Artificial Intelligence

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Contents

1 Motivation

Artificial neural networks are information processing systems, whose structure and operation principles are inspired by the nervous system and the brain of animals and humans.

Artificial neural networks are studied for various reasons.

- Extracting knowledge from data (*phenomena, events, processes, operating environment,...*).
- Understanding the phenomena that I'm observing, extracting the knowledge about that phenomena.
- Automated construction of computational paradigms for problem solving.

The ultimate goal is to be able to have a model which allow to describe the phenomenon that I'm observing and using this model I would like to solve the specific application problem.

There is an huge variety of application, this is the reason which AI now is so popular, and we have so many interested and expertise in this field.

The next evolution of the economy is based on availability of solution which are extracted from the data by analyzing the data reasoning, the only problems is that our capability of reasoning is limited by the fact that our brain is not able to analyze huge quantity of data, with automated system we can exploit this and make more comprehensive models that describe the process of systems we are observing and develop more accurate solutions.

Basically, artificial intelligence is mimicking the nature. We want to take the data analyze the data make a model, and for doing this we use techniques, we want to enrich the analysis we are doing through sensors from environments, we can use other specific sets of techniques.

We have the need of putting together some ideas and observation, we can define rules for reasoning, we extract the knowledge, but we can also build knowledge through reasoning. Basically, what we want to do is to try to replicate how the living beings observe and operate in the environment, how express, interacts.

Not only but we want to observe how the individual evolves, population evolves, in order to understand the trend of the environment. In this broad variety of approaches is to define some techniques which mainly are in two big categories, from the point of view of intelligence :

- **Symbolic approach**
- **Sub-symbolic approach**, which are sub-symbolic techniques for analyze the environment and the systems.

During this course we are focusing on sub-symbolic reasoning techniques:

- **Neural networks**, which is a simulation of a living brain.
- **Fuzzy systems**, which embed the definition of quantities, which are fuzzy (not defined in a very crisp way).
- **Evolutionary computing**, which is a set of techniques which mimics the natural evolution of the species so we can try to optimize the solution by using the basic concept of the natural evolution of the species.

2 Neural networks

2.1 Biological background

Basically, the aim of the artificial neural networks in *mimicking* the behavior of our brain starts from the fields of neural biology and neural physiology. What this discipline tries to do is to analyze the behavior of the biological neurons cells and understand how they behave for retrieving the information from the outer world.

The neurons use sensors and special cells to connect to the external world and get information. As humans or other biological species, we have five senses, taking for example the eyes, they are receptors which are able to see what a round us is, they are able to reconstruct the scene we got around us.

Basically, with artificial neural networks we are trying to replicate what **biology** does for us, in neurobiology we build a model of what is happening in the neurons, this model describes how the neurons are interacting together to extract the knowledge, to build memory, construct reasoning, take decisions.

In computer science we want to build this model in computer just for trying to do something similar, we want to mimic the behavior of the natural brain in order to try to replicate in an artificial environment the same operation.

We are building the *model* for neurons in the computer, in this way we are able to use these artificial models to *learn* the environment and to solve practical problem (predict possible behaviors and solve optimization problem, like we do naturally). We also have some basis in other disciplines like physics and chemistry since we may want to use the neural networks, also for describing physical phenomena, not only to create reasoning in our mind but we want to create models of phenomena, this can be used for various application. We can create an abstract model, and instead of observing the real world we can observe how the model behave in some conditions.

Neural networks and in general artificial intelligence, is a discipline of computer science and engineering, then we use some inspirations from other discipline but the core of the theoretical aspect of the foundation which defines the artificial neural networks this is an area which is been to computer science and engineering.

2.2 Reasons for studying the biological background

The reasons for studying the BB (*biological background*) in computer science are two:

- The **first reason** for studying the neural networks is the fact that they are a very appealing model, since they work in **parallel** means that they have an intrinsically extremely high *parallel process capability*. This is why computer scientist are so attracted to this topic. Our brain in many cases find the solution immediately, this is fascinating, this happens because we are exploiting the parallel capability of our neural networks.
- The **second reason** why we are studying this technology is the fact that there is really a huge amount of *practical application* in broad variety of area : *industrial manufactory, products medicine, finances, economy, social networks, data analysis, ...*

2.3 Neurons

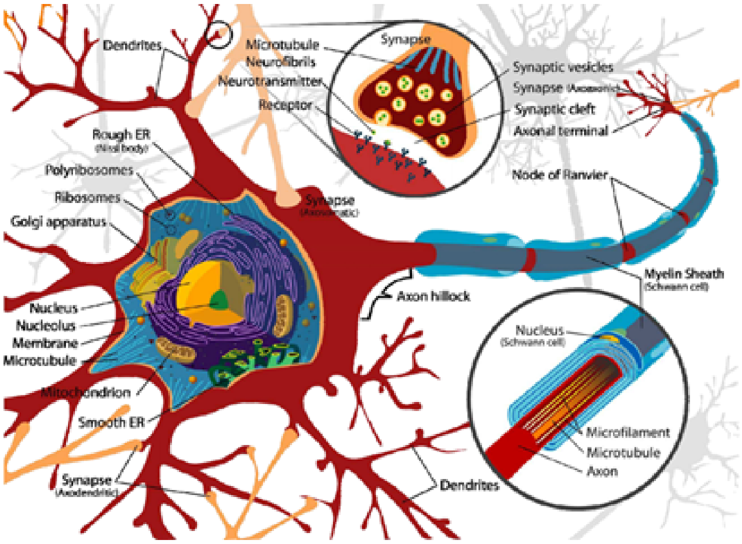


Figure 1: Neuron

The *central* part of the neuron is the part, which is managing the entire cell, this core the nucleus is listening what is happening around the neuron, when I have a **solicitation** from the external (other neurons or special cells related to the five senses).

When there is sufficient stimulation coming from this cells the nucleus is solicited and at a given point the nucleus realizes that the solicitation is so high that he has to take an **action**, the action is to send a *signal* around the *axon* (the long extension covered in blue), this will lead to have a *polarization* of an *electric signal* which is flowing along this connection and this will reach other neurons that are connected to the end of the axon to the synapses.

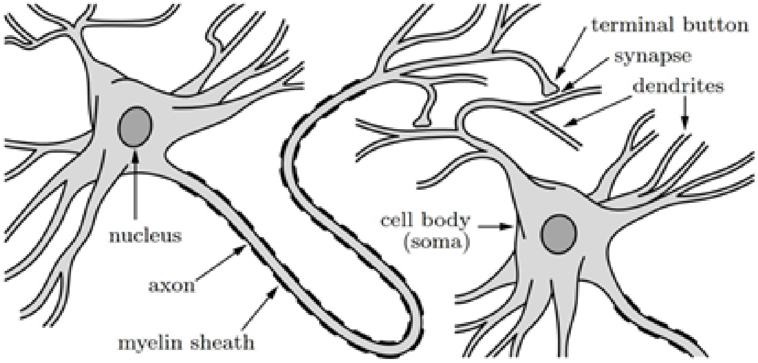


Figure 2: Connection between two neurons

The **axon** is covered by an appropriate *protein* (covered in blue) which protect the axon itself, and make sure that the polarization that occur on the nucleus is transmitted along the axon so that this signal is able to reach the synapse.

Basically, what we see is that the **neuron is exciting the nucleus**, which is generating the excitation along the axon, then it will reach the terminal synapses.

Each synapse is connected to the synapses of *another* neuron, so that the signals which are generated by the nucleus and sent to the axon and then to the synapsis terminal at the terminal the synapses are releasing some chemicals called **neurotransmitters**.

These *substances* are exciting the synapses of the connected neuron, bu stimulating the synapses this excitation is propagated from the **dendrites** to the nucleus of the other neuron, when the other cell is *sufficiently excited* by from the amount of stimulation generated by the neurotransmitter the nucleus will generate again a new stimulation which is going along the axon and reach another neuron (and so on...).

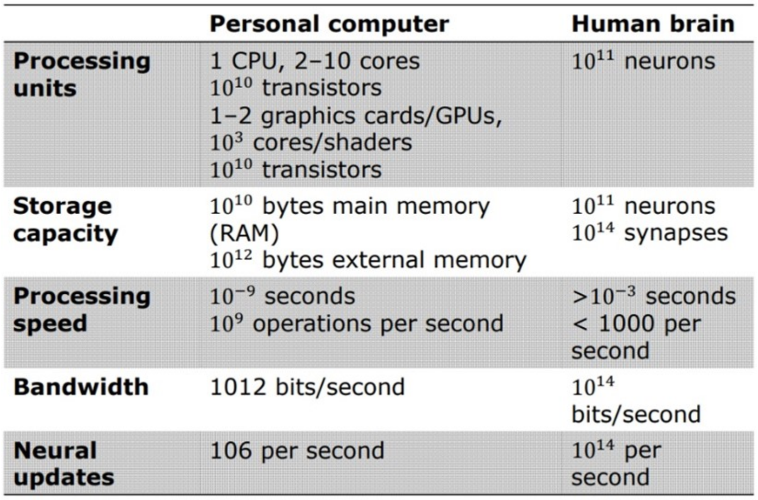
The axon is *depolarized* if there is enough excitatory input, basically this is how the signals are propagated through the brain.

Due to the fact that each neuron can stimulate each other neurons connected to them, this will create the **parallel processing** in our brain, so that each component will take care of analyzing each part of the information and this is a consequence to derive a part of the total computation.

2.4 Computer vs Human brain

When we look to the differences between a computer and the human brain what we notice, is that in the computer we got processors composed by many *transistors*, the human brain counterpart the got $10^{1}1$ *neurons*, the number of the latter overcomes the number of the cores in a processor.

The neurons aren't able to process the same *complex operation* of a core, but they are still so many that they can overcome the limit of the complexity of the individual operation with the fact that they are working significantly in parallel.



	Personal computer	**Human brain**
Processing units	1 CPU, 2–10 cores 10^{10} transistors 1–2 graphics cards/GPUs, 10^{3} cores/shaders 10^{10} transistors	10^{11} neurons
Storage capacity	10^{10} bytes main memory (RAM) 10^{12} bytes external memory	10^{11} neurons 10^{14} synapses
Processing speed	10^{-9} seconds 10^{9} operations per second	$>10^{-3}$ seconds < 1000 per second
Bandwidth	1012 bits/second	10^{14} bits/second
Neural updates	106 per second	10^{14} per second

Figure 3: PC vs Human brain

The **storage** of the neurons has an immense storage potential than any other memory capacity. The **processing speed** seems *much higher* on the computer, but the parallel operation that you can do in parallel in the human brain in the end *overcome* the processing speed of the hardware of a computer.

Basically, what we can observe is that the biological neural networks are able to outperform significantly the processor that we have nowadays, there are some researches carried out which are trying to create processors which are replicating in hardware the operation of the biological neural networks but still the capabilities of this systems are *far* from the capability of human brain.

It may *seem* in some system that they are working faster then humans, it may seem that they are running better, but actually what you have is that you have the ability in the computer to run the algorithms and the explore the possible (deterministic) moves in a fast way but needs some background knowledge in order to that in a very short time.

Advantages of biological neural network:

- High processing speed due to massive parallelism.
- Even if we have a significant amount of the biological neural network damaged, the system is considered **fault tolerance**, it remains functional

even if larger parts of the network get *damaged* (maybe some functions will be disabled). The other cells are able to overcome the death cells, this thanks to the elasticity of the neurons which are able to overcome possible damages in the structures.

- If more neurons are failing, the brain will *degrade the performances* in a *graceful way*, it will not just stop working, will work a bit less not with the same performance and the same functionality but with reduced function. Only when a *really massive* number of neurons is dying at that point a function is not working anymore.

- They are well suited for inductive learning (*learning from examples, generalization from instances*).

What we are trying to do with artificial neural networks is to capture the parallel operation of the brain. The ability to extract the knowledge from the data, we want to replicate these capabilities.

There are some problems due to the **ANN** (artificial neural networks), if we kill part of the architecture which is replicating the **BNN** (biological neural networks), the ANN is **not automated to survives**, we have to assure some physical redundance, this is a problem of the architecture we are using to execute the computation of the ANN.

What we want to do in our model is to construct a *set of abstract models of the neurons* that we call **artificial neurons**, and we like to connect them together to replicate the structure that we have in the natural brain this is why we have the ANN, a connection of neurons that is trying to mimic the behavior of the brain.

The complexity of the brain is so high that is actually difficult to replicate everything in ANN, what we are doing is to replicate a specific function of the brain which is able to solve a specific application problem that we have.

2.5 Threshold Logic Units

This is the first *abstract model* for an artificial neuron of the brain. A **threshold logic unit** (TLU) is a *processing unit* (neuron) with several inputs. It can solve a very simple set of problems.

We have a **core** (the neuron) with several *inputs* that are reaching the neuron, and we have the *output* which is delivered to the subsequential neurons which are connected with it. A TLU is a processing unit in which the output is governed by a threshold θ, if it has a *sufficient excitation* from the inputs, then the TLU became **active** (value 1) and generates the output y.

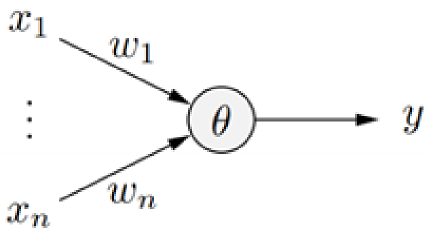


Figure 4: Threshold logic unit

We have n inputs identified by $x_1, ..., x_n$ the unit is generating only one output y each input is **not** delivered directly to the core of the TLU, but each input is **weighted**, some are more relevant, and others are less relevant (exactly how we are doing when we consider the data from the external world).

$$y = \begin{cases} 1, & \text{if} \quad \sum_{i=1}^{n} w_i x_i \geq \theta, \\ 0, & \text{otherwise.} \end{cases}$$

Figure 5: TLU conditions

This means that our problem is depending on the most important information, this is what happens in the real world.

In the ANN we are replicating the relevance of the individual input, we can control how much each input is actually important to influence the generation of the output, to do this we use a weight w for each of the input so that the TLU will not see exactly the input but will see a weighted input, this will allow the modulation of each input by giving to each of them the appropriate importance during the generation of the final output.

When the TLU is solicited enough it will generate an output y that will be delivered to the *terminal synapse* to another neuron.

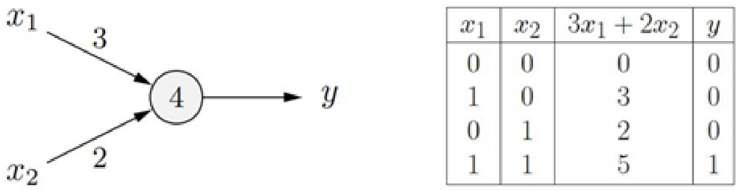
- If the **excitation is enough**, mathematically means that the weighted summation is greater than a thresh θ, we generate 1 (the neuron is active).
- If the **excitation is not enough** for overcoming the threshold θ, we generate 0.

This model that tries to represent what is happening in the BNN from two scientists, also called the **McCulloch-Pitts neuron**.

2.5.1 Conjunction example

The result is equal to 1 only when the two outputs are equal to 1. There is not a standard way to select the threshold θ, we have to choose that in base of the function that we want to implement. In this case I have to select a θ which is greater than the biggest weight.

$$x_1 \wedge x_2$$



x_1	x_2	$3x_1 + 2x_2$	y
0	0	0	0
1	0	3	0
0	1	2	0
1	1	5	1

Figure 6: Conjunction TLU

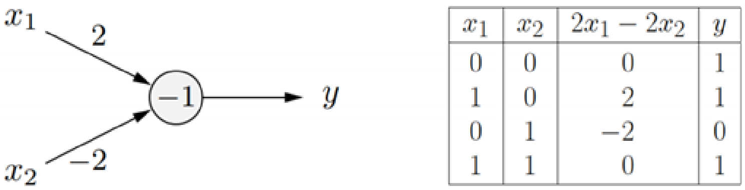
2.5.2 Implication example

I can choose the value of the threshold in order to have the proper function, in this case applies on the same ways. *How can I choose the interconnection weights?*

The problem is that there are no general rules, I choose the weights according to the intrinsic relevance of each input variable.

How can I do that when we have a high number of inputs? we will see that there is a procedure for doing that.

$$x_2 \rightarrow x_1$$

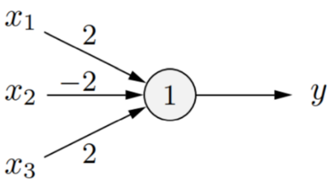


x_1	x_2	$2x_1 - 2x_2$	y
0	0	0	1
1	0	2	1
0	1	-2	0
1	1	0	1

Figure 7: Implication TLU

2.5.3 Multiple inputs example

In this case we can see that we have three possible inputs, we can discriminate the inputs in excitatory input and inhibitory input. The first tries to contributes to the final computation of the neuron in such a way that the results will be greater than the threshold, the other neuron does the opposite.



x_1	x_2	x_3	$\sum_i w_i x_i$	y
0	0	0	0	0
1	0	0	2	1
0	1	0	-2	0
1	1	0	0	0
0	0	1	2	1
1	0	1	4	1
0	1	1	0	0
1	1	1	2	1

Figure 8: Three-input TLU

2.6 Geometric interpretation

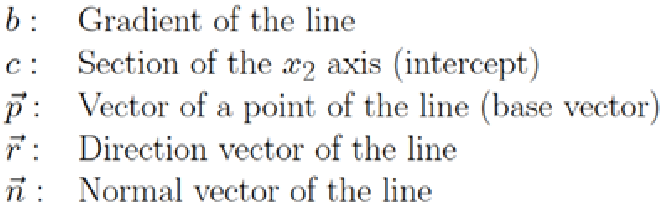
The geometric interpretation is significantly helpful to derive a *method* to configure the threshold and the weights starting from the data. We will consider a single and simple TLU, we will try to understand how we can interpret the behavior of the TLU in a geometrical way.

You know that is possible to represent a straight line on a plane in any of the following forms :

$$\begin{array}{lll}
\text{Explicit Form:} & g \equiv & x_2 = bx_1 + c \\
\text{Implicit Form:} & g \equiv & a_1x_1 + a_2x_2 + d = 0 \\
\text{Point-Direction Form:} & g \equiv & \vec{x} = \vec{p} + k\vec{r} \\
\text{Normal Form:} & g \equiv & (\vec{x} - \vec{p})^\top \vec{n} = 0
\end{array}$$

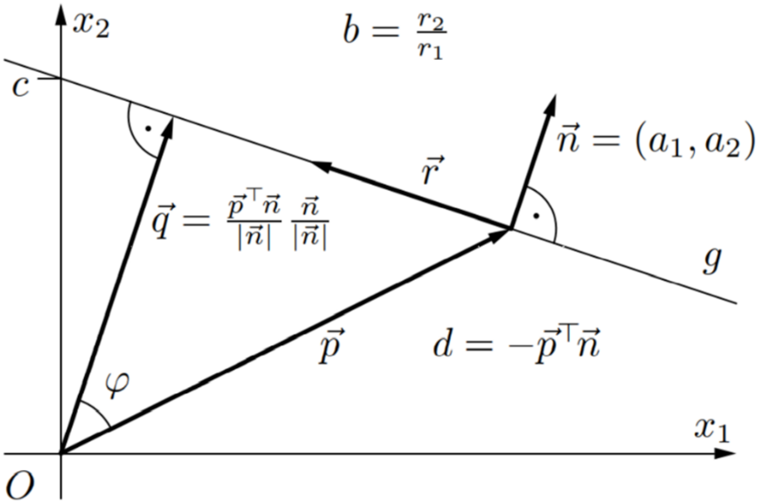
Figure 9: Different form for representing a straight line

If i **implicit form**, where you have a weighted combination of the two variables plus a possible threshold, a vector representation in point-direction form and normal form. Any of this is fine to represent a straight line in the plane, we are considering just two variables x_1 and x_2, and use one of the many representations.



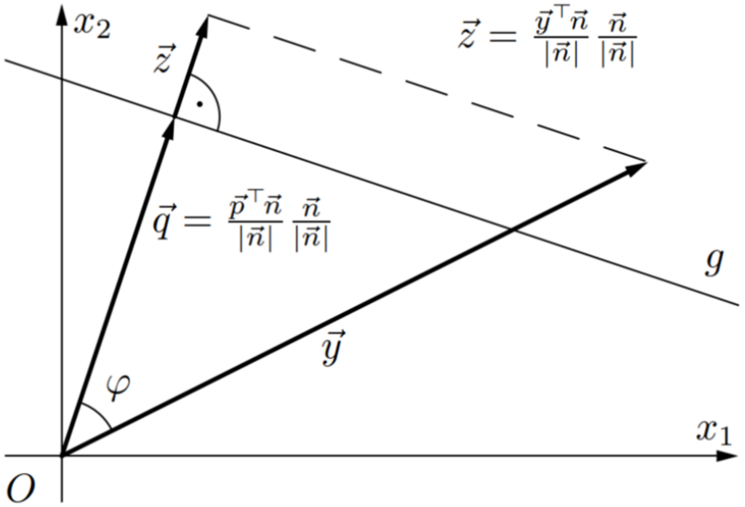
b :	Gradient of the line
c :	Section of the x_2 axis (intercept)
$\vec{p}$:	Vector of a point of the line (base vector)
$\vec{r}$:	Direction vector of the line
$\vec{n}$:	Normal vector of the line

Figure 10: Implicit form representation legend


x_2
$b = \frac{r_2}{r_1}$
c
$\vec{n} = (a_1, a_2)$
$\vec{r}$
$\vec{q} = \frac{\vec{p}^\top \vec{n}}{|\vec{n}|} \frac{\vec{n}}{|\vec{n}|}$
g
$\vec{p}$
$d = -\vec{p}^\top \vec{n}$
φ
x_1
O

In the case of the *explicit/implicit form* the $\vec{b}$ is the **inclination** (or *gradient*) of the straight line in respect of the horizontal axis, and c is the intercept of the vertical axis.

If we look to the normal $\vec{n}$ we want to pick the vector which is *orthogonal* to the straight line. The straight line is represented by all the points which starts from the origin and has a quantity in the direction of the normal. The vector $\vec{p}$ identifies a point in the example, we consider that point belonging to our straight line, the distance of the straight line respect to the origin O is given by $|\vec{q}|$ which is the projection of $\vec{p}$ on straight line g.


x_2
$\vec{z}$
$\vec{z} = \frac{\vec{y}^\top \vec{n}}{|\vec{n}|} \frac{\vec{n}}{|\vec{n}|}$
$\vec{q} = \frac{\vec{p}^\top \vec{n}}{|\vec{n}|} \frac{\vec{n}}{|\vec{n}|}$
g
$\vec{y}$
φ
x_1
O

Considering this other graphical representation it is possible to know on which side a points lands. If we take the vector representing $\vec{y}$ a point, and i compute the projection in the direction of the normal, the projection of this is the vector $\vec{z}$.

To understand on which side the points are, i just need to see if the vector $\vec{z}$ (which is the projection of our point) is shorter or longer than the point i observe on the straight line, which is pointed by $\vec{q}$. This means that all points (expressed by a vector) which have a **module** higher then the projected point onto the straight line ($\vec{q}$), are part of the plane above the straight line (they will *satisfies* the solution), viceversa, they will be below the plane if the module will be shorter then $\vec{q}$ (they won't satisfy the condition).

Basically the straight line which defines the behavior of my TLU, splits the plane in two parts (since i'm considering only x_1 and x_2). All the points which distance is greater then

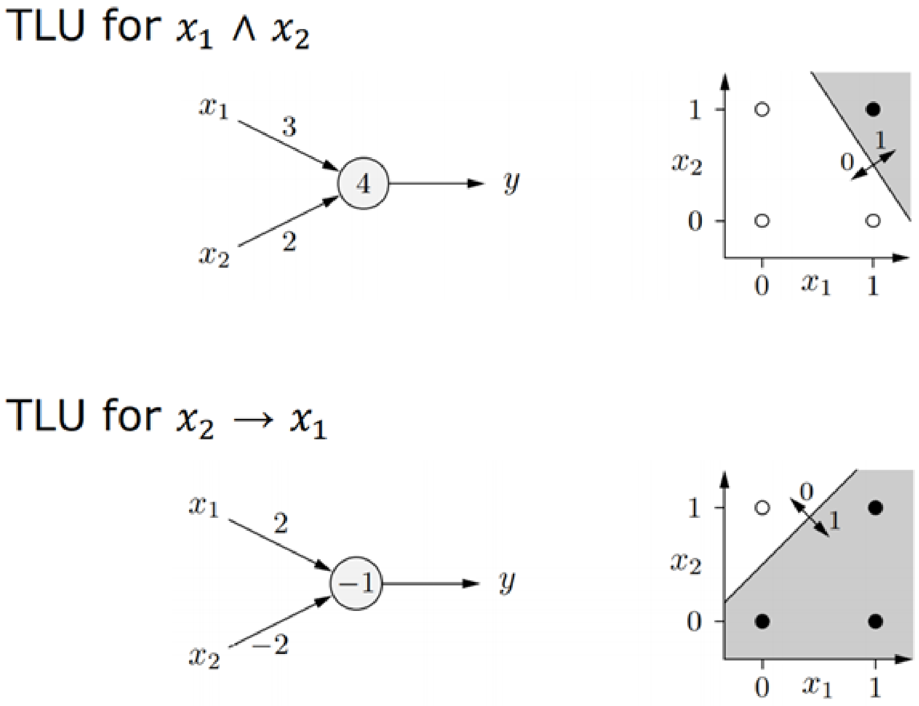


Figure 11: Solution of the *conjunction* and *bi-implication*

Now Let’s go back to the two examples that we have seen before, starting with the conjunction, in this means that I have three points in which the output has to be 0, and one point where the result is 1. This means that if I represent the straight line with $x_1 = 3$, $x_2 = 3$ and the intercept equal to 4 i will draw a line which is actually separating in a clear way the element in which the output is equal to 1 from the values where the output is equal to 0.

For the case of three variables, this is more complex, we need to generalize this idea moving from a plane to a three-dimensional space. Think about the three axis and look at the combination of the dots, you need to set a plane, so you have to separate one set of inputs for which the output has to be equal to 1 from the set of inputs combinations where the output is equal to 0.

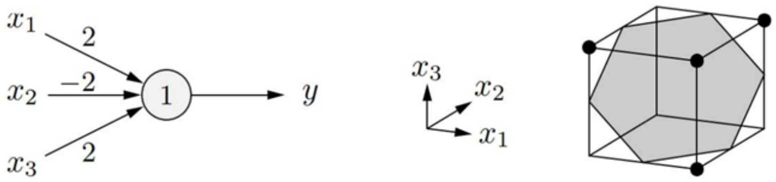


Figure 12: Solution of the complex TLU

Basically, if you represent the plane using these information's you will have this kind of plane (that looks like a hexagon) dividing the solution from the 0 values.

So how we choose the threshold and interconnection weights? I have to look at geometrical distribution of the points for the combination of the input which the output must be equal to 1 and the one where the output must be equal to 0, I have to take a straight line or plane and I need to position the divisor in a way that I clearly separate the two groups. If I can do that, that set of values (inputs and threshold) are the one that I need to use in my ANN.

x_1	x_2	y
0	0	1
1	0	0
0	1	0
1	1	1

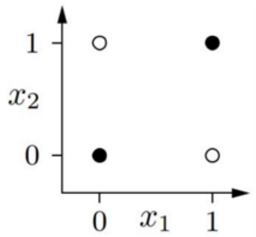


Figure 13: The bi-implication problem

Let's analyze another example, the bi-implication problem, this problem results in this kind of distribution in the plane, as you can see it is not possible to separate these points with a straight line. As a consequence, we don't have any TLU for solving this problem, even if this is a simple problem. We have to introduce some notions for understanding the reasons behind this problem.

2.6.1 Linear separability

Two set of points in the **Euclidean Space**, consider $x_1, x_2, ..., x_n$ as the variable for the TLU, since we have n possible inputs you are analyzing a problem represented in n dimensional Euclidean space.

If you have in this Euclidean space two set of points they are **linearly separable**, if and only if there exists at least one point, line, plane or hyperplane, such that all points of the first set lie on one side and all points of the other set lie on the other side of this point, line, plane or hyperplane.

The point sets can be separated by a linear decision function.

If you are in a mono dimensional space you have one input only, your Euclidean Space is a line, you have one point on this straight line which is separating your space the line in two parts, the output is one, for the other point the output is 0. If you have a plane, we have two input variables, we have to find a plane that separates the two sets of points.

2.6.2 Convex hull

A set of points in the Euclidean Space is called **convex** if it is non-empty and connected and for every pair of points in it every point on the straight-line segment connecting the points of the pair is also in the set.

A **convex hull** of a set of points X in a Euclidean Space is the smallest convex set of points that contains X. Alternatively, the convex hull of a set of points X is the intersection of all convex sets that contain X.

2.7 Solution of the bi-implication problem

Two sets of points in Euclidean Space are linearly separable if and only if their convex hulls are disjoint. In the bi-implication problem, the convex hulls are the diagonal line segments.

They share their intersection point and this means that they are not disjoint, therefore the double implication is not linearly separable.

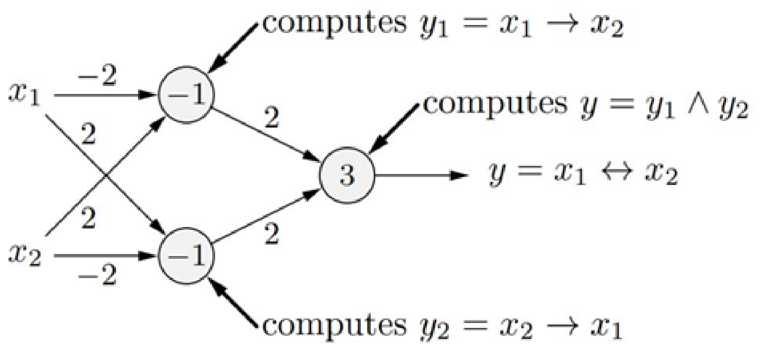

computes $y_1 = x_1 \to x_2$
computes $y = y_1 \wedge y_2$
x_1
-2
-1
2
2
3
$y = x_1 \leftrightarrow x_2$
2
x_2
-2
-1
2
computes $y_2 = x_2 \to x_1$

Figure 14: TLUs to the bi-implication problem

What we can do is putting together more neurons to try to address more complex problem where one neuron can't solve. We are creating a network of TLUs, we are splitting the problem in two sub problems.

The problem of implication can be solved with a single TLU, we create a more complex structure in which are able to solve the problem.

Let's see what happens geometrically, the two points *a* and *c*, are going to be separated from the first two TLUs, I set one of the TLU so that all points which are below the straight line represented by g_2 fives and output equal to 1, and then i set a second straight line represented by g_1 where all points are all over the straight line the values are equal to 1, and then I merge this information.

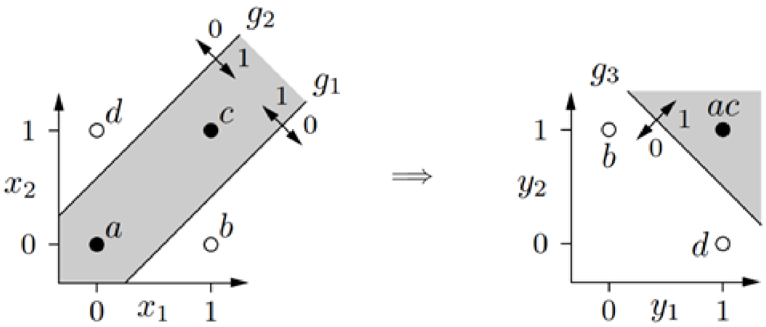


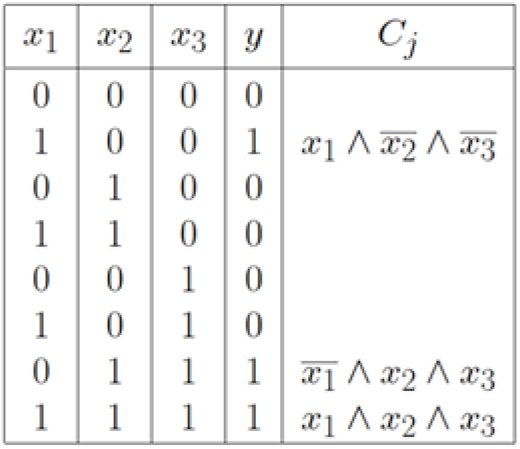
Figure 15: Solution of the bi-implication problem

I combine these information from the previous group in the third neuron so that I transform the representation of the information, I can merge the information of the points *a* and *c*, so that both the output of the two TLU is equal to 1 is represented by one points (in this case they are the same) and then I have the two other points *b* and *d* which are in both the parts above and below the line, for them the solicitation is not enough to generate an output equal to 1, as a consequence I obtained a linear separability.

I transformed the stripe in a semi plane with the third TLU, which identifies the linear separability, I don't have that propriety only with the first TLU but also with the second, both TLUs allow me to partition the first space in three parts.

2.8 Arbitrary boolean functions

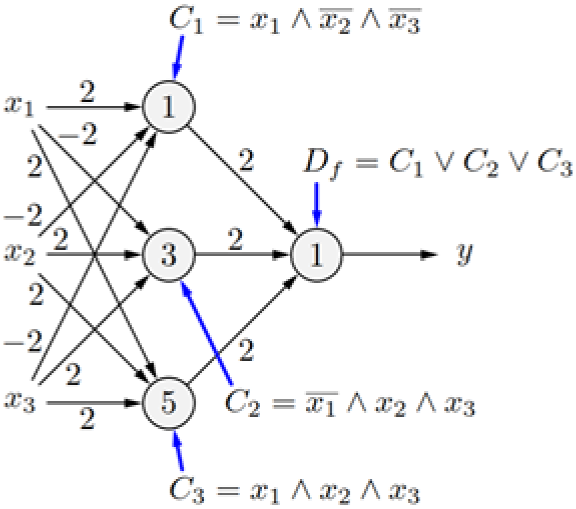
I can work with any arbitrary **Boolean function**; in this example I have a Boolean function of three variables. I have these values of the value *y* according to the formula.



x_1	x_2	x_3	y	C_j
0	0	0	0	
1	0	0	1	$x_1 \wedge \overline{x_2} \wedge \overline{x_3}$
0	1	0	0	
1	1	0	0	
0	0	1	0	
1	0	1	0	
0	1	1	1	$\overline{x_1} \wedge x_2 \wedge x_3$
1	1	1	1	$x_1 \wedge x_2 \wedge x_3$

Figure 16: Table of values

What we can do is to build a network of TLUs that allow me to compute each of the component for which the output has to be 1 and then with a conjunction unit I put together all the possible value with a or for merging the individual TLUs.



$C_1 = x_1 \wedge \overline{x_2} \wedge \overline{x_3}$
x_1
2
−2
2
−2
x_2
2
2
−2
x_3
2
2
1
3
5
2
2
2
$D_f = C_1 \vee C_2 \vee C_3$
1
y
$C_2 = \overline{x_1} \wedge x_2 \wedge x_3$
$C_3 = x_1 \wedge x_2 \wedge x_3$

Figure 17: Network of TLUs solving the boolean function

2.9 Training TLUs

The geometric interpretation that we have seen before about the operation of TLUs gives us the understanding of how we can place the various parameters for our networks in order to construct TLUs with 2 and 3 inputs.

But this makes sense when we are using 2 or 3 input, but this is something that is not feasible when we are having more than three inputs, also this is not an automated method.

We want an automatic method for visualizing the space and points in the space, especially when we have more then 3 inputs.

What we want to do is to have an automatic way which adjusts the weights and the threshold of the network so that I can reach the desired solution (if the two sets are linearly separable).

The **automatic training** of TLUs consist in the fact that we can start from a random value of the weights and threshold, and then when we want to configure a TLU we need to evaluate the error that we are generating at the output (of the TLU) in respect to the input pattern that we have presented.

Basically, we have chosen randomly the threshold, the TLU generates an output, we evaluate the error respect to the desired output, and then we try to adjust the weights and the threshold to reduce the error.

We repeat this operation for all inputs until the error is really reduced or vanished.

1. Start with random values for weights and threshold.

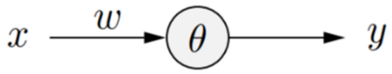
2. Determine the error from the output of the TLU.

3. Consider the error as a function of the weights and the threshold $e = e(w_1, ..., w_n, \theta)$.

4. Adapt weights and threshold so that the error becomes smaller.

5. Iterate adaptation until the error vanishes.

2.9.1 Negation example



x	y
0	1
1	0

Figure 18: TLU that perform negation

$$\neg x$$

In this case we have two really simple parameters, the weights and the threshold. Let's represent the error for all possible weights and all possible threshold at least for a subset that we are interested in analyzing. Let's consider the $x = 0$, in this case the desired output is 1, if we take $w = 2$ and we multiply it by 0 the weighted input will be 0.

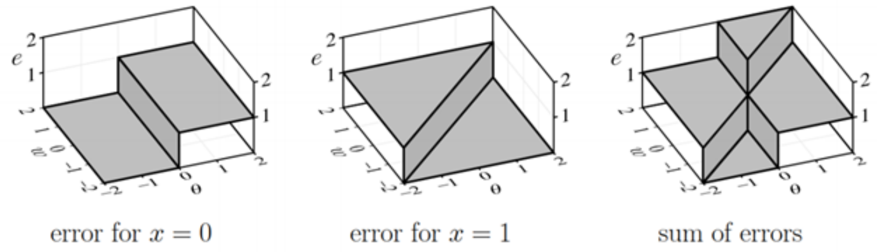


Figure 19: Diagrams of the errors expressed in terms of θ and w

Let's consider the first diagram on the left, with the various values of θ and w, and with an input value of $x = 0$. Let's see the error that we have with the various possible combinations, we see that for any values of the weight where the threshold is *less* than zero, the **error** is zero. Viceversa, for any value of the weight for a θ greater or equal to zero, the error is one (a *plateau*).

Now let's consider $x = 1$, we are on the central diagram, in the left triangular part of the domain there will be the error of 1 defined $\forall w$.

Let's try to sum the errors and see what we obtains: we get an intersection for the error equal to one, and also an intersection for the error equal to *two* (which is strange, since the error in this kind of example is always 1 since the y output is binary, but there we are talking about a sum).

The only part where the error is equal to zero is a small triangle on the bottom. The problem with this definition of the error is that is not suited for define an algorithm which allow me to find the zero error.

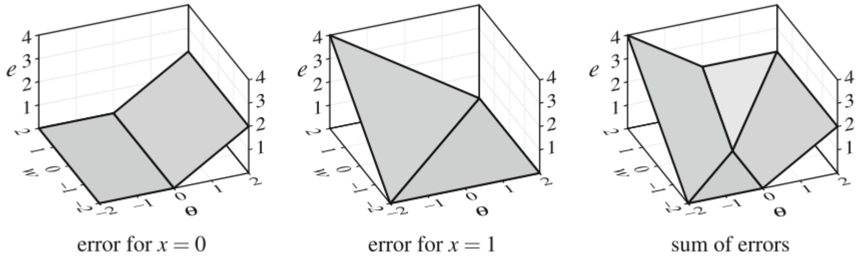


Figure 20: Output error modified as function of weight and threshold

What i can do is modify the description of the error and consider that for each value of the input i will not have just the error which is $1, 0$ or 2, but i will consider a covering and continuos **surface area** (such that is possible to increase progressively the error).

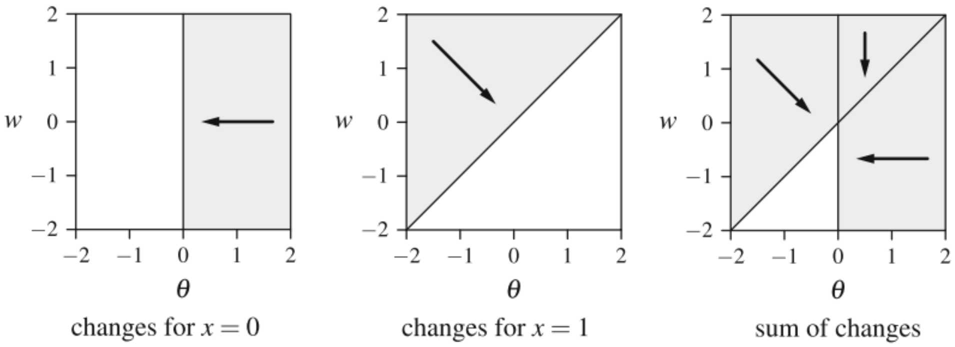


Figure 21: Top view output error modified as function of weight and threshold

So i can start from a random point and iteratively adapt parameters according to the direction corresponding to the current point, i will stop if the error vanishes.

There are two ways of training a neural network:

- **online learning**, we receive the learning pattern at time from the external environment, we compute the parameter corrections for this learning pattern (like we saw in the negation example) and in the end we apply the parameter corrections. In case of the *negation*, first we adapt the weight and the threshold according to the left diagram, then we adapt them according to the middle diagram, then we adapt them again according to the left diagram and so forth until the error vanishes.
- **batch learning**, consists in not applying the changes immediately after every training example, but aggregating them over all training examples. Only at the end of a (learning/training) epoch, that is, after all training examples have been traversed, the aggregated changes are applied. Then the training examples are traversed again and at the end the weight and the threshold are adapted and so forth until the error vanishes.

2.9.2 Delta rule (Widrow-Hoff)

Given:

- $\vec{x} = (x_1, ..., x_n)^T$ be an input vector of TLUs.
- o is the desired output for this input vector.
- y the actual output of the TLU.
- η as learning rate.

If $y \neq o$, then, in order to reduce the error, the threshold θ and the weight vector $\vec{w} = (w_1, ..., w_n)$ are adapted as follow:

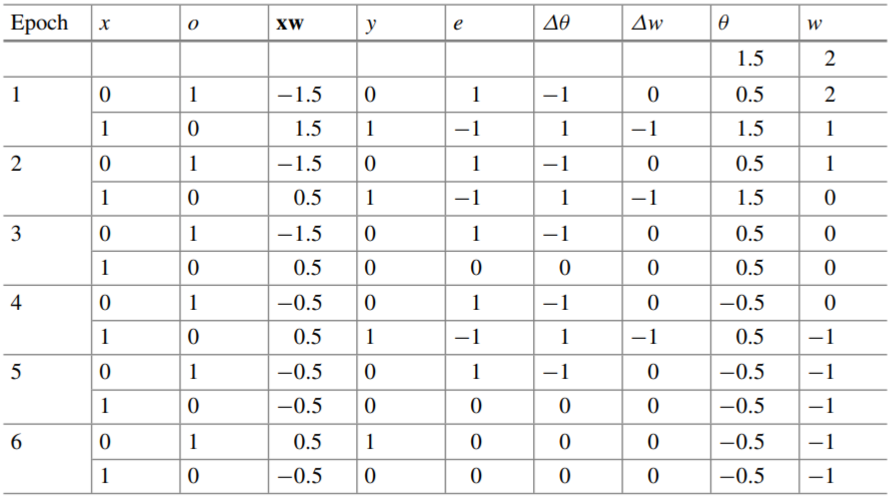
$$\theta^{(new)} = \theta^{(old)} + \Delta\theta, \text{ with } \Delta\theta = -\eta(o - y)$$

$$w_i^{(new)} = w_i^{(old)} + \Delta w_i, \text{ with } \Delta w_i = \eta(o-y)x_i$$
$$\forall i \in \{1, ..., n\}$$

The first equation is correction (delta) of the threshold and the second is the correction of the weight. The variation is given by an expression which is proportional to the difference between the actual and expected output (which is the error).

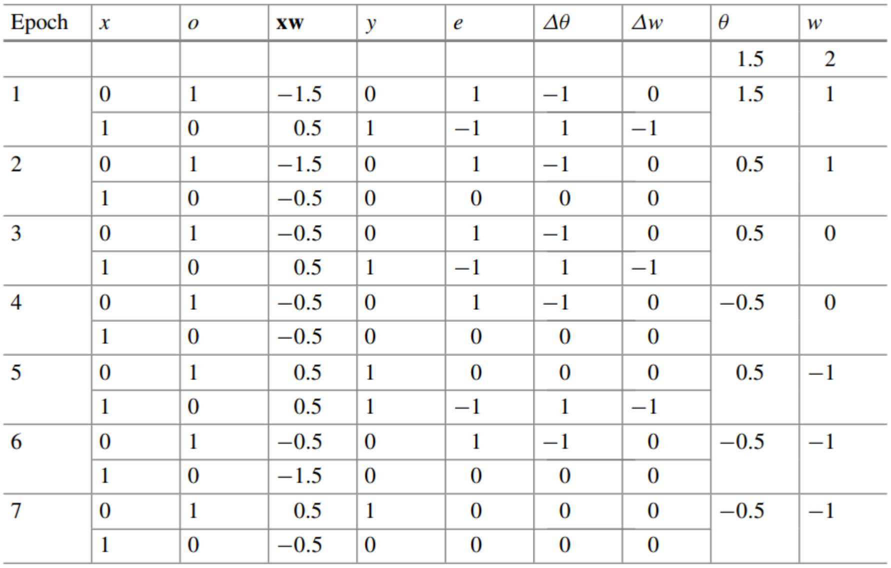
The correction for the weight is proportional not only to the error but also to the input. Essentially, if i have an actual output smaller then the desired one, i take the input that are bigger, and i try to push them to contribute more to the excitation of *threshold logic function* so that the output will be higher and as consequence the error will be lower.

The η controls the speed of updates, the bigger is the bigger will be the update.



Epoch	x	o	**xw**	y	e	$\Delta\theta$	Δw	θ	w
								1.5	2
1	0	1	−1.5	0	1	−1	0	0.5	2
	1	0	1.5	1	−1	1	−1	1.5	1
2	0	1	−1.5	0	1	−1	0	0.5	1
	1	0	0.5	1	−1	1	−1	1.5	0
3	0	1	−1.5	0	1	−1	0	0.5	0
	1	0	0.5	0	0	0	0	0.5	0
4	0	1	−0.5	0	1	−1	0	−0.5	0
	1	0	0.5	1	−1	1	−1	0.5	−1
5	0	1	−0.5	0	1	−1	0	−0.5	−1
	1	0	−0.5	0	0	0	0	−0.5	−1
6	0	1	0.5	1	0	0	0	−0.5	−1
	1	0	−0.5	0	0	0	0	−0.5	−1

Figure 22: Online training with $\theta = \frac{3}{2}, w = 2, \eta = 1$



Epoch	x	o	**xw**	y	e	$\Delta\theta$	Δw	θ	w
								1.5	2
1	0	1	−1.5	0	1	−1	0	1.5	1
	1	0	0.5	1	−1	1	−1		
2	0	1	−1.5	0	1	−1	0	0.5	1
	1	0	−0.5	0	0	0	0		
3	0	1	−0.5	0	1	−1	0	0.5	0
	1	0	0.5	1	−1	1	−1		
4	0	1	−0.5	0	1	−1	0	−0.5	0
	1	0	−0.5	0	0	0	0		
5	0	1	0.5	1	0	0	0	0.5	−1
	1	0	0.5	1	−1	1	−1		
6	0	1	−0.5	0	1	−1	0	−0.5	−1
	1	0	−1.5	0	0	0	0		
7	0	1	0.5	1	0	0	0	−0.5	−1
	1	0	−0.5	0	0	0	0		

Figure 23: Batch training with $\theta = \frac{3}{2}, w = 2, \eta = 1$

Basically what happens in the online training, if i start in the first move i may go here, and so on, i'll move one step at the time since the amount of change is control by the learning rate.

in this case i move in one direction, since i apply together the two errors correction, so i'm moving in combination of the two changes of the secondo batch, then again i'm applying the two changes and i move. I do less move respect to the other since i combine the two correction for the expression that i shown.

I can try to do the same for the more complex case of the TLU, with two inputs. here i have the conjunction with the truth table describing the implementation. What i'm doing basically i have found the straight line that gives the satisfied and unsatisfied area for determining the solution.

2.9.3 Convergence theorem

If we consider a set of training patterns: $L = \{(\vec{x}, o_1), ..., (\vec{x}_m, o_m)\}$, each consisting of an input vector $\vec{x}_i \in \mathbb{R}$ and a desired output $o_i \in \{0, 1\}$.

Furthermore, let's consider $L_0 = \{(\vec{x}, o) \in L | o = 0\}$ and $L_1 = \{(\vec{x}, o) \in L | o = 1\}$. If i can show that L_0 and L_1 are **linearly separable**, then is possible to prove that we have a $\vec{w} \in \mathbb{R}^n$ and $\theta \in \mathbb{R}$ such that:

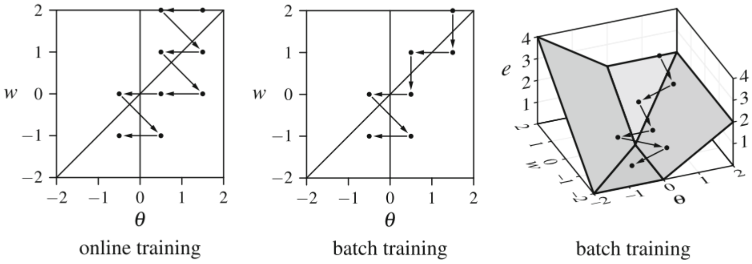
$$\forall (\vec{x}, 0) \in L_0 : \vec{w}^T \vec{x} < \theta$$

and

$$\forall (\vec{x}, 1) \in L_0 : \vec{w}^T \vec{x} \geq \theta$$

This means that is possible to divide the two sets, and then the online or batch training procedure is able to terminate. So if the two sets are linearly separable they will give us a final value in a **finite time**. The final error will e zero.

The problem is that if we are not able to perform the linear separation of L_0 and L_1, the algorithm is **not able to terminate**. The algorithm will oscillate around and we will not be able to find a solution with the zero error.



online training

batch training

batch training

Figure 24: Example of online and batch training (also with summed errors)

The correction of the parameters maybe slowed down due to the fact that we have 0 and 1 to the possible values for our outputs. This implies that if we have an output for our threshold logic function equal to 1, we can find an adjustment and apply it. If we have an input which is 0 whichever weight we have, we may not be able to compute a correction that in the end will reduce the final error.

So when we apply an input which is one we can change the weight for finding a better value for the configuration, if we apply the change on an input which is zero the possible changes actually vanishes since we are multiplying by zero, we are not observing a variation.

To avoid to waste to much time on this issue, we can change the representation of the values, for *true* we are considering 1 and for *false* we are considering -1.

What we can point out, is that a *single* TLU, is able to point out any linearly separable function. We have just to apply the delta rule which is easy and fast and guarantee to find a solution, if one exists.

The problem is given by a more complex structure, like a network of TLUs, in this case we cannot apply directly the delta rule, because we have no clue about which is the output. We need something more complex for managing that.

2.10 Artificial neural network

An ANN in general ha a very simple definition since it is a **directed** graph $G = (U, C)$ composed by nodes and edges, in the graph we have processing nodes that can elaborate the information incoming in, some arcs that are bringing in the network some external information, and others that extract the computation performed by our network (which is a structure that mimic our brain).

The connections are the axon-synaptic connections which connect the nucleus of the neurons. In a general neural network this is the very abstract definition, in practice in order to use this kind of structure we will need to have more regular more focused organization of neurons connections.

The set of vertices U is partitioned into:

- U_{in} is the set of input neurons.
- U_{out} is the set of output neurons, whi are the one delivering the result of the computation to the outside world.
- U_{hidden} is the set of hidden neurons, they don't have any direct connection to the external world.

2.11 General structure of the neuron

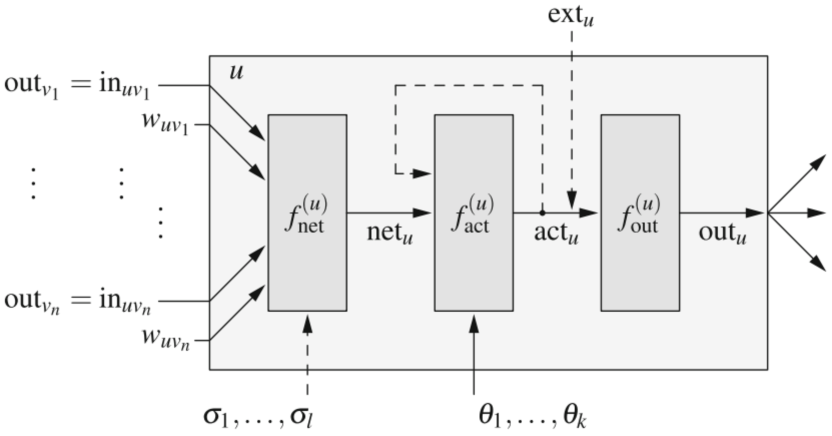


Figure 25: Internal representation of a neuron

We see that we have inputs that are coming in the network and usually this inputs are manipulated in order to understand which is the global stimulus that the neuron receive from the external world.

If an incoming signal from a previous neuron has relevance, we want to multiply the amount o signal incoming in by an appropriate constant in order to have a stronger weight for a subsequent processing in this neuron.

In this example we associate the weight w_{uv_1}, which is the weight for the neuron u respect to the incoming neuron v_1.

These inputs are processed by three stages in which we perform specific operations, we want to see how much the neuron is actually solicited. For these reason we have three stage functions:

- The $f_{net}^{(u)}$, takes the input with the *relative relevance* of the various inputs to generate the **global solicitation** for our neuron. This is a general definition, a specific definition changes in base of the network we are considering.

- The $f_{act}^{(u)}$, the activation functions analyze the network input from the previous function and generate the **excitation status** of our neuron. This will tell us if the neuron is sufficiently excited.

- The $f_{out}^{(u)}$, which takes the excitation status of the neuron and elaborate the final status of the neuron to deliver to the subsequent neurons.

In general we have also an external variable ext_u which tell us how much the excitation should be increased from a stimulus coming directly from the *external world* (not from previous neuron, from the external world).

These are the various inputs that any neuron can have, we may have both the input coming from other neurons and the input coming from the external world, or we can have for a subset of neurons only the stimulus coming from the external world and no other inputs.

We have input neurons coming which are weighted properly, these values are used with the *network input function* which is generating the global excitation status coming from the other neurons, this one is will generate the *activation status* of the neuron (how much it is stimulated by the external neurons).

In the end we have the out function which evaluates the final status of the neuron, which is delivered to the other connected neuron.

2.12 Type of artificial neural network

In the practice we won't use the general structure introduced before, we will have different type of ANN:

- **feed forward network** are ANN that doesn't contains any cycles, the acronym is FNN.

- **recurrent network** are ANN that contains cycles (backward connections), the acronym is RNN.

The operation of a general ANN:

1. **input phase**, where the external input are acquired by input neurons in the network.

2. **work phase**, the external input are disconnect (by freezing the input neurons), we move the excitation generated by the input neurons to the connected neurons, we generate the stimuli for the connected neuron, we compute the output status of them and propagate the output to the neurons which are connected to this one.

During the *working phase* if the input of neurons are steady (input stimuli are not changing), the computation of that neuron doesn't change (every stage function generate the same values, FNN).

This is not the case when we have a RNN, since if one of the outputs connected to a neuron is connected to an input will repeat the computation and this maybe change the output status (due to *recomputation*). I always say *"may"* since the actual change will depend specifically by the function that i'm using. The **recomputation** of a neuron output occurs if any of its input changes, we can't loop forever and not evolving. This means that the working phase continues until the external outputs are steady, or a maximum number of recomputation iterations is reached. The **temporal order** of computation depends by the specific NN.

Feed-forward neural network

1. Computation proceeds from input neurons progressively toward output neurons by following the topological order of the neuron in the network.
2. The external inputs are frozen.
3. Input neuron compute their outputs which are maintained steady and forwarded to the connected neurons.
4. Neurons connected to preceding neurons with steady outputs generate their respective outputs and propagated forward to the subsequent neurons, until the external outputs are generated.

Recurrent neural network

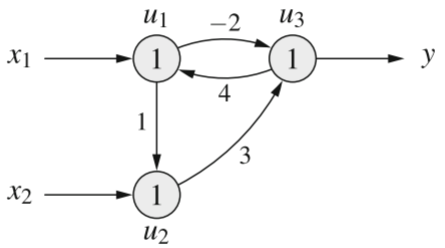
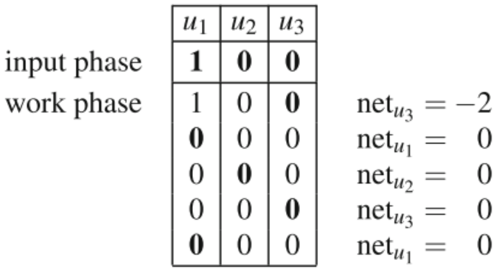


Figure 26: A simple recurrent neural network

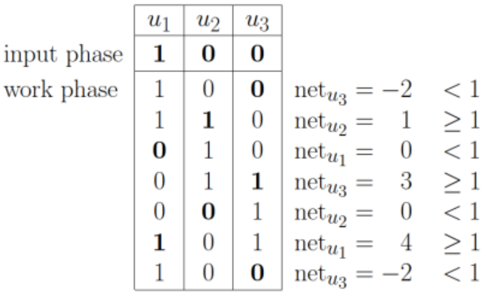
In the neurons there is the threshold which is considered for the operation, and we have some interconnection weights which define the weights to be applied to the output of a neuron when his output is delivered as input to a subsequent neuron.



	u_1	u_2	u_3	
input phase	**1**	**0**	**0**	
work phase	1	0	**0**	$\text{net}_{u_3} = -2$
	0	0	0	$\text{net}_{u_1} = 0$
	0	**0**	0	$\text{net}_{u_2} = 0$
	0	0	**0**	$\text{net}_{u_3} = 0$
	0	0	0	$\text{net}_{u_1} = 0$

Figure 27: Dataset for the previous RNN, for the u_3, u_2, u_1 order

In this case we choice to start from the input $1, 0, 0$ and with an updating order of neurons that is $u_3, u_1, u_2, u_3, u_1, u_2, u_3, ...$ Each bold number in working phase entry of the table is an output of the *ordered* neuron (0 if greater less than θ or viceversa 1). In this case we can reach a steady state, and exit the RNN.



	u_1	u_2	u_3		
input phase	**1**	**0**	**0**		
work phase	1	0	**0**	$\text{net}_{u_3} = -2$	< 1
	1	**1**	0	$\text{net}_{u_2} = 1$	≥ 1
	0	1	0	$\text{net}_{u_1} = 0$	< 1
	0	1	**1**	$\text{net}_{u_3} = 3$	≥ 1
	0	**0**	1	$\text{net}_{u_2} = 0$	< 1
	1	0	1	$\text{net}_{u_1} = 4$	≥ 1
	1	0	**0**	$\text{net}_{u_3} = -2$	< 1

Figure 28: Different dataset of the same RNN with u_3, u_2, u_1 order

Now let's consider a different ordering $u_3, u_2, u_1, u_3, u_2, u_1, u_3, ...$, in this case it is not possible to reach a steady state inside the RNN (**no stable state**, *oscillation* of output).

2.13 Configuration of a neural network

The details of the configuration strictly depends from the structure opf the network, in general we have two categories of learning procedure (or training procedure):

- **fixed learning task**.
- **free learning task**

Fixed learning task
Considering a NN of n input neurons $U_{in} = \{u_1, ..., u_n\}$ and m output neurons $U_{out} = \{v_1, ..., v_m\}$. A fixed learning task is a set of training patterns $l = (\vec{i^{(l)}}, \vec{o^{(l)}})$, each consisting of:

- an input vector $\vec{i^{(l)}} = (ext_{u_1}^{(l)}, ..., ext_{u_n}^{(l)})$
- an output vector $\vec{o^{(l)}} = (o_{v_1}^{(l)}, ..., o_{v_m}^{(l)})$.

At the end of the configuration the network is able to generate the desired output that correspond to the output vector. Since the examples are composed by an input vector and the expected output that we want to get, this is called **supervised learning**.

A fixed learning task is solved when for all training patterns $l \in L_{fixed}$ the neural network computes, from the external inputs contained in the input vector $\vec{i^{(l)}}$ of a training pattern l, the outputs contained in the corresponding output vector $\vec{o^{(l)}}$.

The error of a fixed learning task
The error says how well a neural network solves a given fixed learning task. Essentially it is the difference between desired and actual outputs.

$$e = \sum_{l \in L_{fixed}} e^{(l)} = \sum_{v \in U_{out}} e_v = \sum_{l \in L_{fixed}} \sum_{v \in U_{out}} e_v^{(l)}$$

$$e_v^{(l)} = \left(o_v^{(l)} - out_v^{(l)}\right)^2$$

In order to have a number which tell us the final quality what we need to do we have to consider the module of the error, what we are doing is consider the difference between the actual and the desired output. But in this simple difference could give us a final number which is not reflecting the total accuracy of the NN due to the sign.

A solution to this is to use a squared value, in this way we can avoid the negative sign.

Free learning task
A free learning task is the complementary approach of the fixed learning task, in which the desired behavior is not defined a priori by the pair of vectors for the input and the output.

$$n \text{ input neurons } U_{in} = \{u_1, ..., u_n\}$$
$$\text{one input vector } \vec{i^{(l)}} = \left(ext_{u_1}^{(l)}, ..., ext_{u_1}^{(l)}\right)$$

We only have a set of input vectors which are presented to the network and the learning algorithm will lead to an output vector which is similar to the given input.

Preprocessing
In order to be sure that the learning is working properly, we have to be sure that one of the input is dominating the operation of the network, as consequence we have to do some preprocessing on the data in order to give the same relevance to all neurons.

For each component of the input vector we need to compress the representation in the same range, this is called **normalization** (according to the average of the input value for each component, we need to be sure that the variance σ_k is normalized as well).

$$\mu_k = \frac{1}{|L|} \sum_{l \in L} ext_{u_k}^{(l)}$$

$$\sigma_k = \sqrt{\frac{1}{|L| - 1} \sum_{i \in L} \left(ext_{u_k}^{(l)} - \mu_k \right)^2}$$

This is the standard normalization of the deviation σ_k, we have also another possibility which is called **unbiased standard deviation** (often preferred by statistician since is not polarized on the two direction).

If we apply the normalization this is the external stimuli that we will have after the normalization, basically all the stimuli are recomputed with respect to the average value and they are normalized in dimension dividing them by the standard deviation.

$$\sigma_{u_k}^{(l)(new)} = \frac{ext_{u_k}^{(l)(old)} - \mu_k}{\sigma_k}$$

There is a problem that we have to seriously consider when we are looking to our examples, we need to have *sufficiently descriptive examples*, which have to be well distributed over the domain that i'm considering (not focussing only on a portion of the domain).

So far we have been dealing with integer and real numbers, we want to use symbols for represent a group of examples that are similar together in a concise way.

For doing that we need to associate a group of identifiers to a group of examples. For being able to represent this symbols we consider the **1-in-N encoding**, if we need to represent n symbols we have a string of 0 and 1 and only one bit the one that corresponds to the symbol we want to represent will be 1 (the others will be 0).

2.14 Multi-layer Perceptrons

A **multi-layer perceptrons** it is essentially a feed-forward neural network in which is present a strictly layered structure. They neurons are connected in groups, each groups receives the input only from the previous layer or from the external input. The output is delivered by the subsequent group, there are different kinds of layers:

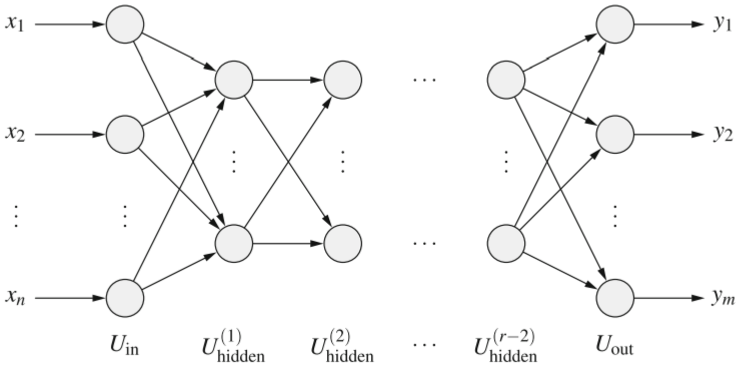

x_1
x_2
x_n
y_1
y_2
y_m
U_{in}
$U^{(1)}_{\text{hidden}}$
$U^{(2)}_{\text{hidden}}$
$U^{(r-2)}_{\text{hidden}}$
U_{out}

Figure 29: General structure of r-layered perceptron

- **input layer**
- **hidden layer**
- **output layer**

Each layers is connected, in multi-layer perceptrons the neurons are strictly connected between layers, jump are not allowed (like in the feed-forward network).

The network input function of each *hidden neuron* and of each *output neuron* is the **weighted sum** of its inputs:

$$f_{net}^{(u)}(\vec{w}_u, \vec{in}_u) = \vec{w}_u \vec{in}_u = \sum_{v \in pred(u)} w_{uv} out_v$$

The activation function of each hidden neuron is a so-called **sigmoid function**, that is, a monotonically non-decreasing function with:

$$f : \mathbb{R} \to [0,1] \text{ with } \lim_{x \to -\infty} f(x) = 0 \text{ and } \lim_{x \to \infty} f(x) = 1$$

It has a shape that allows a minimum and a maximum value (shaped), such that the possible *net status* of the neurons are inside the continuos domain between 0 and 1 of the function (squishification of the net status). If i have enough excitation in the network status the sigmoid function will give a positive excitation of the neuron, viceversa, it will point out a lower value in the function.

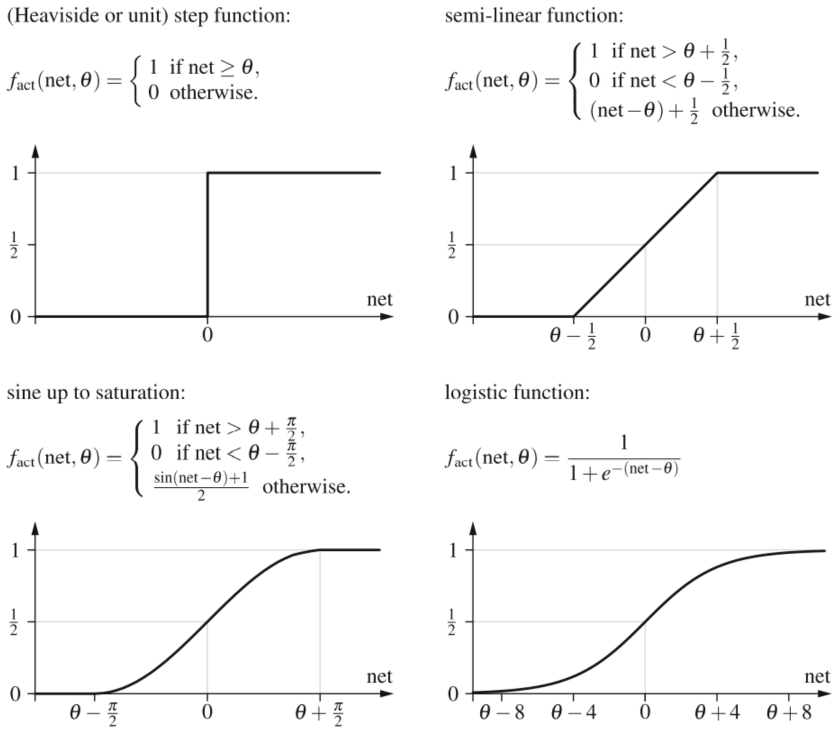


Figure 30: Some **unipolar** sigmoid activation functions

In the contemporary NN the sigmoid function are rarely used, actually the **ReLU** (*Rectified Linear Unit*) function is much more used since it is much easier to train (more similar to the behavior of the biological neurons).

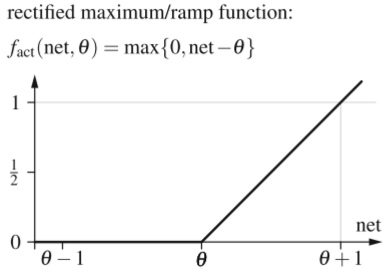


Figure 31: ReLU function

The activation function of each output neuron can be a sigmoid or can be a **linear** function (depends on what we want to achieve). There are many types of sigmoid function for representing the general behavior, the most simple is the **step function**.

I have a 0 value until my network excitation reach the value θ, then the output of excitation jump to the strongest status (the value of minimum and maximum activation are generally 0 and 1).

If you prefer a smoother approach you can use the *sin* approach were the derivative is progressively approaching the maximum value.

A **logistic** function is a function with the same shape but that doesn't reach a saturation at the extremes of the range. In this way it is possible to consider the inverse of the function, otherwise it is not possible.

We may have some problems during the learning operation when using the *step function*, since when we have 0 we won't have any effect on the output of the neuron, even if we change the activation the output will be 0. As solution it is possible to use **bipolar** (opposite to the unipolar, which extends only in one pole) sigmoid functions, which changes the ranging to $[-1, +1]$, like the *hyperbolic tangent*.

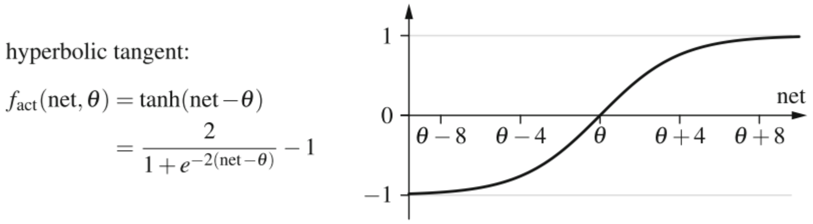


Figure 32: Bipolar sigmoid activation function (*hyperbolic tangent*)

I can describe the group of connections between two *consecutive* layers of a multi-layer perception by using a $n \times m$ matrix. Which is the collection of the connection weights between the layers:

$$\mathbf{W} = \begin{pmatrix} w_{u_1 v_1} & w_{u_1 v_2} & \dots & w_{u_1 v_m} \\ w_{u_2 v_1} & w_{u_2 v_2} & \dots & w_{u_2 v_m} \\ \vdots & \vdots & & \vdots \\ w_{u_n v_1} & w_{u_n v_2} & \dots & w_{u_n v_m} \end{pmatrix}$$

Figure 33: Matrix describing connection weights between two layers

As a consequence the computation can be described in a very simple way, by using the vectors:

$$\vec{net}_{U_2} = \mathbf{W}\vec{in}_{U_2} = \mathbf{W}\vec{out}_{U_1}$$

You just take the vector of the input neurons of the second layer (which are the output of the preceding layer) and multiply by the weight in between the layers.

Then you apply the sigmoid function σ for squish the values between $[0, 1]$, you can also use a **bias** value for each independent values by using a vector $\vec{b}$. The bias tells you *how high* the threshold has to be in order for the neuron to fire.

$$\sigma\left(\mathbf{W}\vec{in_{(U_2)}} + \vec{b}\right)$$

Let's consider an example with the **bi-implication** three-layer perceptron:

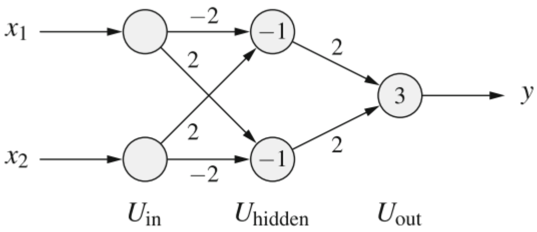


Figure 34: Three-layer perceptron for bi-implication

$$\mathbf{W}_1 = \begin{pmatrix} -2 & 2 \\ 2 & -2 \end{pmatrix} \quad \text{and} \quad \mathbf{W}_2 = \begin{pmatrix} 2 & 2 \end{pmatrix}$$

Figure 35: Weight matrices for the input and hidden layers

The only difference respect the TLUs network of bi-implication is that each neuron can be an input,hidden and output neuron. In this configuration we are dividing everything in layer of neurons, so we have to **add** a input layer for that (in respect to using TLU).

So far we have seen boolean function, but what we want to look now is how we can extend the dimensions of a feed-forward network in order to consider not only the boolean function of the TLUs but we want to consider in a multi-layer perceptron any type of real number (extend the capability of describing the world).

We can see that the multi-layer perceptron, with any input real-number can be used for function approximation.

Function approximation

Consider the function in the diagram, it is very simple and continuos, and let's consider the points $x_1, ..., x_4$ where we want to compute the value of the function and we want to find a method to approximate for any other value x a value in that function.

What i can do is to consider the **midpoint Riemann integration**.

- Approximate a given function by a step function.

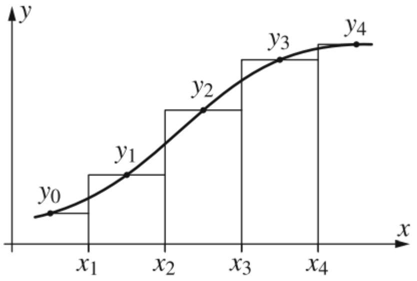


Figure 36: Approximating a continuos function with step functions

- Construct a neural network that computes the step function.
- Error is measured as the area between the functions.

It is possible to prove that if you take any Riemann integrable function, it can be approximated with arbitrary accuracy by a *four-layer perceptron*.

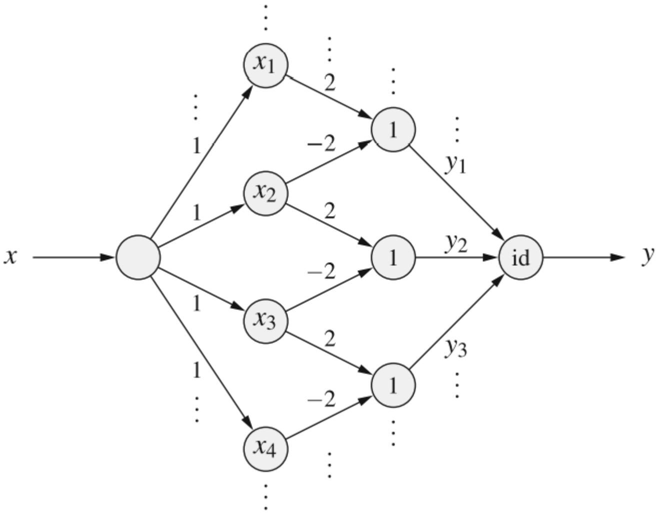


Figure 37: NN that computes the step function for integration

The input x is taken by an input neuron, then we have the first layer composed by the subdivision of the domain in the points x_1, x_2, x_3, x_4.

In the second hidden layer, we create one neuron for each step, which receives input from the two neurons in the first hidden layer that refer to the values x_i and x_{i+1} marking the border of the step. Only one neuron in the second layer can be active, and it will represent the step where the input values lies (this through the **combined excitation** of the neurons in the first hidden layer).

The connection from the neurons of the second layer to the output neuron are weighted with the function values of the stair steps that are represented by the neurons.

Since only one neuron can be active on the second hidden layer, the output neuron receives as input the height of the stair step , in which the input value lies, as result it computes the correct sampling of the function saw in figure 36.

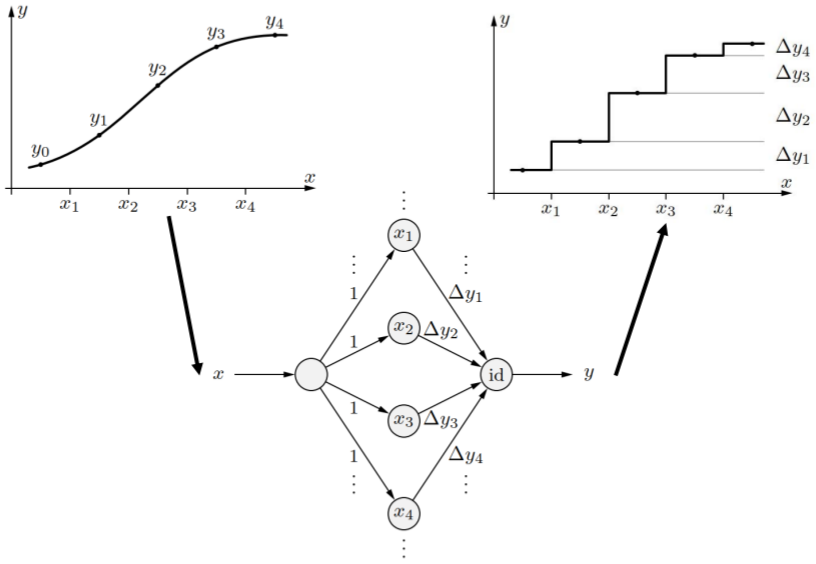
The multi-layer perceptrons can be considered an **universal approximators** of the Riemann integration technique, with the maximum desired error (i can choose the maximum error i want to get for my function by choosing the number of neurons for get that accuracy).

Delta approximation approach

We can actually simplify the error by considering a trick instead of using the combined excitation.

I can split the domain of the function for my network in parts like before, then instead of defining the value of the function for each interval i just use iteratively the Δ variation respect to the value considered.

Figure 38:



The structure of the network (figure 38) will be simpler because i will distribute the input of the hidden neurons, that will tel me if the value x is before x_i or greater than x_i (i don't care where).

For example, if the value is between x_1 and x_2 the first neuron will generate Δy_1 and this will be delivered in output.

If i have a value between x_2 and x_3 i will still have x_1 that will be excited enough and will generate the *contribution* for the output (x_1 and x_2 will be both excited, their contribution will be summed up and then delivered to the output).

This will make simpler the structure of the network.

2.15 Regression

Let's find a way for approximate a function without using the basic calculus approach. In order to do this we have to understand the concept of **regression**. We saw that for training an ANN we need to minimize the error function, which is computed by considering the squared difference between desired output and actual output.

The regression is a technique used in statistical analysis for extrapolating a straight line that better approximate the existing relationship inside a dataset.

Formally, considering the dataset $G = \{(w_0, y_0), ..., (w_n, y_n)\}$ let's imagine it exists a functional relationship between the input vector w_i and the abscissa y, then the regression will help us to find the parameters of that function. Different kind of functions will give us different kind of regressions.

2.15.1 Linear regression

If we expect that our quantities x and y exhibits a linear dependence, then we have to identify the parameters a and b that extrapolate the straight line $y = g(x) = a + bx$. In general, won't be possible to find a straight line that traverse all the points of the dataset. What we will do is finding a straight line which deviates the lest possible, so that minimize the error as follows:

$$F(a,b) = \sum_{i=1}^{n}(g(x_i) - y_i)^2 = \sum_{i=1}^{n}(a + bx_i - y_i)^2$$

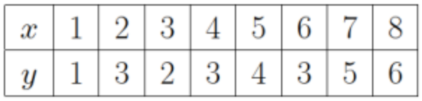
The necessary condition to find the minimum is given us by mathematical, if i take the partial derivatives between the two parameters a and b (which are the variables in the formula) setting this partial derivatives of th error to 0 it will give to me the condition that allow us to find the minimum (*Fermat's theorem*).

$$\frac{dF}{da} = \sum_{i=1}^{n} 2(a + bx_i - y_i) = 0$$

$$\frac{dF}{db} = \sum_{i=1}^{n} 2(a + bx_i - y_i)x_i = 0$$

The *linear algebra* tells me the solution is unique unless i'm so unlucky that all the values x coincides, in that case i have basically one equations but two variable (a and b) and as consequence infinite solutions.

For example, if i need to find the regression of these points:



x	1	2	3	4	5	6	7	8
y	1	3	2	3	4	3	5	6

$$y = \frac{3}{4} + \frac{7}{12}x.$$

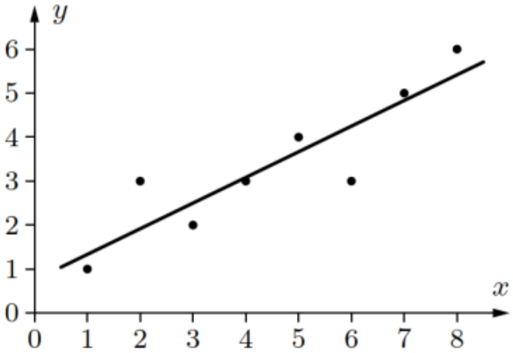


Figure 39: Regression line example

2.15.2 Polynomial regression

The previous method is generalizable to polynomial of arbitrary order. The model i have considered is not a good model, is too approximate, i can look if there is instead a very simple straight line a polynomial. Instead of considering a polynomial of grade one, i consider a polynomial of grade m.

$$y = p(x) = a_0 + a_1 x + ... + a_m x^m$$

The minimization fo the error now can be generalized in this way:

$$F(a_1, ..., a_n) = \sum (p(x_i) - y_i)^2 = \sum (a_0 + a_1 x + ... + a_n x^n - y_i)^2$$

Like in the linear regression, the necessary conditions for the function to be minimized (finding the minimum), are that the partial derivatives respect to the parameters a_i vanishes:

$$\frac{dF}{da_0} = 0, \frac{dF}{da_1} = 0, ..., \frac{dF}{da_m} = 0$$

- This system can be solved by using the standard methods from linear algebra.
- The solution is unique unless the points lie extactly on a polynomial of lower degree.

2.15.3 Multilinear regression

Until now i just tried to make the approximation more accurate going in the direction of polynomial,*what happens if i have a function in multiple variables?*

$$z = f(x, y) = a + bx + cy$$

If i want to do a multi-linear regression (since i'm applying linear regression to a function of two variables), i have just to apply what i wast doing before.

I have to consider the error in the approximated function f, and the actual value given by the samples z_i that i'm collecting (minimizing the sum of squared errors):

$$F(a, b, c) = \sum_{i=1}^{n}$$

What we need to do? again we need to find when the error is going to 0, this happens when the partial derivatives of the parameters are 0.

$$\frac{dF}{da} = \sum_{i=1}^{n} 2(a + bx_i + cy_i - z_i) = 0$$
$$\frac{dF}{da} = \sum_{i=1}^{n} 2(a + bx_i + cy_i - z_i)x_i = 0$$
$$\frac{dF}{da} = \sum_{i=1}^{n} 2(a + bx_i + cy_i - z_i)y_i = 0$$

As already said multiple times, the linear algebra will allow me to solve this problem since i have three parameters a, b, c and three equations.

Except the unfortunate case where all points are on a straight line, because in this case i have a plane that can be rotated in any direction and i have *infinite solutions*.

I can consider trying to approximate with a multi-linear regression a function that is defined on m different variables, this is the generalization of what we have seen previously (difficult to draw):

$$y = f(x_1, ..., x_m) = a_0 + \sum_{k=1}^{m} a_k x_k$$

I have to minimize the sum of squared errors (vectors for parameters and matrices to define the various values):

$$F(\vec{a}) = (\mathbf{X}\vec{a} - \vec{y})^T (\mathbf{X}\vec{a} - \vec{y})$$

where:

$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \dots & x_{m1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{1n} & \dots & x_{mn} \end{pmatrix}, \qquad \vec{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \qquad \text{and} \qquad \vec{a} = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{pmatrix}$$

Figure 40: Various x values and vector parameters

I need to define the **gradient** which is the generalization of the previous definition defined on vectors and not on the partial derivatives of functions as we seen before. We need to look where the gradient is 0 which will give us the *hyperplane* touching the surface in the minimum.

$$\vec{\nabla}_{\vec{a}} F(\vec{a}) = \vec{\nabla}_{\vec{a}} (\mathbf{X}\vec{a} - \vec{y})^T (\mathbf{X}\vec{a} - \vec{y}) = \vec{0}$$

This comes out as set of regular equations and linear algebra will allow us to solve it as usual unless there is the singular case (if i have all points aligned to a single straight line the plane which is minimizing my error is not defined).

The system of normal equations:

$$\mathbf{X}^T \mathbf{X} \vec{a} = \mathbf{X}^T \vec{y}$$

which has solution unless $\mathbf{X}^T\mathbf{X}$ is a singular:

$$\vec{a} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \vec{y}$$

2.15.4 Logistic regression

In the situation in which the dataset is not approximated with sufficient accuracy from a polynomial function, we could use different kind of functions, for example:

$$y = ax^b$$

We can transform this in a linear equation by applying the operation of logarithm:

$$\ln y = \ln a + b \cdot \ln x$$

In the case of ANN we are interested in particular at the **logistic function**:

$$y = \frac{Y}{1 + e^{a+bx}}$$

If we apply the logarithm of this equation we can derive a different expression of our function y so that the description of this function will be a **linear description**.

Since lot of ANN uses as proper neuron activation function the logistic function, if we would find a way for applying the regression method on that we could determine the parameters of any network.

If we would find a way for applying the method of regression om the neurons, we could determine the parameters of any network at two layers of only one point. The value a of the function represent the threshold of the output neuron, while the value of b represent the weight of the input. We can linearize the logistic function by applying the following transformations (called **logit transformation**):

$$y = \frac{Y}{1+e^{a+bx}} \longleftrightarrow \frac{1}{y} = \frac{1+e^{a+bx}}{Y} \longleftrightarrow \frac{Y-y}{y} = e^{a+bx} \longleftrightarrow \ln\left(\frac{Y-y}{y}\right) = a+bx$$

x	1	2	3	4	5
y	0.4	1.0	3.0	5.0	5.6

$$\downarrow$$

$$z = \ln\left(\frac{Y-y}{y}\right), \qquad Y = 6.$$

$$\downarrow$$

x	1	2	3	4	5
z	2.64	1.61	0.00	−1.61	−2.64

Figure 41: Example of logistic regression

The results of the regression line in the example are:

$$z \approx -1.3775x + 4.133, y \approx \frac{6}{1+e^{-1.3775x+4.133}}$$

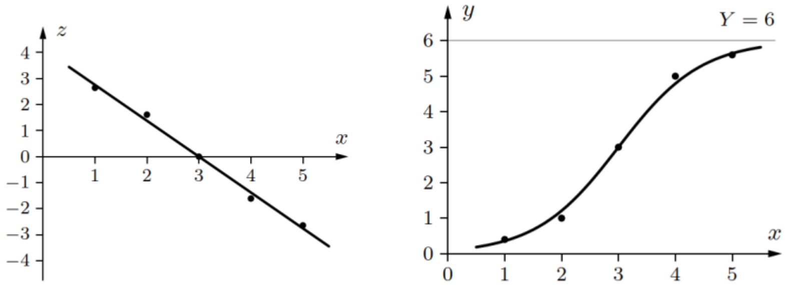


Figure 42: Plot of logistic function

How can we understand the values of this non polynomial approximation by transforming it applying the log transformation, so that we can perform the approximation on a function that appear to be linear and then transform it back on the original function.

We can consider a logistic function defined on two variables, and we have this bi-dimensional shape defined on two arguments. we can apply the same principle that we see before, this can be used to solve a problem of separating two groups of examples of different classes (or group).

$$y = \frac{1}{1 + exp(4 - x_1 - x_2)} = \frac{1}{1 + exp\,(4 - (1,1)^T(x_1, x_2))}$$

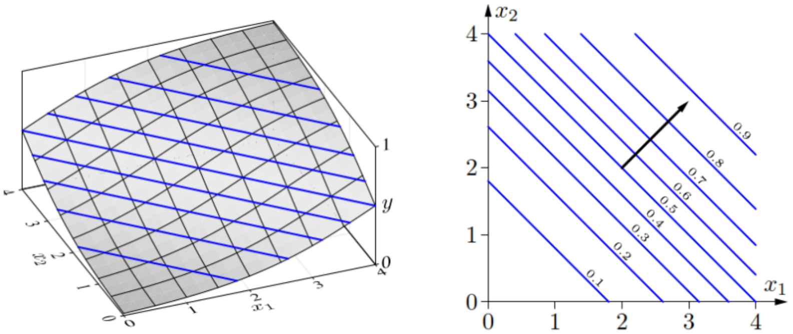


Figure 43: Plot of logistic function with two arguments

2.15.5 Two-class problems

Basically the two class problems can be solved by considering the two attributes, which are the name of the class (C is the class of attributes) and a vector random of m dimension.

$$dom(C) = c_1, c_2$$

We consider the **probability** of belonging to the first class c_1 and the probability to be in the second class c_2.

$$P(C = c_1 | \vec{X} = \vec{x}) = p(\vec{x})$$
$$P(C = c_2 | \vec{X} = \vec{x}) = 1 - p(\vec{x})$$

Given a dataset of points $X = \vec{x_1}, ..., \vec{x_n}$, each of which belongs to one of two classes c_1 and c_2.

Basically i want to get a **simple description of the function** $p(\vec{x})$, if i have this function i can apply the **logistic description**:

$$p(\vec{x}) = \frac{1}{1 + e^{a_0 + \vec{a}\vec{x}}} = \frac{1}{1 + exp(a_0 + \sum_{i=1}^{m} a_i x_i)}$$

Then i can apply the **logistic transformation** so that i can obtain the **formal description** of the probability of being on one or the other class:

$$\ln\left(\frac{1-p(\vec{x})}{p(\vec{x})}\right) = a_0 + \vec{a}\vec{x} = a_0 + \sum_{i=1}^{m} a_i x_i$$

How can i find the specific value of the probability (and so solving the splitting of the example)? We can consider a specific function called **kernel** that describes how strongly a data point influences the probability estimate for neighboring points.

which give us the correlation in the examples, given some examples how can i say that the example that i observed belongs to the group is influenced by similar examples, or belong to the other group which means that is similar to the examples of the other group.

With a kernel we can describe the similarity of a group of examples, the **Gaussian function** is commonly used. A function like this tell me that if the picked data point is similar to the elements in the middle area, in that case i have a significant value of the function, the more i go far from the values which are similar the less is the value of the function.

$$K(\vec{x},\vec{y}) = \frac{1}{(2\pi\sigma^2)} exp\left(-\frac{(\vec{x}-\vec{y})^T(\vec{x}-\vec{y})}{2\sigma^2}\right)$$

If i want to estimate the **probability density** i will use this expression:

$$\hat{f}(\vec{x}) = \frac{1}{n}\sum_{i=1}^{n} K(\vec{x},\vec{x}_i)$$

The kernel estimation applied to a two-class problems:

$$\hat{p}(\vec{x}) = \frac{\sum_{i=1}^{n} c(\vec{x}_i)K(\vec{x},\vec{x}_i)}{\sum_{i=1}^{n} K(\vec{x}, vecx_i)}$$

If it is

$$c(\vec{x}) = 1$$

the x_i will belong to class c_1 if $c(\vec{x}) = 0$ otherwise.

2.16 Training multi-layer perceptrons

2.16.1 Gradient descend

3Blue1Brown Conceptually we think about each neuron to be connected to each neuron of the previous layer, and the weighted sum of this neurons expresses the strength of this connections:

$$\sigma(w_1u_1 + w_2u_2 + ... + w_nu_n + b)$$

If we consider all the weights and bias initialized randomly, the MLP network will perform pretty terrible (he is acting randomly).

What you do is defining a **cost function** that can express if the result of the NN is good or bad (for our objective). The greater the function is the greater is the error of the NN respect to desired output.

$$e_v^{(l)} = \left(o_v^{(l)} - out_v^{(l)}\right)^2$$

So then what you do is considering the average cost function over all the samples inside the NN, it is a cost value that express how good or bad the network is.

We want to use this error in such a way that we can perform better during the next execution, let's consider a function $C(w)$ representing just one cost, if we want to find the input that minimize the cost of this function we just have to take the derivative $\frac{dC}{dw}(w) = 0$, but this is not really feasible for complicate functions. You can find different **local minimum** of the function, so what you find isn't the best possible cost function value that you will find. Find the global minimum is pretty hard.

But our function will be much more complicated, since we are dealing with lot of parameters (like the weights and the biases), let's imagine now a function with two variables where the cost function is graphed as a surface above the *xy* plane. Now, for minimizing the function i should ask my self, in *which direction the $C(x, y)$ function decreases most quickly?*, multi-variable calculus has a concept of **gradient**, which is the direction of the steepest increase $\vec{\nabla} C(x, y)$, and more to that the *length* of that vector expresses how much steep is the increase. The algorithm essentially will be:

- Compute $\vec{\nabla} C$
- Small step in direction $-\vec{\nabla} C$
- Repeat until convergence

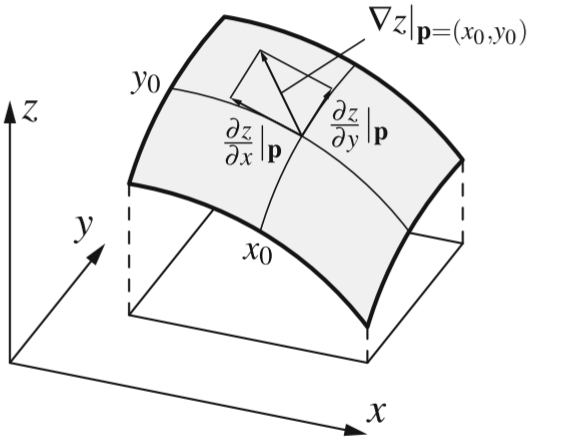
The negative gradient of the cost function will tell you how to change all the weights and biases for all the connections, to efficiently decrease the cost (no overshot). The backpropagation is an algorithm for computing that *crazy* gradient.

The gradient is a vector expressed as n-dimension, where n depends by weights and biases, it is usually a giant number (impossible to visualize). The important thing, is that the magnitude of each component (so the value) will tell you **how sensitive** the cost function output will be respect to the weight and bias (how much it moves respect the previous value).

Lesson notes Now we have to apply this for all the values for all the weights of the network. Essentially when we talk about **training** or the process of learning of a NN it's just about minimizing the cost function (or error function).

More to that, the negative gradient vector will store the relative importance of the weights for each neurons.

What we want to do is to follow the idea of the **gradient descent**, we want to find the *local minimum* of an error function in order to find the proper set of weights.



$\nabla z|_{\mathbf{p}=(x_0,y_0)}$
y_0
z
$\frac{\partial z}{\partial x}|_{\mathbf{p}}$
$\frac{\partial z}{\partial y}|_{\mathbf{p}}$
y
x_0
x

Figure 44: Intuitive interpretation of the gradient of a real-valued function $z = f(x,y)$ at a point (x_0, y_0)

Considering this error surface (figure 44), if we are in the central point we can look to the derivatives of the error function in the two directions, the **gradient** ∇ is the vector tangent to the surface and will tell us the direction where the surface is more or less increasing.

If we want to find the solution for our learning we need to look for the minimum of this error function, so actually we need to look to the opposite direction to the gradient and we look to reach the minimum.

$$e = \sum_{l \in L_{fixed}} e^{(l)} = \sum_{v \in U_{out}} e_v = \sum_{l \in L_{fixed}} \sum_{v \in U_{out}} e_v^{(l)}$$

So we need to evaluate the gradient to find the direction of the decreasing value, and we need to go in the proper direction in order to reduce the error. In the case of the MLP calculate the gradient means compute the partial derivative of the error function in respect of the threshold and the weights taken as parameters.

Given $\vec{w}_u = (-\theta, w_{u_1}, ..., w_{u_k})$ as the vector of weights of a single layer extended with the threshold, then compute the gradient as follow:

$$\vec{\nabla}_{\vec{w}u} e = \frac{\partial e}{\partial \vec{w}_u} = \left(-\frac{\partial e}{\partial \theta_u}, \frac{\partial e}{\partial w_{up1}}, ..., \frac{\partial e}{\partial w_{up_n}} \right)$$

Since the total error e is given by the sum of the individual errors in respect to all neurons and all training patterns l, we get that:

$$\vec{\nabla}_{\vec{w}_u} e = \frac{\partial e}{\partial \vec{w}_u} \sum_{l \in L_{fixed}} e^{(l)} = \sum_{l \in L_{fixed}} \frac{\partial e^{(l)}}{\partial \vec{w}_u}$$

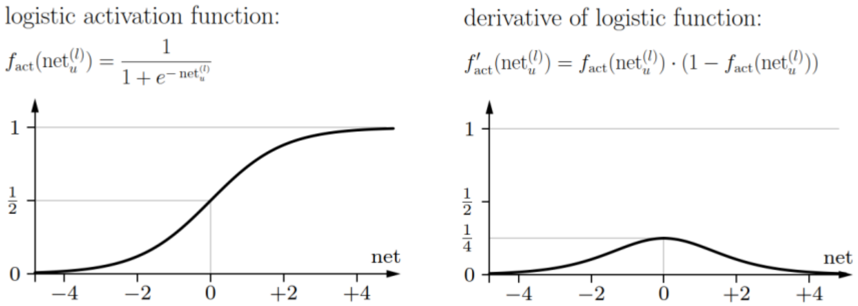


Figure 45: Logistic function as activation function

If we have a **logistic function** as $f_{(act)}$ we will have that the changes performed on the vector $\vec{w}_u$ will be proportional to the derivative of the $f_{(act)}$. More near to 0 the value of the function will be, more precipitous will be the learning.
How we can compute the necessary adjustment for each neurons-weight and threshold after we found the error?
The process that allow this is called **error backpropagation**:

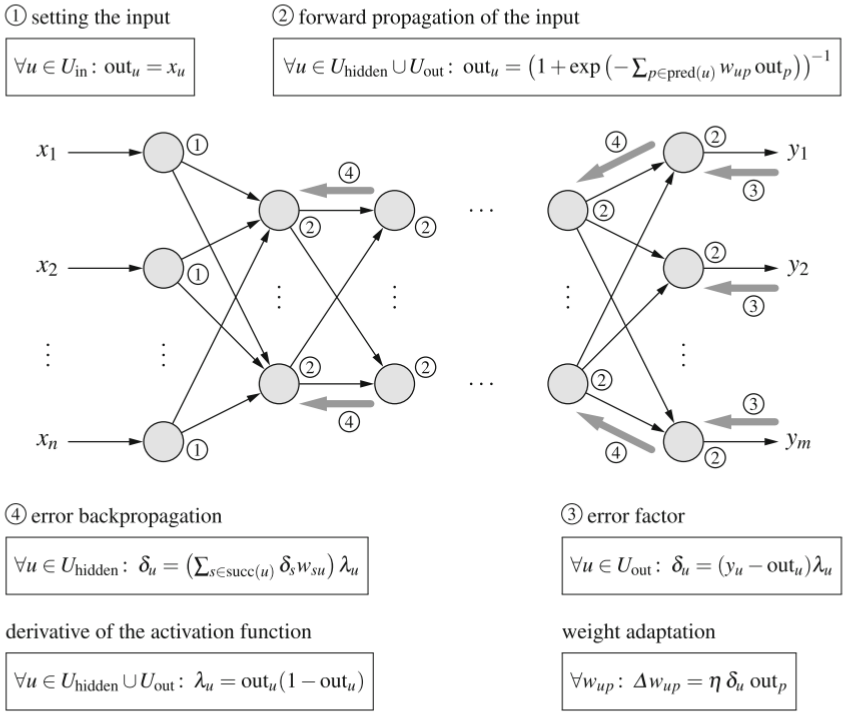

① setting the input
$\forall u \in U_{\text{in}}:\ \text{out}_u = x_u$
② forward propagation of the input
$\forall u \in U_{\text{hidden}} \cup U_{\text{out}}:\ \text{out}_u = \left(1 + \exp\left(-\sum_{p\in\text{pred}(u)} w_{up}\,\text{out}_p\right)\right)^{-1}$
x_1
x_2
x_n
y_1
y_2
y_m
① ② ③ ④
④ error backpropagation
$\forall u \in U_{\text{hidden}}:\ \delta_u = \left(\sum_{s\in\text{succ}(u)} \delta_s w_{su}\right)\lambda_u$
③ error factor
$\forall u \in U_{\text{out}}:\ \delta_u = (y_u - \text{out}_u)\lambda_u$
derivative of the activation function
$\forall u \in U_{\text{hidden}} \cup U_{\text{out}}:\ \lambda_u = \text{out}_u(1 - \text{out}_u)$
weight adaptation
$\forall w_{up}:\ \Delta w_{up} = \eta\,\delta_u\,\text{out}_p$

Figure 46: Schematized structure of the error backpropagation process

We assume that the activation functions is a *logistic function* for each neuron $u \in U_{(hidden)} \cup U_{(out)}$, except for the input neurons.

1. Apply the input at the input neurons that is returned without modifications at the subsequent first hidden layer.

2. We compute for each neuron of the subsequent layers the weighted sum of the inputs and we apply at the result the logistic function, producing the output that will be propagated in all the network until the terminal neurons.

3. Compute the difference between the desired output and the actual output. since it is possible to invert the logistic function $f_{(act)}$, we can know which was the input (error) that has induced that particular error (δ_u).

4. Now that we have transformed the error of the output variable out_u in the error of the input variable net_u, we can distribute the error (with the correction) in a proportional way back to previous neuron, we back propagate the error until the input neurons.

We have to say that given the shape of the logistic function the error can disappear completely, since the gradient will approximate more the **null vector** the more it will be near the zero.

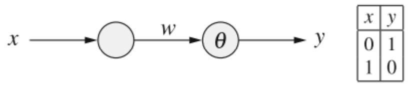
The weight adaptation is performed by the following formula (this tells me how to perform the correction):

$$\forall w_{up} : \delta w_{up} = \eta \delta_u out_p$$

If you initialize the *learning rate* η with a too high value instead of descending the curve we risk to jump from a *"peak"* of the function to another, without ever converging to the minimum. Furthermore, it is not all certain that the minimum reached in this way is the global minimum of the function.

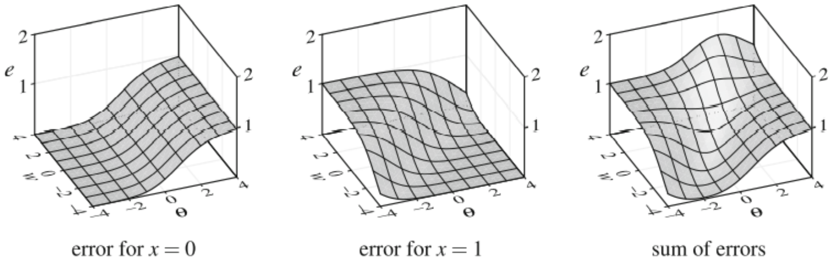
A solution to the problem could consist in *repeating* the learning, initializing the system with a different configuration of weights and threshold, and then choice at the end which configuration result in the better minimum.

Negation example For example let's consider the negation $\neg x$, there is a two-layer perceptron for this function.



x	y
0	1
1	0

Figure 47: Two-layer perceptron with single input and training examples for the negation



error for $x = 0$

error for $x = 1$

sum of errors

Figure 48: Squared errors for computing the negation by using a logic activation function

From a numeric point of view, this procedure won't allow us to reach really the minimum, we will ahave some residual errors due to the computation of the various parameters (this will change according to the process we are adopting).

2.16.2 Variant of Gradient Descend

The variant aim to change the **learning rate** and the **length of the learning step**.

- *Manhattan training*, taking just the sign of the gradient, very fast but you may not reach the optimum.
- *Flat spot elimination*, it tries to limit the culling of the step length when we get near a function plateau by ”lifting” artificially the derivative of the function in that point.
- *Momentum term*, at each successive step we add to the gradient a fraction of the previous with changed weights, so that we can have a sort of memory of how fast it changes respect to the past.
- *Self-adaptive error backpropagation*, i allow to each parameter to have a different learning rate, in this way we can have a grain fine control respect to the characteristic of the single parameter.
- *Resilient error backpropagation*, it’s a combination of the Manhattan variation with the Self-adaptive.
- *Quick propagation*, instead of using the gradient i approximate the function with a parable and i jump directly to the peak of this one.
- *Weight decay*, reduces the weights for avoiding to remain trapped in an already saturated region (avoiding too big weights to keep stuck neurons).

2.17 Number of hidden neurons

For a single hidden layer the following rule of thumb is popular (take as granted):

$$\text{Number of hidden neurons} = \left(\frac{\text{number of inputs} + \text{number of outputs}}{2}\right)$$

The problem is that if we have to few neurons in the hidden layer, we will not be able to achieve a good approximation the function that we need to approximate. We have not enough parameters, this behavior is called **underfitting**.

On the contrary, if we have very large hidden layers we have many neurons, we have many many parameters to train and this may force the NN to learn the examples to much, and this will focus the network on this examples only, we lose the ability of generalizing the desired behavior, this is called **overfitting**.

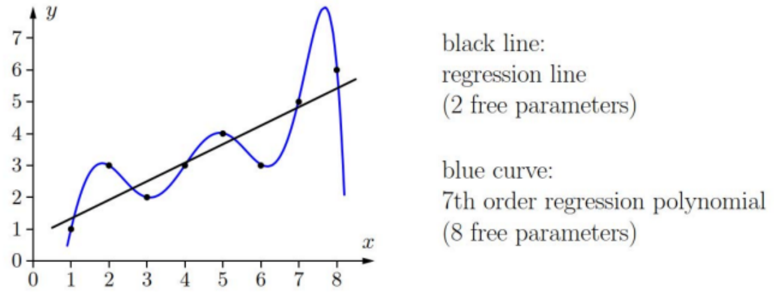


Figure 49: The blue curve fits the data points perfectly, not a good model

For example, the NN learned perfectly the blue line to pass exactly in the points, but this is not what we want to have. Now we can't generalize the abstract view of the black line (too many parameters).

What we need to do in order to understand when we have good quality for our learning? Follow, the next subsection.

2.18 Cross validation

In order to understand if we have a good quality for our learning we need to randomly split our data sets in two parts:

- Training set: used for the training.
- Validation set: used for checking the quality of the result.

This will allow us to see (by using the validation set) if the training makes the NN overfitting the configuration or not, if the error that we have is still reasonable low, we have a good quality of the learning (we still can do good generalization), viceversa we have a bad learning quality.

We can do the splitting in two ways:

- **Cross validation**: splits randomly the data in two subsets (for training and validation), we train the MLP with different numbers of hidden neurons on the training data and evaluate them on the validation data. Then you repeat the split of the data and the training-evaluation many times and average the results. At the end you choose the number of hidden neurons with the best average error.
- **N-fold cross validation**: the data is split in n subsets (called *folds*) of about equal size. The relative frequency of the output values in the folds represent as well as possible the relative frequencies of these values in the data set as a whole (**stratification**). Out of these n data subsets, n pairs of training and validation data set are formed by using 1 fold as a validation and $n-1$ folds for training.

randomly the data in two subsets for training and validation (**cross validation**) and we can repeat this splitting in different phases and at the end we can compare the. or we can split the data set in N-folds (**N-folds validation**) and then use the various n subsets for training and $n-1$ subsets for validation, in this way we can use most of the example for training instead of validation.

The **stopping criterion** is also very important, we stop the training when the validation error is sufficient low.

2.18.1 Sensitivity analysis

Sensitivity of the NN to the various parameters that we have, the variations that we may have to the various parameters influences the behavior of our NN. We want understand how muc hthe learning applied to the NN is really independent from the behavior of the NN.

This is important to understand how much is generalizable the behavior of our NN.

This is a problem for MLP, when we perform the learning (supervised or unsupervised), basically we have a data set presented to the NN and then the learning algorithm adjust the parameters in ordered to find the desired behavior of the NN.

In our hands we have an algorithm, but we don't have an understanding of the why the parameter are configured in this way. We are trying to give an explanation of why a NN is configured in a specific way, this is actually field of research (we still don't have a rational idea).

For the sensitivity analysis which is part of this understanding, we want to answer this question: *How much the output of each neuron is changing if we change the data set for training* (still describing the desired behavior)*?* So essentially, which inputs the output(s) react(s) most sensitively, it hints about which inputs aren't needed and may be discarded.

The approach consists in determine the change of ourput relative to the change of input:

$$\forall u \in U_{in} : s(u) = \frac{1}{|L_{fixed}|} \sum_{l \in L_{fixed}} \sum_{v \in U_{out}} \frac{\partial out_v^{(l)}}{\partial ext_u^{(l)}}$$

2.19 Deep learning

A modern approach to MLP called **Deep learning**, with MLP we can approximate any continuos integrable function, but we have in general a pretty large hidden layer. First problem, *what we can do to simplify the structure?* The second problem, with MLP we have to know the characteristic of the data which are relevant to pick the important data to configure the NN.

It has been experimented that adding 1 or 2 more layers helps to have a concise NN but with the same characteristic of a MLP with a large number of neurons in the hidden layers.

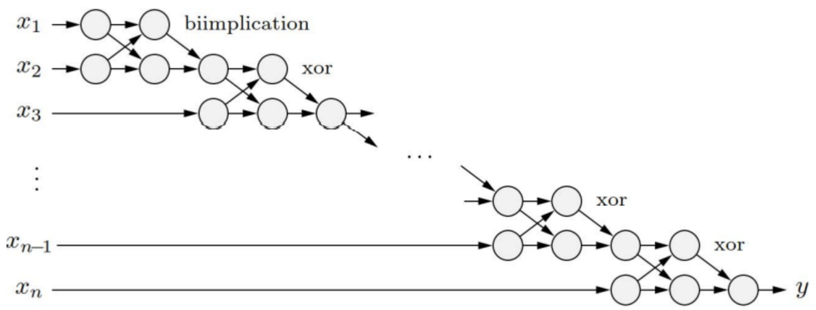


Figure 50: n-bit parity function

The deep learning network is basically a MLP, but with a difference: What we want to do it consists in not having any type of knowledge about the problem and try to force the NN to configure itself with a limited and small number of neurons.

For example, let's consider the n-bit parity function, which output 1 if the n-bit word is even, or viceversa 0. If we want to use an MLP with only one hidden layer, which has 2^{n-1} neurons, the number of hidden neurons grows **exponentially** with the number of inputs. This because the function is a disjunction of 2^{n-1} conjunctions. Instead if we use **multiple** hidden layers, the **linear growth** is possible (respect to the input). This finding bring to the developing of *deep learning*, where the *"depth"* is the one given by the longest path which separates the input neurons from the output neurons.

The rational is to allow a greater deepness of the network in change of better performance in construction and computation of the NN. The deep learning bring some downsides:

- *Overfitting*: the increases of neurons given from the extra hidden layers can multiply the parameters in a disproportional way.
- *Vanishing gradient*: during the propagation of the error the gradient will get reduced until the vanishing.

Some solutions to the overfitting issue:

- *Weight decay*: set a maximum limit to the values which can assume weights this for preventing an adjustment too much dependent from the data set.
- *Sparsity constraint*: introducing some limit to the number of neurons of the hidden layers, or limiting the number of the active neurons.
- *Dropout training*: some neurons of the hidden layers are omtitted during the evolution of the network.

While the issue of the vanishing gradient is given by the fact that the activation function it's a logistic function, which derivative reach at max the value

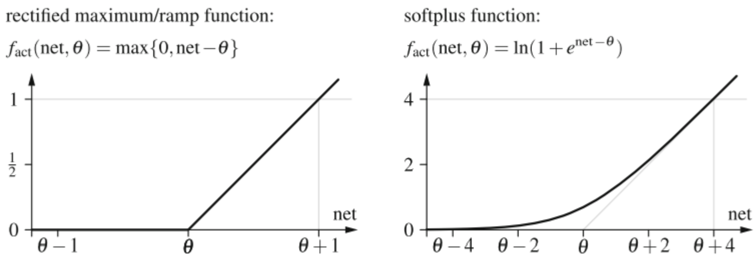


Figure 51: Ramp function and softplus function

of $\frac{1}{4}$. As consequence of this the propagation of the error to a previous layer adds a value, often smaller than 1, and in this way reducing the gradient.

A solution consists in editing slightly the activation function in a way that will be always increasing. Some candidates for that are the *ramp function* and the *softplus function*. A totally different approach consist in building the network *"layer by layer"*. A much used technique consists in think at the NN like a stack of *autoencoder*. An autoencoder is an MLP which maps the input inside an approximation, using an hidden layers of less dimensions. The hidden layer works like an *encoder* by encoding the input in a internal representation which will be decoded to the output layer. The autoencoder, has only one layer, it doesn't suffer about the same limitation and can be traversed normally from the backpropagation.

A problem with this approach is that if there are a lot of neurons in hidden layer as much are in the input layer we are going to propagate with less adjustments, and without the autoencoder extracting any knowledge from the data.

There are three possible solutions:

- *Sparse autoencoder*: provide to use a much smaller number of neurons inside the hidden layers, respect to the input layers. The autoencoder will be forced to extract from the input some features instead of just propagating the data.

- *Sparse activation scheme*: in a similar way for avoiding the overfitting, we decide to *"shutdown"* some neurons during the computation.

- *De-noising autoencoder*: we add randomly some noise to the input.

For obtaining an MLP with multiple layers we combine differente autoencoder. Initially we start by training just one autoencoder. At that time you remove the decoder and you preserve only the internal layer. You use the data processed from this autoencoder for training the second, and so on until you reach a satisfiable number of layers. MLP constructed in this way are really efficient at recognizing with success hand written numbers. If we would want to use similar NN for a more broad class of applications, like, for example, the

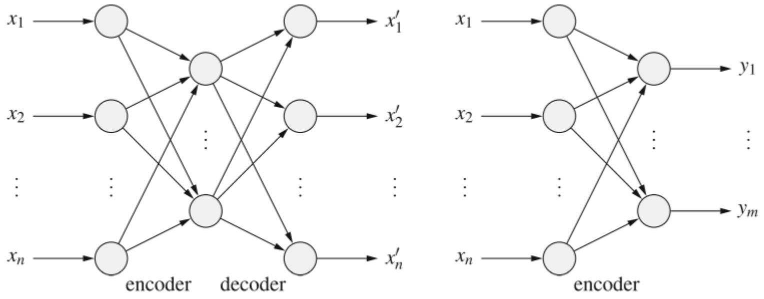


Figure 52: Autoencoder and autoencoder with the decoder removed

feature recognized by the internal layers are not located in a specific portion of the image, we would need to use a CNN (*Convolutional Neural Network*, next topic). This architecture is inspired by the working of the human retina, where the neurons used for the perception has a receptive field, or in other words, a limited region where they can answer to stimulus.

This is simulated inside the CNN by connecting the neurons of the first layer just to some neurons of the input. The weights are partitioned in a way that partial networks can be evaluated from different prospective of the image.

During the computation it will proceed by moving the receptive field on the totality of the image. As result you will obtain a convolution of the weight matrix with the input image.

2.20 Radial Basis Function Networks

This is another NN model, we have a special type of structure for the neurons and a special approach for information we are collecting from images (typically).

I have a 3-layered feed forward network, where the activation function of the hidden layer is a *Radial Basis Function* (RBF).

An RBF is a function which try to point out what is relevant in a very specific area of the information we are observing (an image), and tries to diminish what is in the surrounding area. So it will focus on relevant part of the image where we want to understand the contents.

In this kind of NN we have a set of values for various inputs, we represent this with a vector, we have for example a three dimensional space, where each value represent the input. What i'm considering as input of the hidden layer is the difference between this vector and the weight vector, which is the distance between the vectors.

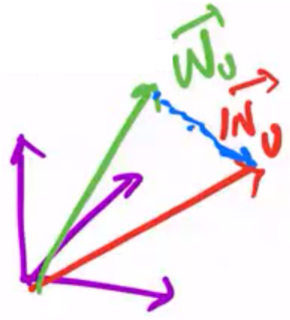


Figure 53: Distance between $\vec{w}$ and $\vec{in}_u$

There are different families of distances, we typical consider the **Minkowski Family**, which are distances defined in general by this formula:

$$d_k(\vec{x}, \vec{y}) = \left(\sum_{i=1}^{n} |x_i - y_i|^k \right)^{\frac{1}{k}}$$

- $k = 1$: Manhattan distance.
- $k = 2$: Euclidean distance.
- $k \to \infty$: Maximum distance.

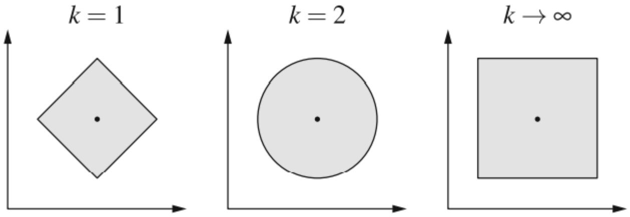


Figure 54: Manhattan, Euclidean and Maximum

The RBF has an activation function in the output layer which is **linear**. Differently, the hidden layer has an activation function which is a **radial function**. A radial function decreases from 0 to ∞ in a monotonically way.

$$f : \mathbb{R}_0^+ \to [0, 1] \text{ with } f(0) = 1 \text{ and } \lim_{x \to \infty} f(x) = 0$$

The size of the *catchment region* of the function is defined by the **reference radius** σ, the bigger is the σ the bigger is the area observed by the neuron. The various parameters and the shape of the function determine the width of this radius. The radial activation function are typically shaped in this way:

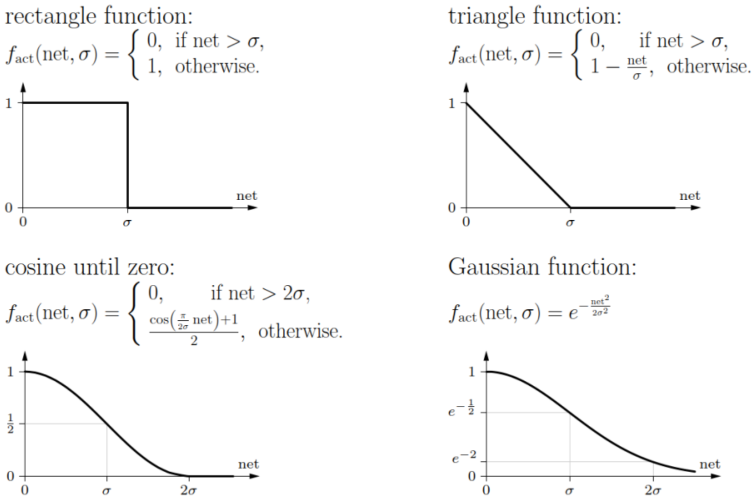


Figure 55: Radial activation functions

As example, let's apply an RBFN for simulating the boolean conjunction $x_1 \wedge x_2$. When i'm around the black point, the input is $(1,1)$, what we want to do is creating a circle around that area where the output is 1 (significant information to extract).

Another approach could consist in considering a RBF in the opposite way, where the interesting data is outside the circle.

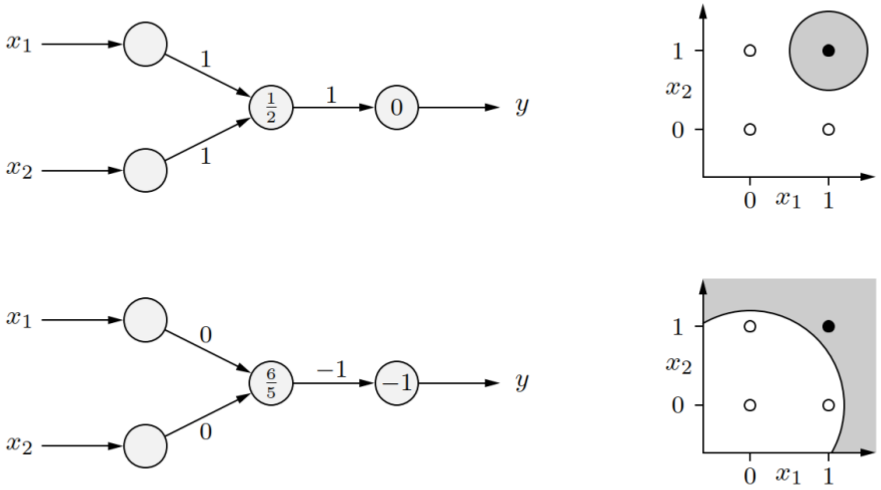


Figure 56: RBFN for conjunction

Another example is with the bi-implication $x_1 \longleftrightarrow x_2$:

$$x_1 \leftrightarrow x_2 \quad \equiv \quad (x_1 \wedge x_2) \vee \neg(x_1 \vee x_2)$$

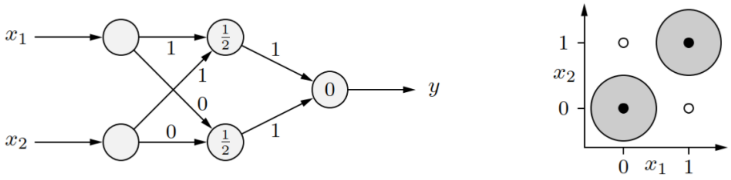
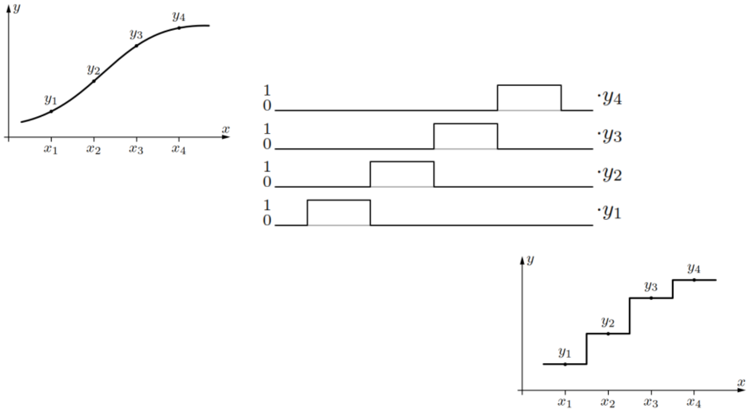


Figure 57: RBFN for bi-implication

Function approximation We have two neurons focusing on the relevant part of the domain, the rest will be 0, and by merging this two information you will get the bi-implication. In general an RBFN as the same expressive power of an MLP, and it can be saw as an universal approximator (can approximate any Riemann integrable function) with a small arbitrary error.

The process is the same of the other NN, the function will get approximated with a step function that can be computed easily by a RBF if we define that as the weighted sum of rectangular functions.



Each pulse can be represented by a neuron of a RBFN: The approximation can be enhanced by increasing the number of points where the function is being evaluated. Furthermore, if instead of using the rectangular function, we use the Gaussian we obtain more ”soft” transitions, avoiding big jumps (like for the MLP).

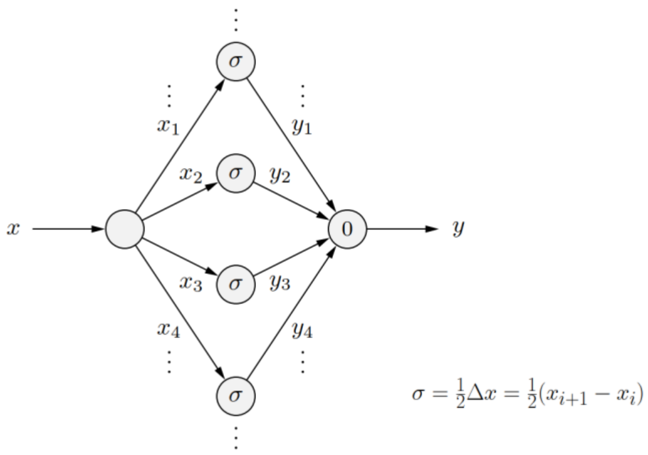


Figure 58: RBFN for the approximation, using the step function

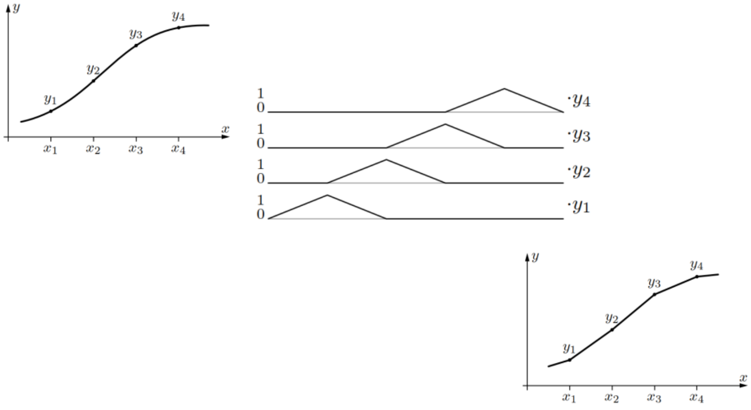


Figure 59: RBFN for the approximation, using the Gaussian function

2.21 Training RBFN

We want to apply in principle a sort of backpropagation in order to perform the configuration, like with the FFN. The principle is always the same, having in mind the *minimization* of the final error, but the problem here is *how we can decline this by taking into account the specific structure of this neurons?* With the others ANN the initialization phase was trivial, because you just had to select some random values, instead with RBFN the same approach conduce to suboptimal results.

Let's consider a **simple radial basis function network**, which is a partial view of the general structure of a RBFN, where each training example is associated with a proper radial function.

We want to apply a **fixed learning task** $L_{fixed} = \{l_1, ..., l_m\}$ with m training patterns $l = (\vec{l}^{(l)}, \vec{o}^{(l)})$ composed by input and desired outputs.

We have one hidden neuron $v_k, k = 1, ..., m$ for each training pattern, let's define the vector of associated weights to the neuron v_k:

$$\forall k \in \{1, ..., m\} \vec{w}_{v_k} = \vec{i}^{l_k}$$

Let's consider the activation function of our neuron equal to the sigma specific to that neuron, the radius can be computed for each of the neuron by considering heuristic approach in which we take the distance between the various input patterns and we take the maximum distance computed between each pair of input vectors (patterns) in our dataset (this value is expressed as d_{max}).

The radius of the neuron σ_k will be choose heuristically if the activation function is Gaussian function:

$$\forall k \in \{1, ..., m\} : \sigma_k = \frac{d_{max}}{\sqrt{2m}}$$

$$d_{max} = maxd \underset{l_j, l_k \in L_{fixed}}{\left(\vec{l}^{(l_j)}, \vec{l}^{(} l_k) \right)}$$

Where d_{max} is the maximum distance between the input vectors. This choice allow to center the various Gaussians in such a way that them doesn't overlap each other, instead they will distributes in an ordered way respect to the input space. Basically we have a structure where we try to learn with each neuron one of the input patterns, one neuron trying to well understanding a specific input pattern.

I can initialize the connections from the hidden to the output neurons by using weights, this can be done by considering this formula:

$$\forall u : \sum_{k=1}^{m} w_{u_{vm}} out_{v_m}^{(l)} - \theta_u = o_u^{(l)}$$

which is the weighted summation of the output of the hidden layer and considering the threshold of the output, which has to be equal to the **desired output**. We know the desired output, we have the threshold and the current output generate by the hidden layer, so the last thing we need is the weights, this can be obtained by multiplying the interconnections weight by the matrix A of the output of the hidden layer (by using $\theta = 0$):

$$\mathbf{A} \cdot \vec{w}_u = \vec{o}_u$$

Where $\mathbf{A}$ is the $m \times m$ matrix that has for components the various output of the neurons in the hidden layer. If the matrix $\mathbf{A}$ has the complete rank, we can invert that and compute the weight vector:

$$\vec{w}_u = \mathbf{A}^{-1} \cdot \vec{o}_u$$

$$\mathbf{A} = \begin{pmatrix} 1 & e^{-2} & e^{-2} & e^{-4} \\ e^{-2} & 1 & e^{-4} & e^{-2} \\ e^{-2} & e^{-4} & 1 & e^{-2} \\ e^{-4} & e^{-2} & e^{-2} & 1 \end{pmatrix} \qquad \mathbf{A}^{-1} = \begin{pmatrix} \frac{a}{D} & \frac{b}{D} & \frac{b}{D} & \frac{c}{D} \\ \frac{b}{D} & \frac{a}{D} & \frac{c}{D} & \frac{b}{D} \\ \frac{b}{D} & \frac{c}{D} & \frac{a}{D} & \frac{b}{D} \\ \frac{c}{D} & \frac{b}{D} & \frac{b}{D} & \frac{a}{D} \end{pmatrix}$$

where

$$\begin{aligned} D &= 1 - 4e^{-4} + 6e^{-8} - 4e^{-12} + e^{-16} &&\approx 0.9287 \\ a &= \phantom{-e^{-2}}1 \; - 2e^{-4} + e^{-8} &&\approx 0.9637 \\ b &= -e^{-2} + 2e^{-6} - e^{-10} &&\approx -0.1304 \\ c &= e^{-4} - 2e^{-8} + e^{-12} &&\approx 0.0177 \end{aligned}$$

$$\vec{w}_u \;=\; \mathbf{A}^{-1} \cdot \vec{o}_u \;=\; \frac{1}{D} \begin{pmatrix} a+c \\ 2b \\ 2b \\ a+c \end{pmatrix} \approx \begin{pmatrix} 1.0567 \\ -0.2809 \\ -0.2809 \\ 1.0567 \end{pmatrix}$$

Figure 60: Example of the computing the weight vector in the bi-implication problem

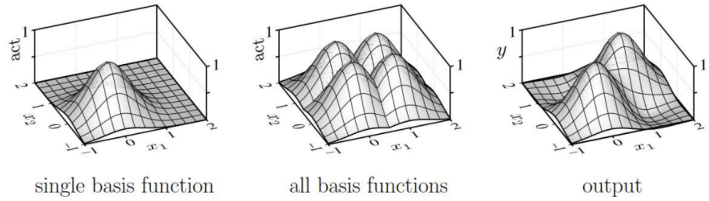


Figure 61: RBFN function centered in the examples

This method guarantee a perfect approximation. This means that is not necessary training a simple radial basis function network. In general, if we don't want to have for each pattern a neuron, we will have to select k subsets from the dataset and find, for each subset, a representative che associeremo to a neuron in the hidden layer.

if we look graphically, for each of the hidden layer we have aRBFN shaped as a Gaussian, which will correspond at each example that the neurons will learn. We will have only two of this Gaussian in the final computation, we will generate an output that will have to be different from 0. This is a RBFN centered in the relevant example that we want to learn.

This is not the general case, if we take a structure like this and we want to create a RBFN having in mind that for each the pattens we have to contribute we need to put a neuron with RBFN as activation function, this implies that if we have many examples that we want to learn we are going to have an incredibile big structure for our network, and this is not smart.

If we are considering the general radial basis function structure in which we don't want to have a neuron with x RBFN network centered on a specific example to learn, we need to try to limit the number of neurons we need to understand which are the neurons which are relevant and understand where to place it. Basically we need to select among the m patterns that we want to learn a subset of k patterns adn then we need to put the neuron centered on this example, then we need to figure out how to build the other outputs by combining this limited number of examples that we learn.

If we want to use this kind of approach we basically need to understand were to place the center, but we need also to understand how large will be the radius in order to be sure that after placing the Gaussians we are able to recreate the examples for which we don't use the Gaussian.

What i can do is splitting the domain of examples, and then for each subdomain find a representative point (not an example) in the subdomain, that will cover the group of the examples (not points) of the subset.

This can be formalized in saying that we select k training patterns as centers, where the connection weights for the hidden neurons are the training pattern, and the connection weights for the output neurons can be obtained by considering this matrix A:

$$\mathbf{A} = \left\{ \begin{matrix} 1 & out_{v_1}^{(l_1)} & out_{v_2}^{(l_1)} & \cdots & out_{v_k}^{(l_1)} \\ 1 & out_{v_1}^{(l_2)} & out_{v_2}^{(l_2)} & \cdots & out_{v_k}^{(l_2)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & out_{v_1}^{(l_m)} & out_{v_2}^{(l_m)} & \cdots & out_{v_k}^{(l_m)} \end{matrix} \right\}$$

Figure 62: Matrix that expresses the connections weights for output neurons

Now i can apply the invert the matrix for computing the weights since system over-determined (not squared), but i can consider the pseudo inverse matrix:

$$A^+ = (A^T A)^{-1} A^T$$

Now we can apply the actual computation for our vector $\vec{w}$ of the weights, given by:

$$\vec{w}_u = A^+ \vec{o}_u$$

So now, *how we can choose the center for creating the configuration for our RBFN?* As for the simple case we can take all points we just need to determine the radius for one single radius and the output weights (considering that we want to use a better structure, which is practicable).

Options of radial basis function centers:

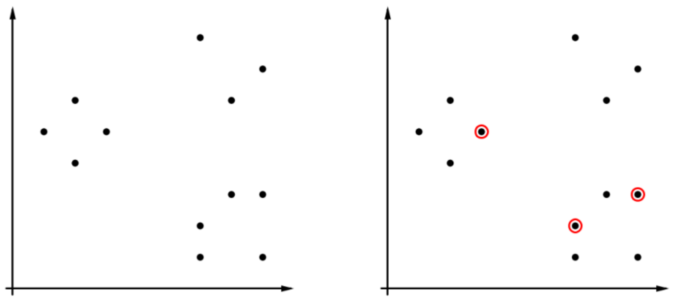
- All data points as centers, the simple case where only radius and output weights need to be determined. The output values ca be achieved exactly, computing the weights is unfeasible.

- Random subset, this is fast, only radius and output weights need to be determined. The performance depends on the choice of data points.
- Clustering, c-means clustering (the centroid point representative for the examples in the subset).

2.21.1 C-means clustering

This is one of the best options for choosing the RBFN centers:

1. Considering a number of c clusters to be found (input).
2. Initialize the cluster centers **randomly**.
3. Assign initially the data points (the examples) to the nearest center (or *centroid*).
4. Adjusting the position of the center considering the position of the assigned data points (mean vectors of the assigned data points, this is called **cluster center update**).
5. Repeat the step 3 and 4 until clusters do not move anymore (converge).



Data set to cluster.

Choose $c = 3$ clusters.
(From visual inspection, can be difficult to determine in general.)

Initial position of cluster centers.

Randomly selected data points.
(Alternative methods include e.g. latin hypercube sampling)

Figure 63: Step 1 with $c = 3$, Step 2 randomly choosing the centroids

Then by using the **Delaunay Triangulation** of the centroids, which leads to the **Voronoi Diagram** by taking the line orthogonal to each one of the three edges. This will result in a tessellation of the domain of the function, basically each tassel of the domain is a cluster.

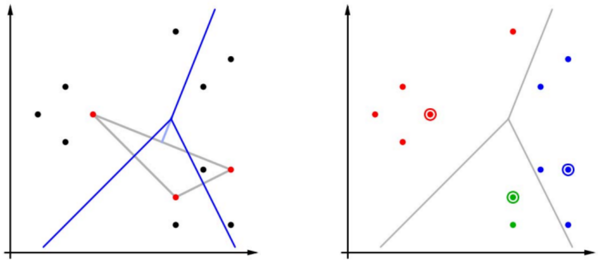


Figure 64: Delunay Trianglulation (left) and Voronoi Diagram (right)

After that i'm going to search for the new centroid of each cluster, where the sum of the distances is minimal, after finding this element i will consider it as the new center. Then i will apply again the same partition (Delunay-Voronoi) as before.

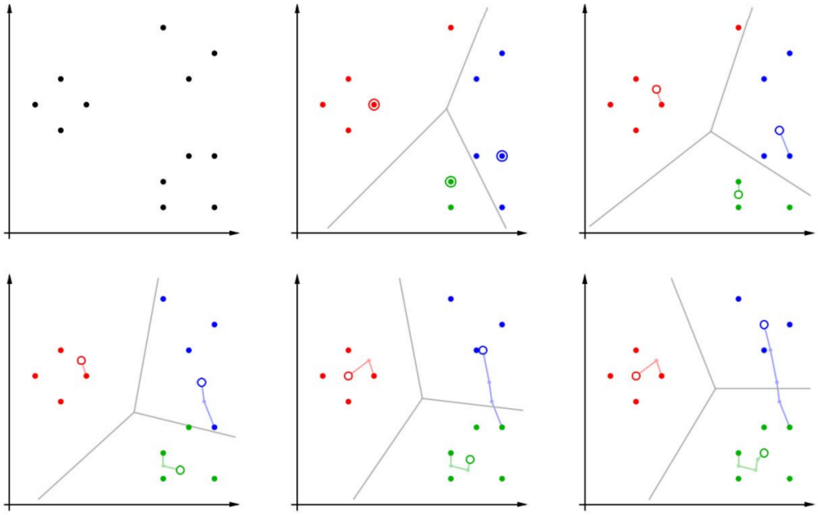


Figure 65: Centroid update

Basically what we can do is to apply some rules for updating the weights that are similar to the backpropagation in the MLP; basically you have just to adjust the weights from the hidden to the output neuron we just need to compute the gradient:

and then we need to find the direction of the maximum slope for the gradient and we need to compute the increase of the decrease in order to go in the d

For the hidden layer we need to place the centers, we need to not only find the interconnection weights for the centers but also the size of the radius which allow to combine together the contribution of the various neurons in the hidden layer for generating the desired output with the requested minimum error.

We have palced the neurons. nwo we need to understand how big the radius is big for the neuron. The gradient of the error with respect to the radius :

Updat raule for enlarge or reduce radius:

special case of Gaussian activation function:

2.22 Learning Vector Quantization

What happen if we don't have examples with a desired output (only the examples)? Basically, until now we saw the fixed-learning task, now we want to see what happens with a free-learning task.

Now i'm going for searching outputs that will be similar to the given input.

We still consider the Delaunay and Voronoi approaches. The problem is that what we want to do is a suitable quantization of the domain in which we have our examples in order to understand the group of the examples which are similar. In the previous example we had given a number of clusters, now we want to find the clusters in a given dataset.

Let's considered the input examples (or data points) as empty circles, and the cluster centers (or points) by the full circles.

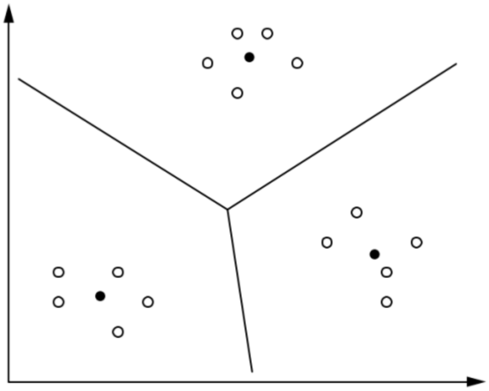


Figure 66: Vector quantization

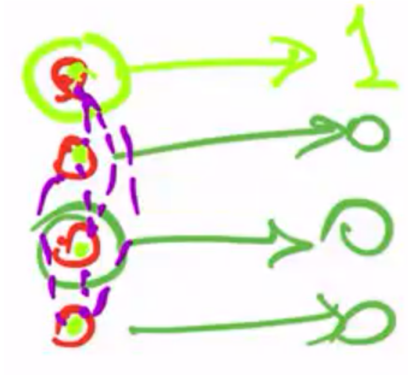
The **Learning Vector Quantization Network** (LVQ/LVQN), is a FFNN with 2-layers that performs this clustering of the examples by similarity, basically from an abstract point of view we see the LVQ as a radial function in which the hidden layer and output layer are collapsed in a single layer.

The network input function of each output neuron is the distance between the input vector and the weight vector. The definition of the distance is the same, we are considering the Mynkowski family and the euclidean distance for represent the behavior of our function,

The output activation function of each neuron is not a simple function of the activation of the neuron: it considers the activation of **all** output neurons.

$$f_{out}^{(u)}(act_u) = \begin{cases} 1 & \text{if } act_u = \max\limits_{v \in U_{out}} act_v \\ 0 & \text{otherwise} \end{cases}$$

We don't just look locally, for example with 4 neurons we will look tothe value of the activation in the activation function of each neuron and we compare the activation value of each on of them. The biggest activation value will lead to an output 1 otherwise 0 (when the activation is smaller). We have one neuron winning over all the other, basically we have a connection between all neurons in the output layer such that each of them is looking to what the other neurons are doing (the activation), this will allow the confrontation.



In the LVQN we can use the same radial functions that are use for any RBFN.