

MACHINE LEARNING

LESSON 9: Neural Networks I

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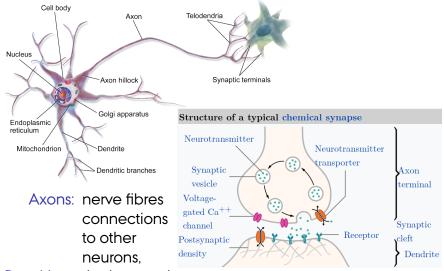




L09: Neural Networks I: Agenda

- ▶ BB | Hand-ins Deadlines: J2, 9 April.
- ▶ J3 custom projects: email a J3-project-description.
- ▶ GPU Cluster: use it, but remember GPU mem trick!
- The Biological Neuron,
 - historical points of neural nets,
 - GPU vs the brain,
 - exercise: L09/neuron.ipynb with ALT OPTIONAL exe.
- ▶ The Perceptron
 - activation functions
 - exercise: L09/perceptron.ipynb
- Multi-layer Perceptrons (MLPs)
 - definitions and more historical points
 - using Keras for building MLPs
 - exercise: L09/keras_mlp_moon.ipynb
 - exercise: L09/keras_mlp_mnist.ipynb

The Biological Neuron



Dendrites: the input points to a neuron

Synapses: connection points btw. neurons.

[https://en.wikipedia.org/wiki/Axon]

History of Neural Networks

Engineered NN Systems Inspired by the Biological Brain

Focus has changed from biology understanding to beyond the neuroscientific perspective:

- began as engineered systems inspired by the biological brain—or as understanding of brain function,
- know as cybernetics in the 1940s-1960s,
- know as connectionism in the 1980s-1990s,
- Now: "a more general principle of learning [..], that are not necessarily neurally inspired", [□L].

Let's look at a history timeline of NNs..

History of Neural Networks

ML Summers and Winters [DL]

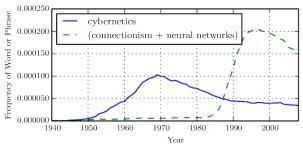


Figure 1.7: The figure shows two of the three historical waves of artificial neural nets research, as measured by the frequency of the phrases "cybernetics" and "connectionism" or "neural networks" according to Google Books (the third wave is too recent to appear). The first wave started with cybernetics in the 1940s–1960s, with the development of theories of biological learning (McCulloch and Pitts, 1943; Hebb, 1949) and implementations of the first models such as the perceptron (Rosenblatt, 1958) allowing the training of a single neuron. The second wave started with the connectionist approach of the 1980–1995 period, with back-propagation (Rumelhart et al., 1986a) to train a neural network with one or two hidden layers. The current and third wave, deep learning, started around 2006 (Hinton et al., 2006; Bengio et al., 2007; Ranzato et al., 2007a), and is just now appearing in book form as of 2016. The other two waves similarly appeared in book form much later than the corresponding scientific activity occurred.

History of Neural Networks

Important Discoveries in the History of NN

```
1670: Leibniz, L'Hôpital, chain rule differentiation
1805/9: Legendre and Gauss, least-squares
1847: Cauchy, numerical gradient descent
1901: Pearson, PCA
1936: Fisher, linear discriminant analysis of iris data
(probability theory: F-distribution)
1943: McCulloch and Pitts neuron
1949: Hebbs rule for self-organized learning
1957: Rosenblatts perceptron and supervised learning
1960-70: Multilayer perceptrons
1969: Minsky and Papert, XOR crisis, first winter
1985-86: BProp. LeCun. Rumelhart et at. second summer
95'ish: second winter
2006'ish: GPUs, start of third summer
2009: Jarrett, reLU activation function
2022'ish: third winter?
```

The GPU vs the Brain

GPU 1080		ine Human Brain			
transistors	$7.2 \cdot 10^9$	neurons	$\sim 86 \cdot 10^{9}$		
physical scale	16nm	physical scale	\sim 0.05 mm		
	(FinFET)	synapses	$\sim 1.5 \cdot 10^{14}$		
		connections	$\sim 10^3 - 10^4$		
		per neuron			
frequency	1.6 GHz	frequency	\sim 10 Hz		
power	180 W	power	\sim 13-20 W		
consumption	(TPD)	consumption			

Cerebral cortex

The Human Drain

NOTE:

African elephant neurons: 257 · 10⁹ Cerebral cortex neurons:

Human: 16 · 10⁹

Long-finned pilot whale: $37 \cdot 10^9$

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[https://hothardware.com/reviews/nvidia-geforce-gtx-1080-pascal-gpu-review]
[https://en.wikipedia.org/wiki/List_of_animals_by_number_of_neurons]

[https://en.wikipedia.org/wiki/Cerebral_cortex]

[https://hypertextbook.com/facts/2004/SamanthaCharles.shtml]

Definition

History:

1943: McCulloch-Pitts: artificial neuron + network.

1957: Rosenblatt: the perceptron. Based on linear regressor + Heaviside activation function.

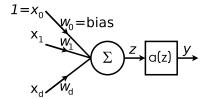
A linear regressor, with $\mathbf{x} \equiv [1 \ x_1 \ x_2 \ \cdots \ x_d]^{\top}$

$$z = \mathbf{w}^{\top} \mathbf{x}$$

= $w_0 \cdot 1 + w_1 x_1 + w_2 x_2 + \dots + w_d x_d$

plus activation function = the Perceptron (linear-threshold unit, LTU)

$$y_{\text{neuron}}(\mathbf{x}; \mathbf{w}) = a(z) = a(\mathbf{w}^{\top}\mathbf{x})$$



The Activation Funtion, $a(\cdot)$

Original Rosenblatt perceptron activation fun

$$a_{\mathsf{Rosenblatt}}(z) = \mathsf{Heaviside}(z) = \left\{ egin{array}{ll} 0, & \mathsf{if}\ z < 0 \ 1, & \mathsf{if}\ z \geq 0 \end{array}
ight.$$

but many other possible

$$a_{\text{sign}}(z) = \text{sgn}(z) = \left\{ egin{array}{ll} -1, & \text{if } z < 0 \\ 0, & \text{if } z = 0 \\ 1, & \text{if } z \geq 0 \end{array} \right.$$

Much debated, and different favorites thought different ML-epochs ...or summers.

More Activation Funtions, $a(\cdot)$

Logistic Sigmoid

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

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

$$= a(z)(1-a(z))$$

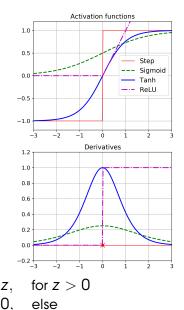
Hyperbolic Tangens

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

Rectified Linear Unit, ReLU

$$a(z) = z^{+} = \max(0, z) = \begin{cases} z, \\ 0, \end{cases}$$

$$\frac{da(z)}{dx} = \begin{cases} 1, & \text{for } z > 0 \\ 0, & \text{else} \end{cases}$$



Properties of the Activation Function

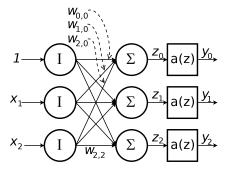
- linear: if multiple layers use identity a(z) = z, the network is equivalent to a single-layer,
- non-linear: two-layer neural network is a universal function approximator,
- (continuously) differentiable: for learning algo,
- monotonic: convex error surf for single layer model.

[https://en.wikipedia.org/wiki/Activation_function]

Name •	Plot •	Equation •	Derivative (with respect to x)	Range •	Order of continuity	Monotonic •	Monotonic derivative
Identity	-/-	f(x) = x	f'(x) = 1	$(-\infty,\infty)$	C^{∞}	Yes	Yes
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$	{0,1}	C^{-1}	Yes	No
Logistic (a.k.a. Sigmoid or Soft step)		$f(x)=\sigma(x)=rac{1}{1+e^{-x}}$ [1]	f'(x) = f(x)(1 - f(x))	(0,1)	C^{∞}	Yes	No
TanH		$f(x) = \tanh(x) = \frac{(e^x - e^{-x})}{(e^x + e^{-x})}$	$f'(x) = 1 - f(x)^2$	(-1, 1)	C^{∞}	Yes	No
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$	$\left(-\frac{\pi}{2},\frac{\pi}{2}\right)$	C^{∞}	Yes	No
ArSinH		$f(x)=\sinh^{-1}(x)=\ln\Bigl(x+\sqrt{x^2+1}\Bigr)$	$f'(x) = \frac{1}{\sqrt{x^2 + 1}}$	$(-\infty,\infty)$	C^{∞}	Yes	No

MLP, but only one layer...

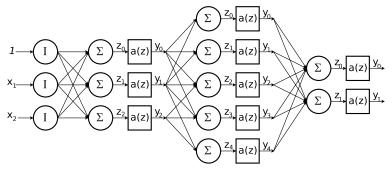
Stacking up neurons or perceptrons into an array



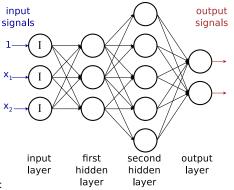
Deep feedforward networks, also often called feedforward neural networks, or multi-layer perceptrons (MLPs), are the quintessential deep learning models. [DL, p167]

MLP, three layers, fully connected...

Stacking arrays of perceptrons into layers



MLP, three layers, fully connected, simplified nodes...



MLP nomenclature:

input layer: handles the input x data,

output layer: only visible output signal from the network,

hidden layer(s): internal layers in the network,

fully connected: all nodes in layer connected to all neurons in the previous/next layer,

feed-forward: the signals flows only forward in the network

(in contrast to feed-backward in BProp),

Backpropagation: or BProp, training algo of NN, more in later lesson, Deep-learning networks: MLP with several hidden layers, say >2?

From Perceptron training to MLP Training

Training perceptrons and Hebb's postulate:

"Cells that fire together wire together."

and

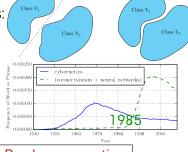
[..] explain synaptic plasticity, the adaptation of brain neurons during the learning process.

[https://en.wikipedia.org/wiki/Hebbian_theory]

 for linearly separable problems: perceptron convergence theorem,

- but what about XOR problems: Minsky/Papert XOR crisis,
- and how do you train MLP's?

No method existed until...



Decision

1985/86: LeCun, Rumelhart et al.: Backpropagation

History: Dataset Size vs Time [DL]

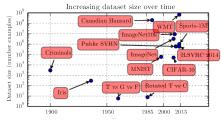


Figure 1.8: Dataset sizes have increased greatly over time. In the early 1900s, statisticians studied datasets using hundreds or thousands of manually compiled measurements (Garson, 1900; Gosset, 1908; Anderson, 1935; Fisher, 1936). In the 1950s through 1980s, the pioneers of biologically inspired machine learning often worked with small, synthetic datasets, such as low-resolution bitmaps of letters, that were designed to incur low computational cost and demonstrate that neural networks were able to learn specific kinds of functions (Widrow and Hoff, 1960; Rumelhart et al., 1986b). In the 1980s and 1990s, machine learning became more statistical in nature and began to leverage larger datasets containing tens of thousands of examples such as the MNIST dataset (shown in Fig. 1.9) of scans of handwritten numbers (LeCun et al., 1998b). In the first decade of the 2000s, more sophisticated datasets of this same size, such as the CIFAR-10 dataset (Krizhevsky and Hinton, 2009) continued to be produced. Toward the end of that decade and throughout the first half of the 2010s, significantly larger datasets, containing hundreds of thousands to tens of millions of examples, completely changed what was possible with deep learning. These datasets included the public Street View House Numbers dataset (Netzer et al., 2011), various versions of the ImageNet dataset (Deng et al., 2009, 2010a; Russakovsky et al., 2014a), and the Sports-IM dataset (Karpathy et al., 2014). At the top of the graph, we see that datasets of translated sentences, such as IBM's dataset constructed from the Canadian Hansard (Brown et al., 1990) and the WMT 2014 English to French dataset (Schwenk, 2014) are typically far ahead of other dataset sizes.

History: MLP Network Size vs Time [DL]

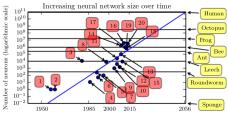


Figure 1.11: Since the introduction of hidden units, artificial neural networks have doubled in size roughly every 2.4 years. Biological neural network sizes from Wikipedia (2015).

- Perceptron (Rosenblatt, 1958, 1962)
 Adaptive linear element (Widrow and Hoff, 1960)
- Neocognitron (Fukushima, 1980)
- L. Early back-propagation network (Rumelhart et al., 1986b)
- Recurrent neural network for speech recognition (Robinson and Fallside, 1991)
- 6. Multilaver 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)
- Echo state network (Jaeger and Haas, 2004)
- Deep belief network (Hinton et al., 2006)
- GPU-accelerated convolutional network (Chellapilla et al., 2006)
- 12. Deep Boltzmann machine (Salakhutdinov and Hinton, 2009a)
- 13. GPU-accelerated deep belief network (Raina et al., 2009)
- Unsupervised convolutional network (Jarrett et al., 2009)
- GPU-accelerated multilayer perceptron (Ciresan et al., 2010)
- OMP-1 network (Coates and Ng, 2011)
- 17. Distributed autoencoder (Le et al., 2012)
- Multi-GPU convolutional network (Krizhevsky et al., 2012)
 COTS HPC unsupervised convolutional network (Coates et al., 2013)
- 20. GoogLeNet (Szegedy et al., 2014a)

History: MLP Neuron Connections vs Time [DL]

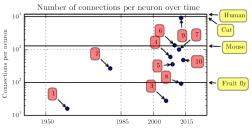


Figure 1.10: Initially, the number of connections between neurons in artificial neural networks was limited by hardware capabilities. Today, the number of connections between neurons is mostly a design consideration. Some artificial neural networks have nearly as many connections per neuron as a cat, and it is quite common for other neural networks to have as many connections per neuron as smaller mammals like mice. Even the human brain does not have an exorbitant amount of connections per neuron. Biological neural network sizes from Wikipedia (2015).

- 1. Adaptive linear element (Widrow and Hoff, 1960)
- 2. Neocognitron (Fukushima, 1980)
- 3. GPU-accelerated convolutional network (Chellapilla et al., 2006)
- 4. Deep Boltzmann machine (Salakhutdinov and Hinton, 2009a)
- Unsupervised convolutional network (Jarrett et al., 2009)
- 6. GPU-accelerated multilayer perceptron (Circsan et al., 2010)
- 7. Distributed autoencoder (Le et al., 2012)
- 8. Multi-GPU convolutional network (Krizhevsky et al., 2012)
- COTS HPC unsupervised convolutional network (Coates et al., 2013)
- 10. GoogLeNet (Szegedy et al., 2014a)

History: MLP Error Rate vs Time [DL]

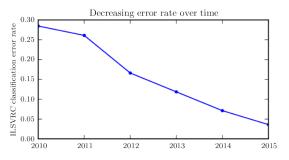
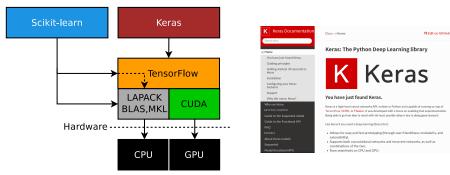


Figure 1.12: Since deep networks reached the scale necessary to compete in the ImageNet Large Scale Visual Recognition Challenge, they have consistently won the competition every year, and yielded lower and lower error rates each time. Data from Russakovsky et al. (2014b) and He et al. (2015).

Keras and Tensorflow



Using the Keras API instead of Scikit-learn or TensorFlow



NOTE:

- documentation: https://keras.io/
- keras provides a fit-predict-interface,
- many similiarities to Scikit-learn,
- but also many differences!

Building Keras MLPs

Using the Keras Sequential class, programatical build up model:

```
ss, — 1
```

```
# Build Keras model
    model = Sequential()
    model.add(Dense(input_dim=2, units=3, activation="tanh", ..)
    model.add(Dense(units=5, activation="relu", ..)
    model.add(Dense(units=2, activation="softmax"))
6
7
    X_train, .. = train_test_split(X, y, .. )
8
9
10
    y_train_categorical = to_categorical(y_train, num_classes=2)
    y_test_categorical = to_categorical(y_test, num_classes=2)
12
14
    history = model.fit(X_train, y_train_categorical, ...
15
16
    score = model.evaluate(X_test, y_test_categorical)
18
```

Input Layer: Categorical Encoding



For MLP Classification

One-hot to_categorical(\cdot) encoding in Keras:

- input layer: one-hot class encoding,
- output layer: one neuron per output class that fires, and use softmax for output neurons
- beware of misformated classes.

```
import numpy as np
    from keras.utils.np_utils import to_categorical
    y = np.array([1, 2, 0, 4, -1])
    y_cat = to_categorical(y)
    print(y_cat)
    \#[[0. 1. 0. 0. 0.]] \Rightarrow i=0, class 1
    # [0. 0. 1. 0. 0.] => i=1, class 2
    \# [1. 0. 0. 0. 0.] \Rightarrow i=2, class 0
  # [0. 0. 0. 0. 1.] => i=3, class 4
    # [0. 0. 0. 0. 1.1] \Rightarrow i=4. also class 4!
                             NOTE: no class 3
14
```

[L09/Extra/keres_to_categorical.ipynb]

Output Layer: Softmax Function



For MLP Classification: Assing a Probability for each Class

Softmax (softargmax/normalized exponential) definition

$$\operatorname{softmax}(\mathbf{x})_i = \frac{\mathbf{e}^{x_i}}{\sum_{i=1}^n \mathbf{e}^{x_i}}$$

softmax: smooth approx. of argmax function.

argmax: the index-of-the-max-value for some data.

 $print(f"np.argmax(softmax(x)) = \{np.argmax(softmax(x))\}"\}$

```
# python demo of softmax/argmax
x = np.array([1, 2, -4, 5, 1])
i = np.argmax(x)

PrintMatrix(x,"x = ")
print(f"np.argmax(x) = {np.argmax(x)}")

def softmax(x):
    z = np.exp(x)
    s = np.sum(z)
    return z / s

PrintMatrix(softmax(x), "softmax(x) = ")
# output
x = [1 2 -4 5 1]
np.argmax(x) = 3
softmax(x) = [0.02 0.05 0. 0.92 0.02]
np.argmax(softmax(x)) = 3
```

[L09/Extra/softmax.ipynb]

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MLP Effect of Number of Hidden Layers

How Many Hidden Layers?

MNIST Search Quest Exercise:

- ► ITMAL Grp10: used a 20-50-70-100-70-50-20 layer MLPClassifier,
- found layers by trial-and-error,
- but what are the optimal hidden layer sizes and neurons per hidden layer?

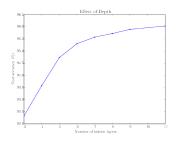


Figure 6.6. Empirical results showing that deeper networks generalize better when used to transcribe multi-digit numbers from photographs of addresses. Data from Goodfellow et al. (2014d). The test set accuracy consistently increases with increasing depth. See Fig. 6.7 for a control experiment demonstrating that other increases to the model size do not yield the same effect.