Expressiveness & Training

Next argument

Expressiveness

Expressiveness

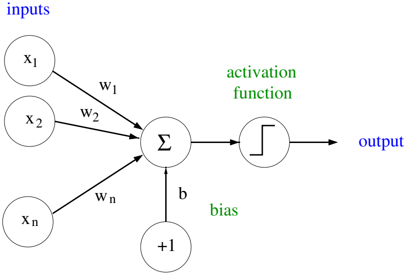
Can we compute any function by means of a Neural Network?

Do we really need **deep** networks?

Can we compute any function with a single neuron?

Single layer case: the perceptron

Binary threshold:



$$output = \begin{cases} 1 & if \sum_i w_i x_i + b \geq 0 \\ 0 & otherwise \end{cases} \qquad output = \begin{cases} 1 & if \sum_i w_i x_i \geq -b \\ 0 & otherwise \end{cases}$$

Remark: the bias set the position of threshold.

Hyperplanes

The set of points

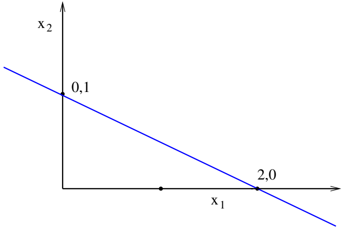
$$\sum_i w_i x_i + b = 0$$

defines a hyperplane in the space of the variables x_i

Example:

$$-\frac{1}{2}x_1 + x_2 + 1 = 0$$

is a line in the bidimensional space



Hyperplanes

The hyperplane

$$\sum_i w_i x_i + b = 0$$

divides the space in two parts: to one of them (above the line) the perceptron gives value 1, to the other (below the line) value 0.

"above" and "below" can be inverted by just inverting parameters:

$$\sum_i w_i x_i + b \leq 0 \iff \sum_i -w_i x_i - b \geq 0$$

Computing logical connectives: NAND

Can we implement this function (NAND) with a perceptron?

x_1	x_2	*output*
0	0	1
0	1	1
1	0	1
1	1	0

Can we find two weights w_1 and w_2 and a bias b such that

$$nand(x_1, x_2) = \begin{cases} 1 & \textit{if } \sum_i w_i x_i + b' \geq 0 \\ 0 & \textit{otherwise} \end{cases}$$

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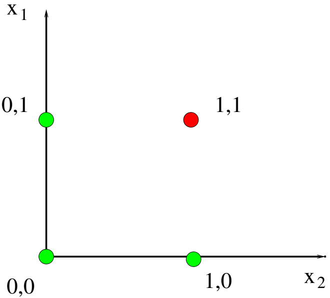
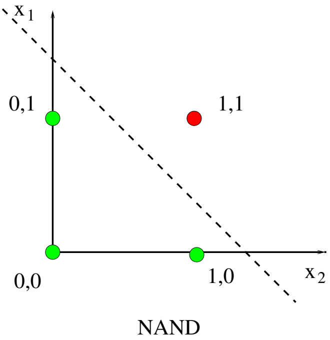
Graphical representation

Same as asking:
can we draw a straight line to separate green and red points?



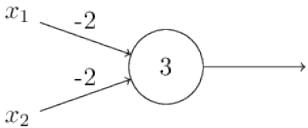
NAND

Yes!



line equation: $1.5 - x_1 - x_2 = 0$ or $3 - 2x_1 - 2x_2 = 0$

The NAND-perpceptron

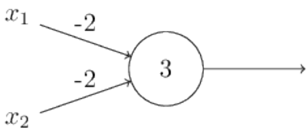


$$output = \begin{cases} 1 & if -2x_1 - 2x_2 + 3 \geq 0 \\ 0 & otherwise \end{cases}$$

x_1	x_2	*output*
0	0	1
0	1	1
1	0	1
1	1	0

Can we compute any logical circuit with a perceptron?

The NAND-perpceptron



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x_1	x_2	*output*
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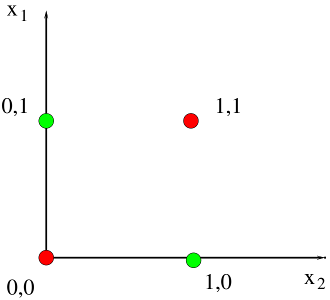
Can we compute any logical circuit with a perceptron?

The XOR case

Can we draw a straight line separating red and green points?



No way!

Single layer perceptrons are not complete!

The XOR case

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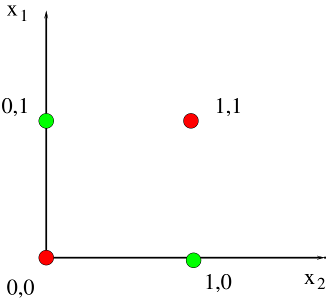

No way!

Single layer perceptrons are not complete!

Multi-layer perceptrons

Question:

- we know we can compute nand with a perceptron
- we know that nand is logically complete
  (i.e. we can compute any connective with nands)

so:

why perceptrons are not complete?

answer:

because we need to compose them and consider
Multi-layer perceptrons

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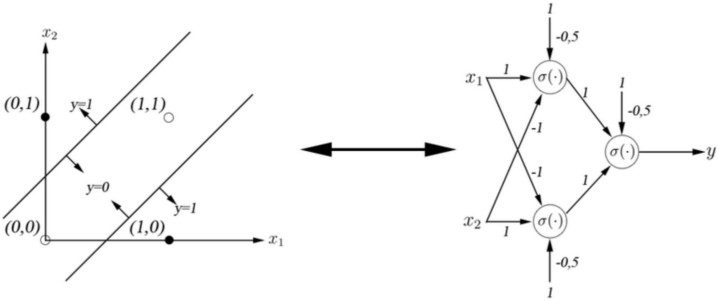
Multi-layer perceptrons

Example: Multi-layer perceptron for XOR

Can we compute XOR by **stacking** perceptrons?



Multilayer perceptrons are logically complete!

Important Points

- shallow nets are already **complete**

  Why going for deep networks?

  With deep nets, the same function may be computed with **less neural units** (Cohen, et al.)

- Activation functions play an **essential role**, since they are the only source of nonlinearity, and hence of the expressiveness of NNs.

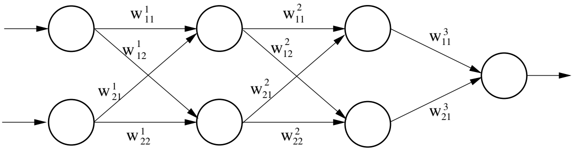
  Composing linear layers not separated by nonlinear activations **makes no sense**!

Next argument

Training

Current loss

Suppose to have a neural network with some configurations of the parameters θ.

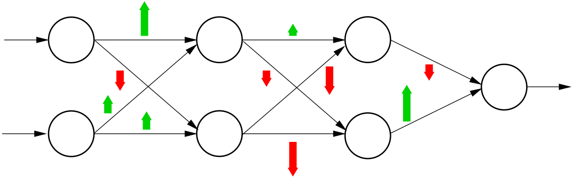


We can take a **batch** of data, pass them (in parallel) through the network, compute the output, and evaluate the current loss relative to θ.

This is a **forward pass** through the network.

Parameter updating

Next, we would like to adjust the parameters in such a way to decrease the current loss.

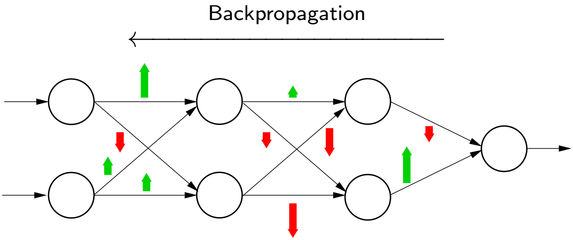


Each parameter should deserve a different adjustment, some of them positive, other negative.

The mathematical tool that allows us to establish in which way parameters should be updated is the **gradient**: a vector of **partial derivatives**.

Backpropagation

The gradient is computed **backward**, **backpropagating** the loss to all neurons inside a networks, and their connections.



This is a **backward pass** through the network.

The algorithm for computing parameters updates is known as **backpropagation algorithm**.

The Backpropagation algorithm (and its problems)

Computing the gradient

A neural network computes a complex function resulting from the composition of many neural layers. How can we compute the gradient w.r.t. a specific parameter (weight) of the net?

We need a mathematical rule know as the chain rule (for derivatives).

The chain rule

Given two derivable functions f, g with derivatives f' and g', the derivative of the composite function $h(x) = f(g(x))$ is

$$h'(x) = f'(g(x)) * g'(x))$$

Equivalently, letting $y = g(x)$,

$$h'(x) = f'(g(x)) * g'(x)) = f'(y) * g'(x)$$

The derivative of a **composition** of a sequence of functions is the **product** of the derivatives of the individual functions.

QUESTION: why binary thresholding is not a good activation function for backpropagation?

The function computed by the net

the artificial neuron at layer ℓ compute the function

$$a^\ell = \sigma(b^\ell + w^\ell \cdot x^\ell)$$

- a^ℓ is the activation vector at layer ℓ
- $z^\ell = b^\ell + w^\ell \cdot x^\ell$ is the weighted input at layer ℓ
- $x^{\ell+1} = a^\ell, x^1 = x$

The function computed by the neural net is

$$\sigma(b^L + w^L \cdot \ldots \sigma(b^2 + w^2 \cdot \sigma(b^1 + w^1 \cdot x^1)))$$

The dimensions of w^ℓ e b^ℓ depend on the number of neurons at layer ℓ (and $\ell - 1$).

All of them are parameters of the models.

Backpropagation rules in vectorial notation

Given some error function E (e.g. euclidean distance) let us define the error derivative at l as the following vector of partial derivatives:

$$\delta^l = \frac{\partial E}{\partial z^l}$$

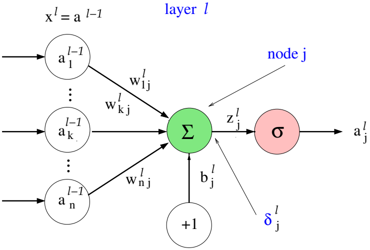
We have the following equations

$$(BP1) \quad \delta^L = \nabla_{a^L} E \odot \sigma'(z^L)$$

$$(BP2) \quad \delta^l = (W^{l+1})^T \delta^{l+1} \odot \sigma'(z^l)$$

$$(BP3) \quad \frac{\partial E}{\partial b_j^l} = \delta_j^l$$

$$(BP4) \quad \frac{\partial E}{\partial w_{jk}^l} = a_k^{l-1} \delta_j^l$$



where $\odot$ is the Hadamard product (component-wise)

The vanishing gradient problem

$$(BP2) \quad \delta^l = (w^{l+1})^T \delta^{l+1} \odot \sigma'(z^l)$$

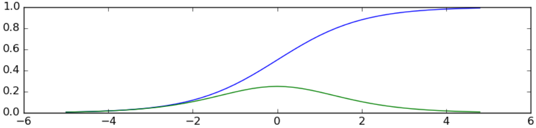
By the chain rule, the derivative is a long sequence of factors, where these factors are, alternately

- derivatives of activation functions
- derivative of linear functions, that are constants (in fact, the transposed matrix of the linear coefficients)

Let's have a look at the derivatives of a couple of activation functions.

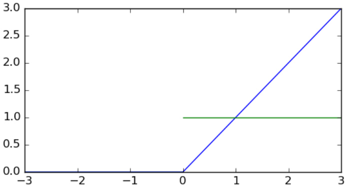
Derivatives of common activation functions

Sigmoid



Observe the flat shape of $\sigma'(x)$, always below 0.25

Relu



The vanishing gradient problem

If you systematically use the sigmoid as activation function in all layers of a deep network, the gradient will contain a lot of factors below 0.25, resulting in a very small value.

If the gradient is close to zero, learning is impossible.

This is known as the **vanishing gradient problem**.

A bit of history

The vanishing gradient problem blocked the progress on neural netwoks for almost 15 years (1990-2005).

It was first bypassed by network pre-training (e.g. with Boltzmann Machines), and later by the introduction on new activation functions, such as Rectified Linear Units (RELU), making pre-training obsolete.

Still, fine-tuning starting from good network weights (e.g. VGG) is a viable approach for many problems (transfer learning).