused with women than men
  - Accuracy is given by the sum of the diagonal over all examples, i.e., $ACC = \frac{13+15+57}{100} = 85\%$, and the error rate is $ERR = 1 - ACC = 15\%$. Again, accuracy alone is not capable to tell us the entire story; in the running example, the algorithm struggles with recognizing women. To better analyze the situation, we can create additional confusion matrices focusing on the correct classification of one class only. See next page for an example for the class “Woman” and “Child”

| | | Actual Class | | |
|---|---|---|---|---|
| | Total Population | Woman ($P=20$) | Not a Woman ($N=80$) | precision |
| Recognized Class | Woman ($19$) | **True Positive** ($TP=13$) | **False Positive** ($FP=6$) | $PPV = \frac{13}{19} = 68\%$ |
| | Not a Woman ($81$) | **False Negative** ($FN=7$) | **True Negative** ($TN=74$) | $NPV = \frac{74}{81} = 91\%$ |
| | | $TPR = \frac{13}{20} = 65\%$<br>recall | $TNR = \frac{74}{80} = 93\%$ | $ACC = \frac{87}{100} = 87\%$ |

| | | Actual Class | | |
|---|---|---|---|---|
| | Total Population | Child ($P=60$) | Not a Child ($N=40$) | precision |
| Recognized Class | Child ($63$) | **True Positive** ($TP=57$) | **False Positive** ($FP=6$) | $PPV = \frac{57}{63} = 90\%$ |
| | Not a Child ($37$) | **False Negative** ($FN=3$) | **True Negative** ($TN=34$) | $NPV = \frac{34}{37} = 92\%$ |
| | | $TPR = \frac{57}{60} = 95\%$<br>recall | $TNR = \frac{34}{40} = 85\%$ | $ACC = \frac{91}{100} = 91\%$ |

– Note that the accuracy for both classes “Woman” and “Child” are high and almost the same. However, it is wrong to conclude that the recognition of both classes works equally good. The reason for the good accuracy of class “Woman” is due to the large number of negative examples that are correctly dismissed. But precision (68%) and recall (65%) are much lower than for class “Child” documenting only mediocre capabilities to recognize women correctly.

- **Binary classification with scores and thresholds:** assume we have an algorithm that decides, based on a metric, whether an object belongs to a class or not. A good example is video shot detection: if the 'distance' between subsequent frames is large enough, we assume that a new shot has started (see application in later chapters of this course). The challenge is to set a threshold value for the distance in such a way, that the smallest number of errors occur (false positives, false negatives). In this scenario, we need:
  - a way to train 'good' thresholds as the overall performance of the method depends on it
  - a way to compare methods regardless of the chosen threshold to assess how well they can separate the positive from the negative cases



Any records below the cut-off number will be predicted as "0".

Any records above the cut-off number will be predicted as "1".

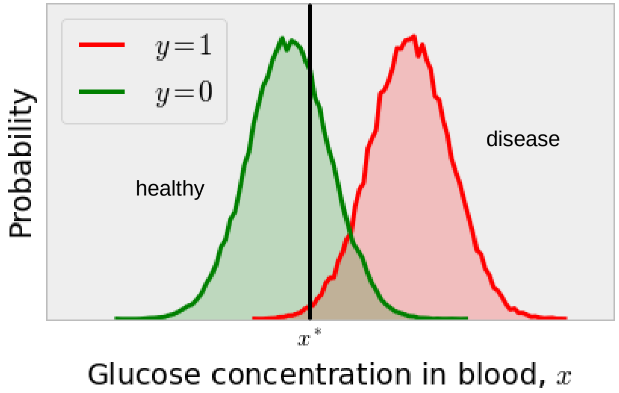
All the true (known/real) answer "0" from your Evaluation Datasource.

All the true (known/real) answer "1" from your Evaluation Datasource.

Striped areas indicate records for which the answer was predicted incorrectly based on the selected cutoff.

source: https://docs.aws.amazon.com/machine-learning/latest/dg/binary-classification.html

**Medical Example:** a new test shall distinguish between 'healthy' and 'disease' based on glucose concentration in the blood. The values of known populations are depicted on the right (green for healthy population on the left, and red for 'disease' population on the right). Given the test, we want to asses how well the test works and what thresholds we employ during medical examinations. Is this a good medical test?



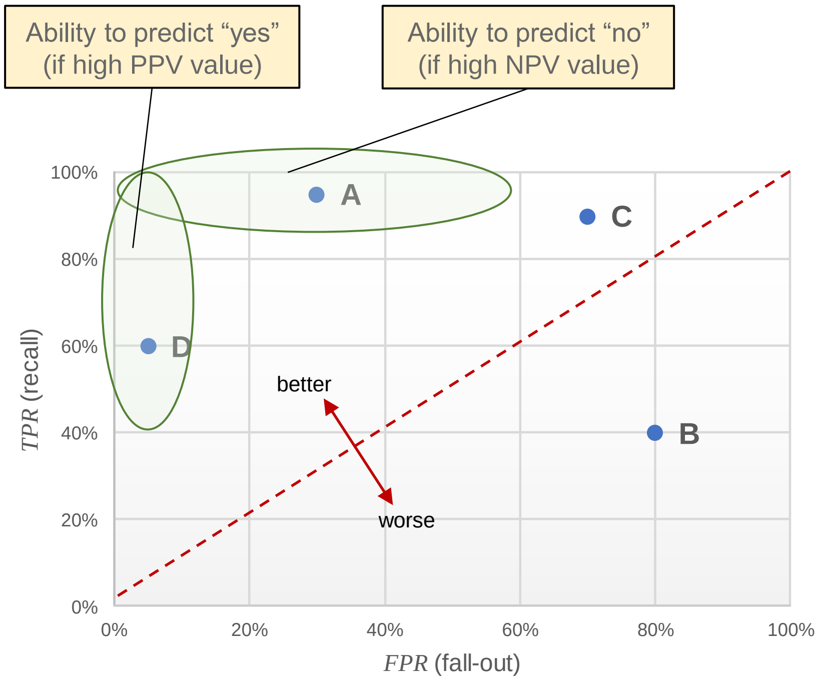
- **Binary classification with scores and thresholds** require an extension to the simple confusion matrix. Firstly, how do we calculate true/false positives/negatives if the algorithm says “Yes” only if the score exceeds a given threshold? Secondly, how do we favor algorithms that assign higher scores for positives (and lower for negatives)? The Receiver Operating Characteristic Curve (ROC Curve) is a simple tool to answer these questions.
  - The ROC curve is a 2-dimensional plot with the x-axis denoting the false positive rate ($FPR$) and the y-axis denoting the true positive rate ($TPR$). The ideal point is $(0,1)$, i.e., the upper-left corner with accuracy ($ACC$), precision ($PPV$), and recall ($TPR$) at 100% and fall-out ($FPR$) and miss rate ($FNR$) at 0%. In general, the more north-west the better, the more south-east the worse the performance is.
  - Example without scores and thresholds:

| A | |
|---|---|
| $TP = 95$ | $FP = 30$ |
| $FN = 5$ | $TN = 70$ |
| $TPR = 95\%$ | $FPR = 30\%$ |
| $PPV = 76\%$ | $NPV = 93\%$ |
| $ACC = 83\%$ | |

| B | |
|---|---|
| $TP = 40$ | $FP = 80$ |
| $FN = 60$ | $TN = 20$ |
| $TPR = 40\%$ | $FPR = 80\%$ |
| $PPV = 33\%$ | $NPV = 25\%$ |
| $ACC = 30\%$ | |

| C | |
|---|---|
| $TP = 90$ | $FP = 70$ |
| $FN = 10$ | $TN = 30$ |
| $TPR = 90\%$ | $FPR = 70\%$ |
| $PPV = 56\%$ | $NPV = 75\%$ |
| $ACC = 60\%$ | |

| D | |
|---|---|
| $TP = 60$ | $FP = 5$ |
| $FN = 40$ | $TN = 95$ |
| $TPR = 60\%$ | $FPR = 5\%$ |
| $PPV = 92\%$ | $NPV = 70\%$ |
| $ACC = 78\%$ | |



Ability to predict “yes” (if high PPV value)

Ability to predict “no” (if high NPV value)

- Adding scores and threshold changes the way the algorithm decides. With binary classification, assume that the prediction is based on a random variable $X$ which is a score for the current instance. The higher the score, the more likely it is a positive case, the lower the score the more likely it is a negative case. A threshold $T$ is required such that the algorithms yields “Yes” if $X > T$ and “No” otherwise.
  - Let $f_p(x)$ denote the probability density of $X$ if the instance belongs to class “positive”
  - Let $f_n(x)$ denote the probability density of $X$ if the instance belongs to class “negative”
- We  can calculate the various rates as a function of the threshold $T$ as follows

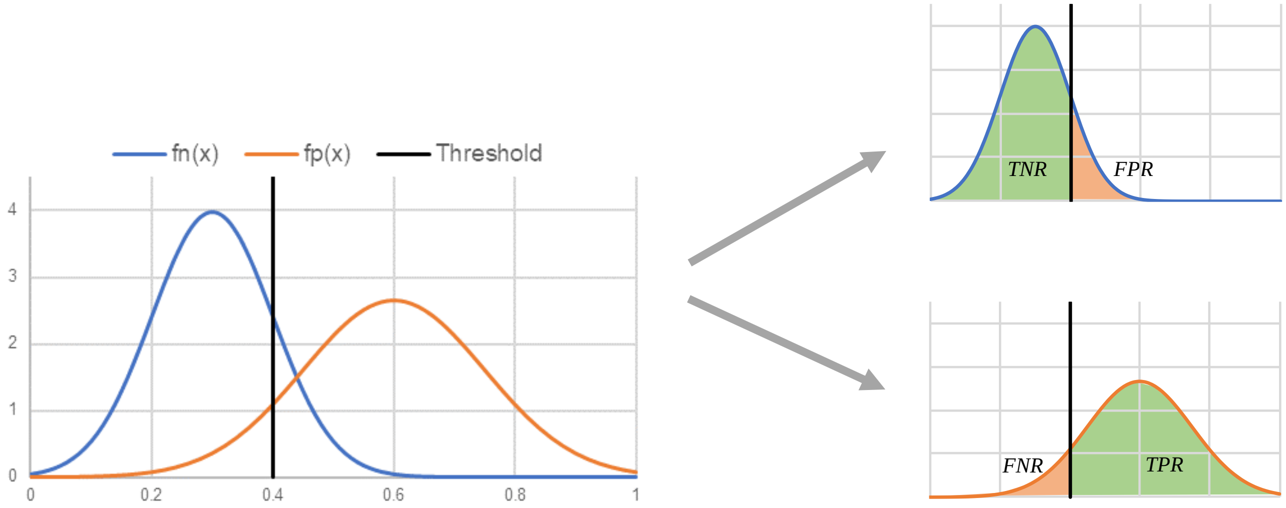
$$TPR(T) = \int_T^\infty f_p(x)\, dx$$

$$FNR(T) = \int_{-\infty}^T f_p(x)\, dx$$

$$TNR(T) = \int_{-\infty}^T f_n(x)\, dx$$

$$FPR(T) = \int_T^\infty f_n(x)\, dx$$

or visually

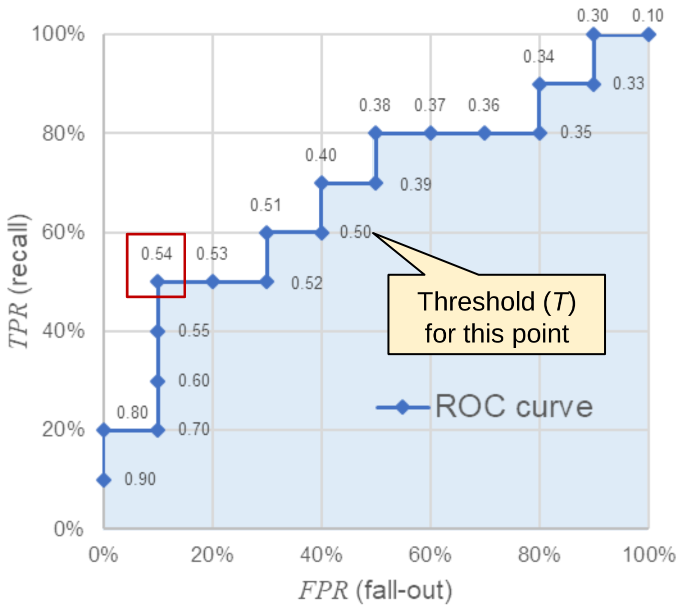


- The ROC curve serves two purposes: 1) optimize the threshold $T$, and 2) assess the performance of the algorithm. Let us consider the following simple example with 20 instances with labels P(“positive”) and N (“negative”). The medical test (in this example) returns a score between 0 and 1, the higher the score the more likely it is positive (i.e., yields a “yes”).

Use score of current row as threshold

Highest accuracy with T=0.54

| Class | Score | TP | FP | FN | TN | TPR | FPR | ACC |
|---|---|---|---|---|---|---|---|---|
| P | 0.90 | 1 | 0 | 9 | 10 | 10% | 0% | 55% |
| P | 0.80 | 2 | 0 | 8 | 10 | 20% | 0% | 60% |
| N | 0.70 | 2 | 1 | 8 | 9 | 20% | 10% | 55% |
| P | 0.60 | 3 | 1 | 7 | 9 | 30% | 10% | 60% |
| P | 0.55 | 4 | 1 | 6 | 9 | 40% | 10% | 65% |
| P | 0.54 | 5 | 1 | 5 | 9 | 50% | 10% | 70% |
| N | 0.53 | 5 | 2 | 5 | 8 | 50% | 20% | 65% |
| N | 0.52 | 5 | 3 | 5 | 7 | 50% | 30% | 60% |
| P | 0.51 | 6 | 3 | 4 | 7 | 60% | 30% | 65% |
| N | 0.50 | 6 | 4 | 4 | 6 | 60% | 40% | 60% |
| P | 0.40 | 7 | 4 | 3 | 6 | 70% | 40% | 65% |
| N | 0.39 | 7 | 5 | 3 | 5 | 70% | 50% | 60% |
| P | 0.38 | 8 | 5 | 2 | 5 | 80% | 50% | 65% |
| N | 0.37 | 8 | 6 | 2 | 4 | 80% | 60% | 60% |
| N | 0.36 | 8 | 7 | 2 | 3 | 80% | 70% | 55% |
| N | 0.35 | 8 | 8 | 2 | 2 | 80% | 80% | 50% |
| P | 0.34 | 9 | 8 | 1 | 2 | 90% | 80% | 55% |
| N | 0.33 | 9 | 9 | 1 | 1 | 90% | 90% | 50% |
| P | 0.30 | 10 | 9 | 0 | 1 | 100% | 90% | 55% |
| N | 0.10 | 10 | 10 | 0 | 0 | 100% | 100% | 50% |



- The table is ordered by the scores of the 20 instances. In each row, we consider the score as the threshold and compute TP, FP, FN, and TN with that threshold across all 20 instances. The resulting TPR and FPR values are then depicted in the ROC cure on the right. In this example, we selected the optimal threshold (0.54) based on the row with highest accuracy (70%)
- In general, higher thresholds tend to be more “conservative” (less false positive) while lower thresholds are more “liberal” (more true positives). Accuracy is only one way to select a threshold. Other values like precision, recall or fall-out can be used as well.
- Performance of an algorithm can be measured regardless of the selected threshold with the **area under the ROC curve** (blue area, right figure); the bigger the area, the better the algorithm.

- **Multi-class Classification with Probabilities** measures the performance based on the probabilities on the class labels of an object. An instance $x$ is part of the class $C_k$ if $c_k(x)=1$, and is not part of that class if $c_k(x)=0$ ($c_k$ denotes the true membership). The algorithm predicts probabilities $y_k(x)$ for an instance $x$ with $y_k(x)$ being large if $x$ is likely to belong to class $C_k$.
  - In information theory, the **cross-entropy H** measures how accurate a model distribution $q$ matches the true distribution $p$ over a set of events $\varepsilon$

$$H(p,q)=-\sum_{\varepsilon} p_\varepsilon \log q_\varepsilon$$

If we do not state otherwise log always refers to the natural logarithm. However, for our purpose, the base is irrelevant as it only scales the result but does not change order

  - The **log-loss** measure is a simplification of the cross-entropy with exactly two events: 1) $x$ is part of class $C_k$, and 2) $x$ is not part of class $C_k$. The true distribution $p$ then becomes $p\in\{c_k(x),1-c_k(x)\}$ and the model distribution $q$ becomes $q\in\{y_k(x),1-y_k(x)\}$. Thus:

$$H_{k,x}(p,q)=-\sum_{\varepsilon} p_\varepsilon \log q_\varepsilon=-c_k(x)\log\big(y_k(x)\big)-\big(1-c_k(x)\big)\log\big(1-y_k(x)\big)$$

  - Summing over all instances $x$ and classes $C_k$, the performance is measured as

$$P=-\sum_{x}\sum_{k}\Big(c_k(x)\log\big(y_k(x)\big)+\big(1-c_k(x)\big)\log\big(1-y_k(x)\big)\Big)$$

  - Note: To improve the numerical stability of the log-calculations, $y_k(x)$ is often adjusted by a small value $\Delta$ (e.g., $\Delta=10^{-15}$): $\hat{y}_k(x)=\max\Big(\Delta,\min\big(1-\Delta,y_k(x)\big)\Big)$

- With **Regression** tasks, we measure the performance as the **mean squared error (MSE)** between the actual values and the predicted ones. Let $\boldsymbol{Y}$ be the vector of observed values with $\boldsymbol{Y} \in \mathbb{R}^N$, thus we have $N$ samples. Let $\widehat{\boldsymbol{Y}}$ be the vector with the predicted values, again with $\widehat{\boldsymbol{Y}} \in \mathbb{R}^N$. The MSE is given as

$$MSE = \frac{1}{N}\sum_{i=1}^{N}\left(\widehat{Y}_i - Y_i\right)^2 = \frac{1}{N}\left\|\widehat{\boldsymbol{Y}} - \boldsymbol{Y}\right\|_2^2$$

  - Regression methods model the prediction with a function $f$ and parameters $\boldsymbol{\theta}$ to map an input vector $\boldsymbol{x}_i$ to an output value $\widehat{Y}_i$, i.e., $\widehat{Y}_i = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$ with $f: \mathbb{R}^M \rightarrow \mathbb{R}$ and $\boldsymbol{\theta} \in \mathbb{R}^D$. The number $D$ of parameters depends on the chosen function. With linear regression, $D = M$ and $f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \boldsymbol{\theta}^\top \boldsymbol{x}$.
  - To find the best solution, a regression algorithm must find the parameters $\boldsymbol{\theta}^*$ which minimize the MSE; in other words. Let $\widehat{Y} = \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{x})$

$$\boldsymbol{\theta}^* = \operatorname{argmin}_{\boldsymbol{\theta}} \|\boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{x}) - \boldsymbol{Y}\|_2^2$$

Note that the factor $1/N$ does not change the solution $\boldsymbol{\theta}^*$, hence we can omit it here

  - To solve the above equation, we need find values for $\boldsymbol{\theta}$ where the gradient is $\boldsymbol{0}$:

$$\nabla_{\boldsymbol{\theta}} \|\boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{x}) - \boldsymbol{Y}\|_2^2 = 0$$

  - With simple regression models, we can use calculus to analytically find the exact solution. In more complex cases, a numeric solution with **gradient descent** is often sufficient even if we find only a local instead of the global minimum (approximate result). The use of squared error simplifies the gradient calculations significantly.
  - Backpropagation in neural networks use a similar method to train the weights in the network through (stoachastic) gradient descent.

# 1.8 Literature and Links

- David A. Grossman, Ophir Frieder, “Information Retrieval Algorithms and Heuristics.“, Kluwer Academic Publishers, 1998
- [TREC] – “Text REtrieval Conference“ http://trec.nist.gov/
- [INEX] – „Initiative for the Evaluation of XML retrieval“ http://qmir.dcs.qmw.ac.uk/INEX/
- Zou, Kelly H.; O'Malley, A. James; Mauri, Laura (2007); *Receiver-operating characteristic analysis for evaluating diagnostic tests and predictive models*, Circulation, 115(5):654–7
- Hanley, James A.; McNeil, Barbara J. (1982). "The Meaning and Use of the Area under a Receiver Operating Characteristic (ROC) Curve". *Radiology*. **143** (1): 29-36. PMID 7063747. doi:10.1148/radiology.143.1.7063747.
- Amazon AWS: https://docs.aws.amazon.com/machine-learning/latest/dg/evaluating-model-accuracy.html