## Introduction to Neural Networks and Deep Learning

Roberto Basili, Danilo Croce Machine Learning, Web Mining \& Retrieval 2020/2021

## Outline

- 2020-21 Course Structure
- Background: from the Statistical Learning Theory to Deep Learning
- Representation and Architectures for Neural Learning
- Convolutional NNs
- Their use in Image Processing and Sentiment Analysis
- Recurrent NeuralNetworks: Long Short Term Memories
- Autoencoders and Language Modeling: embeddings
- Introduction to Transformers
- Laboratory of NN design \& Programming


## Syllabus

- (13/5) From Statistical Learning to Deep learning
- (17/5) Convolutional Networks for Image Processing
- (19/5) Laboratory: Programming neural learners
- (20/5) Recurrent Neural Networks
- $(24 / 5)$ Neural Language Modeling
- $(26 / 5)$ Laboratory: Designing Convolutional Networks in Python
- (27/5) Encoder-Decoder Networks: Transformers
- (31/5) Designing Recurrent Networks for streaming analytics


## Introduction to DL: Outline

- An Al perspective on DL: from Statistical Learning Theory to Deep Learning
- Representation Learning in Deep Learning Architectures
- MLP and non linearity
- History and types of NNs:
- Multilayer Perceptrons
- Autoencoders
- Convolutional NNs
- Recurrent Neural Networks: Long Short Term Memories
- Attentive networks
- Training a Neural Network
- Stochastic Gradient Descent
- The Backpropagation algorithm


## Artificial Intelligence: the pendulum

- "A physical symbol system has the necessary and sufficient means for general intelligent action.
- Symbols are Luminiferous Aether of Al
--Allen Newell \& Herbert Simon



## Neural Networks, Connectionism and Deep Learning


from Goodfellow et al., DL MIT book
very high level representation:
MAN SITTING ...
$\uparrow$
... etc ...
A
slightly higher level representation


## Show \& Tell in italiano

## Current work at UniTV (Croce, Masotti \& Basili,


(a) im2txt+translation: Un gioca-(b) im2txt+translation: Una tore di baseball che oscilla una grande torre dell'orologio che mazza ad una sfera, Italian model: sovrasta una città, Italian model: Un Un giocatore di baseball che tiene grande edificio con un orologio sulla una mazza da baseball su un campo. parte superiore.

(c)
dil dei cht t , uomo che cavalca uno skateboard su una strada.

## A bit of history ...

[- McCollouch \& Pitts 1943 - The logic of the MCP ( $\approx$ Perceptron), through early electronics

- Hebb 1942 - Associative Memories: adaptive storage
- Rosenblatt, 1958 - Perceptron \& on-line learning algorithm
- Minsky \& Papert, 1969 - mathematical limits of the perceptron
- Rumelhart et al., 1986, McClelland et al., 1995 Backpropagation, Distributed representations
- LSTSMs -Hochreiter \& Schmidhuber 1997
- Le Cun et al., 1998-Convolutional Nets
- Hinton et al., 2006 - Deep Belief nets (autoencoders)
- Bengio et al., 2007 - Depth vs. Breadth in NNs
- Nair \& Hinton, 2010 - further training support (e.g. RLU)

- Hinton, 2012 - Dropout

Table 1: Major milestones that will be covered in this paper

| Year | Contributer | Contribution |
| :---: | :---: | :---: |
| 300 BC | Aristotle | introduced Associationism, started the history of human's attempt to understand brain. |
| 1873 | Alexander Bain | introduced Neural Groupings as the earliest models of neural network, inspired Hebbian Learning Rule. |
| 1943 | McCulloch \& Pitts | introduced MCP Model, which is considered as the ancestor of Artificial Neural Model. |
| 1949 | Donald Hebb | considered as the father of neural networks, introduced Hebbian Learning Rule, which lays the foundation of modern neural network. |
| 1958 | Frank Rosenblatt | introduced the first perceptron, which highly resembles modern perceptron. |
| 1974 | Paul Werbos | introduced Backpropagation |
| 1980 | Teuvo Kohonen | introduced Self Organizing Map |
|  | Kunihiko Fukushima | introduced Neocogitron, which inspired Convolutional Neural Network |
| 1982 | John Hopfield | introduced Hopfield Network |
| 1985 | Hilton \& Sejnowski | introduced Boltzmann Machine |
| 1986 | Paul Smolensky | introduced Harmonium, which is later known as Restricted Boltzmann Machine |
|  | Michael I. Jordan | defined and introduced Recurrent Neural Network |
| 1990 | Yann LeCun | introduced LeNet, showed the possibility of deep neural networks in practice |
| 1997 | Schuster \& Paliwal | introduced Bidirectional Recurrent Neural Network |
|  | Hochreiter \& Schmidhuber | introduced LSTM, solved the problem of vanishing gradient in recurrent neural networks |
| 2006 | Geoffrey Hinton | introduced Deep Belief Networks, also introduced layer-wise pretraining technique, opened current deep learning era. |
| 2009 | Salakhutdinov \& Hinton | introduced Deep Boltzmann Machines |
| 2012 | Geoffrey Hinton | introduced Dropout, an efficient way of training neural networks |

## Connections per Neuron


from Goodfellow et al., DL MIT book

## (Vector) Spaces, Functions and Learning



## Structural risk minimization: example



$4^{\text {th }}$ order polynomial

$2^{\text {nd }}$ order polynomial

$8^{t h}$ order polynomial
$y=f^{*}(\vec{x})$
$f^{*}(\vec{x}) \approx h(\vec{x})=g(\vec{x} ; \vec{\theta})$
such that $\forall \vec{x}_{l} \in \mathrm{~L} \quad h\left(\vec{x}_{l}\right) \approx y_{l}$

## Machine Learning: in search of good functions

- Model and Learning

$$
\begin{aligned}
& y=f^{*}(\vec{x}) \\
& f^{*}(\vec{x}) \approx h(\vec{x})=g(\vec{x} ; \vec{\theta}) \\
& \quad \text { such that } \forall \vec{x}_{l} \in \mathrm{~L} \quad h\left(\vec{x}_{l}\right) \approx y_{l}
\end{aligned}
$$

- Linear models

$$
h(\vec{x})=g\left(\sum_{n} \theta_{n} x_{n}+b\right)
$$



## Support Vector Machines

- Support Vector Machines (SVMs) are a machine learning paradigm based on the statistical learning theory [Vapnik, 1995]
- No need to remember everything, just the discriminating instances (i.e. the support vectors, SV)
- The classifier corresponds to the linear combination of SVS



## Linear classifiers and separability

- In a R2 space, 3 point can always be separable by a linear classifier
- but 4 points cannot always be shattered [Vapnik and Chervonenkis(1971)]
- One solution could be a more complex classifier
- Risk of over-fitting



## Linear classifiers and separability (2)

- ... but things change when projecting instances in a higher dimension feature space through a function $\phi$
- IDEA: It is better to have a more complex feature space instead of a more complex function



## SVM First Advantage: making examples linearly separable

- Mapping data in a (richer) feature space where linear separability holds $\vec{x} \rightarrow \Phi(\vec{x})$
(attributes $\rightarrow$ features)



## Perceptron (Rosenblatt, 1958)

- Linear Classifier mimicking a neuron



## The role of Representation

Cartesian coordinates


X

Polar coordinates

$r$

The quintessential example of a representation learning algorithm is the autoencoder. An autoencoder is the combination of an encoder function, which converts the input data into a different representation, and a decoder function, which converts the new representation back into the original format. Autoencoders

## Representation and Learning: the role of depth



## Adding Layers ...

- From simple linear laws ...

$$
h(\vec{x})=g(\vec{x} ; \vec{\theta}, b)=g\left(\sum_{n} \theta_{n} x_{n}+b\right)
$$



- to feedforward structures. It can be made dependent on a sequence of functions $g(1)$ and $g(2), \ldots, g(k)$, that give rise to a structured hypothesis:

$$
\begin{aligned}
h(\vec{x}) & =g^{(2)}\left(g^{(1)}\left(\stackrel{\bar{x}}{ } ; \vec{\theta}^{(1)}, b^{(1)}\right) ; \vec{\theta}^{(2)}, b^{(2)}\right)= \\
& =g^{(2)}\left(W^{(2)} g^{(1)}\left(W^{(1)} \vec{x}+b^{(1)}\right)+b^{(2)}\right)
\end{aligned}
$$

- Hidden layers

$$
h^{(1)}(\vec{x})=g^{(1)}\left(W^{(1)} \vec{x}+b^{(1)}\right)
$$

In our example:

$$
\begin{aligned}
& W^{(1)} \text { is a } 3 \times 3 \text { matrix } \\
& W^{(2)} \text { is a } 3 \times 1 \text { matrix }
\end{aligned}
$$

## Adding Layers ...

- From simple linear laws ...

$$
h(\vec{x})=g(\vec{x} ; \vec{\theta}, b)=g\left(\sum_{n} \theta_{n} x_{n}+b\right)
$$

- to feedforward structures. They depend on a sequence of functions $g^{(1)}, g^{(2)}, \ldots, g^{(k)}$ that give rise to structured hypothesis

$$
\begin{aligned}
h(\vec{x}) & \left.=g^{(k)}\left(g^{(k-1)}\left(\ldots g^{(1)}\left(\vec{x} ; \vec{\theta}^{(1)}, b^{(1)}\right) ; \ldots\right) ; \vec{\theta}^{(k-1)}, b^{(k-1)}\right) ; \vec{\theta}^{(k)}, b^{(k)}\right)= \\
& =g^{(k)}\left(W^{(k)} g^{(k-1)}\left(W^{(k-1)} \ldots g^{(1)}\left(W^{(1)} \vec{x}+b^{(1)}\right) \ldots+b^{(k-1)}\right)+b^{(k)}\right)
\end{aligned}
$$

- Hidden layers

$$
h^{(j)}(\vec{x})=g^{(j)}\left(W^{(j)} g^{(j-1)}\left(\vec{x} ; \vec{\theta}^{(j-1)}, b^{(j-1)}\right)+b^{(j)}\right) \quad j=2, \ldots, k-1
$$

## Neural Networks

- Each circle represent a neuron (or unit)
- 3 input, 3 hidden and 1 output
- $n_{l}=3$ is the number of layers
- $S_{I}$ denotes the number of units in layer 1
- Layers:
- The first layer, i.e. the layer 1 , is denoted as $\mathrm{L}_{1}$
- Layer 1 and $1+1$ are connected by a matrix $W^{(t)}$ of parameters

- $W^{(I)}{ }_{i, j}$ connects the $j$-th neuron in layer $I$ with the $i$ th neuron in layer $1+1$
- $b^{(l)}{ }_{i}$ is the bias associated to neuron I in layer $1+1$


## Forward Step: classification

input layer


## Forward Step: training

 input layer

## Demystifying neural networks

Neural networks come with their own terminological baggage
... just like SVMs

But if you understand how logistic regression or maxent models work

Then you already understand the operation of a basic neural network neuron!

## A single neuron

A computational unit with $n(3)$ inputs and 1 output and parameters $W, b$


Bias unit corresponds to intercept term

$$
h_{w, b}(x)=f\left(w^{\top} x+b\right) \leftarrow \begin{aligned}
& \text { b: We can have an "always on" } \\
& \text { feature, which gives a class prior, } \\
& \text { or separate it out, as a bias term }
\end{aligned}
$$

## A neural network = running several logistic regressions at the same time

If we feed a vector of inputs through a bunch of logistic regression functions, then we get a vector of outputs ...


Layer $L_{1}$

But we don't have to decide ahead of time what variables these logistic regressions are trying to predict!

## What is Deep Learning

- It is a branch of machine learning based on a set of algorithms that attempt to model high-level abstractions in data by using multiple processing layer
- Learning representations of data
- feature hierarchies with features from higher levels of the hierarchy formed by the composition of lower level features


## From Machine Learning...

- Machine Learning in general works well because of human-designed features
- E.g. the so-called "Bag-of-Word" vector
- In this sense, machine learning is optimizing a set of parameters to obtain best performances
- a costly operation
- to be repeated for each new task



## ... to Deep Learning

- Representation Learning attempts at automatically learning the features (as well as the parameters)
- Deep Learning attempts at learning multiple levels (a hierarchy) of features of increasing complexity
- For example, in Face Detection
- A face can be composed by eyes, nose, mouth
- Each of them is composed from simpler shapes
- How to automatically learn these "features"?


Layer 3


Layer 2


## Al desiderata

- Ability to learn complex, highly-varying functions, i.e., with a number of variations much greater than the number of training examples.
- Ability to learn with little human input the low-level, intermediate, and highlevel abstractions that would be useful to represent the kind of complex functions needed for Al tasks.
- Ability to learn from a very large set of examples: computation time for training should scale well with the number of examples, i.e., close to linearly.
- Ability to learn from mostly unlabeled data, i.e., to work in the semisupervised setting, where not all the examples come with complete and correct semantic labels.
- Ability to exploit the synergies present across a large number of tasks, i.e., multi-task learning. These synergies exist because all the Al tasks provide different views on the same underlying reality.
- Strong unsupervised learning (i.e., capturing most of the statistical structure in the observed data), which seems essential in the limit of a large number of tasks and when future tasks are not known ahead of time.


## Basic Notation \& Formalisms

- Basic jargon:
- Vectors spaces, inner products and Topology: Vectors, Matrices and Tensors
- Training vs. Classification
- Forward step, backpropagation,
- Cost Function, Loss \& Regularization
- Input representation
- Dense vs. Discrete
- Embeddings
- Output format
- Tasks: classification aka labeling, autoencoding, encoding-decoding, stacking, multiple task learning


## Non linearity: the MLP

- In order to capture complex non linear functions with can apply a still linear model not to $\underline{x}$ itself but rather to one of its transformed form, e.g. $\Phi(\underline{x})$
- Which mapping $\Phi$ :
- Exploit generic mathematical, domain-independent mappings (e.g. polynomial kernels or RBFs)
- Manually engineering $\Phi$
- Learn the proper $\Phi$ with respect to the task
- The result is a new form of the learning problem

$$
y=f(\underline{x} \cdot \theta, W)=W \cdot \Phi(\underline{x})+b
$$

## A simple MLP: the XOR function

| Input1 | Input2 | Output |  |
| ---: | ---: | ---: | ---: |
| 0 | 0 | 0 | $\square$ |
| 1 | 0 | 1 | $\bigcirc$ |
| 0 | 1 | 1 | 0 |
| 1 | 1 | 0 | $\square$ |



## A MLP for the XOR problem




We can now specify our complete network as $f(\boldsymbol{x} ; \boldsymbol{W}, \boldsymbol{c}, \boldsymbol{w}, b)=\boldsymbol{w}^{\top} \max \left\{0, \boldsymbol{W}^{\top} \boldsymbol{x}+\boldsymbol{c}\right\}+b$.

Figure 6.2: An example of a feedforward network, drawn in two different styles. Specifically, this is the feedforward network we use to solve the XOR example. It has a single hidden layer containing two units. (Left) In this style, we draw every unit as a node in the graph. This style is explicit and unambiguous, but for networks larger than this example, it can consume too much space. (Right) In this style, we draw a node in the graph for each entire vector representing a layer's activations. This style is much more compact. Sometimes we annotate the edges in this graph with the name of the parameters that describe the relationship between two layers. Here, we indicate that a matrix $\boldsymbol{W}$ describes the mapping from $\boldsymbol{x}$ to $\boldsymbol{h}$, and a vector $\boldsymbol{w}$ describes the mapping from $\boldsymbol{h}$ to $y$. We typically omit the intercept parameters associated with each layer when labeling this kind of drawing.

## The solution

We can then specify a solution to the XOR problem. Let

$$
\begin{align*}
\boldsymbol{W} & =\left[\begin{array}{ll}
1 & 1 \\
1 & 1
\end{array}\right]  \tag{6.4}\\
\boldsymbol{c} & =\left[\begin{array}{c}
0 \\
-1
\end{array}\right]  \tag{6.5}\\
\boldsymbol{w} & =\left[\begin{array}{c}
1 \\
-2
\end{array}\right] \tag{6.6}
\end{align*}
$$

Rotazione
Traslazione

Scaling
and $b=0$.

$$
\begin{gathered}
\boldsymbol{X}=\left[\begin{array}{ll}
0 & 0 \\
0 & 1 \\
1 & 0 \\
1 & 1
\end{array}\right] \quad \boldsymbol{X} \boldsymbol{W}=\left[\begin{array}{ll}
0 & 0 \\
1 & 1 \\
1 & 1 \\
2 & 2
\end{array}\right] \quad \boldsymbol{X} \boldsymbol{W}+\boldsymbol{c}\left[\begin{array}{cc}
0 & -1 \\
1 & 0 \\
1 & 0 \\
2 & 1
\end{array}\right. \\
\begin{array}{l}
\text { We can now specify our complete network as } \\
f(\boldsymbol{x} ; \boldsymbol{W}, \boldsymbol{c}, \boldsymbol{w}, b)=\boldsymbol{w}^{\top} \max \left\{0, \boldsymbol{W}^{\top} \boldsymbol{x}+\boldsymbol{c}\right\}+b .
\end{array}
\end{gathered}\left[\begin{array}{l}
0 \\
1 \\
1 \\
0
\end{array}\right]
$$

## The new representation space



.... Break



## Perceptron (Rosenblatt, 1958)

- Linear Classifier mimicking a neuron



## Perceptron and non-linear activation functions

- We can adopt the sigmoid function instead of $g(z)=\frac{1}{1+e^{-z}}$
the $\operatorname{sgn}()$
- to bound the final values between 0 and 1
- can be interpreted as probabilities of belonging to a class
- belonging threshold is $>0.5$
- It remains a linear classifier

$$
h(\vec{x})=g\left(\sum_{n} \theta_{n} x_{n}+b\right)
$$



## Perceptron and non-linear activation functions

Activation Functions


## How to induce $h$ from examples

- Learn the parameters $\theta$ and $b$
- To find these we look at the past data (i.e. training data) optimizing an objective function
- Objective function: the error we make on the training data
- the sum of differences between the decision function $h$ and the label $y$
- also called Loss Function or Cost Function

$$
J(\theta, b)=\sum_{i=1}^{m}\left(h\left(x^{(i)} ; \theta, b\right)-y^{(i)}\right)^{2}
$$

## A general training procedure: Stochastic Gradient Descent

- Optimizing J means minimizing it
- it measures the errors we make on the training data.
- We can iterate over examples and update the parameters in the direction of smaller costs
- we aim at finding the minimum of that function

$$
\theta_{1}=\theta_{1}-\alpha \Delta \theta_{1}
$$

- Concretely, $\theta_{2}=\theta_{2}-\alpha \Delta \theta_{2}$

$$
b=b-\alpha \Delta b
$$

- $\alpha$ is a meta-parameter, the learning rate
- $\Delta$ are the partial derivatives of the cost function wrt each parameter


## Why SGD?

- Weights are updated using the partial derivatives
- Derivative pushes down the cost following the steepest descent path on the error curve



## SGD procedure

- Choose an initial random values for $\theta$ and $b$
- Choose a learning rate
- Repeat until stop criterion is met:
- Pick a random training example $x^{(i)}$
- Update the parameters with

$$
\begin{aligned}
& \theta_{1}=\theta_{1}-\alpha \Delta \theta_{1} \\
& \theta_{2}=\theta_{2}-\alpha \Delta \theta_{2} \\
& b=b-\alpha \Delta b
\end{aligned}
$$

- We can stop
- when the parameters do not change or,
- the number of iteration exceeds a certain upper bound


## Cost Function Derivative

- In order to update the parameters in SGD, we need to compute the partial derivatives wrt the learnable parameters.
- Remember the chain rule:
- if $h$ is a function of $z(x)$, then the derivative of $h$ wrt x is:
- Thus, we need to compute

$$
\frac{\vartheta h}{\vartheta x}=\frac{\vartheta h}{\vartheta z} \frac{\vartheta z}{\vartheta x}
$$

$$
\Delta \vartheta_{1}=\frac{\vartheta}{\vartheta \theta_{1}}\left(h\left(x^{(i)} ; \theta, b\right)-y^{(i)}\right)^{2}
$$

$$
\Delta \vartheta_{2}=\frac{\vartheta}{\vartheta \theta_{2}}\left(h\left(x^{(i)} ; \theta, b\right)-y^{(i)}\right)^{2}
$$

$$
\Delta b=\frac{\vartheta}{\vartheta b}\left(h\left(x^{(i)} ; \theta, b\right)-y^{(i)}\right)^{2}
$$

## Cost Function Derivatives

$\Delta \theta_{1}=\frac{\vartheta}{\vartheta \theta_{1}}\left(h\left(x^{(i)} ; \theta, b\right)-y^{(i)}\right)^{2}=$
$=2\left(\left(h\left(x^{(i)} ; \theta, b\right)-y^{(i)}\right) \frac{\vartheta}{\vartheta \theta_{1}}\left(h\left(x^{(i)} ; \theta, b\right)\right)\right.$
$=2\left(g\left(\theta^{T} x^{(i)}+b\right)-y^{(i)} \frac{9}{\vartheta \theta_{1}}\left(g\left(\theta^{T} x^{(i)}+b\right)\right)\right.$
We have that:

$$
\begin{aligned}
& \frac{\vartheta}{\vartheta \theta_{1}}\left(g\left(\theta^{T} x+b\right)\right)=\frac{\vartheta g\left(\theta^{T} x+b\right)}{\vartheta\left(\theta^{T} x+b\right)} \frac{\vartheta\left(\theta^{T} x+b\right)}{\vartheta \theta_{1}} \\
& \left(1-g\left(\theta^{T} x+b\right)\right) g\left(\theta^{T} x+b\right) \frac{\vartheta\left(\theta_{1} x_{1}+\theta_{2} x_{2}+b\right)}{\vartheta \theta_{1}} \\
& =\left(1-g\left(\theta^{T} x+b\right)\right) g\left(\theta^{T} x+b\right) x_{1}
\end{aligned}
$$

$$
s(x)=\frac{1}{1+e^{-x}} \text { then } \frac{\vartheta s}{\vartheta x}=(1-s(x)) s(x)
$$

$$
\begin{aligned}
& \frac{d}{d x} s(x)=\frac{d}{d x}\left(\left(1+e^{-x}\right)^{-1}\right) \\
& \frac{d}{d x} s(x)=-1\left(\left(1+e^{-x}\right)^{(-1-1)}\right) \frac{d}{d x}\left(1+e^{-x}\right) \\
& \frac{d}{d x} s(x)=-1\left(\left(1+e^{-x}\right)^{(-2)}\right)\left(\frac{d}{d x}(1)+\frac{d}{d x}\left(e^{-x}\right)\right) \\
& \frac{d}{d x} s(x)=-1\left(\left(1+e^{-x}\right)^{(-2)}\right)\left(0+e^{-x}\left(\frac{d}{d x}(-x)\right)\right) \\
& \frac{d}{d x} s(x)=-1\left(\left(1+e^{-x}\right)^{(-2)}\right)\left(e^{-x}\right)(-1)
\end{aligned}
$$

$$
\frac{d}{d x} s(x)=\left(\left(1+e^{-x}\right)^{(-2)}\right)\left(e^{-x}\right)
$$

$$
\frac{d}{d x} s(x)=\frac{1}{\left(1+e^{-x}\right)^{2}}\left(e^{-x}\right)
$$

$$
\frac{d}{d x} s(x)=\frac{e^{-x}}{\left(1+e^{-x}\right)^{2}}=\frac{e^{-x}}{\left(1+e^{-x}\right)}-\frac{1}{\left(1+e^{-x}\right)}
$$

## Cost Function Derivatives

Then,
$\Delta \theta_{1}=2\left[\left(g\left(\theta^{T} x^{(i)}+b\right)-y^{(i)}\right)\right]\left[\left(1-g\left(\theta^{T} x^{(i)}+b\right)\right) g\left(\theta^{T} x^{(i)}+b\right) x^{(i)}{ }_{1}\right]$
and we can do the same for $\theta_{2}$
$\Delta \theta_{2}=2\left[\left(g\left(\theta^{T} x^{(i)}+b\right)-y^{(i)}\right)\right]\left[\left(1-g\left(\theta^{T} x^{(i)}+b\right)\right) g\left(\theta^{T} x^{(i)}+b\right) x^{(i)}{ }_{2}\right]$


## Cost Function Derivatives for b

- For the $b$ parameter, the same steps apply:

$$
\begin{aligned}
& \Delta b=\frac{\vartheta}{\vartheta b}\left(h\left(x^{(i)} ; \theta, b\right)-y^{(i)}\right)^{2}= \\
& =2\left(\left(h\left(x^{(i)} ; \theta, b\right)-y^{(i)}\right) \frac{\vartheta}{\vartheta b}\left(h\left(x^{(i)} ; \theta, b\right)\right)\right. \\
& =2\left(g\left(\theta^{T} x^{(i)}+b\right)-y^{(i)}\right) \frac{\vartheta}{\vartheta b}\left(g\left(\theta^{T} x^{(i)}+b\right)\right)
\end{aligned}
$$

$\frac{\vartheta}{\vartheta b}\left(g\left(\theta^{T} x+b\right)\right)=\frac{\vartheta g\left(\theta^{T} x+b\right)}{\vartheta\left(\theta^{T} x+b\right)} \frac{\vartheta\left(\theta^{T} x+b\right)}{\vartheta b}=\left(1-g\left(\theta^{T} x+b\right)\right) g\left(\theta^{T} x+b\right)$
$\Delta b=2\left[\left(g\left(\theta^{T} x^{(i)}+b\right)-y^{(i)}\right)\right]\left[\left(1-g\left(\theta^{T} x^{(i)}+b\right)\right) g\left(\theta^{T} x^{(i)}+b\right)\right]$

## Learning rate: low values



- make the algorithm converge slowly
- it is a conservative and safer choice
- However, it implies very long training

$$
\begin{aligned}
& \theta_{1}=\theta_{1}-\alpha \Delta \theta_{1} \\
& \theta_{2}=\theta_{2}-\alpha \Delta \theta_{2} \\
& b=b-\alpha \Delta b
\end{aligned}
$$

## Learning rate: high values

- make the algorithm
 converge quickly
- Training time is reduced
- it is a a less safer choice
- risk of divergence

$$
\begin{aligned}
& \theta_{1}=\theta_{1}-\alpha \Delta \theta_{1} \\
& \theta_{2}=\theta_{2}-\alpha \Delta \theta_{2} \\
& b=b-\alpha \Delta b
\end{aligned}
$$



Target: 1.0

Going forward (Regularization, Dropout, Batch Normalization, ...)


Target: 1.0
hidden layer 1 hidden layer 2
Loss Function: $(T-O) \Rightarrow$ Loss: 0.45


Updating the weights using Backpropagation $\frac{\partial E}{\partial w_{j}^{i}}$



By Choosing the Optimizer, new weights will be computed $w_{n e w}=w-\eta \frac{\partial E}{\partial w}$

## Multilayer Networks

- Each circle represent a neuron (or unit)
- 3 inputs, 3 hiddens and 1 output
- $n_{1}=3$ is the number of layers
- $s_{1}$ denotes the number of units in layer 1
- Layers:
- Layer 1 is denoted as $\mathrm{L}_{1}$
- Layer land l+1 are connected by a matrix of parameters $\mathrm{W}^{(1)}$
- $\mathrm{W}^{(\mathrm{I})}{ }_{\mathrm{i}, \mathrm{j}}$ connects neuron j in layer I with neuron $i$ in layer l+1

- $b^{(1)}{ }_{i}$ is the bias associated to neuron $i$ in layer l+1


## Multilayer Networks cont.

- $a^{(1)}{ }_{1}$ is the activation of unit i in layer l
$a_{1}^{(2)}=f\left(W_{11}^{(1)} x_{1}+W_{12}^{(1)} x_{2}+W_{13}^{(1)} x_{3}+b_{1}^{(1)}\right)$
$a_{2}^{(2)}=f\left(W_{21}^{(1)} x_{1}+W_{22}^{(1)} x_{2}+W_{23}^{(1)} x_{3}+b_{2}^{(1)}\right)$
$a_{3}^{(2)}=f\left(W_{31}^{(1)} x_{1}+W_{32}^{(1)} x_{2}+W_{33}^{(1)} x_{3}+b_{3}^{(1)}\right)$
$h_{W, b}(x)=a_{1}^{(3)}=f\left(W_{11}^{(2)} a_{1}^{(2)}+W_{12}^{(2)} a_{2}^{(2)}+W_{13}^{(2)} a_{3}^{(2)}+b_{1}^{(2)}\right.$
- We call $z^{(1)}$ i the weighted sum of inputs to unit i in layer l, i.e.

$$
\begin{aligned}
& z_{i}^{(2)}=\sum_{j=1}^{n} W_{i j}^{(1)} x_{j}+b_{i}^{(1)} \\
& a_{i}^{(l)}=f\left(z_{i}^{(l)}\right)
\end{aligned}
$$

- f is a non-linearity function

- e.g. the sigmoid


## Multilayer Network Classification

- The classification corresponds in getting the value(s) in the output layer
- Propagating the input towards the network given W,b
- This process is called forward propagation

$$
\begin{aligned}
& z^{(l+1)}=W^{(l)} a^{(l)}+b^{(l)} \\
& a^{(l+1)}=g\left(z^{(l+1)}\right)
\end{aligned}
$$

## How to Train a NN?

- We can re-use the gradient descent algorithm
- define a cost function
- compute the partial derivatives wrt to all the parameters

$$
\begin{aligned}
& h(z(x)) \\
& \frac{\vartheta h}{\vartheta x}=\frac{\vartheta h}{\vartheta z} \frac{\vartheta z}{\vartheta x}
\end{aligned}
$$

- As the NN models function composition
- we are going to exploit the chain rule (again)
- Setup:
- we have a training set of $m$ examples
- $\left\{\left(X^{(1)}, y^{(1)}\right), \ldots,\left(X^{(m)}, y^{(m)}\right)\right\}$
- $x$ are the inputs and $y$ are the labels


## Cost Function of a NN

- Given a single training example $(x, y)$ the cost is

$$
J(W, b ; x, y)=\frac{1}{2}\left|h_{W, b}(x)-y\right|^{2}
$$

- For the whole training set $J$ is the mean of the errors plus a regularization term (weight decay)

$$
\begin{aligned}
& J(W, b)=\frac{1}{m} \sum_{i=1}^{m} J\left(W, b ; x^{(i)}, y^{(i)}\right)+\frac{\lambda}{2} \sum_{l=1}^{n_{l}-1} \sum_{i=1}^{s_{l}} \sum_{j=1}^{s_{i+1}}\left(W_{j i}^{(l)}\right)^{2} \\
& =\frac{1}{m} \sum_{i=1}^{m}\left(\frac{1}{2}\left|h_{W, b}\left(x^{(i)}\right)-y^{(i)}\right|^{2}\right)+\frac{\lambda}{2} \sum_{l=1}^{n_{l}-1} \sum_{i=1}^{s_{l}} \sum_{j=1}^{s_{l+1}}\left(W_{j i}^{(l)}\right)^{2}
\end{aligned}
$$

- $\lambda$ controls the importance of the two terms (it has a similar role to the C parameter in SVM)


## ... digression: On regularization

- "any modification we make to a learning algorithm that is intended to reduce its generalization error but not its training error."
- In practical deep learning scenarios: the best fitting model (in the sense of minimizing generalization error) is a large model that has been regularized appropriately
- Many regularization approaches are based on limiting the capacity of models, such as neural networks, linear regression, or logistic regression, by adding a parameter norm penalty $\Omega(\theta)$ to the objective function J
- Regularization methods:
- Weight decay (ridge regression)
- ... Constrained optimization
- Data Augmentation
- Early stopping


## A GD step

- A GD step update the parameters according to

$$
\begin{aligned}
& W_{i j}^{(l)}=W_{i j}^{(l)}-\alpha \frac{\vartheta}{\vartheta W_{i j}^{(l)}} J(W, b) \\
& b_{i}^{(l)}=b_{i}^{(l)}-\alpha \frac{\vartheta}{\vartheta b_{i}^{(l)}} J(W, b)
\end{aligned}
$$

- where $\alpha$ is the learning rate.
- The partial derivatives are computed with the Backpropagation algorithm


## The backpropagation algorithm

- First, we compute for each example $\frac{\vartheta}{\vartheta W_{i j}^{(l)}} J\left(W, b, x^{(i)}, y^{(i)}\right)$
- Backpropagation works as follow:

1. do a forward pass for an example $x^{(i)}, y^{(i)}$
2. for each node i in layer l, compute an error term $\delta_{i}^{1}$
3. it measures how unit i is responsible for the error on the current example
4. The error of an output node is the difference between the true output value and the predicted one
5. For the intermediate layer l, a node receives a portion of the error based on the units it is linked to of the layer l+1

- Partial derivatives will be computed given the error terms


## The backpropagation algorithm cont.

1. Perform a forward propagation for an example
2. For each unit $i$ in the output layer $\left(n_{l}\right)$

$$
\delta_{i}^{(n)}=\frac{\vartheta}{\vartheta z_{i}^{(n)}}\left|y-h_{W, b}(x)\right|^{2}=-\left(y_{i}-a_{i}^{\left(m_{1}\right)}\right) \cdot g^{\prime}\left(z_{i}^{\left(m_{i}\right)}\right)
$$

3. For $l=n_{l}-1, \ldots, 2$
4. for each node $i$ in layer $I \quad \delta_{i}^{(l)}=\left(\sum_{j=1}^{s_{1}} W_{j i}^{(l)} \delta_{j}^{(l+1)}\right) g^{\prime}\left(z_{i}^{(l)}\right)$
5. Compute the partial derivatives as:
$\frac{\vartheta}{\vartheta W_{i j}^{(l)}} J(W, b ; x, y)=a_{j}^{(l)} \delta_{i}^{(l+1)}$
$\frac{\vartheta}{\vartheta b_{i}^{(l)}} J(W, b ; x, y)=\delta_{i}^{(l+1)}$

## The full backpropagation algorithm

1. Set $\Delta W^{(1)}=0, \Delta b^{(1)}=0$ for all l
2. For each examples $(x, y)$, for each layer l
3. Compute $\nabla_{W^{(0)}} J(W, b ; x, y)=\delta^{(+1)}\left(a^{(l)}\right)^{T}, \nabla_{b^{(\prime)}} J(W, b ; x, y)=\delta^{(+1)}$
4. Set $\Delta W^{(l)}=\Delta W^{(t)}+\nabla_{W^{(t)}} J(W, b ; x, y)$

$$
\Delta b^{(l)}=\Delta b^{(l)}+\nabla_{b^{(l)}} J(W, b ; x, y)
$$

3. Update the parameters with:

$$
\begin{aligned}
& W^{(l)}=W^{(l)}-\alpha\left[\left(\frac{1}{m} \Delta W^{(l)}\right)+\lambda W^{(l)}\right] \\
& b^{(l)}=b^{(l)}-\alpha\left[\left(\frac{1}{m} \Delta b^{(l)}\right)\right]
\end{aligned}
$$

## Some considerations

- Randomly initialize the parameters of the network
- for symmetry breaking
- Remember that the function $g$ is a non-linear activation function
- if $f$ is the sigmoid

$$
\begin{aligned}
& g(z)=\frac{1}{1+e^{-z}} \\
& g^{\prime}(z)=(1-g(z)) g(z)
\end{aligned}
$$

- Activations values can be cached from the forward propagation step!

$$
g^{\prime}\left(z_{i}^{(l)}\right)=\left(1-g\left(z_{i}^{(l)}\right)\right) g\left(z_{i}^{(l)}\right)=\left(1-a_{i}^{(l)}\right) a_{i}^{(l)}
$$

- If you must perform multi-classification
- there will be an output unit for each of the labels


## Some considerations

- How to stop and select the best model
- Waiting the iteration in which the cost function doesn't change significantly
- Risk of overfitting
- Early stopping
- Provide hints as to how many iterations can be run before overfitting
- Split the original training set into a new training set and a validation set
- Train only on the training set and evaluate the error on the validation set
- Stop training as soon as the error is higher than it was the last time
- Use the weights the network had in that previous step


## - Dropout

- another form of regularization to avoid overfitting data

- during training (only) randomly "turn off" some of the neurons of a layer
- it prevents co-adaptation of units between layers


## Dropout (Svrivastava et al., 2014)

- Dropout can be interpreted as a way of regularizing a neural network by adding noise to its hidden units.
- It speeds-up the learning algorithm through model averaging
- It helps in reducing the risk of greedily promote simplistic solutions

Randomly setting a fraction rate of input units to $o$ at each update during training time.

(a) Standard Neural Net

(b) After applying dropout.

## Dropout: effects

Fig. 2: parisol of the

(a)

(b)

Fig. 7: Classification error rate on the (a) training and (b) validation sets of the Reuters dataset as learning progresses. The training error is computed using the stochastic nets.

## Next steps ... complex NN architectures

- Convolutional Neural Networks (Neocogitron, Fukushima (1980))
- Recurrent Neural Networks (Jordan, 1986), (Elman, 1990)
- Bidirectional RNNs (Schuster and Paliwal, 1997)
- BP Through-Time (Robinson \& Fallside, 1987)
- Long Short Time Memories LSTMS, (Hochreiter \& Schmidhuber, 1997)
- Attention mechanisms (firstly discussed by (Larochelle \& Hinton, 2010; Denil et al., 2012)).
- Autoencoders (Bengio et al., 2007), Encoder-Decoders (Cho et al., 2015)


## Bibliografia: an historical overview

- Warren S McCulloch and Walter Pitts. A logical calculus of the ideas immanent in nervous activity. The bulletin of mathematical biophysics, 5(4):115\{133, 1943.
- Frank Rosenblatt. The perceptron: a probabilistic model for information storage and organization in the brain. Psychological review, 65(6):386, 1958.
- Donald Olding Hebb. The organization of behavior: A neuropsychological theory. Psychology Press, 1949.
- John J Hopfield. Neural networks and physical systems with emergent collective computational abilities. Proceedings of the national academy of sciences, 79 (8):2554-2558, 1982.
- David E Rumelhart, Georey E Hinton, and Ronald J Williams. Learning internal representations by error propagation. Technical report, DTIC Document, 1985.
- Rumelhart, D. E., McClelland, J. L., and the PDP Research Group (1986). Parallel Distributed Processing: Explorations in the Microstructure of Cognition. MIT Press, Cambridge.
- Teuvo Kohonen. The self-organizing map. Proceedings of the IEEE, 78(9):1464\{1480, 1990.
- David H Ackley, Georey E Hinton, and Terrence J Sejnowski. A learning algorithm for boltzmann machines. Cognitive science, 9(1):147-169, 1985.
- Kunihiko Fukushima. Neocognitron: A self-organizing neural network model for a mechanism of pattern recognition unaected by shift in position. Biological cybernetics, 36(4): 193-202, 1980.
- Le Cun B. Boser, John S. Denker, D. Henderson, Richard E. Howard, W. Hubbard and Lawrence D. Jackel. Handwritten digit recognition with a back-propagation network. In Advances in neural information processing systems. Citeseer, 1990.


## Bibliografia: an historical overview (2)

- Michael I Jordan. Serial order: A parallel distributed processing approach. Advances in psychology, 121:471-495, 1986.
- Jerey L Elman. Finding structure in time. Cognitive science, 14(2):179-211, 1990.
- AJ Robinson and Frank Fallside. The utility driven dynamic error propagation network. University of Cambridge Department of Engineering, 1987.
- Mike Schuster and Kuldip K Paliwal. Bidirectional recurrent neural networks. IEEE Transactions on Signal Processing, 45(11):2673-2681, 1997.
- Sepp Hochreiter and Jurgen Schmidhuber. Long short-term memory. Neural computation, 9(8):1735-1780, 1997.
- Hugo Larochelle and Georey E Hinton. Learning to combine foveal glimpses with a third-order boltzmann machine. In Advances in neural information processing systems, pages 1243-1251, 2010
- Denil, M., Bazzani, L., Larochelle, H., and de Freitas, N. (2012). Learning where to attend with deep architectures for image tracking. Neural Computation, 24 (8), 2151-2184
- Yoshua Bengio, Pascal Lamblin, Dan Popovici, Hugo Larochelle, et al. Greedy layer-wise training of deep networks. Advances in neural information processing systems, 19:153, 2007.
- Kyunghyun Cho, Bart Van Merrienboer, Caglar Gulcehre, Dzmitry Bahdanau, Fethi Bougares, Holger Schwenk, and Yoshua Bengio. Learning phrase representations using rnn encoder-decoder for statistical machine translation. arXiv preprint arXiv:1406.1078, 2014.

