Intelligent Systems

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0 Introduction to Models and Data

0.1 Introduction

When we talk about Artificial Intelligence, we're talking about **building a model**, starting from the available data, that provides some **knowledge** about the world: this knowledge must be **readable**, **interpretable** and **tangible**, with a practical use in various fields. Each IA algorithm on the following operational pillars:

- **exploration**;
- **modeling**,
- **evaluation**.

0.1.1 Exploration

In this first step, data are crucial, serving as the main focus of the algorithm to begin its analysis and the **hypothesis generation**. The data, stored in databases, represent the reality, and the effectiveness of the AI algorithm is based on the ability to **utilize data**, to inform strategic decision trough a process called **business intelligence**. Obviously, to have an effective algorithm, we require data that are logically consistent with themselves, and that are **representative** of the reality: to achieve that, a good strategy could be to gather data from different sources; this could be challenging, but it's a necessary step to have a good model. Lastly, it's crucial to understand how to **leverage data**, both for validation and the testing phases of the model.

0.1.2 Modeling

In this phase, the figure of the **knowledge engineer** appears: it has a good understanding of the data, the principles over them and their defining parameters. The aim of this phase is to **estimate** the parameters of the model, using statistics and machine learning techniques. It' also important to **define the model**: based on the goal of the analysis, different possibilities are available.

0.1.2.1 Descriptive models

These models are typically identified by **clustering** and **association rules mining** algorithms; they're used to **describe the organizational structure and the data distribution**, and the main goal is a **deeper understanding** of the data and its knowledge.

0.1.2.2 Predictive models

These models are usually implemented for **classification** and **regression** problems, and they're used to **predict** the future behavior of the data, based on the past one. This is made by exploiting **parameters** and **mechanisms** within the data, predicting how they will behave in the future.

0.1.2.3 Unsupervised learning

This is a type of learning where the algorithm is given a set of data and must find patterns and relationships within it, without any prior knowledge, such as labels; it's related to the descriptive models and it's used for **building a model**.

0.1.2.4 Supervised learning

Typical of predictive models, where the data are labeled, and it's a method used to **train the model**.

0.1.3 Evaluation

In this phase, we want want to **evaluate the validity** of the model. When we're dealing with predictive models, performances are assessed by appropriate **accuracy metrics**; if instead we're dealing with descriptive ones, we have to evaluate the **quality** of the model trough **model-specific metrics**. Part of this phase is also the **comparison between models**, made by knowledge engineers, trough statistical tests and analysis of the results. At the end of this step, we can both decide to **deploy** the model, or to refine it in order to obtain better results.

0.1.4 Remarks

- Achieving a good model is a **complex process**, that requires a meticulous approach to all the steps, such as leading to a multiple execution of the same step for multiple times;
- the knowledge of the application domain can aids during the modeling phase, adding some **domain-specific knowledge** to the model that could be not clear by simply analyzing the data;

- the process of **knowledge elicitation**, where the knowledge engineer has to **extract the knowledge** from the domain expert, is crucial to have a good model;

0.2 Data and transactions

Before going deep into the AI models, we have to understand what are the data, and define a common way to refer to them. *Data* is usually a general term that refers to the **raw facts**, but in fact we call **data set** the collection of **data objects**, which are the information that represent an **entity**.

> Example: in a database of students, the data set is the collection of all the students, and the data objects are the single students.

0.2.1 Data objects

Data objects are also called **samples**, **instances** or **records**, and they're defined by **atributes**: we can image a samples as a **row of a table**, and the attributes as the **columns**. The attributes are also called **features**, they're the **characteristics** of the data object and they can be expressed with different types.

0.2.2 Attribute types

The attributes can be of different types, such as:

- **nominal**;
- **binary**;
- **numeric**, and we can distinguish between **interval** and **ratio**.

0.2.2.1 Nominal attributes

Intuitively, we define a nominal attribute as a **category**, a **name** or a *name of a thing**:

> Example: possible hair colors are blonde, brown, black, red, etc.

Dealing with nominal attributes, we can define the **distance** between two attributes $d(i, j)$ as $d(i, j) = \frac{p-m}{p}$ where p is the number of attributes and m is the number of matching attributes.

> Example: given the variables *eye color* and *hair color* and two elements $i = $ {green, blonde} and $j = $ {gree, black}, we have $d(i, j) = \frac{2-1}{2} = 0.5$.

0.2.2.2 Binary attributes

These are a particular case of nominal attributes, where we have only two possible values, usually 0 and 1. If the possible outcomes are equally important, they're called **symmetric**; if instead one of the two outcomes is more important, they're called **asymmetric**, and we'll use the convention to assign the value 1 to the most important outcome.

0.2.2.3 Ordinal attributes

These are attributes that have a **natural order**, but with a **not defined distance** between them. They're used to represent **rankings** or **grades**.

> Example: *size = {small, medium, large}*.

Notice the **importance** of the order, and for this reason we can treat them as **interval-scaled** attributes, by mapping them into a set of **integer values**, and this could be done with this algorithm:

1. assign a number to each value, starting from 1;
2. convert the values into a number between 0 and 1 using this formula: $v = \frac{x_i - 1}{x_M - 1}$, where x_i is the value of the attribute and x_M is the maximum value.

In this way, we can compute the **distance** using the same methods of the interval-scaled attributes.

0.2.2.4 Interval-scaled attributes

They are some sort of **quantity**, measured in a scale of equal-sized units. Values have an order, but they lacks on the definition of a **zero point**.

> Example: *temperature* measured in Celsius, where the 0 doesn't mean the absence of temperature.

0.2.2.5 Ratio-scaled attributes

They're similar to the interval-scaled attributes, but they have a **true zero point** (usually **naturally defined**) and this allows us to compute the **ratio** between two values.

> Example: *weight* measured in kilograms, where the 0 means the absence of weight.

0.2.3 Distance of numeric attributes

A popular measurement for the distance between two numeric attributes is the **Minkowski distance**, defined as $d(i,j) = \sqrt[h]{\sum_{k=1}^{n} |x_{ik} - x_{jk}|^h}$. When $h = 1$, we have the **Manhattan distance**, when $h = 2$ we have the **Euclidean distance**.

0.3 Working with models

When operating with models, we have to **extract** the knowledge from the data; an example is the **data mining** process, in which we have to **extract patterns** and knowledge from massive data sets. In general, this process can be summarized as follows:

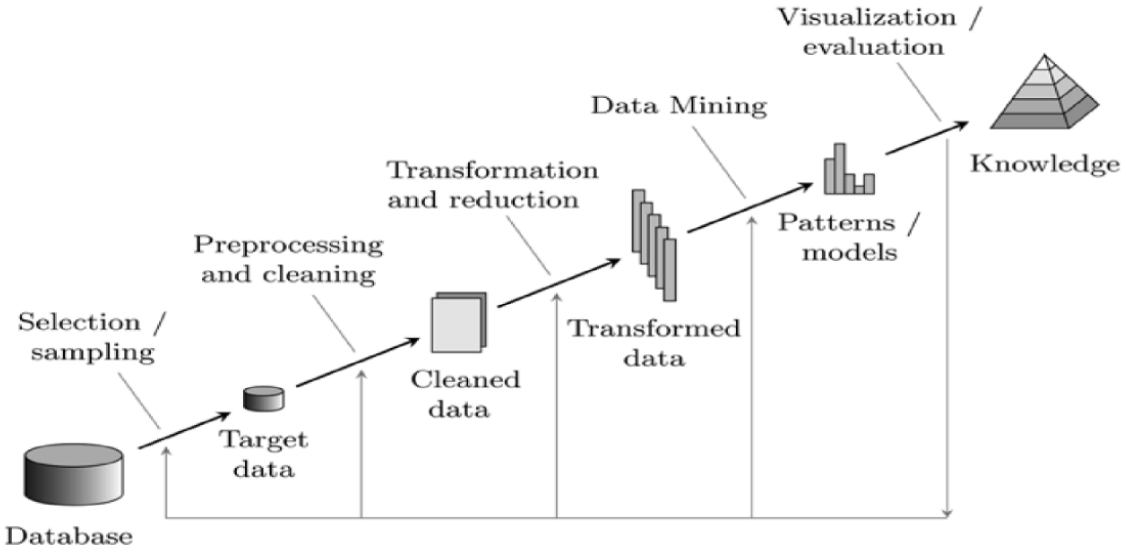


Figure 1: The knowledge extraction process

0.3.1 Training and generalization

We start knowing that **training data contain the knowledge** that we want to extract: any AI algorithm is dependent on these data, and the aim is to create a model that **mirror the data** as close as possible, both for predictive and descriptive models. Now appears clear that the **quality of the data** is crucial in order to made the extraction process effective. When we build a system, we must include a

training phase, where the data are used to **estimate the parameters** of the model: the effectiveness of this phase is evaluated by the **capacity of the model to generalize** the knowledge, that is,classify correctly new data that are not part of the training set.

0.3.2 Data sampling

Given a set of data, not all the records are used to create the model, and this for two main reasons:

- for certain datasets, there are too much data available, and this could lead to very long training times;
- part of the data have to be used in the evaluation phase, to test the model.

A sampling strategy is used to select the data that will be used in the training phase, considering the fact that our model should have a good **generalization capacity**.

0.3.3 Overfitting

In statistics, the **overfitting** problem arises when the model has **to many parameters** relative to the amount of data, leading to a model that is **too complex**: we should avoid this situation, because **simpler models have a better generalization capacity**. The overfitting problem is usually solved by **reducing the number of parameters** of the model, or by **increasing the amount of data**.

0.3.4 Using the model

Once the model is created, it's ready to be used, following its purpose.

0.3.4.1 Usage of predictive models

Predictive model can be used, where the functions are like **boxes** with different **opacity** (black, which is a neural network, grey, which is a rule-based system, or white), that based on their structure and complexity can produce outputs from the given input. The output of these models are obtained by mechanisms, called **inference engines**, that use the parameters obtained in the training.

0.3.4.2 Usage of descriptive models

These models use their parameters to **describe** the characteristics of the data, such as **centroid** or **clusters**, to represent similar data objects; we can use these models to categorize new data objects,

assigning them to the most similar cluster. The accuracy of that classification, when data aren't labeled, is evaluated by the **domain expert**.

0.3.5 Training and testing

Only a portion of the data (that have to be **labeled** in order to create a predictive model), known as **training set**, is used to train the model, while the remaining part, the **testing set**, is used to evaluate the model. The testing set is used to evaluate the **generalization capacity** of the model, and it's crucial to have a good model. Labeled data allow us to evaluate the model, computing values such as **average error** or **accuracy**.

Dealing with classification models, we instead use **misclassification rate**, while for **regression models** we use the **error metrics**.

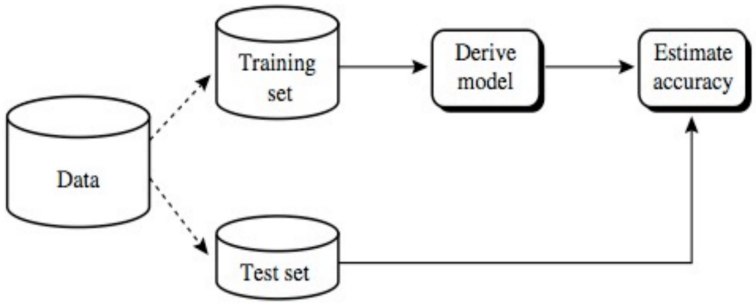


Figure 2: Model evaluation

The training and test set have to be carefully, in order to ensure randomness and to avoid **bias** towards a particular class. In general:

- we must assure the **independence** of the training and test set;
- the ratio between sets is unbalanced, with the training set that is usually larger than the test set.

0.4 Useful techniques

0.4.1 K-fold cross-validation

This is one the most robust, and also used, approach used to **evaluate a model**. Remember the fact that this is only an evaluating procedure: it doesn't gave any clue about how to improve the model!.

The technique is employed to **reduce the model dependence** on data for both identification and evaluation.

Suppose to have a dataset, splittable in N instancies, the dataset is divided in K random partitions, also called **folds**. The model is then trained and evaluated K times, using for each iteration $K-1$ folds for training and the remaining one for testing: this results in having K different models, each one evaluated against a different test set, to assess the model's generalization capacity. The output of the procedure is K different values of **error**, or **accuracy**, corresponding to the K different models: the average of these values gives the **cross-validation error**.

Some general consideration about the standard deviation can be made: if the **standard deviation** of the error is high, this means that the model is **sensitive** to the data used for training; on the other hand, if the **standard deviation** is low, this means that the model appears to be **insensitive** to the data used for training.

It's important to remember that **we cannot compare results obtained with different evaluation techniques**: the **cross-validation error** is only a measure of the model's generalization capacity, and it's not a measure of the model's quality. Lastly, remember that the **cross-validation error** isn't suitable in every situation, and it's not always the best choice.

0.4.1.1 Example of K-fold cross-validation

The following figure shows an example of a 5-fold cross-validation, where the dataset is divided into 4 folds:

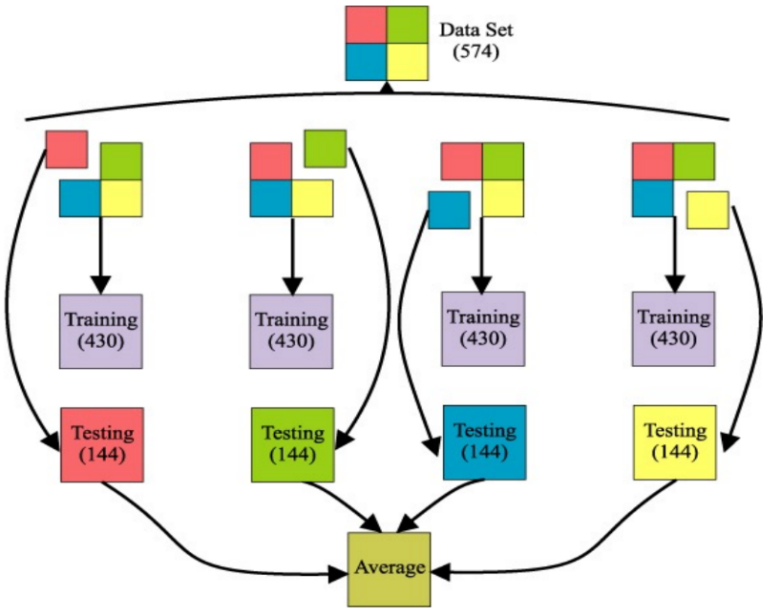


Figure 3: K-fold cross-validation

Every color represents a different fold, and we can clearly see the creation of 4 different models, where each of them is created using 3 different folds for training and the remaining one for testing.

In output, we have 4 different statistics, that are used to evaluate the model's generalization capacity.

0.4.2 Stratified cross-validation and leave-one-out

Stratified CV is an extension of the standard cross-validation, and it's often applied when we're dealing with classification problems.

In this technique, the subsets are partitioned in a way such that the **initial distribution of instancies** of every class is **preserved** in every fold. In case where the partitions K are equal to the number of instancies N (the number of available instancies), the strategy is to **leave one instance out**.

Then, $N - 1$ instancies are iteratively used to train the model, and the generalization capacity is evaluated for each of them. In the end, **average error** is computed, considering the N results of the test set (which is the single instance left out).

0.4.3 Bagging

This technique is used to **reduce the overtraining**: we train a set of T models, such that they are of different types but aiming to solve the same problem. Each of them is trained on a **unique training set**, drawn from the total data available, using the **bootstrap sampling**. The latter let, for the same instance, to appears multiple times in a single training set, while other instances could not appear at all.

For each model n_i, the number of training samples N_i is such that $N_i \leq N$, where N is the total number of instances available. After the training phase of all the T models, we can combine the outcomes to classify new instances:

- each model predicts the class of the new instance;
- the final class will be the one that appears most frequently, using the principle of **majority voting**.

0.4.4 Boosting

Boosting is in fact an **ensemble technique**, which have the aim to **create a strong model** from a set of weak models. The idea is to build a model using **the entire training set**, and then creating a **second model** that attempts to **correct the errors** of the first one. Models can be created and added sequentially, and new models focus on the instances that were **misclassified** by the previous ones.

This technique wants to give more importance to the instances that are **hard to classify**; it also differs from the bagging technique because the models aren't trained in parallel (which results in a independent training), but they're trained **sequentially**, where the new model is trained based on the performance of the previous one.

The final model is made by taking the weighted vote, or average, of the models created during the boosting process, where the weights are assigned based on the individual performance of the models, having the best models a higher weight.

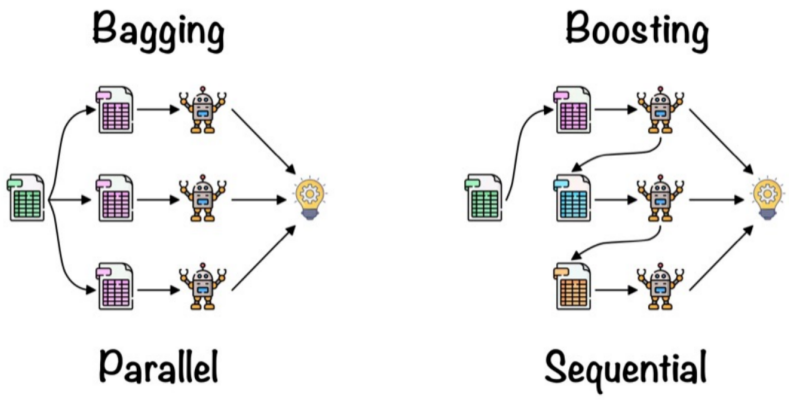


Figure 4: Visual comparison between bagging and boosting

0.5 Essential Statistical Concepts

In order to deal correctly with data, it is important to understand some basic statistical and analysis concepts. In this section, we will cover some fundamental concepts that will help you to understand the data exploration process.

0.5.1 Dispersion of data

Dispersion is a measure of how much the data points in a dataset differ from the mean. We'll use the k**-th percentile** to measure the dispersion of data that are numerically sorted. We say that *value* x_i *has the property that* k *percent of the data points are less than or equal to* x_i. From the previous we obtain that the **median** is the 50-th percentile, and we also define **quartiles** Q_1 and Q_3 as the 25-th and 75-th percentiles, respectively. The **interquartile range (IQR)** is defined as $Q_3 - Q_1$.

0.5.2 Box plot

A box plot is a graphical representation of the dispersion of data. It is composed of a box that represents the interquartile range, and two whiskers that represent the range of the data. The box plot also shows the median as a line inside the box, as we can see in the following figure.

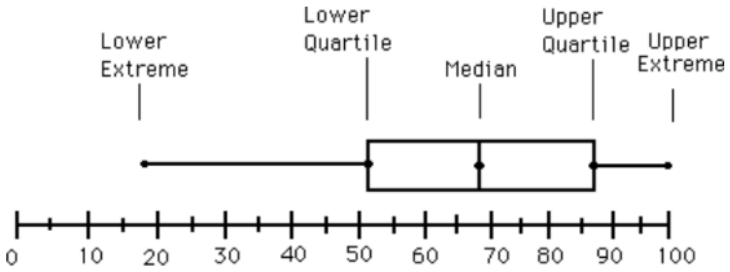


Figure 5: Box plot

0.5.3 Histogram analysis

A histogram is a graphical representation of the distribution of data. It is composed of bars that represent the frequency of data points in a given range, where the bars are called **bins**. The main purpose of a histogram is to show the distribution of data, and it is useful to identify patterns in the data. An example of a histogram is shown in the following figure.

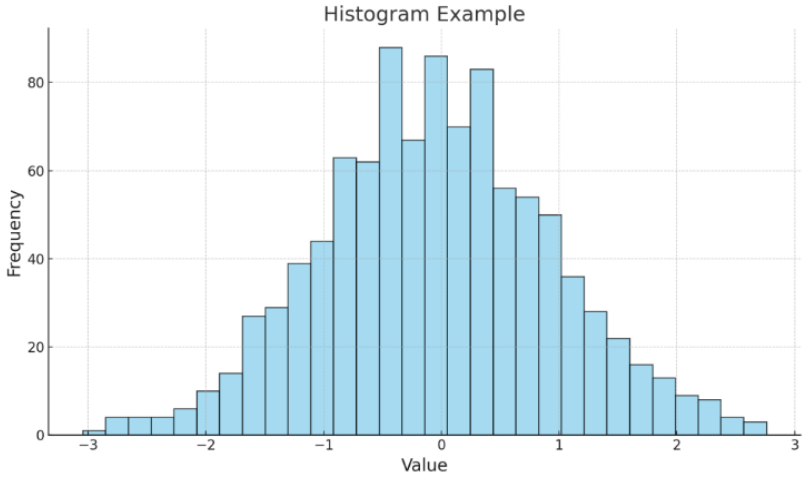


Figure 6: Histogram

0.5.4 Scatter plot

A scatter plot is a graphical representation of the relationship between two variables. It is composed of points that represent the values of the two variables, where the x-axis represents one variable and

the y-axis represents the other. The main purpose of a scatter plot is to show the relationship between the two variables, and it is useful to identify patterns in the data. An example of a scatter plot is shown in the following figure.

Figure 7: Scatter plot

0.5.5 X^2 (Chi-squared) test

The χ^2 test is a statistical test that is used to determine if two categorical variable, that are independent by hypothesis, A and B are somehow related in a given population. The **correlation coefficient**, also called **Pearson's correlation coefficient**, is a measure of the strength and direction of the linear relationship between two variables. The correlation coefficient ranges from -1 to 1, where -1 indicates a perfect negative linear relationship, 0 indicates no linear relationship, and 1 indicates a perfect positive linear relationship, and it's calculated as $r = \frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2 \sum_{i=1}^{n}(y_i-\bar{y})^2}}$.

1 Data exploration and preprocessing - Data mining process

The data mining process is a systematic approach to extract knowledge from data. It is composed of several steps that are executed in a sequence, which are shown in the following figure.

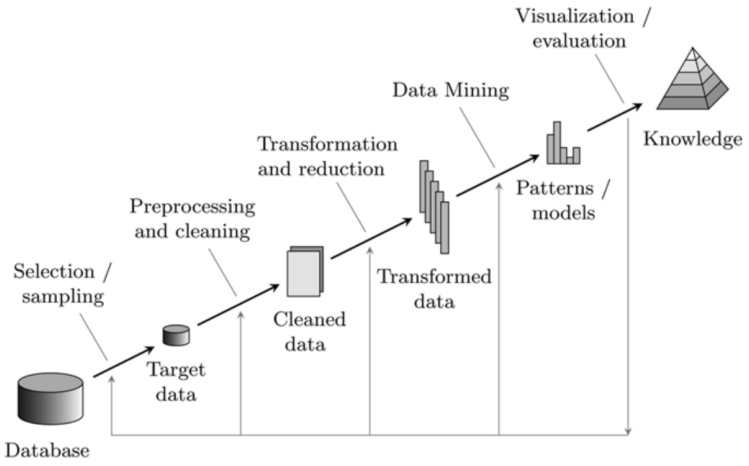


Figure 1.1: Data mining process

1.1 Data cleaning

Data that are extracted from the real world are **dirty**. Different classes of *dirtiness* exist, and they differ in the way they affect the data, and how they can be detected and corrected.

1.1.1 Incomplete data

Those are data that lack one or more attribute values: this might be due to several reasons, such as the data collection process, equipment failures, or human errors. In this case, missing data **may need to be inferred**:

- **Ignore the tuple**: this is usually done when class label is missing, but it's not an effective method when the percentage of missing values varies from attribute to attribute;
- **Fill in the missing value manually**: this is usually done when the percentage of missing values is small. Infeasible when the number of missing values is large;
- **automatic filling in of missing values**: this can be done using:
  - a **global constant**, such as "unknown" or even a new class;
  - the **attribute mean** (or median, or mode);
  - the **attribute mean** for all samples belonging to the **same class**;
  - the **most probable value** (e.g., using a decision tree);

1.1.2 Noisy data

We define the noise as *random error or variance in a measured variable*. This can be due to several reasons, such as data collection errors, data transmission errors, or data entry errors. We can deal with noisy data considering the source of the data that are usually affected by noise, and the nature of the noise. Typical data affected by noise are those from ambient intelligence, sensor networks, and data streams: here the true signal amplitude (the y-value) change **rather smoothly**, compared to the x-value. We can operate a process called **smoothing** to remove the noise from the data: data points of a signal are modified so that individual points that are higher than the adjacent points are reduced, and those that are lower are increased, naturally preserving the shape of the signal, while reducing the noise and being naturally smoothed.

> Example: the simplest smoothing algorithm is the **moving average**. We can use the **rectangular sliding-average smooth**, that simply replace the point i with the mean of the m points around it, where m is called **smooth width**. The formula for a 3-point rectangular sliding-average smooth is $y_i = \frac{1}{3}(x_{i-1} + x_i + x_{i+1})$.

1.2 Data discrepancy detection

Data discrepancy detection is the process of identifying and correcting discrepancies in the data. Different methods can be used to detect discrepancies, such as:

- checking the **metadata** of the data;
- check the **field overload**, typically results when developers squeeze new attribute definitions into unused portions of existing fields;
- check the **uniqueness rule**: each value of a certain attribute must be different from all the others;

- check the **consecutive rule**: there cannot be missing values between the lowest and the highest value of an attribute;
- check the **null rule**: specifies the conditions under which an attribute value can be null;
- use commercial tools for both **data scrubbing** and **data auditing**.

1.3 Data redundancy

Redundancy may appears when an integration of multiple databases is performed:

- an attribute, or an object, may have different names in different databases, also known as **object identification problem**;
- an attribute can be a **derived attribute**, that is, it can be computed from other attributes;

Redundant attributes can be also detected trough **correlation analysis**; in general, extra care must be taken when dealing during a data integration process, to reduce or entirely remove redundancy.

1.4 Data reduction

Data reduction strategies are used to get a reduced representation of the data set, while maintaining the same analytical power. This could be done by several reason, such as no enough data storage, or to reduce the time needed to perform the analysis. Two are the main strategies to reduce data: **dimensionality reduction** and **numerosity reduction**.

1.4.1 Dimensionality reduction

We start defining the dimensionality as the *number of attributes in the data set*: adding dimensions to data, they become increasingly **sparse**, and this lead to the **curse of dimensionality**. This is a problem that arises when the data set has a large number of dimensions, and it is difficult to analyze and visualize the data: when dimensions increase, analysis such as density, critical in clustering and outlier detection, become less powerful, and this because the combinations of subspaces grow exponentially with the number of dimensions.

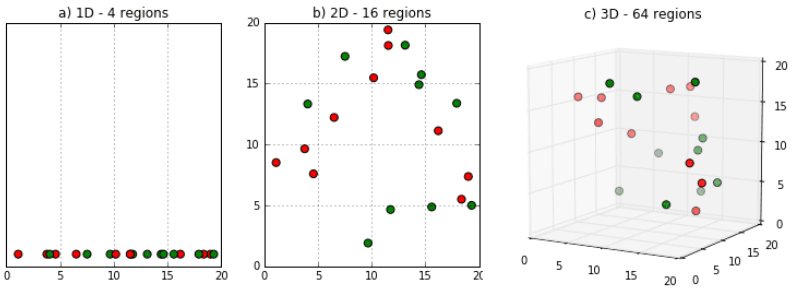


Figure 1.2: Visualization od the *curse of dimensionality*

Understood the problem, we can now define the **dimensionality reduction** as the process of reducing the number of dimensions in the data set. Note that the process also helps to **reduce the noise** in the data, and **remove redundant information**. The main techniques to reduce the dimensionality are divided in two main classes: the supervised ones, such as **PCA** or **Wavelet Transform**, and the unsupervised ones, that are in matter of fact kind of optimization problems, such as **feature selection** or **feature extraction**.

1.4.1.1 Principal Component Analysis (PCA)

The aim of this process is to project relevant attributes in a different space, with a *hopefully* reduced space than the original one. The projection should capture the largest amount of variation in data, and this is done by finding the **eigenvectors** of the **covariance matrix** of the data. Using this technique we have to deal with the **loss of the feature meaning**, that is explained in the further example.

> Example: loss of feature meaning. Having a dataset containing data about the weather, such as temperature, humidity, and wind speed, we can apply PCA to reduce the dimensionality of the data. Reducing the dataset dimensionality, we're going to lose some features, that will be replaced by a **linear combination** of the original features. This means that the new features will be a mix of the original ones, and they will not have a clear meaning.

1.4.1.2 Attribute and feature selection

This selection involves a search trough all possible combinations of attributes, in order to find which subset of attributes is the most relevant for the analysis, leading in fact to an optimization problem. The main used algorithms are:

- **evaluator algorithms**: they evaluate the goodness of a subset of attributes using a **quality function**;

- **search algorithms**: they search for the best subset of attributes using a **search strategy**, exploiting heuristics to reduce the search space.

1.4.1.3 Metrics for feature importance

We know that features aren't independent when we're using them to predict a result; however, we can use some metrics to understand which features are more important than others. The most used metrics are the **correlation**, the **information gain**, and the **Gini index**, that show how much data entropy exists between a given feature and the result.

Dealing with **multiple feature evaluation**, we use the **mRMR** approach: *maximal Relevance, Minimal Redundancy*. This approach is based on a filter feature measurement criterion, which computes **redundancy** between features in the subset, and **correlation** between features, and class based on the **mutual information**, in order to estimate the capability of making a good prediction for a given group of features.

1.4.1.4 Filter and wrapper methods

These are common optimization methods used to select the best subset of features.

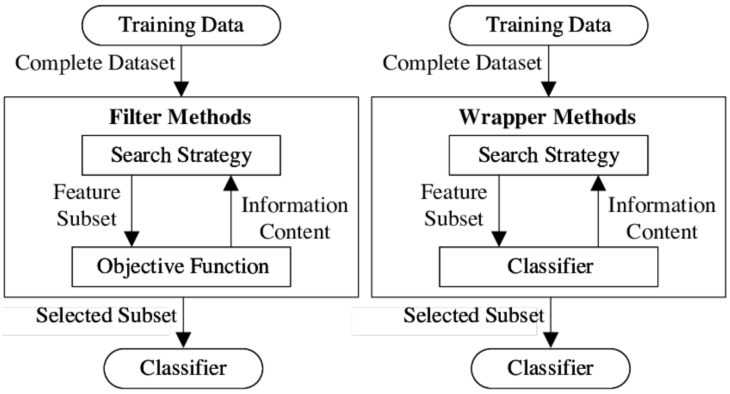


Figure 1.3: Filter and wrapper methods

The **search strategy** is common on both methods, and it's based on heuristics: it identifies a subset which goes as input in different modules, based on the method used. Using the **filter method**, the subset is evaluated using a **objective function**, that returns to the search module the goodness of the subset, and other possibly useful statistics. The **wrapper method** instead uses a **predictive model** to evaluate the subset, and this model is trained on the subset, and then tested on a validation set.

Take care of the model used in the wrapper method: we're using a classifier to obtain parameters for another classifier! The one used during this evaluation phase should be very simple, using few (and possibly different) parameters, compared to the one used in the final model.

In both cases, we can stop the search when the **quality function**, or the **predictive model**, reaches a certain given stop condition.

1.4.1.5 Ranking method

This is the fastest method to select the best subset of features, but also the one with the worst results. We can see the phases of the ranking method in the following figure.

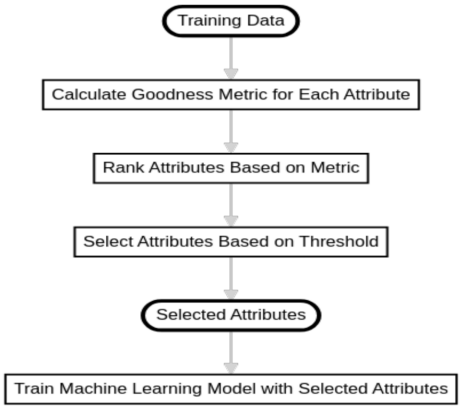


Figure 1.4: Ranking method

Examples of threshold can be, for instance, the **number of features** to select, or a minimum **quality function** value.

1.4.2 Numerosity reduction

The aim of this process is to reduce the number of data instances, while maintaining the same analytical power. The first operation we can make is the **sampling**: we can select a subset of the data, and use it for the analysis; this is typically done when dealing with skewed data. Another methods are available: they're called **mining algorithms**, and they should be potentially **sub-linear** in the size of the data set. The key idea to have in mind is choose a representative subset of the data: operating a random selection could lead to a non-representative subset, and this could lead to a wrong analysis. To achieve a good results, different sampling methods can be used:

- **random sampling**: each data instance has the same probability to be selected;

- **sampling without replacement**: each data instance can be selected only once;
- **sampling with replacement**: each data instance can be selected multiple times;
- **stratified sampling**: the data set is divided into strata, and then a random sample is selected from each stratum.

The latter is particularly useful when dealing with skewed data, because it ensure that even the smallest stratum is represented in the sample.

1.5 Advices for attribute selection

The most important thing to understand is that **we never want to touch the training set**. Suppose to have a dataset, and a certain reduction is being applied to it. We consider the training set as a *part of the future*, because our model should never see the test set during the training phase. If we included the test set during the analysis for the attribute selection, we're somehow **including the test set inside the model**, and this is a **bad practice**. We're, in fact, introducing a bias in the model, using *future data* that are impossible to obtain in the real world. Given that rationale, we'll refer at the following figure, that shows the correct way to perform the attribute selection, as the **golden rule**.

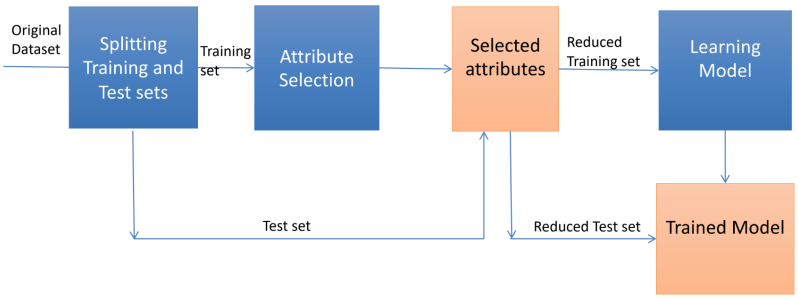


Figure 1.5: Golden rule for attribute selection

1.6 Heuristic search in Attribute Selection

1.6.1 Decision tree induction

The decision tree induction is an automatic way to perform a search; to explain the concept, we can consider the following example.

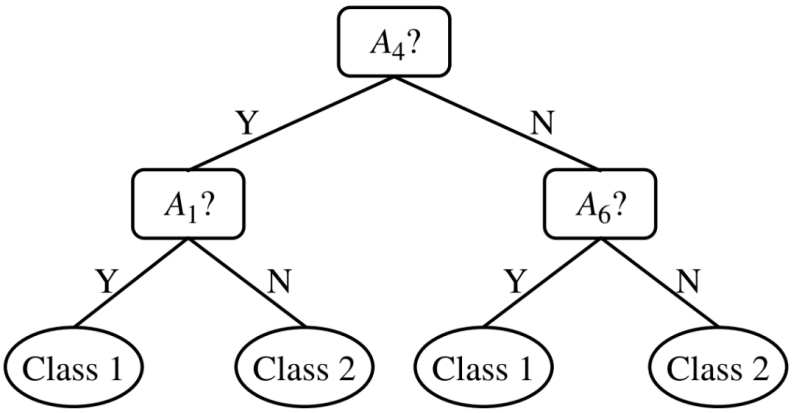


Figure 1.6: Decision tree induction

Take an initial set of attributes $\{A_1, A_2, A_3, A_4, A_5, A_6\}$, and compute metrics on these attributes (e.g., the **information gain**, usually chosen based on the problem we're dealing with), and we choose an attribute based on that metric. Then we start to build our tree from the root: it will have a condition based on the chosen attribute, and the branches will develop themselves based on other attributes. The aim of the technique is to find the **splitting point** as the point such that we split the attribute set in two parts, and we chose the one that represents better the data. The process is repeated until we reach a stopping condition, that could be the **maximum depth** of the tree, or the **minimum number of samples** in a leaf. Following the example, the reduced attribute set will be $\{A_1, A_4, A_5\}$.

1.6.2 Backward elimination

This is a **greedy** algorithm, that starts with the full set of attributes, and then removes one attribute at a time, based on a certain criterion such as the **information gain**. The process is repeated until a stopping condition is reached, such as the **minimum number of attributes**.

1.6.3 Forward selection

This is another **greedy** algorithm, that starts with an empty set of attributes, and then adds one attribute at a time, based on a certain criterion. The pseudo-code for the algorithm is the following:

1. initialize: set $F = \{f_i | i = 1, \dots, N\}$ the initial set of the features, and $S = \emptyset$;
2. calculate, for each attribute, the importance metric $M(f_i, Y)$ with respect to the input Y;
3. select the first feature f_i that maximizes $M(f_i, Y)$, and set $F = F \setminus \{f_i\}$, and $S = S \cup \{f_i\}$;

4. **greedy selection**: repeat the process until a stopping condition is reached, such as the **minimum number of attributes**.
    1. calculate the importance metric $M(f_i \cup S, Y)$ for each attribute $f_i \in F$;
    2. select the next feature f_i that maximizes $M(f_i \cup S, Y)$, and set $F = F \setminus \{f_i\}$, and $S = S \cup \{f_i\}$.
5. output the set S.

1.7 Data transformation

Data transformation is the process of **changing the format, the structure or the values of the data**. These techniques are usually applied to ensure **more efficient data analysis** and better **knowledge extraction**.

1.7.1 Normalization

The aim of this process is to scale the data in a certain range, usually $[0, 1]$, or $[-1, 1]$. This is done to avoid that some attributes have a **higher weight** in the analysis, compared to others. The most used normalization techniques are:

- **min-max normalization**: the data are scaled in the range $[\text{new-min}_A, \text{new-max}_A]$, using the formula $x' = \frac{v - \text{min}_A}{\text{max}_A - \text{min}_A} \cdot (\text{new-max}_A - \text{new-min}_A) + \text{new-min}_A$;
- **z-score normalization**: the data are scaled using the formula $x' = \frac{v - \mu_A}{\sigma_A}$, where μ_A is the mean of the attribute A, and σ_A is the standard deviation of the attribute A.

2 Introduction to Artificial Neural Networks

2.1 Introduction

2.1.1 What is a Neural Network?

An **Artificial Neural Network (ANN)** is an abstract simulation of a human nervous system, that contains a collection of neurons connected with each other trough connections called **axons**. The aim of a neural network is to simulate neurons and connections, resembling the human brain.

2.1.2 Neuron model

Many neurons have a structure called **dendrites** that receive signals from other neurons trough **synapses**. The neuron processes the signals and sends the output signal through the **axon**, which is basically an electrical impulse: it can be **excitatory** or **inhibitory**, and in case of excitatory signals, the neuron will generate informational messages to other neurons.

It's estimated that around 100 billion neurons are in the human brain, and each neuron can be connected to thousands of other neurons: their switching time is significantly slower than the switching time of a computer, but the connectivity is much higher, up to hundreds times more.

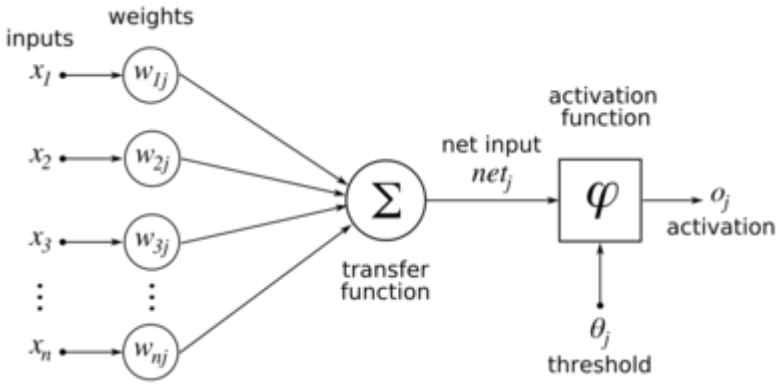
2.2 Artificial Neural Networks

2.2.1 Structure of an ANN

An NNN is composed by a set of **neurons** and **weighted connections** between them, plus a series of thresholds or **activation levels**. During the design of an ANN, we have to take into account the **number and type of neurons**, the **morphology of the network**, the **weights** and the **training examples**, in terms of network inputs and outputs.

2.2.2 Artificial Neuron

The scheme of an artificial neuron is shown in the following image:



{width=400px}

Note that the artificial neuron has a set of **inputs** $x_1, x_2, \dots, x_n$ and a set of **weights** $w_1, w_2, \dots, w_n$, which are real number such that, if positive, they are excitatory, and if negative, they are inhibitory; these weights are related to the corresponding inputs. The neuron computes the **weighted sum** of the inputs and weights as a linear combination $a = \sum_{i=1}^{n} w_i \cdot x_i$, that goes into an **activation function** $\phi(a)$. The output of the neuron can be a real number, both non-limited or limited to a certain range, or even a discrete value. Lastly, there also is a binary threshold function such that, if the output is above a certain threshold θ_i, the neuron will fire. In fact, the latter is a generalization of a **step function** for a given threshold. Typically, the threshold is also subtracted from the weighted sum, in order to have the function $y = f(\sum_{i=1}^{n} w_i \cdot x_i - \theta_i) = f(\sum_{i=0}^{n} w_i \cdot x_i)$ **centered in zero**. If a threshold assumes a negative value, is called **bias**, and it's considered as a weight connected to a unit that always outputs 1 (note that in the previous equation we added the index 0 to the sum, which is the bias).

2.2.3 Activation functions

In the following image, we can see some examples of activation functions:

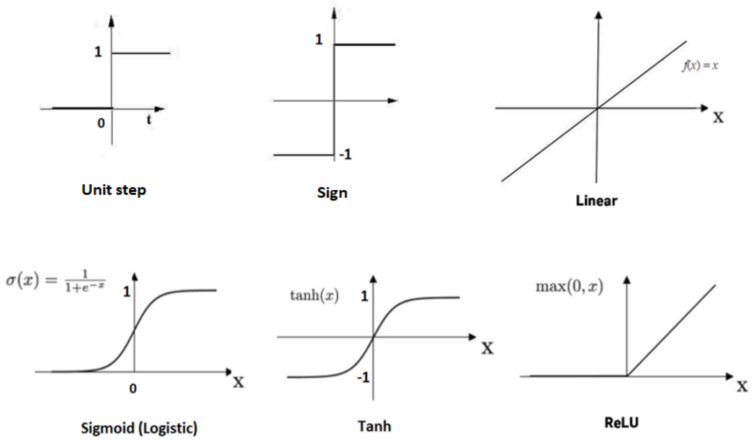


Figure 2.1: Activation functions

2.2.4 Network topology

The topology depends on **how neurons are connected which each other**: if they're arranged in a **hierarchical** way, such that the neurons are connected only with **adjacent layers**, we have a **feedforward network**. If the neurons are connected with **non-adjacent layers**, we have a **recurrent network**. We can see an example of these two types of networks in the following image:

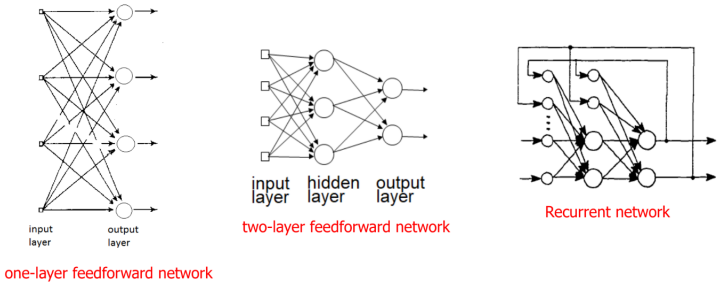


Figure 2.2: Feedforward and Recurrent Networks

Note how the firsts neurons are connected only with the second layer in the feedforward network, while in the recurrent network they this rule is not respected; in particular, in this case, the network is implementing a sort of *memory*, with a structure that resembles a **flip-flop**.

2.3 Network training

When we want to use a neural network to deal with classification and regression problems, we resort to a **supervised learning** process, which modifies the weights of the network by applying a set of **labeled training examples**: each sample consists of an input and the corresponding target output. During the training phase, the network is fed with the input, and the output is compared with the target output, then the weights are adjusted in order to **minimize the error**. The training process is repeated until there are no significant changes in the weights.

2.3.1 Delta rule

The **delta rule** is a simple algorithm that modifies the weights of the network in order to minimize the error. The rule is based on the **gradient descent** method, which is a method to find a local minimum of a function. The delta rule says that the adjustment to be made is $\Delta w_i = \eta \cdot \delta \cdot x_i$, where η is the **learning rate**, and δ is defined as $\delta = t - y$, t is the target output, y is the actual output, and x_i is the input. Note that this is a **recursive rule**, and the formula can be rewritten as $w_i(n+1) = w_i(n) + \Delta w_i(n)$.

We define the **error for the k-th sample** as $E_k = \frac{1}{2}\sum_{i=1}^{n}(t_i - y_i)^2$, where t_i is the target output and y_i is the actual output. The **total error** is defined as $E = \sum_{k=1}^{m} E_k$, where m is the number of samples.

2.3.1.1 Main idea

TO understand the main idea behind the delta rule, we have to give a mathematical interpretation of the error function, that is the fact that it lies in the same space of the weights. This is crucial because, after the start where the weights are randomly assigned, the algorithm adjusts them in a direction **towards a lower overall error**: in other words, the weights are modified in the direction of the **steep descent** of the error surface, and we'll prove the convergence of the algorithm in the next section.

2.3.1.2 Proof of convergence

For the proof, we start rewriting the delta rule as $\Delta w_{ij} = -G = -\frac{\partial E}{\partial w_{ij}}$, and we can visually interpret this in the following image:

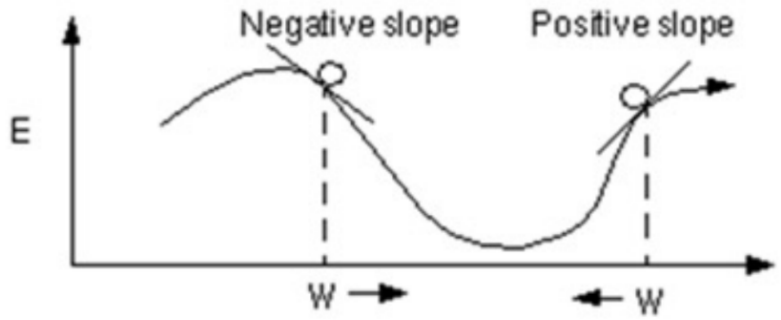


Figure 2.3: Visualization of the delta rule

Iterating the rule, we move *downhill* in E, until we reach a minimum $G = 0$.

Now we write the actual output of the network as $y_i = \sum_i x_i w_{ij}$, so as a linear combinations of the inputs and weights. We can now compute the partial derivative, applying the *chain rule*, and we obtain $\frac{\partial E}{\partial w_{ij}} = \frac{\partial E}{\partial y_i} \cdot \frac{\partial y_i}{\partial w_{ij}}$. Then, we write $-\delta = \frac{\partial E}{\partial y_i}$, and we can compute the partial derivative of the output with respect to the weights as $\frac{\partial y_i}{\partial w_{ij}} = x_i$. So, we can rewrite the delta rule, adding the **learning rate** η, as $\Delta w_{ij} = \eta \cdot \delta \cdot x_i$, and we can prove that the algorithm converges to a minimum.

The definition of δ came out by calculating the partial derivative of the error with respect to the output, considering a single instance: $\frac{\partial E}{\partial y_i} = \frac{\partial}{\partial y_i} \frac{1}{2}(t_i - y_i)^2 = -(t_i - y_i) = -\delta$.

2.3.1.3 The learning rate

The learning rate η is a crucial parameter in the delta rule, because it determines the **step size** of the algorithm. If the learning rate is too high, the algorithm may oscillate around the minimum, and if it's too low, the algorithm may take too long to converge. In real cases, its value is determined experimentally, and it can vary overtime, getting smaller as the training progresses.

2.3.2 Momentum

In real-world problems, it can happens that the error surface is not smooth, and the algorithm may get stuck in a local minimum. To overcome this issue, we can introduce a **momentum** m term in the delta rule, such that the new formula is $\Delta w_{ij}(n+1) = \eta \cdot \delta \cdot x_i + m \cdot \Delta w_{ij}(n)$. The momentum term is a fraction of the previous weight update, and it's domain is $]0, 1[$, and the actual value is determined by trial and error.

2.3.3 Learning algorithms

We divide the learning algorithms in three categories:

- **online learning**, where the weights are updated after each sample;
- **batch learning** (or *offline*), where the gradient is computed for all the samples, and the weights are updated at the end of the process;
- **mini-batch learning**, where the gradient is computed for a subset of the samples, and the weights are updated at the end of the process.

The last two methods provide both a more precise estimation of the gradient vector, and possibly a faster computation, given the fact that these processes can be parallelized; on the other hand, the online learning is more flexible, because it doesn't need a fixed training set, requires less memory and, lastly, it has the ability to escape from local minima under certain conditions.

2.4 Perceptron

A perceptron is a **single neuro**n with an hard limiter as activation function, such as sign or step function , and it's used to solve **binary classification** problems. It can be trained to correctly classify training examples from classes C_1 abd C_2 by assigning inputs to C_1 if the output is positive, and to C_2 if the output is negative.

The classification is made by using a **straight line** in the input space, that represents the **decision boundary** between the two classes, which are the regions that are separated by the line.

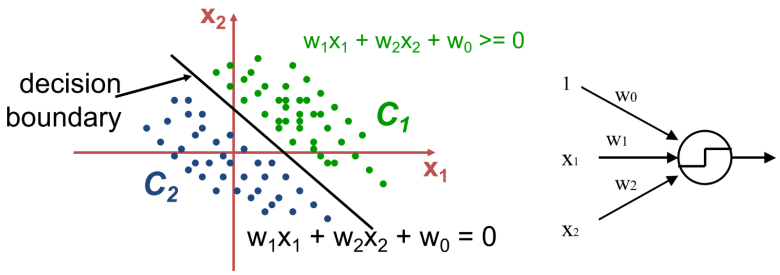


Figure 2.4: Perceptron

2.4.1 Perceptron learning algorithm

A pseudo-code of the perceptron learning algorithm is the following:

1. Initialize the weights to 0 or small random values;
2. choose an appropriate learning rate η;
3. until the stopping criterion is met (such as the number of iterations or the fact that weights don't change significantly):

    1. for each training sample (x_i, t_i):

        1. compute the output $y_i = f(w, x)$;
        2. if $y_i = t_i$, continue;
        3. if $y_i \neq t_i$, update the weights as $w = w + \eta \cdot (t_i - y_i) \cdot x_i$, where t_i is the target output.

2.4.2 Decision boundary

We can make a mathematical consideration about the points that lie in the decision boundary: they all have the same inner product with the weight vector. From this, we can say that they have the **same projection** on the weight vector, so they must lie on a line that is **orthogonal** to the weight vector. Look at these two images:

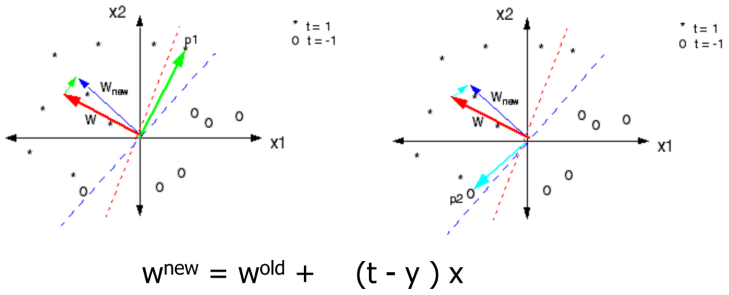


Figure 2.5: Decision boundary

The red dashed line is the decision boundary, so note that both points p_1 and p_2 are incorrectly classified. What happens if we choose one of the as training sample to update the weights?

- choosing p_1, it has target $t = 1$, so weights are slightly updated in the direction of p_1;
- choosing p_2, it has target $t = -1$, so weights are slightly updated in the direction of p_2.

Note that in both cases, the new boundary is better than the previous one, and this because **the perceptron learning algorithm is a linear algorithm is guaranteed to converge in a finite number of steps, if the problem us linearly separable**.

2.4.3 XOR problem with perceptron

The XOR problem is a problem that can't be solved by a single perceptron, because the classes are not linearly separable. In fact, the XOR problem is a **non-linear** problem, and it can be solved by adding a **hidden layer** to the network, or by using a specific activation function.

If we want to resolve the problem by using two separating lines, we'll need **two perceptrons** to represents the two lines, and a third neuron to combine the outputs of the first two neurons. We'll obviously need a **threshold** for each neuron, and the output of the third neuron will be the final output of the network.

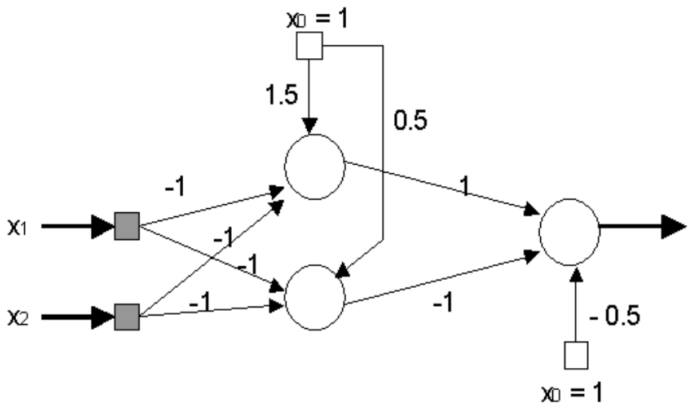


Figure 2.6: Network with hidden layer

The effect of the first layer on the weights is such that now the problem that goes into the second layer is linearly separable, and the second layer will be able to solve the problem.

2.4.4 Hidden layers

In general, we observe that adding a hidden layer to the network, the network itself became able to model regions with a number of sides at most equal to the number of neurons in the hidden layer. In fact, the hidden layer is able to model **non-linear** regions, and the output layer is able to combine the results of the hidden layer to solve the problem. If we instead add a second hidden layer, the network will be able to model regions that are arbitrarily complex.

2.4.5 Improving the fitting

Observe the following image:

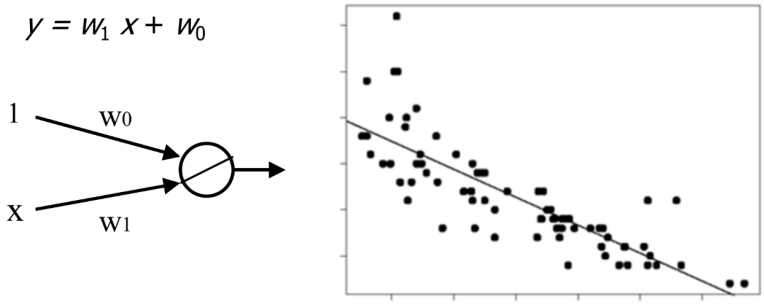


Figure 2.7: An example of linear fitting

We can clearly see that data are not evenly distribuited around the straight line, so we can achieve a better approximation by using a **hidden layer**, consisting in a single neuron with **tanh** as activation function. The result is shown in the following image:

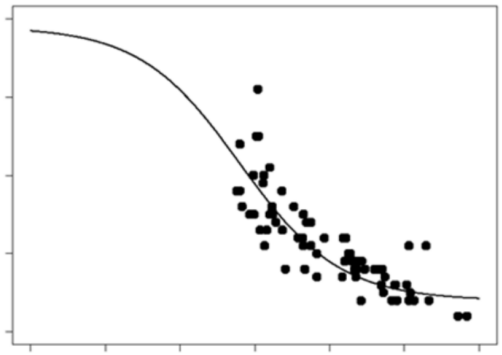


Figure 2.8: An example of non-linear fitting

This approach can be used to approximate even more complex functions, simply adding more neurons to the hidden layer. However, we need to consider the negative aspect of this approach: too **many neurons** in a single hidden layer, or simply too **many hidden layers**, can have a **negative impact on the network performance**. The best practice is to start with a network with a reasonable minimum number of hidden neurons, and then increase the number of neurons only if the network doesn't perform well. Remember that a network with a hidden layer that contains enough neurons can approximate any continuous function.