Neural networks

Friday, 21 May 2021 04:35

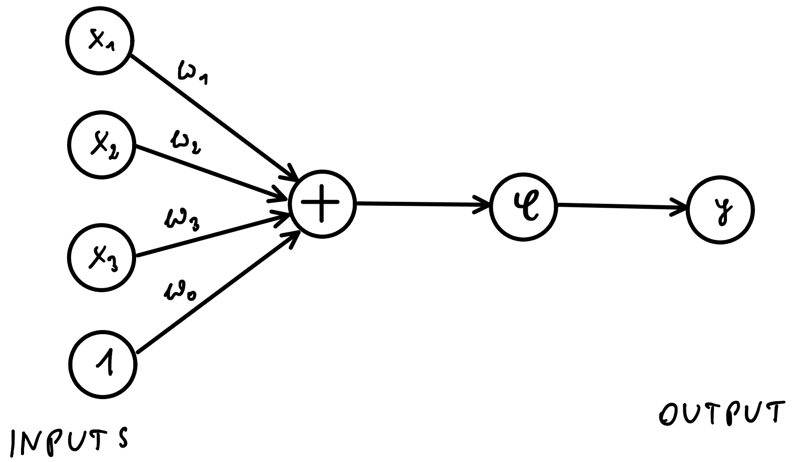
A neural network (NN), just as any other ML model, represents a function $f: \mathbb{R}^n \to \mathbb{R}^m$:

$$y = f(x \mid \theta)$$

dependent on some parameters θ. It is also characterized by its typically large number of parameters and its unique training method - backpropagation.

Neurons

A neuron has the form



and performs the following operation

$$y = \varphi\left(\sum_{k=1}^{n} w_k x_k + w_0\right)$$

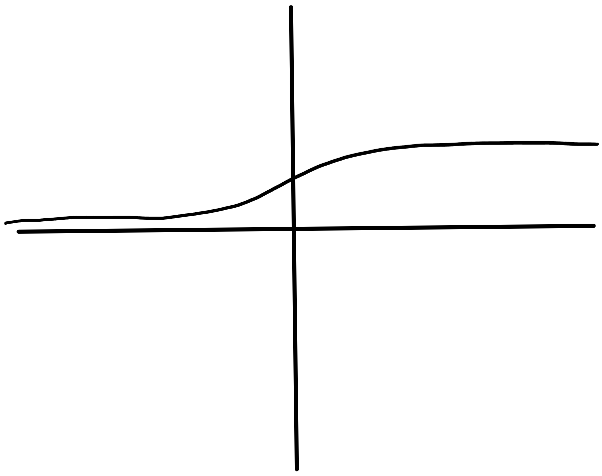
where φ is a non-decreasing differentiable function (except for possibly one point) and is called an activation function.

Examples of activation functions:

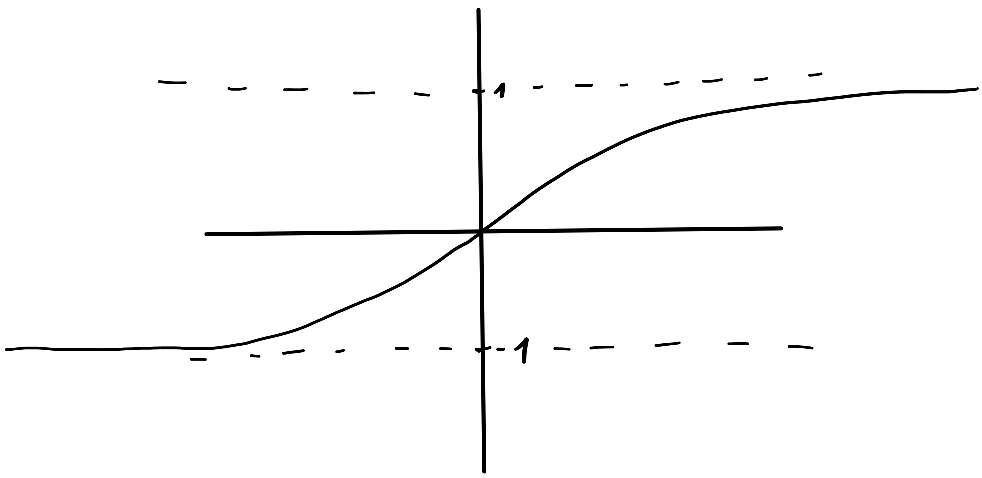
- $\varphi(x) = ax + b$ (linear) (with a linear activation function NN becomes Linear Regression)

(favorite activation ...

- $\varphi(x) = \dfrac{1}{1+e^{-x}}$ (sigmoid or logistic curve) (favorite activation function in the 80's and 90's)

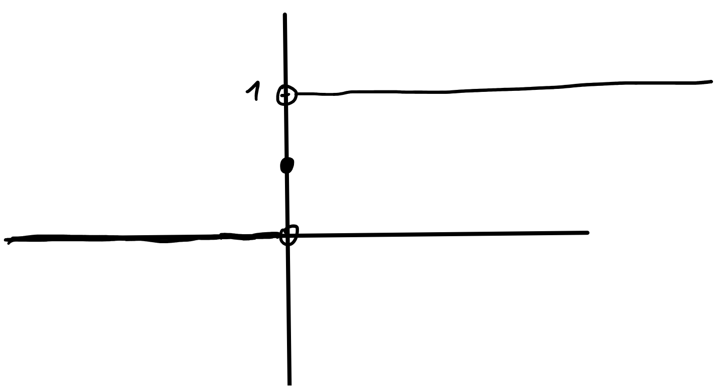


- $\varphi(x) = \dfrac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$ (hyperbolic tangent)



- $\varphi(x) = \begin{cases} 0 & : x < 0 \\ 0.5 & : x = 0 \\ 1 & : x > 0 \end{cases}$ (Heaviside function)

(this function is closest to how the brain neurons actually work, but was used only in the early days of neural networks as it makes training very hard)



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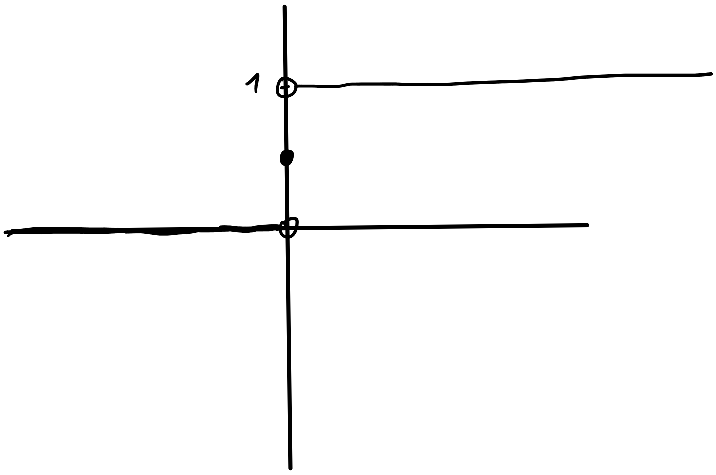
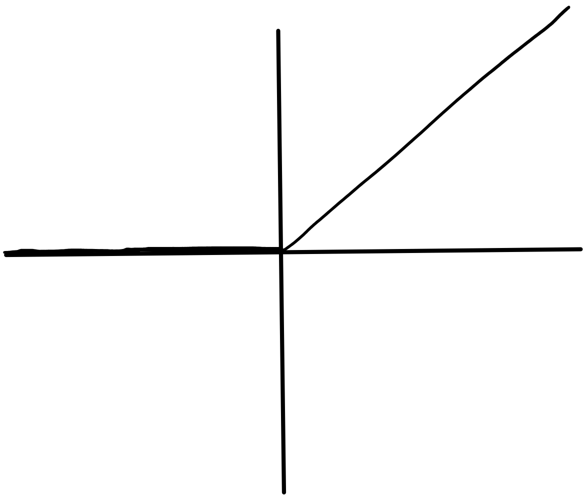


- $\varphi(x) = \begin{cases} x & : x > 0 \\ 0 & : x \leq 0 \end{cases}$ (Rectified Linear Unit - ReLU)

(this is the most commonly used activation function in the modern days)

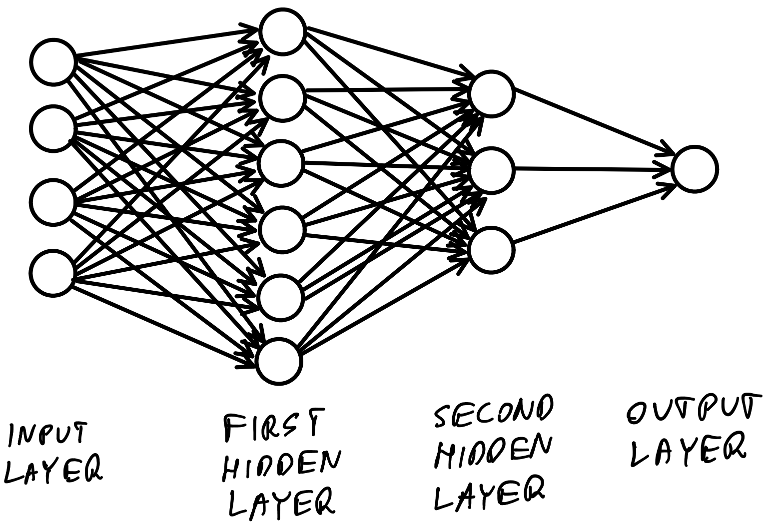


A neuron can be thought of as the most basic non-linear model built on top of a linear model.

A neuron is a primary building block of a neural network.

Structure of a neural network

Every neural network consists of layers of neurons where the outputs of the previous layer form the input for the next layer.



Fully connected layer

Layers with all possible connections to the previous layer are called fully connected layers.

A neural network which consists of fully connected layers is called artificial neural network (ANN)

There exist other types of layers, e.g.:

- dropout
- normalization (e.g. batch, spectral)
- convolution
- deconvolution
- recurrent
- embedding
- self-attention

There are also many neural network architectures. The most common include:

- artificial neural networks (ANN)
- convolutional neural networks (CNN)
- recurrent neural networks (RNN)
- long short-term memory (LSTM)
- encoder-decoder
- generative adversarial networks (GAN)

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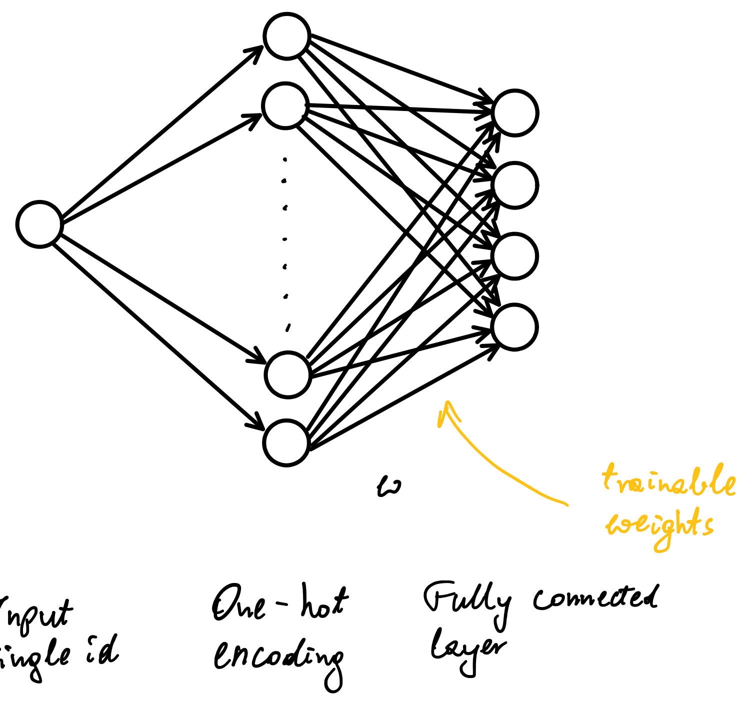
ANN with just one layer is called perceptron.

ANN with more than one layer is called multi-layer perceptron (MLP)

A neural network with many layers is called deep neural network (DNN)

In many real-world applications many types of layers and architectures are mixed into a larger network.

Embedding layer



Training a neural network

Learning the parameters of a neural network is always performed by minimizing a loss function.

The minimization process is typically done using backpropagation.

The two most common loss functions are:

- mean squared error (MSE) - for regression problems
- cross-entropy loss - for classification problems

MSE

$$loss(\theta) = \frac{1}{|D|} \sum_{(x_n, y_n) \in D} \left(y_n - f(x_n \mid \theta) \right)^2$$

Cross-entropy

$$loss(\theta) = \frac{1}{|D|} \sum_{(x_n, y_n) \in D} \left(-\sum_c y_{nc} \ln(f_c(x_n \mid \theta)) + (1 - y_{nc}) \ln(1 - f_c(x_n \mid \theta)) \right)$$

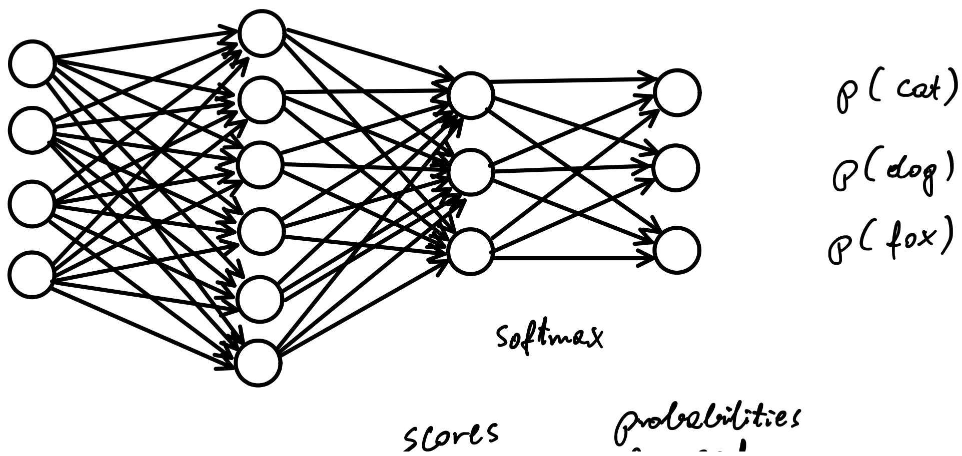
where $y_{nc} \in \{0, 1\}$.

In the case of cross-entropy the neural network must return probabilities for all classes in the output layer.

Typically this is achieved by applying softmax to the final layer of a neural network:

$$p(c) = \frac{e^{f(c \mid \theta)}}{\sum_{c'} e^{f(c' \mid \theta)}}$$

where c is an index of a neuron in the final layer



scores for each class

probabilities for each class

Backpropagation

Backpropagation relies on stochastic gradient descent to minimize the loss, which means in every step it shifts every network parameter in the direction opposite to the loss derivative with respect to that parameter, i.e.

$$\theta_i^{(n)} = \theta_i^{(n-1)} - \alpha \frac{\partial\, \text{loss}}{\partial \theta_i}$$

But the network parameters are in different layers and the formula for calculating the value of the network and then the loss can be very complex, hence also the derivative will be extremely complex.

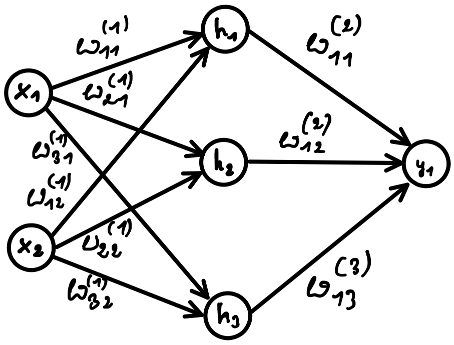
The clever idea in backpropagation is how to calculate those derivatives and parameter updates efficiently.

Consider the case of MSE loss

$$\text{loss}(\theta) = \sum_{(x_n, y_n) \in D} \left(y_n - f(x_n \mid \theta) \right)^2$$

(We omit $\frac{1}{|D|}$ as it does not affect the optimization problem)

and a one hidden layer network



$$\Theta = \left(\omega_{11}^{(1)}, \omega_{12}^{(1)}, \omega_{21}^{(1)}, \omega_{22}^{(1)}, \omega_{31}^{(1)}, \omega_{32}^{(1)}, \omega_{11}^{(2)}, \omega_{12}^{(2)}, \omega_{13}^{(2)} \right)$$

We can denote

$$\omega^{(1)} = \begin{bmatrix} \omega_{11}^{(1)} & \omega_{12}^{(1)} \\ \omega_{21}^{(1)} & \omega_{22}^{(1)} \\ \omega_{31}^{(1)} & \omega_{32}^{(1)} \end{bmatrix} \qquad \omega^{(2)} = \left[\omega_{11}^{(2)}, \omega_{12}^{(2)}, \omega_{13}^{(2)} \right]$$

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad h = \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} \qquad y = [y_1]$$

Then

$$h = \varphi(\omega^{(1)} x)$$

$$y = \varphi(\omega^{(2)} h) = \underbrace{\varphi(\omega^{(2)} \varphi(\omega^{(1)} x))}_{\text{function composition}}$$

Calculating the value of a neural network on a given input using such chained matrix operations is called

feed forward

We can use the chain rule to calculate the derivative of this composition.

In the case of bigger networks the formula just contains more identical terms

$$y = \varphi(\omega^{(n)} \varphi(\omega^{(n-1)} \varphi(\dots \omega^{(2)} \varphi(\omega^{(1)} x) \dots)$$

We have

$$\frac{\partial\, loss(\theta)}{\partial\, \omega_{ij}^{(2)}} = \frac{\partial}{\partial \omega_{ij}^{(2)}} \left(y_n - f(x_n|\theta) \right)^2$$

$$= 2\left(y_n - f(x_n|\theta)\right) \cdot \left(-\frac{\partial}{\partial \omega_{ij}^{(2)}} f(x_n|\theta)\right)$$

$$= -2\, e \frac{\partial}{\partial \omega_{ij}^{(2)}} \varphi(\omega^{(2)} h)$$

$e = (y_n - f(x_n|\theta))$

$$= -2\, e \frac{\partial}{\partial \omega_{ij}^{(2)}} \varphi\left(\omega_{11}^{(2)} h_1 + \omega_{12}^{(2)} h_2 + \omega_{13}^{(2)} h_3\right)$$

$$= -2e\, \varphi'(\omega^{(2)} h) \cdot \frac{\partial}{\partial \omega_{ij}^{(2)}} \left(\omega_{11}^{(2)} h_1 + \omega_{12}^{(2)} h_2 + \omega_{13}^{(2)} h_3\right)$$

Consider $i=1$, $j=1$. Then

$$\frac{\partial\, loss(\theta)}{\partial\, \omega_{11}^{(2)}} = -2e\, \varphi'(\omega^{(2)} h) \cdot \frac{\partial}{\partial \omega_{11}^{(2)}} \left(\omega_{11}^{(2)} h_1 + \omega_{12}^{(2)} h_2 + \omega_{13}^{(2)} h_3\right)$$

$$= -2e\, \varphi'(\omega^{(2)} h) \cdot h_1$$

Therefore

$$\begin{bmatrix} \Delta \omega_{11}^{(2)} \\ \Delta \omega_{12}^{(2)} \\ \Delta \omega_{13}^{(2)} \end{bmatrix} = -\alpha \begin{bmatrix} \frac{\partial\, loss(\theta)}{\partial\, \omega_{11}^{(2)}} \\ \frac{\partial\, loss(\theta)}{\partial\, \omega_{12}^{(2)}} \\ \frac{\partial\, loss(\theta)}{\partial\, \omega_{13}^{(2)}} \end{bmatrix} = \underbrace{2\alpha e}_{\text{single value}}\, \underbrace{\varphi'(\omega^{(2)} h)}_{\text{single value}} \cdot \underbrace{\begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix}}_{3\times 1}$$

For the sigmoid function

$$\varphi'(x) = \varphi(x)\left(1 - \varphi(x)\right)$$

hence

$$\varphi'(\omega^{(2)} h) = \underbrace{\varphi(\omega^{(2)} h)}\left(1 - \underbrace{\varphi(\omega^{(2)} h)}\right)$$

$$\varphi'(\omega^{(2)}h) = \underbrace{\varphi(\omega^{(2)}h)}(1 - \underbrace{\varphi(\omega^{(2)}h)})$$

this is the output
from the second layer

Therefore for the second layer

for the second layer
these are just 1x1 matrices

$$\begin{bmatrix} \Delta\omega_{11}^{(2)} \\ \Delta\omega_{12}^{(2)} \\ \Delta\omega_{13}^{(2)} \end{bmatrix} = 2\alpha\,[\text{error\_term}]\begin{bmatrix}\text{gradient in} \\ \text{this layer result}\end{bmatrix}\begin{bmatrix}\text{previous} \\ \text{layer} \\ \text{result}\end{bmatrix}$$

In other words we propagate the error term backwards into the network with weights derived from the previous layer and this layer results

Symbolically it could be expressed as

$$\Delta\omega = f^{-1}(\text{error\_term} \mid \Psi(x|\Theta))$$

To calculate the first layer parameter updates compare

$$y = \varphi(\omega^{(2)}h)$$

$$y = \varphi(\omega^{(2)}\varphi(\omega^{(1)}x))$$

For the second layer we had

$$\frac{\partial\,\text{loss}(\theta)}{\partial\omega_{ij}^{(2)}} = -2\,e\,\frac{\partial}{\partial\omega_{ij}^{(2)}}\varphi(\omega^{(2)}h)$$

Hence for the first layer

$$\frac{\partial\,\text{loss}(\theta)}{\partial\omega_{ij}^{(1)}} = -2\,e\,\frac{\partial}{\partial\omega_{ij}^{(1)}}\varphi(\omega^{(2)}\varphi(\omega^{(1)}x))$$

$$\frac{\partial \, loss(\theta)}{\partial \omega_{ij}^{(1)}} = -2 \, e \, \frac{\partial}{\partial \omega_{ij}^{(1)}} \varphi(\omega^{(2)} \varphi(\omega^{(1)} x))$$

We have

$$\frac{\partial}{\partial \omega_{ij}^{(1)}} \varphi(\omega^{(2)} \varphi(\omega^{(1)} x)) = \underbrace{\varphi'(\omega^{(2)} \overbrace{\varphi(\omega^{(1)} x)}^{h})} \frac{\partial}{\partial \omega_{ij}^{(1)}} (\omega^{(2)} \varphi(\omega^{(1)} x))$$

This expression is equal to $\varphi'(\omega^{(2)} h)$ and we already calculated it for updates in the second layer

Again we can „propagate" information backward

Then

$$\frac{\partial}{\partial \omega_{ij}^{(1)}} (\omega^{(2)} \varphi(\omega^{(1)} x)) = \frac{\partial}{\partial \omega_{ij}^{(1)}} \left([\omega_{11}^{(2)}, \omega_{12}^{(2)}, \omega_{13}^{(2)}] \, \varphi\left(\begin{bmatrix} \omega_{11}^{(1)} & \omega_{12}^{(1)} \\ \omega_{21}^{(1)} & \omega_{22}^{(1)} \\ \omega_{31}^{(1)} & \omega_{32}^{(1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right) \right)$$

$$= \frac{\partial}{\partial \omega_{ij}^{(1)}} \left([\omega_{11}^{(2)}, \omega_{12}^{(2)}, \omega_{13}^{(2)}] \begin{bmatrix} \varphi(\omega_{11}^{(1)} x_1 + \omega_{12}^{(1)} x_2) \\ \varphi(\omega_{21}^{(1)} x_1 + \omega_{22}^{(1)} x_2) \\ \varphi(\omega_{31}^{(1)} x_1 + \omega_{32}^{(1)} x_2) \end{bmatrix} \right)$$

$$= \frac{\partial}{\partial \omega_{ij}^{(1)}} \left(\omega_{11}^{(2)} \varphi(\omega_{11}^{(1)} x_1 + \omega_{12}^{(1)} x_2) + \omega_{12}^{(2)} \varphi(\omega_{21}^{(1)} x_1 + \omega_{22}^{(1)} x_2) + \omega_{13}^{(2)} \varphi(\omega_{31}^{(1)} x_1 + \omega_{32}^{(1)} x_2) \right)$$

For $i = 1$, $j = 1$ we have

$$\frac{\partial}{\partial \omega_{11}^{(1)}} (\omega^{(2)} \varphi(\omega^{(1)} x))$$

$$= \frac{\partial}{\partial \omega_{11}^{(1)}} \left(\omega_{11}^{(2)} \varphi(\omega_{11}^{(1)} x_1 + \omega_{12}^{(1)} x_2) + \omega_{12}^{(2)} \varphi(\omega_{21}^{(1)} x_1 + \omega_{22}^{(1)} x_2) + \omega_{13}^{(2)} \varphi(\omega_{31}^{(1)} x_1 + \omega_{32}^{(1)} x_2) \right)$$

$$^{(2)} \varphi'(\omega_{11}^{(1)} x_1 + \omega_{12}^{(1)} x_2) \cdot \frac{\partial}{\partial \omega_{11}^{(1)}} (\omega_{11}^{(1)} x_1 + \omega_{12}^{(1)} x_2)$$

$$= \omega_{11}^{(2)} \varphi'\left(\omega_{11}^{(1)} x_1 + \omega_{12}^{(1)} x_2\right) \cdot \frac{\partial}{\partial \omega_{11}^{(1)}} \left(\omega_{11}^{(1)} x_1 + \omega_{12}^{(1)} x_2\right)$$

$$= \omega_{11}^{(2)} \varphi'\left(\omega_{11}^{(1)} x_1 + \omega_{12}^{(1)} x_2\right) x_1$$

Hence

$$\frac{\partial}{\partial \omega_{ij}^{(1)}} \varphi\left(\omega^{(2)} \varphi\left(\omega^{(1)} x\right)\right) = \varphi'\left(\omega^{(2)} h\right) \omega_{1i}^{(2)} \varphi'\left(\omega_i^{(1)} x\right) x_j$$

and

$$\frac{\partial \, loss(\theta)}{\partial \omega_{ij}^{(1)}} = -2 \, e \, \varphi'\left(\omega^{(2)} h\right) \omega_{1i}^{(2)} \varphi'\left(\omega_i^{(1)} x\right) x_j$$

Therefore

$$\begin{bmatrix} \Delta \omega_{11}^{(1)} & \Delta \omega_{12}^{(1)} \\ \Delta \omega_{21}^{(1)} & \Delta \omega_{22}^{(1)} \\ \Delta \omega_{31}^{(1)} & \Delta \omega_{32}^{(1)} \end{bmatrix} = -\alpha \begin{bmatrix} \frac{\partial loss(\theta)}{\partial \omega_{11}^{(1)}} & \frac{\partial loss(\theta)}{\partial \omega_{12}^{(1)}} \\ \frac{\partial loss(\theta)}{\partial \omega_{21}^{(1)}} & \frac{\partial loss(\theta)}{\partial \omega_{22}^{(1)}} \\ \frac{\partial loss(\theta)}{\partial \omega_{31}^{(1)}} & \frac{\partial loss(\theta)}{\partial \omega_{32}^{(1)}} \end{bmatrix} = 2\alpha \underset{\text{single value}}{e} \, \underbrace{\varphi'\left(\omega^{(2)} h\right)}_{\text{single value}} \cdot \underbrace{\underbrace{\omega^{(2)} \odot \varphi'\left(\omega^{(1)} x\right)}_{3 \times 1} \cdot \underbrace{x^T}_{1 \times 2}}_{3 \times 2}$$

Again we just propagate the error term e backwards into the network. We also „propagate" the gradient from the next layer to the previous layer.

Symbolically

$$\begin{bmatrix} \Delta \omega_{11}^{(1)} & \Delta \omega_{12}^{(1)} \\ \Delta \omega_{21}^{(1)} & \Delta \omega_{22}^{(1)} \\ \Delta \omega_{31}^{(1)} & \Delta \omega_{32}^{(1)} \end{bmatrix} = 2\alpha \left[\text{error-term}\right] \left[\begin{array}{c}\text{gradient} \\ \text{in the next} \\ \text{layer result}\end{array}\right] \left[\begin{array}{c}\text{weighted} \\ \text{gradient in} \\ \text{this layer result}\end{array}\right] \left[\begin{array}{c}\text{previous} \\ \text{layer} \\ \text{result}\end{array}\right]$$

All the necessary values for backpropagation can be calculated ... except for the error term.

All the necessary values for backpropagation can be calculated in the forward network run except for the error term.
But the error term is the same for each weight update, therefore all weight updates can be calculated simultanously.