EE-559 – Deep learning

3b. Multi-Layer Perceptrons

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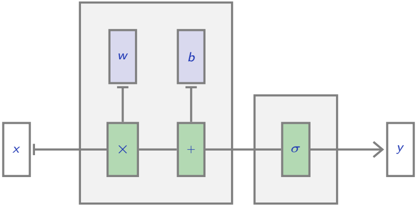
Combining multiple layers

For flexibility, we will separate the linear operators and the non-linearities in different blocks in our figures.



We can combine several "layers":

With $x^{(0)} = x$,

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

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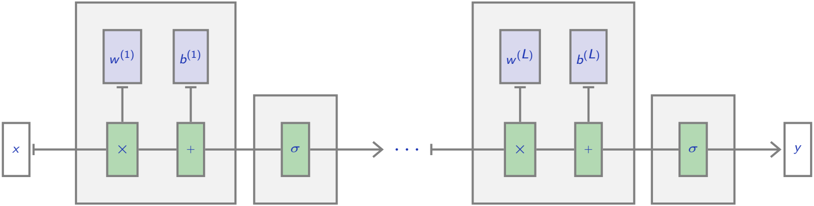

Such a model is a **Multi-Layer Perceptron (MLP).**

Note that if σ is a linear transformation,

$$\forall x \in \mathbb{R}^N, \ \sigma(x) = \alpha x + \beta \mathbb{I}$$

with $\alpha, \beta \in \mathbb{R}$, we have

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and the whole mapping is an affine transform

$$f(x; w, b) = A^{(L)} x + B^{(L)}$$

where $A^{(0)} = \mathbb{I}, B^{(0)} = 0$ and

$$\forall l < L,\ \begin{cases} A^{(l)} = \alpha\, w^{(l)} A^{(l-1)} \\ B^{(l)} = \alpha\, w^{(l)} B^{(l-1)} + \alpha\, b^{(l)} + \beta \mathbb{I} \end{cases}$$

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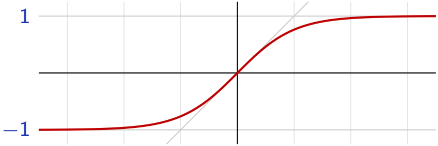
⚠ Consequently, **the activation function should be non-linear**, or the resulting MLP is an affine mapping with a peculiar parametrization.

The two classical activation functions are the hyperbolic tangent

$$x \mapsto \frac{2}{1+e^{-2x}} - 1$$



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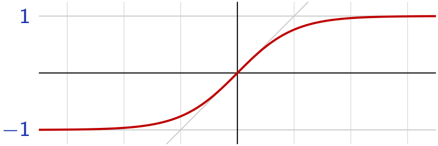

and the rectified linear unit (ReLU)

$$x \mapsto \max(0, x)$$

Universal approximation

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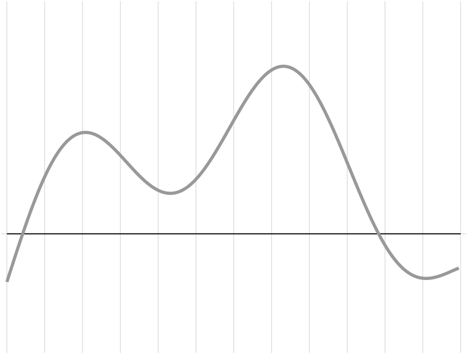

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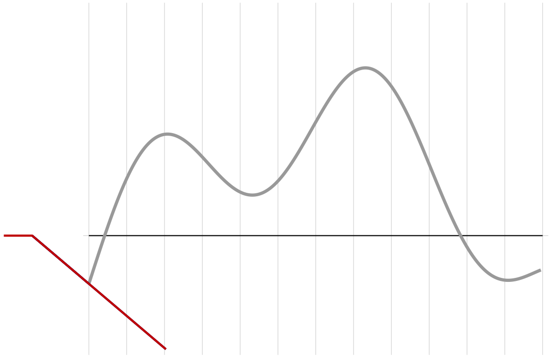

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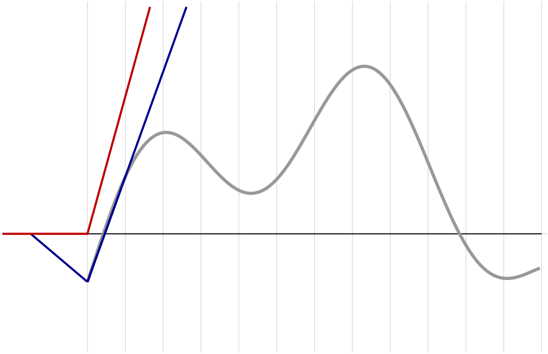

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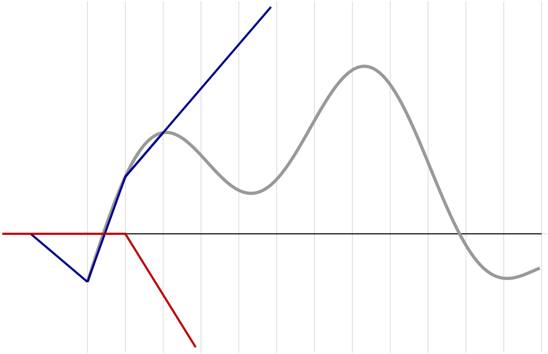

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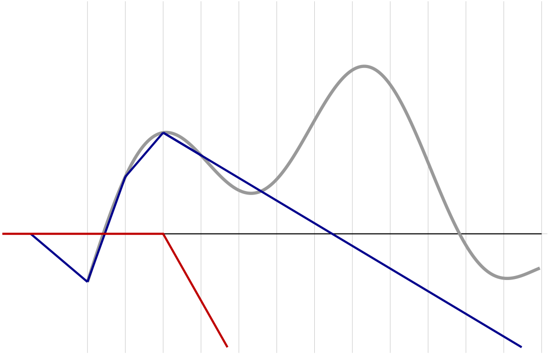

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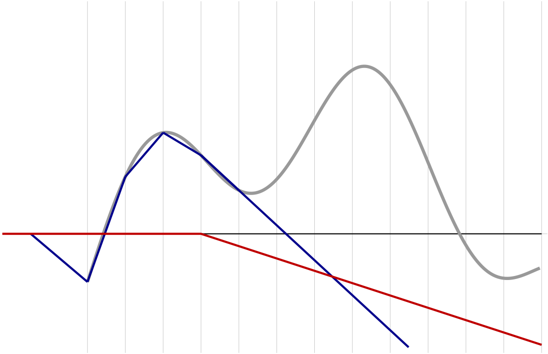

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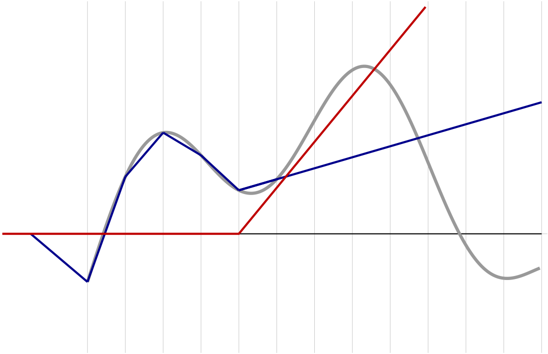

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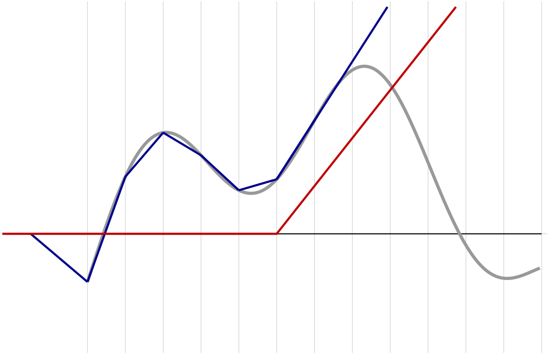

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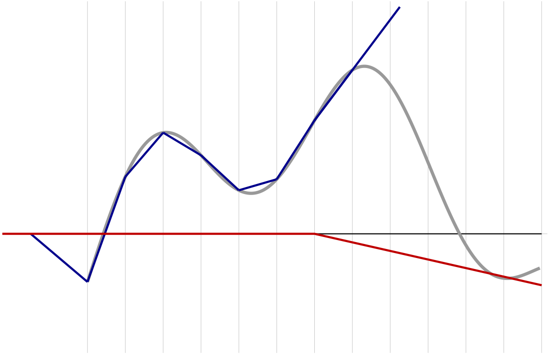

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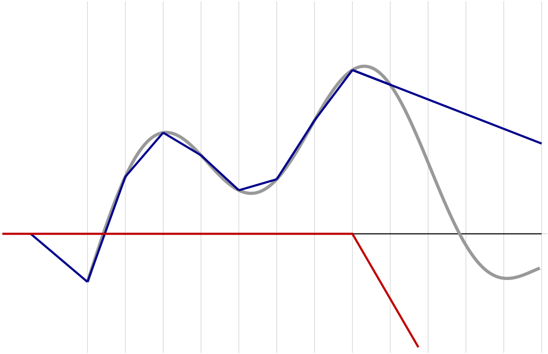

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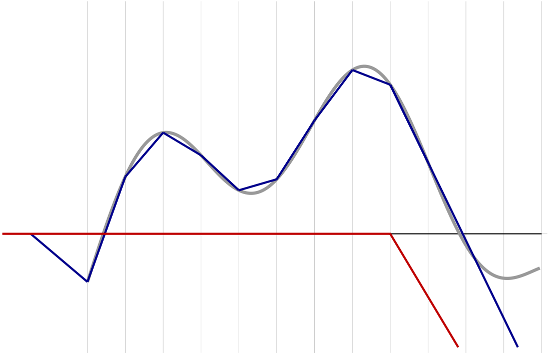

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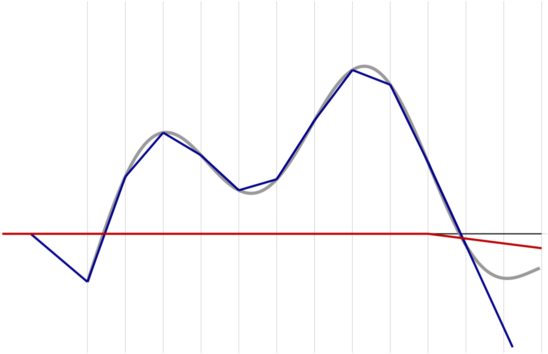

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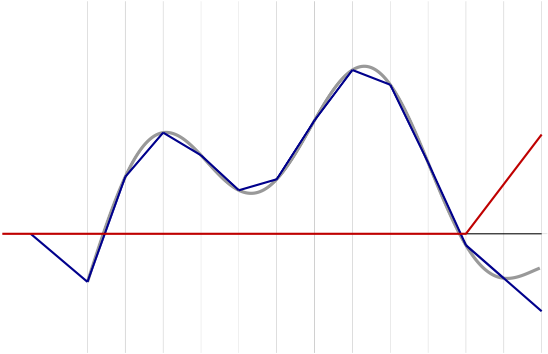

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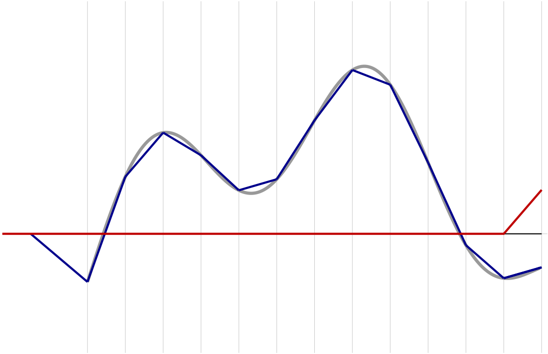

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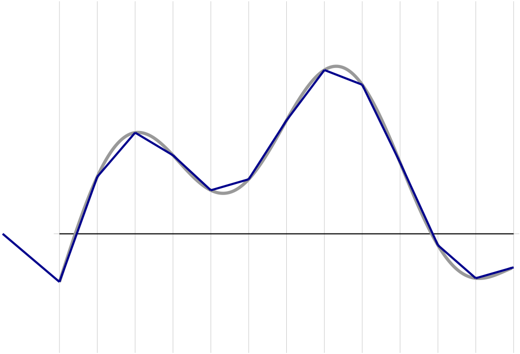

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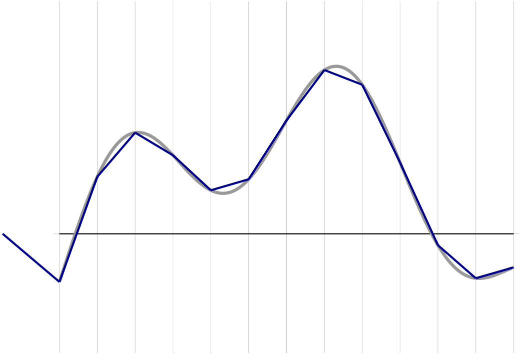

This is true for other activation functions under mild assumptions.

Extending this result to any $\psi \in \mathscr{C}([0,1]^D, \mathbb{R})$ requires a bit of work.

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First, we can use the previous result for the sin function

$$\forall A > 0, \epsilon > 0,\ \exists N,\ (\alpha_n, a_n) \in \mathbb{R} \times \mathbb{R}, n = 1, \dots, N,$$

$$\text{s.t.} \max_{x \in [-A,A]} \left| \sin(x) - \sum_{n=1}^{N} \alpha_n \sigma(x - a_n) \right| \leq \epsilon.$$

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And the density of Fourier series provides

$$\forall f \in \mathscr{C}([0,1]^D, \mathbb{R}), \delta > 0, \exists M, (v_m, \gamma_m, c_m) \in \mathbb{R}^D \times \mathbb{R} \times \mathbb{R}, m = 1, \dots, M,$$

$$\text{s.t.} \max_{x \in [0,1]^D} \left| \psi(x) - \sum_{m=1}^{M} \gamma_m \sin(v_m \cdot x + c_m) \right| \leq \delta.$$

So, $\forall \xi > 0$, with

$$\delta = \frac{\xi}{2}, A = \max_{1 \leq m \leq M} \max_{x \in [0,1]^D} |v_m \cdot x + c_m|, \text{ and } \epsilon = \frac{\xi}{2 \sum_m |\gamma_m|}$$

we get, $\forall x \in [0,1]^D$,

$$\begin{aligned}
&\left| \psi(x) - \sum_{m=1}^{M} \gamma_m \left(\sum_{n=1}^{N} \alpha_n \sigma(v_m \cdot x + c_m - a_n) \right) \right| \\
&\leq \underbrace{\left| \psi(x) - \sum_{m=1}^{M} \gamma_m \sin(v_m \cdot x + c_m) \right|}_{\leq \frac{\xi}{2}} \\
&\quad \underbrace{+ \sum_{m=1}^{M} |\gamma_m| \underbrace{\left| \sin(v_m \cdot x + c_m) - \sum_{n=1}^{N} \alpha_n \sigma(v_m \cdot x + c_m - a_n) \right|}_{\leq \frac{\xi}{2 \sum_m |\gamma_m|}}}_{\leq \frac{\xi}{2}}
\end{aligned}$$

So we can approximate any continuous function

$$\psi : [0,1]^D \to \mathbb{R}$$

with a mapping of the form

$$x \mapsto \omega \cdot \sigma(w\,x + b),$$

where $b \in \mathbb{R}^K$, $w \in \mathbb{R}^{K \times D}$, and $\omega \in \mathbb{R}^K$,

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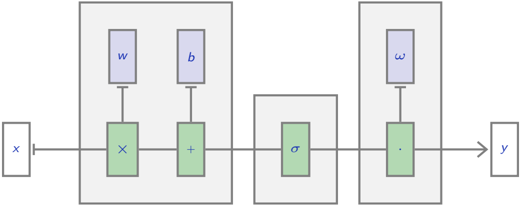

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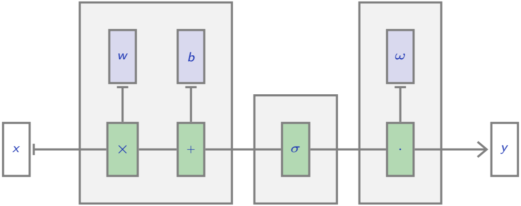

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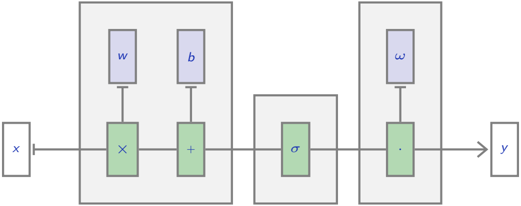

This is the **universal approximation theorem.**

A better approximation requires a larger hidden layer (larger K), and this theorem says nothing about the relation between the two. We will come back to that later.

Training and gradient descent

We saw that training consists of finding the model parameters minimizing an empirical risk or loss, for instance the mean-squared error (MSE)

$$\mathscr{L}(w, b) = \frac{1}{N} \sum_n \ell \left(f(x_n; w, b) - y_n \right)^2 .$$

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In our previous examples we minimized the loss either with an analytic solution for the MSE, or with *ad hoc* recipes for the empirical error rate (k-NN and perceptron).

There is generally no *ad hoc* method. The logistic regression for instance

$$P_w(Y = 1 \mid X = x) = \sigma(w \cdot x + b), \text{ with } \sigma(x) = \frac{1}{1 + e^{-x}}$$

leads to the loss

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The general minimization method used in such a case is the **gradient descent**.

Given a functional

$$\begin{aligned} f : \mathbb{R}^D &\to \mathbb{R} \\ x &\mapsto f(x_1, \dots, x_D), \end{aligned}$$

its gradient is the mapping

$$\begin{aligned} \nabla f : \mathbb{R}^D &\to \mathbb{R}^D \\ x &\mapsto \left(\frac{\partial f}{\partial x_1}(x), \dots, \frac{\partial f}{\partial x_D}(x) \right). \end{aligned}$$

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$$\mathscr{L} : \mathbb{R}^D \to \mathbb{R}$$

the gradient descent uses local linear information to iteratively move toward a (local) minimum.

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$$\tilde{\mathscr{L}}_{w_0}(w) = \mathscr{L}(w_0) + \nabla \mathscr{L}(w_0)^T (w - w_0) + \frac{1}{2\eta} \|w - w_0\|^2.$$

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We have

$$\nabla \tilde{\mathscr{L}}_{w_0}(w) = \nabla \mathscr{L}(w_0) + \frac{1}{\eta}(w - w_0),$$

which leads to

$$\operatorname*{argmin}_w \tilde{\mathscr{L}}_{w_0}(w) = w_0 - \eta \nabla \mathscr{L}(w_0).$$

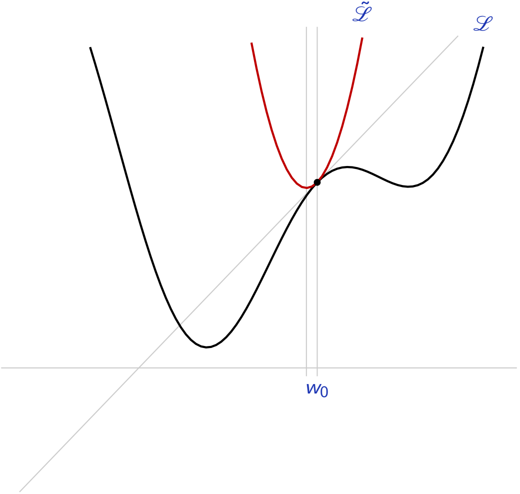
The resulting iterative rule, which goes to the minimum of the approximation at the current location, takes the form:

$$w_{t+1} = w_t - \eta \nabla \mathscr{L}(w_t).$$

Which corresponds intuitively to "following the steepest descent".

This finds a **local** minimum, and the choices of w_0 and η are important.

$\eta = 0.125$



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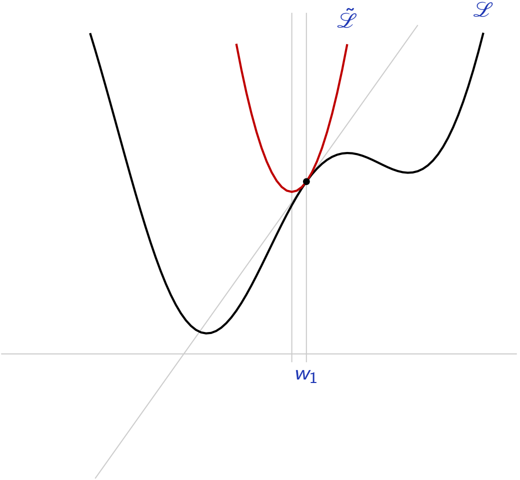

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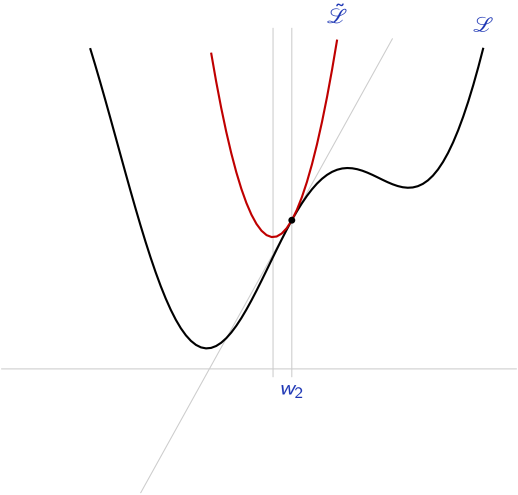

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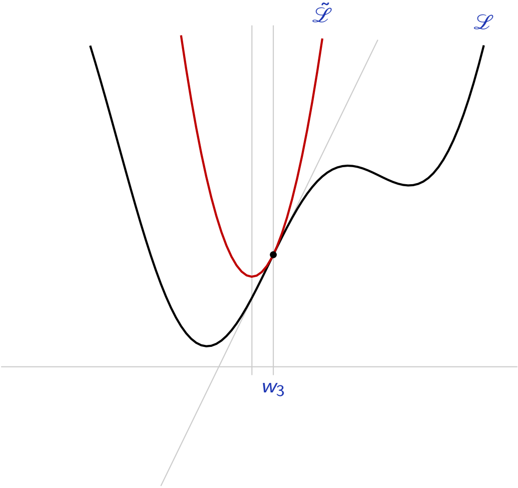

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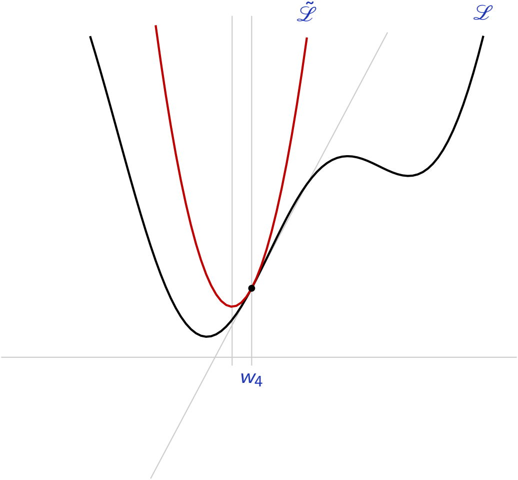

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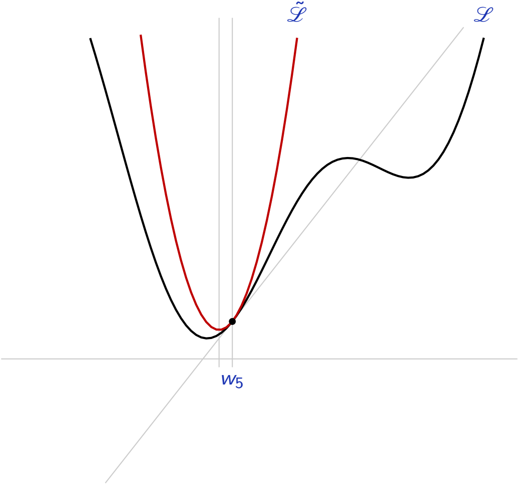

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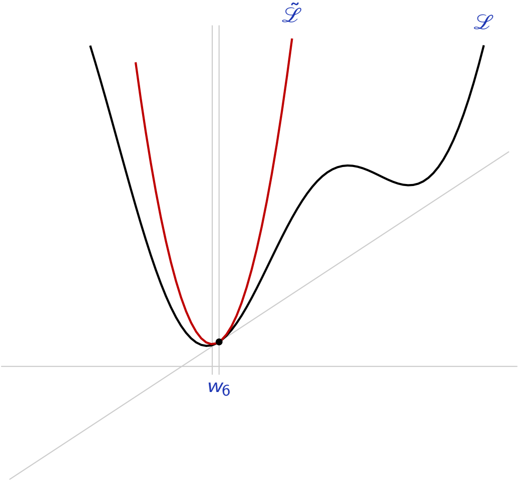

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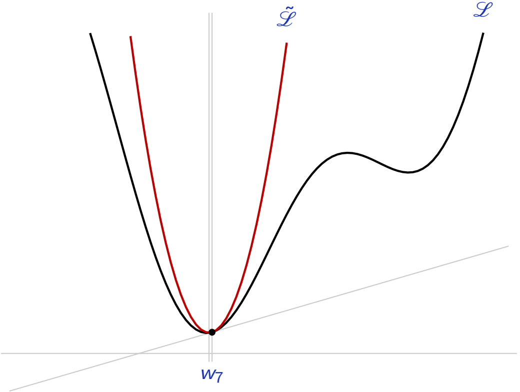

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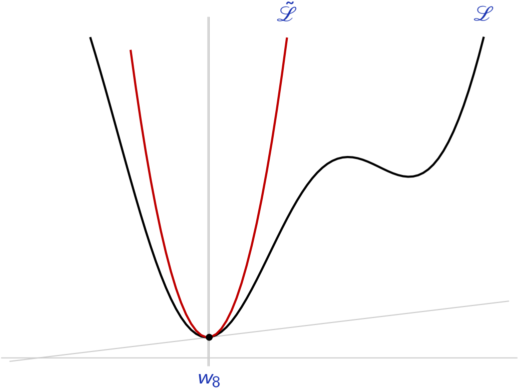

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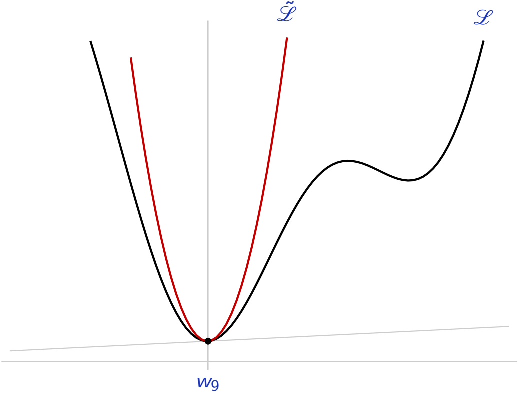

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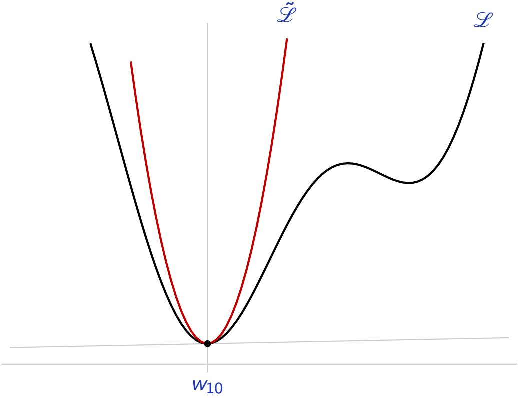

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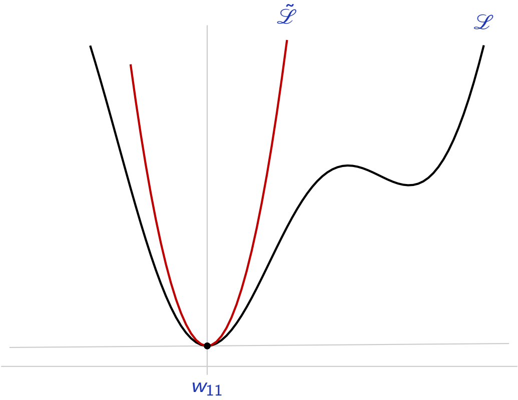

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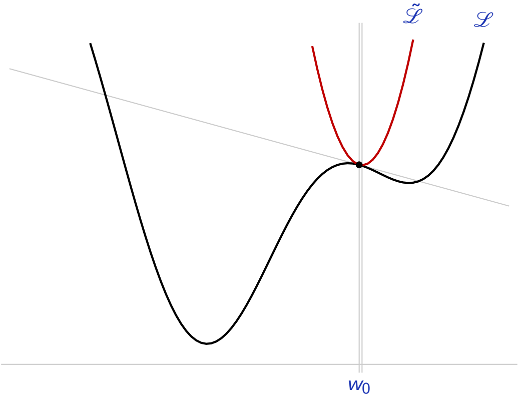

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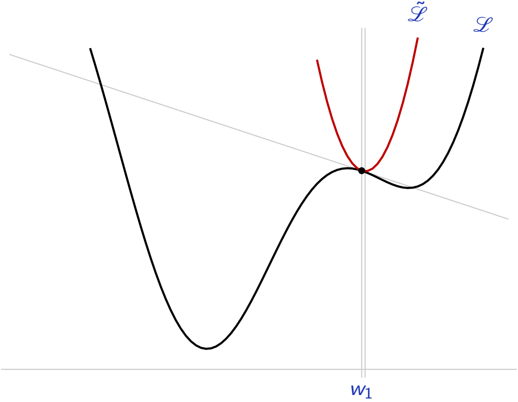

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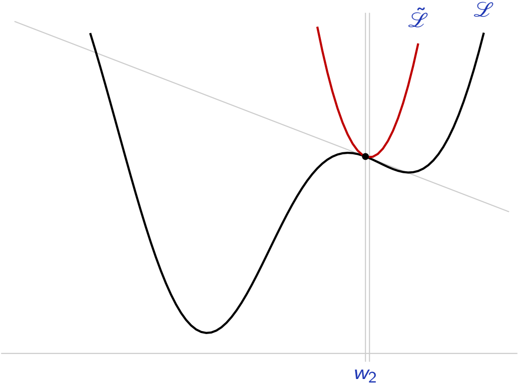

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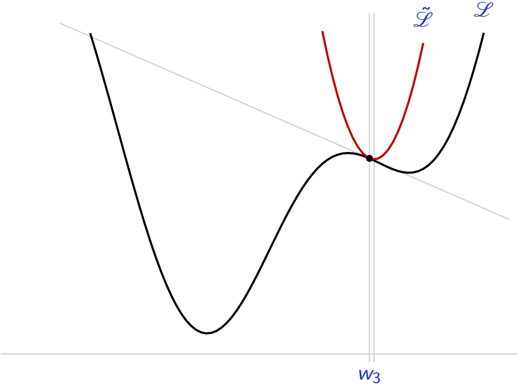

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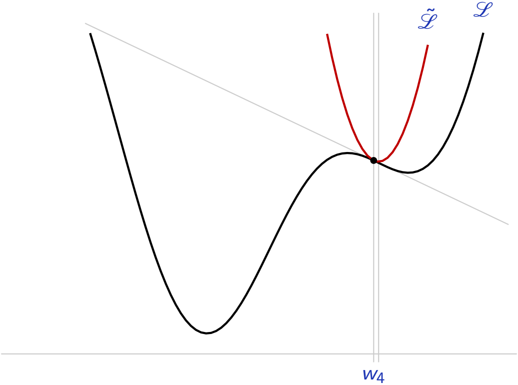

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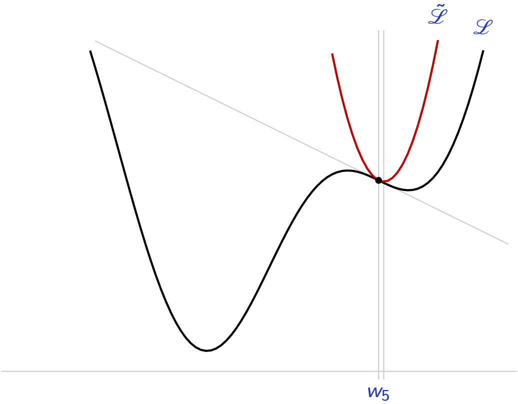

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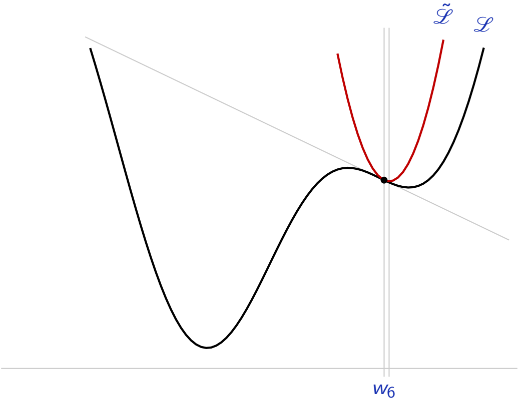

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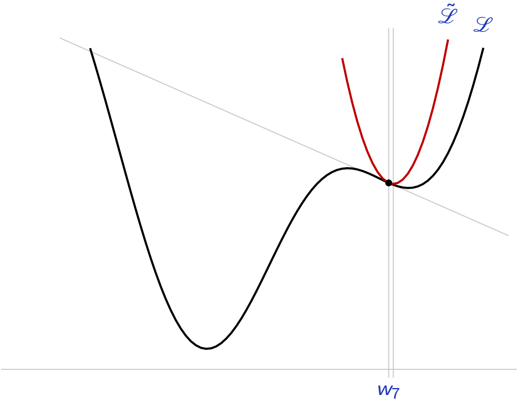

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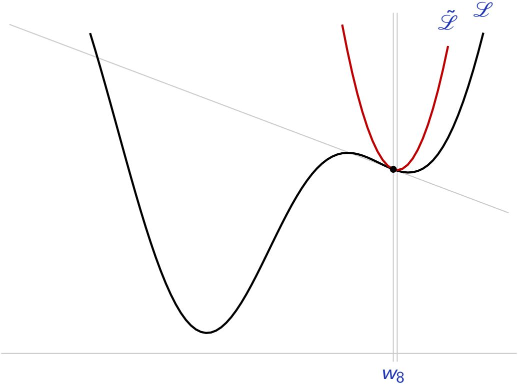

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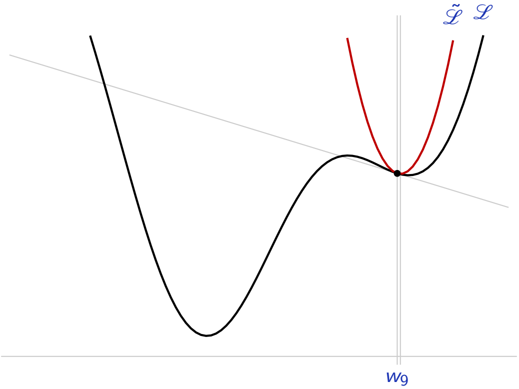

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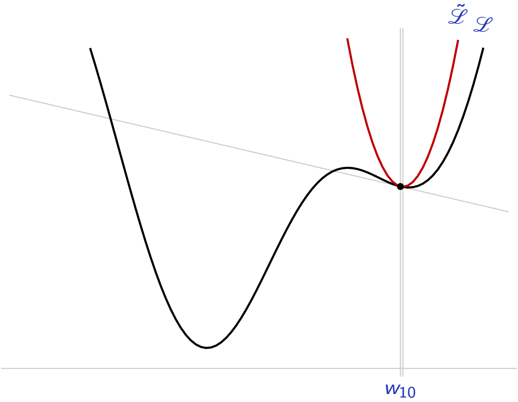

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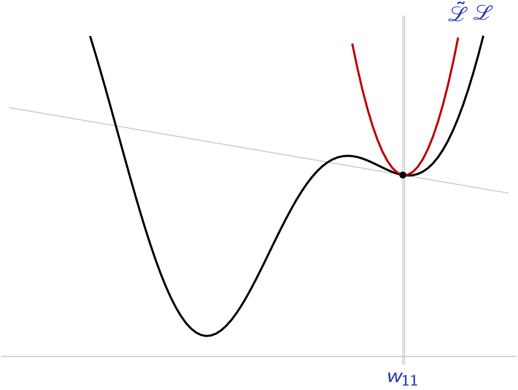

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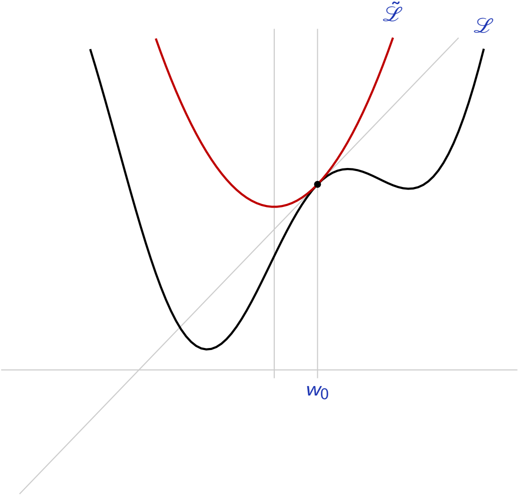

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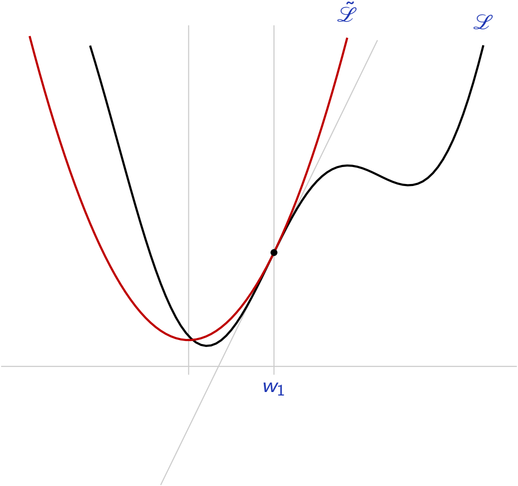

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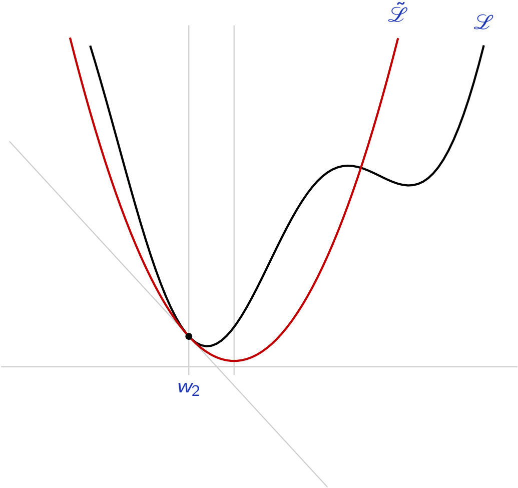

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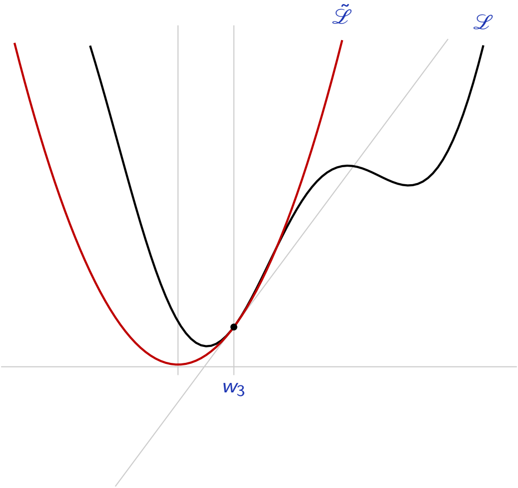

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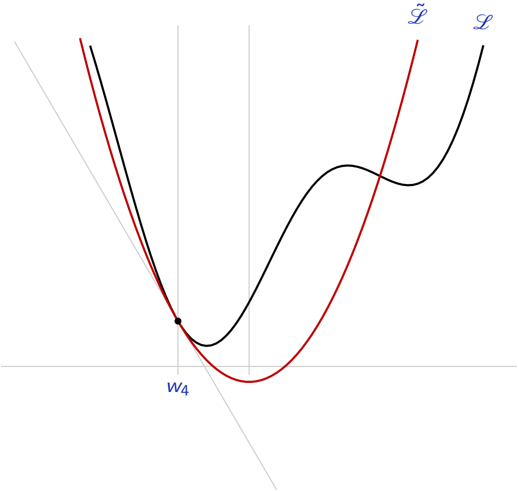

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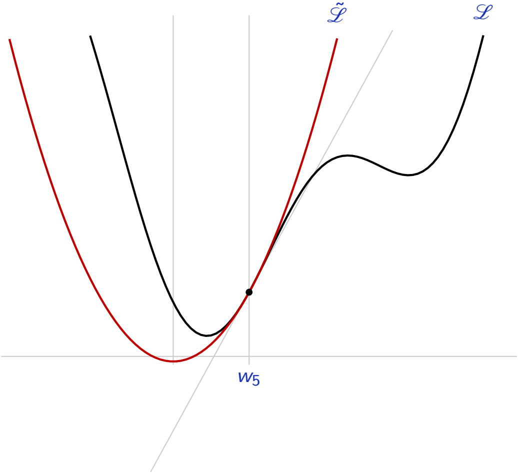

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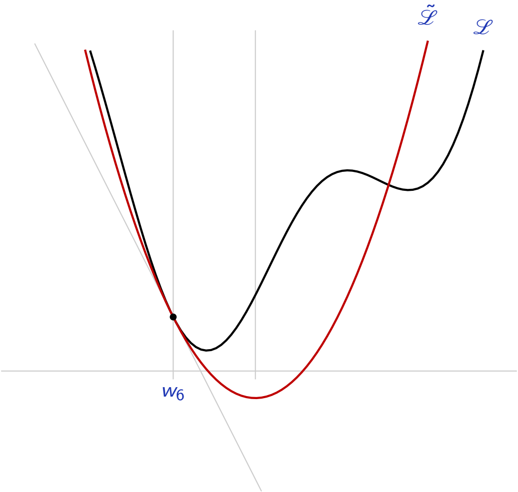

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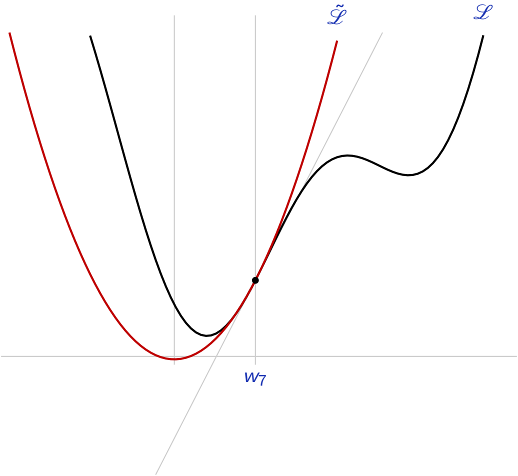

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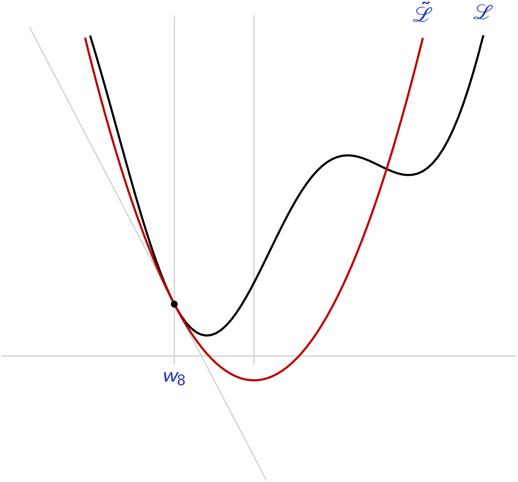

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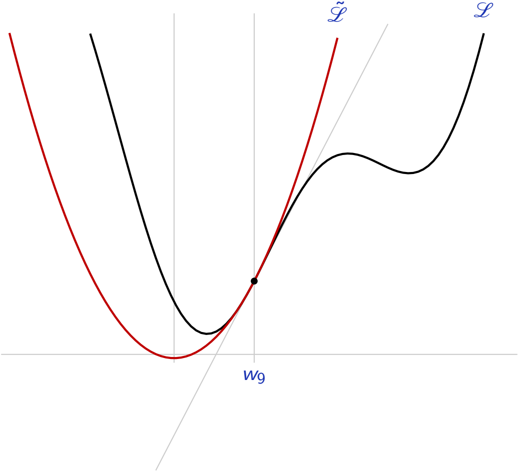

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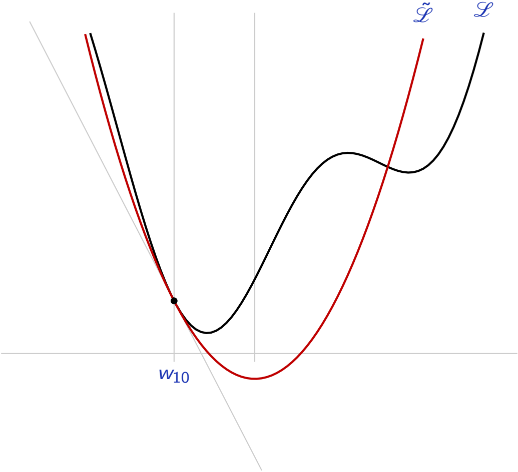
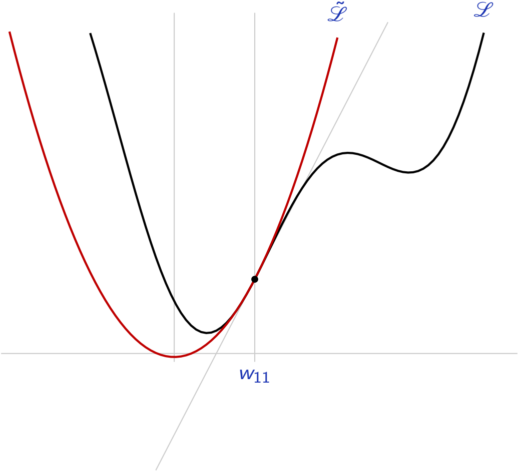
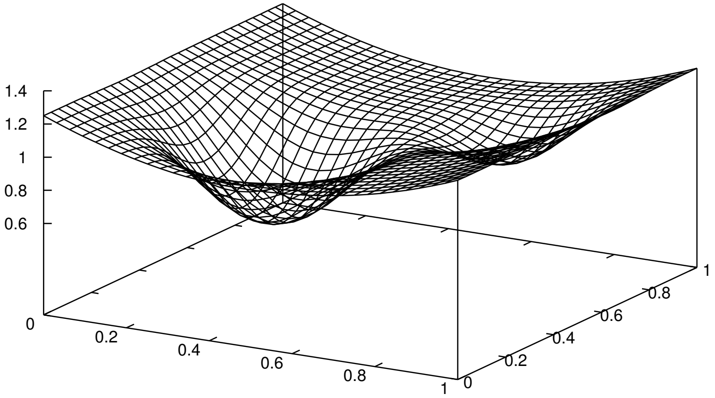


$$\eta = 0.5$$





1.4
1.2
1
0.8
0.6
0
0.2
0.4
0.6
0.8
1
0
0.2
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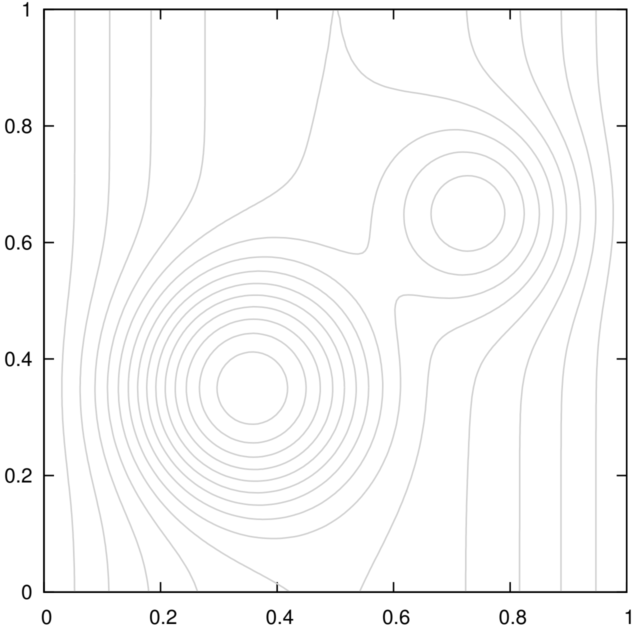
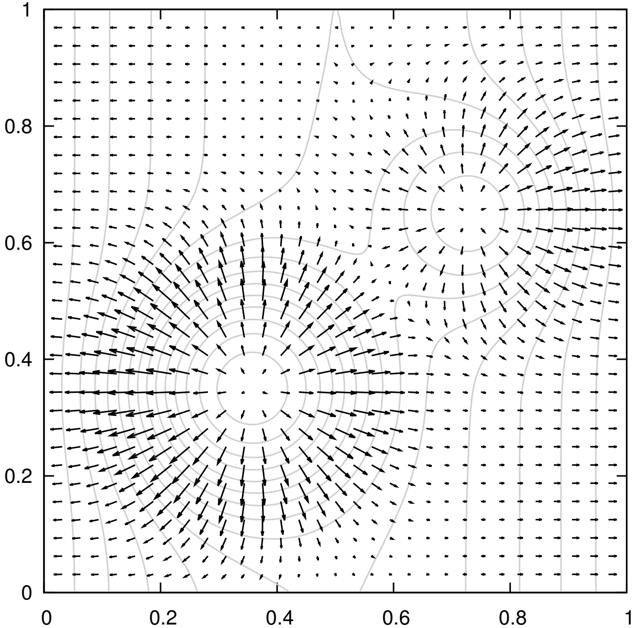
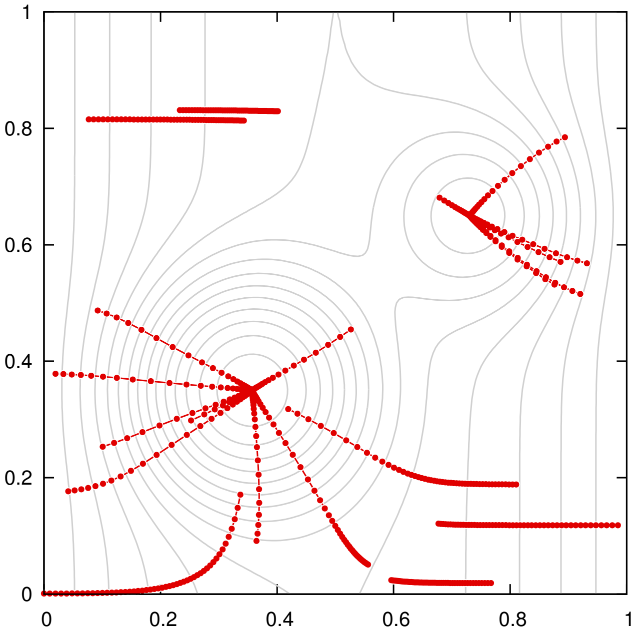
0.6
0.8
1


1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1


1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1



1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1

We saw that the minimum of the logistic regression loss

$$\mathscr{L}(w, b) = -\sum_n \log \sigma(y_n(w \cdot x_n + b))$$

does not have an analytic form.

We can derive

$$\frac{\partial \mathscr{L}}{\partial b} = -\sum_n \underbrace{y_n \, \sigma(-y_n(w \cdot x_n + b))}_{u_n},$$

$$\forall d, \; \frac{\partial \mathscr{L}}{\partial w_d} = -\sum_n \underbrace{x_{n,d} \, y_n \, \sigma(-y_n(w \cdot x_n + b))}_{v_{n,d}}.$$

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$$\forall d, \; \frac{\partial \mathscr{L}}{\partial w_d} = -\sum_n \underbrace{x_{n,d} \, y_n \, \sigma(-y_n(w \cdot x_n + b))}_{v_{n,d}}.$$

Which can be implemented as

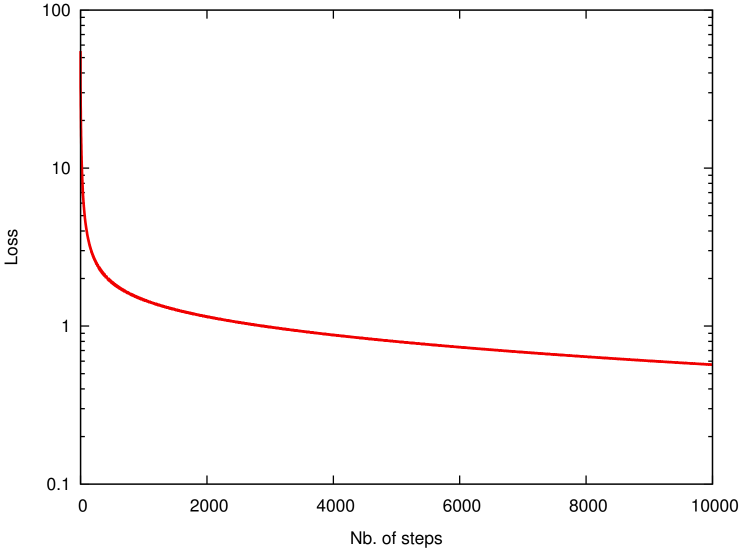
```
def gradient(x, y, w, b):
    u = y * ( - (x.mv(w) + b) * y).apply_(sigmoid)
    v = x * u.view(-1, 1) # Broadcasting
    return - v.sum(0), - u.sum()
```

and the gradient descent as

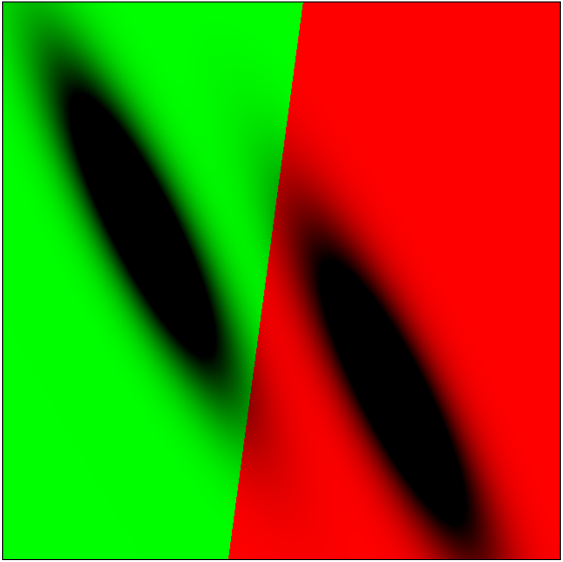
```
w = Tensor(dimension).normal_()
b = 0

eta = 1e-1

for k in range(nb_iterations):
    dw, db = gradient(x, y, w, b)
    w = w - eta * dw
    b = b - eta * db
```

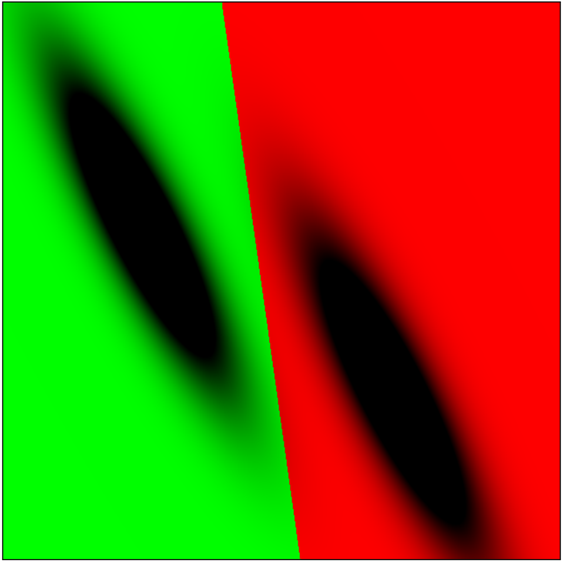

100
10
1
0.1
Loss
0
2000
4000
6000
8000
10000
Nb. of steps

With 100 training points and $\eta = 10^{-1}$.



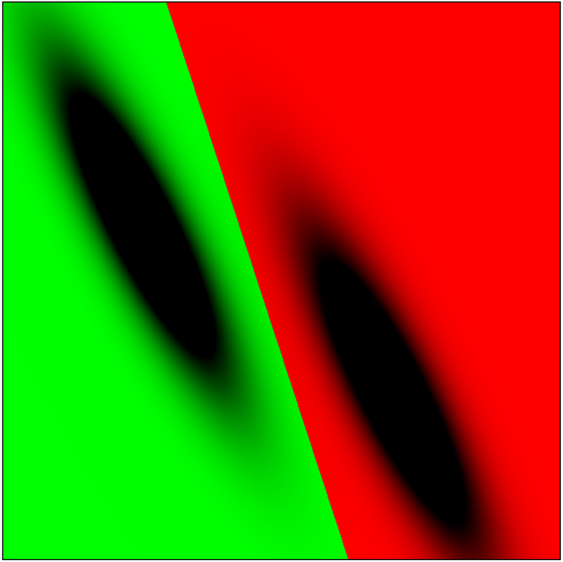
$n = 0$

With 100 training points and $\eta = 10^{-1}$.



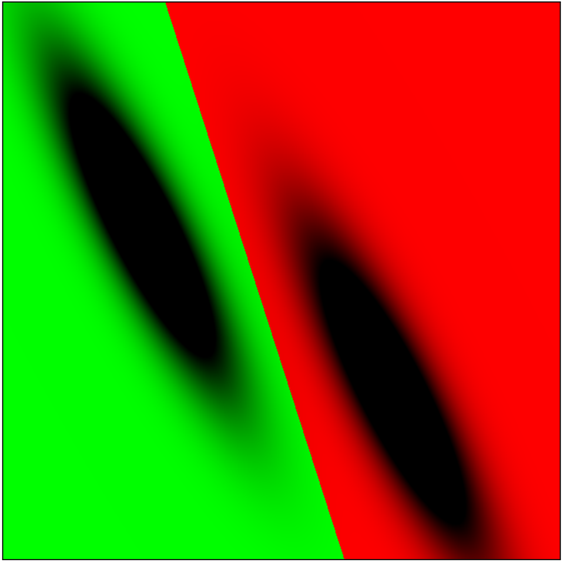
$n = 10$

With 100 training points and $\eta = 10^{-1}$.



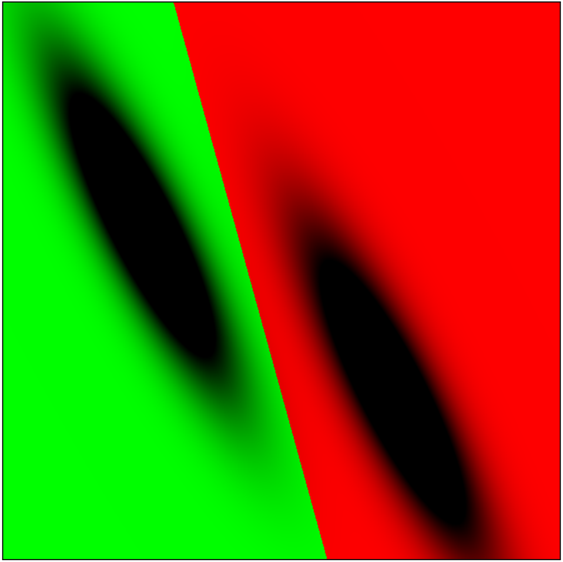
$n = 10^2$

With 100 training points and $\eta = 10^{-1}$.

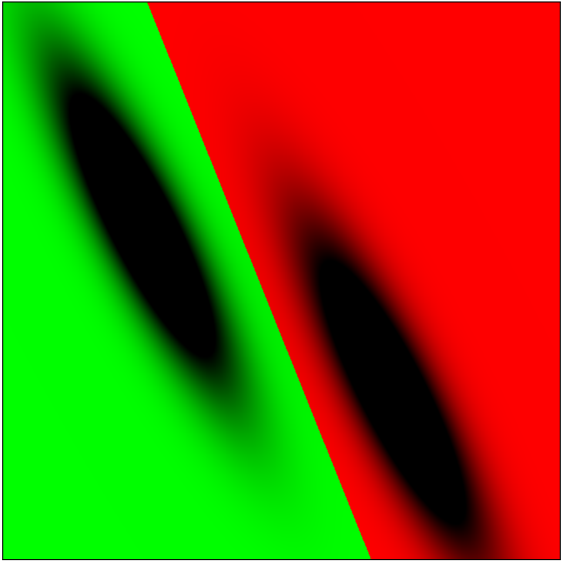


$n = 10^3$

With 100 training points and $\eta = 10^{-1}$.



$n = 10^4$



LDA

Back-propagation

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

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

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

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

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

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.

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

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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 $f(x; w, b) = x^{(L)}$.

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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.

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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

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

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

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

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

$$\frac{\partial \ell}{\partial w_{i,j}^{(l)}}$$

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

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

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and similarly

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

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

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

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We have

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

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

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

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

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

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

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

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.

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

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

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

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

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

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$$\frac{\partial \ell}{\partial x_i^{(l)}} = \sum_h \frac{\partial \ell}{\partial s_h^{(l+1)}} \frac{\partial s_h^{(l+1)}}{\partial x_i^{(l)}}$$

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

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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

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

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

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

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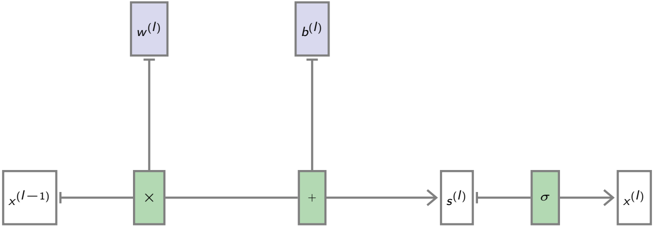
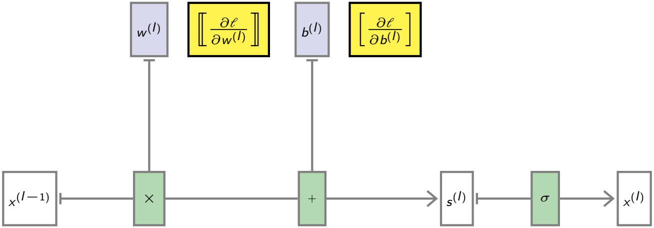

$w^{(l)}$
$b^{(l)}$
$x^{(l-1)}$
$\times$
$+$
$s^{(l)}$
σ
$x^{(l)}$



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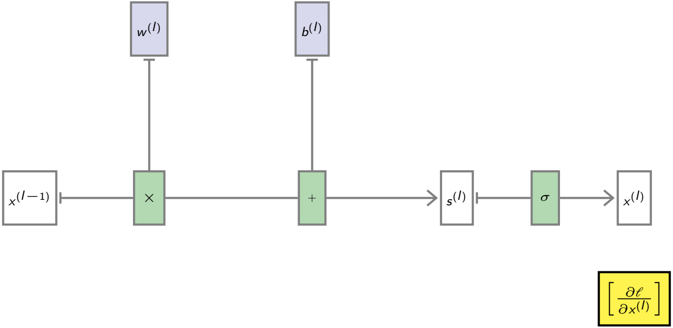
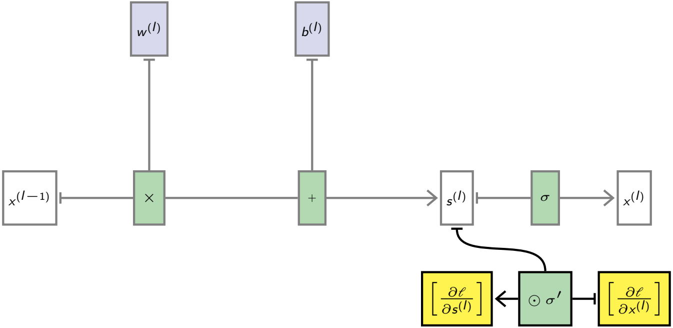
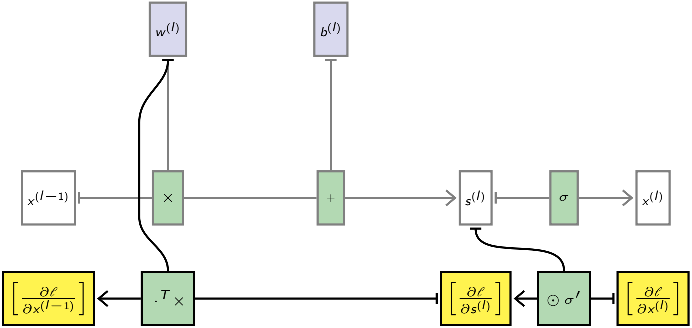
$x^{(l)}$

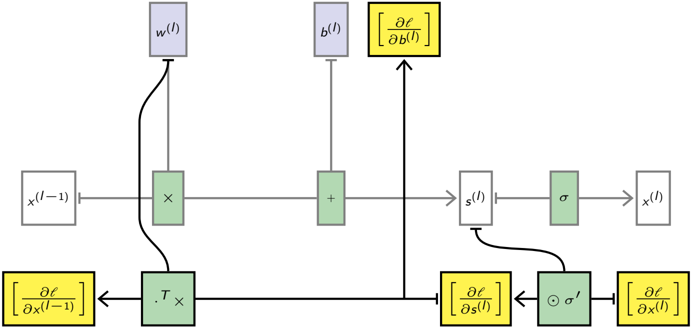

$w^{(l)}$
$b^{(l)}$
$x^{(l-1)}$
$\times$
$+$
$s^{(l)}$
σ
$x^{(l)}$
$\left[\frac{\partial \ell}{\partial x^{(l)}}\right]$



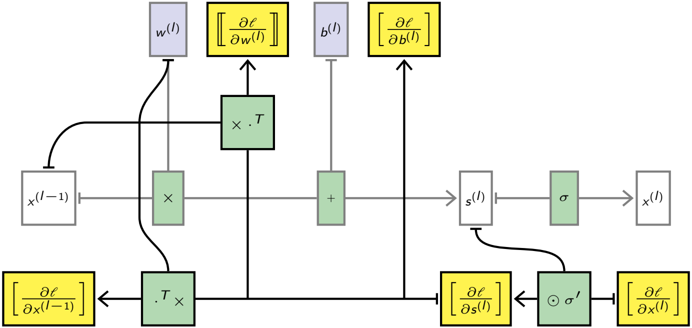
$$\frac{\partial \ell}{\partial s_i^{(l)}} = \frac{\partial \ell}{\partial x_i^{(l)}} \sigma'\left(s_i^{(l)}\right)$$



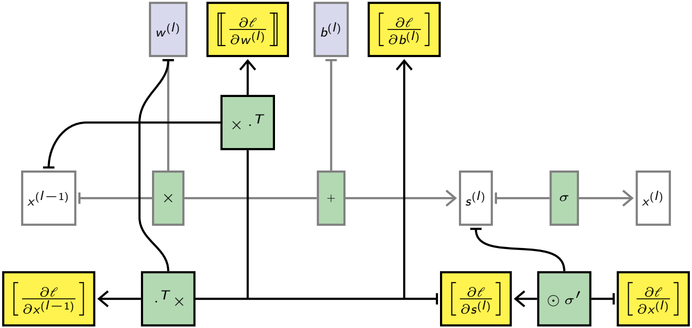
$$\frac{\partial \ell}{\partial x_j^{(l-1)}} = \sum_i w_{i,j}^{(l)} \frac{\partial \ell}{\partial s_i^{(l)}}$$



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



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


$w^{(l)}$
$\left[\!\left[\frac{\partial \ell}{\partial w^{(l)}}\right]\!\right]$
$b^{(l)}$
$\left[\frac{\partial \ell}{\partial b^{(l)}}\right]$
$\times \, .^T$
$x^{(l-1)}$
$\times$
$+$
$s^{(l)}$
σ
$x^{(l)}$
$\left[\frac{\partial \ell}{\partial x^{(l-1)}}\right]$
$.^T \times$
$\left[\frac{\partial \ell}{\partial s^{(l)}}\right]$
$\odot \, \sigma'$
$\left[\frac{\partial \ell}{\partial x^{(l)}}\right]$

Forward pass

Compute the activations.

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

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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.

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

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

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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.

Practical session:

https://fleuret.org/dlc/dlc-practical-3.pdf

The end