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

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

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

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

So, with $\ell_n = \ell(f(x_n; w, b), y_n)$, 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 $x^{(0)} = x$,

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

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.

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

We have

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

so $w_{i,j}^{(l)}$ influences ℓ 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 $\frac{\partial \ell}{\partial s_i^{(l)}}$.

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

We have

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

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

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

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

$$\ldots \xrightarrow{\sigma} x^{(l-1)} \xrightarrow{w^{(l)}, b^{(l)}} s^{(l)} \xrightarrow{\sigma} x^{(l)} \xrightarrow{w^{(l+1)}, b^{(l+1)}} s^{(l+1)} \xrightarrow{\sigma} \ldots$$

Finally, we have

$$\frac{\partial \ell}{\partial x_i^{(L)}} = (\nabla_1 \ell)_i$$

where $\nabla_1 \ell$ is the gradient of ℓ with respect to its first parameter, that is the predicted value.

Also, $\forall l = 1, \ldots, L-1$, since

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

and $x_i^{(l)}$ influences ℓ 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 $\psi : \mathbb{R}^N \to \mathbb{R}^M$, we will use the standard Jacobian notation

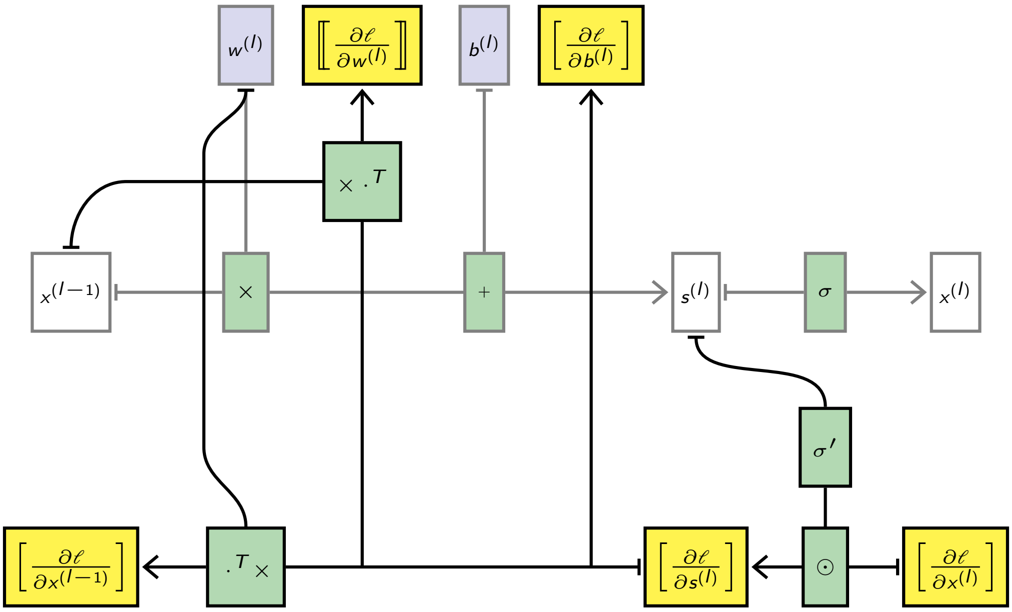
$$\left[\frac{\partial \psi}{\partial x}\right] = \begin{pmatrix} \frac{\partial \psi_1}{\partial x_1} & \ldots & \frac{\partial \psi_1}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial \psi_M}{\partial x_1} & \ldots & \frac{\partial \psi_M}{\partial x_N} \end{pmatrix},$$

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

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

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.

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

Backward pass

Compute the derivatives of the loss wrt the activations.

$$\begin{cases} \left[\frac{\partial \ell}{\partial x^{(L)}}\right] = \nabla_1 \ell\left(x^{(L)}\right) \\ \text{if } l < L, \left[\frac{\partial \ell}{\partial x^{(l)}}\right] = \left(w^{(l+1)}\right)^T \left[\frac{\partial \ell}{\partial s^{(l+1)}}\right] \end{cases} \qquad \left[\frac{\partial \ell}{\partial s^{(l)}}\right] = \left[\frac{\partial \ell}{\partial x^{(l)}}\right] \odot \sigma'\left(s^{(l)}\right)$$

Compute the derivatives of the loss wrt the parameters.

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

Gradient step

Update the parameters.

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

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

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

and for the backward

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

and

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

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