INSTITUT NATIONAL DES SCIENCES APPLIQUÉES TOULOUSE

Machine Learning – 4A
Neural Networks

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Université Fédérale Toulouse Midi-Pyrénées

Section 1

Multi-layer perceptron (MLP)

Limitation of the perceptron

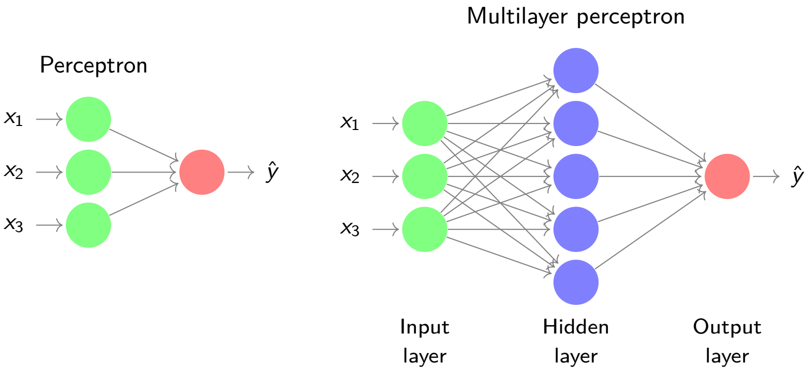
So far, we limited ourselves to functions of the form :

$$h_w(x) = w \cdot x \text{ or}$$
$$h'_w(x) = Logistic(w \cdot x)$$

Main limitations :

- each feature contributes to the output **independently of the others**.
- our hypothesis space is **linear**.

From one to multi-layers perceptron
Feedforward networks



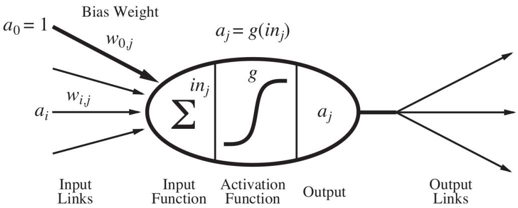
N.B. : some NN can feed their output (or intermediate results) back into their inputs $\Longrightarrow$ Recurrent Neural Networks (RNN).

Neural unit

A neural unit j has :

- an output a_j
- a weight $w_{i,j}$ for each unit i it takes as input
- an non-linear **activation function** g_j

$$a_j = g_j(\sum_i w_{i,j} \times a_i)$$



Common activation functions

- **logistic** or **sigmoid** function

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

- the **rectified linear unit** function (**ReLu**)

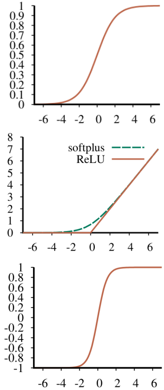
$$ReLU(z) = max(0, z)$$

- the **softplus** function

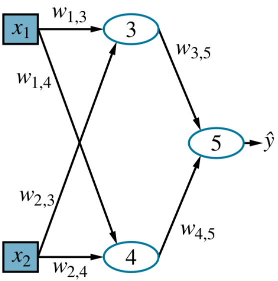
$$softplus(z) = log(1 + e^{z})$$

- the **tanh** function

$$tanh(z) = \frac{e^{2z} - 1}{e^{2z} + 1}$$



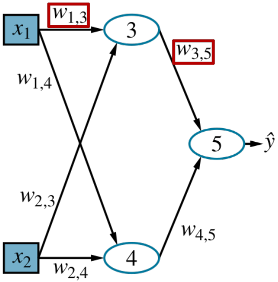
Neural network : training



$$\hat{y} = h_w(x) = g_5(w_{0,5} + w_{3,5}a_3 + w_{4,5}a_4)$$

where $a_3 = g_3(w_{0,3} + w_{1,3}x_1 + w_{2,3}x_2)$ and $a_4 = g_4(w_{0,4} + w_{1,4}x_1 + w_{2,4}x_2)$

Training network with $L2$-loss
Updating weights



$$\hat{y} = h_w(x) = g_5(in_5) \text{ with } in_5 = w_{0,5} + w_{3,5}a_3 + w_{4,5}a_4$$
$$a_3 = g_3(in_3) \text{ with } in_3 = w_{0,5} + w_{3,5}a_3 + w_{4,5}a_4$$
$$Loss(w) = \frac{1}{2}(y - \hat{y})^2$$

We remind that the weights are updated as :

$$w \leftarrow w - \alpha \times \vec{\nabla} Loss(w)$$

How to compute the gradients ? **Use the chain rule recursively !**

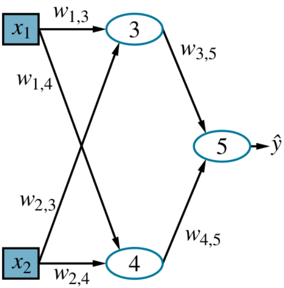
Output layer :

$$\frac{\partial Loss(w)}{\partial w_{3,5}} = \frac{\partial Loss(w)}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial in_5} \cdot \frac{\partial in_5}{\partial w_{3,5}} = -(y - \hat{y}).g_5'(in_5).a_3 = \Delta_5.a_3$$

Hidden layer :

$$\frac{\partial Loss(w)}{\partial w_{1,3}} = \frac{\partial Loss(w)}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial in_5} \cdot \frac{\partial in_5}{\partial a_3} \cdot \frac{\partial a_3}{\partial in_3} \cdot \frac{\partial in_3}{\partial w_{1,3}} = -(y - \hat{y}).g_5'(in_5).w_{3,5}.g_3'(in_3).x_1 = \Delta_3.x_1$$

Error associated to a particular node



In the output node (here 5), we say that the modified error is :

$$\Delta_5 = -(y - \hat{y}) \times g_5'(in_5)$$

The error contributed by a link $j \to k$ is :

$$g_j'(in_j) \times w_{j,k} \times \Delta_k$$

The error of a hidden unit j is the sum of its contribution to the errors in the next layer :

$$\Delta_j = g'(in_j) \sum_k w_{j,k} \Delta_k$$

Backpropagation

We can now define what's needed for a single iteration of gradient descent :

function $\textsc{Backprop-Iter}(E, \text{Network})$
  for each example $(x, y) \in E$ **do**
    for each node i in the input layer **do**
      $a_i \leftarrow x_i$
    for $\ell = 2$ to N **do**
      for each node j in layer ℓ **do**
        $in_j \leftarrow \sum_i w_{i,j} \times a_i$
        $a_j \leftarrow g_j(in_j)$

...
for each node j in the output layer **do**
  $\Delta_j \leftarrow g'(in_j) \times (y_j - a_j)$
for $\ell = N - 1$ to 1 **do**
  for each node i in layer ℓ **do**
    $\Delta_i \leftarrow g_i'(in_i) \sum_j w_{i,j} \Delta_j$
for each weight $w_{i,j}$ in the network **do**
  $w_{i,j} \leftarrow w_{i,j} - \alpha \times a_i \times \Delta_j$

Gradient descent

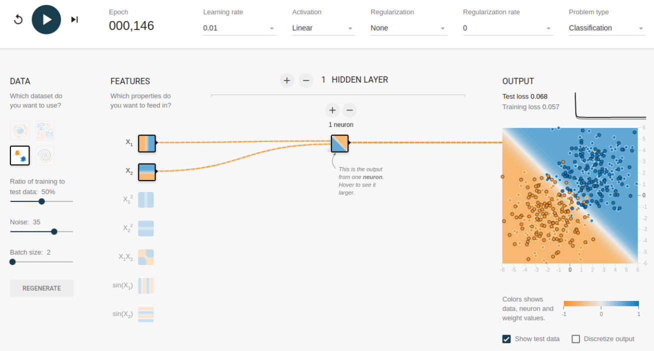
Network $\leftarrow$ neural network with initial weights
while not converged **do**
    BACKPROP-ITER(E, Network)

Remaining questions :

- how to choose the network structure ?
- how to initial the weights ? (critical in deep learning)

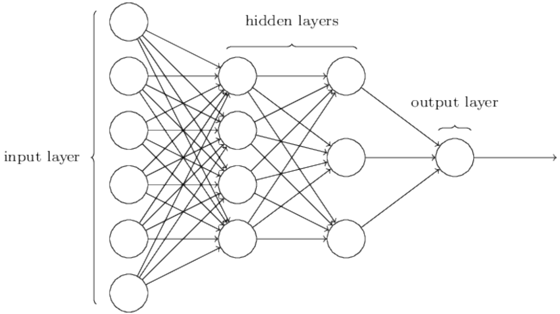
Tensorflow Playground

https://playground.tensorflow.org/



Network structure : MLP

A **multi-layer perceptron** is a network with **fully connected** hidden layers : each unit is connect to all unit of the previous layer.



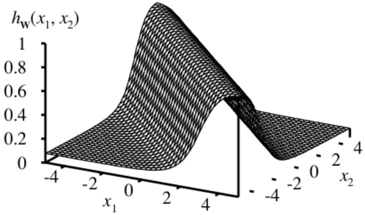
MLP : Universal approximators

*The **Universal Approximation Theorem** states that a neural network with 1 hidden layer can approximate any **continuous** function for inputs within a specific range.*

Caveats :

- The hidden layer might be arbitrary large
- If the function jumps around or has large gaps, we won't be able to approximate it.

Behind the universal approximation theorem



Combining two sigmoids produces a ridge, combining two ridges produce a bump

Beyond the MLP

There are many possible settings for a MLP :

- depth
- width
- connectivy (full/local)
- activation function (sigmoid/relu/tanh)

And there are even more network topologies beyond the MLP

To this day, choosing the right topology remains a difficult process based on experience and trial and error. [1]

1. This process is sometime called the "graduate student descent".

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Section 2

Learning Algorithms

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Gradient descent

Network $\leftarrow$ neural network with initial weights
while not converged **do**
    $\textsc{Backprop-Iter}(E, \text{Network})$

Problems :

- slow
- overfits
- requires the derivatives

Stochastic gradient descent

Problem :

- gradient computation is costly
  and increases with
  - number of weight
  - number of examples

$$O(|w| \times |E|)$$

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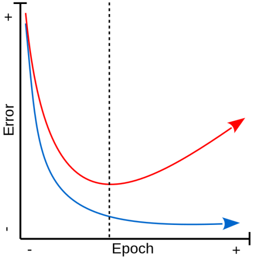
$$O(|w| \times |E|)$$

Solution : select a small subset of example on which to propagate the error

Network $\leftarrow$ neural network with initial weights
while not converged **do**
  $MiniBatch \leftarrow sample(E, k)$
  $\textsc{Backprop-Iter}(MiniBatch,$ Network$)$

This is called **stochastic gradient descent (SGD)** or **mini-batch gradient descent**.

Stopping criterion

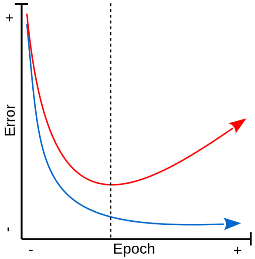


Error on training set (blue) and test set (red)

Problem :

- training tend to overfit the data

Stopping criterion



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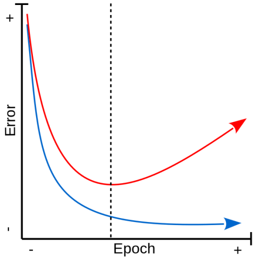
Stopping criterion



Error on training set (blue) and test set (red)

Problem :

- training tend to overfit the data
- we cannot touch the test data

Solution :

- in the training algorithm, reserve a small portion of the test data for internal **validation**
- do not use it for training
- stop when performance decreases on the validation set

The problem of differentiation

What's f'(z)

Symbolic differentiation (manual or computed) is not always possible/tractable as it can lead to very large computation graphs

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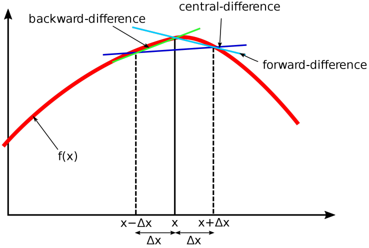
What's f'(z)

Symbolic differentiation (manual or computed) is not always possible/tractable as it can lead to very large computation graphs

However :

- we do **not** need to know f'
- we could compute $f'(z)$ on demand for the current z



Finite differences

Automatic differentiation

In practice, finite difference is too costly as it requires repeated evaluations for all parameters

Machine learning libraries (and in optimization tools in general) use **automatic differentiation (AD)**

Reverse mode AD computes, for a function f and a scalar z :

$$(f(z), f'(z))$$

with low overhead.

Key in enabling neural networks to be trained with complex and arbitrary functions. [2]

2. but beyond the scope of this course.

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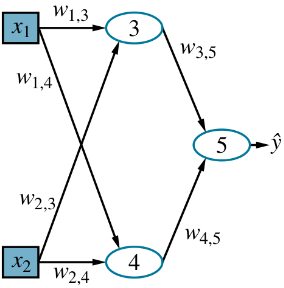
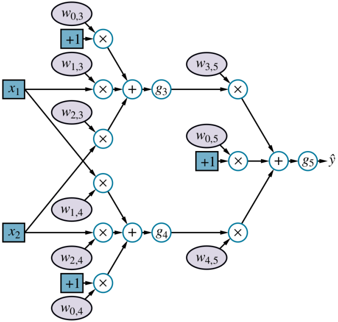
Automatic differentiation : computation graph





Section 3

Convolutional neural networks

Convolutional neural networks

Is there a left turn in the following images ?

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Convolution Kernel

$$input = \begin{bmatrix} x_1 & x_2 & x_3 \\ x_4 & x_5 & x_6 \\ x_7 & x_8 & x_9 \end{bmatrix}$$

$$kernel = \begin{bmatrix} w_1 & w_2 & w_3 \\ w_4 & w_5 & w_6 \\ w_7 & w_8 & w_9 \end{bmatrix}$$

$$f_w(x) = \sum_i w_i x_i$$

Kernel (manually defined)

$$kernel = \begin{bmatrix} -1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & -1 \end{bmatrix}$$

$$f_w(\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix}) = 3 \quad f_w(\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}) = 2 \quad f_w(\begin{bmatrix} 0 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix}) = 1 \quad f_w(\begin{bmatrix} 0 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 0 \end{bmatrix}) = 2$$

- When $f_w(x) = 3$ our kernel is able to detect a "right turn" in a 3x3 image. [4]
- Our kernel is essentially a neural unit (perceptron).
- The weights could be learned

4. It could be combined with an activation function to get an answer between 0 and 1.

Scaling up to 4x4

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 \end{bmatrix}$$

$$TL = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad TR = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$

$$BL = \begin{bmatrix} 0 & 1 & 1 \\ 0 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \quad BR = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}$$

Convolutional layer

Key idea : apply the convolutional unit to each 3x3 sub-images.

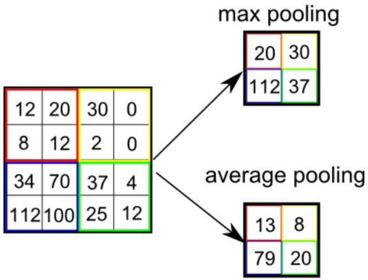
$$\begin{bmatrix} f_w(TL) & f_w(TR) \\ f_w(BL) & f_w(BR) \end{bmatrix} = \begin{bmatrix} 3 & -3 \\ -1 & -4 \end{bmatrix} = \begin{bmatrix} a_{17} & a_{18} \\ a_{19} & a_{20} \end{bmatrix}$$

Interpretation : there is a "right turn" in the top left corner, the rest is garbage.

Key insight :

- in this convolutional layer, we have 4 (2x2) output nodes
- each uses the **same** function, with the **same weights**
- the kernel is trained to detect a feature independently of its location in the source image

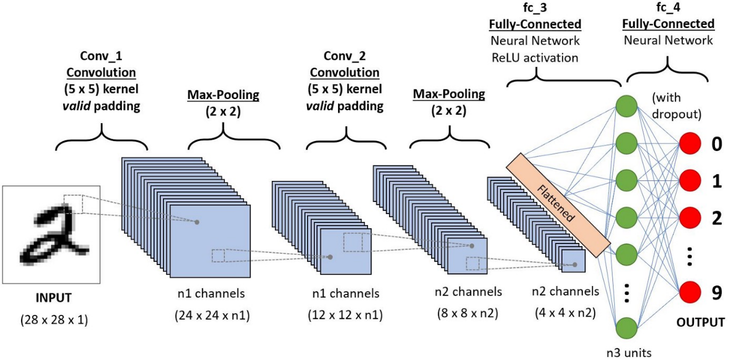
Pooling



2x2 pooling

- reduces dimensionality and variance
- suppresses the noise

A full network



Section 4

Conclusion

Subsection 1

History

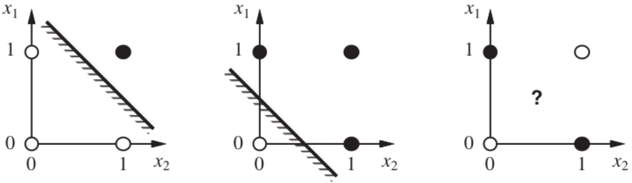
In the old days

- Least-square linear regression
  - Legendre (1805) and Gauss (1809)
  - Initially applied for the prediction of planetary movement

- 1958 : discovery of the **perceptron** and the associated **perceptron learning rule** by F. Rosenblatt

"The Navy revealed the embryo of an electronic computer today that it expects will be able to walk, talk, see, write, reproduce itself an be conscious of its existence . . . Dr. Frank Rosenblatt, a research psychologist at the Cornell Aeronautical Laboratory, Buffalo, said Perceptrons might be fired to the planets as mechanical space explorers"

The first AI winter



(a) x_1 **and** x_2 (b) x_1 **or** x_2 (c) x_1 **xor** x_2

- As noted by Marvin Minsky (Perceptrons)
  - we need to use MLPs even to represent simple nonlinear functions such as the XOR mapping
  - no one on earth had found a viable way to train MLPs good enough to learn such simple functions

Work restarts

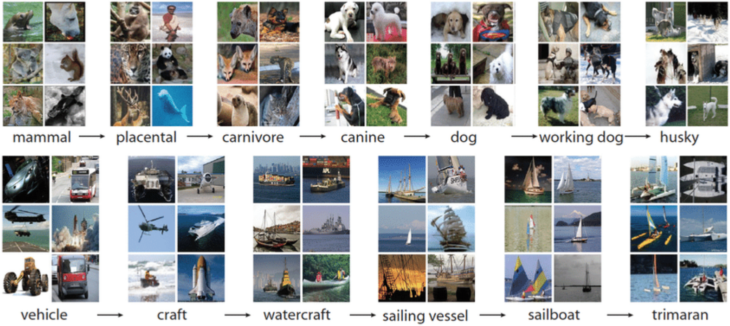
- 1982 J. Hopfield (a reknown physicist) advocates the use of neural networks
- 1986 : Rumelhart and McClelland apply the backpropagation algorithm to train **multi-layer neural networks**
- 1989 : universal approximatin theorem
- 1989 : first uses of the convolutional neural networks
- First success story : hand-written digit recognition [5]

5. LeCun et al. *Backpropagation Applied to Handwritten Zip Code Recognition (1989)*

Second winter (of neural networks)

- deep neural networks remain hard to train (vanishing gradient, weight initiallization)
- Support Vector Machines (SVM) dominate the machine learning world
- neural networks are undesirable (de facto excluded from AI conferences)

2009 ImageNet



15M images / 22 000 categories / 62 000 cats

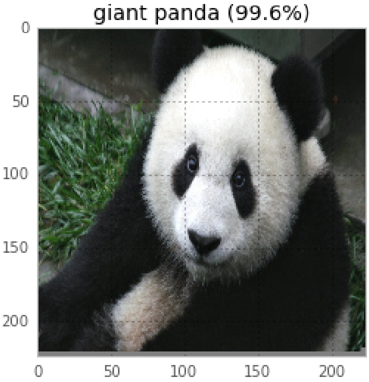
Early 2010s : the advent of deep learning

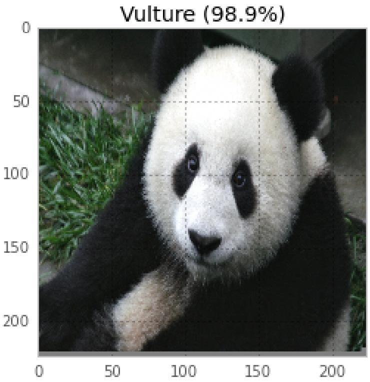
- Several breakthrough in the early 2010s :
  - weight initialization
  - Big Data
  - GPU
  - ReLU

- Deep neural networks become state of the art
  - 2012 : image classification [6]
  - 2015 : Natural language processing (NLP)

6. ImageNet Classification with Deep Convolutional Neural Networks (2012)

Some work left





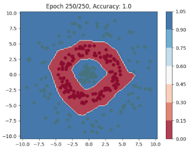
Subsection 2

In practice

How to use neural networks ?

Use existing libraries ! Also contains all elements to develop new machine learning methods (used in research) :

- Scikit-learn
- Keras + Tensorflow




```python
# Création du modèle de réseau de neurones
model = tf.keras.Sequential([
    tf.keras.layers.Dense(8, activation='relu', input_shape=(2,)),
    tf.keras.layers.Dense(8, activation='relu'),
    tf.keras.layers.Dense(2, activation='softmax')
])
# Compilation du modèle
model.compile(optimizer='adam', loss='categorical_crossentropy', metrics=['accuracy'])
# Entraînement sur data avec labels
model.fit(data, labels, epochs=250, verbose=0)
# Prédiction sur data_test
predicted_labels = model.predict(data_test)
```

To go further...

Introduction to Deep Learning : https://fidle.cnrs.fr/ / https://www.youtube.com/@CNRS-FIDLE