EE-559 – Deep learning

3.1. The perceptron

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 $(w = 1, b = -0.5)$
 $and(u,v) = \mathbf{1}_{\{u+v-1.5 \ge 0\}}$ $(w = 1, b = -1.5)$
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$$\begin{array}{ll} \textit{or}(u,v) = \mathbf{1}_{\{u+v-0.5 \geq 0\}} & (w=1,b=-0.5) \\ \textit{and}(u,v) = \mathbf{1}_{\{u+v-1.5 \geq 0\}} & (w=1,b=-1.5) \\ \textit{not}(u) = \mathbf{1}_{\{-u+0.5 \geq 0\}} & (w=-1,b=0.5) \end{array}$$

Hence, any Boolean function can be build with such units.

(McCulloch and Pitts, 1943)

The perceptron is very similar

$$f(x) = \begin{cases} 1 & \text{if} & \sum_{i} w_i \, x_i + b \ge 0 \\ 0 & \text{otherwise} \end{cases}$$

but the inputs are real values and the weights can be different.

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This model was originally motivated by biology, with w_i being the *synaptic* weights, and x_i and f firing rates.

It is a (very) crude biological model.

(Rosenblatt, 1957)

To make things simpler we take responses ± 1 . Let

$$\sigma(x) = \begin{cases} 1 & \text{if } x \ge 0 \\ -1 & \text{otherwise.} \end{cases}$$

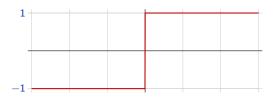


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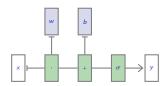
For neural networks, the function σ that follows a linear operator is called the activation function.

We can represent this "neuron" as follows: Value Parameter Operation x_2

*x*₃

We can also use tensor operations, as in

$$f(x) = \sigma(w \cdot x + b).$$



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$$(x_n, y_n) \in \mathbb{R}^D \times \{-1, 1\}, \quad n = 1, \dots, N,$$

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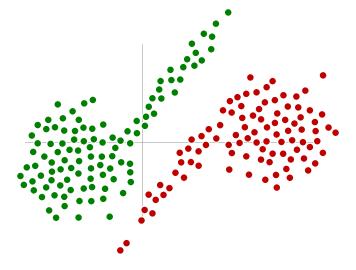
The bias b can be introduced as one of the ws by adding a constant component to x equal to 1.

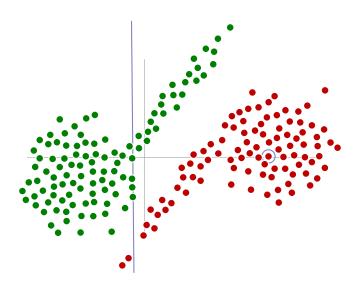
(Rosenblatt, 1957)

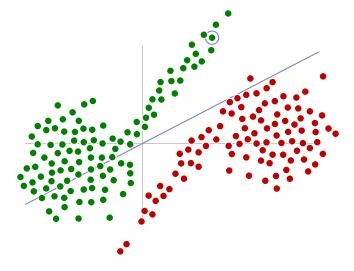
```
def train_perceptron(x, y, nb_epochs_max):
    w = torch.zeros(x.size(1))

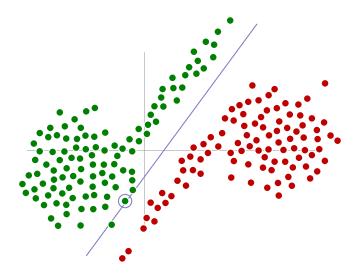
for e in range(nb_epochs_max):
    nb_changes = 0
    for i in range(x.size(0)):
        if x[i].dot(w) * y[i] <= 0:
            w = w + y[i] * x[i]
            nb_changes = nb_changes + 1
    if nb_changes == 0: break;

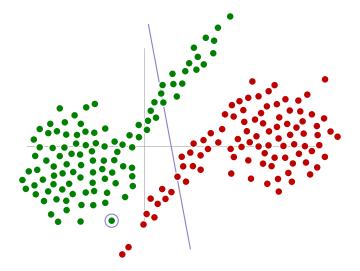
return w</pre>
```

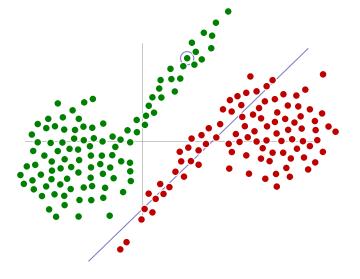


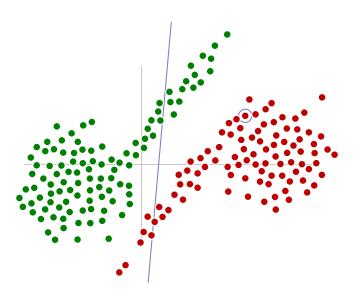


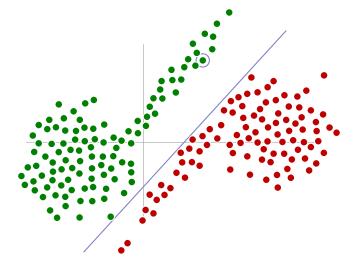




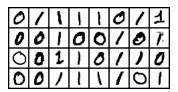




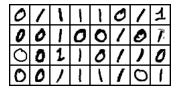




This crude algorithm works often surprisingly well. With MNIST's "0"s as negative class, and "1"s as positive one.

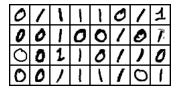


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epoch 0 nb_changes 64 train_error 0.23% test_error 0.19% epoch 1 nb_changes 24 train_error 0.07% test_error 0.00% epoch 2 nb_changes 10 train_error 0.06% test_error 0.05% epoch 3 nb_changes 6 train_error 0.03% test_error 0.14% epoch 4 nb_changes 5 train_error 0.03% test_error 0.14% epoch 5 nb_changes 4 train_error 0.02% test_error 0.14% epoch 6 nb_changes 3 train_error 0.01% test_error 0.14% epoch 8 nb_changes 2 train_error 0.00% test_error 0.14% epoch 8 nb_changes 0 train_error 0.00% test_error 0.14% epoch 8 nb_changes 0 train_error 0.00% test_error 0.14%

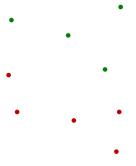
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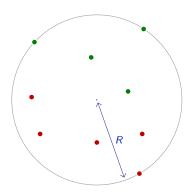
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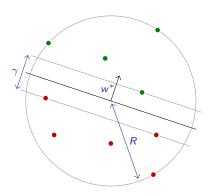


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- 1. The x_n are in a sphere of radius R:
 - $\exists R > 0, \ \forall n, \ \|x_n\| \leq R.$
- 2. The two populations can be separated with a margin $\gamma > 0$. $\exists w^*, \|w^*\| = 1, \exists \gamma > 0, \forall n, y_n(x_n \cdot w^*) \ge \gamma/2$.

To prove the convergence, let us make the assumption that there still is a misclassified sample at iteration k, and w^{k+1} is the weight vector updated with it. We have

$$w^{k+1} \cdot w^* = \left(w^k + y_{n_k} x_{n_k}\right) \cdot w^*$$

$$= w^k \cdot w^* + y_{n_k} \left(x_{n_k} \cdot w^*\right)$$

$$\geq w^k \cdot w^* + \gamma/2$$

$$\geq (k+1)\gamma/2.$$

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Since

$$||w^k|||w^*|| \ge w^k \cdot w^*,$$

we get

$$\|w^{k}\|^{2} \ge (w^{k} \cdot w^{*})^{2} / \|w^{*}\|^{2}$$

 $\ge k^{2} \gamma^{2} / 4.$

And

$$||w^{k+1}||^{2} = w^{k+1} \cdot w^{k+1}$$

$$= \left(w^{k} + y_{n_{k}} \times_{n_{k}}\right) \cdot \left(w^{k} + y_{n_{k}} \times_{n_{k}}\right)$$

$$= w^{k} \cdot w^{k} + 2 \underbrace{y_{n_{k}} w^{k} \cdot x_{n_{k}}}_{\leq 0} + \underbrace{\|x_{n_{k}}\|^{2}}_{\leq R^{2}}$$

$$\leq ||w^{k}||^{2} + R^{2}$$

$$\leq (k+1) R^{2}.$$

Putting these two results together, we get

$$k^2 \gamma^2 / 4 \le ||w^k||^2 \le k R^2$$

hence

$$k \leq 4R^2/\gamma^2$$
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hence no misclassified sample can remain after $\left\lfloor 4R^2/\gamma^2\right\rfloor$ iterations.

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This result makes sense:

- The bound does not change if the population is scaled, and
- the larger the margin, the more quickly the algorithm classifies all the samples correctly.

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Other algorithms maximize the distance of samples to the decision boundary, which improves robustness to noise.

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Support Vector Machines (SVM) achieve this by minimizing

$$\mathscr{L}(w,b) = \lambda ||w||^2 + \frac{1}{N} \sum_{n} \max(0, 1 - y_n(w \cdot x_n + b)),$$

which is convex and has a global optimum.

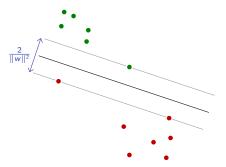
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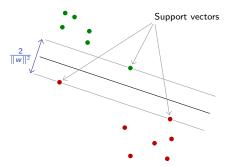


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Minimizing $\max(0, 1 - y_n(w \cdot x_n + b))$ pushes the *n*th sample beyond the plane $w \cdot x + b = y_n$, and minimizing $||w||^2$ increases the distance between the $w \cdot x + b = \pm 1$.

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At convergence, only a small number of samples matter, the "support vectors".

The term

$$\max(0, 1 - \alpha)$$

is the so called "hinge loss"





References

W. S. McCulloch and W. Pitts. A logical calculus of the ideas immanent in nervous activity.

F. Rosenblatt. The perceptron-A perceiving and recognizing automaton. Technical Report

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85-460-1, Cornell Aeronautical Laboratory, 1957.

EE-559 – Deep learning

3.2. Probabilistic view of a linear classifier

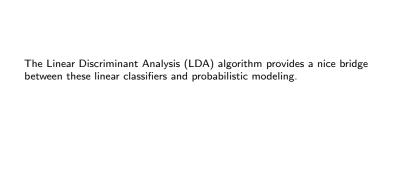
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The Linear Discriminant Analysis (LDA) algorithm provides a nice bridge between these linear classifiers and probabilistic modeling.

Consider the following class populations

$$\forall y \in \{0, 1\}, x \in \mathbb{R}^{D},$$

$$\mu_{X|Y=y}(x) = \frac{1}{\sqrt{(2\pi)^{D}|\Sigma|}} \exp\left(-\frac{1}{2}(x - m_{y})\Sigma^{-1}(x - m_{y})^{T}\right).$$

That is, they are Gaussian with the same covariance matrix Σ . This is the homoscedasticity assumption.

$$P(Y=1 \mid X=x)$$

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It follows that, with

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we get

$$P(Y = 1 \mid X = x) = \sigma \left(\log \frac{\mu_{X|Y=1}(x)}{\mu_{X|Y=0}(x)} + \log \frac{P(Y = 1)}{P(Y = 0)} \right).$$

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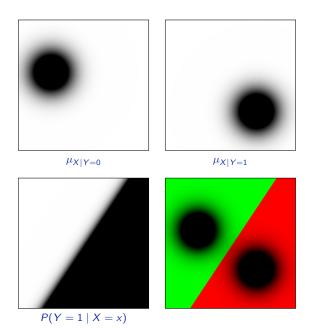
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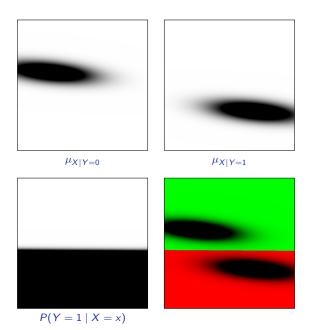
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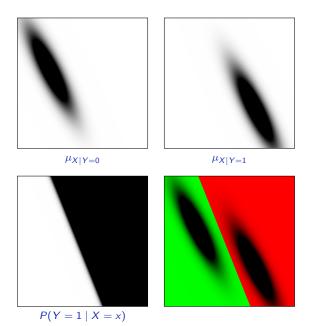
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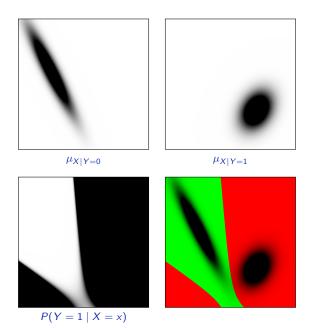
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The homoscedasticity makes the second-order terms vanish.





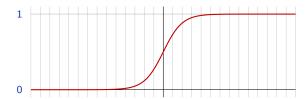




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$$\sigma(x) = \frac{1}{1 + e^{-x}},$$

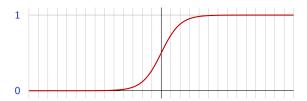
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looks like a "soft heavyside"



So the overall model

$$f(x; w, b) = \sigma(w \cdot x + b)$$

looks very similar to the perceptron.

We can use the model from LDA

$$f(x; w, b) = \sigma(w \cdot x + b)$$

but instead of modeling the densities and derive the values of w and b, directly compute them by maximizing their probability given the training data.

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but instead of modeling the densities and derive the values of w and b, directly compute them by maximizing their probability given the training data.

First, to simplify the next slide, note that we have

$$1 - \sigma(x) = 1 - \frac{1}{1 + e^{-x}} = \sigma(-x),$$

hence if Y takes value in $\{-1,1\}$ then

$$\forall y \in \{-1,1\}, \quad P(Y=y \mid X=x) = \sigma(y(w \cdot x + b)).$$

$$\log \mu_{W,B}(w,b \mid \mathcal{D} = \mathbf{d})$$

$$= \log \frac{\mu_{\mathcal{D}}(\mathbf{d} \mid W = w, B = b) \mu_{W,B}(w,b)}{\mu_{\mathcal{D}}(\mathbf{d})}$$

$$= \log \mu_{\mathcal{D}}(\mathbf{d} \mid W = w, B = b) + \log \mu_{W,B}(w,b) - \log Z$$

$$= \sum_{n} \log \sigma(y_n(w \cdot x_n + b)) + \log \mu_{W,B}(w,b) - \log Z'$$

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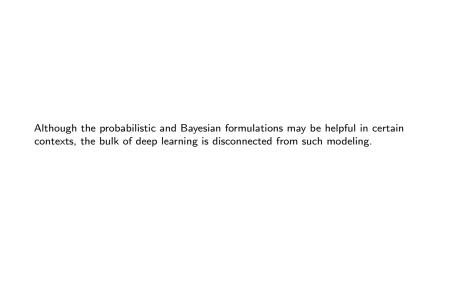
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$$= \sum_{n} \log \sigma(y_n(w \cdot x_n + b)) + \log \mu_{W,B}(w,b) - \log Z'$$

This is the logistic regression, whose loss aims at minimizing

$$-\log \sigma(y_n f(x_n)).$$





Although the probabilistic and Bayesian formulations may be helpful in certain contexts, the bulk of deep learning is disconnected from such modeling.

We will come back sometime to a probabilistic interpretation, but most of the methods will be envisioned from the signal-processing and optimization angles.



EE-559 - Deep learning

3.3. Linear separability and feature design

François Fleuret

https://fleuret.org/ee559/

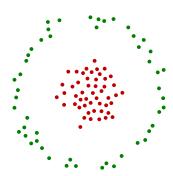
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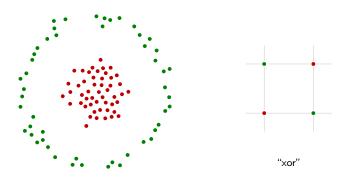


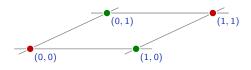
The main weakness of linear predictors is their lack of capacity. For classification, the populations have to be **linearly separable**.

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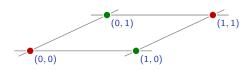


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$$\Phi: (x_u, x_v) \mapsto (x_u, x_v, x_u x_v).$$



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$$(1, 1, 1)$$

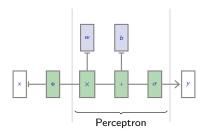
$$(0, 0, 0)$$

$$(1, 0, 0)$$

$$\Phi: (x_{u}, x_{v}) \mapsto (x_{u}, x_{v}, x_{u}x_{v}).$$

$$(1, 1, 1)$$

$$(0, 0, 0)$$



This is similar to the polynomial regression. If we have

$$\Phi: x \mapsto \left(1, x, x^2, \dots, x^D\right)$$

and

$$\alpha = (\alpha_0, \dots, \alpha_D)$$

then

$$\sum_{d=0}^{D} \alpha_d x^d = \alpha \cdot \Phi(x).$$

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and

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then

$$\sum_{d=0}^{D} \alpha_d x^d = \alpha \cdot \Phi(x).$$

By increasing D, we can approximate any continuous real function on a compact space (Stone-Weierstrass theorem).

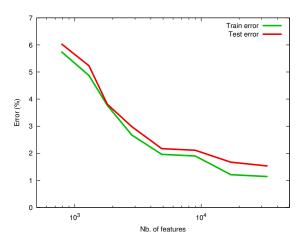
It means that we can make the capacity as high as we want.

We can apply the same to a more realistic binary classification problem: MNIST's "8" vs. the other classes with a perceptron.

The original 28×28 features are supplemented with the products of pairs of features taken at random.

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The original 28×28 features are supplemented with the products of pairs of features taken at random.



Remember the bias-variance tradeoff:

$$\mathbb{E}((Y-y)^2) = \underbrace{(\mathbb{E}(Y)-y)^2}_{\text{Bias}} + \underbrace{\mathbb{V}(Y)}_{\text{Variance}}.$$

The right class of models reduces the bias more and increases the variance less.

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Beside increasing capacity to reduce the bias, "feature design" may also be a way of reducing capacity without hurting the bias, or with improving it.

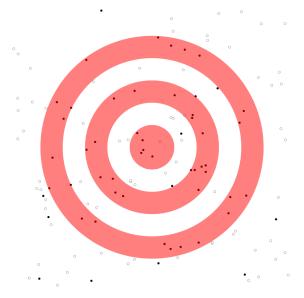
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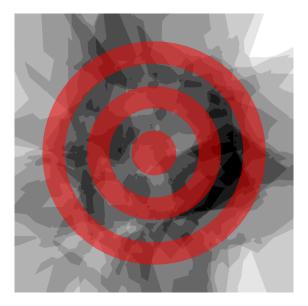
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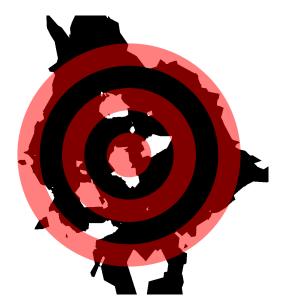
In particular, good features should be invariant to perturbations of the signal known to keep the value to predict unchanged.



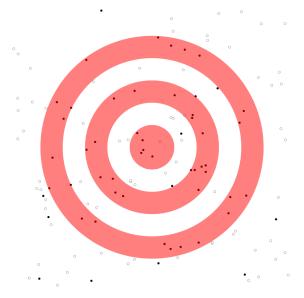
Training points



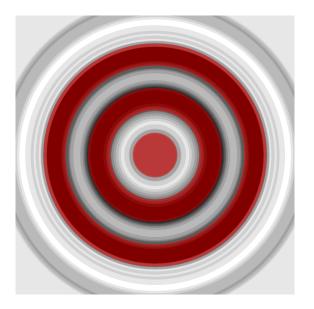
Votes (K=11)



Prediction (K=11)



Training points



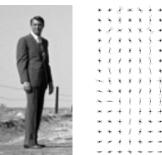
Votes, radial feature (K=11)



Prediction, radial feature (K=11)

A classical example is the "Histogram of Oriented Gradient" descriptors (HOG), initially designed for person detection.

Roughly: divide the image in 8×8 blocks, compute in each the distribution of edge orientations over 9 bins.



Dalal and Triggs (2005) combined them with a SVM, and Dollár et al. (2009) extended them with other modalities into the "channel features".

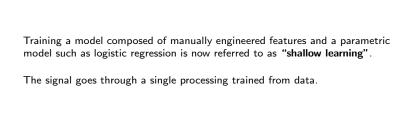
Many methods (perceptron, SVM, k-means, PCA, etc.) only require to compute $\kappa(x,x') = \Phi(x) \cdot \Phi(x')$ for any (x,x').

So one needs to specify κ alone, and may keep Φ undefined.

Many methods (perceptron, SVM, k-means, PCA, etc.) only require to compute $\kappa(x,x')=\Phi(x)\cdot\Phi(x')$ for any (x,x').

So one needs to specify κ alone, and may keep Φ undefined.

This is the kernel trick, which we will not talk about in this course.





References

Vision Conference, pages 91.1-91.11, 2009.

N. Dalal and B. Triggs. Histograms of oriented gradients for human detection. In Conference on Computer Vision and Pattern Recognition (CVPR), pages 886-893, 2005. P. Dollár, Z. Tu, P. Perona, and S. Belongie. Integral channel features. In British Machine

EE-559 - Deep learning

3.4. Multi-Layer Perceptrons

François Fleuret

https://fleuret.org/ee559/

Mon Feb 18 13:34:07 UTC 2019





So far we have seen linear classifiers of the form

$$\mathbb{R}^D \to \mathbb{R}$$
$$x \mapsto \sigma(w \cdot x + b),$$

with $w \in \mathbb{R}^D$, $b \in \mathbb{R}$, and $\sigma : \mathbb{R} \to \mathbb{R}$.

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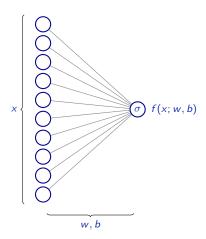
with $w \in \mathbb{R}^D$, $b \in \mathbb{R}$, and $\sigma : \mathbb{R} \to \mathbb{R}$.

This can naturally be extended to a multi-dimension output by applying a similar transformation to every output, which leads to

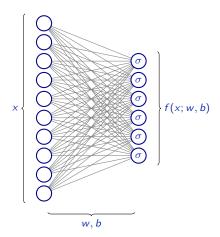
$$\mathbb{R}^D \to \mathbb{R}^C$$
$$x \mapsto \sigma(wx + b),$$

with $w \in \mathbb{R}^{C \times D}$, $b \in \mathbb{R}^C$, and σ is applied component-wise.

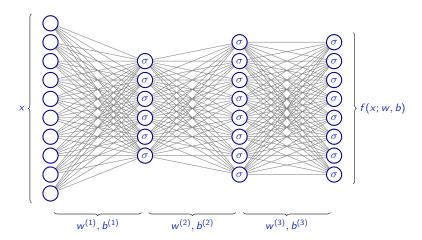
Even though it has no practical value implementation-wise, we can represent such a model as a combination of units, and extend it.



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This latter structure can be formally defined, with $x^{(0)} = x$,

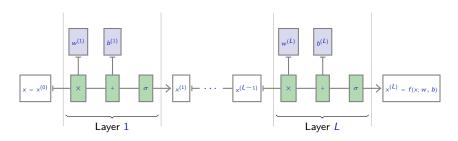
$$\forall l = 1, ..., L, \ x^{(l)} = \sigma \left(w^{(l)} x^{(l-1)} + b^{(l)} \right)$$

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

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

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



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

Note that if σ is an affine transformation, the full MLP is a composition of affine mappings, and itself an affine mapping.

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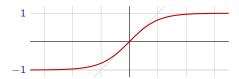
Consequently:



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

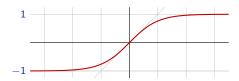
The two classical activation functions are the hyperbolic tangent

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



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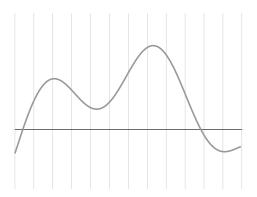


and the rectified linear unit (ReLU)

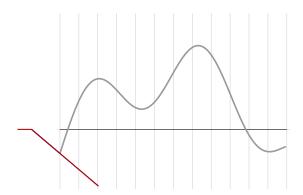
$$x \mapsto \max(0, x)$$



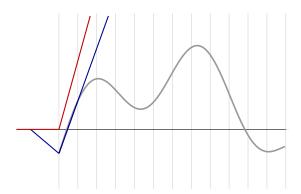
Universal approximation



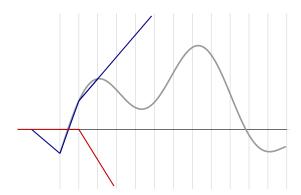
$$f(x) = \sigma(w_1 x + b_1)$$



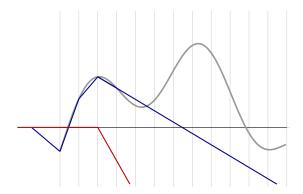
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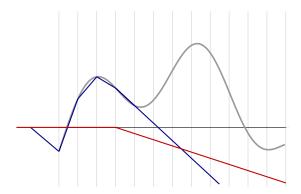
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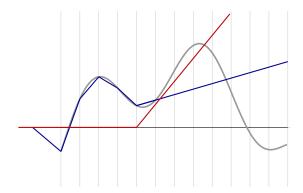
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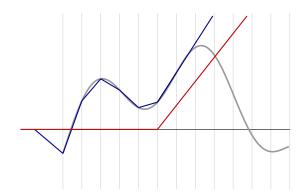
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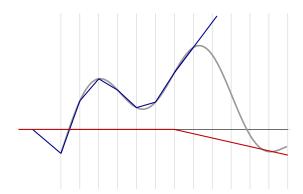
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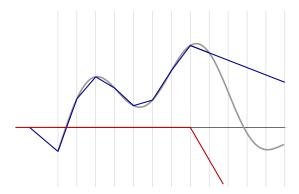
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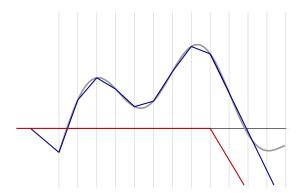
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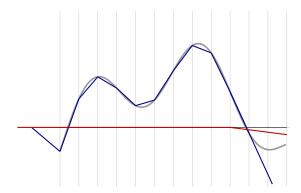
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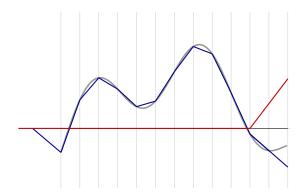
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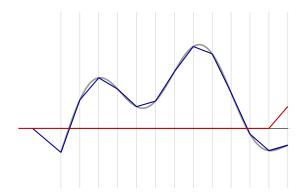
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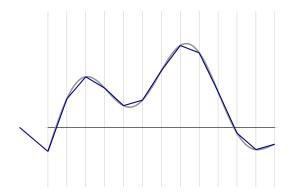
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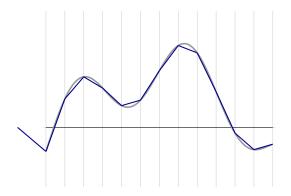
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This is true for other activation functions under mild assumptions.

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

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

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

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And the density of Fourier series provides

$$\begin{split} \forall \psi \in \mathscr{C}([0,1]^D,\mathbb{R}), \delta > 0, \exists M, (v_m,\gamma_m,c_m) \in \mathbb{R}^D \times \mathbb{R} \times \mathbb{R}, m = 1,\ldots,M, \\ \text{s.t.} \ \max_{x \in [0,1]^D} \left| \psi(x) - \sum_{m=1}^M \gamma_m \sin(v_m \cdot x + c_m) \right| \leq \delta. \end{split}$$

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

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

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

$$\left| \psi(x) - \sum_{m=1}^{M} \gamma_m \left(\sum_{n=1}^{N} \alpha_n \sigma(v_m \cdot x + c_m - a_n) \right) \right|$$

$$\leq \underbrace{\left| \psi(x) - \sum_{m=1}^{M} \gamma_m \sin(v_m \cdot x + c_m) \right|}_{\leq \frac{\xi}{2}}$$

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

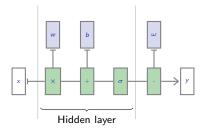
So we can approximate any continuous function

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

with a one hidden layer perceptron

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

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



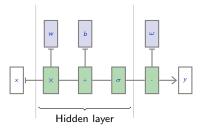
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This is the universal approximation theorem.

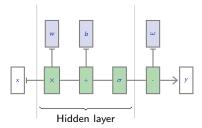
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This is the universal approximation theorem.



A better approximation requires a larger hidden layer (larger K), and this theorem says nothing about the relation between the two.



EE-559 – Deep learning

3.5. Gradient descent

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

$$\mathscr{L}(w,b) = \frac{1}{N} \sum_{n} (f(x_n; w, b) - y_n)^2.$$

Other losses are more fitting for classification, certain regression problems, or density estimation. We will come back to this.

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Other losses are more fitting for classification, certain regression problems, or density estimation. We will come back to this.

So far 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

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

which cannot be minimized analytically.

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

which cannot be minimized analytically.

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

Given a functional

$$f: \mathbb{R}^D \to \mathbb{R}$$

 $x \mapsto f(x_1, \dots, x_D),$

its gradient is the mapping

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

To minimize a functional

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

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

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

For $w_0 \in \mathbb{R}^D$, consider an approximation of \mathscr{L} around w_0

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

Note that the chosen quadratic term does not depend on \mathcal{L} .

To minimize a functional

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

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

For $w_0 \in \mathbb{R}^D$, consider an approximation of \mathscr{L} around w_0

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

Note that the chosen quadratic term does not depend on \mathcal{L} .

We have

$$abla ilde{\mathscr{L}}_{w_0}(w) = \nabla \mathscr{L}(w_0) + \frac{1}{n}(w - w_0),$$

which leads to

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

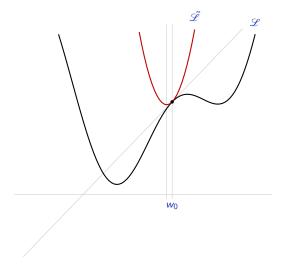
The resulting iterative rule, which goes to the minimum of the approximation at the current location, takes the form:

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

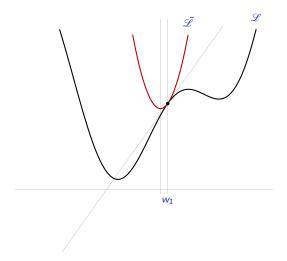
which corresponds intuitively to "following the steepest descent".

This [most of the time] eventually ends up in a **local** minimum, and the choices of w_0 and η are important.

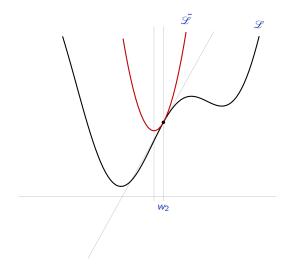




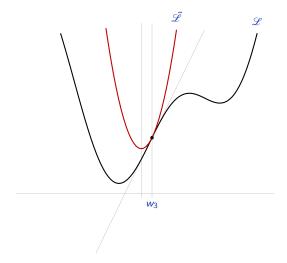




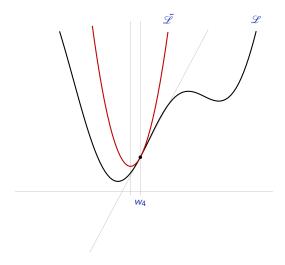




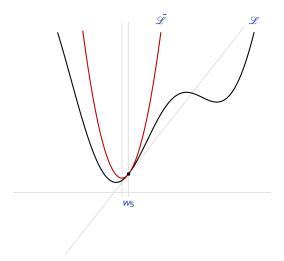




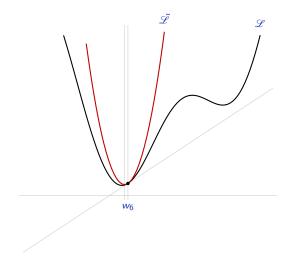




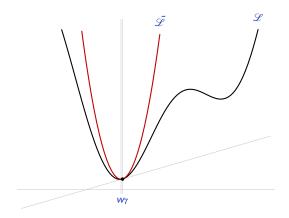




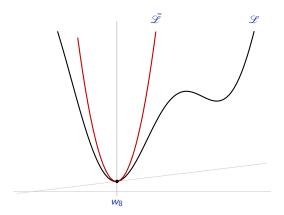




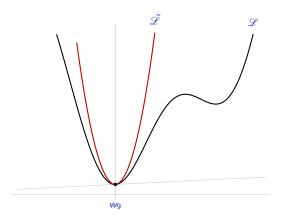




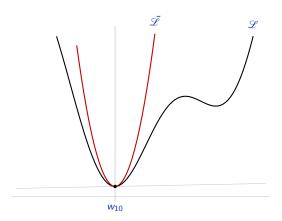




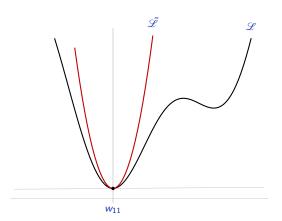




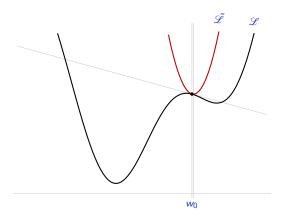




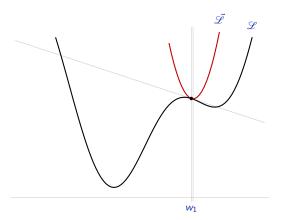




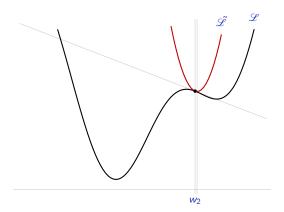




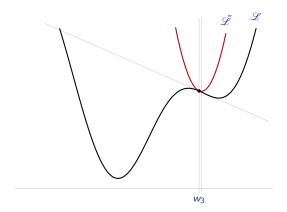




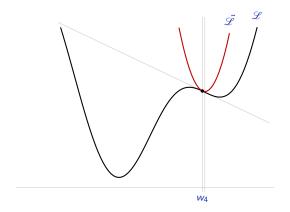




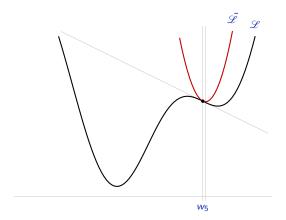




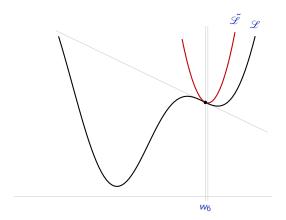




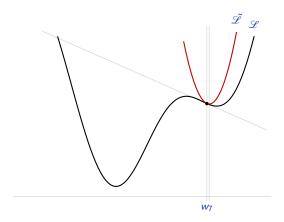




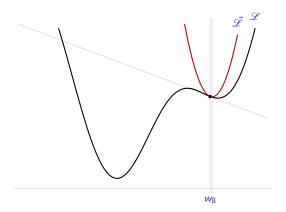




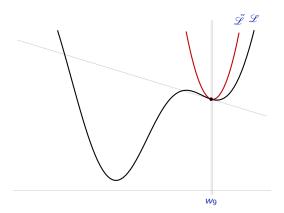




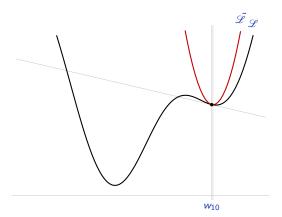




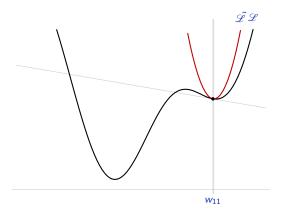




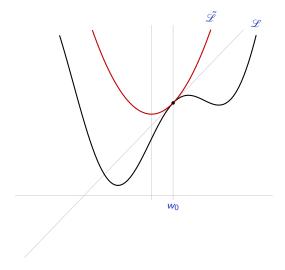




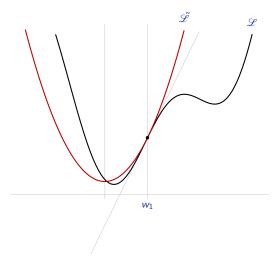




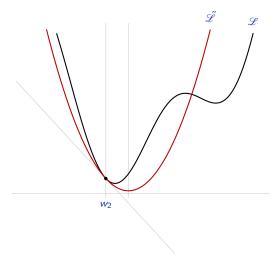




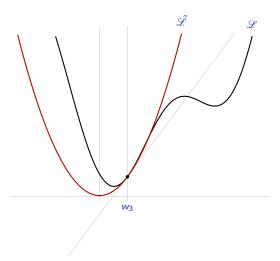




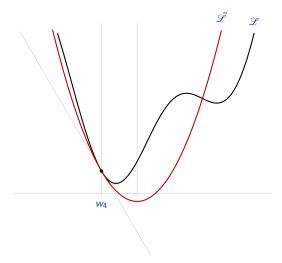




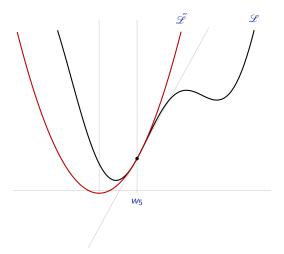




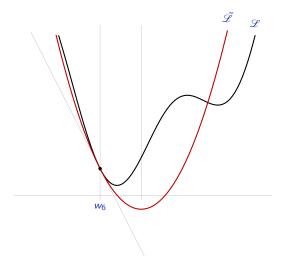




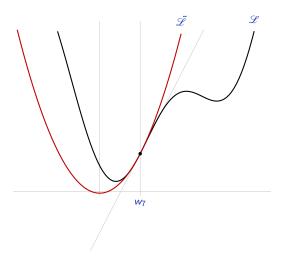




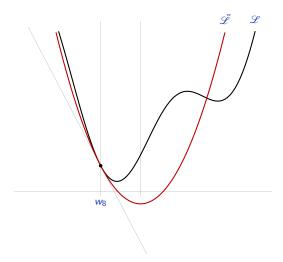




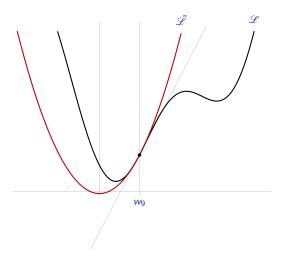




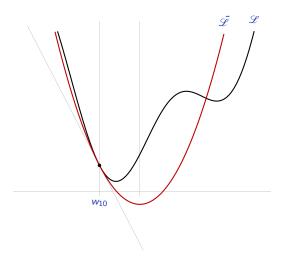




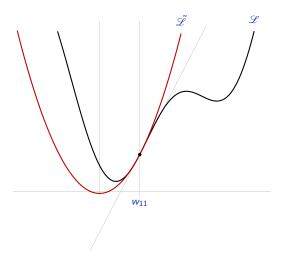


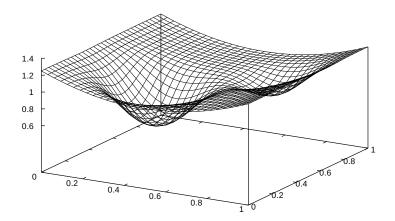


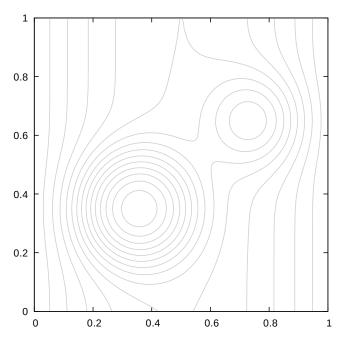




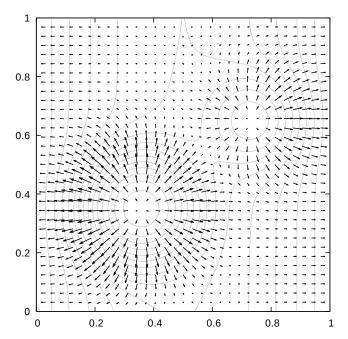


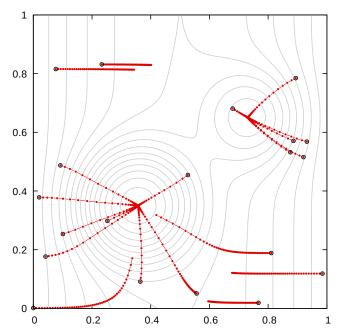






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We saw that the minimum of the logistic regression loss

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

does not have an analytic form.

We can derive

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{n} \underbrace{y_{n} \, \sigma(-y_{n}(w \cdot x_{n} + b))}_{u_{n}},$$

$$\forall d, \ \frac{\partial \mathcal{L}}{\partial w_{d}} = -\sum_{n} \underbrace{x_{n,d} \, y_{n} \, \sigma(-y_{n}(w \cdot x_{n} + b))}_{v_{n,d}},$$

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which can be implemented as

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

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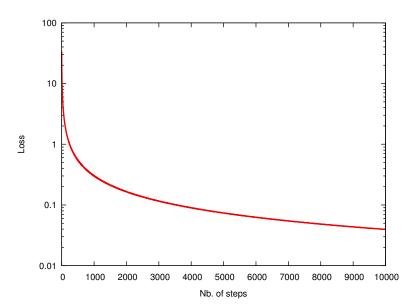
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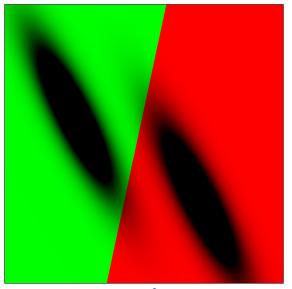
and the gradient descent as

```
w, b = torch.empty(x.size(1)).normal_(), 0
eta = 1e-1

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

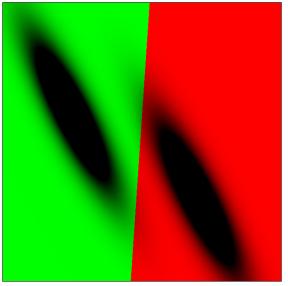


With 100 training points and $\eta = 10^{-1}$.



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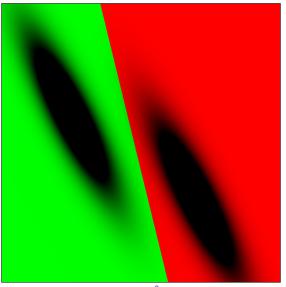
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n = 10

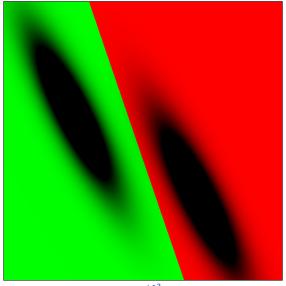
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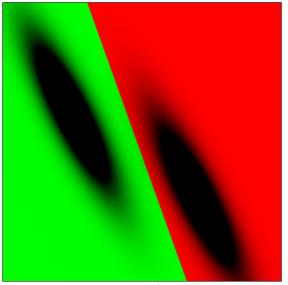
 $n = 10^2$

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

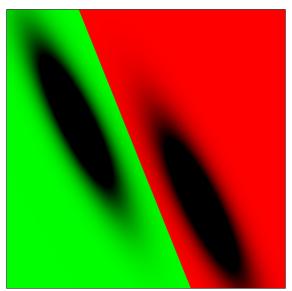


 $n = 10^3$

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



 $n = 10^4$



LDA



EE-559 - Deep learning

3.6. Back-propagation

François Fleuret

https://fleuret.org/ee559/

Shell escape disabled





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

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

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$$\mathscr{L}(w,b) = \sum_{n} \mathscr{E}(f(x_n; w, b), y_n).$$

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

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

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

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

For clarity, we consider a single training sample x, and introduce $s^{(1)}, \ldots, s^{(\ell)}$ 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 $x^{(0)} = x$.

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

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

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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

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

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.

$$\dots \xrightarrow{\sigma} \overset{\chi^{(l-1)}}{\underset{\longrightarrow}{w^{(l)},b^{(l)}}} \overset{w^{(l)},b^{(l)}}{\underset{\longrightarrow}{\sigma}} \overset{\sigma}{\underset{\longrightarrow}{s^{(l)}}} \xrightarrow{w^{(l+1)},b^{(l+1)}} s^{(l+1)} \xrightarrow{\sigma} \dots x^{(L)} \xrightarrow{\sigma} \ell$$

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

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

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

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

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

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

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

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

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

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

$$\frac{\partial \ell}{\partial w_{i:i}^{(I)}} = \frac{\partial \ell}{\partial s_{i:}^{(I)}} \frac{\partial s_{i}^{(I)}}{\partial w_{i:i}^{(I)}} = \frac{\partial \ell}{\partial s_{i:}^{(I)}} x_{j}^{(I-1)},$$

and similarly

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

$$\dots \xrightarrow{\sigma} \overset{(l-1)}{\underset{\sim}{x}} \xrightarrow{w^{(l)},b^{(l)}} \overset{s^{(l)}}{\underset{\sim}{\sigma}} \times \overset{\sigma}{\underset{\sim}{x}} \overset{(l)}{\underset{\sim}{w}} \xrightarrow{w^{(l+1)},b^{(l+1)}} \overset{\sigma}{\underset{\sim}{s}} \dots \overset{(l-1)}{\underset{\sim}{\sigma}} \xrightarrow{w^{(l)}} \overset{\sigma}{\underset{\sim}{s}} \dots \overset{(l)}{\underset{\sim}{s}} \to \mathscr{E}$$

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and similarly

$$\frac{\partial \ell}{\partial b_{:}^{(I)}} = \frac{\partial \ell}{\partial s_{:}^{(I)}}.$$

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

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

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

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

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

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

$$\frac{\partial \ell}{\partial s_{:}^{(l)}}$$

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

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

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

We have

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

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

$$\frac{\partial \ell}{\partial s_{\cdot}^{(l)}} = \frac{\partial \ell}{\partial x_{\cdot}^{(l)}} \frac{\partial x_{i}^{(l)}}{\partial s_{\cdot}^{(l)}} = \frac{\partial \ell}{\partial x_{\cdot}^{(l)}} \sigma' \left(s_{i}^{(l)}\right),$$

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

We have

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

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

$$\frac{\partial \ell}{\partial \mathbf{s}_{i}^{(l)}} = \frac{\partial \ell}{\partial \mathbf{x}_{i}^{(l)}} \frac{\partial \mathbf{x}_{i}^{(l)}}{\partial \mathbf{s}_{i}^{(l)}} = \frac{\partial \ell}{\partial \mathbf{x}_{i}^{(l)}} \sigma' \left(\mathbf{s}_{i}^{(l)} \right),$$

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

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

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

from the definition of ℓ

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

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

from the definition of ℓ , and $\forall l = 1, ..., L-1$, 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

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

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

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

from the definition of ℓ , and $\forall l = 1, ..., L-1$, 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

$$\frac{\partial \ell}{\partial x_{i}^{(l)}} = \sum_{h} \frac{\partial \ell}{\partial s_{h}^{(l+1)}} \frac{\partial s_{h}^{(l+1)}}{\partial x_{i}^{(l)}}$$

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

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

from the definition of ℓ , and $\forall l = 1, ..., L-1$, 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

$$\frac{\partial \ell}{\partial x_{\cdot}^{(l)}} = \sum_{h} \frac{\partial \ell}{\partial s_{h}^{(l+1)}} \frac{\partial s_{h}^{(l+1)}}{\partial x_{\cdot}^{(l)}} = \sum_{h} \frac{\partial \ell}{\partial s_{h}^{(l+1)}} w_{h,i}^{l+1}.$$

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

$$\begin{bmatrix} \frac{\partial \psi}{\partial x} \end{bmatrix} = \begin{pmatrix} \frac{\partial \psi_1}{\partial x_1} & \cdots & \frac{\partial \psi_1}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial \psi_M}{\partial x_1} & \cdots & \frac{\partial \psi_M}{\partial x_N} \end{pmatrix},$$

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

$$\begin{bmatrix} \frac{\partial \psi}{\partial w} \end{bmatrix} = \begin{pmatrix} \frac{\partial \psi}{\partial w_{1,1}} & \cdots & \frac{\partial \psi}{\partial w_{1,M}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \psi}{\partial w_{N,1}} & \cdots & \frac{\partial \psi}{\partial w_{N,M}} \end{pmatrix}.$$

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

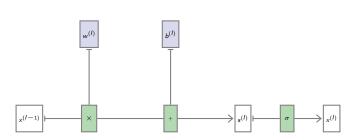
$$\begin{bmatrix} \frac{\partial \psi}{\partial x} \end{bmatrix} = \begin{pmatrix} \frac{\partial \psi_1}{\partial x_1} & \dots & \frac{\partial \psi_1}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial \psi_M}{\partial x_1} & \dots & \frac{\partial \psi_M}{\partial x_N} \end{pmatrix},$$

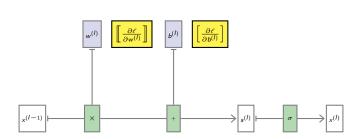
and if $\psi: \mathbb{R}^{N \times M} \to \mathbb{R}$, we will use the compact notation, also tensorial

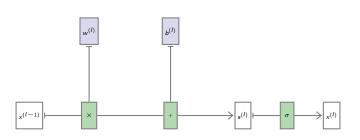
$$\begin{bmatrix}
\frac{\partial \psi}{\partial w}
\end{bmatrix} = \begin{pmatrix}
\frac{\partial \psi}{\partial w_{1,1}} & \cdots & \frac{\partial \psi}{\partial w_{1,M}} \\
\vdots & \ddots & \vdots \\
\frac{\partial \psi}{\partial w_{N,1}} & \cdots & \frac{\partial \psi}{\partial w_{N,M}}
\end{pmatrix}.$$

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

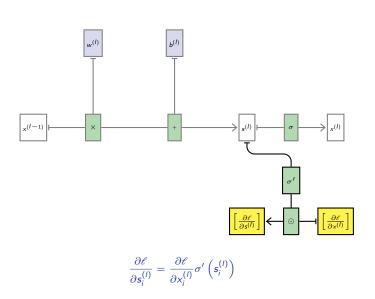
$$\left[\frac{\partial \ell}{\partial x^{(l)}}\right] = \nabla_{\!\! x^{(l)}} \ell \quad \left[\frac{\partial \ell}{\partial s^{(l)}}\right] = \nabla_{\!\! s^{(l)}} \ell \quad \left[\frac{\partial \ell}{\partial b^{(l)}}\right] = \nabla_{\!\! b^{(l)}} \ell \quad \left[\frac{\partial \ell}{\partial w^{(l)}}\right]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

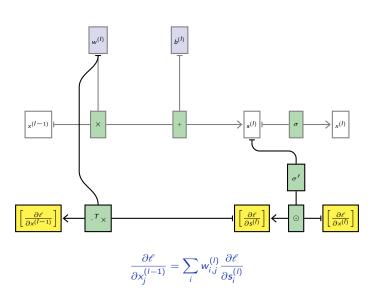


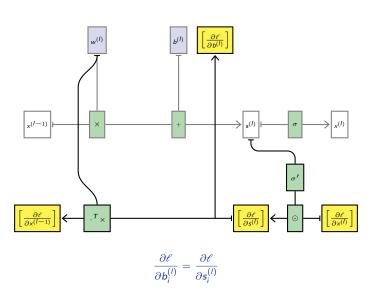


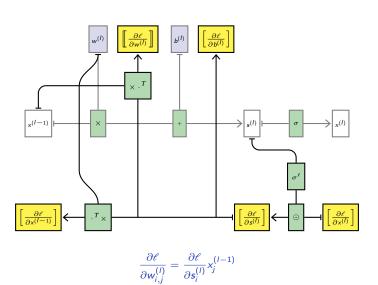


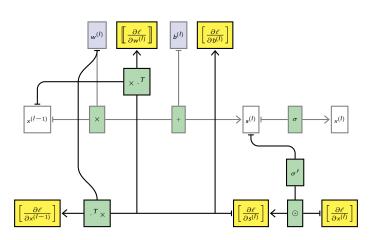
 $\left[\frac{\partial \ell}{\partial x^{(l)}}\right]$











Forward pass

Compute the activations.

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

Forward pass

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

Backward pass

Compute the derivatives of the loss wrt the activations.

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

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.

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

Backward pass

Compute the derivatives of the loss wrt the activations.

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

Compute the derivatives of the loss wrt the parameters.

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

Gradient step

Update the parameters.

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

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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

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

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

