Artificial Intelligence:
Machine Learning and Pattern Recognition

Year: 2017/2018

Afternotes Artificial Intelligence

24th October 2019

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1 Information Theory

Information theory studies the quantification, storage, and communication of information. It was originally proposed by Claude E. Shannon in 1948 and it includes the study of transmission, processing, extraction, and utilization of information. One of the first representation of a communication system, given by Shannon, can be seen in the following image:

Figure 1: Shannon representation communication system.

This representation is composed by some components as:

- **Two agents** that, in general, are called *sender* and *receiver*. Normally, sender is the agent that enters a particular message in the channel, instead receiver is the entity that receives message. These two entities are not necessary different.
- **Channel** is the means that allows the transmission of messages between two entities. It is possible that a message is written in a certain language but it travels in the channel with another understandable one (usually binary language).

Usually sender and receiver use a different language respect to the channel, and so it is necessary to expand the original model introducing some **translator** entities as following:

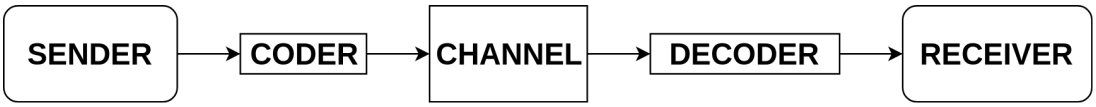


Figure 2: Extensive Shannon representation.

Coder and **Encoder** are instruments that allow us to translate a language to another one. They should provide:

- **efficiency**, senders sends a message as soon as possible, with a compression provided by the coder.
- **reliability**, receiver is sure about the message received from sender.

Despite that, in real life this model is not completely true and reliability is not easy to reach. The final model, therefore, is provided in this way:

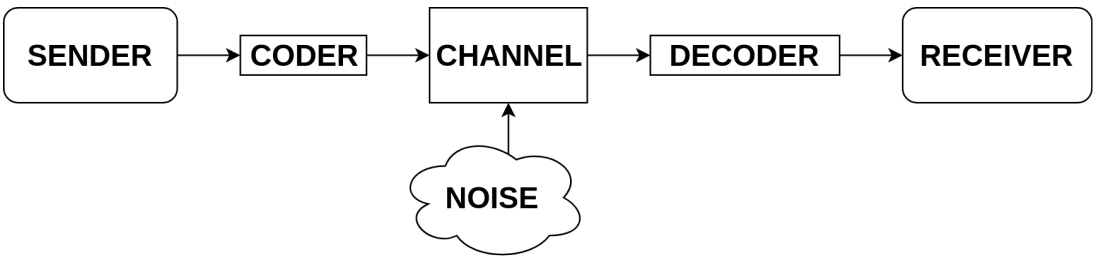


Figure 3: Shannon representation information theory.

Noise is a known component of the channel that creates interference inside it and it can affect the communication. Several techniques are used in order to guarantee the correctness of transmissions.

Figure 4: Noise effect on a communication system.

As said in the previous lines, because of the presence of noise inside the channel, *coder* and *decoder* have the task to ensure efficiency and reliability of messages but, ensuring these two properties, another problem is introduced: **redundancy**.
In order to have efficiency it is necessary to remove redundancy from the message, using compression, on the other hand, if we want to improve the reliability it is necessary that receiver will be able to make inference about the original message, this possibility is given only by adding redundancy.
As we can see there is a kind of contrast for the two requirements and so it is necessary to find a good trade-off. A possible solution, for instance, is to send more bits (better if odd) to codify a single symbol, like `"0"` is encoded in `"000"`. In this way decoder will have greater possibility to correct the received message, this will increase reliability but also redundancy.

1.1 Information

We can consider 3 different levels of information:

1. **Syntactical level** deals only with symbols and it does not consider the semantic (meaning) of the message. In this level we approach the information not from a syntactical point of view (set of rules), but from a statistical point of view. For example, if we have the letter `"h"`, which is now the probability that the next letter will be an `"e"`, an `"i"` or a `"q"`?

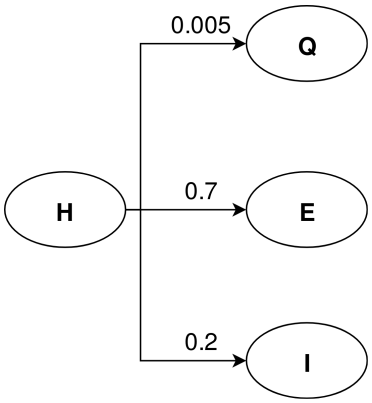


Figure 5: Probability Analysis.

2. **Semantic level** deals with the meaning of the sended message, it tries to understand the semantic. It is very complex.
3. **Pragmatic level** deals with the intention of the speaker. It's something more complex than a semantic level.

Information theory works at syntactical level.

1.2 Quantify Information

Quantify information refers to the necessity of finding a measure to quantify the **amount of information** that travels inside the channel. However, firstly, it is necessary to give a definition of information. One of the purposes of Shannon consists to tie the notion of $information$ with the notion of "$surprise$" and the probability of an event.
Suppose we have an event E and associated with this event we have its probability $P(E)$. Let us consider two extreme situations:

- $P(E) = 1$, we won't be surprised of the fact that this particular event happens. In this case the amount of information given by event E is 0.
- $P(E) = 0$, it is impossible this fact happens. However we cannot consider the probability exactly equal to 0, but more or less equal to $10^{-\cdot\cdot}$. We must left the possibility that in a rare case this fact could happen. In this case the amount of information given by the event E is ∞.

1.2.1 Shannon function

After the premises made till now, we can consider information as a probability function, that mathematically speaking, we can write as $I(E)$. Where:

- E is the event.
- $I(..)$ is the amount of information provided by the event.

The function $I(E) = f(P(E))$ from a graphical point of view could be seen as below.

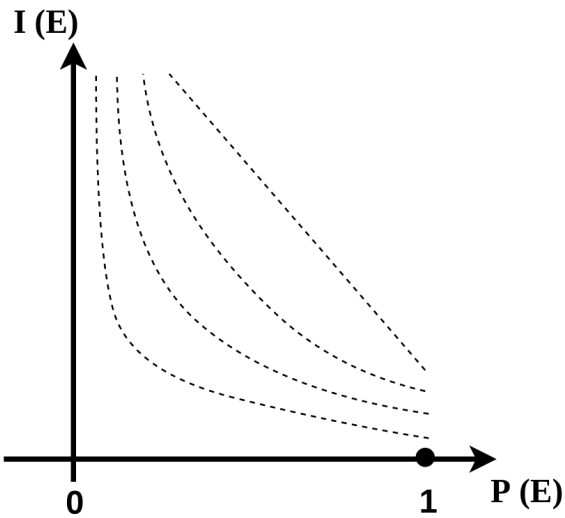


Figure 6: Possible configurations of function $I(E)$.

Notice that writing $I(E) = f(P(E))$ we are saying that the information is a function of probability. The unique information that we have from the previously definition is that:

$$\text{if } P(E) = 1 \text{ then } I(E) = 0 \qquad \longrightarrow \qquad I(E) = 0 \text{ iff } P(E) = 1$$

in the other extreme case we can say that:

$$\lim_{P(E)\to 0} I(E) = +\infty$$

We don't know however which is the behavior of the $I(E)$ in the middle but, surely, it must be positive and monotonically decreasing. Shannon provided that there is a **unique function** that satisfy these assumptions and respect its definition:

$$I(E) = -\log(P(E)) = \log\left(\frac{1}{P(E)}\right)$$

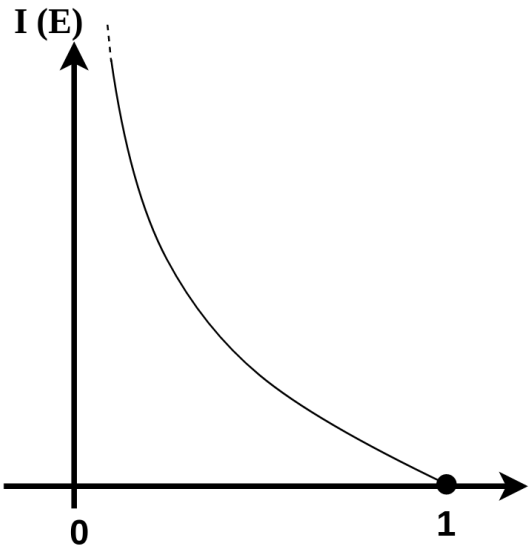


Figure 7: Graphical representation of $I(E)$ $(-\log(P(E)))$.

1.2.2 Definition of Entropy

Source is a random variable or, in a more precise way, it can be defined as a **stochastic process**. We know the source only if we know the probability distribution of its symbols. We define X as a random variable valid in the following set:

$$\mathcal{X} = \{x_1, x_2, \cdots, x_n\} \text{ with probabilities } \{P(x_1), P(x_2), \cdots, P(x_n)\}$$

Given a source it can be interesting to evaluate the amount of information provided, and so we introduce the concept of **entropy**.
The **entropy** $H(x)$ of a random variable represents an average of the amount of information provided by the source $\mathcal{X}$, or a measure of uncertainty, and it is defined as:

$$H(x) = \sum_{x\in\mathcal{X}} P(x)I(x) = \sum_{x\in\mathcal{X}} p(x) \underbrace{\log\left(\frac{1}{p(x)}\right)}_{I(x)} = -\sum_{x\in\mathcal{X}} p(x)\log(p(x))$$

As said before, we can see that entropy is nothing else than the expected value of X. The base of logarithm define the measure of information:

$\log_2$	bit
$\log_e$	nat
$\log_{10}$	Hartley

Table 1: Measure of Entropy.

A problem that rises immediately dealing with logarithmic functions is the handling of $p(x) = 0$, indeed, in this case we will have the problem with $\log(0)$ and at least two possible solutions can be adopted. The first one consists in removing the symbol from the source, since $p(x) = 0$ this operation doesn't affect the communication. The other solution, instead, is to adopt an internal convention: $\lim_{x \to 0} x \log x = 0 \qquad 0 \cdot \log(0) = 0$.

Example 1.1. Thinking at the flip of a coin, we can say that the random variable associated with this event follows the following distribution:

$$\text{FAIR COIN} = \begin{cases} 0 & p(\text{"Tail"}) = p(0) = 0.5 \\ 1 & p(\text{"Head"}) = p(1) = 0.5 \end{cases}$$

Thanks to the function $H(x)$, it is possible to compute the entropy of this random variable, which means how much information we can get. Entropy can be defined as a measure of uncertainty.

$$H(x) = \frac{1}{2}\underbrace{\log 2}_{1} + \frac{1}{2}\underbrace{\log 2}_{1} = 1 \text{ bit}$$

This is a case in which we have a fair coin but if we had an unfair coin (unbalanced), the *entropy* function will change. As in the previous case the set of possible outcomes will be similar to the previous case, $\mathcal{X} = \{x_1, x_2\}$ and it will follow this distribution:

$$\text{UNFAIR COIN} = \begin{cases} x_1 & p(\text{"Tail"}) = p(x_1) = p \\ x_2 & p(\text{"Head"}) = p(x_2) = 1 - p \end{cases}$$

Now, the *entropy* function $H(x)$ will be equal to:

$$H(x) = -p \cdot \log p - (1 - p) \cdot \log(1 - p) = H(p)$$

A general graphical representation of the entropy function is:

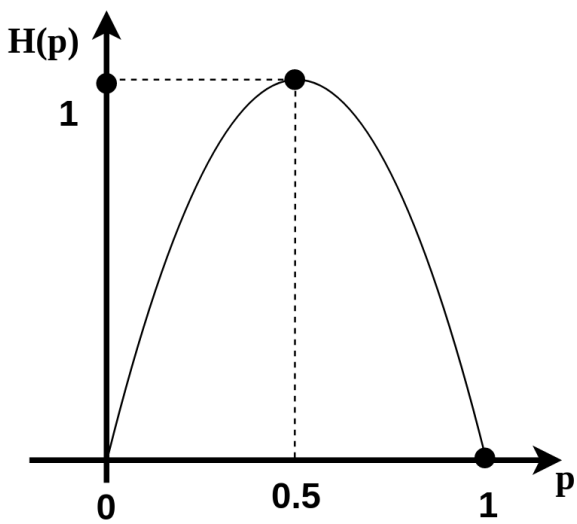


Figure 8: $H(p)$ in relation to p.

As it is possible to see, we have a symmetric and concave function, in which the maximum is reached in the point of maximum uncertainty $p = 0.5$. This is reasonable since there is more surprise for the receiver. Imagine instead that $p(x) = 0.8$, the receiver is likely to expect tail, since it has a large probability, and so the surprise tend to 0.

1.2.3 Entropy properties

In the previous section we have introduced the concept of entropy and its relation to uncertainty, measure of uncertainty of a source. We now want to discuss its properties:

$$X \text{ source} \qquad \mathcal{X} = \{x_1, x_2, \cdots, x_n\} \qquad P(x_1), P(x_2), \cdots, P(x_n)$$
$$P_r(X = x_i) = p(x_i) \qquad n = |\mathcal{X}|$$

At a first glance, we can notice that function $H(x)$ is limited inside the following interval:

$$0 \leq H(x) \leq \log(n)$$

First of all, it is obviously to ask us which is the meaning of $H(x)$ when it reaches the extreme values of 0 or $\log(n)$.

$\mathbf{H(x) = 0}$:
this limit is reached when there's no uncertainty and from a statistically point of view, we've got a probability distribution with only one point with value equal to 1 and the others have $p(x) = 0$. Formally we can say:

$$H(x) = 0 \iff \exists x \in \mathcal{X} \text{ such that } p(x) = 1$$

$\mathbf{H(x)} = \log(\mathbf{n})$:
this limit is reached when the probability distribution is uniform and in this way, the maximum level of uncertainty is provided. Every solution has probability $\frac{1}{n}$. Geometrically speaking, the point in which function reaches the maximum value ($\log(n)$) is the **baricentre** of the probability space.

$$H(X) = -\sum_{x \in \mathcal{X}} p(x) \log(p(x)) = -\sum_{x \in \mathcal{X}} \frac{1}{n} \log\left(\frac{1}{n}\right) = \log n$$

According to the possible number of outcomes, different probability space can be created inside a space $\mathbb{R}^n$.

$$\triangle = \{p \in \mathbb{R}^n \mid p_i \geq 0 \quad \forall i = 1, \cdots n \text{ and } \sum_i p_i = 1\}$$

When we have only two outcomes, **n=2**. This is the space of all possible probability distributions:

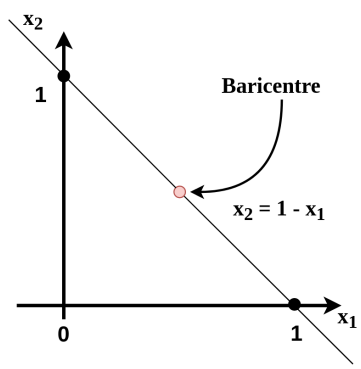


Figure 9: Probability space with n=2.

In case we will have three outcomes, this will generate a space in which each vertex is the point with the minimum information value. It will have the following structure:

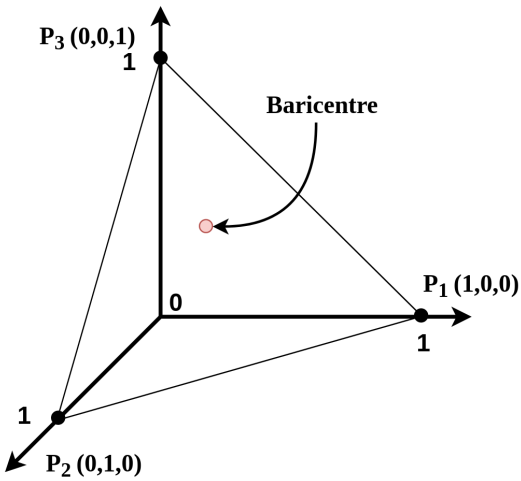


Figure 10: Probability space with n=3.

1.2.4 Entropy of two random variables

If we talk about the entropy of two random variables, we have so, X and Y that are defined in the following set of solutions:

$$\mathcal{X} = \{x_1, \cdots, x_n\} \quad \text{and} \quad \mathcal{Y} = \{y_1, \cdots, y_n\}$$

$p(x)$ and $p(y)$ represent the two marginal probability distributions for source X and Y.
Given two random variables X and Y, it is possible to consider:

- **Marginal entropy:** $H(X)$ and $H(Y)$.
- **Joint entropy:** $H(X, Y)$ provides the amount of information given by joint of the two distributions. It is defined as:

$$H(X,Y) = -\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x,y) \cdot \log p(x,y) \quad \text{where} \quad p(x,y) = p(x) \cdot p(y|x) = p(y) \cdot p(x|y)$$

- **Conditional entropy:** $H(y|x)$ provides the amount of information given by y fixed a value of x. In the particular case in which x has a precise constant value, the conditional entropy is:

$$H(Y|X = x) = -\sum_{y} p(y|x) \cdot \log(p(y|x))$$

  On the average, the information that we obtain from X is:

$$\begin{aligned} H(Y|X) &= \sum_{x} p(x) \cdot H(Y|X = x) \\ &= -\sum_{x} \sum_{y} p(x) \cdot p(y|x) \cdot \log p(y|x) \\ &= -\sum_{x} \sum_{y} p(x,y) \cdot \log p(y|x) \end{aligned}$$

Regarding the average conditional entropy is possible to notice that values can vary in a precise range, in fact:

$$0 \leq H(X|Y) \leq H(X)$$

$\mathbf{H(X|Y) = 0}$ when X is a deterministic function of Y such that:

$$\forall y \in \mathcal{Y} \qquad \exists!\ x \in \mathcal{X} \text{ such that } p(x|y) = 1$$

Choosing the value of y, we know the result of x.

$\mathbf{H(X|Y) = H(X)}$ when X and Y are two independent random variables.

$$p(x, y) = p(x) \cdot p(y)$$

- **Chain rule:** it defines a relationship between joint entropy, marginal entropy and condition entropy. It is defined as:

  $$H(X, Y) = H(X) + H(Y|X) = H(Y) + H(X|Y)$$

  This chain rule is derived from the fact that:

  $$p(x, y) = p(x) \cdot p(y|x) = p(y) \cdot p(x|y)$$

  and applying a $\log(\cdots)$ products become sums.

1.2.5 Entropy of n random variables

What is possible to say instead if we deal with n random variables? Considering n different sources $X_1, X_2, \cdots, X_n$, the entropy function is so defined:

$$\begin{aligned} H(X_1, X_2, \cdots, X_n) &= -\sum_{x_1 \in \mathcal{X}_1} \sum_{x_2 \in \mathcal{X}_2} \cdots \sum_{x_n \in \mathcal{X}_n} p(x_1, \cdots, x_n) \cdot \log p(x_1, \cdots, x_n) \\ &= H(X_1) + H(X_2|X_1) + H(X_3|X_1, X_2) + \cdots + H(X_n|X_1, \cdots, X_{n-1}) \\ &= \sum_{i=1}^{n} H(x_i|x_1, \cdots, x_{i-1}) \end{aligned}$$

1.3 Mutual information

The mutual information of two random variables is a measure of the **mutual dependence** between the two variables. More specifically, it quantifies the "amount of information" (in units such as shannons, commonly called bits) obtained about one random variable through observing the other random variable.

In a space $\mathbb{R}^n$ it is possible to have two points $\bar{x}$ and $\bar{y}$ where:

$$\bar{x} = (x_1, \cdots, x_n) \in \mathbb{R}^n \qquad \text{and} \qquad \bar{y} = (y_1, \cdots, y_n) \in \mathbb{R}^n$$

Euclidean distance The distance between this two points can be computed using the **euclidean distance**:

$$E(\bar{x}, \bar{y}) = ||\bar{y} - \bar{x}||^2 = \sum_{i=1}^{n} (x_i - y_i)^2$$

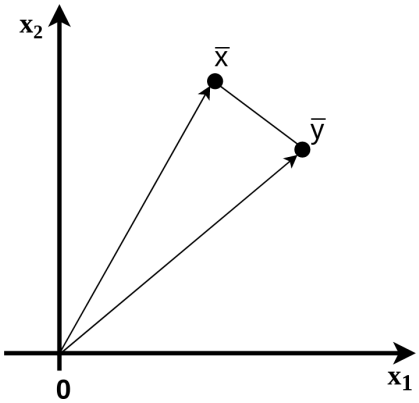


Figure 11: Euclidean distance.

This value represents the length of the segment that connects the point $\bar{x}$ to $\bar{y}$. In relation to euclidean distance, four properties can be defined:

1. $E(\bar{x}, \bar{y}) \geq 0$
2. $E(\bar{x}, \bar{y}) = 0 \iff \bar{x} = \bar{y}$
3. $E(\bar{x}, \bar{y}) = E(\bar{y}, \bar{x})$
4. $E(\bar{x}, \bar{z}) \leq E(\bar{x}, \bar{y}) + E(\bar{y}, \bar{z})$ (Triangular inequality)

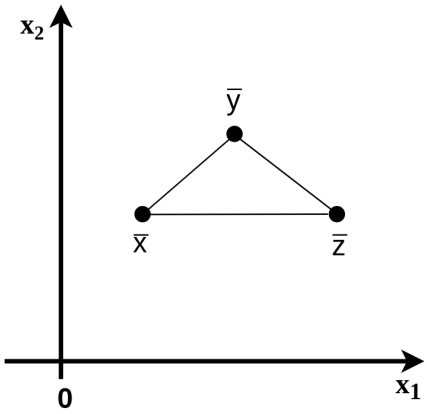


Figure 12: Triangular inequality property.

Only if these four properties are satisfied then we can consider any measure as a **metric**, so in this case Euclidean distance is a metric.

Kullback-Leibler divergence Kullback-Leibler defines a distance between probability distributions. If we have two points $\bar{p}$ and $\bar{q} \in \triangle$.

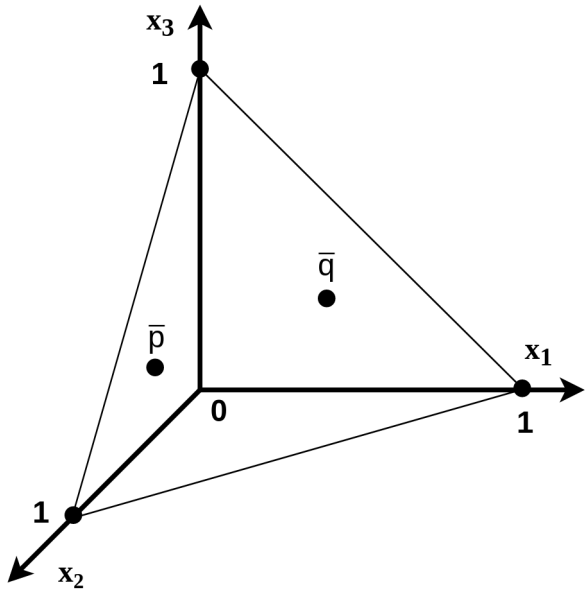


Figure 13: Point $\bar{p}$ and $\bar{q} \in \triangle$.

The **Kullback-Leibler divergence** between $\bar{p}$ and $\bar{q}$ is defined as:

$$D(\bar{p}||\bar{q}) = \sum_{i=1}^{n} p_i \cdot \log\left(\frac{p_i}{q_i}\right)$$

As in the euclidean distance case, *KLD* has properties like:

1. $D(\bar{p}||\bar{q}) \geq 0$
2. $D(\bar{p}||\bar{q}) = 0 \iff \bar{p} = \bar{q}$

On the other hand *KLD* doesn't hold other properties as:

1. $D(\bar{p}||\bar{q}) \neq D(\bar{q}||\bar{p})$ (KLD is not symmetric)
2. $D(\bar{p}||\bar{r}) \nleq D(\bar{p}||\bar{q}) + D(\bar{q}||\bar{r})$ (Triangular inequality doesn't always hold)

1.3.1 Compute Mutual Information

Through the computation of mutual information between X and Y, we can have access to different interpretations. One of them is surely understanding if two random variables are dependent or not.

$$\begin{aligned} I(x;y) &= D(p(x,y)||p(x)p(y)) \\ &= \sum_x \sum_y p(x,y) \cdot \log\left(\frac{p(x,y)}{p(x)p(y)}\right) \end{aligned}$$

As seen above, it is possible to compute the mutual information applying the concept of *Kullback-Leibler divergence*. Paying attention at the ending part of the computed formula we can understand an important property that is, the lower is $\log\left(\frac{p(x,y)}{p(x)p(y)}\right)$ and the more independent are the two random variables.

The mutual information of two random variables is 0 if and only if the two random variables are independent.
$D(p(x,y)||p(x)p(y)) = 0$ when x and y are independent $p(x,y) = p(x) \cdot p(y)$, meaning that:

$$\log \frac{p(x,y)}{p(x)p(y)} = \log 1 = 0$$

Mutual information is also useful when we want to measure how much information travels on the channel.

1.4 Channel

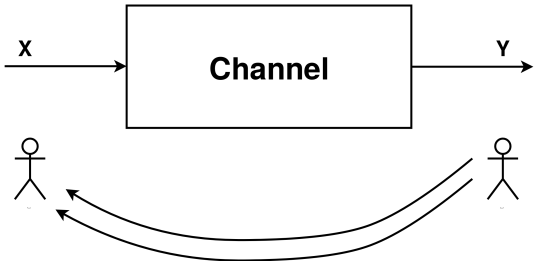


Figure 14: Channel model.

When we deal with the transmission of information, it is important to take into account two different moments: *before* transmission arrives to receiver and *after* transmission is arrived to receiver.

- **Before:** uncertainty of the receiver before to see the output from the channel. In this phase the value of information is $H(X)$.
- **After:** uncertainty of the receiver given the channel output Y. It is $H(X|Y)$, it could be 0 if we don't consider noise on the channel.

Computing the difference between $before$ and $after$ information it is possible to obtain the mutual information that travels in the channel.

$$I(X,Y) = H(X) - H(X|Y)$$

If $X \perp Y$ we have $H(X|Y) = H(X)$ so $I(X,Y) = 0$.

Theorem 1.2 (Before - After information)**.** *Taking into account the before and after information, it is possible to define the mutual information as:*

$$I(X,Y) = H(X) - H(X|Y) \qquad \textit{if we consider the role of the receiver}$$

or

$$I(X,Y) = H(Y) - H(Y|X) \qquad \textit{if we consider the role of the sender}$$

Theorem 1.3.

$$H(X) = I(X,X)$$

Theorem 1.4.

$$I(X,Y) = H(X) + H(Y) - H(X,Y)$$

We will see later further meanings of these values, especially we can say that:

- $H(X)$ is related to the **efficiency** of the information channel.
- $I(X,Y)$ is related to the **reliability** of the information channel.
- $I(X,Y) \geq 0$.
- $I(X,Y) = 0$ if and only if X and Y are independent.

Since $I(X,Y) \geq 0$ we have $H(X) - H(X|Y) \geq 0 \rightarrow H(X) \geq H(X|Y)$ with equality if and only if X and Y are independent.

1.5 Data compression - Source coding theorem

In the following subsection we will focus on the first part of the communication, that is related to sender and encoder entities. We want so introduce the notion of **source code**.

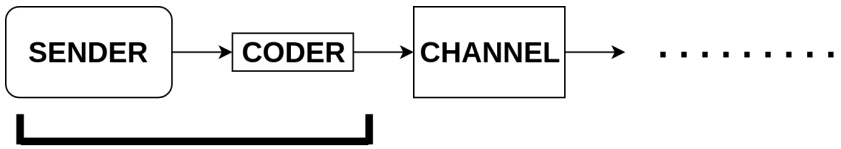


Figure 15: Souce coding theorem is focused on the first part of the channel.

Suppose we have a random variable (source) X and $\mathcal{X}$ is the range of all possible symbols.

$$\mathcal{X} = \{x_1, \cdots, x_n\} \qquad and \qquad p(x) = Pr\{X = x\}$$

We define $\mathcal{D}$ as the channel alphabet and we define a code such a function that executes the following transformation:

$$c : \mathcal{X} \rightarrow \mathcal{D}^*$$

Code is a map that maps strings from the source code to the channel code $\mathcal{D}$.

Example 1.5. Suppose you have the following data:

$$\mathcal{X} = \{a, b, c, d\} \qquad \mathcal{D} = \{0, 1\}$$

with the following probabilities:

$$p(a) = \frac{1}{2} \qquad p(b) = \frac{1}{4} \qquad p(c) = \frac{1}{8} \qquad p(d) = \frac{1}{8}$$

With this conditions it is possible to generate a pretty large number of codes, for example, we can generate two codes as $\mathcal{D}_1^*$ and $\mathcal{D}_2^*$ as we can see in the below table.

$\mathcal{X}$	$\mathcal{D}_1^*$	$\mathcal{D}_2^*$
a	0	111001
b	10	01
c	110	111
d	111	01000

Table 2: Coding example.

From the previous example it is possible to understand that not all codes can be defined as a good code but, there are some rules that can help us in order to define a good one:

- It must be as **short** as possible in order to ensure the *efficiency* of transmission.
- There must not be presence of codes that are prefixes of other ones. For example, in code $\mathcal{D}_2^*$, letter `"b"` is encoded into `"01"` and letter `"d"` into `"01000"`. As we can see, one encoding is **prefix** of the other one. This leads problems with *efficiency* because receiver must wait until the third bit in order to understand if sender has sent letter `"b"` or `"d"`.

It is also possible to have an efficient code that is useless, because receiver can't understand what is transmitted in the channel. An example is the following table in which **ambiguity** appears.

$\mathcal{X}$	$\mathcal{D}^*$
a	0
b	0
c	0
d	0

Table 3: Ambiguous code.

In a more general way we can say that a particular coding function must be **injective**.

1.5.1 Non-singular codes

Non-singular codes are codes in which the coding function is injective. Is it possible, in this case, to have again ambiguity?
An example of this can be seen below.

$\mathcal{X}$	$\mathcal{D}^*$
a	a
b	c
c	ad
d	abb
e	bad
f	deb
g	bbcde

Table 4: Example of ambiguous non-singular code.

A code like this can generate a message as `"abbcdebad"`, in which decoder can generate more than one decoded message. It is possible to generate for example:

$$\underbrace{\texttt{abb}}_{\texttt{d}}\ \underbrace{\texttt{c}}_{\texttt{b}}\ \underbrace{\texttt{deb}}_{\texttt{f}}\ \underbrace{\texttt{ad}}_{\texttt{c}}$$

or

$$\underbrace{\texttt{a}}_{\texttt{a}}\ \underbrace{\texttt{bbcde}}_{\texttt{g}}\ \underbrace{\texttt{bad}}_{\texttt{e}}$$

As we can see, even if we are in an optimal situation without noise, the receiver can't understand the message send (two configurations are possible).
We can define so, as **unique decodable codes**, all the codes in which receiver is always sure of the decomposition done.

1.5.2 Prefix code

With a **prefix code**, none code is prefix of other codes. Any prefix code is also a *uniquely decodable code*.

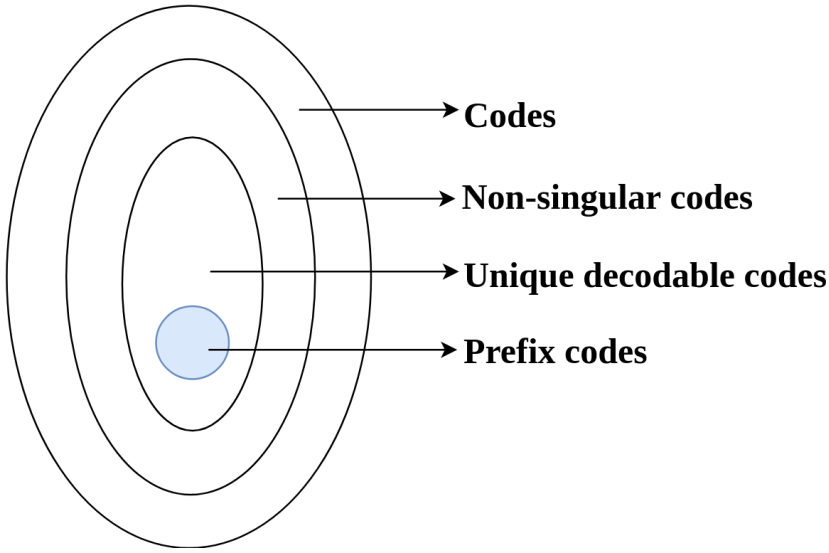


Figure 16: Codes classification.

As we can see also from the previous picture all the prefix codes are also unique decodable codes. An example of a non prefix code is so provided:

$\mathcal{X}$	$\mathcal{D}_1^*$	$\mathcal{D}_2^*$
a	0	111001
b	10	01
c	110	111
d	111	01000

Table 5: Non-prefix code.

We can see that there are two pairs of codewords that have the same prefix.

1.6 Quantify Efficiency

While we define a code, it is also useful to consider the efficiency given by it. If we consider a code like this:

$\mathcal{X}$	$\mathcal{D}_1^*$	$\mathcal{D}_2^*$
a	0	0
b	10	10001
c	110	1100110
d	111	1110010

Table 6: Non-efficient code.

We can see immediately that the codewords use too many bits to codify the original symbol of the source. So we could consider the length of codewords as a possible metric to quantify efficiency of a code, but we will find out in the next example that this is not a good metric.

Example 1.6. Consider the following example:

$$\mathcal{X} = \{a, b, c, d\} \qquad \mathcal{D} = \{0, 1\}$$

with the following probabilities:

$$p(a) = \frac{1}{2} \qquad p(b) = \frac{1}{4} \qquad p(c) = \frac{1}{8} \qquad p(d) = \frac{1}{8}$$

We can define two possible codes to convert symbols from $\mathcal{X}$ to $\mathcal{D}$.

$\mathcal{X}$	$\mathcal{D}_1^*$	$\mathcal{D}_2^*$
a	0	111
b	10	110
c	110	10
d	111	0

Table 7: Comparing codes.

The second code is the reversed version of the first one. If we consider only the length of the codewords we can say that in terms of efficiency they are equal, but this is not true. When we talk about efficiency it is necessary to consider also the probability distribution. In this case the symbol `a` is very likely to appears and the second code associates the largest codeword to it, instead symbol `d` is very unlikely and it is associated to the smallest one. The first code is more efficient since $p(a)$ is the greater probability, instead, the second code uses a lot of bit to codify it.
So we can define the *measure of efficiency of a code* with the following formula:

$$L(c) = \sum_{x \in \mathcal{X}} p(x) \cdot l(x)$$

where $l(x)$ is the length of the codeword associated to the symbol x.

Example 1.7. Considering the previous example we want to compute the efficiency of each code:

$$L(c_1) = \frac{1}{2} \cdot 1 + \frac{1}{4} \cdot 2 + \frac{1}{8} \cdot 3 + \frac{1}{8} \cdot 3 = \frac{7}{4} = 1.75$$

On average the codewords sent using the first code have length 1.75.

$$L(c_2) = \frac{1}{2} \cdot 3 + \frac{1}{4} \cdot 3 + \frac{1}{8} \cdot 2 + \frac{1}{8} \cdot 1 = \frac{21}{8} = 2.625$$

On average the codewords sended using the second code have length 2.625. This bring us to consider the first code as the more efficient one, since, considering the same symbols and probabilities, it spends less bits to codify them, improving in this way the speed of transmission.

Another interesting consideration is given by the relationship between efficiency of a code and the entropy given by the source.

Example 1.8. Considering the previous example we want to compute entropy, on base 2, of source X and compare it with the length of the code:

$$H(x) = \frac{1}{2} \cdot \log 2 + \frac{1}{4} \cdot \log 4 + \frac{1}{8} \cdot \log 8 + \frac{1}{8} \cdot \log 8 = \frac{7}{4} = 1.75$$

We can see that $H(x) = L(c_1)$. There is a theorem which affirms that entropy is a lower bound for $L(c)$, considering a **noise free channel**.

Theorem 1.9 (Relationship between $H(x)$ and $L(c)$)**.** *Let X be a random variable (source), with range $\mathcal{X}$ and probability distribution $p(x)$. Let $\mathcal{D}$ be the channel's alphabet, $c \cdot \mathcal{X} \to \mathcal{D}^*$ an uniquely decodable code for X and $D = |\mathcal{D}|$.*
Then, with the assumption of noise free channel:

$$L(c) \geq H_D(x)$$

where D indicate the base of the logarithm.
Moreover:

$$L(c) = H_D(x) \iff \forall x \in \mathcal{X} : \quad l(x) = -\log_D p(x) = \log_D \frac{1}{p(x)}$$

Example 1.10.

$$\mathcal{X} = \{a, b, c, d\} \qquad \mathcal{D} = \{0, 1\}$$

with the following probabilities:

$$p(a) = \frac{1}{2} \qquad p(b) = \frac{1}{4} \qquad p(c) = \frac{1}{8} \qquad p(d) = \frac{1}{8}$$

$$\begin{aligned} p(a) &= \frac{1}{2} \quad \log_2 2 = 1 \\ p(b) &= \frac{1}{4} \quad \log_2 4 = 2 \\ p(c) &= \frac{1}{8} \quad \log_2 8 = 3 \\ p(d) &= \frac{1}{8} \quad \log_2 8 = 3 \end{aligned}$$

When the probability distribution $p(x)$ has the property:

$$\log_D \frac{1}{p(x)} \in \mathbb{N} \setminus \{0\}$$

the probability distribution $p(x)$ is called **D-Adic**.

1.7 Fano-Shannon Coding

Fano-Shannon coding is a technique for constructing a prefix code based on a set of symbols and their probabilities.

$$\left\lceil \log_D \frac{1}{p(x)} \right\rceil = l(x)$$

If $\log_D \frac{1}{p(x)}$ is not an integer value, it is approximated to the upper integer value.

Example 1.11. Fano-Shannon Algorithm:

$$\mathcal{X} = \{1, 2, 3\} \qquad \mathcal{D} = \{0, 1\} \qquad |\mathcal{D}| = 2$$

$\mathcal{X}$	$p(x)$	$-\log_2 p(x)$	$l(x)$	c_{sf}	c^*
1	2/3	0.58	1	0	0
2	2/9	2.17	3	110	10
3	1/9	3.17	4	1111	11

Table 8: Comparing codes.

Where $l(x)$ is computed considering Fano-Shannon approximation. We can see that p(x) is not 2-Adic.

$$H(x) = 1.22$$

$$L(c_{sf}) = 1.78 \qquad L(c_{sf}) > H(x)$$

$$L(c_{sf}) = 1.33 \qquad L(c^*) > H(x)$$

Code c_{sf} is not optimal but it is a good approximation, the length of c^* is lower meaning that is more efficient.

1.8 Huffman Coding

Huffman coding is a greedy algorithm used to build/define the best code.

Example 1.12. Huffman coding with $\mathcal{X} = \{x_1, \dots, x_6\}$ and $p(x) = (0.4, 0.3, 0.1, 0.1, 0.06, 0.04)$.

$\mathcal{X}$	$p(x)$	c_5	$p(x)^1$	c_4	$p(x)^2$	c_3	$p(x)^3$	c_2	$p(x)^4$	c_1
$x1$	0.4	1	0.4	1	0.4	1	0.4	1	0.6	0
$x2$	0.3	0	0.3	00	0.3	00	*0.3	00	0.4	1
$x3$	0.1	011	*0.1	011	*0.2	010	*0.3	01		
$x4$	0.1	010	*0.1	0100	*0.1	011				
$x5$	*0.06	01010	0.1	0101						
$x6$	*0.04	01011								

Table 9: Comparing codes.

1.9 Channel

In the previous sections, we covered the topic of coding. However, two different definitions of codes can be indicated:

- **Lossless codes:** codes that don't lose any information from the initial source. It is possible to reconstruct completely the original message.
- **Lossy codes:** codes that lose information. After compression some information are lost (jpg, ...).

Related to coding, we have talk about **source coding** which is related to *efficiency* and **channel coding**, that is, instead, related to *reliability*. In the following lines, we will focus exactly on this last topic.

1.9.1 Definition of channel

A channel can be formally defined as:

$$\mathcal{C} = (\mathcal{X}, p(y|x), \mathcal{Y})$$

where:

- $\mathcal{X}$ is the input alphabet.
- $p(y|x)$ is the channel's probability distribution. It represents the probability that symbol x is translated into y. It is the most important component of the channel and it is defined as:

$$p(y|x) = Pr(Y = y|X = x)$$

- $\mathcal{Y}$ is the output alphabet.

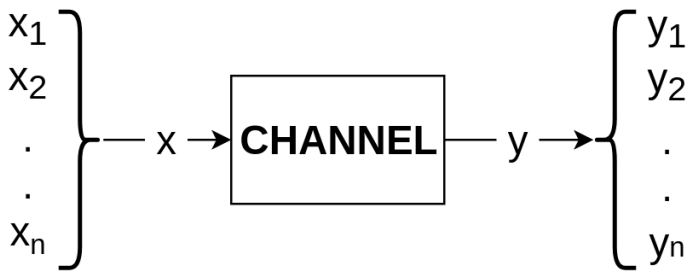


Figure 17: Channel definition.

1.9.2 Channel representation

In order to graphically represent and analyze a channel there are two possible ways, a **channel graph** or a **channel matrix**.

Channel graph. This kind of representation is defined according to the acronym **BSC**, that stands for **Binary Symmetric Channel**.
Binary means that both the input and the output alphabets are binary.

$$\mathcal{X} = \mathcal{Y} = \{0, 1\}$$

Instead *symmetric* means that the probability that an error occurs in the channel is the same for every possibles input message. Probability that an error occurs is the same both in the case input is 0 or 1.
With this properties, we generate a **bipartied graph** as:

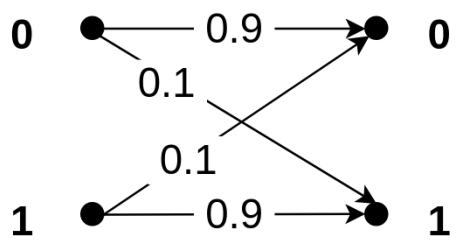


Figure 18: Channel graph representation.

In this representation we can see the probability that in 90% of the cases symbols 0 and 1 are translated respectively into 0 and 1, they represent the probability of a right transmission. With only 10% of probability the transmission is affected by noise and symbols 0 and 1 are translated into 1 and 0. On this representation if there is no arc from x_1 to y_1 we assume that $P(y_1|x_1) = 0$.

Channel matrix. Another possible representation of the channel is provided by a matrix usage. As it is possible to see, p is the probability that during transmission an error occurs.

$$\begin{array}{cc} & \begin{array}{cc} & \mathbf{Y} \\ & \begin{array}{cc} \mathbf{0} & \mathbf{1} \end{array} \end{array} \\ \mathbf{X} \begin{array}{c} \mathbf{0} \\ \mathbf{1} \end{array} & \begin{bmatrix} \mathbf{1 - p} & \mathbf{p} \\ \mathbf{p} & \mathbf{1 - p} \end{bmatrix} \end{array}$$

Figure 19: Channel matrix representation.

1.9.3 n-th extension of the channel

Before moving to a more general topic, we need to define the **n-th extension** of $\mathcal{C}$ which is an additional definition of the channel. It can be defined as:

$$\mathcal{C}^n = (\mathcal{X}^n, p(y^n|x^n), \mathcal{Y}^n) \qquad where \qquad p(y^n|x^n) = \prod_{i=1}^{n} p(y_i|x_i)$$

Now $\mathcal{X}^n$ represents a packet of symbols transmitted by the source X. Knowing that several products of $p(y_i|x_i)$ are made, it is possible to understand that an important assumption of independence has been made, meaning that the channel has no memory of the past messages and each packet is independent from the others.

1.9.4 Capacity of a channel

Let us consider a channel $\mathcal{C}$, we want to analyze the mutual information $I(X;Y)$. We have defined the mutual information as:

$$I(X;Y) = H(X) - H(X|Y)$$

where:

- $H(X)$ is considered as $f(p(x))$ function of the probability distribution of the source.
- $H(X|Y) = -\sum_x \sum_y p(x,y) \log p(x|y)$, where:
  - $p(x,y) = p(x)p(y|x)$ in which $p(x)$ is related to the *source* and $p(y|x)$ is related to the *channel*. Generally, it is possible to say that $p(x,y)$ depends both on the source and on the channel.
  - From Bayes Theorem we also know that

    $$p(x|y) = \frac{p(y|x)p(x)}{p(y)}$$

    in which again $p(y|x)$ is related to the *channel* and instead $p(x)$ is related to the *source*.

    $$p(y) = \sum_x p(x,y) = \sum_x \underbrace{p(x)}_{source} \underbrace{p(y|x)}_{channel}$$

The mutual information that travels on the channel depends both on the source and on the channel.

$$I(X;Y) = f(p(x), p(y|x)) = f(source, channel)$$

where:

- $p(x)$ is the a priori probability.
- $p(y|x)$ is the posteriori probability.

So we can't use mutual information to give capacity information of the channel since $I(x, y)$ depends also from the source. After all these premises, we are able to define the **capacity of channel** as:

$$C = max_{p(x)} I(X; Y)$$

Capacity is the maximum value of mutual information given by all the possible probability distributions (source).

Example 1.13. Compute the capacity of the following BSC:

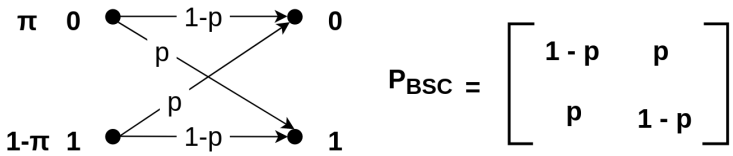


Figure 20: Channel representation.

We know that $Pr\{X = 0\} = \pi$ and $Pr\{X = 1\} = 1 - \pi$ (with $\pi \in [0, 1]$), so starting from the classic definition of *mutual information*

$$I(X; Y) = H(Y) - H(Y|X)$$

we can compute:

- $H(Y)$ where $Pr\{Y = 0\} = \pi(1 - p) + (1 - \pi)p$ and $Pr\{Y = 1\} = \pi p + (1 - \pi)(1 - p)$
  $H(Y)$ can be defined so as:

  $$H(Y) = H(\pi p + (1 - \pi)(1 - p), \pi(1 - p) + (1 - \pi)p)$$

  But since here $H(Y)$ is a function of only one variable we can simply write:

  $$H(Y) = H(\pi p + (1 - \pi)(1 - p))$$

- $H(Y|X) = \sum_x p(x)H(Y|X = x) = \pi \underbrace{H(Y|X = 0)}_{\text{first matrix row}} + (1 - \pi) \underbrace{H(Y|X = 1)}_{\text{second matrix row}}$

  Since rows of the matrix are written in function of parameter p we can simply write:

  $$H(Y|X) = \pi H(p) + (1 - \pi)H(p) = H(p)$$

  From the result, we can understand that $H(Y|X)$ depends only on their probabilities and not on the input.

After computing the values of $H(Y)$ and $H(Y|X)$ we can finally write:

$$I(X; Y) = \underbrace{H(\pi p + (1 - \pi)(1 - p))}_{H(Y)} - \underbrace{H(p)}_{H(Y|X)}$$

The **capacity** of the channel is computed as:

$$C_{BSC} = max_{0 \leq \pi \leq 1} I(X; Y)$$

The maximum is reached when $H(\pi p + (1-\pi)(1-p))$ is maximum, which is given in correspondence of 0.5, when so $\pi p + (1-\pi)(1-p) = 1/2$, for which the solution is $\pi = 1/2$.

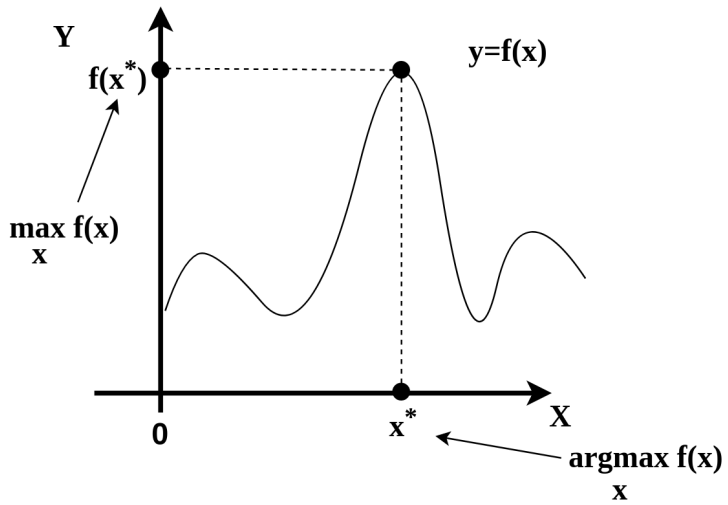


Figure 21: Channel Capacity as a function of the source X.

After this example, it is possible to specify the general capacity for BSC with $\pi = 1/2$ that is:

$$C_{BSC} = 1 - H(p)$$

At point $\pi = 1/2$ the entropy of $H(y)$ is maximum, equal to 1. Below it is possible to see the graphical representation of C_{BSC} compared to the mutual information representation.

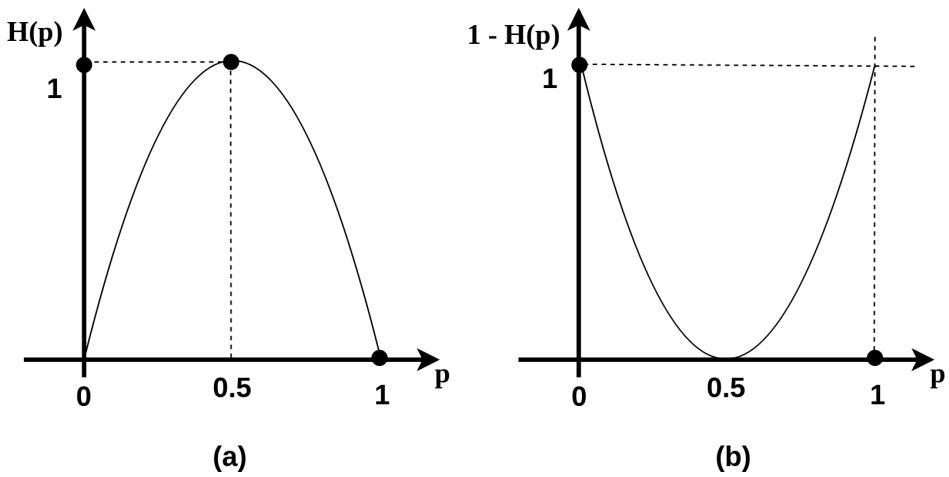


Figure 22: (a) Entropy graph - (b) Channel capacity graph.

What could happen in the different extreme cases, it is explained in the following lines:

- $p = 0$, we have that the channel is **perfect** and its capacity is 1. This represent the ideal case in which the channel is not affected by noise and receiver knows that the messages are correct. No loosing of information.

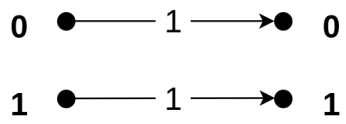


Figure 23: Channel representation when $p = 0$.

- $p = 1$, we have that the channel is again **perfect**. Receiver always knows how to reconstruct the right message. The message is always modified during the transmission on the channel. The channel's capacity is again 1.

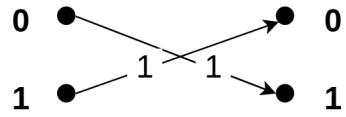


Figure 24: Channel representation when $p = 1$.

- $p = 0.5$ is the worst scenario for the receiver. We can consider the starting message X and the final message Y as independent messages.

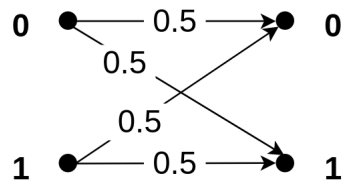


Figure 25: Channel representation when $p = 0.5$.

Here there is a strong assumption: **Receiver knows the probability distribution of the channel.** The best case for receiver is to know channel distribution and sender distribution, but this is not always available. Probabilities of the channel, in fact, can be specified only after several trials and they are not fixed, they could change during the time.

1.10 Reliability

How is it possible to use the channel in such a way that reliability is ensured?
Considering a channel with an error probability of 0.1, it is possible that, because of noise intervention, some errors could occur. A basic channel, as the one below, does not ensure, indeed, any form of reliability.

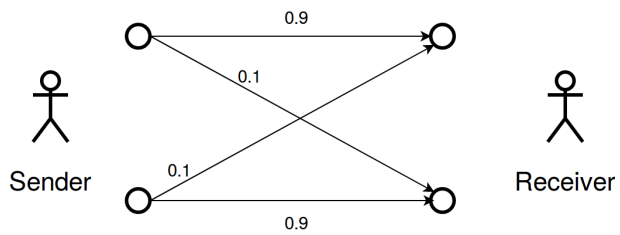


Figure 26: Unreliable communication channel.

Receiver can make an error when it takes a decision based on its inference about the right message transmitted by the source. This probability to make a mistake can be quantified and can be improved. One possibility is surely the technique of code replication, in order to improve the probability of success *coder* includes **redundancy**. Instead of transmitting a single bit, a packet of bits is sent. In this way we will use a third extension of the channel.

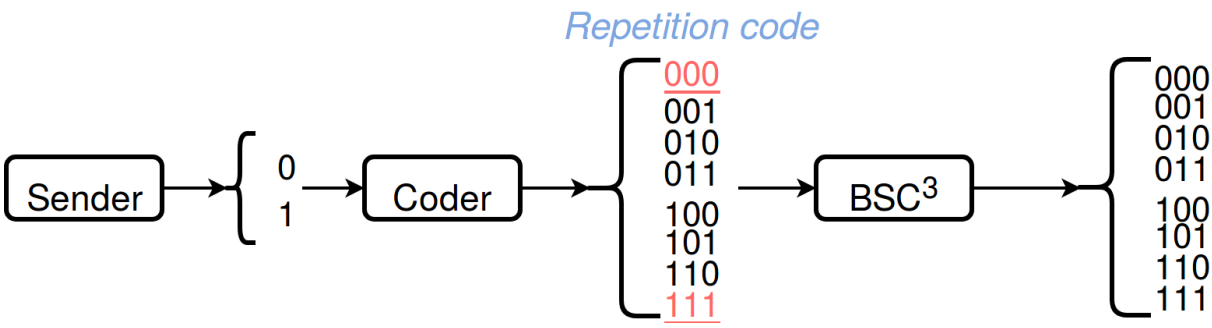


Figure 27: Third extension Binary Symmetric Channel: 1 bit.

This strategy improve the **reliability**, since the probability of making a mistake for the receiver is lower. The drawback is that this strategy reduces the rate, speed of sending data. Here we have a rate of 1/3, instead of transmitting one single bit coder extends the codewords and it transmits 3 bit.

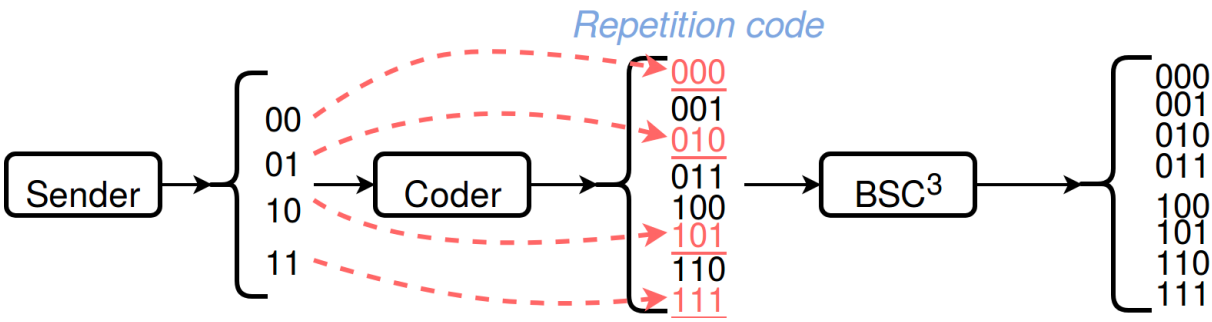


Figure 28: Third extension Binary Symmetric Channel: 2 bit.

Now we want to consider the case in which the sender's alphabet is composed by couples of bits $\mathcal{X} = \{\texttt{00}, \texttt{01}, \texttt{10}, \texttt{11}\}$, and instead of considering only codewords `111` and `000` to codify `1` and `0` now 4 possible choices are available: $\{\texttt{000}, \texttt{010}, \texttt{101}, \texttt{111}\}$.
Now respect to the previous case the sender transmit messages of 2 bits, for which the coder select $M = 4$ possible choices to codify them. The channel transmits $n = 3$ bits instead of $n = 2$ in order to improve the reliability. The final rate of this communication system is given by:

$$R = \frac{\log_2 M}{n} = \frac{\log_2 4}{3} = \frac{2}{3}$$

With M equal to the number of possible choices made by the coder and n number of bits sent by the channel. Respect to the previous case the rate is greater.
What if we consider $n \to \infty$? We define P_e as the probability of making a mistake: When $n \to \infty$ we have that $P_e \to 0$ but $R \to 0$, meaning that a more reliable code produces a slower

communication system. It is necessary to find a right trade-off to maintain a good level of reliability and speed.

1.11 Channel Coding Theorem - Shannon's 2nd Theorem

Shannon Theorem says that if $R < C$ (R is the transmission rate), it is possible to define a reliable code with fixed R. Instead, if $R > C$ it's impossible to guarantee that the information is transmitted in a reliable way.
The capacity of the channel is an upper bound for R if we want to define a reliable code.

Theorem 1.14 (Channel Coding Theorem)**.** *Let $\mathcal{C}$ be a channel with capacity C.*

- *If $R < C$ then there exists a sequence of $(2^{nR}, n)$ codes such that:*

$$P_e \underset{n\to\infty}{\to} 0$$

  $(2^{nR}, n) = (M, n)$ represents codes with the same rate R: $R = \frac{\log_2 M}{n} = \frac{\log_2 2^{nR}}{n} = \frac{nR}{n} = R$
- $\forall \varepsilon > 0 \quad \exists n_0 \in \mathcal{N} \quad s.t. \quad \forall n \geq n_0 : \quad P_e < \varepsilon$
  We choose ε as the maximum error probability. Shannon Theorem says that it is possible to define a code with redundancy $n > n_0$.
- *Any sequence of $(2^{nR}, n)$ codes such that $P_e \underset{n\to\infty}{\to} 0$ must have $R < C$. Comparing this with point 1 we can see that it is an if and only if.*

2 Neural Networks

A Neural Network is an information processing paradigm that is inspired by the way biological nervous systems, such as the brain, process information. The key element of this paradigm is the new structure of the information processing system. It is composed of a large number of highly interconnected processing elements (**neurons**) working in unison to solve specific problems. A NN is configured for a specific application, such as pattern recognition or data classification, through a learning process.
Two key features distinguish neural networks from any other sort of computing developed:

- **Neural networks are adaptive or trainable**. Neural networks are not so much programmed as they are trained with data, the more data they are fed, the more accurate or complete is their response.
- **Neural network are naturally massively parallel**. This suggests they should be able to make decisions at high-speed and be fault tolerant (information is stored in a distributed fashion). There are more interconnections than processing units and the processing power of a neural network corresponds to the number of interconnection updates per second.

The Neuron. The biological neural network is composed by the following elements:

- **Cell body (Soma)**: 5-10 microns in diameter, it is the *computational unit*.
- **Axon**: Output mechanism for a neuron.
- **Dendrites**: Receive incoming signals from other nerve axons via synapse.

The neural dynamics. The transmission of signal in the cerebral cortex is a complex process:

$$\text{Electrical} \rightarrow \text{Chemical} \rightarrow \text{Electrical}$$

Simplifying:

1. The cellular body performs a "*weighted sum*" of the incoming signals.
2. If the result exceeds a certain threshold value, then it produces an "action potential" which is sent down the axon (cell has "fired"), otherwise it remains in a rest state.
3. When the electrical signal reaches the synapse, it allows the “neuro-transmitter” to be released and these combine with the “receptors” in the post-synaptic membrane.
4. The post-synaptic receptors provoke the diffusion of an electrical signal in the post-synaptic neuron.

In other words computations by neuron are performed thanks to a combination of electrical and chemical processes.

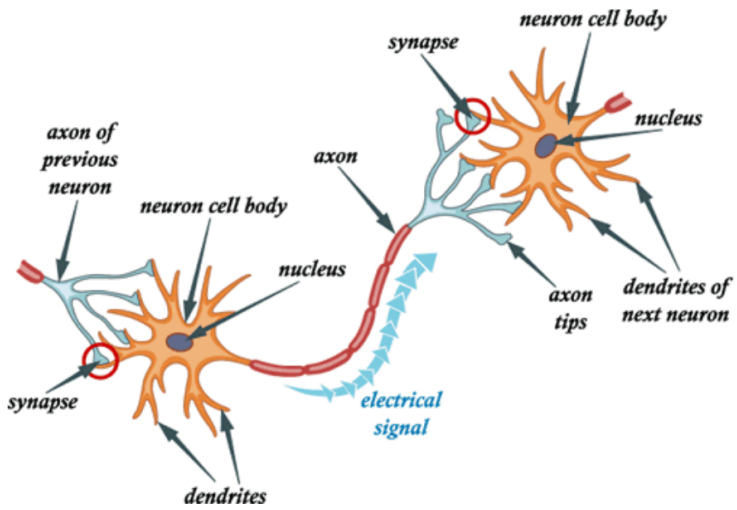


Figure 29: Neural dynamics.

Synaptic Efficacy. Synapses are connecting point between neurons. It's the amount of electricity that enters into the post-synaptic neuron, compared to the action potential of the pre-synaptic neuron. The **learning step** takes place by modifying the synaptic efficacy. Two different types of synapses are present:

- **Excitatory**: favor the generation of action potential in the post-synaptic neuron.
- **Inhibitory**: hinder the generation of action potential.

2.1 The McCulloch and Pitts Model

Neural network simulations appear to be a recent development, however, this field was established before the advent of computers and the first model was created in the 1943, it is called **McCulloch and Pitts Model**.
The McCulloch-Pitts (MP) neuron is a simple process unit modeled as a binary threshold unit.

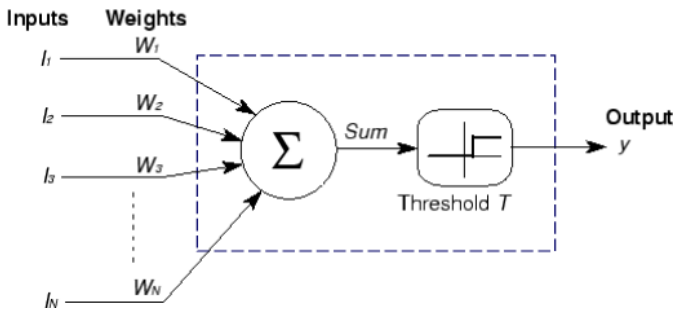


Figure 30: McCulloch and Pitts neuron representation.

The unit fires if the **net input** $\sum_j w_j I_j$ reaches (or exceeds) the unit's threshold T:

$$y = g\left(\sum_j w_j I_j - T\right) \qquad \text{where } g \text{ is the unit step function}$$

If neuron is firing, then its output y is 1, otherwise it is 0.

$$g \text{ is the unit step function such that} \quad \rightarrow \quad g(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$$

The weight w_{ij} represents the strength of the synapse between neuron j and neuron i. The function $g(x)$ is also called **activation function**.

Properties of MP networks. Combining the MP neurons, it is possible to simulate the behavior of any Boolean circuit.

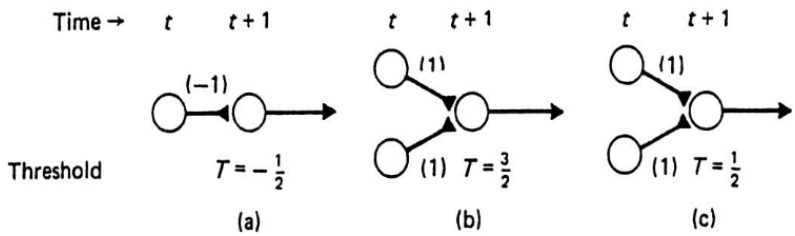


Figure 31: These elementary logical operations (a) **negation**, (b) **and**, (c) **or**. In each diagram the states of the neurons on the left are at time t and those on the right at time $t + 1$.

2.2 Network Topologies and Architectures

There are different network topologies and the main differences are highlighted below.

Feedforward only allow signals to travel one way only: from input to output. There are no feedback (loops). The output of any layer does not affect that same layer. This type of organization is also referred to as bottom-up or top-down.	**Feedback networks** (*or Recurrent networks*) can have signals traveling in both directions by introducing loops in the network. Feedback networks are powerful and can get extremely complicated.
Fully connected has each neuron connected to every neuron in the previous layer, and each connection has it's own weight.	**Sparsely connected** has fewer links than the possible maximum number of links within that network.
Single layer	**Multilayer**

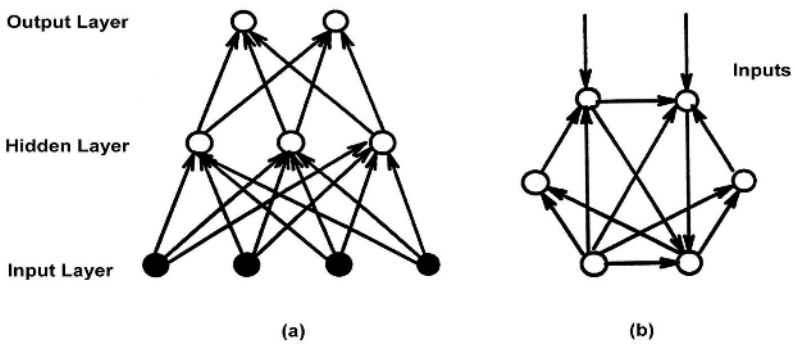


Figure 32: *(a)* feedforward network - *(b)* feedback network

2.3 Classification problems

Given:

1. **Features**, attributes that describe our objects. $f_1, f_2, \ldots, f_n$
2. **Classes**, categories in which the objects are divided. $c_1, \ldots, c_m$

What we desire is to classify our objects according to its features. A neural networks can be used as a classification device and it can be configured as follow:

- The *input* of the network are the object's features to classify.
- The *output*, returned by the network, is the class predicted for the input object.

Before going on we assume that features are numbers, and remember that we cannot mapping categorical features into numbers, since otherwise we can introduce an order which can make confusion or error. Example: red = 0, blu = 1, green = 2, is not a correct coding since we are imposing an incorrect order between colors. We propose a simple model of neural network:

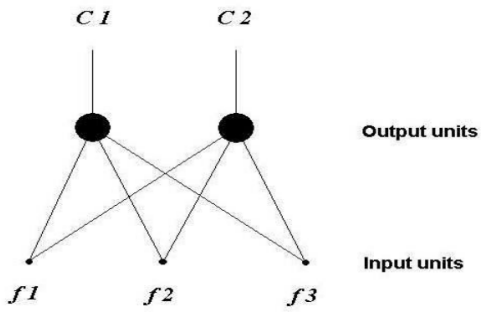


Figure 33: Example of NN with 3 features input and 2 class labels as output.

The application of a learning algorithm of a network configuration consists on finding the best configuration of weights of the income connection and the threshold. In these classification problems we can get rid of the **thresholds** (also called bias) associated to neurons by adding an extra unit **permanently clamped at -1**. Doing this, thresholds become weights and can be adaptively adjusted during learning phase, otherwise we have to tune manually the right threshold. Since it is just a simple parameter we can learn it taking advantage on the learning procedure.

$$NET_i = \sum w_{ij} x_j - 1 w_0$$

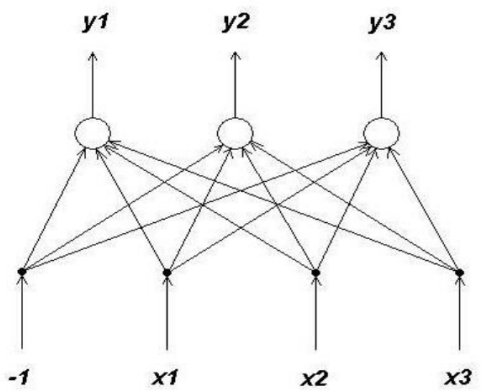


Figure 34: Thresholds

2.4 The Perceptron

The perceptron is an algorithm for **supervised learning** of binary classifiers (functions that can decide whether an input, represented by a vector of numbers, belongs to some specific class or not). It is a type of linear classifier, that is a classification algorithm that makes its predictions based on a linear predictor function combining a set of weights with the feature vector. A simple perceptron can only solve linearly separable problems, this make the model very limited in terms of computational power. However, it is possible to say that for the problems that it can solve, it is able to learn from example and it can be considered as the **simplest feedforward neural network**. It is implemented as a network of one layer of M&P neurons connected in a feedforward way.

The Perceptron Learning Algorithm. It is an iterative algoritnm characterized by the following variables and parameters:

- Inputs vector: $x(n) = (m+1)$-by-1 input vector $= [-1, x_1(n), x_2(n), \ldots, x_m(n)]^T$
  Objects are described with m features and -1 as the threshold, that is the reason of the $m+1$.
- Weights vector: $w(n) = (m+1)$-by-1 weight vector $= [b, w_1(n), w_2(n), \ldots, w_m(n)]^T$
- $b =$ bias
- $y(n) =$ actual response (quantized). $+1/-1$
- $d(n) =$ desired response. $+1/-1$
- $\eta =$ learning-rate parameter, a positive constant less than unity. It affects the convergence of the learning algorithm.

It is structured with the following steps:

1. **Initialization.** Set $w(0) = 0$ and then perform the following computations for time-step $n = 1, 2, \ldots$.
2. **Activation.** At time-step n, activate the perceptron by applying continuous-valued input vector $x(n)$ and desired response $d(n)$. Pick element from the training set.
3. **Computation of Actual Response.** Compute the actual response of the perceptron as:

   $$y(n) = sgn[w^T(n)x(n)] \qquad w^T x = \sum_i w_i x_i$$

   where $sgn(\cdot)$ is the signum function. Until this phase there's not learning.
4. **Adaptation of Weight Vector.** Update the weight vector of the perceptron to obtain.

   $$w(n+1) = w(n) + \eta[d(n) - y(n)]x(n)$$

   where

   $$d(n) = \begin{cases} +1 & \text{if } x(n) \text{ belongs to class } \varphi_1 \\ -1 & \text{if } x(n) \text{ belongs to class } \varphi_2 \end{cases}$$

   In this point there's the learning phase. In case of wrong classification, the current configuration will change modifying $d(n) - y(n)$. The convergence of the algorithm is ensured by $x(n)$.If the network classify correctly then there is no learning $d(n) - y(n) = 0$. Note that $x(n)$ is included to be sure that the new prediction is correct but it can fail with the previous one.

5. **Continuation.** Increment time step n by one and go back to step 2.

Through this algorithm we are looking for a straight line which separates the good examples from bad ones. The decision boundary is described such that $w_1x_1 + w_2x_2 = 0$ and in a general way each point is classified according the following formula:

$$\text{net}_i = \sum_i w_i x_i \rightarrow \begin{cases} \text{if } > 0 \rightarrow +1 \\ \text{if } < 0 \rightarrow -1 \end{cases}$$

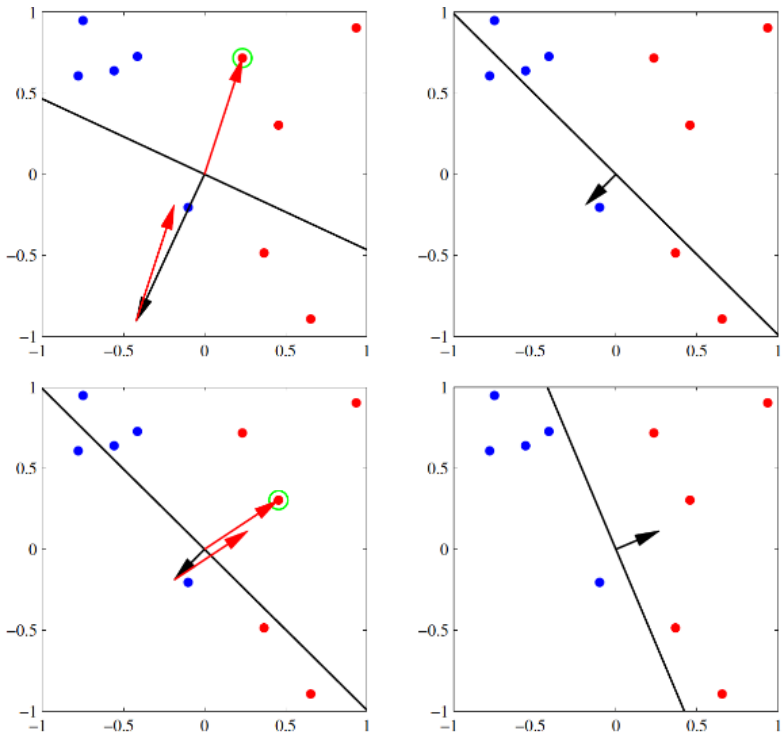


Figure 35: Perceptron learning algorithm procedure.

From a geometrical point of view, finding w means find the line (or hyperplane) which separates the two regions. As it is possible to see from the previous image, some examples can be misclassified. Each time a precise error is correct but other mistakes can be produced, continuing to correct the errors found, the final situation can be reached.
It is possible to define a **decision region** as an area wherein all examples of ones class fall. A classification problem is said to **linearly separable** if the decision regions can be separated by an hyperplane. These concepts allows us to introduce the fact that one important **limitation of perceptrons** is that they can only solve linearly separable problems.

The Perceptron Convergence Theorem. This theorem was formulated by Rosenblatt in 1960. It said that:
If the training set is **linearly separable**, the perceptron learning algorithm **always converges** to a consistent hypothesis after a **finite** number of epochs, for any $\eta > 0$ (It doesn't say anything about the number of steps).
If the training set is **not linearly separable**, after a certain number of epochs the weights start oscillating. In this situation surely some points will be misclassified. The learning algorithm will

never converge to a stable configuration, due to the fact that perceptron can't solve non-linear classification problem.

2.5 Multi-Layer Feedforward Networks

In the following image it is possible to find some properties of the different structures that can create a neural network.

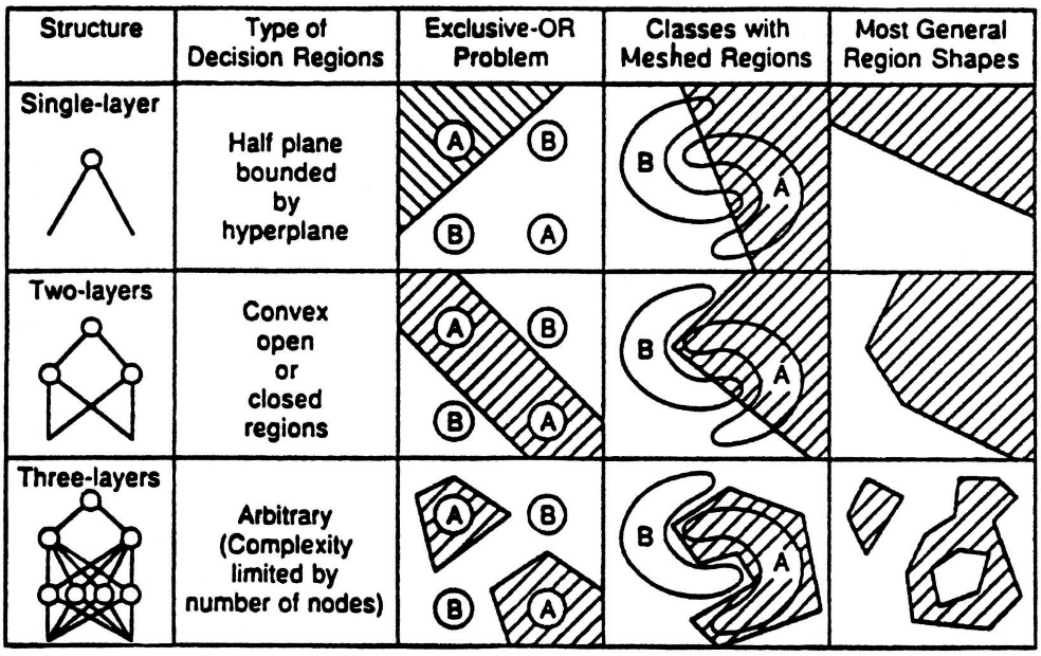


Figure 36: A view of the Role of Units

A single layer represents the structure of a perceptron and as we said before it can implement only linearly separable functions. In order to overcome these limitations, the introduction of multi-layer feedforward networks allows us to improve our networks through the adding of **hidden layers** between the input and the output layer. This can allow us to reach a good approximation of our classification problem, it is possible to notice that a network with just one hidden layer can represent any Boolean functions including XOR. From the **Universal approximation power** we also know that a two-layer network (only one hidden layer) can approximate any smooth function (valid for regression problem). But this power does not give us information about how large should be this network. This model here is static, meaning that we have no feedback.

$$f : I \to \mathbb{R}^m \qquad I \subseteq \mathbb{R}^n$$

$$f(x_1, \ldots, x_n) = \bar{y} \in \mathbb{R}^m$$

We want that the estimated function $NN(X)$ satisfies the following property:

$$||\mathrm{NN}(\bar{X}) - f(\bar{X})|| \leq \varepsilon$$

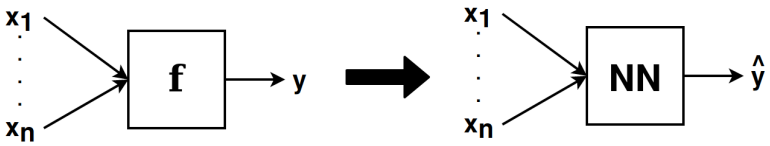


Figure 37: Neural Network function model.

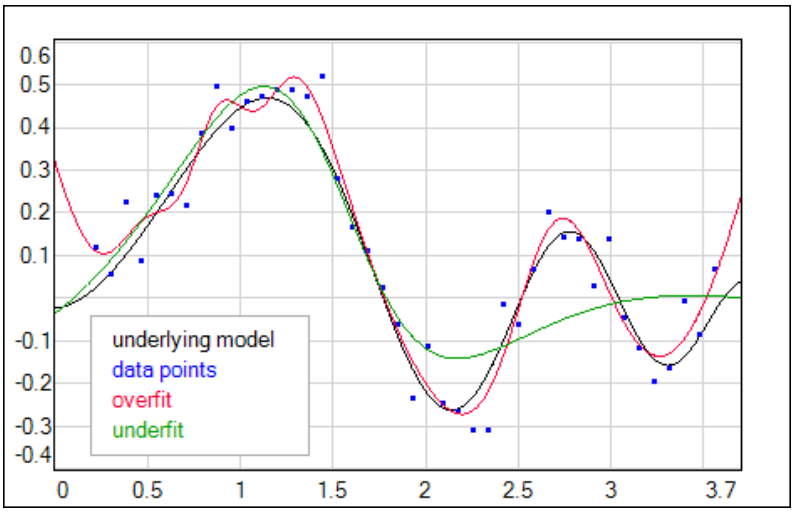


Figure 38: Neural Network function approximation.

Note that the Universal approximation power works only for regression problems, since usually classification problems are more difficult (3 layers instead of 2).

Continuous-Valued Units. The usage of continuous-valued units allows us to introduce calculus and derivatives procedures that will give us several advantages.
Sigmoid (or logistic), this is the rate of firing of the neurons, they can fire more or less, so they are not Boolean 0 or 1 but instead they are float values from 0 to 1. They are often interpreted as probabilities.

$$g \to \sigma(x) = \frac{1}{1 + e^{-f(x)}} \in (0, 1)$$

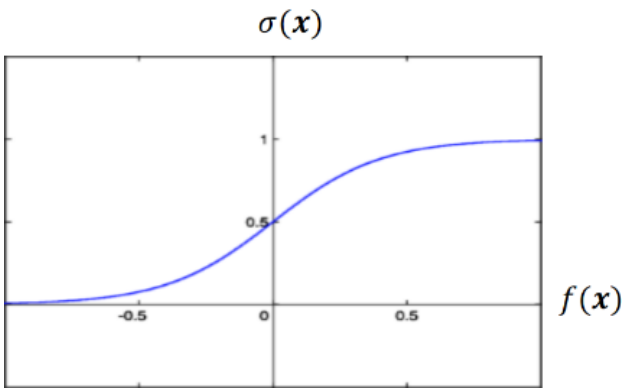


Figure 39: Sigmoid function.

Continuous-Valued discriminant functions allows us to have a confidence about the prediction. We will see later one that they are used for finding optimal solutions using the gradient descent technique. In particular, when the $g(z)$ is close to zero (less confidence about the prediction) the gradient will be greater then the situation in which $|g(x)| >> 0$ (more confidence, weights could remain stable).

Hyperbolic tangent is a rescaling of the logistic sigmoid such that its output range is from -1 and 1. This type of function could be better because the length of the interval has length 2 and so it has more degrees of freedom.

$$g \to \sigma(x) = \frac{e^{f(x)} - e^{-f(x)}}{e^{f(x)} + e^{-f(x)}} \in (-1, 1)$$

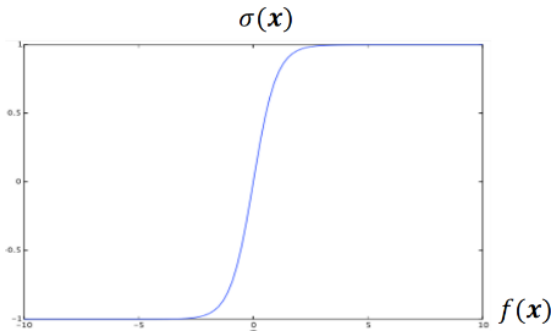


Figure 40: Hyperbolic tangent function.

2.6 Back-propagation Learning Algorithm

It is an algorithm for learning the weights in a feed-forward network, solving the learning in multilayers neural networks (respect to the one provided by the perceptron). We've got a training set $\mathcal{L} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ in which each pair is an input/output behavior. The algorithm is based on gradient descent method, it can be considered as a greedy algorithm with infinite possible solutions where each time the best solution is chosen. The algorithm is guarantee to converge only to a local maximum and during the execution we move along the gradient through a predetermined step-size. This property is due to the fact that this algorithm is just an approximation based on a greedy solution.

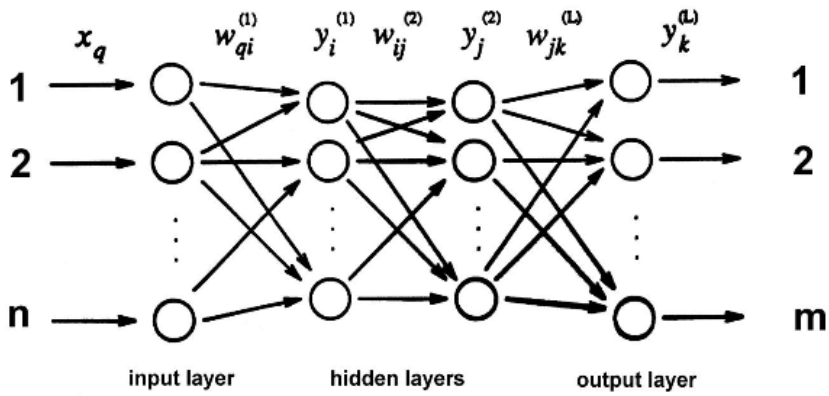


Figure 41: Back-propagation schema. W_{ij}^{l} represents the weight on connection between the ith unit in layer $(l-1)$ to j^{th} unit in layer l.

Supervised Learning. Supervised learning algorithms require the presence of a previous knowledge that makes possible to provides the right answers to the input questions. Technically this means that we need a **training set** of the form:

$$\mathcal{L} = \left\{ \left(x^1, y^1\right), \ldots, \left(x^p, y^p\right) \right\}$$

where:

$$x^\mu (\mu = 1, \ldots, p) \text{ is the network input vector}$$

$$y^\mu (\mu = 1, \ldots, p) \text{ is the desired network output vector}$$

The learning (or training) phase consists of determining a configuration of weights in such a way that the network output be as close as possible to the desired output, for all the examples in the training set. Normally, this amounts to minimizing an **error function** such as:

$$E(w) = \frac{1}{2} \sum_\mu \sum_k \left(y_k^\mu - O_k^\mu(w)\right)^2$$

where $O_k^\mu(w)$ is the output provided by the output unit k when the network is given example μ as input. In other words, $O_k^\mu(w)$ represents the prediction of the kth unit when the input is μ. The loss function computes the difference between the network output and the expected output and of course, our aim is to **minimize the loss function** $min_w E(w)$ that means finding the set of weights that minimize the function. It is possible to say so that we are in a minimization (optimization) problem. If the network is performing well $E(\omega)$ is close to zero.
In order to minimize the error function E, we can use the classic **gradient-descent** algorithm. Gradient gives information about the best path to follow in order to increase/decrease our objective function. Without any kind of direction information it would be extremely complex to find the solution since we have to search along an infinite number of directions in a continuous domain. Gradient descent is a very well-known greedy algorithm, but it does not guarantee to find an optimal solution, but at least a local one. It is a first-order iterative optimization algorithm for finding the minimum of a function. It can be defined as:

$$w_{ji} \leftarrow w_{ji} - \eta \frac{\partial E_k}{\partial w_{ji}} \qquad \text{where } \eta \text{ is the learning rate.}$$

In back-propagation algorithm, we have an initial configuration of the network and at each step we update the weights as:

$$w_{new} = w_{old} - \eta \nabla E(w_{old})$$

To compute the partial derivatives we use the **error back propagation** algorithm, it consists of two stages:

- **Forward pass**: the input of the network is propagated layer after layer in forward direction.
- **Backward pass**: the "error" made by the network is propagated backward and weights are updated properly.

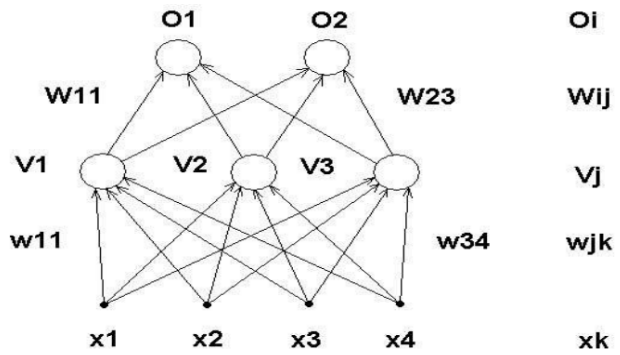
In a more informal way it is possible to say that we determine the gradient direction and then we will move in the opposite direction since we want to minimize the error.

Notations. Before start understanding in which way the weights are updated, it is important to fix some notations that will be used later.
Given a pattern μ, hidden unit j receives a net input

$$h_j^\mu = \sum_k w_{jk} x_k^\mu$$

and produces as output:

$$V_j^\mu = g\left(h_j^\mu\right) = g\left(\sum_k w_{jk} x_k^\mu\right)$$



Updating Hidden-to-Output Weights. The updating rules of the back-propagation algorithm are nothing but a long series of chain rules, for this reason, the objective function is not linear and so the output is highly non linear, indeed, it is a product of chain of non linear functions.

$$\begin{aligned}
\Delta w_{ij} &= -\eta \frac{\partial E}{\partial w_{ij}} \\
&= -\eta \frac{\partial}{\partial w_{ij}} \left[\frac{1}{2} \sum_\mu \sum_k (y_k^\mu - O_k^\mu)^2\right] \quad \text{First application of the chain rule} \\
&= \eta \sum_\mu \sum_k \left(y_k^\mu - O_k^\mu\right) \frac{\partial O_k^\mu}{\partial w_{ij}} \quad \text{The sum over } k \text{ disappers because the partial derivative is} \\
&\qquad \text{different from 0 only when } k = i \\
&= \eta \sum_\mu \left(y_i^\mu - O_i^\mu\right) \frac{\partial O_i^\mu}{\partial w_{ij}} \quad \text{Again we apply the chain rule. Partial derivative can be} \\
&\qquad \text{written as } w_{ij} \to h_i^\mu \to g'(h_i^\mu) \\
&= \eta \sum_\mu \left(y_i^\mu - O_i^\mu\right) g'\left(h_i^\mu\right) V_j^\mu \quad \text{That is } \frac{\partial h_i^\mu}{\partial w_{ij}} = \frac{\partial}{\partial w_{ij}} \left(\sum_l w_{il} V_l\right) = V_j \frac{\partial w_{ij}}{\partial w_{ij}} = V_j \\
&= \eta \sum_\mu \delta_i^\mu V_j^\mu \qquad where: \quad \delta_i^\mu = \left(y_i^\mu - O_i^\mu\right) g'\left(h_i^\mu\right)
\end{aligned}$$

In $\eta \sum_\mu \delta_i^\mu V_j^\mu$, the component δ_i^μ represents the error made by the i-th neuron and instead V_j^μ is the output of the neuron.

Updating Input-to-Hidden Weights.

$$\begin{aligned}
\Delta w_{jk} &= -\eta \frac{\partial E}{\partial w_{jk}} \\
&= \eta \sum_{\mu} \sum_{i} \left(y_i^{\mu} - O_i^{\mu}\right) \frac{\partial O_i^{\mu}}{\partial w_{jk}} \qquad \text{Chain rule} \\
&= \eta \sum_{\mu} \sum_{i} \left(y_i^{\mu} - O_i^{\mu}\right) g'\left(h_i^{\mu}\right) \frac{\partial h_i^{\mu}}{\partial w_{jk}} \qquad \text{Chain rule}
\end{aligned}$$

We have that the partial derivative is:

$$\begin{aligned}
\frac{\partial h_i^{\mu}}{\partial w_{jk}} &= \sum_{l} w_{il} \frac{\partial V_l^{\mu}}{\partial w_{jk}} \\
&= w_{ij} \frac{\partial V_j^{\mu}}{\partial w_{jk}} \\
&= w_{ij} \frac{\partial g\left(h_j^{\mu}\right)}{\partial w_{jk}} \\
&= w_{ij} g'\left(h_j^{\mu}\right) \frac{\partial h_j^{\mu}}{\partial w_{jk}} \\
&= \frac{\partial}{\partial w_{jk}} \sum_{m} w_{jm} x_m^{\mu} \\
&= x_k^{\mu}
\end{aligned}$$

Hence coming back to the original equation we have that:

$$\begin{aligned}
\Delta w_{jk} &= \eta \sum_{\mu,i} \left(y_i^{\mu} - O_i^{\mu}\right) g'\left(h_i^{\mu}\right) w_{ij}\ g'\left(h_j^{\mu}\right) x_k^{\mu} \\
&= \eta \sum_{\mu,i} \delta_i^{\mu} w_{ij} g'\left(h_j^{\mu}\right) x_k^{\mu} \qquad (1) \\
&= \eta \sum_{\mu} \hat{\delta}_j^{\mu} x_k^{\mu} \qquad where: \quad \hat{\delta}_j^{\mu} = g'\left(h_j^{\mu}\right) \sum_{i} \delta_i^{\mu} w_{ij}
\end{aligned}$$

$\sum_i \delta_i^{\mu} W_{ij}$ is the average error performed by the output layer and i is the reference to the i-th neuron.
In the following image it is possible to understand the error back-propagation in which the black line means the forwarded signal instead the red lines indicate the error that is back-propagated.

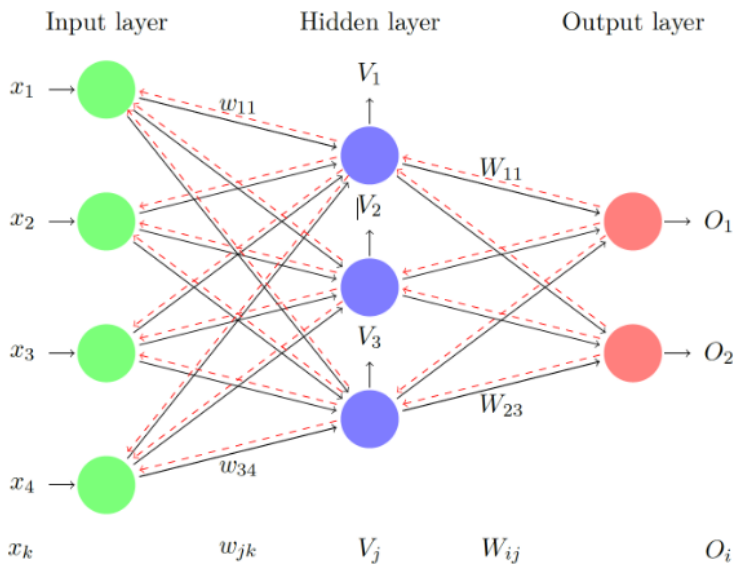


Figure 42: Error Back-propagation representation.

Locality of Back-Propagation. Another important aspect is the locality of the back-propagation.

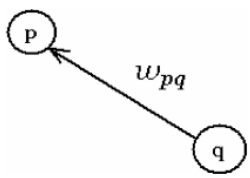


Figure 43: Locality of back-propagation

Off-line: In this way we compute the gradient exactly. It is done a sum over all the possible μ. Normally this procedure is not used because it is computational expensive and also because if we start search in a bad region we can't escape from it.

$$\Delta\omega_{pq} = \eta \sum_{\mu} \delta_p^{\mu} V_q^{\mu} \qquad \text{off-line}$$

$$\delta_p^{\mu} = \text{Error} \quad V_q^{\mu} = \text{Output of neurons}$$

On-line: In this other situation some noise is introduced. It allows to escape a bad region and to reach a better solution through the exploration of regions that otherwise we won't visit.

$$\Delta\omega_{pq} = \eta \delta_p^{\mu} V_q^{\mu} \qquad \text{on-line}$$

A possible compromise between the two techniques is to use the first technique with a small training set, this third option is called (**stochastic gradient descent**).

The Back-Propagation Algorithm. In this algorithm we will use the on-line rule.
The general structure of the algorithm:

1. Initialize the weight to (*small*) random values. Small because otherwise derivative of logistic function will be all zeros.

2. Choose a pattern $\bar{x}^\mu$ and apply it to the input layer ($m = 0$).

$$V_k^0 = x_k^\mu \qquad \forall k$$

3. Propagate the signal forward, remember that g is a continuous function:

$$V_i^m = g\left(h_i^m\right) = g\left(\sum_j w_{ij} V_j^{m-1}\right)$$

4. Compute the δ's for the output layer:

$$\delta_i^m = g'\left(h_i^m\right)\left(y_i^m - V_i^m\right)$$

5. Compute the δ's for all preceding layers (for each neuron):

$$\delta_i^{m-1} = g'\left(h_i^{m-1}\right) \sum_j w_{ji}^m \delta_j^m$$

6. Update connection weights according to the error, with learning rate η:

$$w_{ij}^{NEW} = w_{ij}^{OLD} + \Delta w_{ij} \qquad \text{where} \qquad \Delta w_{ij} = \eta \delta_i^m V_j^{m-1}$$

7. Go back to step 2 until convergence.

One of the most important problem is the fact that η (learning step) should be initialized in a correct way. When η is small the algorithm will converge but it will be too slow, on the other hand when it is too big, there will be an oscillating problem that won't bring the algorithm to the convergence.
In the following image four trajectories can be found, the only significant difference between them is the value of η they used. From left to right they are $0.02, 0.0476, 0.049, 0.0505$.

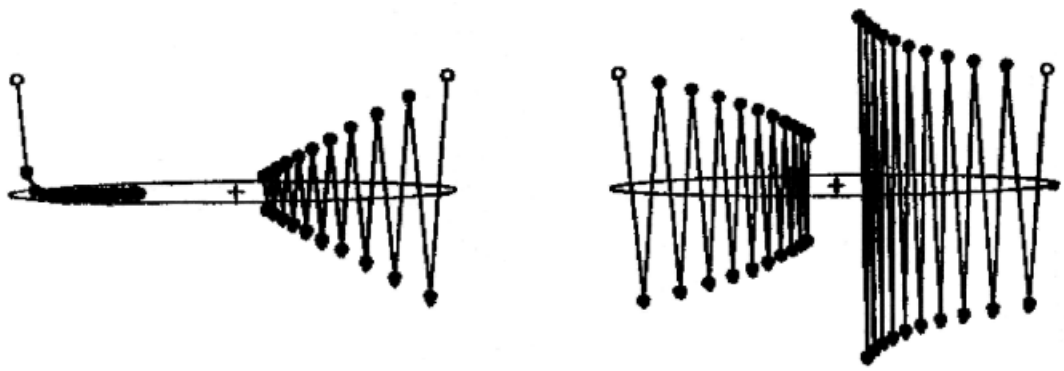


Figure 44: The Role of the Learning Rate. The minimum is at the + and the ellipse shows a constant error contour.

The first case is too slow in reaching the minimum, in the second and in the third case the oscillation becomes smaller and smaller, instead in the last case the algorithm won't converge, the oscillation is larger and larger.
As said before, one of the most limitations of the **gradient descent** method is the fact that:

- It converges too slowly if η is too small.

- It oscillates if η is too large.

One possible remedy to this problem is in introducing the **momentum term**, a simple heuristic that can help to find a good value for learning rate. One of the most advantages of this improvement is the fact that it will introduce a correction that is based also on the step at time $t-1$, on the contrary the original idea produces a correction related only to the current point.

$$\Delta\omega_{pq}(t+1) = -\eta\frac{\partial E}{\partial w_{pq}} + \underbrace{\alpha\Delta w_{pq}(t)}_{\text{momentum}}$$

- If $\alpha = 0$ we come back to the original formula $\Delta = f(w^T)$
- Otherwise $\Delta = f(w^T, w^{t-1})$

The momentum term introduces dependency with the previous step. Surely, a negative aspect is the fact that we need to set two parameters but on the other hand the momentum term allows us to use large values of η avoiding the introduction of the oscillatory phenomena. The application of the momentum term can be seen in the following image.

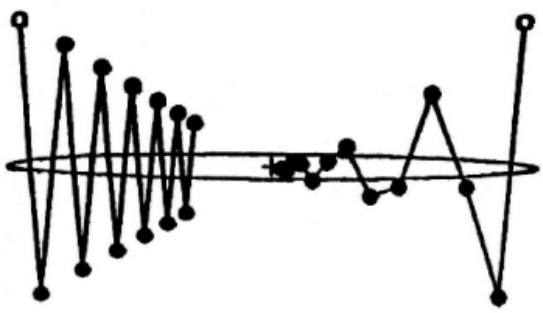


Figure 45: Momentum term application.

Both trajectories uses $\eta = 0.0476$ that is the best value of learning rate in the absence of momentum. On the left example there is not application of momentum ($\alpha = 0$), while on the right $\alpha = 0.5$. The application of momentum, hence, brings a clear improvement in the convergence.

The Problem of Local Minima. One of the most important disadvantages is the fact that back-propagation cannot avoid the problem of local minima. For this reason the choice of initial weights is very important, if they are too large the nonlinearities tend to saturate since the beginning of the learning process.
A common heuristic for the choice of the initial weights is:

$w_{ij} \simeq 1/\sqrt{K_i}$ Where k_i is the number of units that feed unit i (the "fan-in" of i)

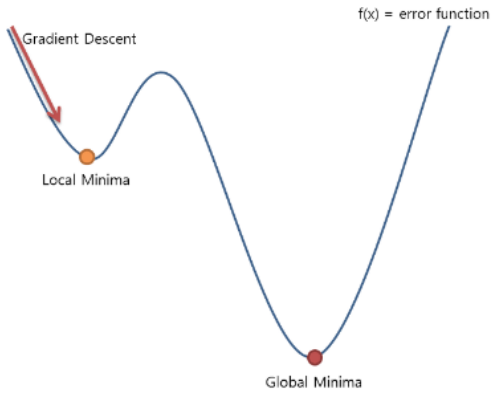


Figure 46: The problem of local minima.

2.7 Theoretical / Practical Questions

- How many layers are needed for a given task?
- How many units per layer?
- To what extent does representation matter?
- What do we mean by generalization?
- What can we expect a network to generalize?
    - **Generalization:** performance of the network on data not included in the training set. One of the major advantages of neural nets is their ability to generalize. This means that a trained net could classify data from the same class as the learning data that it has never seen before. In real world applications developers normally have only a small part of all possible patterns for the generation of a neural net. To reach the best generalization, the dataset should be split into three parts: training set, validation set and test set.
      The learning should be stopped in the minimum of the validation set error. At this point the net generalizes best. When learning is not stopped, overtraining occurs and the performance of the net on the whole data decreases, despite the fact that the error on the training data still gets smaller. After finishing the learning phase, the net should be finally checked with the third data set, the test set.
    - Size of the training set: how large a training set should be for "good" generalization?
    - Size of the network: too many weights in a network result in poor generalization.

2.8 Model evaluation

When we talk about the model evaluation, it is important to understand specially in which way the goodness of the model can be evaluated. Surely the lower is the error generated by the model and the best is the fit created by the model. It is possible to differentiate between two different types of errors:

- The **true error** (denoted $error_{\mathcal{D}}(h)$) of hypothesis h with respect to target function f and distribution $\mathcal{D}$, is the probability that h will misclassify an instance drawn at random according to $\mathcal{D}$.
$$error_{\mathcal{D}}(h) \equiv \Pr_{x \in \mathcal{D}} [f(x) \neq h(x)]$$

In other words it measures the probability of committing error in the real life, but notice that for computing this quantity it is necessary to have knowledge of the probability distribution (which in general in unknown).

- The **sample error** (denoted $error_s(h)$) of hypothesis h with respect to target function f and data sample S is:

$$error_S(h) \equiv \frac{1}{n} \sum_{x \in S} \delta(f(x), h(x))$$

Where n is the number of examples in S, and the quantity $\delta(f(x), h(x))$ is 1 if $f(x) \neq h(x)$, and 0 otherwise. It comes from the idea that since in general we don't know the probability distribution of our data we estimate it using the samples.

The true error is unknown (and will remain so forever...). In order to compute the sample error, it is possible to subdivide the dataset in a percentage for the training set and a percentage for the test set.

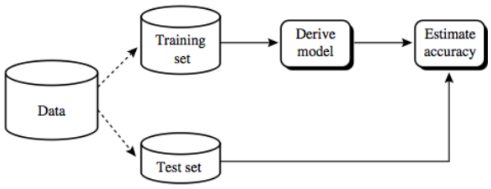


Figure 47: Training set vs Test set.

Cross-Validation Cross-validation is a technique to evaluate predictive models by partitioning the original sample into a training set to train the model, and a test set to evaluate it. It avoids that test and training set affect the model evaluation.

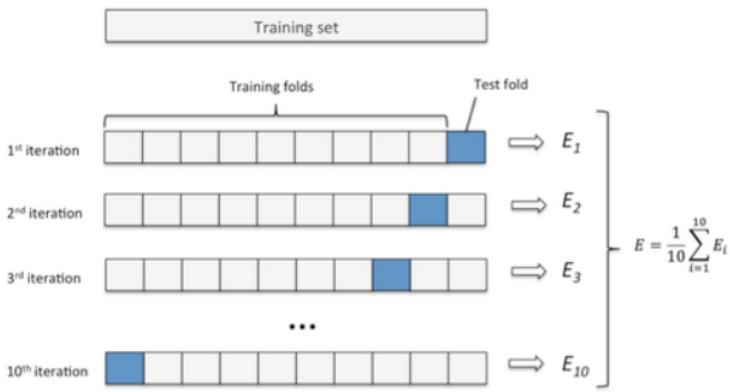


Figure 48: Cross validation example using **leave-one-out** technique (size of the test fold = 1).

Cross validation is an useful method to evaluate the performance of a neural network. The drawback is the time required to run it.

Overfitting Even if the cross-validation technique can give us a good evaluation of the model, it is possible that this score is due to a particular problem called **overfitting**. In the following image, it is possible to see in the right image its phenomenon.

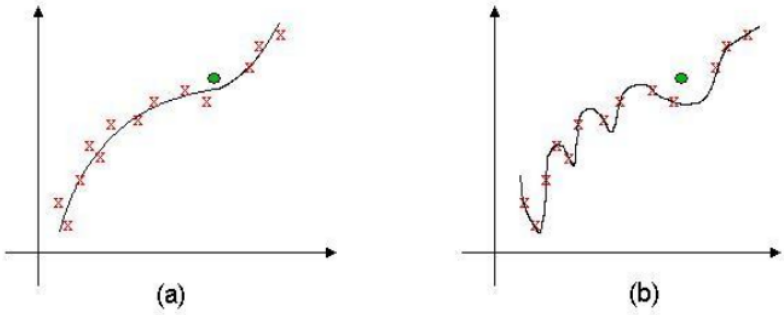


Figure 49: Example of overfitting.

In the image **(a)**, a good fit to noisy data and the model uses less parameters capturing the general trend behavior. Instead in the image **(b)** overfitting of the same data is performed, the fit is perfect on the "training set", but it is likely to be poor on "test set" represented by the circle. Following the concept of the **Occam's razor** the simplest model is preferable.
The different steps in the model definition are reached through the separation of the starting set in:

- **Training set:** for the execution of the learning algorithm.
- **Validation set:** it is used to stop the learning algorithm
- **Test set:** to evaluate the performance of the learning algorithm.

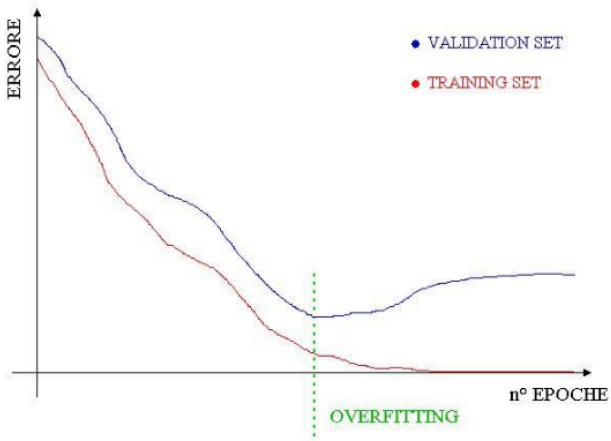


Figure 50: Early stopping.

Epoches of a learning algorithms represents the steps of machine learning algorithm. After the green line (overfitting line) during the next epochs the model start to learn noisy. Note also that the greater global optimum represents the overfit of the model, meaning that the error function is equal to zero since the model works well with training data points. The stop of the learning algorithm is executed when the fit starts deteriorating.

The size of the NN. The size of a NN (the number of hidden neurons) affects both its functional capabilities and its generalization performance.

- A **big network** leads to poor generalization performance. It has a lot of parameters and for this reason it's a too complex model.

- A **small network** could not be able to realize the desired input/output mapping and for this reason it won't be able to learn nothing.

However, it is hard to tell when the algorithm should stop because it is impossible to tell if the addiction of a further unit will dramatically decrease the error. This problem is known as **horizon effect**. A common strategy is called **growing**, it starts with one neuron and then it tries to train. It will add neurons until we will reach the right size.

The Pruning Approach. This approach is based on the idea of training an over-dimensioned network and then removing **redundant** nodes and connections. In pruning, indeed, we have a large number of neurons than the necessary and we will search to reduce the size. Pruning reduces the final complexity of the classifier and hence, it improves predictive accuracy by the reduction of overfitting.
The most important advantages of this technique are:

- Arbitrarily complex decision regions.
- Faster training.
- Independence of the training algorithm.

The pruning approach has anyway some disadvantages: in a network with the perfect number of neurons backpropagation can fail, since the number of degree of freedom is limited. In general it is not a good idea to apply learning algorithms on a network with the exact number of neurons due to the limitation on the degrees of freedom. If we have more degrees of freedom we have more chance and different ways to reach the desired objective.
We can have two types of pruning algorithm:

- **Online pruning:** during the training process it will decrease the size of the network.
- **Offline pruning:** it's preferable because it is possible to train the network in whatever way and the pruning is done only after the training process.

Suppose (for simplicity) a network with one hidden layer and suppose that unit h is to be removed.

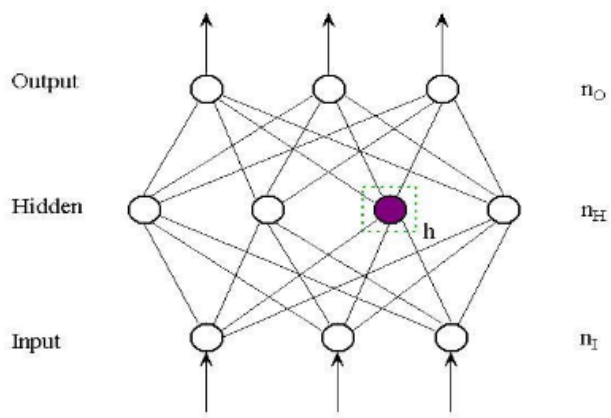


Figure 51: Example of the pruning approach.

As a consequence of this action we have to remove the incoming/outgoing connections and update the weights of the other connections such that the output remains the same. We focus on the input because if the input remains the same also the output remains unchanged.

This is equivalent to solving the system:

$$\underbrace{\sum_{j=1}^{n_h} w_{ij} y_j^{(\mu)}}_{\text{Before removing } h} = \underbrace{\sum_{\substack{j=1 \\ j\neq h}}^{n_h} (w_{ij} + \delta_{ij})\, y_j^{(\mu)}}_{\text{After removing } h} \qquad i = 1 \dots n_0 \text{ (\# output nodes)},\ \mu = 1 \dots P \text{ (network levels)}$$

Which is equivalent to the following linear system (in the unknown δ's):

$$\sum_{j\neq h} \delta_{ij} y_j^{(\mu)} = w_{ih} y_h^{(\mu)} \qquad i = 1, \dots n_0,\ \mu = 1, \dots, P$$

We can observe that $\sum_{j\neq h} \delta_{ij} y_j^{(\mu)}$ is a linear system of equations and instead $w_{ih} y_h^{(\mu)}$ represents b.

$$\begin{aligned}
\sum_{j=1}^{n_h} w_{ij} y_j^{(\mu)} &= \sum_{\substack{j=1 \\ j\neq h}}^{n_h} (w_{ij} + \delta_{ij})\, y_j^{(\mu)} \\
&= \sum_{\substack{j=1 \\ j\neq h}}^{n_h} w_{ij} y_j^{(\mu)} + \sum_{\substack{j=1 \\ j\neq h}}^{n_h} \delta_{ij} y_j^{(\mu)}
\end{aligned}$$

In order to satisfy this equation is necessary that $\sum_{j\neq h} \delta_{ij} y_j^{(\mu)} = w_{ih} y_h^{(\mu)}$ since the rest of the weights remains the same, the unique contribution that was deleted is the one provided by the neuron h.

In a more compact notation, it is possible to write the previous linear system as:

$$Ax = b \qquad \text{where } A \in \mathbb{R}^{P n_o \times n_o (n_h - 1)}$$

A is a matrix that represents the weights of the nodes in the output layer fed by the node h, x are the feature vectors and b means the contribution to the network.
The **Least Squares solution** is:

$$min_{\bar{x}} ||A\bar{x} - b||$$

A solution not always exists.
An important aspect is to detect which is the right neuron to prune. Residual reducing-methods start with an initial solution x_0 and produces some sequences of points $\{x_k\}$ so that the residuals are computed as:

$$\begin{aligned}
||Ax_0 - b|| &= r_0 \\
||Ax_1 - b|| &= r_1 \\
&\vdots \\
||Ax_k - b|| &= r_k \qquad \text{where } r_k \leq r_{k-1}
\end{aligned}$$

The starting point is in $x_0 = 0 \rightarrow r_0 = ||b||$. From this previous observation it is possible to say that excessive units can be detected so that $||b||$ is minimum.

The algorithm instead of computing all the system considers only the initial contribution $||b||$ for each neuron, and then uses it as an estimate of the true contribution. Once the neuron with the smallest contribution is detected, the real linear system is computed and weights on the net are updated. It is an heuristic procedure that hopes that the initial contribution $||b||$ will be not to far from the real one.

Example $b = w_{ih} y_n$ and $A = \sum \delta_{ij} y_j^{(\mu)}$

$$h1 : ||A_1 x_1 - b_1|| = 0.1$$
$$h2 : ||A_2 x_1 - b_2|| = 1.6$$
$$h3 : ||A_3 x_1 - b_3|| = 7.6$$

From this example we can see that h_1 should be removed since the contribution of that neuron is the smallest one and it is very small. We can see that $||A_h x_h - b_h||$ measures how difference it the network removing the neuron h. The problem of this procedure is that we have to compute a lot of linear systems, one for each neuron.

The Pruning Algorithm. The pruning algorithm follows these steps:

1. Start with an over-sized trained network.
2. Repeat

   2.1 Find the hidden unit h for which $||b||$ is minimum.
   2.2 Solve the corresponding system.
   2.3 Remove unit h.

   Until Perf(pruned) − Perf(original) $< \varepsilon$
3. Reject the last reduced network.

We can formulate the goal al the pruning algorithm in this way:

$$\min_x ||Ax + b||$$

2.9 Deep Neural Networks

The philosophy based on Deep Learning is to learn a feature hierarchy from the initial pixel image in order to obtain a classifier. Each layer extracts features from the output of previous layer and it trains all layers jointly.

Figure 52: Example of deep learning process.

Shallow vs Deep Networks. Shallow architectures are inefficient at representing deep functions. A shallow network, indeed, has less number of hidden layers. A shallow network with a large enough single hidden layer can fit any function (universal approximator), but on the other hand this produces a very large hidden layer and increase a lot the number of parameters. A deep network can fit functions better with less parameters than a shallow network, increasing the number of hidden layers but decreasing the number of required parameters. Deep networks try to simulate the brain behavior, in which the electronic signals traversal different layers.

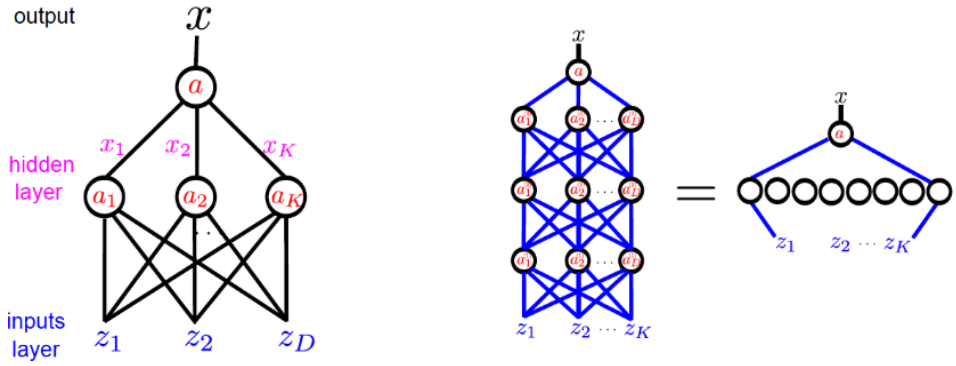


Figure 53: Shallow vs Deep Networks.

Another important aspect to notice is the fact that there's an improvement of the performances with the presence of more data.

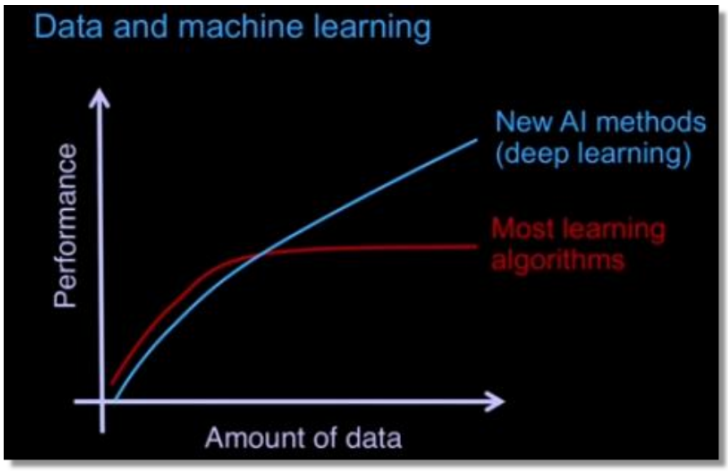


Figure 54: Performances improves with more data.

The usage of deep networks is not a current idea, it is indeed an old idea, but it has been made possible only nowadays thanks to the fact that we have more data and we have more computing power (GPUs are really good at this).
The **image classification** consists in predicting a single label (or a distribution over labels as shown here to indicate our confidence) for a given image. Images are 3-dimensional arrays of integers from 0 to 255 of size Width x Height x 3. The 3 represents the three color channels Red, Green and Blue.

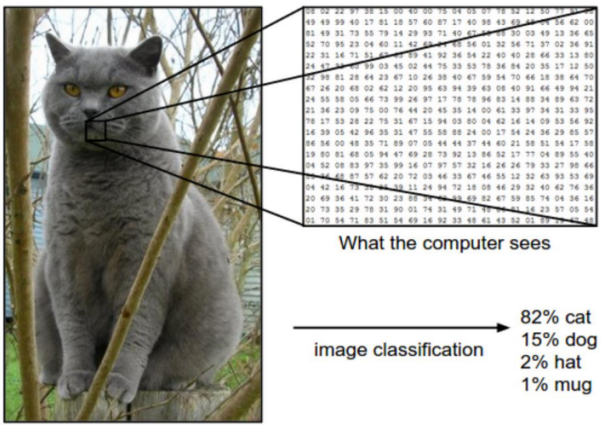


Figure 55: Image classification example.

In image classification, the most important challenges are:

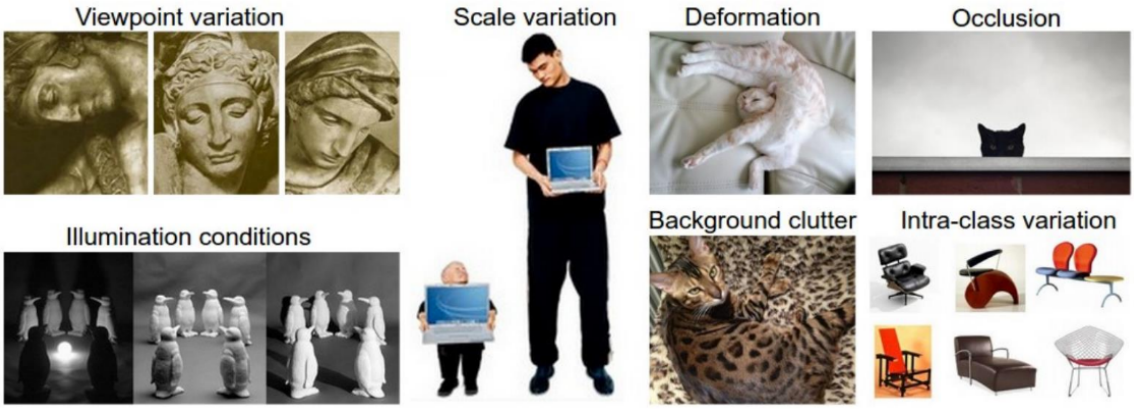


Figure 56: Challenges in image classification.

For this reason, in order to face these challenges, what we need is a data-driven approach in which we have thousands of categories and hundreds of thousand of images for each category.
As it is possible to understand, there's a difference between **traditional approach** and **deep learning**, indeed, in the first one we extract meaningful features from images through a manual process, in the second case instead, everything is automatic and there's a bunch of layers in which the final ones are useful for classification.

Convolutional Neural Networks (CNNs). Convolutional Neural Networks are used to solve OCR problems. A neural network can be defined as a **fully-connected network** or a **local-connected network**. A local-connected layer is much more specialized, and efficient, than a fully-connected layer. In a fully-connected layer each neuron is connected to every neuron in the previous layer, and each connection has it's own weight. This is a totally general purpose connection pattern and makes no assumptions about the features in the data. It's also very expensive in terms of memory (weights) and computations (connections).
In contrast, in a local-connected layer, each neuron is only connected to a few nearby neurons in the previous layer, and the same set of weights (and local connection layout) is used for every neuron. This connection pattern only makes sense for cases where the data can be interpreted as spatial with the features to be extracted being spatially local and equally likely to occur at any input position. The typical use case for local-connected layers is for image data where, as

required, the features are local (e.g. a "nose" consists of a set of nearby pixels, not spread all across the image). The fewer number of connections and weights make local-connected layers relatively cheap in terms of memory and computing power needed.

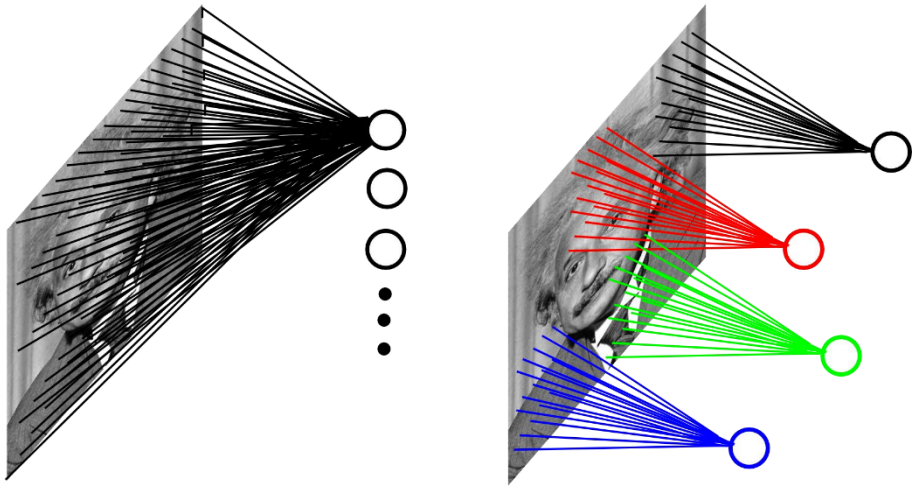


Figure 57: Fully vs local-connected networks.

Normally, several filters are packed together and learnt automaticaly during training.

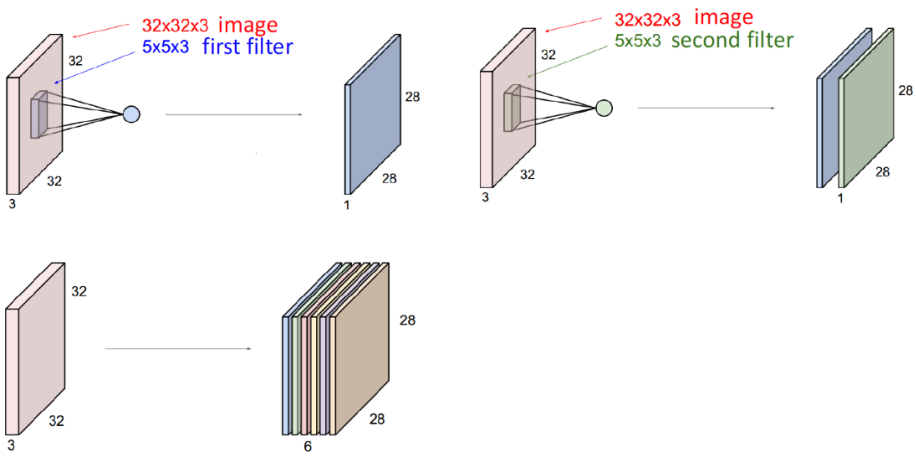


Figure 58: Using Several Trainable Filters.

Max pooling is a way to simplify the network architecture, by downsampling the number of neurons resulting from the filtering operations. In other words, the image is partitioned in small squares and for each square the maximum value pixel is taken.

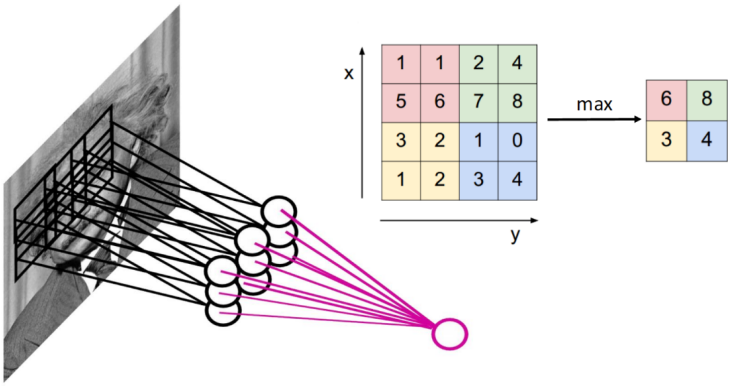


Figure 59: Max Pooling.

As we can see in the next image, a deep neural network is a combination of feature extraction and classification processes. In input we have an image, then there are some initial layers locally-connected that extract features from the image. In the final part there's the classification part and it is fully-connected.

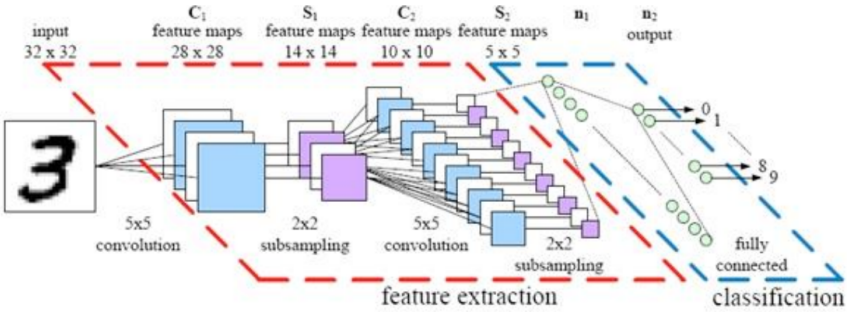
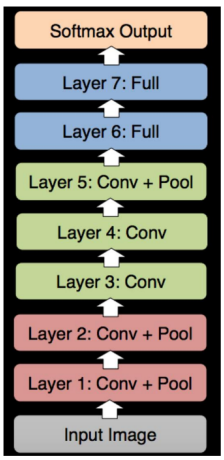


Figure 60: Combining Feature Extraction and Classification.

AlexNet Architecture. AlexNet presents 8 layers total that follows the following schema:



Going more in deep inside these layers, we can notice that:

- **1st layer:** 96 kernels ($11 \times 11 \times 3$).
- **2nd layer:** 256 kernels ($5 \times 5 \times 48$).

- **3rd layer:** 384 kernels ($3 \times 3 \times 256$).
- **4th layer:** 384 kernels ($3 \times 3 \times 192$).
- **5th layer:** 256 kernels ($3 \times 3 \times 192$).
- **6th layer:** fully connected layer with 4096 neurons.
- **7th layer:** fully connected layer with 4096 neurons.
- **8th layer:** 1000-way **SoftMax** layer.

The graphical representation of the AlexNet can be seen in the following image. There are two independent GPUs that runs in parallel and it can be noticed that there are connections between the two GPUs. The last *SoftMax* layer gives as output:

$$y_i = \frac{e^{\text{net}_i}}{\sum_j e^{\text{net}_i}}$$

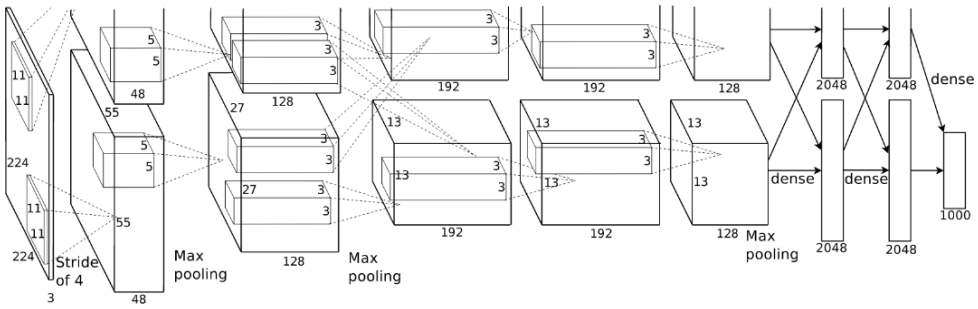


Figure 61: AlexNet architecture.

ReLU's. **ReLU** is an acronym that stands for *Rectified Linear Units*, they are used to solve the problem that sigmoid activation takes only values in $(0, 1)$. Propagating the gradient back to the initial layers, it tends to become 0 (*vanishing gradient problem*). From a practical perspective, this slows down the training procedure of the initial layers of the network. Indeed, with sigmoid the gradient will be close to 0 and the algorithm won't make progresses, in order to speed up the progress of learning, ReLU is used.

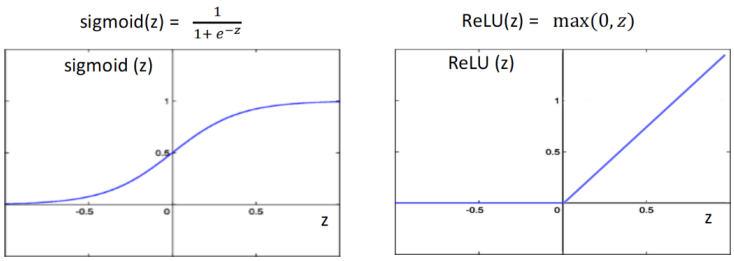


Figure 62: Comparison between sigmoid and ReLU functions.

It is possible to notice also that ReLU reaches the same results but much faster than sigmoid function. As it can be seen in the following image, the solid line represents the convergence of a 4 layer CNN with ReLUs, the dashed line instead represents an equivalent network with *tanh* neurons. It can be noticed that the CNN with ReLUs converges six times faster.

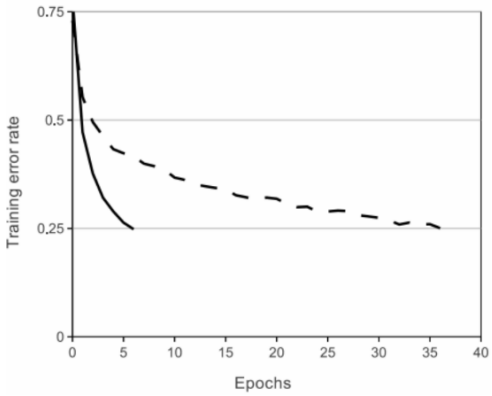


Figure 63: Convergence of ReLU neurons.

Mini-batch Stochastic Gradient Descent. We extract a random sample and we compute the gradient on it. Each time we execute it we have a different result. At each loop these steps are done:

1. Sample a batch of data (the dimension is an hyper parameter to choose).
2. Forward prop it through the graph, get loss.
3. Backprop to calculate the gradients.
4. Update the parameters using the gradient.

The easiest and most common method to reduce the overfitting on image data is to artificially enlarge the dataset using label-preserving transformations.
AlexNet uses two forms of this **data augmentation**:

- The first form consists of generating image translations and horizontal reflections (translations, scaling or rotations of the images).
- The second form consists of altering the intensities of the RGB channels in training images (introduce random noise inside the images).

Dropout. Set to 0 the output of each hidden neuron with probability 0.5. The neurons which are *"dropped out"* in this way do not contribute to the forward pass and do not participate in back-propagation. So every time an input is presented, the neural network samples a different architecture, but all these architectures share weights.
Dropout reduces complex co-adaptations of neurons, since a neuron cannot rely on the presence of particular other neurons.

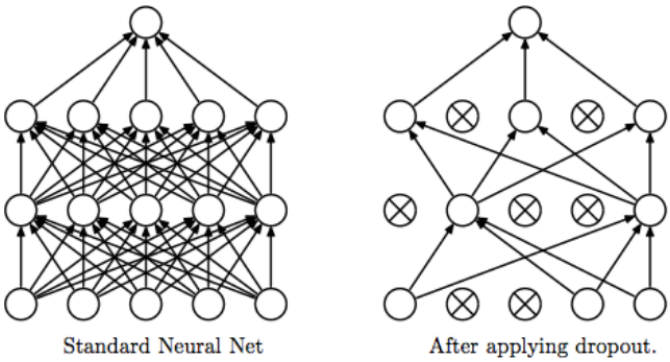


Figure 64: Dropout results

3 Statistical Learning Theory and Support Vector Machines

Statistical learning theory deals mainly with **supervised learning** problems, such that, given:

- an input (feature) space: $\mathcal{X}$
- an output (label) space: $\mathcal{Y}$ (typically $\mathcal{Y} = \{-1, +1\}$)

The question of learning amounts to estimating a functional relationship between the input and the output spaces:

$$f : \mathcal{X} \to \mathcal{Y}$$

such mapping f is called a **classifier**. In order to do this, we have access to some (labeled) training data:

$$(x_1, y_1), \ldots, (x_n, y_n) \in \mathcal{X} \times \mathcal{Y}$$

A classification algorithm is a procedure that takes the training data as input and outputs a classifier f.
In statistical learning theory, the following **assumptions** are made:

- There exists a joint probability distribution P on $\mathcal{X} \times \mathcal{Y}$. The P distribution is unknown at the time of learning.
- The training examples (x_i, y_i) are sampled independently from P (iid sampling).

Moreover:

- No assumption on the unknown distribution P.
- P is fixed.
- Non-deterministic labels due to label noise or overlapping.

What is needed is also a measure of "how good" a function f is when used as a classifier. A **loss function** measures the "cost" of classifying instance $x \in \mathcal{X}$ as $y \in \mathcal{Y}$. In other words, a loss function measures the cost of classification and miss-classification of an element. The simplest loss function in classification problems is the $0 - 1$ loss (or miss-classification error):

$$\ell(X, Y, f(X)) = \begin{cases} 1 & \text{if } f(X) \neq Y \\ 0 & \text{otherwise} \end{cases}$$

The **risk** of a function is the average loss over data points generated according to the underlying distribution P:

$$R(f) = E(\ell(X, Y, f(X)))$$

The best classifier is the one with the smallest risk $R(f)$, since it gives us a measure of goodness of the classifier.

$$R(f) = \sum_{x \in X} p(x)\ell(x, y, f(x))$$

This theoretical result cannot be computed in real experiments since the underlying distribution is unknown, and estimating it can be very expensive in a high dimensional space.
Among all possible classifiers, the best one is the **Bayes classifier**:

$$f_{\text{Bayes}}(x) = \begin{cases} 1 & \text{if } P(Y = 1|X = x) \geq 0.5 \\ -1 & \text{otherwise} \end{cases}$$

In practice, it is impossible to directly compute the Bayes classifier as the underlying probability distribution P is unknown to the learner, the idea of estimating P from data doesn't usually work.

Bayes' Theorem. The Bayes' theorem is defined by the following formula:

$$P(h|e) = \frac{P(e|h)P(h)}{P(e)} = \frac{P(e|h)P(h)}{P(e|h)P(h) + P(e|\neg h)P(\neg h)}$$

where:

- $P(h)$: prior probability of hypothesis h.
- $P(h|e)$: posterior probability of hypothesis h (in the light of evidence e).
- $P(e|h)$: "likelihood" of evidence e on hypothesis h.

3.1 The classification problem

Given:

- A set of training points $(x_1, y_1), \ldots, (x_n, y_n) \in \mathcal{X} \times \mathcal{Y}$ drawn iid from an unknown distribution P.
- A loss function.

Determine a function $f : \mathcal{X} \to \mathcal{Y}$ which has risk $R(f)$ as close as possible to the risk of the Bayes classifier. Since we don't known the distribution of P it is impossible to compute the Bayes error and the risk of a function f.

NN Classifier It is a non-parametric method used for classification. Given a new point to be classified x, the NN classifier search in the training set for the closest point z to x and assign the same label of z to x. Positions in the space of the training points define a partition of the input space (decision regions). The resulting partition follows the property of the **Voronoi Tessellation**. The assumption made by the NN classifier is that the training set is fixed, no updates are done during test, otherwise it is necessary to re-train it.
An extension of this classifier is called **KNN** which, instead of considering only the closest point, it considers the k-closest points to x and assigns the class with the greater number of voting. This is done in order to improve the robustness of the classifier.
In summary we have the following variations of NN:

- k-NN rule: use the k nearest neighbors and take a majority vote.
- k_n-NN rule: the same as above, for k_n growing with n.

With the NN classifier basically we don't have learning and so we have two fundamental problems:

- **Search problem**, require an efficient algorithm to find the closest points.
- **Storage**, in order to work with the entire training set it must be loaded in memory.

Estimate P One of the assumptions that we said at the beginning is that the probability distribution P is unknown, but we can think to estimate it. A good estimator is:

$$P(x) = \frac{\frac{K}{n}}{V}$$

where V is the volume and K is the number of observations in V. We know that each observation has probability $\frac{1}{nv}$. From this we can think that when $n \to \infty$ and $K(n) \to \infty$ the estimate density is equal to the real density, of course it can be computationally expensive in very high dimensional space.

3.2 How good is the NN rule?.

Cover and Thomas showed that:

$$R(f_{bayes}) \leq R_\infty \leq 2R(f_{Bayes})$$

where R_∞ denotes the expected error rate of NN when the sample size tends to infinity. Remember that $R(f_{bayes})$ is the lower bound since we said that the Bayes classifier is the best one. We cannot say anything stronger as there are probability distributions for which the performance of the NN rule achieves either the upper or lower bound.

Theorem 3.1 (Stone Theorem (1977))**.** *If $n \to \infty$ and $k \to \infty$, such that $k/n \to 0$, then for all probability distributions $R(k_n\text{-}NN) \to R(f_{Bayes})$ (that is, the k_n-NN rule is "universally Bayes consistent")*

The Empirical Risk Minimization principle. Instead of looking for a function which minimizes the true risk $R(f)$, we try to find one which minimizes the **empirical risk**:

$$R_{\text{emp}}(f) = \frac{1}{n}\sum_{i=1}^{n} \ell\left(X_i, Y_i, f\left(X_i\right)\right)$$

Given training data $(x_1, y_1), \ldots, (x_n, y_n) \in \mathcal{X} \times \mathcal{Y}$, a function space $\mathcal{F}$, and a loss function, we define the classifier f_n as:

$$f_n = \operatorname*{argmin}_{f \in \mathcal{F}} \mathrm{R}_{\text{emp}}(f)$$

This approach is called the **empirical risk minimization** (ERM) induction principle, the motivation of which comes from the law of large numbers.

3.3 Estimation vs approximation

Ideally we want to make $R(f_n) - R(f_{Bayes})$ as small as possible, as $n \to \infty$. Denoting by $f_{\mathcal{F}}$ the best classifier in $\mathcal{F}$, the difference can be decomposed as:

$$R\left(f_n\right) - R\left(f_{Bayes}\right) = \underbrace{\left(R\left(f_n\right) - R\left(f_{\mathcal{F}}\right)\right)}_{\text{estimation error}} + \underbrace{\left(R\left(f_{\mathcal{F}}\right) - R\left(f_{\text{Bayes}}\right)\right)}_{\text{approximation error}}$$

- $R(f_n)$ is the risk of my classifier.
- $R(f_{\mathcal{F}})$ is the risk of the best classifier f on the family $\mathcal{F}$.
- $R\left(f_{\text{Bayes}}\right)$ is the risk of the best classifier.

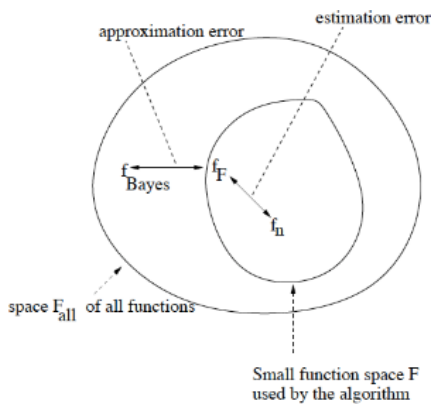


Figure 65: Estimation vs approximation.

According to the complexity of $\mathcal{F}$ we can have:

- small complexity of $\mathcal{F}$: small estimation error, large approximation error (*underfitting*)
- large complexity of $\mathcal{F}$: large estimation error, small approximation error (*overfitting*)

The best overall risk is achieved for "moderate" complexity.

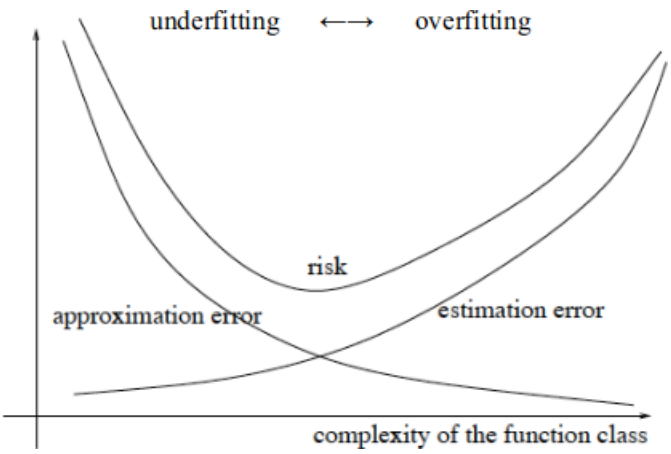


Figure 66: Underfitting vs Overfitting graph

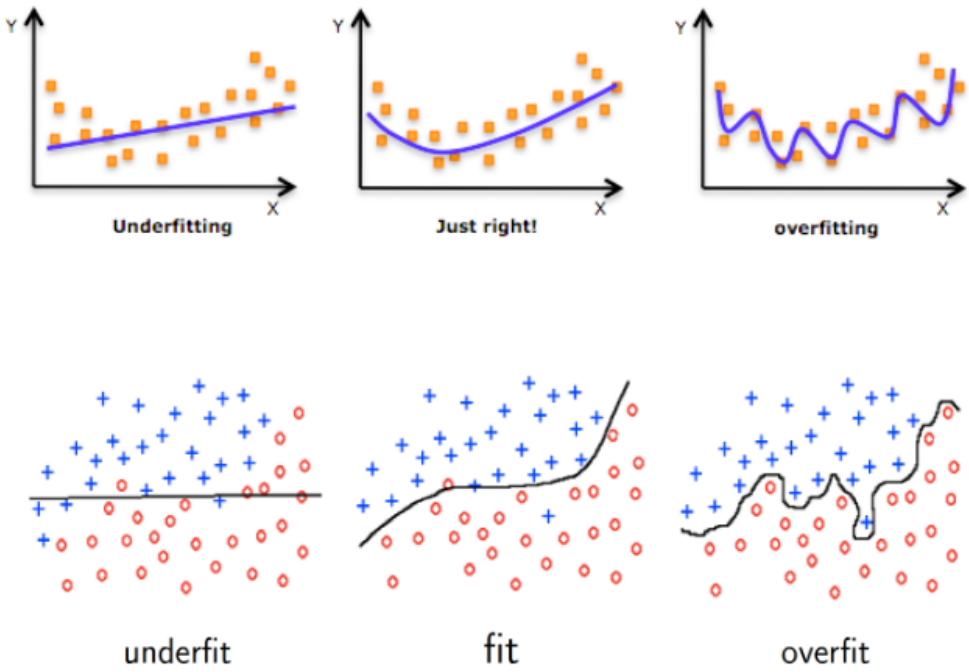
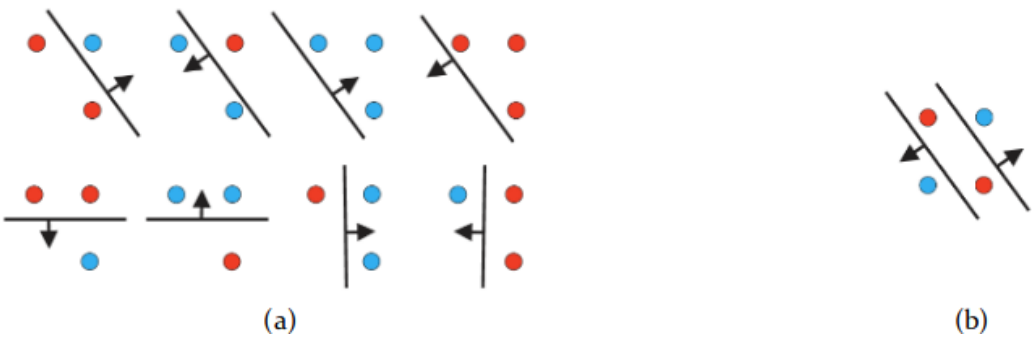


Figure 67: Model selection.

Shattering. A set of n instances $x_1, \ldots, x_n$ from the input space $\mathcal{X}$ is said to be *shattered* by a function class $\mathcal{F}$ if all the 2^n labelings of them can be generated using functions from $\mathcal{F}$.
For instance, with $\mathcal{F}$ as a linear decision functions (straight lines) in the plane, we can have:

(a) Any set of 3 non-collinear points shatters $\mathcal{F}$

(b) No set of 4 points can shatter $\mathcal{F}$



The VC dimension. The **VC dimension** of a function class $\mathcal{F}$, denoted $VC(\mathcal{F})$, is the largest integer h such that there exists a sample of size h which is shattered by $\mathcal{F}$. It is a measure of complexity of a function class.
If arbitrarily large samples can be shattered, then $VC(\mathcal{F}) = \infty$.
For example:

- $\mathcal{F}$ = linear decision functions in $\mathbb{R}^2 \to VC(\mathcal{F}) = 3$
- $\mathcal{F}$ = linear decision functions (hyperplanes) in $\mathbb{R}^n \to VC(\mathcal{F}) = n + 1$
- $\mathcal{F}$ = multi-layer perceptrons with W weights $\to VC(\mathcal{F}) = O(W \ \log(W))$
- $\mathcal{F}$ = nearest neighbor classifiers $\to VC(\mathcal{F}) = \infty$

The VC dimension for the classifier depends on the dimension of space that your data points belong to. In your problem, if your mean $x \in \mathbb{R}^2$, then the VC dimension is 3. For $\mathbb{R}^2$, you can always shatter any three general position points ("general position" means they do not coincidentally lie on the same line). For instance, consider three points $(0,0)$, $(0,1)$, $(1,0)$. No matter how you assign labels to them, you can always separate them by a line. If you consider three points $(0,0)$, $(0,1)$, $(1,0)$, $(1,1)$ with label $[+,-,-,+]$, this is the "xor" case which cannot be separated by a line. For $x \in \mathbb{R}$, then the VC dimension is 2 because you cannot separate $+-+$. In general for $x \in \mathbb{R}^d$, the VC dimension for a linear classifier is $d + 1$.

The VC dimension is in general not related to the number of free parameters of a model.
For all $f \in \mathcal{F}$, with probability at least $1 - \delta$, we have:

$$R(f) \leq R_{\text{emp}}(f) + \underbrace{\sqrt{\frac{h(\log(2n/h) + 1) - \log(\delta/4)}{n}}}_{\text{VC confidence}}$$

where $h = VC(\mathcal{F})$ is the VC dimension of the family F, δ is a tolerant parameter, and n is the sample size. We can read this results as:

With probability approaching 1, no matter what the unknown probability distribution, given more and more data, the expected error for the functions that ERM endorses at each stage eventually approaches the minimum value of expected error of the functions in $\mathcal{F}$ if and only if $\mathcal{F}$ has finite VC dimension. If VC dimension is equal to ∞, like in the KNN case, we have that $R_{emp}(f) = 0$ and so $R(f) \leq \infty$ which is meaningless.

Another key of reading is that since the second term $R_{\text{emp}} \ldots$ is an upper bound, if it is small so also $R(f)$ will be. This result is fundamental due to the fact that we have no knowledge about P and so we cannot compute $R(f)$, but we can have a bound for it using the second quantity. Indirectly we want to reduce the bound so that at the end the resulting risk is minimized.

Structural Risk minimization. It is a general framework for choosing the best classifier. Empirical Risk Minimization takes only care of the *estimation* error (variance) but it is not concerned with the **approximation error** (bias). The optimal model is found by striking a balance between the empirical risk and the capacity of the function class $\mathcal{F}$ (ex: the VC dimension).
The basic idea of *Structural Risk Minimization* (SRM) is:

1. Construct a nested structure for family of function classes $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \dots$ with non-decreasing VC dimension ($VC(\mathcal{F}_1) \leq VC(\mathcal{F}_2) \leq \dots$)
2. For each class $\mathcal{F}_i$, find the solution f_i that minimizes the empirical risk.
3. Choose the function class $\mathcal{F}_i$, and the corresponding solution f_i that minimizes the risk bound (= empirical risk + VC confidence)

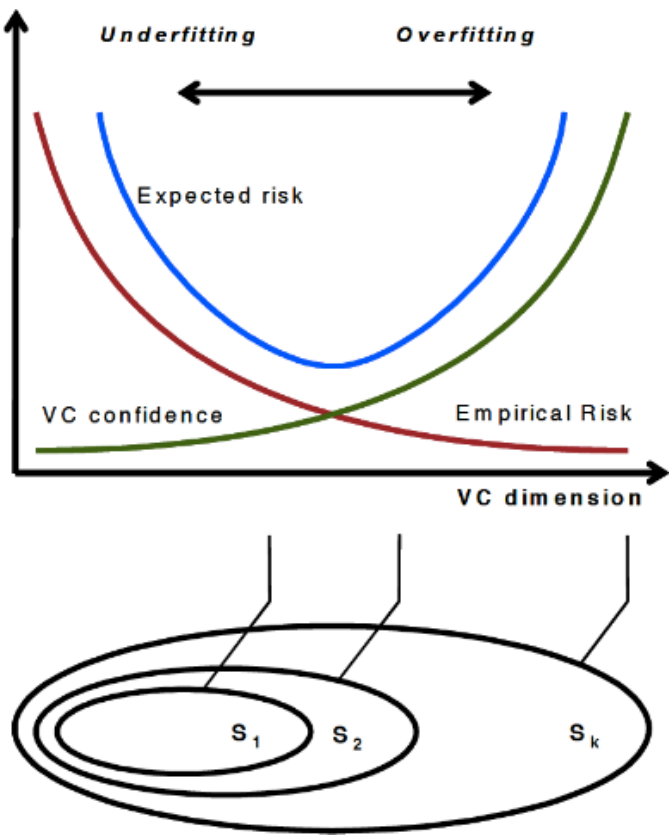


Figure 68: Structural risk minimization.

3.4 Support Vector Machine

In this section we are going to deal with a very well known supervised learning algorithm, called **Support Vector Machine**. We will see that it can be written as an intuitive optimization problem and can be easily extended to work very well with non-linear patterns or in high dimensional spaces.

SVM belongs to the class of discriminative classifiers since its goal consists on learning the class boundary between the two classes y starting from features x. From now, we'll use $y \in \{-1, 1\}$ to denote the class labels. We can formally define the SVM linear classifier in this way:

$$h_{w,b}(x) = g(w^T x + b)$$

$$g(z) = \begin{cases} 1 & \text{if} \quad z \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

Where $w^T + b$ represents a **separating hyperplane** for the two classes, and $g(z)$ is the decision function which returns the predicted class for the observation x. In our problem the classifier would then predict 1 if $h_{w,b}(x) \geq 0$, which is equivalent of considering $w^T x + b \geq 0$, and -1 otherwise. We define the probability of classification given an observation x as:

$$p(y = 1|x; w, b)$$

This quantity over here represent the confidence of our classifier on assigning the label 1 to the input value x. We can also say that the larger $w^T x + b$ is, the higher is the confidence that the label is 1. Remember that the function g is our decision function, so if we are strongly distant from the 0 we have high confidence of the class 1, otherwise if we are close to the 0 the function g assigns the label 1 but now the confidence is lower. In other words this probability represent the confidence about the algorithm classification.
This result is a consequence of the fact that if $w^T x + b$ increase then also $h_{w,b}(x) = p(y = 1|x; w, b)$ becomes larger. The same thing is valid with label -1, in this case we would like to have $w^T x + b$ as small as possible $w^T x + b \ll 0$.

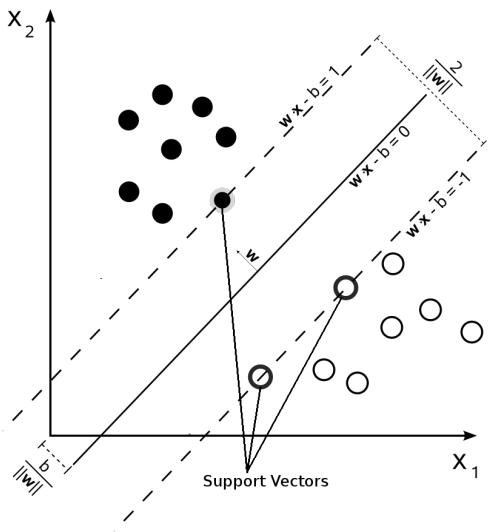


Figure 69: Support Vector Machines classifier

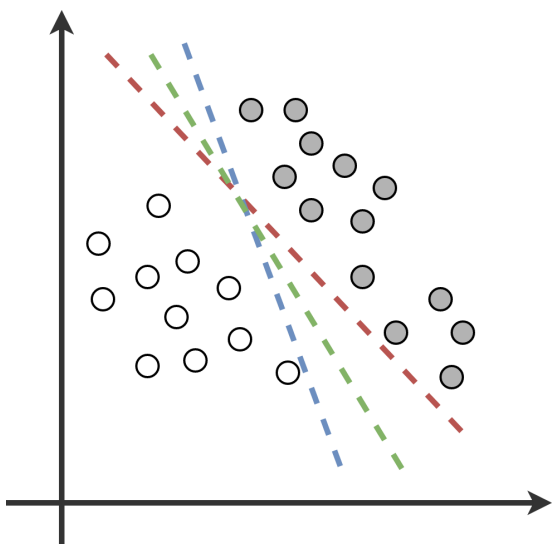


Figure 70: Possible separating hyperplanes

Figure 69 shows an application of a SVM classifier. In this example we have two classes 1 and -1 represented in a 2 dimensional space using respectively filled points and empty ones. The line given by the equation $w^T x + b = 0$ defines the **separate hyperplane** which works as a **decision boundary** of our problem. Points that below the plane are labeled with $y = -1$, since $w^T x + b < 0$, otherwise they are labeled with $y = 1$.

Considering Figure 70 we can notice that we can define different separating hyperplanes, and all of them provides 100% of accuracy on this training set. This concept introduces a problem which must be considered: *Which is the right hyperplane?* In general it is possible to find an infinite number of hyperplanes that separate the two classes, but they can produce different results/performance and also they can have effects on the robustness of the classifier.
Before going in details of the best hyperplane it is necessary to introduce the following concepts: **functional margin** and **geometric margin**.

Functional margin It is a testing function that verifies if a particular point is properly classified or not.

$$\hat{\gamma}^{(i)} = y^{(i)}(w^T x^{(i)} + b)$$

When $\hat{\gamma}^{(i)} > 0$ the prediction of the observation i is correct, and the larger is the functional margin result the greater is the confidence of the current prediction. However it cannot be considered as a very good measure of confidence since it is affected by the length of the two vectors w, b. In fact, considering the pair $(\alpha w, \alpha b)$ we can notice that the new functional margin is multiplied by the factor α. For that reason could be reasonable to set $||w||_2 = 1$, but we will discuss about it later.

Geometric margin It represents the euclidean distance between a point and the decision boundary.

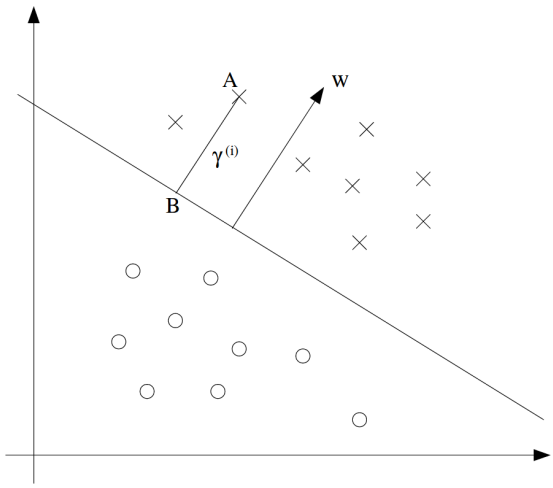


Figure 71: Geometric margin

Considering the previous figure, A is a point representing the ith observation and B is a point on the straight line defined by $w^T B + b = 0$. We can so define the geometrical margin $\gamma^{(i)}$ as the length of the segment AB.

Now that we have defined the notion of geometric and functional margin it is possible to give an idea of which is the best hyperplane. This concept, as we are going to see, is strictly related to

the two margins. We define the **geometric margin** γ and the **functional margin** $\hat{\gamma}$ respect to the training set $S = \{(x^{(i)}, y^{(i)}); i = 1, \dots, m\}$ the following value:

$$\gamma = \min_{i=1,\dots,m} \gamma^{(i)}$$

$$\hat{\gamma} = \min_{i=1,\dots,m} \hat{\gamma}^{(i)}$$

This values γ represents the distance from the decision boundary to the closest point, and it is also called **margin**. Distance to the closest training point is called the margin. An interesting property of the geometric margin is that it is related with the functional margin by the following definition: $\gamma = \frac{\hat{\gamma}}{||w||}$.
The idea of an SVM classifier is to find a separating hyperplane which **maximizes the geometric margin**. The resulting hyperplane is so considered as the best one since it separates better then other ones the two classes. Intuitively, the farthest is the boundary from the points, the greater is the confidence.
Formally speaking the main goal of Support Vector Machine is to solve the following optimization problem:

$$\begin{aligned} &\max_{\gamma,w,b} \quad \gamma \\ &\text{s.t.} \quad y^{(i)}(w^T x^{(i)} + b) \geq \gamma \qquad i = 1, \dots, m \\ &||w|| = 1 \end{aligned}$$

where $y^{(i)}(w^T x^{(i)} + b) \geq \gamma$ means that points must have minimum distance γ from the decision boundary. The constraint $||w|| = 1$, that we have seen previously, is now introduced to enforce that the functional margin is equal to the geometric one, so that the problem can be rewritten as:

$$\begin{aligned} &\max_{\hat{\gamma},w,b} \quad \frac{\hat{\gamma}}{||w||} \\ &\text{s.t.} \quad y^{(i)}(w^T x^{(i)} + b) \geq \hat{\gamma} \qquad i = 1, \dots, m \end{aligned}$$

Now the non-convex constraint $||w|| = 1$ is introduced directly inside the target function and instead of considering the geometric margin the optimization problem is re-formulated in terms of functional margin. Now imposing the scaling constraint $\hat{\gamma} = 1$ it is possible to rewrite the same optimization problem as a minimization of $||w||^2$:

$$\begin{aligned} &\min_{\gamma,w,b} \quad \frac{1}{2}||w||^2 \\ &\text{s.t.} \quad y^{(i)}(w^T x^{(i)} + b) \geq 1 \qquad i = 1, \dots, m \end{aligned} \tag{1}$$

This formulation represent an optimization problem on a convex function and with only linear constraints. Due to the nature of the problem we have a unique minimum solution which represents **optimal margin classifier**. An interesting thing of SVM is that it does not require to check for all the points, but it considers only the support vectors. They are showed in Figure 69 and they represents the points with distance equal to the minimum margin from the decision boundary. SVM is only affected by these points, all the other ones can move freely. The advantage of SVM is that instead of considering all the possible points SV from the training set it considers only these points to determine the decision boundary.

In order to solve constrained Problem 1 we introduce the concept of Lagrange multipliers. Using the **Lagrange** function with N Lagrange multipliers $\Lambda = (\lambda_1, \dots, \lambda_N)$ it is possible to rewrite the correspondent optimization problem, with parameters w and b, into an identical one but with

parameters $(\lambda_1, \ldots, \lambda_N)$. Taking advantage of the dual representation, that allows to convert an original min/max problem into another one which is equivalent but with max/min formulation, we can write the new optimization problem as follow:

$$L(w, b, \Lambda) = \frac{1}{2}||w||^2 - \underbrace{\sum_{i=1}^{N} \lambda_i [y_i(w^T x_i + b) - 1]}_{\text{Sum of constraints}} \tag{2}$$

Note that thanks to the dual representation we have converted a constrained problem into an unconstrained one (which is easier to solve).

Convert constrained P into an unconstrained one Given the following constrained optimization problem:

$$\begin{aligned} &\min \ f(x) \\ &\text{s.t. } x \in \mathcal{D} \end{aligned} \tag{3}$$

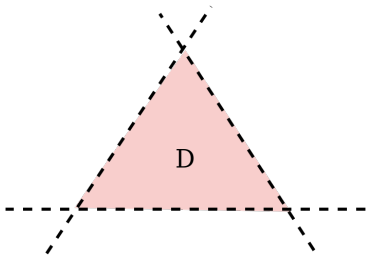


Figure 72: Constrained space for the Optimization Problem 3.

The unconstrained version can be defined:

$$\begin{aligned} &\min \ f(x) \\ &\text{s.t. } x \in \mathbb{R}^n \end{aligned} \tag{4}$$

Of course the solutions of problems 3 and 4 can be different. For that reason we can introduce a new formulation that tries to produce the same results:

$$\begin{aligned} &\min \ f(x) + \lambda p(x) \\ &\text{s.t. } x \in \mathbb{R}^n \end{aligned} \tag{5}$$

where $p(x)$ is a penalty function equal to 0 if $x \in \mathcal{D}$, otherwise it is greater than 0. The greater is the distance from $\mathcal{D}$ the greater is the penalty. The advantage of this formulation is that now we have an unconstrained problem. The same idea is adopted by the dual representation with Lagrangian Multipliers.

The goal is to find a function parameterized only by Lagrangian Multipliers. Setting the derivatives of $L(w, b, \Lambda)$ to zero:

$$\frac{\partial L(w, b, \Lambda)}{\partial w} = w - \sum_{i=1}^{N} \lambda_i y_i x_i = 0 \qquad \Longrightarrow \qquad w = \sum_{i=1}^{N} \lambda_i y_i x_i$$

$$\frac{\partial L(w, b, \Lambda)}{\partial b} = \sum_{i=1}^{N} \lambda_i y_i = 0$$

We obtain a new formulation of the optimization problem expressed with only lagrangian multipliers:

$$\begin{aligned} \max \quad & L_D(\lambda_1, \ldots, \lambda_m) = \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \lambda_i \lambda_j y_i y_j x_i^T x_j \\ \text{s.t.} \quad & \sum_{i=1}^{m} \lambda_i y_i = 0 \qquad \lambda_i \geq 0, \forall i = 1, \ldots, m \end{aligned}$$

Note that the training vectors appears only as *dot products*, and the advantage of using this formulation is that only support vectors will have Lagrange multipliers such that $\lambda_i > 0$ and the others will be essentially equal to zero (sparse solution). The SVM complexity is given only by the support vectors. Now the maximum margin hyperplane is given by:

$$\sum_{i=1}^{m} y_i \lambda_i x_i^T x + b = 0$$

If $\Lambda = (\lambda_1, \ldots, \lambda_N)$ is the solution of the dual optimization problem, then:

- The weight vector of the maximum margin hyperplane is: $w = \sum_{i=1}^{N} y_i \lambda_i x_i$
- The corresponding discriminant function (separating hyperplane) is:

$$f(x) = w^T x + b = \sum_{i=1}^{N} y_i \lambda_i x_i^T x_i + b$$

- The linear SVM classifier $g : \mathbb{R}^n \to \{-1, 1\}$ is:

$$g(x) = \text{sign}(w^T x + b = \sum_{i=1}^{N} y_i \lambda_i x_i^T x_i + b)$$

For support vector we have:

$$y_i(\sum_{i=1}^{N} y_i \lambda_i x_i^T x_i + b) = \gamma$$

For simplicity we consider $\gamma = 1$. Since SVM is affected only by support vectors we can derive:

$$b = \frac{1}{|SV|} \sum_{i \in SV} (y_i - \sum_{j=1}^{N} y_j \lambda_j x_j^T x_i)$$

where SV is the set of support vectors.

3.4.1 SVM error function

The generic loss function adopted for training a support vector machine is the **Hinge loss function**.

$$L_{\text{hinge}} = \max\{0, 1 - y_i f(x_i)\}$$

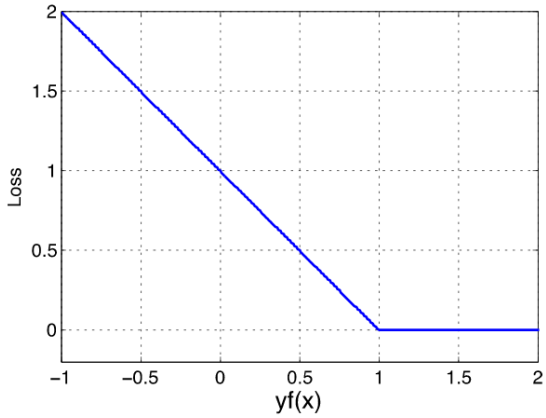


Figure 73: Hinge loss function.

$$E = \sum_{i=1}^{N} \max\{0, 1 - y_i f(x_i)\} + \frac{1}{2} \sum_{j=1}^{d} w_j^2$$

- $\sum_{i=1}^{N} \max\{0, 1 - y_i f(x_i)\}$, hinge loss function over all data points.
- $\frac{1}{2} \sum_{j=1}^{d} w_j^2$, proportional to the inverse of the margin.

Notice that the hinge loss function is not differentiable on 1, we can't apply the gradient descent procedure. The solution of this problem consists on using **quadratic programming (QP)** algorithms, since E is a quadratic function with linear constraints.

3.4.2 SVM's and the VC dimension

Theorem (Vapnik) Consider hyperplanes $w^T x + b = 0$ in canonical form, that is such that:

$$\min_{1 \leq i \leq N} |w^T x_i + b| = \gamma = 1$$

Then the set of decision functions $g(x) = sgn(w^T x + b = 0)$ that satisfy the constraint $||w|| < \gamma$ has a VC dimension h satisfying:

$$h \leq R^2 \gamma^2$$

where R is the smallest radius of the sphere around the origin containing all the training points. Note that dropping the condition $||w|| < \gamma$ leads to a VC dimension equal to $n + 1$. Hence, the constraint allows us to work in high-dimension spaces.
From the previous theorem and from:

$$R(f) \leq R_{\text{emp}}(f) + \sqrt{\frac{h(\log(\frac{2n}{h}) + 1) - \log(\frac{\sigma}{4})}{n}}$$

we have:

- By maximizing the margin, or equivalent by minimizing $||w||$, we are in fact minimizing the VC dimension of the SVM.

- The minimization of the expected risk depends on both minimizing the empirical risk and the confidence interval.
- The confidence interval depends mainly on the ratio $\frac{h}{n}$.
- SVM algorithm minimizes both the empirical risk and the confidence interval.
- SVM directly implements the structural risk minimization principle.

3.4.3 Outliers: soft margins

One of the problem of SVM is to make decisions in presence of outliers.

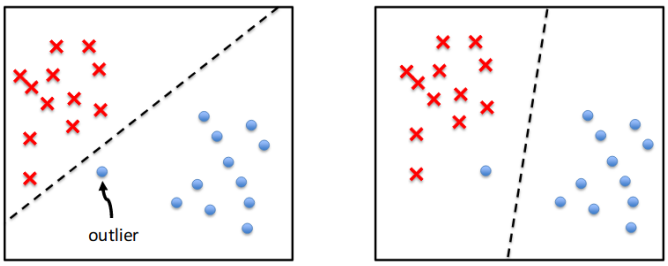


Figure 74: Outliers effects on an SVM.

In the previous image is showed the effect that can have a single outlier. We can make two types of decision: correct classify it reducing the robustness of the classifier, or leave it miss-classified. The strategy which is commonly adopted is the second one, otherwise with the first one we can find decision boundaries that work very well on the training set, but they does not provide optimal performance during testing. In order to reduce the effects of miss-classification we adopt some **slack variables**, useful for allowing some errors in the boundary.

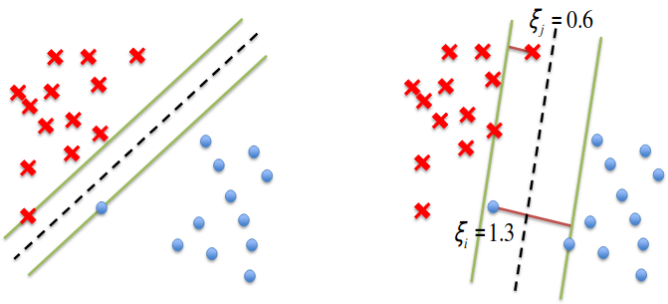


Figure 75: Outliers effects on an SVM with slack variables.

Now the optimization problem can be re-formulated:

$$\begin{aligned}
&\text{minimize} \frac{1}{2}||w||^2 + C\sum_{i=1}^{N}\xi_i \\
&\text{subject to } y_i(w^T x_i - b) \geq 1 - \xi_i \\
&\xi_i \geq 0 \qquad i = 1, \ldots, N
\end{aligned}$$

The only parameter C controls the tradeoff between the accuracy with respect to the training data and the maximization of the margin. It can be interpreted also as a regularization term:

- small C allows constraints to be easily ignored *(large margin)*.

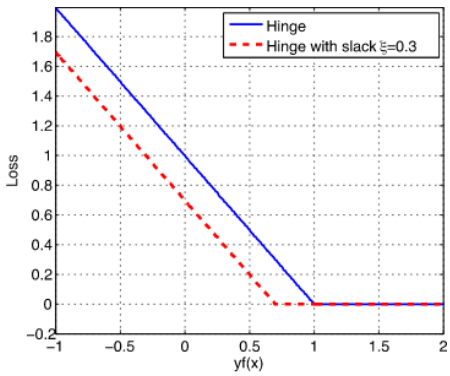
- large C makes constraints hard to ignore *(narrow margin)*.
- $C = \infty$ enforces all constraints *(hard margin)*.

The dual representation of the problem can be reformulated as follows:

$$\begin{aligned}
\max \quad & L_D(\lambda_1, \ldots, \lambda_m) = \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \lambda_i \lambda_j y_i y_j x_i^T x_j \\
\text{s.t.} \quad & \sum_{i=1}^{m} \lambda_i y_i = 0 \qquad \lambda_i \geq 0, \forall i = 1, \ldots, m \\
& 0 \leq \lambda_i \leq C \qquad \forall i = 1, \ldots, N
\end{aligned}$$

The hyperplanes whose weights vector solves this quadratic optimization problem are called the **soft margin hyperplanes**. The soft-margin optimization problem is equivalent to that of the maximum margin hyperplanes with the additional constraint $\lambda_i \leq C$ (box constraints). This approach limits the effect of the outliers (for which λ_i tends to be large).

$$L_{hinge} = \max \left\{ 0, 1 - y_i f(\mathbf{x}_i) - \xi_i \right\},$$



$$E = \sum_{i=1}^{N} \max \left\{ 0, 1 - y_i f(\mathbf{x}_i) - \underbrace{\xi_i}_{\text{slack}} \right\} + \frac{1}{2} \sum_{j=1}^{d} w_j^2 + \underbrace{C \sum_{i=1}^{N} \xi_i}_{\text{penalty for using slack}}$$

Figure 76: Hinge loss function with slack variables.

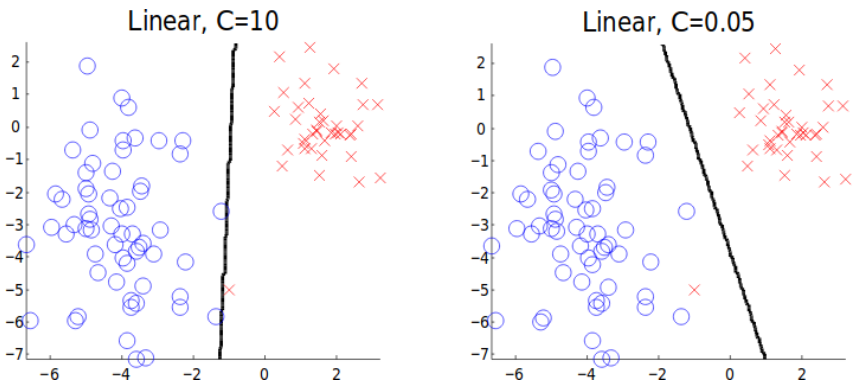


Figure 77: Effect of C on the decision boundary.

3.4.4 Kernel Trick

Until now we worked with the assumption that the space is linearly separable, but SVM allows a strategy called **kernel trick** for learning a possible separating hyperplane in a new space. In some cases could be interesting or evaluating not the original space but a transformation of it, for instance when in the original space data points are not linearly separable. We define a function $\phi(x)$ as the function that applies a mapping of a feature vector to another one. The SVM algorithm now instead of considering the vector x learns using the resulting vector of $\phi(x)$. A **kernel** function is nothing else that an inner product between feature mappings of ϕ:

$$K(x, z) = \phi(x)^T \phi(z)$$

Cover's Theorem *A complex pattern-classification problem cast in a high-dimensional space non-linearly is more likely to be linearly separable than in a low-dimension space.*

The power of SVM's resides in the fact that they represent a robust and efficient implementation of Cover's theorem. Informally speaking a kernel function is a similarity measure between the feature mapping x and z. The advantage of using this technique is that it allows to learn in the high dimensional feature space of a transformation of it defining a function ϕ. Since the SVM algorithm works with only inner products between input vectors (x,z), then we can replace the simple inner product with a kernel function in order to learn in a different feature space that in some cases could be more efficient. But there is a restriction on the function K, it must satisfy the following property in order to be considered a **valid kernel**:

$$K(x, z) = \phi(x)^T \phi(z) \qquad \forall x, z \in S$$

This property of the kernel is also called **Mercer's condition**.
Another interesting property is the positivity of a kernel:

Definition A symmetric function $K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is said to be **positive definite kernel** if:

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j K(x_i, x_j) \geq 0 \qquad c_i, c_j \in \mathbb{R}$$

It will be possible to deal with several positive definite kernels, for instance:

- **Linear**: $K(x_i, x_j) = x_i^T x_j$
- **Polynomial of degree 2**: $K(x_i, x_j) = (1 + x_i^T x_j)^2$
- **Gaussian Radial Basis Function** (RBF): $K(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right)$

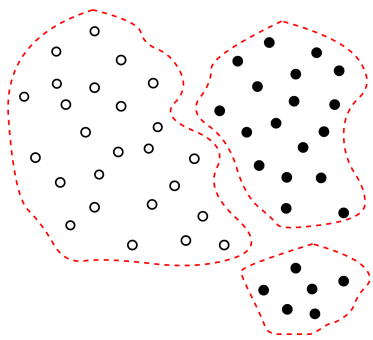


Figure 80: SVM: Radial Basis Function Kernel

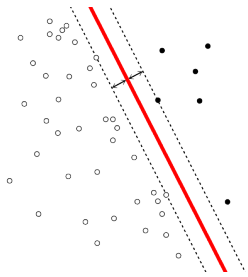


Figure 78: SVM: Linear Kernel

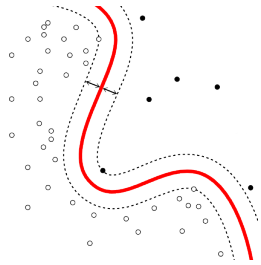


Figure 79: SVM: Polynomial Kernel

Nonlinear SVM's operate in two stages:

- Perform a non-linear mapping of the feature vector x onto a high-dimensional space that is hidden from the inputs or the outputs.
- Construct an optimal separating hyperplane in the high-dimensional space.

$$\begin{aligned} \max \quad & L_D(\lambda_1, \ldots, \lambda_N) = \sum_{i=1}^{N} \lambda_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \lambda_i \lambda_j y_i y_j x_i^T x_j \\ \text{s.t.} \quad & \sum_{i=1}^{N} \lambda_i y_i = 0 \qquad 0 \leq \lambda_i \leq C, \quad \forall i = 1, \ldots, N \end{aligned}$$

The discriminant function obtained from the solution is:

$$f(x) = \sum_{i=1}^{N} y_i \lambda_i x_i^T x + b$$

Suppose we first mapped the data to some other (possibly infinite dimensional) Euclidean space, using a mapping:

$$x \to \phi(x) \qquad K(x, y) = \phi(x)^T \phi(y)$$

$$\begin{aligned} \max \quad & L_D(\lambda_1, \ldots, \lambda_N) = \sum_{i=1}^{N} \lambda_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \lambda_i \lambda_j y_i y_j K(x_i, x_j) \\ \text{s.t.} \quad & \sum_{i=1}^{N} \lambda_i y_i = 0 \qquad 0 \leq \lambda_i \leq C, \quad \forall i = 1, \ldots, N \end{aligned}$$

$$f(x) = \sum_{i=1}^{N} y_i \lambda_i K(x_i, x) + b$$

Note that is not necessary to compute $\phi(x)$.

3.5 Multi-class problems

Until now we have discussed about the application of an SVM just using two labels $y \in \{-1, 1\}$. But in real case we can have more than two classes and we have to make an SVM which is able to assign input vector to one of the K classes. In other words, we have to find a decision rule that divides the input space into K decision regions separated by decision boundaries.

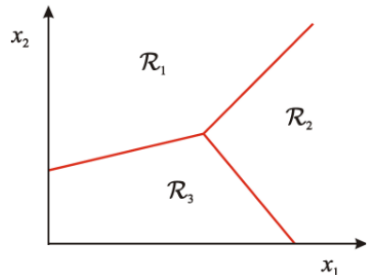


Figure 81: Space separation for 3 classes.

We can apply to distinct strategies:

- **One-vs-the rest classifiers**, train $K-1$ classifiers each of which solves a two-class problem of separating points in a particular class from points not in that class.
- **One-vs-one classifiers**, train $k(k-1)/2$ binary classifiers, one for every possible pairs of classes.

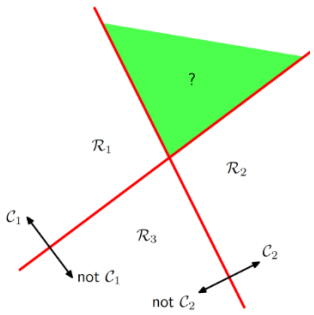


Figure 82: One-vs-the-rest classifiers.

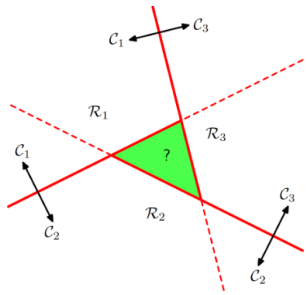


Figure 83: One-vs-one classifier.

The classical approach consists on training K one-vs-the rest classifiers and then the classification is done choosing the class with the most positive score.

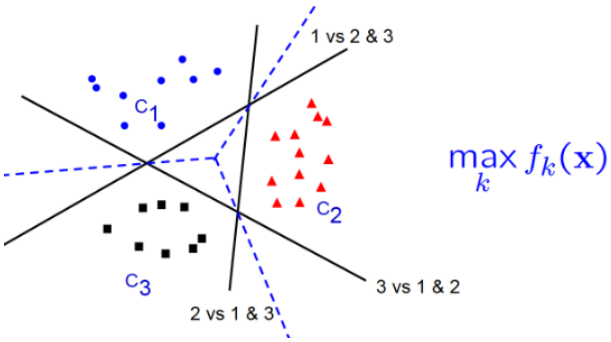


Figure 84: Decision boundaries on typical approaches.

4 Unsupervised Learning

The classical clustering problem starts with a set of n objects and an $n \times n$ matrix A of pairwise similarities that gives us an edge-weighted graph G. The goal of the clustering problem is to partition the vertices of G into maximally homogeneous groups (clusters). Usually the graph G is an undirected graph.

Figure 85: The "classical" clustering problem.

4.1 K-means

K-means is an iterative clustering algorithm that follows these steps:

- **Initialize:** pick K random points as cluster centers.

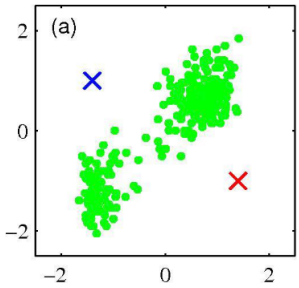


Figure 86: Initialization with $K = 2$.

- **Alternate:**
  1. assign data points to closest cluster center.
  2. change the cluster center to the average of its assigned points.

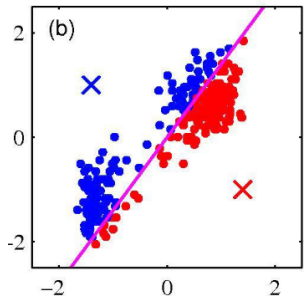


Figure 87: Iterative step 1.

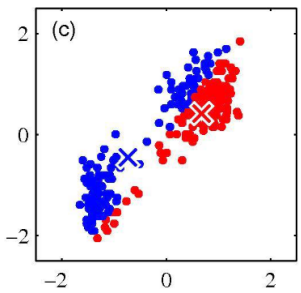


Figure 88: Iterative step 2.

- **Stop:** when no points' assignments change.

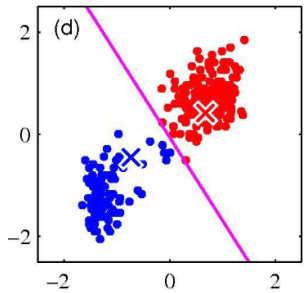


Figure 89: Repeat until convergence.

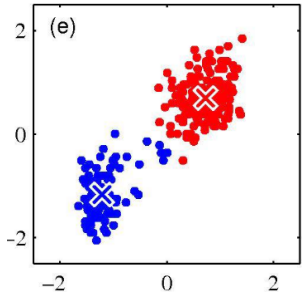


Figure 90: Final output.

Properties of K-means. K-means has the following properties:

- It is guaranteed to converge in a finite number of steps.
- It minimizes an objective function (compactness of clusters):

$$\sum_{i \in \text{clusters}} \left\{ \sum_{j \in \text{elements of i-th cluster}} ||x_j - \mu_i||^2 \right\}$$

  where μ_i is the center of cluster i.
- It assigns data points to closest cluster center in $O(Kn)$ and it changes the cluster center to the average of its points in $O(n)$.

It is possible to say that K-means is a very simple and efficient method but, on the other hand, it converges to a local minimum of the error function and it needs to pick K initial points and for this reason, it is sensitive to the initialization.

4.2 Images as graphs

It is possible to consider also images as graphs, they can be described in the following way:

- A node for every pixel.
- An edge between every pair of pixels (or every pair of "sufficiently close" pixels).
- Each edge is weighted by the affinity or similarity of the two nodes.

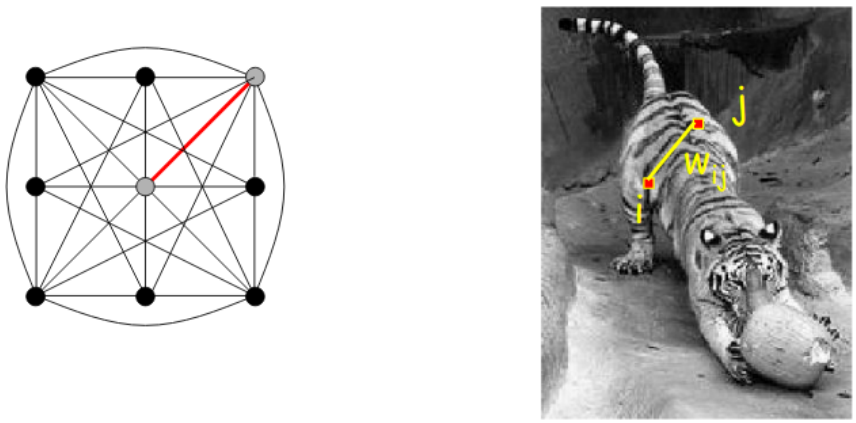


Figure 91: Image as a graph.

If we suppose to represent each pixel by a feature vector x and to define a distance function appropriate for this feature representation, then we can convert the distance between two feature vectors into an **affinity** with the help of a Guassian kernel:

$$exp\left(-\frac{1}{2\sigma^2}dist(x_i, x_j)^2\right)$$

The scale affects the affinity:

- Small σ: group only nearby points.
- Large σ: group far-away points.

4.3 Eigenvector-based clustering

Let us represent a cluster using a vector x whose k-th entry captures the participation of node k in that cluster. If a node does not participate in a cluster, the corresponding entry is zero.
We also impose the restriction that $x^T x = 1$.
We want to maximize:

$$\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}x_i x_j = x^T A x$$

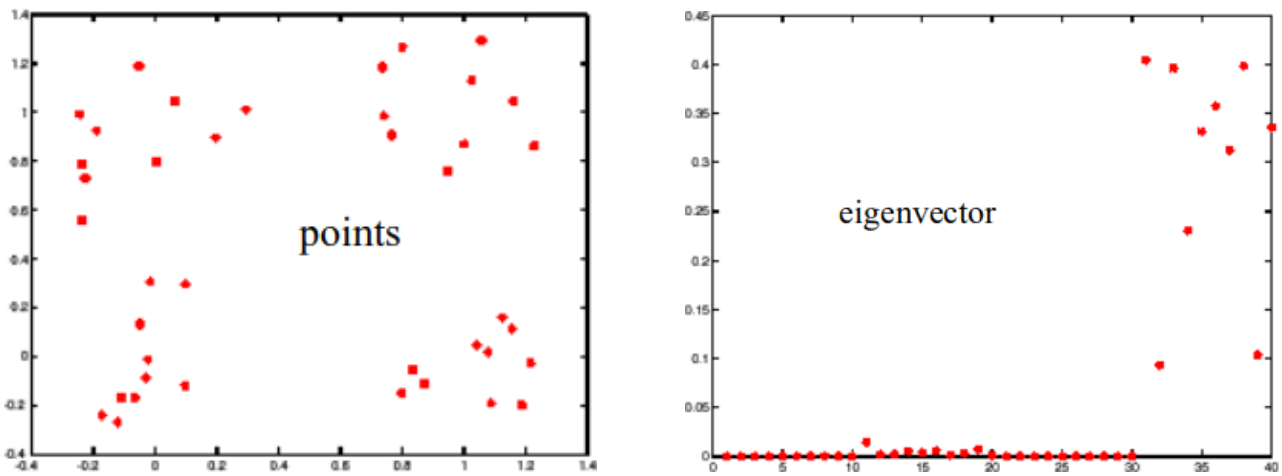
which measures the cluster's cohesiveness.
This is an **eigenvalue problem**, that is choosing the eigenvector of A with largest eigenvalue.
We have that A is the affinity matrix (square matrix) $n \times n$ where n is the number of nodes.
There are important theorems:

1. if $A = A^T$ then A is symmetric and A possesses only "*real*" eigenvalues.
2. if A is symmetric then $x^T A x$ is the largest eigenvalue.

x_i, x_j represent the measure of centrality to the cluster and it is defined as:

$$x_i = \begin{cases} \neq 0 \text{ if } i \in C \\ = 0 \text{ if } i \notin C \end{cases}$$

Also from the following image it is possible to understand that just looking at the eigenvectors it is possible to find clusters.



In case we must extract from eigenvectors more than two clusters we can recursively split each side to get a tree, continuing till the eigenvalues are too small.

Clustering by eigenvectors: Algorithm. The algorithm that builds the clusters through the eigenvectors is composed by the following steps:

1. Construct (or take as input) the affinity matrix A
2. Compute the eigenvalues and eigenvectors of A
3. Repeat
4. Take the eigenvector corresponding to the largest unprocessed eigenvalue.
5. Zero all the components corresponding to elements that have already been clustered
6. Threshold the remaining components to determine which elements belong to this cluster
7. If all elements have been accounted for, there are sufficient clusters
8. Until there are sufficient clusters

4.3.1 Clustering as graph partitioning

Let $G = (V, E, w)$ is an undirected weighted graph (affinity matrix is symmetric). Given a *cut* (A, B), with $B = V \backslash A$, define:

$$cut(A, B) = \sum_{i \in A} \sum_{j \in B} w(i, j)$$

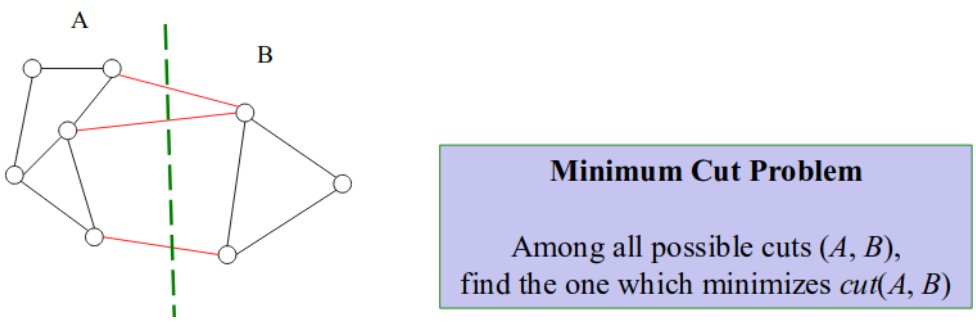


Figure 92: Minimum cut problem.

In the MinCut problem, the weights of the edges which cross the cut should be as small as possible.
The MinCut clustering is advantageous because is solvable in polynomial time but, on the other hand, it favors highly unbalanced clusters (often with isolated vertices), indeed, it only measures what happens between the clusters and not what happens within the clusters.

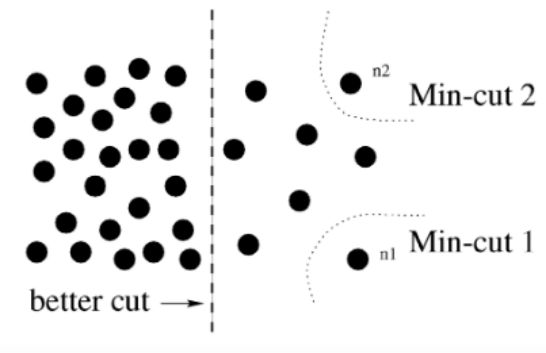


Figure 93: Minimum cut disadvantage.

4.3.2 Normalized Cut

In order to overcome the problem of unbalanced clusters, **Normalized Cut** is used and it is defined by:

$$Ncut(A,B) = \underbrace{cut(A,B)}_{\text{Between A and B}} \left(\underbrace{\frac{1}{vol(A)} + \frac{1}{vol(B)}}_{\text{Within A and B}} \right)$$

where $vol(A)$ is the volume of the set A given by $vol(A) = \sum_{i \in A} d_i,\ A \subseteq V$ and $d_i = \sum_j w_{i,j}$ is the degree of nodes (sum of weights).
Normalized cut has the advantage of taking into consideration what happens within clusters, indeed, considering $vol(A)$ and $vol(B)$ it takes into account what's going on within A and B.

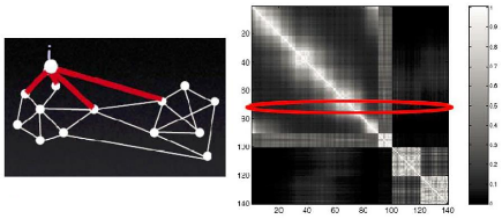


Figure 94: Degree of nodes.

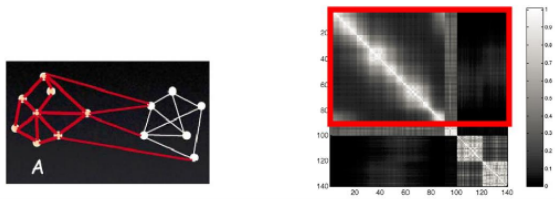


Figure 95: Volume of a set.

4.3.3 Graph Laplacians

The main tools for spectral clustering are graph Laplacian matrices, there exists a whole field dedicated to the study of those matrices, called spectral graph theory. In this section we want to define different graph Laplacians and point out their most important properties.

The unnormalized graph Laplacian. The **unnormalized graph Laplacian** matrix is defined as:

$$L = D - W$$

where:

- D is a diagonal matrix where on the main diagonal there are the degrees of our nodes.
- W is the affinity matrix, it contains $1s$ or $0s$ and its diagonal elements are all $0s$.

This is an example of the degree matrix D and the affinity matrix W in relation to the graph of the next page.

$$D = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

Figure 96: Degree matrix D.

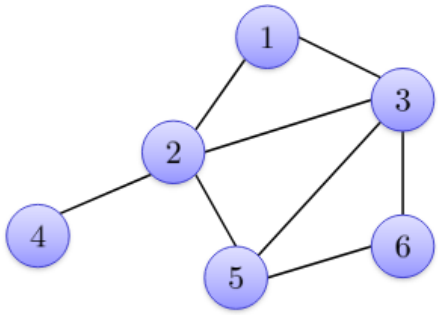
$$W = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}$$

Figure 97: Affinity matrix W.

The elements of L are given by:

$$L_{i,j} = \begin{cases} \mathrm{d}\left(v_i\right) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise} \end{cases}$$

where $d(v_i)$ is the degree of the vertex i.



$$L = \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & -1 & 0 \\ -1 & -1 & 4 & 0 & -1 & -1 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & -1 & 0 & 3 & -1 \\ 0 & 0 & -1 & 0 & -1 & 2 \end{pmatrix}$$

Assume the weights of edges are 1

Figure 98: Example of laplacian graph.

The matrix L satisfies the following properties:

1. For all vectors f in $\mathbb{R}^n$, we have:

$$f^\top L f = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} \left(f_i - f_j\right)^2$$

   This is proved by the definition of d_i:

$$\begin{aligned} f^\top L f = f^\top D f - f^\top W f &= \sum_{i=1}^{n} d_i f_i^2 - \sum_{i,j=1}^{n} f_i f_j w_{ij} \\ &= \frac{1}{2} \left(\sum_{i=1}^{n} \left(\sum_{j=1}^{n} w_{ij} \right) f_i^2 - 2 \sum_{i,j=1}^{n} f_i f_j w_{ij} + \sum_{j=1}^{n} \left(\sum_{i=1}^{n} w_{ij} \right) f_j^2 \right) \\ &= \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} \left(f_i - f_j\right)^2 \end{aligned}$$

2. L is symmetric (by assumption) and positive semi-definite. The symmetry of L follows directly from the symmetry of W and D. The positive semi-definiteness is a direct consequence of the first property, which shows that $f^T L f \geq 0$
3. The smallest eigenvalue of L is 0, the corresponding eigenvector is the constant 1 vector.
4. L has n non-negative, real-valued eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$

First relation between spectrum and clusters:

- Multiplicity of eigenvalue $\lambda_1 = 0$ is the number of connected components of the graph.
- Eigenspace is spanned by the characteristic function of these components (so all eigenvectors are piecewise constant).

The normalized graph Laplacians. There are two matrices which are called normalized graph Laplacians in the literature. Both matrices are closely related to each other and are defined as:

$$L_{\text{sym}} = D^{-1/2} L D^{-1/2} = I - D^{-1/2} W D^{-1/2}$$
$$L_{\text{rw}} = D^{-1} L = I - D^{-1} W$$

We denote the first matrix by L_{sym} as it is a symmetric matrix, and the second one by L_{rw} as it is closely connected to a random walk.

4.3.4 Solving Ncut

Any cut (A, B) can be represented by a binary indicator vector x:

$$x_i = \begin{cases} +1 \text{ if } i \in A \\ -1 \text{ if } i \in B \end{cases}$$

It can be shown that:

$$min_x \; Ncut(x) = min_y \underbrace{\frac{y'(D-W)y}{y'Dy}}_{\text{Rayleigh quotient}}$$

subject to the constraint that $y'D1 = \sum_i y_i d_i = 0$ (with $y_i \in \{1, -b\}$ (relaxation introducing also real values), indeed y is an indicator vector with 1 in the i-th position if the i-th feature point belongs to A, negative constant $(-b)$ otherwise). This is **NP-Hard**!
The huge Ncut time complexity brings us to take into consideration an approximation of it. If we relax the constraint that y be a discrete-valued vector and allow it to take on real values, the original problem

$$\min_y \frac{y'(D-W)y}{y'Dy}$$

will be equivalent to:

$$\min_y y'(D-W)y \quad \text{subject to } y'Dy = 1$$

This amount to solve a *generalized* eigenvalue problem:

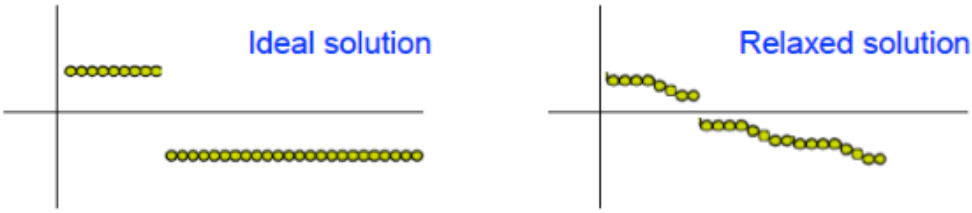
$$\underbrace{(D-W)}_{Laplacian} y = \lambda D y$$

It is possible then, to sum up the different steps of the Normalized Cut algorithm as:

1. Represent the image as a weighted graph $G = (V, E)$, compute weight of each edge and summarize in D and W.
2. Solve $(D - W)y = \lambda D y$ for the eigenvector with the second smallest eigenvalue.
3. Use the entries of the eigenvector to bipartition the graph.

We started from an NP-Hard problem and through relaxation we reached a feasible solution. However, we have not the guaranteed that the relaxed solution is in one to one correspondence.

The effect of relaxation. Through the relaxation we loose some precision in the final solution.



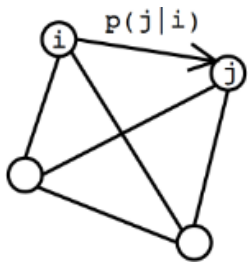
Note that the original problem returns binary values $(-1, 1)$, indicating the clustering membership. The relaxed version, on the right, returns continuous values of it can be the case that some points are not so clear to assign (close to the margin between the two). For that reason relaxed solution not always is in one-to-one correspondence with the original problem.

4.3.5 Random walk interpretation

The Ncut problem can be formalized also in terms of random walk, since we want to find a cut that reduces probability of jumping between nodes of different clusters. It can be defined building a Markov chain where each data point is a state, connected to all other states with some probability. With our affinity W and degree D, the stochastic matrix is:

$$P = D^{-1}W$$

which is the row-normalized version of W, so each entry $P(i, j)$ is a probability of "*walking*" to state j from state i.



Probability of a walk through states $(s_1, \ldots, s_m)$ is given by:

$$P(s_1, \ldots, s_2) = P(s_1) \prod_{i=2}^{m} P(s_i, s_{i-1})$$

Suppose we divide the states into two groups, and minimize the probability of jumping between the two groups. Formulate this as an eigenvector problem:

$$Py = \lambda y$$

where the component of vector y will give the segmentation.
We can precise also that:

- P is a stochastic matrix.
- The largest eigenvalue is 1, and its eigenvector is the all-one vector 1. Not very informative about segmentation.

- The second largest eigenvector is orthogonal to the first, and its components indicate the strongly connected sets of states.
- Meila and Shi (2001) showed that minimizing the probability of jumping between two groups in the Markov chain is equivalent to minimizing Ncut.

Theorem 4.1 (Random Walk Proposition)**.** (λ, y) *is a solution to* $Py = \lambda y$ *if and only if:*

- $1 - \lambda$ *is an eigenvalue of* $(D - W)y = \lambda Dy$
- y *is an eigenvector of* $(D - W)y = \lambda Dy$

Proof:

$$\begin{aligned} Py = \lambda y \quad &\Leftrightarrow \quad -Py = -\lambda y \\ &\Leftrightarrow \quad y - Py = y - \lambda y \\ &\Leftrightarrow \quad (I - P)y = (1 - \lambda)Iy \\ &\Leftrightarrow \quad \left(D^{-1}D - D^{-1}W\right) y = (1 - \lambda)D^{-1}Dy \\ &\Leftrightarrow \quad D^{-1}(D - W)y = D^{-1}(1 - \lambda)Dy \\ &\Leftrightarrow \quad (D - W)y = (1 - \lambda)Dy \end{aligned}$$

The problem is to find a cut (A, B) in a graph G such that a random walk does not have many opportunities to jump between the two clusters.
This is equivalent to the Ncut problem due to the following relation:

$$Ncut(A, B) = P(A|B) + P(B|A)$$

4.3.6 2-way Ncut

1. Compute the affinity matrix W, compute the degree matrix D. D is diagonal and $D_{i,i} = \sum_{j \in V} W_{i,j}$
2. Solve the generalized eigenvalue problem $(D - W)y = \lambda Dy$
3. Use the eigenvector associated to the second smallest eigenvalue to bipartition the graph into two parts.
   Why the second smallest eigenvalue? Remember, the smallest eigenvalue of Laplacians is always 0 (corresponds to the trivial partition $A = V, B = \{\}$).

Sometimes there's not a clear threshold to split based on the second vector since it takes continuous values. In which way it is possible to choose the splitting point?

- Pick a constant value (0 or 0.5).
- Pick the median value as splitting point.
- Look for the splitting point that has minimum Ncut value:
  1. Choose n possible splitting points.
  2. Compute Ncut value.
  3. Pick minimum.

4.3.7 Ncut with more than 2 clusters

There are two possible approaches if we desire to have more than 2 clusters:

Approach # 1. It is a recursive two-way cuts:

1. Given a weighted graph $G = (V, E, w)$, summarize the information into matrices W and D.
2. Solve $(D - W)y = \lambda Dy$ for eigenvectors with the smallest eigenvalues.
3. Use the eigenvector with the second smallest eigenvalue to bipartition the graph by finding the splitting point such that Ncut is minimized.
4. Decide if the current partition should be subdivided by checking the stability of the cut, and make sure Ncut is below the prespecified value.
5. Recursively repartition the segmented parts if necessary.

Note: The approach is computationally wasteful, only the second eigenvector is used, whereas the next few small eigenvectors also contain useful partitioning information.

Approach #2. Using the first k eigenvectors:

1. Construct a similarity graph and compute the unnormalized graph Laplacian L.
2. Compute the k smallest **generalized** eigenvectors $u_1, u_2, \ldots, u_k$ of the generalized eigenproblem $Lu = \lambda Du$.
3. Let $U = [u_1, u_2, \ldots, u_k] \in \mathbb{R}^{n \times k}$.
4. Let $y_i \in \mathbb{R}^k$ be the vector corresponding to the ith row of U.

$$U = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1k} \\ u_{21} & u_{22} & \cdots & u_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ u_{n1} & u_{n2} & \cdots & u_{nk} \end{bmatrix} = \begin{bmatrix} y_1^T \\ y_2^T \\ \vdots \\ y_n^T \end{bmatrix}$$

5. Thinking of y_i's as points in $\mathbb{R}^k$, cluster them with k-means algorithms.

4.3.8 Spectral Clustering vs k-means

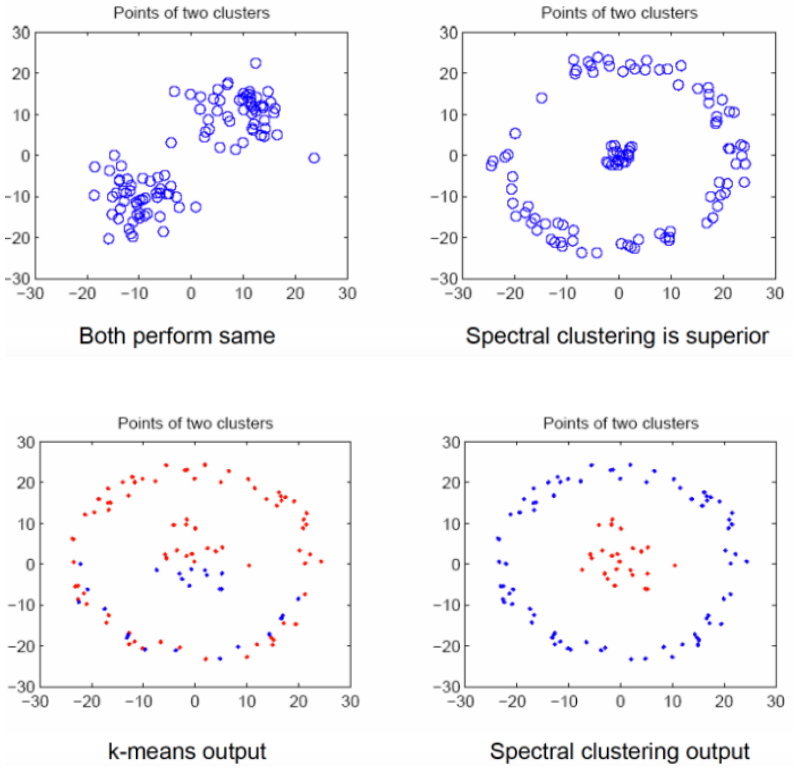
First of all, let us define the **spectral clustering**, its goal is to cluster data that is connected but not necessarily compact or clustered within convex boundaries. The algorithm has in input the similarity matrix $S \in \mathbb{R}^{n \times n}$ and the k number of clusters to construct. It returns in output the k clusters. It follows these steps:

1. Construct a similarity graph and compute the normalized graph Laplacian L_{sym}.
2. Embed data points in a low-dimensional space (spectral embedding), in which the clusters are more obvious, computing the k smallest eigenvectors $v_1, \ldots, v_k$ of L_{sym}.
3. Let $V = [v_1, \ldots, v_k] \in \mathbb{R}^{n \times k}$.
4. Form the matrix $U \in \mathbb{R}^{n \times k}$ from V by normalizing the row sums to have norm 1, that is:

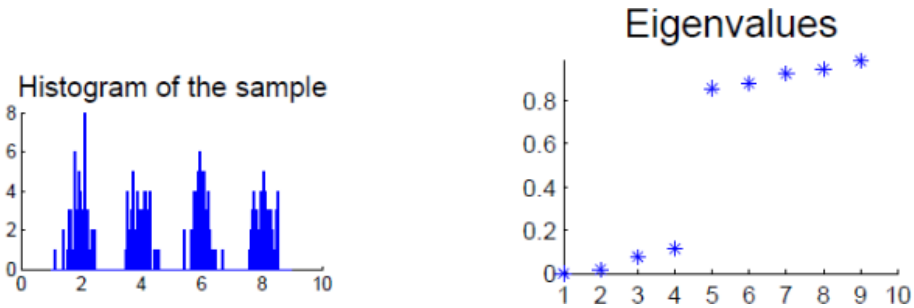
$$u_{ij} = \frac{v_{ij}}{\left(\sum_k v_{ik}^2\right)^{1/2}}$$

5. For $i = 1, \ldots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the ith row of U.
6. Cluster the points y_i with $i = 1, \ldots, n$ with the k-means algorithm into clusters $C_1, \ldots, C_k$.

Applying k-means to Laplacian eigenvectors allows us to find cluster with non-convex boundaries.



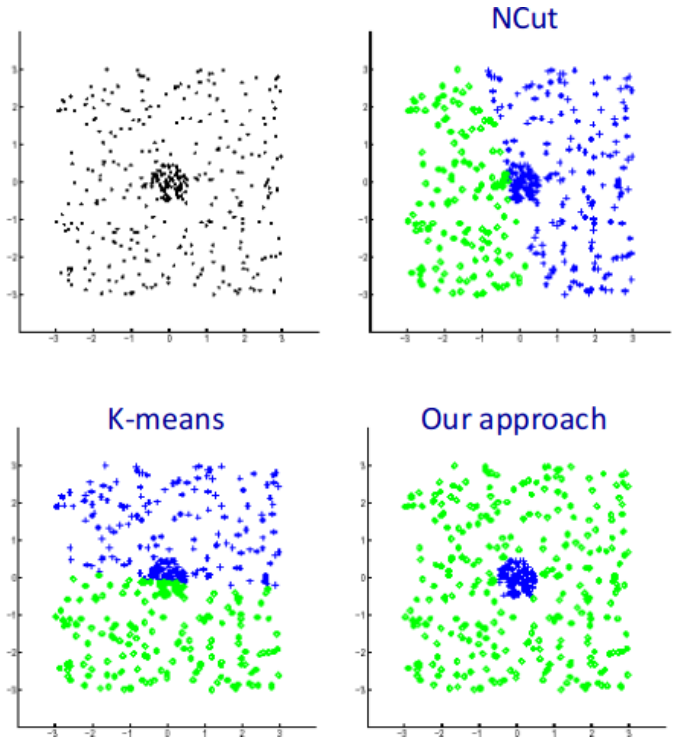
One of the possible problems that could appear in spectral clustering is choosing k such that all eigenvalues $\lambda_1, \ldots, \lambda_k$ are very small, but λ_{k+1} is relatively large. In this way, the choosing of k maximizes the eigengap (difference between consecutive eigenvalues) $\delta_k = |\lambda_k - \lambda_{k-1}|$.



5 Dominant Sets

In some applications, data are more likely to be represented as weighted graphs rather than in a **features-based way**. In this context, a common approach is to construct a **similarity graph** of the data, in which data are represented by nodes in the graph and the edges represent the similarity relation between nodes. This way of presenting data is very common since it allows to codify and use complex structured and unstructured data, and, since we are using graphs, a very strong graph theory literature is provided.
Coming back to the clustering problem, some authors argue to the fact that a cluster can be seen as a **maximal clique**[1] of a graph, indeed the concept of clique is related to the internal cluster criteria, instead maximal clique responds to the external criteria. Problems raise because maximal clique problem cannot be applied to weighted graphs. For this reason, dominant set is introduced as an evolution of the continuous formulation of the maximal clique problem.

The notion of **dominant set** provides measures of cohesiveness of a cluster and vertex participation of different clusters. Clusters can be found by using continuous optimization technique, the replicator. An interesting property that will be discussed later on, is that dominant set is strongly connected to the graph theory, game theory and quadratic optimization. Thanks to this strong connection it is possible to establish a connection between dominant sets and local extrema (max or min) of a quadratic form over the standard simplex. The other methods are not able to capture a particular cloud of data distinguishing it from the other points that are considered noise. In other words, a cluster is nothing else that a set of maximally homogeneous points.



This new approach allows us, for example, also to consider nodes belonging to two different clusters considering so the hypothesis of overlapping clusters.

[1] A **clique** is a subset of mutually adjacent vertices.
A **maximal clique** is a clique that is not contained in a larger one.

5.1 Graph-theoretic definition of a cluster

Data to be clustered are represented as an undirected weighted graph with no self-loops: $G = (V, E, \omega)$, where $V = \{1, \ldots, n\}$ is the vertex set, $E \subseteq V \times V$ is the edges set and $w : E \to \mathbb{R}^*_+$ is the positive weight function. Vertices represent data points, edges neighborhood relationships and edge-weights similarity relations. G is then represented with an adjacency matrix A, such that $a_{ij} = \omega(i, j)$. Since there are not self-loops we have that $\omega(i, i) = 0$ (main diagonal equal to 0).
There is not a unique and well define definition of cluster, but in literature we agree that a cluster should satisfy two conditions:

- **High internal homogeneity**, also named *Internal criterion*. It means that all the objects inside a cluster should be highly similar(or low distance) to each other.
- **High external in-homogeneity**, also named *External criterion*. It means that objects coming from different clusters have low similarity (or high distance).

The idea of the criterion is that clusters are groups of objects which are strongly similar to each other if they become to the same cluster, otherwise they have an highly dissimilarity.
Informally, a cluster is a set of entities which are alike, and entities from different clusters are not alike.
Let $S \subseteq V$ be a nonempty subset of vertices and $i \in S$. The average weighted degree of i with regard to S is defined as:

$$\text{awdeg}_S(i) = \frac{1}{|S|} \sum_{j \in S} a_{ij} \tag{1}$$

Informally, it represents the average similarity between entity i and the rest of the entities in S. It can be observed that $\text{awdeg}_{\{i\}}(i) = 0 \; \forall i \in V$, since we have no self-loops.
We now introduce a new quantity ϕ such that if $j \notin S$:

$$\phi_S(i, j) = a_{ij} - \text{awdeg}_S(i) \tag{2}$$

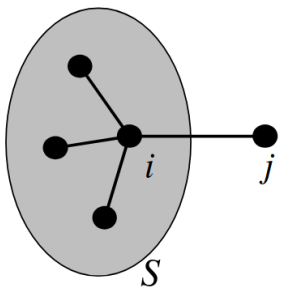


Figure 99: ϕ measure.

Note that $\phi_{\{i\}}(i,j) = a_{ij}\ \forall i,j \in V$ with $i \neq j$. $\phi_S(i,j)$ measures the relative similarity between i and j with respect to the average similarity between i and its neighbors in S. This measures can be either positive or negative.

Definition. Let $S \subseteq V$ be a nonempty subset of vertices and $i \in S$. The weight of i with regard to S is:

$$w_S(i) = \begin{cases} 1 & \text{if } |S| = 1 \\ \sum\limits_{j \in S \setminus \{i\}} \phi_{S \setminus \{i\}}(j,i) w_{S \setminus \{i\}}(j) & \text{otherwise} \end{cases} \tag{3}$$

Further, the total weight of S is defined to be $W(S) = \sum_{i \in S} w_S(i)$.

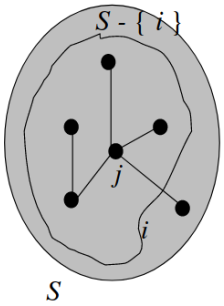


Figure 100: Weight of i respect to elements in S.

Note that $w_{\{i,j\}}(i) = w_{\{i,j\}}(j) = a_{ij}\ \forall i,j \in V \wedge i \neq j$. Then, $w_S(i)$ is calculated simply as a function of the weights on the edges of the sub-graph induced by S.

Intuitively, $w_S(i)$ gives a measure of the similarity between i and $S \setminus \{i\}$ with respect to the overall similarity among the vertices of $S \setminus \{i\}$. In other words, how similar (important) is i respect to the entities in S. An important property of this definition is that it induces a sort of natural ranking among vertices of the graph.

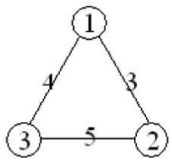


Figure 101: Similarity graph example.

Considering the graph proposed in Figure 101, we can put ranking:

$$w_{\{1,2,3\}}(1) < w_{\{1,2,3\}}(2) < w_{\{1,2,3\}}(3)$$

.

Definition. A nonempty subset of vertices $S \subset V$ such that $W(T) > 0$ for any nonempty $T \subseteq S$, is said to be a **dominant set** if:

- $w_S(i) > 0\ \forall i \in S$ (*internal homogeneity*)
- $w_{S \cup \{i\}}(i) < 0\ \forall i \notin S$ (*external homogeneity*)

These conditions correspond to cluster properties (**internal homogeneity** and **external inhomogeneity**). Informally we can say that the first condition requires that all the nodes in the clusters are important for it. The second one assumes that if we consider a new point in the cluster, the cluster cohesiveness will be lower, meaning that the current cluster should be already maximal.
By definition, dominant sets are expected to capture compact structures. Moreover, this definition is equivalent to the one of maximal clique problem when applied to unweighted graphs.

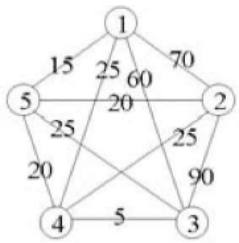


Figure 102: The set {1,2,3} is dominant.

5.2 From dominant set to local optima

Clusters are commonly represented as an n-dimensional vector expressing the participation of each node to a cluster. Large numbers denote a strong participation, while zero values no participation. The cohesiveness of a cluster can be computed using:

$$f(x) = x^\top A x \tag{1}$$

where A is a symmetric real-valued matrix with null diagonal.
Clustering can be formulated now as the problem of finding x that maximizes f. The objective function has to be normalized. For this aim simplex constraints are imposed. This yields the following standard quadratic problem which local solution corresponds to a maximally cohesive cluster:

$$\begin{array}{ll} \text{maximize} & f(x) \\ \text{subject to} & x \in \Delta \end{array} \tag{2}$$

where

$$\Delta = \{x \in \mathbb{R}^n : x \geq 0 \wedge e^\top x = 1\} \tag{3}$$

is the standard simplex of $\mathbb{R}^n$.

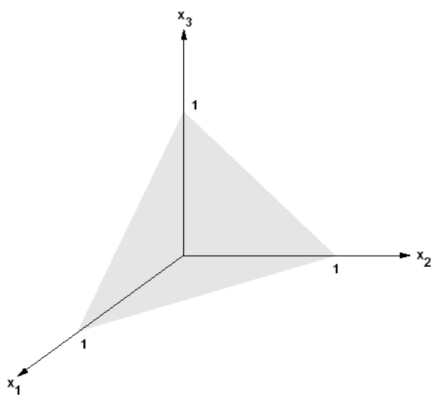


Figure 103: Standard Simple on $\mathbb{R}^3$.

The entity x is a strict local solution of problem 2 if there exists a neighborhood $U \subset \Delta$ of x such that $f(x) > f(z)\ \forall z \in U \setminus \{x\}$. The support $\sigma(x)$ of $x \in \Delta$ is defined as the index set of the positive components in x.

$$\sigma(x) = \{i \in V : x_i > 0\}$$

Definition. A non-empty subset $C \subseteq V$ and C is a dominant set, admits a weighted **characteristic vector** $x^c \in \Delta$ if it has positive total weight $W(C)$, in which:

$$x_i^C = \begin{cases} \frac{W_c(i)}{W(C)} & \text{if } i \in C \\ 0 & \text{otherwise} \end{cases}$$

Note that by definition dominant sets always admit a characteristic vector. In conclusion dominant sets can be put in one-to-one correspondence (modulo a technical condition) with strict local maximizers of a quadratic function over the simplex. As opposed to many other clustering algorithms, which try to find the global optimum of some energy function, dominant sets can be found by mining local solutions.

5.3 Link to Game theory

Game theory is the study of mathematical models of strategic interaction between rational decision-makers. In this sense we can model a new **clustering game** with the following properties:

- **Symmetric game**, the payoffs for playing a particular strategy depend only on the other strategies employed, not on who is playing them.
- **Complete knowledge**, payoffs, strategies and types of players are known.
- **Non-cooperative game**, players cannot form alliances or if all agreements need to be self-enforcing (e.g. through credible threats). Player takes independent decisions about the strategy to play.
- Pre-existing set of **pure strategies**. Players do not behave "rationally" but act according to a pre-programmed behavioral pattern (pure strategy).

Data points V are the pure strategies available to the players and the similarity matrix A represents the **payoff matrix**, which resumes the revenues that each player obtains when a pair of strategies is played. The values A_{ij} and A_{ji} are the revenues obtained by player 1 and player 2 considering that they have player strategies $(i, j) \in V \times V$. A **mixed strategy** $x = (x_1, \ldots, x_n)^T \in \Delta$ is a probability distribution over the set of pure strategies, which models a stochastic playing strategy of a player. If player 1 and 2 play mixed strategies $(x_1, x_2) \in \Delta \times \Delta$, then the expected payoffs for the players are: $\mathbf{x_1^T A x_2}$ and $\mathbf{x_2^T A x_1}$ respectively. The goal of the two players of course is to maximize as much as possible their resulting revenue. During the game each player extract an object (i, j) and the resulting revenue is associated according to the payoff matrix A. Since we are considering A equal to the similarity matrix we can say that in order to maximize their revenue the two players would coordinate their strategies so that the extracted objects belong to the same cluster. In other words, only by selecting objects belonging to the same cluster, each player is able to maximize his expected payoff. The unique difference is that the similarity between two equal entities is 0, meaning that $A_{ii} = 0$. The desired condition is that the two players reach the **symmetric Nash equilibrium**, state in which the two players agree about the cluster membership. A **Nash Equilibrium** is a mixed-strategy profile $(x_1, x_2) \in \Delta \times \Delta$ such that no player can improve the expected payoff by changing his playing

strategy, given the opponent's strategy being fixed. In other words, it's a configuration of strategies for which none player will deviate from it for its convenience since there is no incentive to change choice. This concept can be expressed with the following expression:

$$y_1^T Ax_2 \leq x_1^T Ax_2 \qquad y_2^T Ax_1 \leq x_2^T Ax_1 \qquad \forall (y_1, y_2) \in (V \times V).$$

A Nash equilibrium is **symmetric** if $x_1 = x_2$, meaning that considering a symmetric Nash Equilibrium $x \in \Delta$ the two conditions hold in a unique one:

$$y^T Ax \leq x^T Ax$$

This condition over here satisfies the internal homogeneity criterion required inside the dominant set definition, but it does not include any kind of constraint that guarantees the maximality condition. In order to satisfy this condition it is necessary to look for a different type of Nash Equilibrium, known as **Evolutionary Stable Strategy (ESS)**.

Definition. A symmetric Nash equilibrium $x \in \Delta$ is an ESS if it satisfies also:

$$y^T Ax = x^T Ax \implies x^T Ay > y^T Ay \qquad \forall y \in \Delta \setminus \{x\}$$

$$y^T Ax = x^T Ax \implies x^T Ay < x^T Ax \qquad \forall y \in \Delta \setminus \{x\}$$

Even if the strategy y provides the same payoff of the strategy x, it is better to play x since the payoff against itself is greater than the one provided by y. The two strategies x and y represents two Nash Equilibrium, but only x is an ESS.
In conclusion we can say that the ESSs of the clustering game with affinity matrix A are in **correspondence** with dominant sets of the same clustering problem instance. However, we can also conclude that ESS's are in one-to-one correspondence to (strict) local solutions of StQP.
It is possible to say that ESS's abstract well the main characteristic of a cluster:

- **Internal coherency:** High mutual support of all elements within the group.
- **External incoherency:** Low support from elements of the group to elements outside the group.

5.4 Extracting dominant sets

One of the major advantages of using dominant sets is that it can be written with few lines of code. There are several dominant set clustering approaches:

- To get a single dominant set cluster use replicator dynamics.
- To get a partition use a simple *peel-off* strategy: iteratively find a dominant set and remove it from the graph, until all vertices have been clustered.
- To get overlapping clusters, enumerate dominant sets.

The **Replicator Dynamics** (RD) are deterministic game dynamics that have been developed in evolutionary game theory. It considers an idealized scenario whereby individuals are repeatedly drawn at random from a large, ideally infinite, population to play a two-player game. In contrast to classical game theory, here players are not supposed to behave rationally or to have complete knowledge of the details of the game. They act instead according to an inherited behavioral pattern, or pure strategy, and it is supposed that some evolutionary selection process operates over time on the distribution of behaviors.

Let $x_i(t)$ the population share playing pure strategy i at time t. The state of the population at time t is: $x(t) = (x_1(t), \ldots, x_n(t)) \in \Delta$.
We define an evolution equation, derived from Darwin's principle of nature selection:

$$\dot{x_i} = x_i \; g_i(x)$$

where g_i specifies the rate at which pure strategy i replicates.

$$\frac{\dot{x_i}}{x_i} \propto \text{payoff of pure strategy } i \text{ - average population payoff}$$

which yields:

$$\dot{x_i} = x_i[(Ax)_i - x^T Ax]$$

where $(Ax)_i$ is the i-th component of the vector and $x^T Ax$ is the average payoff for the population. If we have a result better than the average strategy there's an improvement.

Theorem. A point $x \in \Delta$ is a Nash equilibrium if and only if x is the limit point of a replicator dynamics trajectory starting from the interior of Δ. Furthermore, if $x \in \Delta$ is an ESS, then it is an asymptotically stable equilibrium point for the replicator dynamics.

Assuming that the payoff matrix A is symmetric ($A = A^T$), we call this type of game as a doubly symmetric game. Thanks to this assumption we can derive some conclusions:

- (***Fundamental Theorem of Natural Selection***.) For any doubly symmetric game, the average population payoff $f(x) = x^T Ax$ is strictly increasing along any non-constant trajectory of replicator dynamics, meaning that $\frac{df(x(t))}{dt} \geq 0 \; \forall t \geq 0$, with equality if and only if $x(t)$ is a stationary point.
- (***Characterization of ESS's***.) For any doubly symmetric game with payoff matrix A, the following statements are equivalent:
  - $x \in \Delta^{ESS}$
  - $x \in \Delta$ is a strict local maximizer of $f(x) = x^T Ax$ over the standard simplex Δ.
  - $x \in \Delta$ is asymptotically stable in the replicator dynamics.

A well-known discretization of replicator dynamics, which assumes non-overlapping generations, is the following (assuming a non-negative A):

$$x_i(t+1) = x_i(t) \frac{A(x(t))_i}{x(t)^T Ax(t)}$$

which inherits most of the dynamical properties of its continuous-time counterpart.

```
distance=inf;
while distance>epsilon
    old_x=x;
    x = x.*(A*x);
    x = x./sum(x);
    distance=pdist([x,old_x]');
end
```

Figure 104: MATLAB implementation of discrete-time replicator dynamics

The components of the **converged vector** give us a measure of the **participation** of the corresponding vertices in the cluster, while the value of the objective function provides of the cohesiveness of the cluster.

5.5 Application to Image Segmentation

An image is represented as an edge-weighted undirected graph, where vertices correspond to individuals pixels and edge-weights reflect the similarity between pairs of vertices.
The clustering problem consists on extracting dominant sets from an input image, below is proposed the pseudo-code version of the solution with dominant sets:

```
Partition_into_dominant_sets(G)
Repeat
   find a dominant set
   remove it from graph
until all vertices have been clustered
```

Figure 105: Pseudo-code for Image Segmentation.

Remember that to find a single dominant set we used replicator dynamics.
Given an input image with $H \times W$ pixels we construct a similarity matrix ω such that the similarity between the pixels i and j is measured by:

$$\omega(i,j) = \exp\left(\frac{-||F(i) - F(j)||_2^2}{\sigma^2}\right)$$

where σ is a positive real number which affects the decreasing rate of ω and:

- $F(i)$, is the normalized intensity of pixel i (for *intensity segmentation*).
- $F(i) = [v, vs\sin(h), vs\cos(h)](i)$ where h, s, v are the HSV values of pixel i (for *color segmentation*).
- $F(i) = [|I * f_1|, \ldots, |I * f_k|](i)$ is a vector based on texture information at pixel i, the f_i being DOOG filters at various scales and orientations (for *texture segmentation*).

5.6 Extensions

Path-based measure. The similarity matrix can be computed in different ways, and a very well known application consists on using the **path-based measure**, which defines the distance between two entities i and j as:

$$D_{ij}^{path} = \min_{p \in \mathcal{P}_{ij}(O)} \left\{ \max_{1 \le l \le |p|} D_{p(l)l(l+1)} \right\}$$

where $\mathcal{P}_{ij}(O)$ is the set of all paths from i to j. Thereby, the effective distance between i and j is the largest gap of the path $p*$, where $p*$ is the path with the minimum largest gap among all admissible paths between i and j.

Building a Hierarchy: A family of quadratic programs. Another interesting extension is introduced re-formulating the optimization problem such that the goal of the clustering problem consists on:

$$\begin{array}{ll} \text{maximize} & f_\alpha(x) = x'(A - \alpha I)x \\ \text{subject to} & x \in \Delta \end{array} \tag{1}$$

where $\alpha \ge 0$ is a parameter and I is the identity matrix.
The objective function f_α consists of:

- a **data term** ($x'Ax$) which favors solutions with high internal coherency.
- a **regularization term** ($-\alpha x'x$) which acts as an entropic factor: it is concave and, on the simplex Δ, it is maximized at the barycenter and it attains its minimum value at the vertices of Δ.

The effect of α can be seen in the number of different clusters found. With an huge value of α each point will be classified in the same cluster, instead decreasing the value of α the number of cluster will increase.
For any fixed α, the energy landscape of f_α is populated by two kinds of solutions:

- solutions which correspond to dominant sets for original matrix A.
- solutions which don't correspond to any dominant set for the original matrix A, although they are dominant for the scaled matrix $A + \alpha(ee' - I)$. In other words it allows to find subsets of points that are not sufficiently coherent to be dominant with respect to A, and hence they should by split.

This algorithm has the basic idea of starting with a sufficiently large α and adaptively decrease it during the clustering process following these steps:

1. Let α be a large positive value (ex: $\alpha > |V| - 1$).
2. Find a partition of the data into α-clusters.
3. For all the α-clusters that are not 0-clusters recursively repeat step 2 with decreasing α.

Dealing with High-Order Similarities. Dominant set can be applied also to hypergraphs. A weighted hypergraph is a triplet $H = (V, E, \omega)$ where:

- V is a finite set of vertices.
- $E \subseteq 2^V$ is the set of (hyper)-edges, where 2^V is the power set of V.
- $\omega : E \to \mathbb{R}$ is a real-valued function assigning a weight to each edge.

We focus on a particular class of hypergraphs, called **k-graphs**, whose edges have fixed cardinality $k \geq 2$.

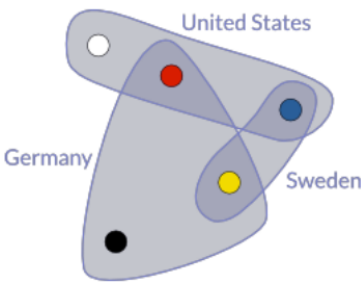


Figure 106: A hypergraph where the vertices are flag colors and the hyperedges are flags.

For solving this problem we come back to the clustering game. Given a weighted k-graph representing an instance of a hypergraph clustering problem, we cast it into a k-player (hypergraph) clustering game where:

- There are K players;
- The objects to be clustered are the pure strategies;
- The payoff function is proportional to the similarity of the objects/strategies selected by the players;

Definition (ESS-cluster). Given an instance of a hypergraph clustering problem $H = (V, E, \omega)$, an **ESS-cluster** of H is an ESS of the corresponding hypergraph clustering game.

5.7 Properties

- **Well separation between structure and noise.** In such situations it is often more important to cluster a small subset of the data very well, rather than optimizing a clustering criterion over all the data points, particularly in application scenarios where a large amount of noisy data is encountered.
- **Overlapping clustering**. In some cases we can have that two distinct clusters share some points, but partitional approaches impose that each element cannot be long to more than one cluster.
- Dominant sets can be found by mining **local solutions**, so it is not necessary to look for global solutions.
- Deal very well in presence of noise.
- Strong connection with theoretical results.
- Makes no assumptions on the structure of the affinity matrix, being it able to work with asymmetric and even negative similarity functions.
- Does not require a priori knowledge on the number of clusters (since it extracts them sequentially).
- Leaves clutter elements unassigned (useful, e.g., in figure/ground separation or one-class clustering problems).
- Generalizes naturally to hypergraph clustering problems.

6 Supplementary material

6.1 Evolutionary Stable Strategy (ESS)

An ESS is an extension of the Nash equilibrium definition. In a Nash equilibrium, if all players adopt their respective parts, no player can benefit by switching to any alternative strategy. In a two player game, it is a strategy pair. Let $P(S,T)$ represent the payoff for playing strategy S against strategy T. The strategy pair (S,S) is a Nash equilibrium in a two player game if and only if this is true for both players and:

$$\forall_{T \neq S} \quad P(S,S) \geq P(T,S)$$

In this definition, strategy T can be a neutral alternative to S, scoring equally well. A Nash equilibrium is presumed to be **stable** even if T scores equally, on the assumption that there is no long-term incentive for players to adopt T instead of S. This fact represents the point of departure of the ESS.
We have two definition of ESS:

John Maynard Smith and George R. Price S is an ESS if $\forall_{T \neq S}$:

- $P(S,S) > P(T,S)$, **OR**
- $P(S,S) = P(T,S)$ and $P(S,T) > P(T,T)$.

The first condition is sometimes called a **strict Nash equilibrium**. The second is sometimes called **Maynard Smith's second condition**. The second condition means that although strategy T is neutral with respect to the payoff against strategy S, the population of players who continue to play strategy S has an advantage when playing against T.

Bernhard Thomas S is an ESS if $\forall_{T \neq S}$:

- $P(S,S) \geq P(T,S)$ **AND**
- $P(S,T) > P(T,T)$

The payoff of the first player when both players play strategy S is higher than (or equal to) the payoff of the first player when he changes to another strategy T and the second players keeps his strategy S and the payoff of the first player when only his opponent changes his strategy to T is higher than his payoff in case that both of players change their strategies to T. In this formulation, the first condition specifies that the strategy is a Nash equilibrium, and the second specifies that Maynard Smith's second condition is met. Note that the two definitions are not precisely equivalent.

	A	B
A	2, 2	1, 2
B	2, 1	2, 2

Figure 107: Harm thy neighbor payoff matrix.

Considering the example of the harm thy neighbor game, we have two Nash equilibrium (A, A) and (B, B), since players cannot do better by switching away from either. However, only B is an ESS and a strong Nash. A is not an ESS, so B can neutrally invade a population of A strategists and predominate, because B scores higher against B than A does against B.

6.2 Replication Equation

In mathematics, the **replicator equation** is a deterministic monotone non-linear and non-innovative game dynamic used in evolutionary game theory.This important property allows the replicator equation to capture the essence of selection, does not incorporate mutation and so is not able to innovate new types or pure strategies (strategies are fixed). The most general continuous form is given by the differential equation:

$$\dot{x_i} = x_i[f_i(x) - \phi(x)], \quad \phi(x) = \sum_{j=1}^{n} x_j f_j(x)$$

where x_i is the proportion of type i in the population, $x = (x_1, \ldots, x_n)$ is the vector of the distribution of types in the population, $f_i(x)$ is the fitness of type i (which is dependent on the population), and $\phi(x)$ is the average population fitness (given by the weighted average of the fitness of the n types in the population).

- $\dot{x_i}$, grow rate of strategy i.
- x_i, current fit for strategy i.
- $[f_i(x) - \phi(x)]$,fit for i relative to the average fit.

If $x_i > 0$ and $f_i(x) > \phi(x)$ then the grow rate of strategy i increase, meaning that i will be increased in the population. Since the elements of the population vector x sum to unity by definition, the equation is defined on the n-dimensional simplex. In application, populations are generally finite, making the discrete version more realistic, but in contrast it is more expensive to compute. To simplify analysis, fitness is often assumed to depend linearly upon the population distribution, which allows the replicator equation to be written in the form:

$$\dot{x_i} = x_i \left((Ax)_i - x^T Ax \right)$$

where the payoff matrix A holds all the fitness information for the population: the expected payoff can be written as $(Ax)_i$ and the mean fitness of the population as a whole can be written as $x^T Ax$.

6.3 Spectral Clustering

In the following lines is possible to find other important notions linked to the spectral clustering chapter.

Theorem 6.1 (The k smallest eigenvalue)**.** *If A is an $n \times n$ real symmetric matrix, then for all $1 \leq k \leq n$, we have:*

$$\lambda_k(A) = \min_{x \in \mathbb{R}^n \setminus \{0\}} \frac{x^T A x}{x^T x}$$

Theorem 6.2 (Properties for Laplacian matrices and normalized ones)**.** *In relation to Laplacian matrices, it is possible to notice that, let L be the Laplacian of a graph $G = (V, E)$. Then, $L \geq 0$, indeed:*
$\forall x = (x_1, \ldots, x_n)$,

$$\begin{aligned} x^T L x &= x^T \sum_{e \in E} L_e x \\ &= \sum_{e \in E} x^T L_e x \\ &= \sum_{i,j \in E} (x_i - x_j)^2 \geq 0 \end{aligned}$$

In relation instead to the normalized Laplacian Matrix we have that:

$$\forall x \in \mathbb{R}^n \quad x^T L x = \sum_{i,j} \left(\frac{x(i)}{\sqrt{d(i)}} - \frac{x(j)}{\sqrt{d(j)}} \right)^2 \geq 0$$

The following proof will explain how we come to the fact that $\min_x \mathrm{Ncut}(x) = \min_y \frac{y'(D-W)y}{y'Dy}$

Theorem 6.3 (Solving Ncut proof)**.**

$$\lambda_2 = \min_x \frac{x^T L x}{x^T x} = \min_x \frac{x^T D^{-1/2} L D^{-1/2} x}{x^T x} \qquad \textit{Remember } L_{sym} = D^{-1/2} L D^{-1/2}$$

Considering the change of variables obtained by setting $y = D^{-1/2}x$ and $x = D^{1/2}y$:

$$\lambda_2 = \min_y \frac{y^T L y}{(D^{1/2}y)^T (D^{1/2}y)} = \min_y \frac{y^T L y}{y^T D y}$$