CSCI-UA 9472. Artificial Intelligence, Neural Networks

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Fall 2020

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So far

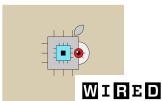
- Simple reflex, random agents, Utility based, Goal based
- Improvement through Search Methods (uninformed (DFS, BFS), informed (BS, A*)).
- Logical Reasoning, Propositional logic + First Order Logic, Inference
- Learning
 - Decision trees, regression, classification
 - Neural Networks

- Neural Networks
 - Current applications
 - History
 - Universal Approximation Properties
 - Training/Backpropagation
 - Local mins and symmetries/ regularization

DarwinAl raises \$3 million for Al that optin HOW APPLE MAKES THE neural networks







FINANCIAL TIMES

Special Report Artificial intelligence + Add to mvFT

Neural networks allow us to 'read faces' in a new way

Facial analysis software is being used to predict sexuality and security



Always Learning, Always Growing: How Neural works Do The Hard Work



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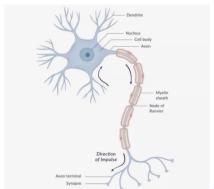
Neural Networks: The biological inspiration

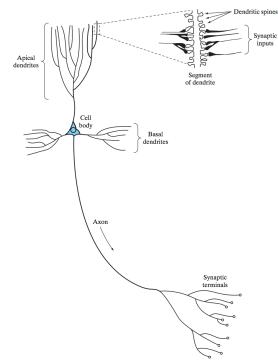
(E. Roberts, Stanford, C. Stergiou & D. Siganos, Imperial College)

- Much is still unknown about how the brain train itself to process information
- A biological neuron collects signals from other neurons through fine structures called dendrites
- The neuron then sends spikes of electrical activity through a long stand named axon which splits into thousands of branches
- At the end of each branch, a structure called synapse converts the activity from the axon into electrical effects that inhibit or excite acitivity in the connected neuron

Neural Networks: The biological inspiration

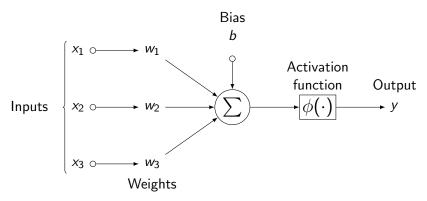
- When a neuron receives excitatory input that is sufficiently large compared to its inhibitory inputs, it sends a spike of electrical activity down its axon
- Learning results from changes in the strength of the synapse (e.g. past patterns of use)



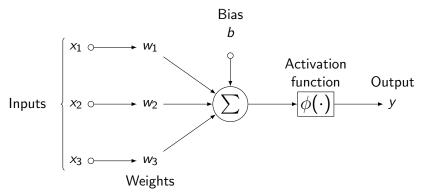


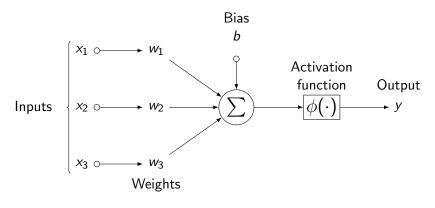
Haykin, Neural Networks Learning Machines

 The original idea is to extract the original features of neurons and their interconnections. An artificial neuron is a device with many inputs and one output



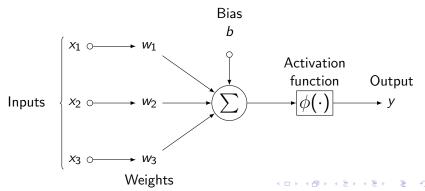
- Just as other ML algorithms, the artificial neuron has two modes of operation: a training mode and a test mode
- In training mode, the neuron learns to fire or not for specific input patterns. In the test mode, the firing is controlled by the firing rule which was learned at training



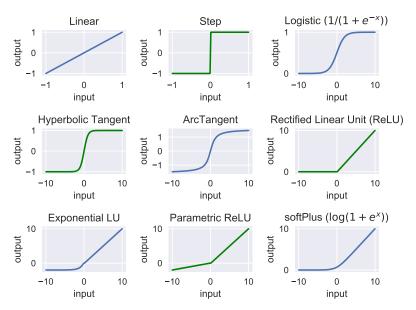


(Single Unit)
$$y = \phi \left(\sum_{j=1}^{3} w_j x_j + b \right)$$

- The function $\phi(\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b)$ is called Ridge function and it varies only in the direction defined by \boldsymbol{w}
- The general regression model $y = \sum_{m=1}^{M} \phi_m(\boldsymbol{w}_m^T \boldsymbol{x})$ is known as Projection pursuit Regression (PPR) as the input to ϕ is the projection of \boldsymbol{x} onto \boldsymbol{w}



Neural Networks: activation functions



How to choose the activation function?

- A good choice is the Relu
- If the network suffers from dead neurons during training, then you can switch to leaky ReLu or Maxout

1962

1969

McCulloch and Pitts



Bernard Widrow



Marcian Hoff

Marvin Minsky



Seymour Papert

- 1943. In order to describe how neurons in the brain might work, McCulloch and Pitts model a simple neuron using electrical circuits (thresholded logic unit)
- 1958. Rosenblatt develops the perceptron (first precursor to modern neural nets)

1962

1969

McCulloch and Pitts



Bernard Widrow



Marcian Hoff

Marvin Minsky



Seymour Papert

• 1958. Together with Rosenblatt's perceptron come the learning rule and the convergence Theorem (1962).

"[The perceptron is] the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence."





Bernard Widrow



Marcian Hoff

Marvin Minsky

1969



Seymour Papert

 1959-1962. Widrow and Hoff develop models called ADALINE and MADALINE ((Multiple ADAptive LINear Elements)) to recognize bineary patterns. The system is still in commercial use.

1958

Rosenblatt

1962

1969

McCulloch and Pitts



Bernard Widrow



Marcian Hoff

Marvin Minsky



Seymour Papert

• 1969. Marvin Minsky questions the ability of the percetron [...] I started to worry about what such a machine could not do. [...] it could tell 'E's from 'F's, and '5's from '6's. But when there were disturbing stimuli near these figures that weren't correlated with them the recognition was destroyed.

1969

McCulloch and Pitts



Bernard Widrow



Marcian Hoff

Marvin Minsky



Seymour Papert

- 1969 (cont.). Together with Seymour Papert, Minsky writes the book "Perceptrons" that kills the perceptron. They prove that the perceptron is unable to learn the XOR function.
- Not clear yet how to train Multi-layers perceptrons.
- Research and funding go down.





Bernard Widrow



Marcian Hoff

Marvin Minsky



Seymour Papert

• (1963). In parallel to those more difficult times, the idea of backpropagation starts to appear (through the work of Arthur Bryson) but does not receive a lot of attention at the time.

Progression Degression 1995 1986 1998



Ronald Williams David Rumelhart

Learning representations by back-propagation errors. published in Nature by Rumelhart, Williams and Hinton. Neural Networks with many hidden layers can be effectively trained by a relatively simple procedure. New extension to the perceptron (which had no ability to learn non linear functions)

Progression Degression
1986 1995 1998







V.Vapnik Y. LeCun

- 1986. Around the same time, it is shown that neural networks have the ability to learn any function (Universal Approximation Theorem)
- Neural nets get back on track
- But there are still many open questions: Overfitting? Optimal structure (Number of neurons, layers) Bad local mins?





1986





v.vapnik C.Cortes

V. Vapnik Y. LeCun

- (1995). Support Vector Machines are introduced by V. Vapnik and C. Cortes. SVMs have shallow architectures.
- Graphical models are becoming increasingly popular
- Together Graphical models and SVMs almost kill research on Artificial Neural Networks







Y. LeCun

- Training deeper networks give poor results..
- (1998) LeCun introduces deep convolutional neural networks.



Y. Bengio Ian Goodfellow





2012

Alex Krizhevsky Geoffrey Hinton Ilya Sutskever



- (2006). Deep Learning appears as a rebranding of ANN
- (2006). Deep Belief Networks (Hinton et al.)
- (2007) Deep Autoencoders (Bengio et al.)



Y. Bengio Ian Goodfellow



Alex Krizhevsky Geoffrey Hinton Ilya Sutskever

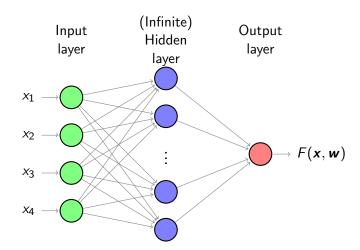


- Neural networks become increasingly popular following massive usage of GPUs
- (2012). This trend is illustrated by the use of AlexNet for image classification (Krizhevsky, Sutskever and Hinton)

Universal approximation

- For M sufficiently large, The simple Projection Pursuit Regression model (PPR) can approximate any function in \mathbb{R}^p .
- This result is known as the Universal Approximation Theorem
- The combination "non linear activation function" + "linear function of the inputs" is part of a class of functions called universal approximators

Universal approximation



Universal Approximation Theorem (Haykin 1994)

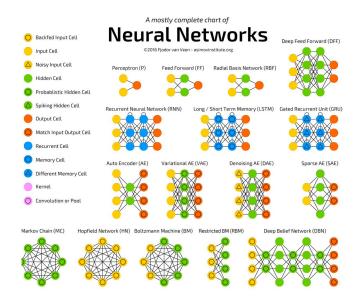
- Let $\phi(\cdot)$ denote a nonconstant, bounded and monotone-increasing continuous function.
- Let I_{m_0} denote the m_0 dimensional unit hypercube $[0,1]^{m_0}$.
- Let $C(I_{m_0})$ denote the space of continuous functions on I_{m_0} .

Then for any function $f \in \mathcal{C}(I_{m_0})$ and $\varepsilon > 0$, there exists an integer \overline{M} and sets of real constants α_i, b_i and w_{ij} where $i = 1, \ldots, M$ and $J = 1, \ldots, d$ such that if we define

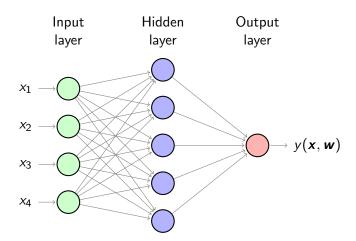
$$F(x_1,\ldots,x_d) = \sum_{i=1}^{\overline{M}} \alpha_i \phi \left(\sum_{j=1}^d w_{ij} x_j + b_i \right)$$
 we have
$$|F(x_1,\ldots,x_d) - f(x_1,\ldots,x_d)| < \varepsilon$$

for all x_1, x_2, \ldots, x_d that lie in the input space.

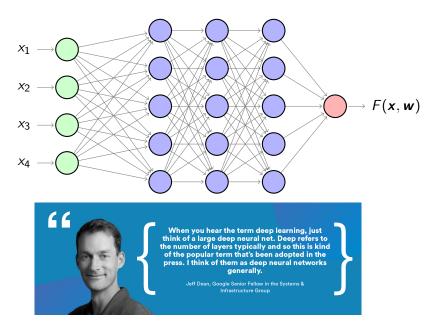
Many possible architectures



One (hidden) layer



Deep neural network



How do we train? (I)

• To train the network, we minimize the empirical risk function. For a given training set $\{x_i, y_i\}$ and a network with weights \boldsymbol{w} , the loss/Empirical risk reads as (as usual there is a statistical intuition for that loss)

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} \|y(\mathbf{x}_i, \mathbf{w}) - t_i\|^2$$

• The general approach at minimizing functions such as $\ell(\mathbf{w})$ is to start from some initial value \mathbf{w} and then follow the gradient to minimize E.

$$\mathbf{w}^{k+1} \leftarrow \mathbf{w}^{(k)} - \eta \nabla E(\mathbf{w}^{(k)})$$

How do we train? (II)

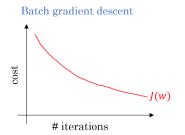
- Minimizing the empirical risk directly is often expensive because the training set of input-output pairs can be very large
- When dealing with practical problems, we will in general not apply gradient descent directly on those function.
- An alternative known as stochastic gradient descent or sequential gradient descent (due to LeCun) relies on the independence of the samples and view the empirical risk as a sum of N independent contributions.
- This approach then optimizes each of those terms sequentially rather than jointly resulting in iterations of the form

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \nabla E_n(\mathbf{w}^{(k)}), \quad n = 1, \dots, N.$$



How do we train? some vocabulary

- Batch gradient descent = use all the data at once
- Minibatch = use subsets
- Epoch = one pass over the full training data



Mini-batch gradient descent

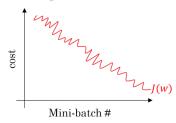
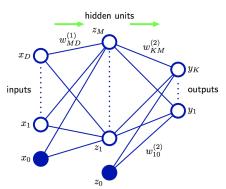


Figure 5.1 Network diagram for the twolaver neural network corresponding to (5.7). The input, hidden, and output variables are represented by nodes, and the weight parameters are represented by links between the nodes, in which the bias parameters are denoted by links coming from additional input and hidden variables x_0 and z_0 . Arrows denote the direction of information flow through the network during forward propagation.



Bishop, Pattern Recognition and ML

• Consider the simple two layers neural net

$$y_k(\mathbf{x}, \mathbf{w}) = \sigma \left(\sum_{j=1}^N w_{k,j}^{(2)} \sigma \left(\sum_{i=1}^D w_{ji}^{(1)} x_i + w_{j0}^{(1)} \right) + w_{k0}^{(2)} \right)$$



- Computing the gradient of a complex nested function involving a large number of layers is painful.
- In practice, optimization relies on an idea called backpropagation. In backpropagation, the information is propagated through the network first forward and then backwards in order to update the weights.
- The method proceeds in two steps,
 - During the first step, the error vector containing the residuals is propagated backwards in the network to evaluate the derivatives
 - During the second step, the derivatives that were computed in the first step are used to update the weights.

 For an empirical risk function which reads as a sum of M independent contributions,

$$E=\sum_{m=1}^M E_m,$$

• In the sequential framework, we can focus on a single E_m . In a NN, each unit computes a weighted sum s_i of the inputs,

$$a_j^{(\ell)} = \sum_i w_{ji}^{\ell} z_i^{(\ell-1)}$$

The sum is then transformed through the activation function σ as $z_i^\ell = \sigma(a_i^\ell)$.

Applying the chain rule, we get

$$\frac{\partial E_m}{\partial w_{ji}^{(\ell)}} = \frac{\partial E_m}{\partial a_j^{(\ell)}} \frac{\partial a_j^{(\ell)}}{\partial w_{ji}}$$



Notice that

$$\frac{\partial a_j^{(\ell)}}{\partial w_{ji}} = z_i^{(\ell-1)}$$

• If we let E_m to denote the log-loss or the RSS loss, we have

$$E_{m,\ell_2} = \frac{1}{2} \sum_{k} (y_{n,k}(\mathbf{x}, \mathbf{w}) - t_{n,k})^2$$

$$E_{m,LL} = -t_{n,k} \log(y_{n,k}(\mathbf{x}, \mathbf{w})) + (1 - t_{n,k}) \log(1 - y_{n,k}(\mathbf{x}, \mathbf{w}))$$

• The gradient w.r.t the weights appearing in the last layer can read as

$$\frac{\partial E_m}{\partial a_{\nu}^{\text{out}}} = (y_{n,k} - t_{n,k}) = \delta_{\text{out},k}$$

• Moreover, all the other derivatives w.r.t the $a_n^{(\ell)}$ (of layer ℓ) can be computed using the chain rule

$$\frac{\partial E_m}{\partial a_j^{(\ell-1)}} = \sum_{k=1}^K \frac{\partial E_m}{\partial a_k^{(\ell)}} \frac{\partial a_k^{(\ell)}}{\partial a_j^{\ell-1}}$$

• The relation between the inputs $a_{\vec{k}}^\ell$ from the ℓ^{th} layer and the inputs $a_j^{(\ell-1)}$ from the previous $(\ell-1)$ layer reads as

$$a_k^\ell = \sum_{j=1}^D w_{kj}^\ell \sigma(a_j^{(\ell-1)})$$

 $a_j^{\ell-1}$ appears in each of the a_k^{ℓ} for $k=1,\ldots,K$. When taking the derivative, we must therefore take eah of those contributions into account.



• The relation between the inputs a_k^ℓ from the ℓ^{th} layer and the inputs $a_j^{(\ell-1)}$ from the previous $(\ell-1)$ layer reads as

$$a_k^\ell = \sum_{j=1}^D w_{kj}^\ell \sigma(a_j^{(\ell-1)})$$

• From this, we get the equation

$$rac{\partial \mathsf{a}_k^{(\ell)}}{\partial \mathsf{a}_j^{(\ell-1)}} = \mathsf{w}_{kj}^\ell \sigma'(\mathsf{a}_j^{(\ell-1)})$$

• Which we can substitute in the gradient $\frac{\partial E_m}{\partial a_i^{(\ell-1)}}$

$$\delta_{j}^{\ell-1} = \frac{\partial E_{m}}{\partial a_{j}^{(\ell-1)}} = \sum_{k=1}^{K} \frac{\partial E_{m}}{\partial a_{k}^{(\ell)}} \frac{\partial a_{k}^{(\ell)}}{\partial a_{j}^{\ell-1}} = \sum_{k=1}^{K} \sigma'(a_{j}^{(\ell-1)}) w_{k,j}^{(\ell)} \delta_{k}^{(\ell)}$$

Backpropagation (summary)

- Propagate the feature vectors from the training set forward and compute all the outputs to the activation functions $a_j^{(\ell)}$, $\sigma(a_j^{(\ell)})$ as well as the derivatives $\sigma'(a_j^{(\ell)})$.
- Evaluate the output $\delta_k^{\mathrm{out}} = (t_k y_k)$
- Backpropagate those $\delta_k^{({
 m out})}$ to get the $\delta_j^{(\ell)}$ for all layers ℓ
- Once you have the $\delta_j^{(\ell)}$ for all layers ℓ and indices j, compute the derivatives of the empirical risk by using

$$\frac{\partial E_m}{\partial w_{ij}^{(\ell)}} = \frac{\partial E_m}{\partial a_j^{\ell}} \frac{\partial a_j^{(\ell)}}{\partial w_{ji}^{(\ell)}} = \delta_j^{(\ell)} \sigma(a_i^{(\ell)})$$