Introducción a Redes Neuronales

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Diplomado Ciencia de Datos con Python

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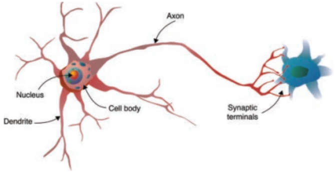
Introduction

Neural Networks

Artificial neural networks are machine learning techniques that simulate the mechanism of learning in biological organisms. The human nervous system contains cells, referred to as neurons. The neurons are connected to one another by of axons and dendrites, and the connecting regions between axons and dendrites are called synapses. The strengths of synaptic connections often change in response to external stimuli. This change is how learning takes place in living organisms.



El modelo lineal de clasificación

- The Perceptrón algorithm (Rosenblatt, 1961) played an important role in Machine Learning history. It was first simulated in a computer IBM 704 at Cornell in 1957. By the early 60s, a dedicated hardware was designed to implement the learning algorithm.

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- It was criticized by Marvin Minsky, who showed the limitations of the perceptron algorithm when dealing with a non linear separable set of points. This caused a void in the neural computation research lasting until the mid 80s.

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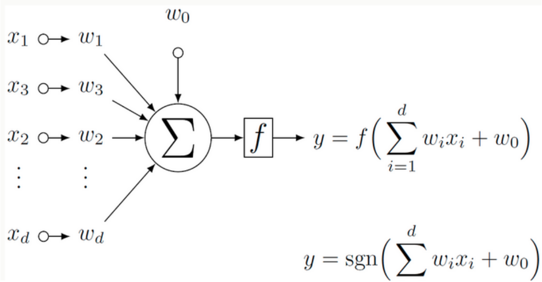
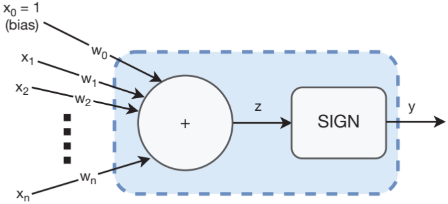
The Rosenblatt Perceptron





The Algorithm

We iterate over the training set

$$(x_1, y_1), (x_2, y_2) \cdots , (x_N, y_N).$$

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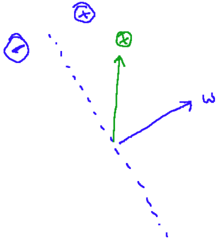

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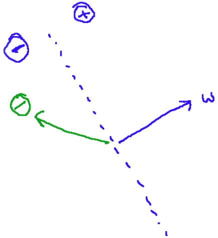

(b) If $y = -1$

The Algorithm

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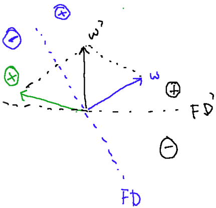

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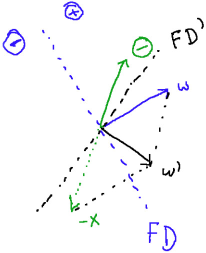

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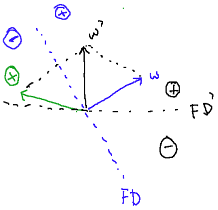

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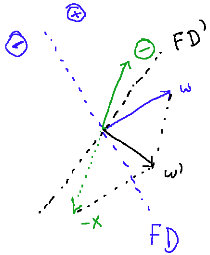

(b) If $y = -1$

We update the vector w with $w + yx$

The Algorithm

For each epoch, the algorithm is summarized as follows:

Data: A: training set of points, $X = \{x_1, ..., x_N\} \subset \mathbb{R}^{D+1}$,
$Y = \{y_1, ..., y_N\}$: set of labels
$\eta > 0$: learning rate.
Result: $\mathbf{w}$: weight vector defining the decision frontier.

Function `Perceptron`(X, y, η)**:**
- $\mathbf{w} = 0$;
- converged $=$ `False`;
- **while** *converged* $==$ `False` **do**
  - **for** $i \in \{1, ..., N\}$ **do**
    - **if** $y_i \langle \mathbf{w}, x \rangle \leq 0$ **then**
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$\mathbf{w}$ is a linear combination of $x_1, \dots, x_N$.

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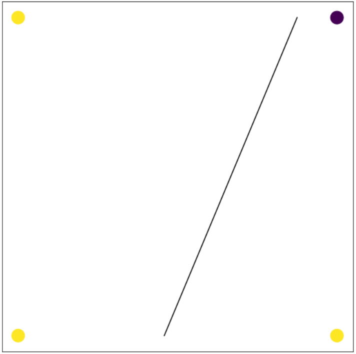

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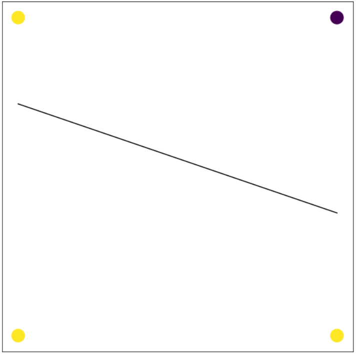

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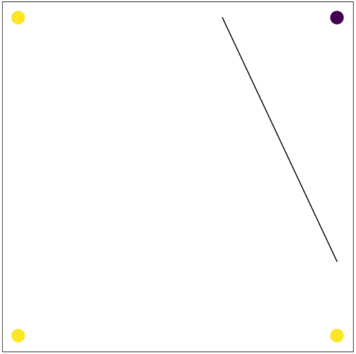

Limitations of the Perceptron

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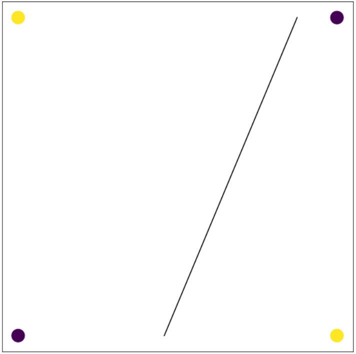

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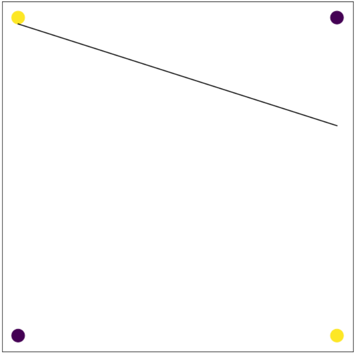

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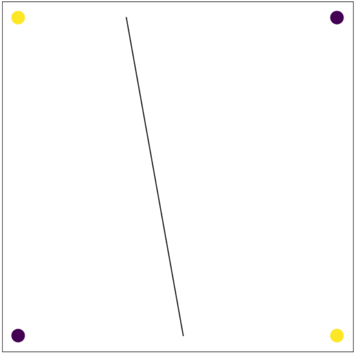

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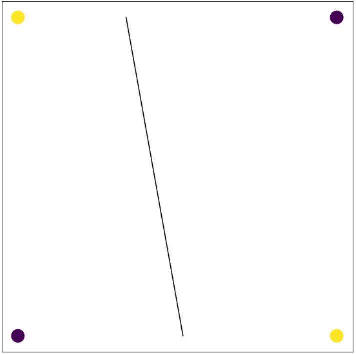

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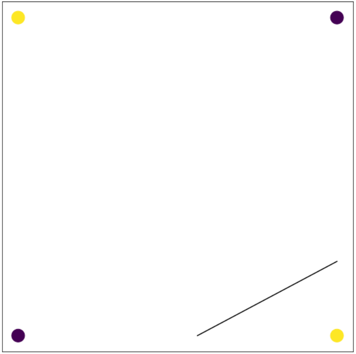

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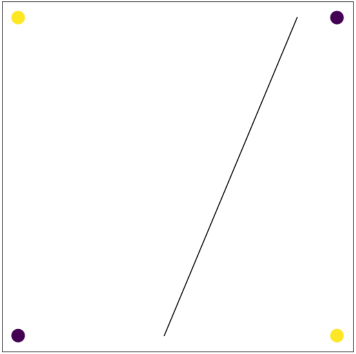

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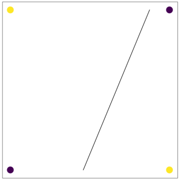
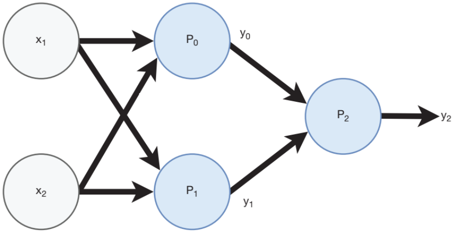


Alternatives:

- We change the model of a neuron or
- We combine multiple of them to solve this limitation.

Combining Perceptrons



$$
\begin{array}{r|c}
-1 & (-1,-1) \\
+1 & (1,-1) \\
+1 & (-1,1) \\
-1 & (1,1)
\end{array}
$$

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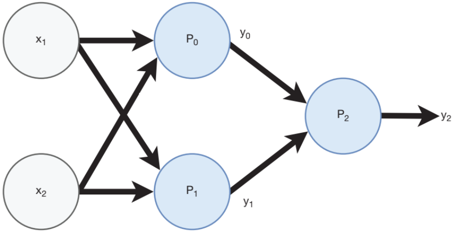

This neural network is one of the simplest examples of a fully connected feedforward network. Fully connected means that the output of each neuron in one layer is connected to all neurons in the next layer. Feedforward means that there are no backward connections. A multilevel neural network has an input layer, one or more hidden layers, and an output layer. The input layer does not contain neurons but contains only the inputs themselves.

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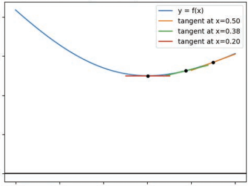

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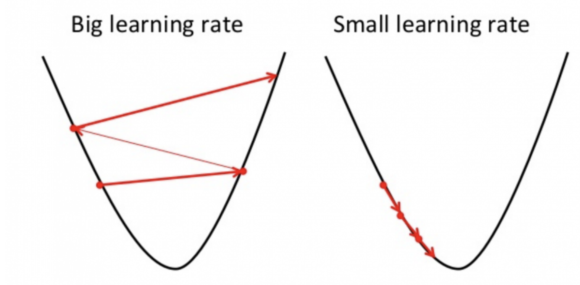
- The algorithm is not guaranteed to find the global minimum because it can get stuck in a local minimum.

Learning Rate



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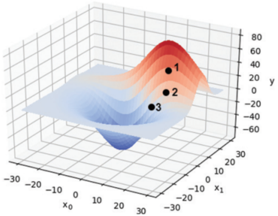

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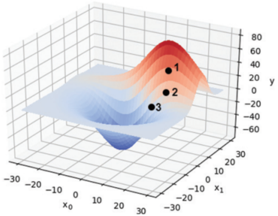

- If we are at the point $\mathbf{x_n} = (x_0^{(n)}, x_1^{(n)})$ and want to minimize y, then we choose our next point as

$$\mathbf{x_{n+1}} = \mathbf{x_n} - \eta \nabla f(\mathbf{x_n})$$

Gradient-based Learning

When applying gradient descent to our neural network, we consider input values $\mathbf{x}$ to be constants, with our goal being to adjust the weights $\mathbf{w}$.

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When applying gradient descent to our neural network, we consider input values $\mathbf{x}$ to be constants, with our goal being to adjust the weights $\mathbf{w}$.

- Which function we want to minimize? A loss function.
- In the context of an optimization algorithm, the function used to evaluate a candidate solution is referred to as the objective function. With neural networks, we seek to minimize the error. As such, the objective function is often referred to as a cost function or a loss function.

Gradient-based Learning

- In the case of the Perceptron, the loss function is given by

$$L^{(0/1)}(\mathbf{w}) = (y_i - \mathrm{sign}\langle \mathbf{w}, \mathbf{x}_i \rangle)^2$$

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$$L^{(0/1)}(\mathbf{w}) = \frac{1}{2}(y_i - \text{sign}\langle \mathbf{w}, \mathbf{x}_i \rangle)^2 = 1 - y_i \text{sign}\langle \mathbf{w}, \mathbf{x}_i \rangle$$

- This function is not smooth, we use the smooth surrogate loss function

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- Applying gradient descent

$$\begin{aligned} \mathbf{w}_{n+1} &= \mathbf{w}_n - \eta \nabla L(\mathbf{w}) \\ &= \begin{cases} \mathbf{w}_n + \eta y_i \mathbf{x}_i, & \text{well classified} \\ \mathbf{w}_n, & \text{misclassified} \end{cases} \end{aligned}$$

Loss Functions

Other examples of loss functions

Keras Losses

Loss Functions: MSE

Mean Square Error (MSE)

$$L(y, t) = (t - y)^2.$$

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- Trivial derivative for gradient descent.

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Loss Functions: Hinge

Hinge Loss

$$L = \max\{-y_i \hat{y}_i, 0\}.$$

- Used in SVMs and Perceptron.
- Penalizes errors, but also correct predictions of low confidence (probabilities).
- Good for binary classification tasks.

Loss Functions: Categorical cross entropy

Categorical cross entropy

$$L = \sum_{i}^{n} y_i \log\left(\hat{y}_i\right).$$

- Good for multi-class classification problems.
- Considers y to be a one-hot encoding vector in n classes.

Optimizers: Gradient Descent

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Advantages:

- Easy computation.
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Disadvantages:

- May trap at local minima.
- Weights are changed after calculating gradient on the whole dataset. May take a long time to converge.
- Requires large memory to calculate gradient on the whole dataset.

Optimizers

- Gradient Descent
- Stochastic Gradient Descent
- Stochastic Gradient descent with momentum
- Mini-Batch Gradient Descent
- Adagrad
- RMSProp
- AdaDelta
- Adam

Keras Optimizers

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- Due to an increase in the number of iterations, the overall computation time increases. Still, the computation cost is still less than that of the gradient descent optimizer.
- If the data is enormous and computational time is an essential factor, stochastic gradient descent should be preferred over batch gradient descent algorithm.

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- One downside of AdaGrad optimizer is that it decreases the learning rate aggressively and monotonically. There might be a point when the learning rate becomes extremely small.

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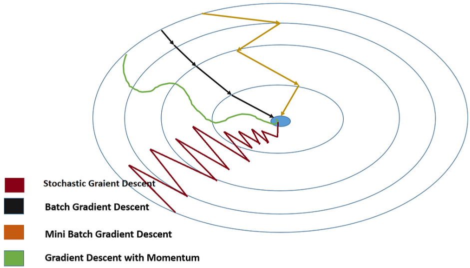
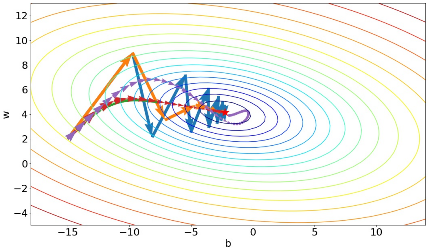
- It tends to focus on faster computation time, it might not generalize the data well enough.

Optimizers


Stochastic Graient Descent
Batch Gradient Descent
Mini Batch Gradient Descent
Gradient Descent with Momentum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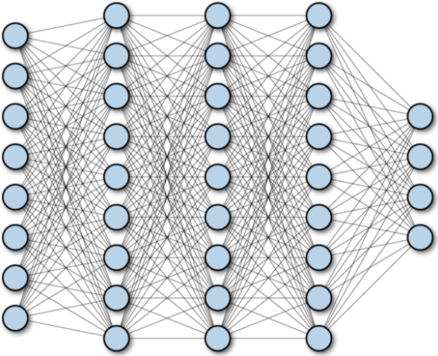
Fully Connected Networks



A fully connected neural network consists of a series of fully connected layers that connect every neuron in one layer to every neuron in the other layer.

Advantages and Disadvantages

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- While being structure agnostic makes fully connected networks very broadly applicable, such networks do tend to have weaker performance than special-purpose networks tuned to the structure of a problem space.

The Algorithm

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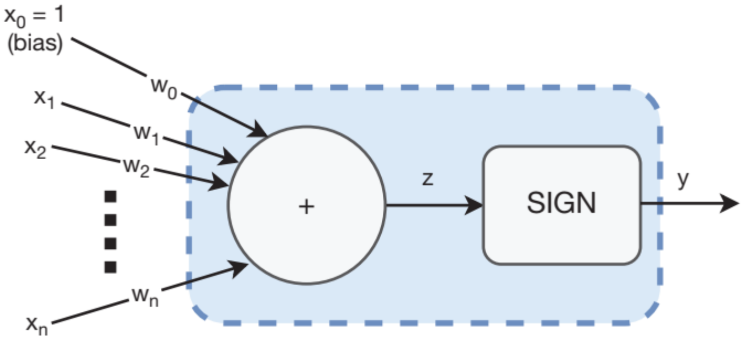
- Finally, adjust the weights to make the output get closer to the desired value using gradient descent: Back propagation.

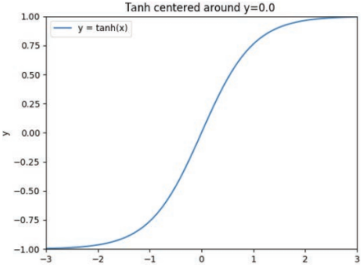
Feed-Forward



The sign function is an activation function of the neuron. It is not smooth because of the discontinuity in 0.

Other Activation Functions

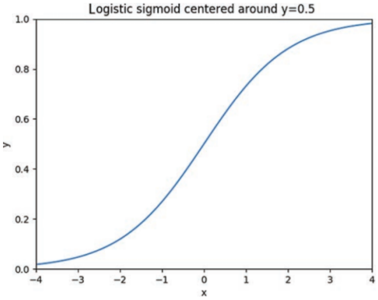
$$\tanh(x) = \frac{e^{2x} - 1}{e^{2x} + 1}$$



$$\tanh'(x) = 1 - \tanh^2(x)$$

Other Activation Functions

$$S(x) = \frac{e^x}{e^x + 1}$$

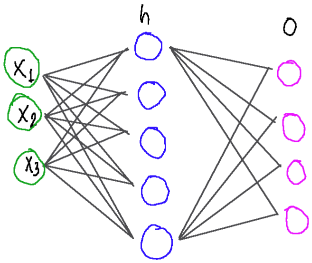


$$S'(x) = S(x)(1 - S(x))$$

Choice of Activation Functions

There exist a large number of activation functions. Two popular choices are tanh and the logistic sigmoid function. When picking between the two, choose tanh for hidden layers and logistic sigmoid for the output layer.

Feed-Forward: An Example



$$X = \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & x_3^{(1)} \\ & \cdots & & \\ 1 & x_1^{(N)} & x_2^{(N)} & x_3^{(N)} \end{pmatrix}$$

$$h = \Phi_1 (X \cdot W_1^T)$$

$$o = \Phi_2 (\bar{h} \cdot W_2^T)$$

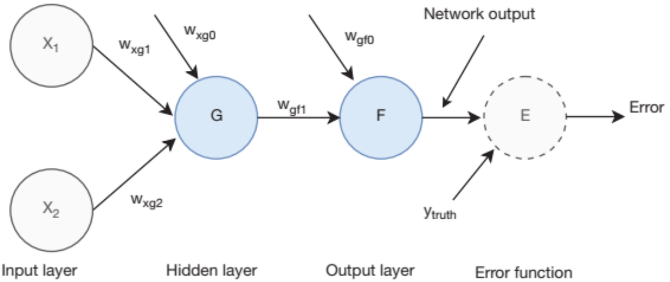
$W_1 \in M_{5 \times 4}$ $\quad$ $W_2 \in M_{4 \times 6}$

$X \in M_{N \times 4}$

$h \in M_{N \times 5}$

$\bar{h} \in M_{N \times 6}$

Example: Back-propagation



This neural network implements

$$\hat{y} = S\left(w_{gf0} + w_{gf1}\tanh(w_{xg0} + w_{xg1}x_1 + w_{xg2}x_2)\right)$$

We use the MSE:

$$e(f) = \frac{(y-f)^2}{2}.$$

Example: Back-propagation

- The error is given by

$$\text{Error} = \frac{1}{2}\left(y - S\left(w_{gf0} + w_{gf1}\tanh(w_{xg0} + w_{xg1}x_1 + w_{xg2}x_2\right)\right)$$

- We write it as:

$$\begin{aligned} e(f) &= \frac{1}{2}(y - f)^2 \\ f(z_f) &= S(z_f) \\ z_f(w_{gf0}, w_{gf1}, g) &= w_{gf0} + w_{gf1}g \\ g(z_g) &= \tanh(z_g) \\ z_g(w_{xg0}, w_{xg1}, w_{xg2}) &= w_{xg0} + w_{xg1}x_1 + w_{xg2}x_2 \end{aligned}$$

Example: Back-propagation

$$\frac{\partial e}{\partial w_{gf0}} = -(y-f)\cdot S'(z_f)$$

$$\frac{\partial e}{\partial w_{gf1}} = -(y-f)\cdot S'(z_f)\cdot g$$

$$\frac{\partial e}{\partial w_{xg0}} = -(y-f)\cdot S'(z_f)\cdot w_{gf1}\cdot tanh'(z_g)$$

$$\frac{\partial e}{\partial w_{xg1}} = -(y-f)\cdot S'(z_f)\cdot w_{gf1}\cdot tanh'(z_g)\cdot x_1$$

$$\frac{\partial e}{\partial w_{xg2}} = -(y-f)\cdot S'(z_f)\cdot w_{gf1}\cdot tanh'(z_g)\cdot x_2$$

Example: Back-propagation

Finally, we update the weights, via gradient descent

$$w_{gf0} \leftarrow w_{gf0} + \eta \frac{\partial e}{\partial w_{gf0}}$$
$$w_{gf1} \leftarrow w_{gf1} + \eta \frac{\partial e}{\partial w_{gf1}}$$
$$w_{xg0} \leftarrow w_{xg0} + \eta \frac{\partial e}{\partial w_{xg0}}$$
$$w_{xg1} \leftarrow w_{xg1} + \eta \frac{\partial e}{\partial w_{xg1}}$$
$$w_{xg2} \leftarrow w_{xg2} + \eta \frac{\partial e}{\partial w_{xg2}}$$