

## EE-559 – Deep learning

### 3.6. Back-propagation

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We want to train an MLP by minimizing a loss over the training set

$$\mathcal{L}(w, b) = \sum_n \ell(f(x_n; w, b), y_n).$$

To use gradient descent, we need the expression of the gradient of the loss with respect to the parameters:

$$\frac{\partial \mathcal{L}}{\partial w_{i,j}^{(l)}} \quad \text{and} \quad \frac{\partial \mathcal{L}}{\partial b_i^{(l)}}.$$

So, if we define  $\ell_n = \ell(f(x_n; w, b), y_n)$ , what we need is

$$\frac{\partial \ell_n}{\partial w_{i,j}^{(l)}} \quad \text{and} \quad \frac{\partial \ell_n}{\partial b_i^{(l)}}.$$

For clarity, we consider a single training sample  $x$ , and introduce  $s^{(1)}, \dots, s^{(L)}$  as the summations before activation functions.

$$x^{(0)} = x \xrightarrow{w^{(1)}, b^{(1)}} s^{(1)} \xrightarrow{\sigma} x^{(1)} \xrightarrow{w^{(2)}, b^{(2)}} s^{(2)} \xrightarrow{\sigma} \dots \xrightarrow{w^{(L)}, b^{(L)}} s^{(L)} \xrightarrow{\sigma} x^{(L)} = f(x; w, b).$$

Formally we set  $x^{(0)} = x$ ,

$$\forall l = 1, \dots, L, \begin{cases} s^{(l)} = w^{(l)}x^{(l-1)} + b^{(l)} \\ x^{(l)} = \sigma(s^{(l)}), \end{cases}$$

and we set the output of the network as  $f(x; w, b) = x^{(L)}$ .

**This is the forward pass.**

The core principle of the back-propagation algorithm is the “chain rule” from differential calculus:

$$(g \circ f)' = (g' \circ f)f'$$

which generalizes to longer compositions and higher dimensions

$$J_{f_N \circ f_{N-1} \circ \dots \circ f_1}(x) = \prod_{n=1}^N J_{f_n}(f_{n-1} \circ \dots \circ f_1(x)),$$

where  $J_f(x)$  is the Jacobian of  $f$  at  $x$ , that is the matrix of the linear approximation of  $f$  in the neighborhood of  $x$ .

The linear approximation of a composition of mappings is the product of their individual linear approximations.

What follows is exactly this principle applied to a MLP.

$$\dots \xrightarrow{\sigma} \underbrace{x^{(l-1)} \xrightarrow{w^{(l),b^{(l)}}} s^{(l)}} \xrightarrow{\sigma} x^{(l)} \xrightarrow{w^{(l+1),b^{(l+1)}}} s^{(l+1)} \xrightarrow{\sigma} \dots \rightarrow x^{(L)} \rightarrow \ell$$

We have

$$s_i^{(l)} = \sum_j w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)},$$

so  $w_{i,j}^{(l)}$  influences  $\ell$  only through  $s_i^{(l)}$ , and we get

$$\frac{\partial \ell}{\partial w_{i,j}^{(l)}} = \frac{\partial \ell}{\partial s_i^{(l)}} \frac{\partial s_i^{(l)}}{\partial w_{i,j}^{(l)}} = \frac{\partial \ell}{\partial s_i^{(l)}} x_j^{(l-1)},$$

and similarly

$$\frac{\partial \ell}{\partial b_i^{(l)}} = \frac{\partial \ell}{\partial s_i^{(l)}}.$$

Since we know  $x_j^{(l-1)}$  from the forward pass, we only need  $\frac{\partial \ell}{\partial s_i^{(l)}}$ .

$$\dots \xrightarrow{\sigma} x^{(l-1)} \xrightarrow{w^{(l),b^{(l)}}} \underbrace{s^{(l)} \xrightarrow{\sigma} x^{(l)}} \xrightarrow{w^{(l+1),b^{(l+1)}}} s^{(l+1)} \xrightarrow{\sigma} \dots \rightarrow x^{(L)} \rightarrow \ell$$

We have

$$x_i^{(l)} = \sigma(s_i^{(l)}),$$

and since  $s_i^{(l)}$  influences  $\ell$  only through  $x_i^{(l)}$ , the chain rule gives

$$\frac{\partial \ell}{\partial s_i^{(l)}} = \frac{\partial \ell}{\partial x_i^{(l)}} \frac{\partial x_i^{(l)}}{\partial s_i^{(l)}} = \frac{\partial \ell}{\partial x_i^{(l)}} \sigma'(s_i^{(l)}),$$

Since we know  $\frac{\partial \ell}{\partial x_i^{(l)}}$  from the forward pass, we only need  $\frac{\partial \ell}{\partial x_i^{(l)}}$ .

$$\dots \xrightarrow{\sigma} x^{(l-1)} \xrightarrow{w^{(l),b^{(l)}}} s^{(l)} \xrightarrow{\sigma} x^{(l)} \xrightarrow{w^{(l+1),b^{(l+1)}}} s^{(l+1)} \xrightarrow{\sigma} \dots \rightarrow \underbrace{x^{(L)} \rightarrow \ell}$$

We know

$$\frac{\partial \ell}{\partial x_i^{(L)}}$$

from the definition of  $\ell$ , and  $\forall l = 1, \dots, L - 1$ , since

$$s_h^{(l+1)} = \sum_i w_{h,i}^{l+1} x_i^{(l)} + b_h^{l+1},$$

and  $x_i^{(l)}$  influences  $\ell$  only through the  $s_h^{(l+1)}$ , we have

$$\frac{\partial \ell}{\partial x_i^{(l)}} = \sum_h \frac{\partial \ell}{\partial s_h^{(l+1)}} \frac{\partial s_h^{(l+1)}}{\partial x_i^{(l)}} = \sum_h \frac{\partial \ell}{\partial s_h^{(l+1)}} w_{h,i}^{l+1}.$$

To write all this in tensorial form, if  $\psi : \mathbb{R}^N \rightarrow \mathbb{R}^M$ , we will use the standard Jacobian notation

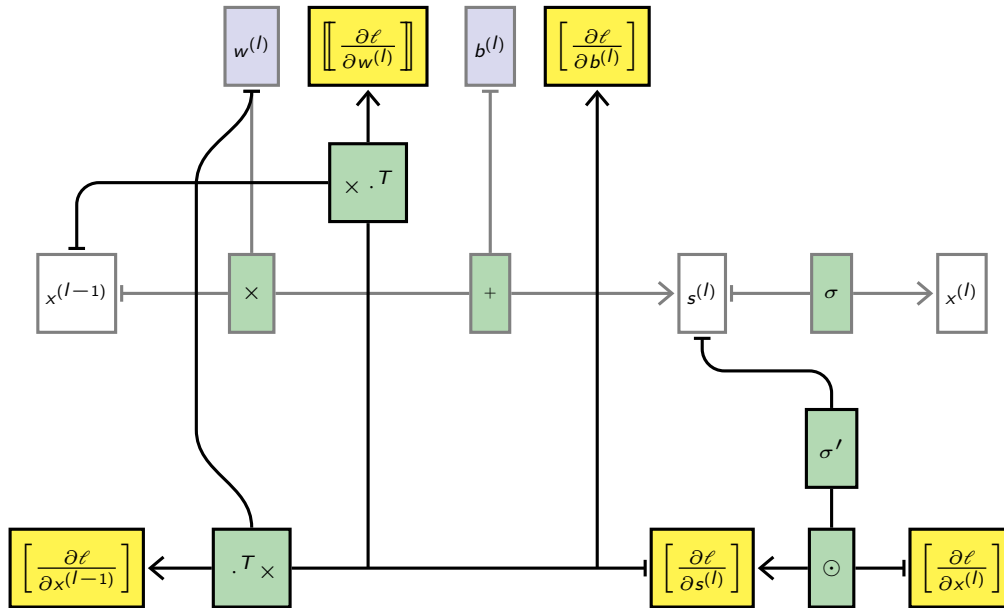
$$\left[ \frac{\partial \psi}{\partial x} \right] = \begin{pmatrix} \frac{\partial \psi_1}{\partial x_1} & \dots & \frac{\partial \psi_1}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial \psi_M}{\partial x_1} & \dots & \frac{\partial \psi_M}{\partial x_N} \end{pmatrix},$$

and if  $\psi : \mathbb{R}^{N \times M} \rightarrow \mathbb{R}$ , we will use the compact notation, also tensorial

$$\left[ \left[ \frac{\partial \psi}{\partial w} \right] \right] = \begin{pmatrix} \frac{\partial \psi}{\partial w_{1,1}} & \dots & \frac{\partial \psi}{\partial w_{1,M}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \psi}{\partial w_{N,1}} & \dots & \frac{\partial \psi}{\partial w_{N,M}} \end{pmatrix}.$$

A standard notation (that we do not use here) is

$$\left[ \frac{\partial \ell}{\partial x^{(l)}} \right] = \nabla_{x^{(l)}} \ell \quad \left[ \frac{\partial \ell}{\partial s^{(l)}} \right] = \nabla_{s^{(l)}} \ell \quad \left[ \frac{\partial \ell}{\partial b^{(l)}} \right] = \nabla_{b^{(l)}} \ell \quad \left[ \left[ \frac{\partial \ell}{\partial w^{(l)}} \right] \right] = \nabla_{w^{(l)}} \ell.$$



### Forward pass

Compute the activations.

$$x^{(0)} = x, \quad \forall l = 1, \dots, L, \quad \begin{cases} s^{(l)} = w^{(l)} x^{(l-1)} + b^{(l)} \\ x^{(l)} = \sigma(s^{(l)}) \end{cases}$$

### Backward pass

Compute the derivatives of the loss wrt the activations.

$$\begin{cases} \left[ \frac{\partial \ell}{\partial x^{(L)}} \right] \text{ from the definition of } \ell & \left[ \frac{\partial \ell}{\partial s^{(l)}} \right] = \left[ \frac{\partial \ell}{\partial x^{(l)}} \right] \odot \sigma'(s^{(l)}) \\ \text{if } l < L, \left[ \frac{\partial \ell}{\partial x^{(l)}} \right] = (w^{(l+1)})^T \left[ \frac{\partial \ell}{\partial s^{(l+1)}} \right] & \end{cases}$$

Compute the derivatives of the loss wrt the parameters.

$$\left[ \frac{\partial \ell}{\partial w^{(l)}} \right] = \left[ \frac{\partial \ell}{\partial s^{(l)}} \right] (x^{(l-1)})^T \quad \left[ \frac{\partial \ell}{\partial b^{(l)}} \right] = \left[ \frac{\partial \ell}{\partial s^{(l)}} \right].$$

### Gradient step

Update the parameters.

$$w^{(l)} \leftarrow w^{(l)} - \eta \left[ \frac{\partial \ell}{\partial w^{(l)}} \right] \quad b^{(l)} \leftarrow b^{(l)} - \eta \left[ \frac{\partial \ell}{\partial b^{(l)}} \right]$$

In spite of its hairy formalization, the backward pass is a simple algorithm: apply the chain rule again and again.

As for the forward pass, it can be expressed in tensorial form. Heavy computation is concentrated in linear operations, and all the non-linearities go into component-wise operations.

Regarding computation, since the costly operation for the forward pass is

$$\mathbf{s}^{(l)} = \mathbf{w}^{(l)} \mathbf{x}^{(l-1)} + \mathbf{b}^{(l)}$$

and for the backward

$$\left[ \frac{\partial \ell}{\partial \mathbf{x}^{(l)}} \right] = \left( \mathbf{w}^{(l+1)} \right)^T \left[ \frac{\partial \ell}{\partial \mathbf{s}^{(l+1)}} \right]$$

and

$$\left[ \left[ \frac{\partial \ell}{\partial \mathbf{w}^{(l)}} \right] \right] = \left[ \frac{\partial \ell}{\partial \mathbf{s}^{(l)}} \right] \left( \mathbf{x}^{(l-1)} \right)^T,$$

the rule of thumb is that the backward pass is twice more expensive than the forward one.