Neural Networks

Réda DEHAK
http://ia.dehak.org

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Contents

- Origins/History
- Human Brain / Biological Neuron
- Perceptron
- Neural Networks Topology
- Learning:
  - Perceptron
  - Multi Layers Neural Networks: Backpropagation Algorithm
- Conclusions

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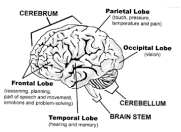
Origins

- Many machine learning methods inspired by biology, e.g., the (human) brain
- Neural Networks:
  - Algorithms that try to mimic the brain
  - Produce artificial systems capable of complex calculation similar to the human brain



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History

1943 : McCulloch and Pitts proposed the McCulloch-Pitts neuron model
1949 : Hebb published his book The Organization of Behavior, in which the Hebbian learning rule was proposed.
1958 : Rosenblatt introduced the simple single layer networks now called Perceptrons.
1969 : Minsky and Papert's book Perceptrons demonstrated the limitation of single layer perceptrons, and almost the whole field went into hibernation.
1982 : Hopfield published a series of papers on Hopfield networks.
1982 : Kohonen developed the Self-Organising Maps that now bear his name.
1986 : The Back-Propagation learning algorithm for Multi-Layer Perceptrons was rediscovered and the whole field took off again.
1990s : The sub-field of Radial Basis Function Networks was developed.
2000s : The power of Neural Networks, Support Vector Machines, and Bayesian Techniques methods become apparent.
2009- : DNNs outperform other Machine Learning Methods in different competitions

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Human brain

- Our brain has ~ 10^{11} neurons, each of which communicates (is connected) to ~ 10^{4} other neurons
- The brain can fire all the neurons in a single step (parallelism).
- The human brain is extremely energy efficient, using approximately 10^{-16} joules per operation per second.
- Brains have been evolving for tens of millions of years

	Processing Elements	Element size	Energy use	Processing speed	Style of computation	Fault Tolerant	Learns	Intelligent, conscious
	10^{14} synapses	10^{-6} m	30 W	100 Hz	parallel, distributed	yes	yes	usually
	10^{8} transistors	10^{-6} m	30 W (CPU)	10^{9} Hz	serial, centralized	no	a little	not (yet)

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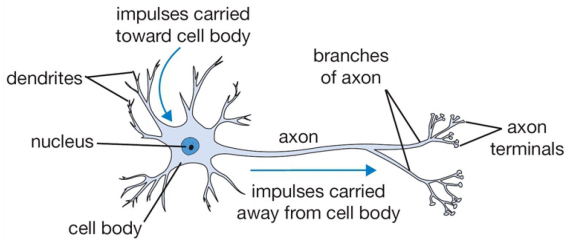
Biological Neuron



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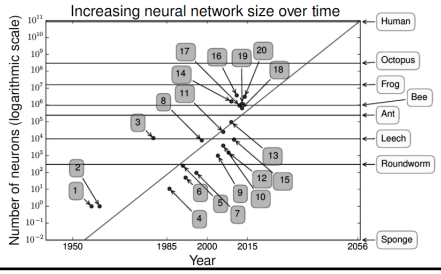
Neural Network Sizes



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1. Perceptron (Rosenblatt, 1958, 1962)
2. Adaptive Linear Element (Widrow and Hoff, 1960)
3. Neocognitron (Fukushima, 1980)
4. Early backpropagation network (Rumelhart *et al.*, 1986b)
5. Recurrent neural network for speech recognition (Robinson and Fallside, 1991)
6. Multilayer perceptron for speech recognition (Bengio *et al.*, 1991)
7. Mean field sigmoid belief network (Saul *et al.*, 1996)
8. LeNet-5 (LeCun *et al.*, 1998b)
9. Echo state network (Jaeger and Haas, 2004)
10. Deep belief network (Hinton *et al.*, 2006)
11. GPU-accelerated convolutional network (Chellapilla *et al.*, 2006)
12. Deep Boltzmann machines (Salakhutdinov and Hinton, 2009a)
13. GPU-accelerated deep belief network (Raina *et al.*, 2009)
14. Unsupervised convolutional network (Jarrett *et al.*, 2009b)
15. GPU-accelerated multilayer perceptron (Ciresan *et al.*, 2010)
16. OMP-1 network (Coates and Ng, 2011)
17. Distributed autoencoder (Le *et al.*, 2012)
18. Multi-GPU convolutional network (Krizhevsky *et al.*, 2012a)
19. COTS HPC unsupervised convolutional network (Coates *et al.*, 2013)
20. GoogLeNet (Szegedy *et al.*, 2014a)

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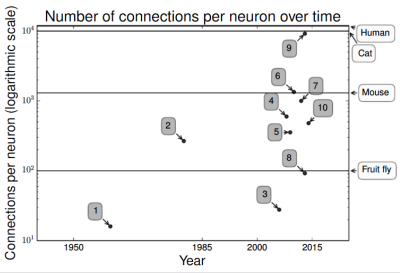
Number of connections



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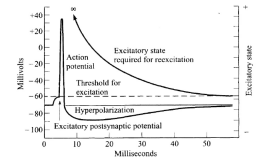
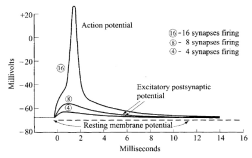
Biological Neuron Activation



From: Principles of Neurocomputing for Science & Engineering, Ham & Kostanic, McGraw-Hill



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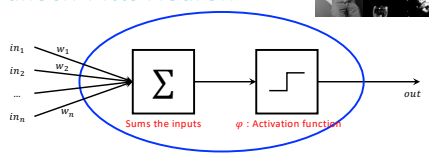
McCulloch-Pitts Neuron



- A set of synapses (i.e. connections) brings in activations from other neurons.
- A processing unit sums the inputs, and then applies a non-linear activation function (i.e. squashing/transfer/threshold function).
- An output line transmits the result to other neurons.
- Any number of McCulloch-Pitts neurons can be connected together in any way we like

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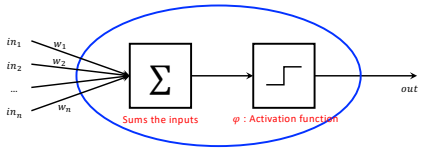
McCulloch-Pitts Neuron



$$out = \begin{cases} 1 & if \sum_{i=1}^{n} w_i in_i \geq \theta \\ 0 & else \end{cases}$$

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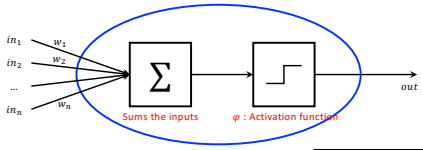
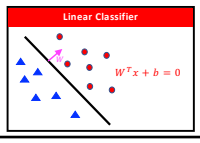
McCulloch-Pitts Neuron



$$out = \varphi\left(\sum_{i=1}^{n} w_i in_i - \theta\right)$$

$$out = sign\left(\sum_{i=1}^{n} w_i in_i - \theta\right)$$



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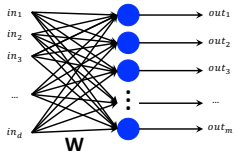
Perceptron

(Rosenblatt, 1958)

- An arrangement of one layer of McCulloch-Pitts neurons is known as a Perceptron (Dense Layer).



$$out_j = sign\left(\sum_{i=1}^{d} in_i w_{ij} - \theta_j\right)$$

$$\text{Out} = sign(W^T In)$$

$$In = \qquad \widetilde{In} = \begin{bmatrix} 1 \\ in_1 \\ in_2 \\ \vdots \\ in_d \end{bmatrix}$$

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Perceptron

(Rosenblatt, 1958)

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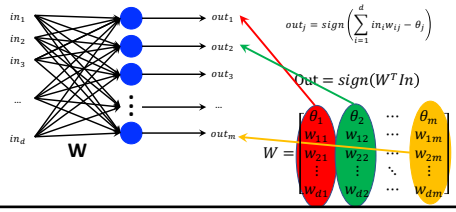

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Perceptron

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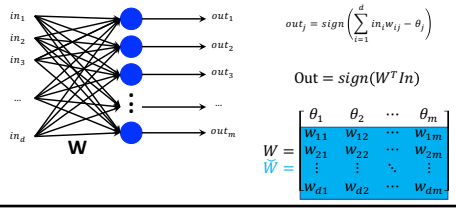

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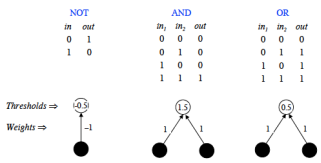
Implementation of Logical operator



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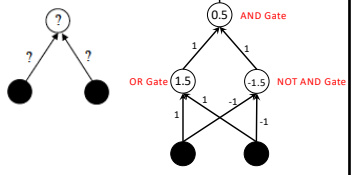
XOR

XOR		
in_1	in_2	out
0	0	0
0	1	1
1	0	1
1	1	0



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Architectures, Structures or Topology

- Single-Layer Feed-forward NNs: One input layer and one output layer of processing units. No feed-back connections. (For example, a simple Perceptron.)
- Multi-Layer Feed-forward NNs: One input layer, one output layer, and one or more hidden layers of processing units. No feed-back connections. The hidden layers sit in between the input and output layers, and are thus hidden from the outside world. (For example, a Multi-Layer Perceptron.)
- Recurrent NNs: Any network with at least one feed-back connection. It may, or may not, have hidden units. (For example, a Simple Recurrent Network.)

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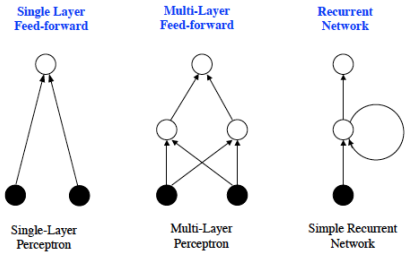
Examples



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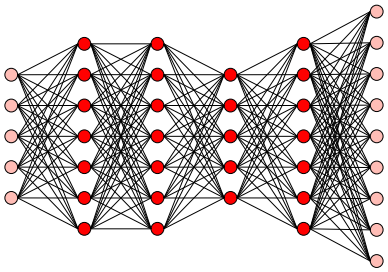
Deep Neural Networks



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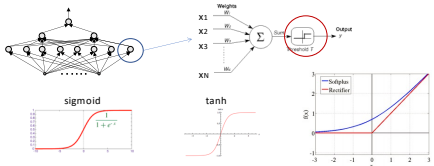
A note on activations



- Previous explanations assumed network units used a threshold function for "activation"
- In reality, we use a number of other *differentiable* functions
  - Mostly, but not always, "squashing" functions

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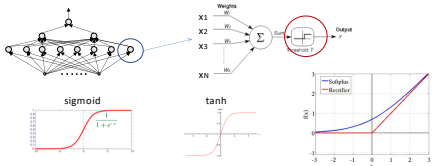
A note on activations



- Composing/learning networks using threshold "activations" is a combinatorial problem
  - Exponentially hard to find the right solution
- The smoother *differentiable* activation functions enable learning through optimization

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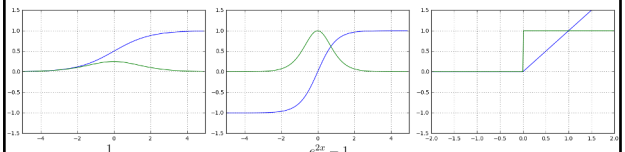
Activation functions



$\text{sigm}(x) = \frac{1}{1+e^{-x}}$ $\quad \tanh(x) = \frac{e^{2x}-1}{e^{2x}+1}$ $\quad \text{relu}(x) = \max(0,x)$

$\text{sigm}'(x) = \text{sigm}(x)(1-\text{sigm}(x))$ $\quad \tanh'(x) = 1-\tanh(x)^2$ $\quad \text{relu}'(x) = 1_{x>0}$

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Softmax function

$$softmax(\mathbf{x}) = \frac{1}{\sum_{i=1}^{n} e^{x_i}} \cdot \begin{bmatrix} e^{x_1} \\ e^{x_2} \\ \vdots \\ e^{x_n} \end{bmatrix}$$

$$\frac{\partial softmax(\mathbf{x})_i}{\partial x_j} = \begin{cases} softmax(\mathbf{x})_i \cdot (1 - softmax(\mathbf{x})_i) & i = j \\ -softmax(\mathbf{x})_i \cdot softmax(\mathbf{x})_j & i \neq j \end{cases}$$

- Vector of values in $[0,1]$ that add up to 1
- $\mathrm{P}(Y = k|X = x) = \mathrm{softmax}(\mathrm{z}(x))_k$
- The pre-activation vector $\mathrm{z}(x)$ is often called "the logits"

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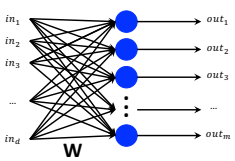
Learning: 1-Perceptron



$$\mathrm{Out}(in) = \varphi(W^T In)$$

Learning: Gradient Descent

Given a training set: $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$
$x_1, x_2, \dots, x_n$ are the input vectors
$y_1, y_2, \dots, y_n$ are the desired output (target)
Minimize MSE :

$$E = \frac{1}{N}\sum_{n=1}^{N} \|e_n\|^2$$

$$E = \frac{1}{N}\sum_{n=1}^{N} \|Out(x_n) - y_n\|^2$$

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Derivatives: Chain Rule

1. $z = u(v(x))$ with $v(x)$ is a vector

$$\frac{\partial z}{\partial x_{ij}} = \sum_k \frac{\partial z}{\partial v_k}\frac{\partial v_k}{\partial x_{ij}} = \left(\frac{\partial v}{\partial x_{ij}}\right)^T @ \frac{\partial z}{\partial v}$$

2. $z = u(v(x))$ with $v(x)$ is a matrix

$$\frac{\partial z}{\partial x_{ij}} = \sum_k \sum_l \frac{\partial z}{\partial v_{kl}}\frac{\partial v_{kl}}{\partial x_{ij}}$$

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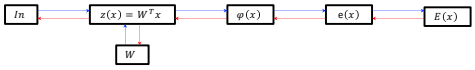
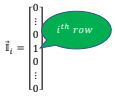
Learning: 1-Perceptron



- $\frac{\partial E(x)}{\partial e(x)_i} = \frac{\partial (e^T e)}{\partial e(x)_i} = 2\, e(x)_i$
- $\frac{\partial e(x)_j}{\partial \varphi(x)_i} = \frac{\partial (\varphi(x)_j - y_j)}{\partial \varphi(x)_i} = \mathbb{I}_{i=j}$
- $\frac{\partial E(x)}{\partial \varphi(x)_i} = 2(\vec{\mathbb{I}}_i)^T @\, e(x) = 2e(x)_i$

$$\frac{\partial E(x)}{\partial e(x)} = 2e(x)$$
$$\frac{\partial e(x)}{\partial \varphi(x)_i} = \vec{\mathbb{I}}_i$$
$$\frac{\partial E(x)}{\partial \varphi(x)} = 2e(x)$$

$\vec{\mathbb{I}}_i =$ 

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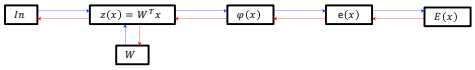
Learning: 1-Perceptron



- $\frac{\partial \varphi(z(x))_j}{\partial z(x)_i} = \frac{\partial (\varphi(z(x))_j)}{\partial z(x)_i} = \varphi'(z(x)_j)\mathbb{I}_{i=j} = \varphi'(z(x))_j \,.\, \mathbb{I}_{i=j}$

$$\frac{\partial \varphi(x)}{\partial z(x)_i} = \varphi'(z(x)) \,.\, \vec{\mathbb{I}}_i$$
$$\frac{\partial E(x)}{\partial z(x)_i} = 2(\varphi'(z(x)) \,.\, \vec{\mathbb{I}}_i)^T @ e(x) = 2e(x)_i \varphi'(z(x))_i$$
$$\frac{\partial E(x)}{\partial z(x)} = 2e(x) \,.\, \varphi'(z(x))$$

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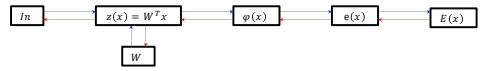
Learning: 1-Perceptron



$$\frac{\partial z(x)_k}{\partial w_{ij}} = \frac{\partial (W^T in)_k}{\partial w_{ij}} = \frac{\partial \sum_{d=1}^{D} W_{dk} in_d}{\partial w_{ij}} = in_i \mathbb{I}_{k=j} \qquad \frac{\partial z(x)}{\partial W_{ij}} = in_i \vec{\mathbb{I}}_j$$

$$\frac{\partial E(x)}{\partial W_{ij}} = 2\left(in_i \vec{\mathbb{I}}_j\right)^T @ \left(e(x) \cdot \varphi'(z(x))\right)$$

$$\frac{\partial E(x)}{\partial W_{ij}} = 2in_i \left(e(x) \cdot \varphi'(z(x))\right)_j$$

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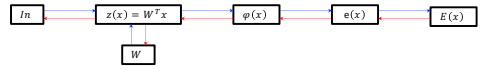
Learning: 1-Perceptron



$$\frac{\partial z(x)_k}{\partial w_{ij}} = \frac{\partial (W^T in)_k}{\partial w_{ij}} = \frac{\partial \sum_{d=1}^{D} W_{dk} in_d}{\partial w_{ij}} = in_i \mathbb{I}_{k=j} \qquad \frac{\partial z(x)}{\partial W_{ij}} = in_i \vec{\mathbb{I}}_j$$

$$\frac{\partial E(x)}{\partial W_{ij}} = 2\left(in_i \vec{\mathbb{I}}_j\right)^T @ \left(e(x) \cdot \varphi'(z(x))\right)$$

$$\frac{\partial E(x)}{\partial W} = 2In @ \left(e(x) \cdot \varphi'(z(x))\right)^T$$

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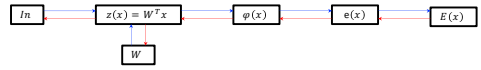
Learning: 1-Perceptron



$$\frac{\partial z(x)_k}{\partial w_{ij}} = \frac{\partial (W^T in)_k}{\partial w_{ij}} = \frac{\partial \sum_{d=1}^{D} W_{dk} in_d}{\partial w_{ij}} = in_i \mathbb{I}_{k=j} \qquad \frac{\partial z(x)}{\partial W_{ij}} = in_i \vec{\mathbb{I}}_j$$

$$\frac{\partial E(x)}{\partial W_{ij}} = 2\left(in_i \vec{\mathbb{I}}_j\right)^T @ \left(e(x) \cdot \varphi'(z(x))\right)$$

$$\frac{\partial E(x)}{\partial W} = In @ \left(\frac{\partial E(x)}{\partial z(x)}\right)^T$$

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Learning Multi Mayers Neural Networks

Backpropagation Algorithm

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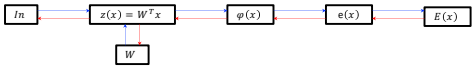
Learning: 2-Multilayers Neural Networks

Backpropagation Algorithm



- $\frac{\partial z(x)_k}{\partial \widetilde{In}_i} = \frac{\partial (W^T In)_k}{\partial \widetilde{In}_i} = \frac{\partial \sum_{d=1}^{D} W_{dk} in_d}{\partial \widetilde{In}_i} = \widetilde{W}_{ik}$ $\quad \frac{\partial z(x)}{\partial \widetilde{In}_i} = (\widetilde{W}_{i\bullet})^T$

$$\frac{\partial E(x)}{\partial In_i} = 2\widetilde{W}_{i\bullet} @ \left(e(x) . \varphi'(z(x))\right)$$

$$\boxed{\frac{\partial E(x)}{\partial \widetilde{In}} = \widetilde{W} @ \frac{\partial E(x)}{\partial z(x)}}$$

Réda DEHAK 35

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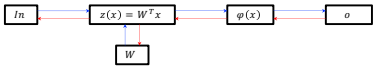
Learning: 2-MultiLayers Neural Networks

Backpropagation Algorithm



- $\frac{\partial o_j}{\partial z(x)_i} = \frac{\partial \left(\varphi(z(x))\right)_j}{\partial z(x)_i} = \varphi'(z(x)_j)\mathbb{I}_{i=j} = \varphi'(z(x))_j . \mathbb{I}_{i=j}$

$$\frac{\partial o}{\partial z(x)_i} = \varphi'(z(x)) . \vec{\mathbb{I}}_i$$

$$\frac{\partial E(x)}{\partial z(x)_i} = \left(\varphi'(z(x)) . \vec{\mathbb{I}}_i\right)^T @ \frac{\partial E(x)}{\partial o} = \left(\frac{\partial E(x)}{\partial o}\right)_i \varphi'(z(x))_i$$

Réda DEHAK 36

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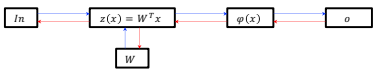
Learning: 2-MultiLayers Neural Networks
Backpropagation Algorithm



- $\frac{\partial o_j}{\partial z(x)_i} = \frac{\partial(\varphi(z(x)))_j}{\partial z(x)_i} = \varphi'(z(x)_j)\mathbb{I}_{i=j} = \varphi'(z(x))_j.\mathbb{I}_{i=j}$

$$\frac{\partial E(x)}{\partial z(x)} = \left(\frac{\partial E(x)}{\partial o}.\varphi'(z(x))\right)$$

$$\frac{\partial E(x)}{\partial z(x)} = \left(\frac{\partial E(x)}{\partial In_+}.\varphi'(z(x))\right)$$

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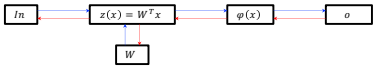
Learning: 2-MultiLayers Neural Networks
Backpropagation Algorithm



$$\frac{\partial z(x)_k}{\partial w_{ij}} = \frac{\partial(w^T In)_k}{\partial w_{ij}} = \frac{\partial \sum_{d=1}^{D} W_{dk} in_d}{\partial w_{ij}} = in_i \mathbb{I}_{k=j} \qquad \frac{\partial z(x)}{\partial W_{ij}} = in_i \vec{\mathbb{I}}_j$$

$$\frac{\partial E(x)}{\partial W_{ij}} = 2\left(in_i \vec{\mathbb{I}}_j\right)^T @ \left(\frac{\partial E(x)}{\partial z(x)}\right)$$

$$\frac{\partial E(x)}{\partial W} = In @ \left(\frac{\partial E(x)}{\partial z(x)}\right)^T$$

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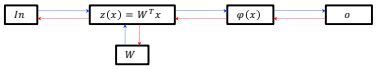
Learning: 2-MultiLayers Neural Networks
Backpropagation Algorithm



- $\frac{\partial z(x)_k}{\partial In_i} = \frac{\partial(W^T In)_k}{\partial In_i} = \frac{\partial \sum_{d=1}^{D} W_{dk} in_d}{\partial In_i} = \widetilde{W}_{ik} \qquad \frac{\partial z(x)}{\partial In_i} = (\widetilde{W}_{i\bullet})^T$

$$\frac{\partial E(x)}{\partial In_i} = 2\widetilde{W}_{i\bullet} @ \left(e(x).\varphi'(z(x))\right)$$

$$\frac{\partial E(x)}{\partial In} = \widetilde{W} @ \frac{\partial E(x)}{\partial z(x)}$$

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Learning: 2-MultiLayers Neural Networks
Backpropagation Algorithm

For a Multilayer NN with L Layers

- First Step: Forward Propagation of the input
  - Compute and store the activation and the output of each layer in order from the input layer to the output layer

$$in^{(l)} = \begin{bmatrix} 1 \\ o^{(l-1)} \end{bmatrix}$$

$$z^{(l)} = W^{(l)^T} in^{(l)}$$

$$o^{(l)} = \varphi\left(z^{(l)}\right)$$

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Learning: 2-MultiLayers Neural Networks
Backpropagation Algorithm

For a Multilayers NN with L Layers

- Second Step: Backward Propagation of the gradient
  - Compute and store the gradient of each layer in order from the ouput layer to the input layer

Compute : $\frac{\partial E(X)}{\partial o^{(L)}} = 2e$ with $e = o^{(L)} - y$ in the case of *MSE*

and $\delta^{(L)} = \frac{\partial E(x)}{\partial z(x)^{(L)}} = \frac{\partial E(X)}{\partial o^{(L)}} . \varphi'\left(z(x)^{(L)}\right)$

Iterate: $\frac{\partial E(x)}{\partial W^{(l)}} = in^{(l)} @ \left(\delta^{(l)}\right)^T$

$$\delta^{(l-1)} = \frac{\partial E(x)}{\partial z(x)^{(l-1)}} = \varphi'\left(z(x)^{(l-1)}\right) . \left(\bar{W}^{(l)} @ \delta^{(l)}\right)$$

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Loss Function

- Regression:
  - Use MSE cost function with a Identity activation function for output layer.

$$E = \frac{1}{N} \sum_{i=1}^{N} \left\| o^{(L)}(x_i) - y_i \right\|^2 \quad \frac{\partial E(x)}{\partial o^{(L)}} = 2\left(o^{(L)} - y\right)$$

- Classification:
  - Use Cross Entropy cost function with sigmoid (in the case of binary classifier) or softmax (in the case of multiclass classifier) activation function for output layer

$$E = -\frac{1}{N} \sum_{i=1}^{N} \sum_{k=1}^{K} \mathbb{I}_{y_i=k} \log\left(o^{(L)}(x_i)\right)_k \quad \frac{\partial E(x)}{\partial o^{(L)}} = -\frac{\mathbb{I}_y}{o^{(L)}}$$

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Gradient descent variants

- Three variants of gradient descent:
  - Stochastic gradient descent: uses one random sample of the training dataset to compute the gradient at each iteration
  - Batch gradient descent: uses the full trainning dataset to compute the gradient at each iteration
  - Mini-batch gradient descent: use a small random portion of the training dataset to compute the gradient at each iteration

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Heuristic for making the Back Propagation algorithm perform better

It is more of an art than a science

- Input data should be normalized to have approx. same range: standardization or quantile normalization
- Initializing W^h and W^o:
  - Zero is a saddle point: no gradient, no learning
  - Constant init: hidden units collapse by symmetry
  - Solution: random init, ex: $W \sim \mathcal{N}(0; 0.01)$
  - Better inits:
    - Xavier Glorot and Kaming He
    - orthogonal
- Biases can (should) be initialized to zero

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Conclusions:

- Neural Networks is a complex function.
- NN Learning is based on Gradient Descent and Backpropagation algorithm.
- New Regulation algorithms were proposed recently: dropout, …
- New topologies emerge recently.

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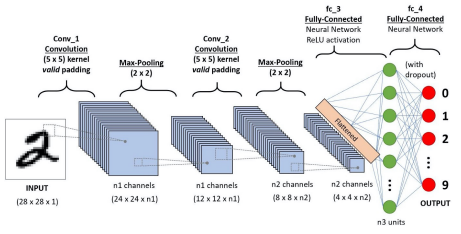
CNN: Convolutional Neural Networks



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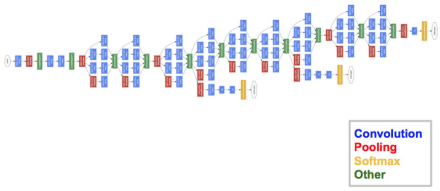
Googlenet/Inception(2014)



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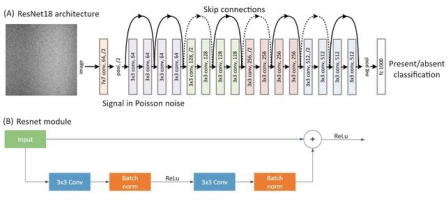
ResNet48



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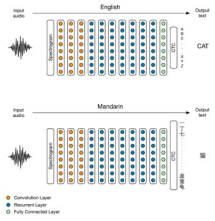
DL Applications: Speech to Text



[Baidu 2014]

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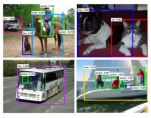
DL Applications: Vision

[Krizhevsky 2012]

[Ciresan et al. 2013]



[Faster R-CNN - Ren 2015]

[NVIDIA dev blog]

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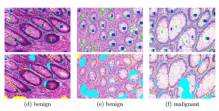
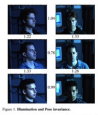
DL Applications: Vision

[Stanford 2017]



[Nvidia Dev Blog 2017]



[FaceNet - Google 2015]

[Facial landmark detection CUHK 2014]

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DL Applications: NLP

[Google Translate System - 2016]

[Socher 2015]

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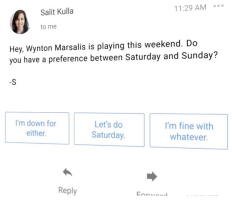
DL Applications: NLP



[Google Inbox Smart Reply]

ChatGPT, MISTRAL, ...

[Amazon Echo / Alexa]

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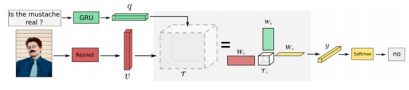
DL Applications: Vision and NLP



[VQA - Mutan 2017]

[Karpathy 2015]

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DL Applications: Image translation

[DeepDream 2015]

[Gatys 2015]

[Ledig 2016]

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DL Applications: Generative Models

Sampled celebrities [Nvidia 2017]

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DL Applications: Generative Models

StackGAN v2 [Zhang 2017]

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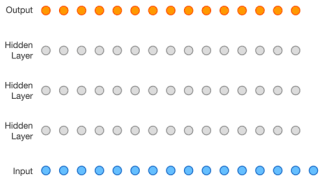
DL Applications: Generative Models



Sound generation with WaveNet
[DeepMind 2017]

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DL Applications: Generative Models

- Guess which one is generated?

- *Tacotron 2 Natural TTS Synthesis by Conditioning WaveNet on Mel Spectrogram Predictions, 2017*

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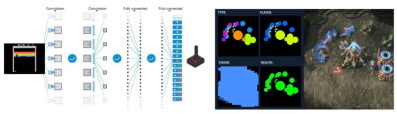
DL Applications: Games

[Deepmind AlphaGo / Zero 2017]



[Atari Games - DeepMind 2016]

[Starcraft 2 for AI research]

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