

Foundations of Machine Learning in Python

Moritz Wolter

September 23, 2022

High-Performance Computing and Analytics Lab

Neural networks

Classification with neural networks

Neural networks

The wonders of the human visual system



Figure: Most humans effortlessly recognize the digits 5 0 4 1 9 2 1 3.

Biological motivation

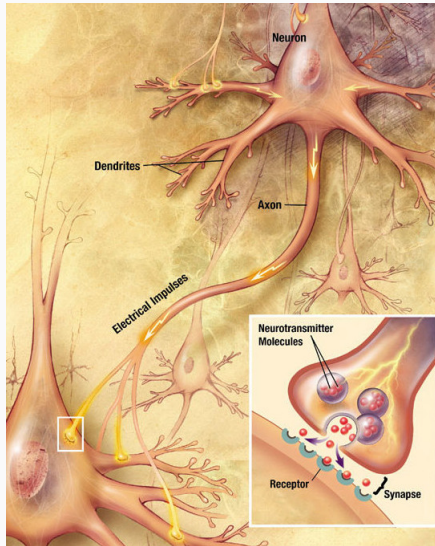


Image source: en.wikipedia.org

Foundations of Machine Learning in Python

└ Neural networks

└ Biological motivation

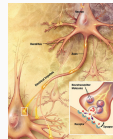
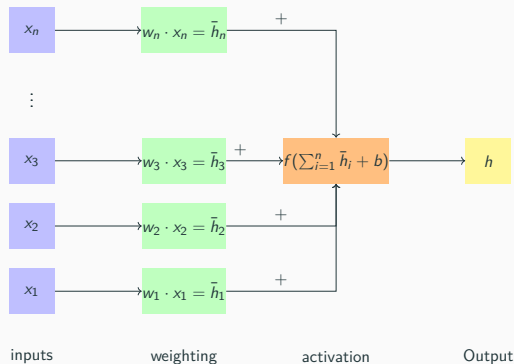


Image source: en.wikipedia.org

- A Human brain contains approximately 86 billion neurons.
- 10^{14} to 10^{15} synapses connect these neurons.
- Neurons receive inputs from dendrites.
- and can produce output signals along its axon.
- Axons connect neurons, modelled by weighting inputs wx .
- Neuron inputs can be inhibitive (negative weight) or
- excitatory (positive weight).
- If enough inputs excite a neuron it fires.
- The activation function aims to mimic this behaviour.
- Even though neural networks started out as biologically motivated,
- engineering efforts have since diverged from biology.

The perceptron

Can computers recognize digits? Mimic biological neurons,



Formally a single perceptron is defined as

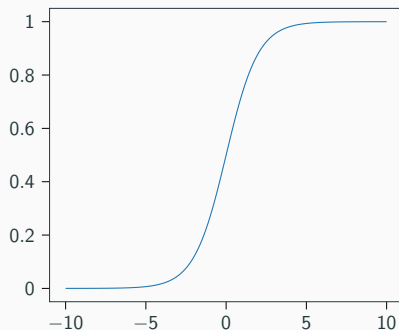
$$f(\mathbf{w}^T \mathbf{x}) = h \quad (1)$$

with $\mathbf{w} \in \mathbb{R}^n$, $\mathbf{x} \in \mathbb{R}^n$ and $h \in \mathbb{R}$.

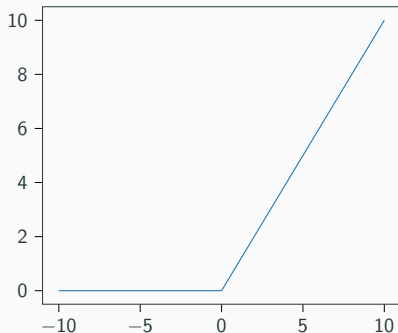
The activation function f

Two popular choices for the activation function f .

Sigmoid $\sigma(x)$

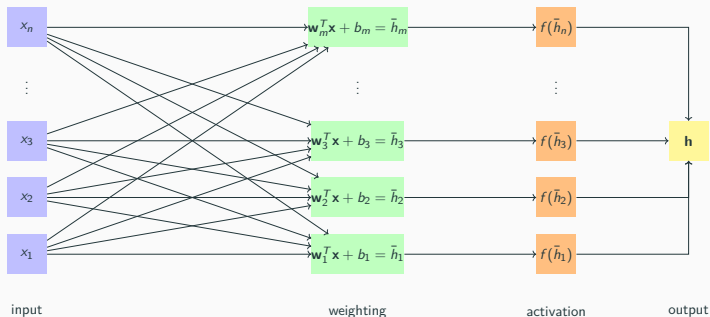


ReLU(x)



Arrays of perceptrons

Let's extend the definition to cover an array of perceptrons:



Every input is connected to every neuron. In matrix language, this turns into

$$\bar{\mathbf{h}} = \mathbf{W}\mathbf{x} + \mathbf{b}, \quad \mathbf{h} = f(\bar{\mathbf{h}}). \quad (2)$$

With $\mathbf{W} \in \mathbb{R}^{m,n}$, $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^m$, and $\mathbf{h}, \bar{\mathbf{h}} \in \mathbb{R}^m$.

The loss function

To choose weights for the network, we require a quality measure. We already saw the mean squared error cost function,

$$C_{\text{mse}} = \frac{1}{2} \sum_{k=1}^n (\mathbf{y}_k - \mathbf{h}_k)^2 = \frac{1}{2} (\mathbf{y} - \mathbf{h})^T (\mathbf{y} - \mathbf{h}) \quad (3)$$

This function measures the squared distance from each desired output. \mathbf{y} denotes the desired labels, and \mathbf{h} represents network output.

The gradient of the mse-cost-function

Both the mean squared error loss function and our dense layer are differentiable.

$$\frac{\partial C_{\text{mse}}}{\partial \mathbf{h}} = \mathbf{h} - \mathbf{y} = \triangle_{\text{mse}} \quad (4)$$

The \triangle symbol will re-appear. It always indicates incoming gradient information from above. If the labels are a vector of shape \mathbb{R}^m , \triangle and the network output \mathbf{h} must share this dimension.

The gradient of a dense layer

The chain rule tells us the gradients for the dense layer [Nie15]

$$\delta \mathbf{W} = [f'(\bar{\mathbf{h}}) \odot \Delta] \mathbf{x}^T, \quad \delta \mathbf{b} = f'(\bar{\mathbf{h}}) \odot \Delta, \quad (5)$$

$$\delta \mathbf{x} = \mathbf{W}^T [f'(\bar{\mathbf{h}}) \odot \Delta], \quad (6)$$

where \odot is the element-wise product. δ denotes the cost function gradient for the value following it [Gre+16].

Modern libraries will take care of these computations for you!

You can choose to verify these equations yourself by completing the optional deep learning project.

Foundations of Machine Learning in Python

└ Neural networks

└ The gradient of a dense layer

The chain rule tells us the gradients for the dense layer [Nie15]

$$\partial \mathbf{W} = [f'(\bar{\mathbf{h}}) \odot \Delta] \mathbf{x}^T, \quad \partial \mathbf{b} = f'(\bar{\mathbf{h}}) \odot \Delta, \quad (5)$$

$$\delta \mathbf{x} = \mathbf{W}^T [f'(\bar{\mathbf{h}}) \odot \Delta], \quad (6)$$

where \odot is the element-wise product. δ denotes the cost function gradient for the value following it [Gre+16].

Modern libraries will take care of these computations for you! You can choose to verify these equations yourself by completing the optional deep learning project.

On the board, derive: Recall the chain rule $(g(h(x)))' = g'(h(x)) \cdot h'(x)$.

For the activation function, we have,

$$\bar{\mathbf{h}} = f(\bar{\mathbf{h}}) \quad (7)$$

$$\Rightarrow \delta \bar{\mathbf{h}} = f'(\bar{\mathbf{h}}) \odot \Delta \quad (8)$$

For the weight matrix,

$$\bar{\mathbf{h}} = \mathbf{W}\mathbf{x} + \mathbf{b} \quad (9)$$

$$\Rightarrow \delta \mathbf{W} = \delta \bar{\mathbf{h}} \mathbf{x}^T = [f'(\bar{\mathbf{h}}) \odot \Delta]^T \mathbf{x} \quad (10)$$

For the bias,

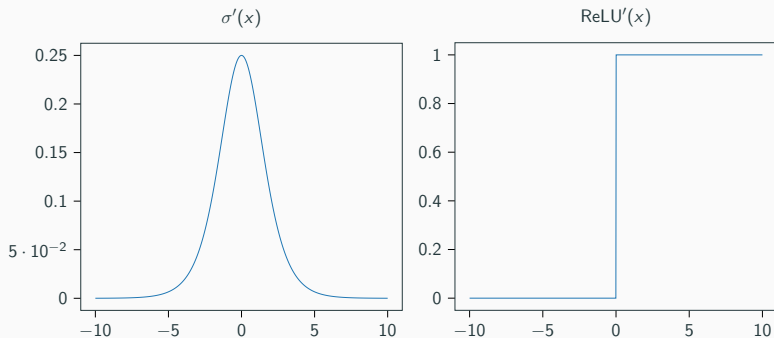
$$\bar{\mathbf{h}} = \mathbf{W}\mathbf{x} + \mathbf{b} \quad (11)$$

$$\Rightarrow \delta \mathbf{b} = 1 \odot \delta \bar{\mathbf{h}} = [f'(\bar{\mathbf{h}}) \odot \Delta] \quad (12)$$

Derivatives of our activation functions

$$\sigma'(x) = \sigma \cdot (1 - \sigma(x)) \quad (13)$$

$$\text{ReLU}' = H(x) \quad (14)$$



Perceptrons for functions

The network components described this far already allow function learning. Given a noisy input signal $\mathbf{x} \in \mathbb{R}^m$ and a ground through output $y \in \mathbb{R}^m$, define,

$$\mathbf{h} = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b}) \quad (15)$$

$$\mathbf{y}_{\text{net}} = \mathbf{W}_y \mathbf{h} \quad (16)$$

With $\mathbf{W} \in \mathbb{R}^{m,n}$, $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{b} \in \mathbb{R}^m$. m and n denote the number of neurons and the input signal length. For signal denoising, input and output have the same length. Therefore $\mathbf{W}_y \in \mathbb{R}^{n,m}$.

Denoising a cosine

Training works by iteratively descending along the gradients. For \mathbf{W} the weights at the next time step τ are given by,

$$\mathbf{W}_{\tau+1} = \mathbf{W}_{\tau} + \epsilon \cdot \delta \mathbf{W}_{\tau}. \quad (17)$$

The step size is given by ϵ . At $\tau = 0$ matrix entries are random. $\mathcal{U}[-0.1, 0.1]$ is a reasonable choice here. The process is the same for all other network components.

Denoising a cosine

Optimization for 500 steps leads to the output below:

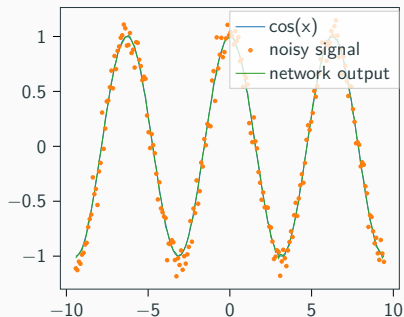
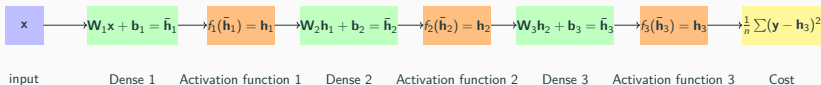


Figure: The cosine function is shown in blue. A noisy network input in orange, and a denoised network output in green.

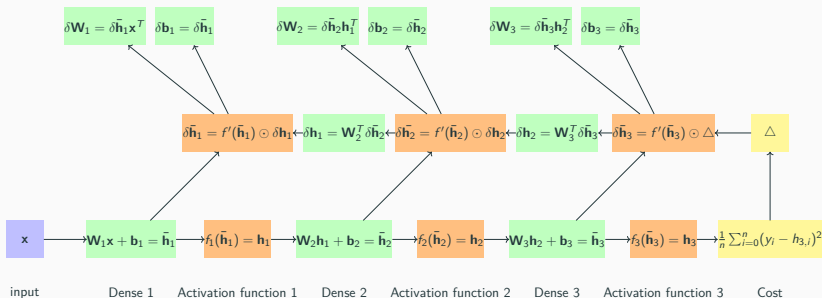
Classification with neural networks

Deep multi-layer networks

Stack dense layers and activations to create deep networks.



Backpropagation



The cross-entropy loss

The cross entropy loss function is defined as [Nie15; Bis06]

$$C_{ce}(\mathbf{y}, \mathbf{o}) = - \sum_k^{n_o} (\mathbf{y}_k \ln \mathbf{o}_k) + (\mathbf{1} - \mathbf{y}_k) \ln(\mathbf{1} - \mathbf{o}_k). \quad (18)$$

If a sigmoidal activation function produced \mathbf{o} the gradients can be computed using [Nie15; Bis06]

$$\frac{\partial C_{ce}}{\partial \mathbf{h}} = \sigma(\mathbf{o}) - \mathbf{y} = \Delta_{ce} \quad (19)$$

Foundations of Machine Learning in Python

└ Classification with neural networks

└ The cross-entropy loss

The cross entropy loss function is defined as [Nie15; Bia06]

$$C_{ce}(\mathbf{y}, \mathbf{a}) = - \sum_k \left[y_k \ln a_k + (1 - y_k) \ln(1 - a_k) \right]. \quad (18)$$

If a sigmoidal activation function produced \mathbf{o} the gradients can be computed using [Nie15; Bia06]

$$\frac{\partial C_{ce}}{\partial \mathbf{a}} = \sigma(\mathbf{o}) - \mathbf{y} = \Delta_{ce} \quad (19)$$

TODO: find the proof.

The MNIST-Dataset



Figure: The MNIST-dataset contains 70k images of handwritten digits.

Validation and Test data splits

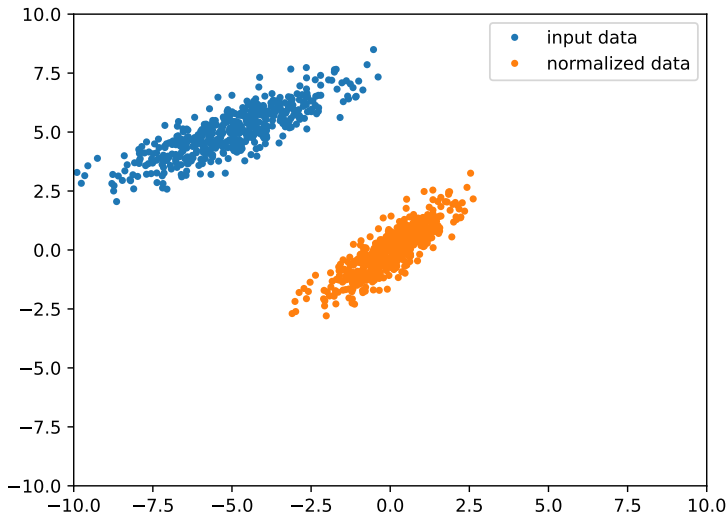
- To ensure the correct operation of the systems we devise, it is paramount to hold back part of the data for validation and testing.
- Before starting to train, split off validation and test data.
- The 70k MNIST samples could, for example, be partitioned into 59k training images. 1k validation images and 10k test images.

Standard initializations and learning algorithms assume an approximately standard normal distribution of the network inputs. Consequently we must rescale the data using,

$$\mathbf{X}_n = \frac{\mathbf{X} - \mu}{\sigma} \quad (20)$$

With μ and σ the training set mean and standard deviation. And the data matrix $\mathbf{X} \in \mathbb{R}^{b,n}$ with a row for each data point. b denotes the number of data points and n the data dimension.

The effect of normalization



Whitening the inputs

Instead of deviding by the standard deviation, rescale the centered data with the singular values of the covariance matrix.

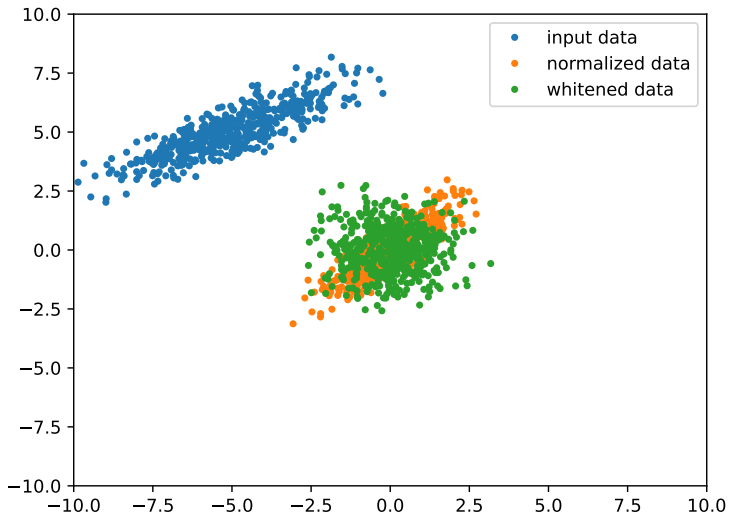
$$\mathbf{C} = \frac{1}{n}(\mathbf{X} - \mu)^T(\mathbf{X} - \mu) \quad (21)$$

With n as the total number of data points. Whitening now uses the singular values of \mathbf{C} to rescale the data,

$$\mathbf{x}_w = \frac{(\mathbf{x} - \mu)}{\sqrt{\sigma} + \epsilon} \quad (22)$$

With ϵ i.e. equal to $1e^{-8}$ for numerical stability.

The effect of Whitening



Label-encoding

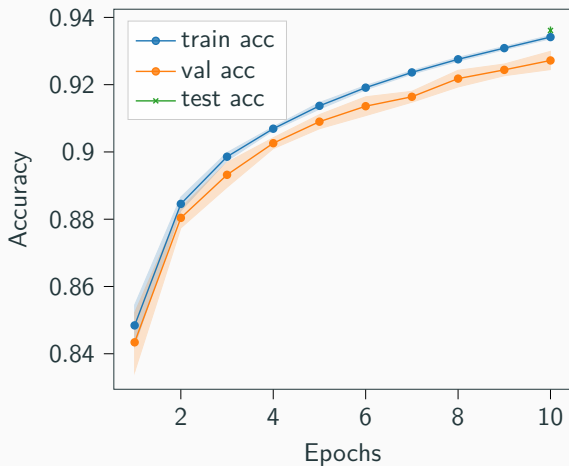
It has proven useful to have individual output neurons produce probabilities for each class. Given integer labels $1, 2, 3, 4, \dots \in \mathbb{Z}$. One-hot encoded label vectors have a one at the labels positions and zeros elsewhere. I.e.

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}, \dots \quad (23)$$

for the integer label sequence above.

MNIST-Classification

Training a three-layer dense network on mnist for five runs leads to:



Conclusion

- Preprocessing followed by forward-passes, backward-passes, and testing form the classic training pipeling.
- Using the pipeline, artificial neural networks enable computers to make sense of images.
- The optimization result depends on the initialization.
- The initialization depends on the pseudo-randomness-seed.
- Seed-values must be recorded.

References



Christopher M Bishop. *Pattern recognition and machine learning*. springer, 2006.



Klaus Greff, Rupesh K Srivastava, Jan Koutnik, Bas R Steunebrink, and Jürgen Schmidhuber. “LSTM: A search space odyssey.” In: *IEEE transactions on neural networks and learning systems* 28.10 (2016), pp. 2222–2232.



Michael A Nielsen. *Neural networks and deep learning*.
Vol. 25. Determination press San Francisco, CA, USA,
2015.