Introduction to Deep Learning

Machine Learning basics

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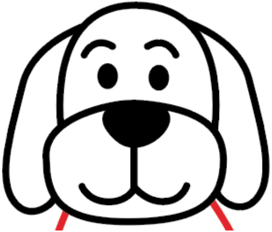
Outline

Outline

Starter: a “simple” question

What it is ?

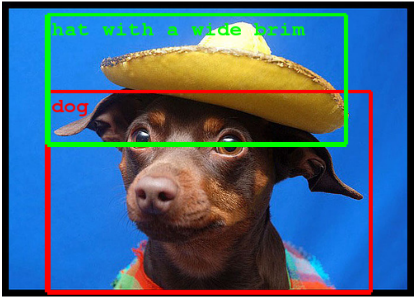


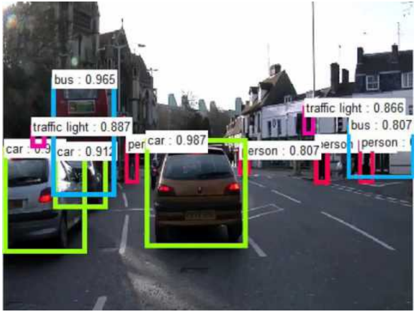
Can you write an algorithm to answer ?

- What is the input space ?
- What do you want to predict ?
- The output space ?

And more questions ?

Object detection



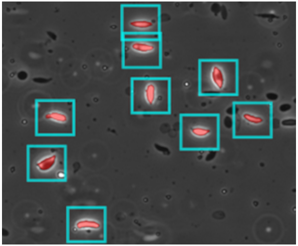


- A review: (Liu et al.2020)
- Real time detection in video, e.g Yolo (Redmon and Farhadi2018)

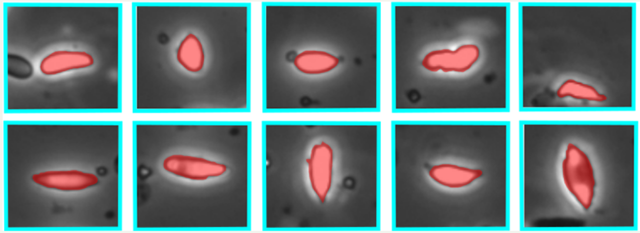
Cells classification / detection (Praljak et al.2020)

Red blood cell detection

- Images from a biochip (microfluidic assay)
- Detect and count sickle cells



Red Blood Cell classification



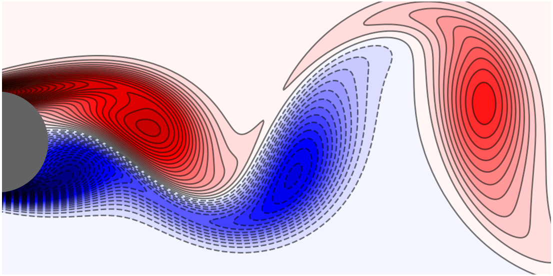
Sequence classification and generation

Classification

$$\boxed{\begin{array}{c} \text{A T C G A T T C} \\ \cdots \text{ G T A A T C G} \end{array}} \;:\; \mathbf{x} \in \mathbb{R}^D \longrightarrow c \in \{0,1\}$$

- Enhancer Identification in DNA Sequences (Min et al.2017; Cohn et al.2018)
- Predicting sequence specificities (Alipanahi et al.2015)

Generation



The "Machine Learning" way

How to make a 'computer' do a specific task?

Traditional approach (old AI)

A program is:

- hand-coded
- specific set of instructions to complete the task
- can be explained and proved, "always" gives the correct answer

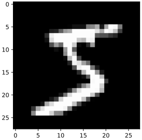
Machine Learning

A program is:

- trained or learnt
- from large amount of annotated data
- algorithm + inductive bias
- it works ... on average

Machine learning: the main tasks

Supervised classification



$$: \quad \mathbf{x} \in \mathbb{R}^{784} \longrightarrow c \in \{0, 1, 2, \ldots, 9\}$$

- $\mathcal{D} = (\mathbf{x}_{(i)}, c_{(i)})_{i=1}^{N}$
- **Supervised** learning of a **classification** task

Machine learning: the main tasks

Supervised binary classification or regression

my wonderful friend took me to see this movie for our anniversary. it was terrible.

$: \ \mathbf{x} \in \mathbb{R}^D \ \longrightarrow \ c \in \{0, 1\}$

- $\mathcal{D} = (\mathbf{x}_{(i)}, c_{(i)})_{i=1}^{N}$
- Supervised learning of a **binary** classification task

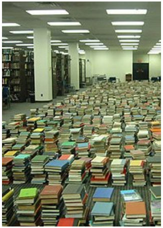
Supervised regression

$$\mathbf{x} \in \mathbb{R}^D \ \longrightarrow \ y \in \mathbb{R} \text{ (e.g } [0, 1]) \text{ or } \mathbf{y} \in \mathbb{R}^m$$

Machine learning: the main tasks

Unsupervised learning / Clustering

$\Longrightarrow$



$$\mathbf{x} \in \mathbb{R}^D \longrightarrow \boldsymbol{z} \in \mathbb{R}^M$$

- A set of observations $\mathcal{D} = (\mathbf{x}_{(i)})_{i=1}^N$ must be assigned to a cluster $\rightarrow z$
- The model infer a hidden/latent structure in the $\mathcal{D}$
- The *guidelines*: the structure of the model, the assumptions (distance, similarty between the $\mathbf{x}$, ...)
- Dimensionality reduction, data mining, ...

Overview in 3 ingredients

The NNet (in one equation)

$$\mathbf{y} = f_{\boldsymbol{\theta}}(\mathbf{x})$$

- $\mathbf{x}$ and $\mathbf{y}$ (structured, in high dimension, ...)
- $f_{\boldsymbol{\theta}}$ is the NNet
- $\boldsymbol{\theta}$ its parameters

The training dataset

$$\mathcal{D} = (\mathbf{x}_i, \mathbf{y}_i)_{i=1}^{N}$$

- For supervised learning
- N can (should be) large

Optimisation

$$\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}, \mathcal{D})$$

- Require time and tricks
- and GPUs !

The structure of f_θ

For image

- Matrices (one per channels) with a spatial structure
- Convolutional NNet

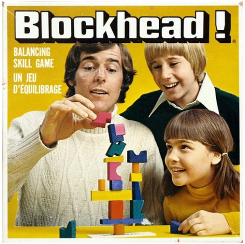
Sequence and time series

- Convolutional NNet (1D)
- Recurrent architectures, Transformers

Graph

- Graph convolutional NNet
- Graph Transformer based attention

A deep NNet:



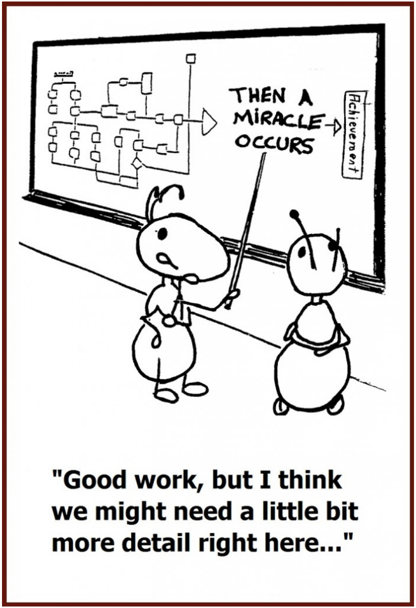
A success story

Since 2009, deep learning approaches won several challenges

- Image classification, object detection, ...
- Handwritting recognition since 2009
- Machine translation, Automatic Speech Recognition
- ...

But it started a bit earlier

- 1943: The artificial neuron by McCulloch & Pitts
- 1949: Hebb's rule for update
- 1958: Rosenblatt and the perceptron
- ...
- 2006: "Deep learning"
- 2018: "Transformers"


THEN A MIRACLE OCCURS
Achievement
"Good work, but I think we might need a little bit more detail right here..."

Outline

Outline of the course

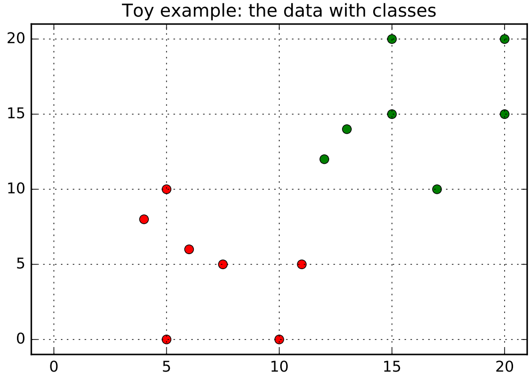
- Machine Learning Basics
- Feed-forward Neural Network: going deep
- Tools for deep-learning
- Convolution and Recurrent Nets
- Transformers

Outline

The A simple example: binary classification in 2D

The dataset $\mathcal{D}$

$$\mathcal{D} = \begin{pmatrix} x_1 = & 17 & 12 & 13 & 15 & 15 & 20 & 20 & 4 & 7.5 & 10 & 11 & 5 & 5 & 6 \\ x_2 = & 10 & 12 & 14 & 15 & 20 & 15 & 20 & 8 & 5 & 0 & 5 & 0 & 10 & 6 \\ c = & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$



Example of binary classification

Goal:

- Predict whether a candidate is hired ($c = 1$) or not ($c = 0$)
- knowing his results $\mathbf{x}$
- a candidate = 2 grades $\rightarrow \mathbf{x} = (x_1, x_2)$

The simplest model

$$c = 1 \text{ if } w_1 x_1 + w_2 x_2 > \alpha \text{ otherwise } c = 0$$
$$c = 1 \text{ if } w_0 + w_1 x_1 + w_2 x_2 > 0 \text{ otherwise } c = 0$$
$$c = 1 \text{ if } w_0 + \mathbf{w}^t \mathbf{x} > 0 \text{ otherwise } c = 0 \text{ (with } \mathbf{w} = (w_1, w_2))$$

Learning

- Given $\mathcal{D} = (\mathbf{x}_{(i)}, c_{(i)})_{i=1}^{n}$ find $\boldsymbol{\theta} = (w_0, \mathbf{w})$
- $c_{(i)}$ is the good answer (the supervision)

Binary classification or separation

- Given $\mathcal{D} = (\mathbf{x}_{(i)}, c_{(i)})_{i=1}^{n}$ find $\boldsymbol{\theta} = (w_0, \mathbf{w})$
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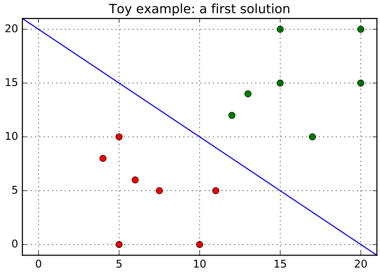

- $\boldsymbol{\theta}$ defines the separation
- $w_0 + \mathbf{w}^t\mathbf{x} = 0$: on the line
- $w_0 + \mathbf{w}^t\mathbf{x} > \mathbf{0}$ or $< \mathbf{0}$
- $\frac{w_0 + \mathbf{w}^t\mathbf{x}}{||\mathbf{w}||}$: the distance between the line and $\mathbf{x}$

Binary classification or separation

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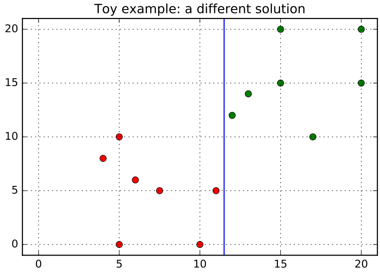

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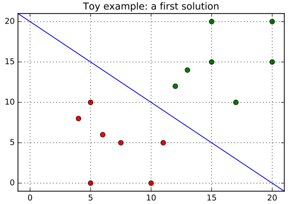
Regression or classification

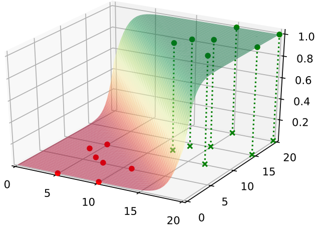
The class c is the outcome of the binary random variable C

$$y = P(C = 1|\mathbf{x}) = \sigma(w_0 + \mathbf{w}^t\mathbf{x})$$

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

$$a = w_0 + \mathbf{w}^t\mathbf{x}, a \in \mathbb{R}$$





Machine Learning

- Learn the parameters $\boldsymbol{\theta} = (w_0, \mathbf{w})$ from $\mathcal{D} = (\mathbf{x}_{(i)}, c_{(i)})_{i=1}^n$
- By minimizing a loss function ($a.k.a$ empirical risk)

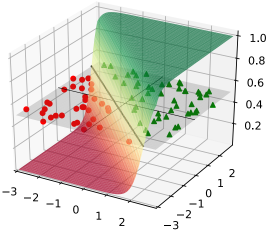
From Maximum-Likelihood to loss minimization

Given $\mathcal{D} = (\mathbf{x}_{(i)}, c_{(i)})_{i=1}^{n} = (\mathcal{X}, \tilde{\mathcal{C}})$ and a logistic regression model, $\boldsymbol{\theta} = (w_0, \mathbf{w})$.

Maximize the Log-Likelihood

$$\log P(\tilde{\mathcal{C}}|\mathcal{X}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \log P(C = c_{(i)}|\mathbf{x}_{(i)}, \boldsymbol{\theta})$$

$$= \sum_{i=1}^{n} \underbrace{c_{(i)} log(y_{(i)})}_{c_{(i)}=1} + \underbrace{(1 - c_{(i)}) log(1 - y_{(i)})}_{c_{(i)}=0}$$



Minimize the loss

$$\mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) = \frac{1}{N} \sum_{i=1}^{N} l(\boldsymbol{\theta}, \mathbf{x}_{(i)}, c_{(i)}), \text{ with}$$

$$l(\boldsymbol{\theta}, \mathbf{x}_{(i)}, c_{(i)}) = -c_{(i)} log(y_{(i)}) - (1 - c_{(i)}) log(1 - y_{(i)})$$

Optimization with Gradient Descent

Setup

$$\operatorname*{argmin}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) = \operatorname*{argmin}_{\boldsymbol{\theta}} \frac{1}{N} \sum_{i=1}^{N} l(\boldsymbol{\theta}, \mathbf{x}_{(i)}, c_{(i)})$$

This function is convex.

Gradient Descent

- Start with an initial value $\boldsymbol{\theta}^{(0)}$ and set $k = 1$
- Repeat until convergence:

$$\boldsymbol{\theta}^{(k)} = \boldsymbol{\theta}^{(k-1)} - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}), \text{ with}$$

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) = \frac{\partial \mathcal{L}(\boldsymbol{\theta}; \mathcal{D})}{\partial \boldsymbol{\theta}}$$

$$\eta > 0, \text{ the } \textit{learning rate} \text{ or } \textit{gradient step}$$

Very efficient (in time) with matrix-matrix operations

Bias or not bias

A matter of notation

The bias can be explicit:

$$w_0 + \mathbf{w}^t\mathbf{x} = w_0 + w_1 x_1 + \cdots + w_D x_D$$

or implicit:

$$\mathbf{w} \cdot \mathbf{x} = \begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \\ w_4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

$$= w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3 + w_4 x_4$$

Summary

Machine Learning overview

- A model defines a **function**: $\mathbf{x} \rightarrow \boldsymbol{y}$
- The output is then used by a decision rule.
- This function is defined by the parameters $\boldsymbol{\theta}$.
- **Training/Learning** finds the good values for $\boldsymbol{\theta}$
- How ? by minimizing a **loss function** $\mathcal{L}(\boldsymbol{\theta}; \mathcal{D})$.
- How ? by **Stochastic Gradient Descent**
- The **learning rate** is an **hyper-parameter**.

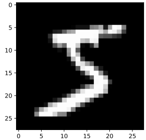
From logistic regression to artificial neurone

- An artificial neurone is a **linear model** followed by a non-linear **activation**
- With the sigmoid activation, it is similar to the **logistic regression**

Outline

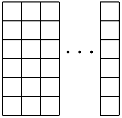
The MNIST dataset

The task



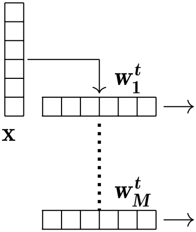
$\longrightarrow$  $\mathbf{x}_{(i)} \in \mathbb{R}^D, D = 784 \longrightarrow c_{(i)} \in \{0, 1, 2, \dots, 9\}$

The dataset

- $\mathcal{D} = (\mathbf{X}, \mathbf{c})$
- $\mathbf{X} =$  is a (D, N) matrix
- The labels $\mathbf{c}$ is $(N, 1)$
- $N = 50\ 000$

The model

From binary classification to a multiclass problem



$$y_1 = f(\mathbf{w_1}^t\mathbf{x})$$

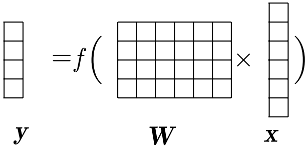
$$y_M = f(\mathbf{w_M}^t\mathbf{x})$$

$$y_k = f(a_k = \mathbf{w_k}^t\mathbf{x}) = P(C = k|\mathbf{x}, \boldsymbol{\theta})$$

$$= \frac{e^{a_k}}{\sum_{k'=1}^{M} e^{a_{k'}}} = \frac{e^{a_k}}{Z(\mathbf{x})}$$

$$\sum_{k=1}^{M} y_k = \sum_{k=1}^{M} P(c = k|\mathbf{x}) = 1$$

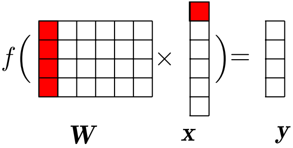
The matrix view



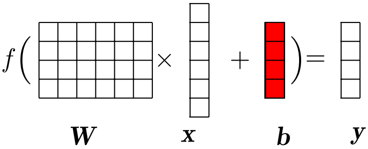
- $\mathbf{x} : (D, 1)$
- $\mathbf{W} : (M, D)$
- $\mathbf{y} : (M, 1)$

Bias or not bias

Implicit Bias



Explicit bias



Loss function

The parameters

$$\boldsymbol{\theta} = \mathbf{W}$$

The negative log-likelihood loss (or Cross-entropy)

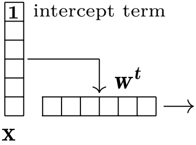
$$\mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) = -\sum_{i=1}^{N} \log P(C = c_{(i)} | \mathbf{x}_{(i)}, \boldsymbol{\theta})$$

(Mini-)Batch training

$$\mathbf{Y} = f(\mathbf{W} \times \mathbf{X}) \rightarrow \text{ inference for all the batch in once}$$

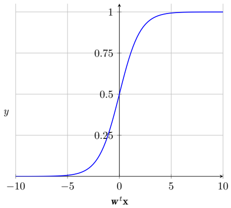
A choice of terminology

Logistic regression (binary classification)

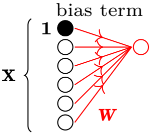


$\longrightarrow \quad y = f(\mathbf{w}^t\mathbf{x})$

$$f(a = \mathbf{w}^t\mathbf{x}) = \frac{e^a}{1+e^a} = \sigma(a)$$



A single artificial neuron

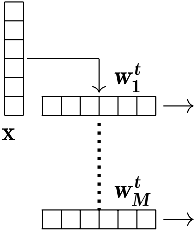


$y = f(\mathbf{w}^t\mathbf{x})$

- pre-activation : $a = \mathbf{w}^t\mathbf{x}$
- f: activation function
- Input values = input “neurones”
- $\mathbf{x}$: a vector of values, a layer

A choice of terminology - 2

From binary classification to M classes (Maxent)



$$y_1 = f(\mathbf{w_1}^t\mathbf{x})$$

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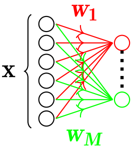
A simple neural network

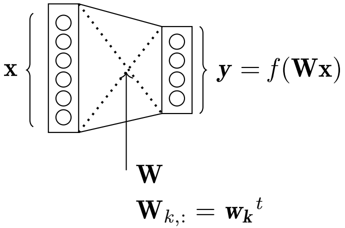


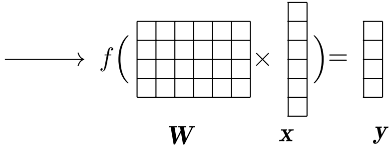
$$y_1 = f(\mathbf{w}_1^t\mathbf{x})$$

$$y_M = f(\mathbf{w}_M^t\mathbf{x})$$

- $\mathbf{x}$: *input layer*
- $\boldsymbol{y}$: *output layer*
- each y_k has its parameters $\boldsymbol{w}_k$
- f is the **softmax** function

Two layers fully connected





Activation f:

- f is usually a non-linear function
- f is a component wise function
- tanh, sigmoid, relu, ...

$e.g$ the softmax function:

Dimensions:

- $\mathbf{x} : D \times 1$
- $\boldsymbol{W} : M \times D$
- $\boldsymbol{y} : (M \times \cancel{D) \times (D} \times 1) = M \times 1$

$$y_k = P(c = k|\mathbf{x}) = \frac{e^{\boldsymbol{w_k}^t\mathbf{x}}}{\sum_{k'} e^{\boldsymbol{w_{k'}}^t\mathbf{x}}} = \frac{e^{\mathbf{W}_{k,:}\mathbf{x}}}{\sum_{k'} e^{\mathbf{W}_{k',:}\mathbf{x}}}$$

Classification with a simple and shallow network

Binary classification

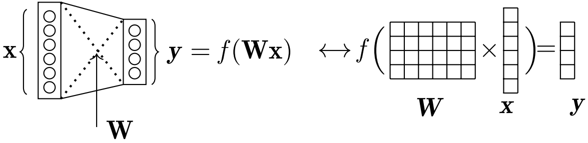
- The input layer is a vector ($\mathbf{x}$), it encodes the data
- A single output neuron transform $\mathbf{x}$, $\boldsymbol{w}$ are its parameters
- With a sigmoïd activation, the loss function is the binary cross entropy, the log-loss, minus the log-likelihood, ...

Multiclass

- The input layer is a vector ($\mathbf{x}$)
- The output layer $\mathbf{y}$ contains one neuron per class
- It transforms $\mathbf{x}$, $\mathbf{W}$ are the parameters of the output layer
- $\mathbf{W}$ gathers the $\boldsymbol{w}_k = \mathbf{W}_{k,:}$
- With a softmax activation, the loss function is the cross entropy, the log-loss, minus the log-likelihood, ...

Other loss functions exist for classification

Two layers fully connected: another view

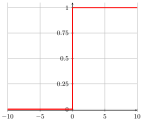


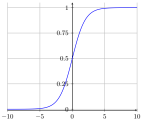
This basic brick implements a transformation of $\mathbf{x}$ in $\boldsymbol{y} = f(\mathbf{Wx})$:

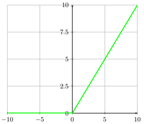
- A linear transformation $\mathbf{Wx}$
- Followed by a non-linear function

Example: a candidate made 6 interviews $\rightarrow \mathbf{x} \in \mathbb{R}^6$

- First compute 4 new scores : $\mathbf{Wx} \in \mathbb{R}^4$, each is a linear combination of $\mathbf{x}$
- Apply a non-linearity to get $\boldsymbol{y}$

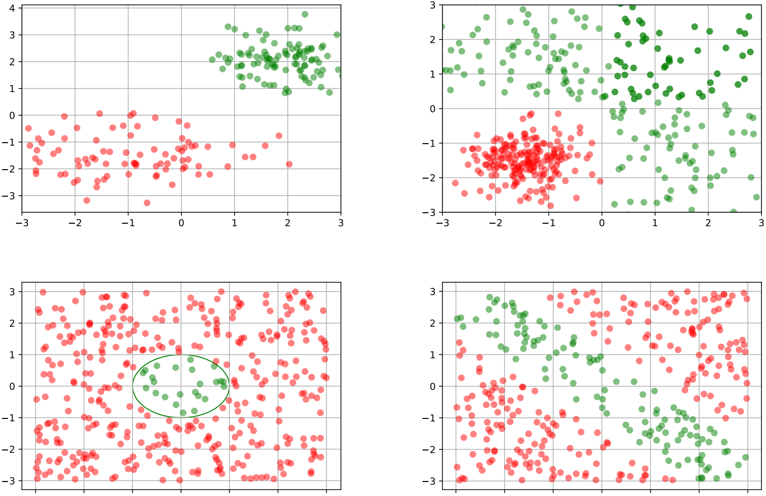






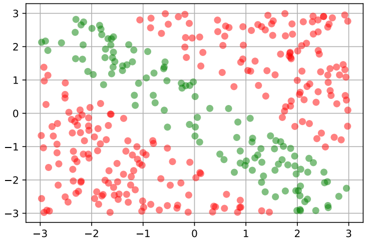
Outline

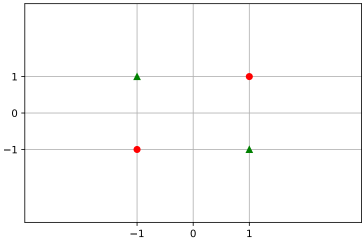
Limits of the linear separation



Case study : X-or

Starting point



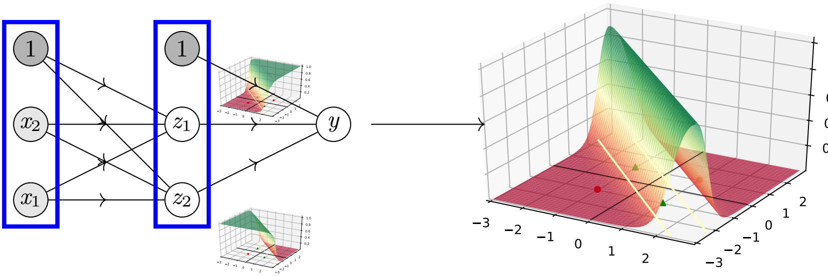


Hint

Try two linear separations instead of one !

A first neural network

The multi-layer architecture



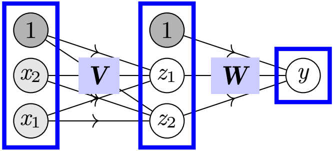
- The network is organized by layers: input ($\mathbf{x}$), hidden ($\mathbf{z}$), and output ($\mathbf{y}$)
- Two layers are fully connected
- The propagation of the input is sequential:

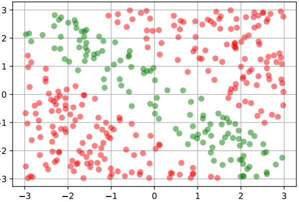
$$z_1 = g(\mathbf{v}_1^t\mathbf{x}) \text{ and } z_2 = g(\mathbf{v}_2^t\mathbf{x})) \qquad \Rightarrow \boldsymbol{z} = g(\boldsymbol{V}\mathbf{x})$$

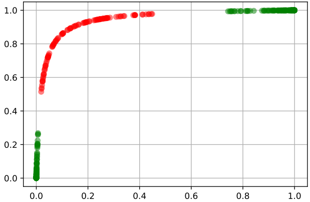
$$y = f(\mathbf{w}^t\boldsymbol{z}) \qquad \Rightarrow y = f(\boldsymbol{W}\boldsymbol{z})$$

Another view of the neural network

Representation learning







- The network learns its own representation $\boldsymbol{z}$.
- The final decision is linear.

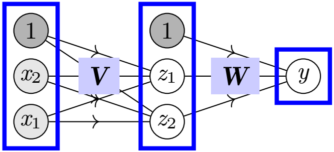
Summary

The multi-layer or feed-forward architecture

- 1 neuron = 1 value; 1 layer = 1 vector
- Two layers $(\boldsymbol{x}, \boldsymbol{z})$ fully connected:

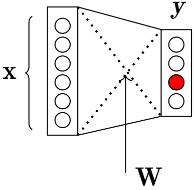
$$\boldsymbol{z} = g(\boldsymbol{V}\boldsymbol{x})$$

- Inference: a sequential propagation
- Hidden layer $(\boldsymbol{z})$: the internal representation



Outline

For a shallow network, with a single layer



$\boldsymbol{y} = f(\mathbf{W}\mathbf{x})$

$y_k = P(c = k|\mathbf{x})$

$\boldsymbol{\theta} = (\mathbf{W})$

Forward (inference) ↑		Backward (gradient) ↓
$l(\boldsymbol{\theta}, \mathbf{x}_{(i)}, c_{(i)})$	$\leftarrow \boldsymbol{y}$	$\dfrac{\partial l(\boldsymbol{\theta}, \mathbf{x}_{(i)}, c_{(i)})}{\partial \mathbf{W}} = \dfrac{\partial l(\boldsymbol{\theta}, \mathbf{x}_{(i)}, c_{(i)})}{\partial \boldsymbol{y}}$
$\boldsymbol{y}$	$= f(\boldsymbol{a})$	$\times \dfrac{\partial \boldsymbol{y}}{\partial \boldsymbol{a}}$
$\boldsymbol{a}$	$= \mathbf{W}\mathbf{x}$	$\times \dfrac{\partial \boldsymbol{a}}{\partial \mathbf{W}}$

Review of the gradient computation

Without hidden layer (shallow net)

l is the shortcut for $l(c_{(i)}, \mathbf{x}_{(i)}, \boldsymbol{\theta}_{(i)})$

$$\frac{\partial l}{\partial \mathbf{W}} = \frac{\partial l}{\partial y_{(i)}} \times \frac{\partial y_{(i)}}{\partial \mathbf{a}} \times \frac{\partial \mathbf{a}}{\partial \mathbf{W}}$$

Supervision

loss *vs* output

activation

gradient of **W**

Error signal from supervision and output

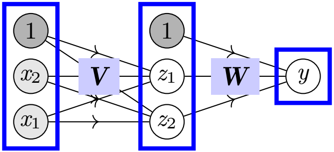
Contribution of **W** $\rightarrow \mathbf{x}$

In the matrix form

$$
\begin{aligned}
\nabla_{\mathbf{W}} = \frac{\partial l}{\partial \mathbf{W}} &= \frac{\partial l}{\partial y_{(i)}} \times \frac{\partial y_{(i)}}{\partial \mathbf{a}} \times \frac{\partial \mathbf{a}}{\partial \mathbf{W}} \\
&= \boldsymbol{\delta}_{\mathbf{W}} \times \mathbf{x}^t \\
&= (M, 1) \times (1, D) \\
&= \text{Gradient up to the pre-activation} \times \text{input of the layer}
\end{aligned}
$$

- $\nabla_{\mathbf{W}}$ is a matrix of size (M, D)
- $\nabla_{\mathbf{W}}[i, j] = \boldsymbol{\delta}[i] \times \mathbf{x}[j]$

Gradient computation with one hidden layer



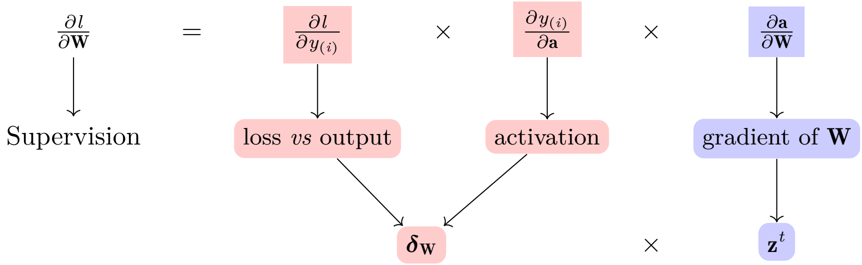
- $\boldsymbol{b} = \boldsymbol{V}\mathbf{x}$
- $\boldsymbol{z} = g(\boldsymbol{b})$
- $\boldsymbol{a} = \boldsymbol{W}\mathbf{z}$
- $\boldsymbol{y} = f(\boldsymbol{a})$

Two questions (or gradients):

- $\frac{\partial l}{\partial \mathbf{W}} = \ ?$
- $\frac{\partial l}{\partial \mathbf{V}} = \ ?$

Gradient computation with one hidden layer

Step 1: **W**



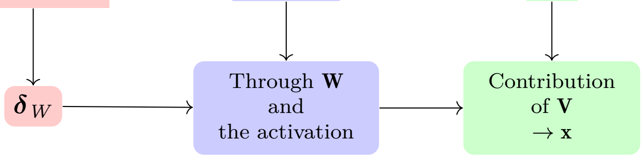
- Very similar to the shallow network, but the “input” is $\mathbf{z}$ instead of $\mathbf{x}$
- But $\mathbf{z}$ is computed by the network (parameters $\mathbf{V}$)

Gradient computation with one hidden layer

Step 2 : $\mathbf{V}$

Denote the pre-activation of the input layer $\mathbf{b} = \mathbf{V}\mathbf{x}$

$$\frac{\partial l}{\partial \mathbf{V}} = \frac{\partial l}{\partial y_{(i)}} \times \frac{\partial y_{(i)}}{\partial \mathbf{a}} \times \frac{\partial \mathbf{a}}{\partial \mathbf{z}} \times \frac{\partial \mathbf{z}}{\partial \mathbf{b}} \times \frac{\partial \mathbf{b}}{\partial \mathbf{V}}$$



- The error signal $\boldsymbol{\delta}_W$ is back-propagated through $\mathbf{W}$,
- to get $\boldsymbol{\delta}_V$
- The update for $\mathbf{V}$ is $\nabla_{\mathbf{V}} = \boldsymbol{\delta}_V \mathbf{x}^t$

The back-propagation algorithm for a feed-forward network with one hidden layer

Introduced in (Rumelhart et al.1986)

One iteration of the online version, for a given value of $\boldsymbol{\theta}$:

1. Foward propagation of $\mathbf{x}_{(i)}$ ($\rightarrow$ $\mathbf{z}$ and $\mathbf{y}_{(i)}$)
2. Compute the loss
3. Back-propagation and collect of the gradients:
   - output layer: $\boldsymbol{\delta}_W$ and $\nabla_{\mathbf{W}} = \boldsymbol{\delta}_W \mathbf{z}^t$
   - input layer: $\boldsymbol{\delta}_V$ and $\nabla_{\mathbf{V}} = \boldsymbol{\delta}_V \mathbf{x}^t$
4. Update parameters:

$$\mathbf{W} = \mathbf{W} - \eta \nabla_{\mathbf{W}}$$
$$\mathbf{V} = \mathbf{V} - \eta \nabla_{\mathbf{V}}$$

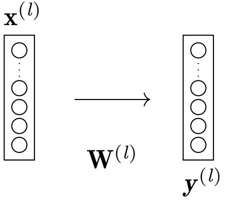
One training iteration: forward and backward propagation

Forward	Backward	
$\boldsymbol{b} = \boldsymbol{V}\mathbf{x}$	$\dfrac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$	$\rightarrow \dfrac{\partial l}{\partial \boldsymbol{b}} \dfrac{\partial \mathbf{b}}{\partial \boldsymbol{V}}$
$\downarrow$	$\uparrow$	
$\boldsymbol{z} = g(\boldsymbol{b})$	$\dfrac{\partial \mathbf{a}}{\partial \boldsymbol{z}}$	
$\downarrow$	$\uparrow$	
$\boldsymbol{a} = \boldsymbol{W}\mathbf{z}$	$\dfrac{\partial y_{(i)}}{\partial \mathbf{a}}$	$\rightarrow \dfrac{\partial l}{\partial \mathbf{a}} \dfrac{\partial \mathbf{a}}{\partial \boldsymbol{W}}$
$\downarrow$	$\uparrow$	
$\boldsymbol{y} = f(\boldsymbol{a})$	$\dfrac{\partial l}{\partial y_{(i)}}$	
$\searrow$	$\nearrow$	

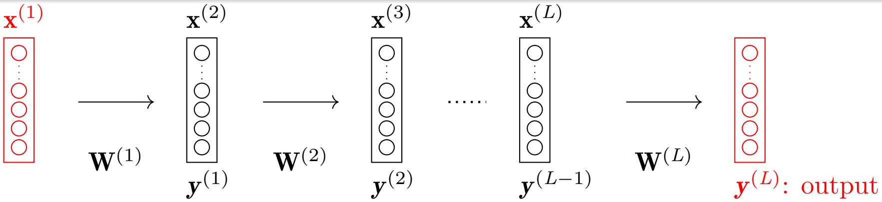
$$l$$

Notations for a multi-layer neural network (feed-forward)

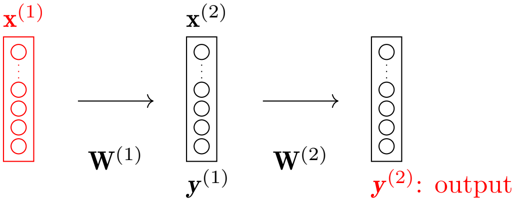
One layer, indexed by l



- $\mathbf{x}^{(l)}$: input of the layer l
- $\boldsymbol{y}^{(l)} = f^{(l)}(\mathbf{W}^{(l)}\ \mathbf{x}^{(l)})$
- stacking layers: $\boldsymbol{y}^{(l)} = \mathbf{x}^{(l+1)}$
- $\mathbf{x}^{(1)}$ = a data example



Example : with one hidden layer



$$\boldsymbol{\theta} = (\mathbf{W}^{(1)}, \mathbf{W}^{(2)})$$

To learn, we need the gradients for:

- the output layer: $\nabla_{\mathbf{W}^{(2)}}$
- the hidden layer: $\nabla_{\mathbf{W}^{(1)}}$

Back-propagation: generalization

For a hidden layer l:

- The gradient at the pre-activation level:

$$\boldsymbol{\delta}^{(l)} = f'^{(l)}(\mathbf{a}^{(l)}) \circ \left(\mathbf{W}^{(l+1)}{}^{t} \boldsymbol{\delta}^{(l+1)}\right)$$

- The update is as follows:

$$\mathbf{W}^{(l)} = \mathbf{W}^{(l)} - \eta_t \boldsymbol{\delta}^{(l)} \mathbf{x}^{(l)}{}^{t}$$

The layer should keep:

- $\mathbf{W}^{(l)}$: the parameters
- $f^{(l)}$: its activation function
- $\mathbf{x}^{(l)}$: its input
- $\mathbf{a}^{(l)}$: its pre-activation associated to the input
- $\boldsymbol{\delta}^{(l)}$: for the update and the back-propagation to the layer $l-1$

Back-propagation: one training step

Pick a training example: $\mathbf{x}^{(1)} = \mathbf{x}_{(i)}$

Forward pass

For $l = 1$ to $(L-1)$

- Compute $\boldsymbol{y}^{(l)} = f^{(l)}(\mathbf{W}^{(l)}\mathbf{x}^{(l)})$
- $\mathbf{x}^{(l+1)} = \boldsymbol{y}^{(l)}$

$\boldsymbol{y}^{(L)} = f^{(L)}(\mathbf{W}^{(L)}\mathbf{x}^{(L)})$

Backward pass

Init: $\boldsymbol{\delta}^{(L)} = \nabla_{\boldsymbol{a}^{(L)}}$
For $l = L$ to 2 // all hidden units

- $\boldsymbol{\delta}^{(l-1)} = f'^{(l-1)}(\boldsymbol{a}^{(l-1)}) \circ \left(\mathbf{W}^{(l)^t}\boldsymbol{\delta}^{(l)}\right)$
- $\mathbf{W}^{(l)} = \mathbf{W}^{(l)} - \eta_t \boldsymbol{\delta}^{(l)}\mathbf{x}^{(l)^t}$

$\mathbf{W}^{(1)} = \mathbf{W}^{(1)} - \eta_t \boldsymbol{\delta}^{(1)}\mathbf{x}^{(1)^t}$

Conclusion on back-propagation for one layer l

Training a NNet relies on forward-backward propagation.

Forward:

- get $\mathbf{x}^{(l)}$ for the previous layer;
- compute and send $\boldsymbol{y}^{(l)} = f^{(l)}(\mathbf{W}^{(l)}\mathbf{x}^{(l)})$.

Backward:

- get $\boldsymbol{\delta}^{(l)}$ as input from the up-coming layer;
- compute and send $\boldsymbol{\delta}^{(l-1)}$ to the previous layer;
- update parameters $\mathbf{W}^{(l)}$

Outline

Summary

Multi-layered Perceptron (MLP) or feed-forward NNet

- Artificial neurons are organizes in **layers**: $\rightarrow$ a vector
- Two layers are in general **fully connected**
  - A linear transformation parametrized by a matrix
  - followed by a pointwise non-linear function, the activation function
- A **feed-forward** architecture is a stack of layers fully connected

$\rightarrow$ Can approximate any functions depending on the number of hidden units.

Training by back-propagation

- After a forward pass (inference from input to the output)
- Backward pass (compute the gradients of each layer from the output to the input)

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