

Foundations of Machine Learning in Python

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September 7, 2022

High-Performance Computing and Analytics Lab

Neural networks

Classification with neural networks

Neural networks

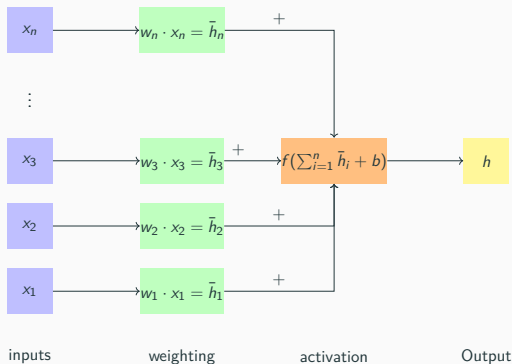
The wonders of the human visual system



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

The perceptron

Can computers recognize digits? Mimic biological neurons,



Formally a single perceptron is defined as

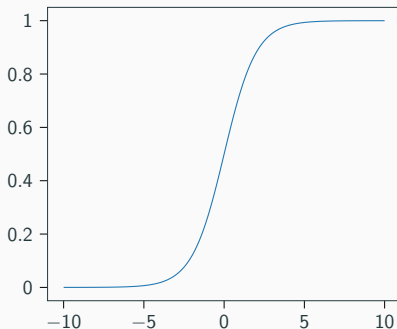
$$f(\mathbf{w}^T \mathbf{x}) = h \quad (1)$$

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

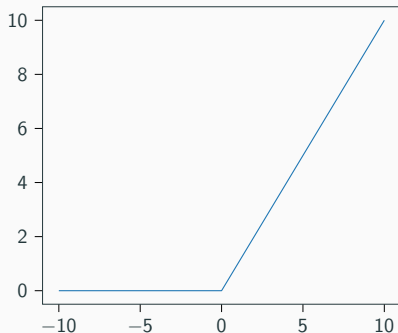
The activation function f

Two popular choices for the activation function f .

Sigmoid $\sigma(x)$

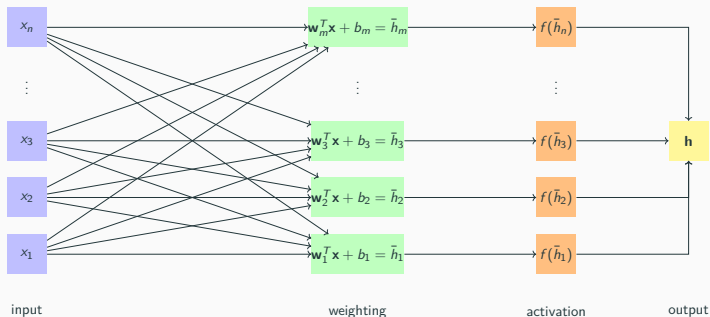


ReLU(x)



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.

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└ Neural networks

└ The gradient of a dense layer

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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,

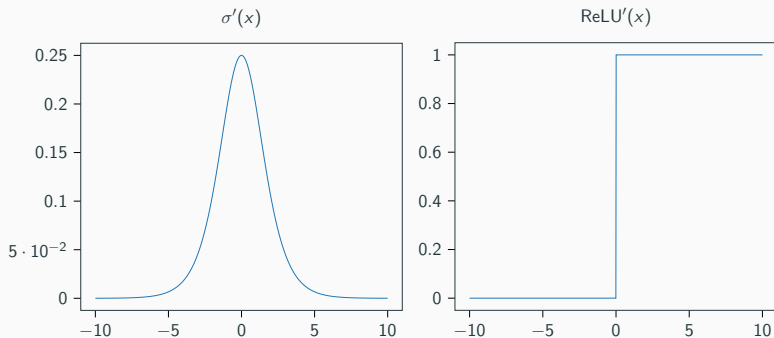
$$\bar{\mathbf{h}} = \mathbf{W}\mathbf{x} + \mathbf{b} \quad (11)$$

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

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 $\mathbf{x} \in \mathbb{R}^n$ and a ground through output $\mathbf{y} \in \mathbb{R}^m$, 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:

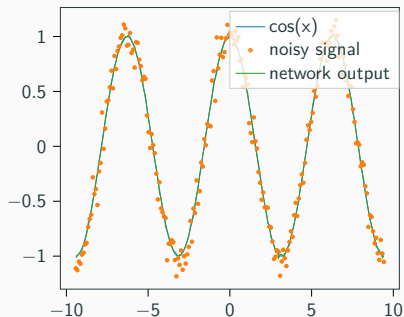
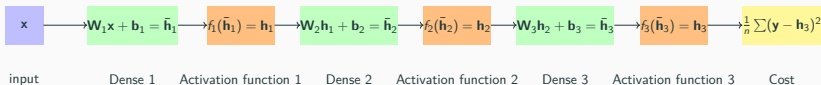


Figure: The cosine function is shown in blue. A noisy network input in orange, and a denoised network output in green.

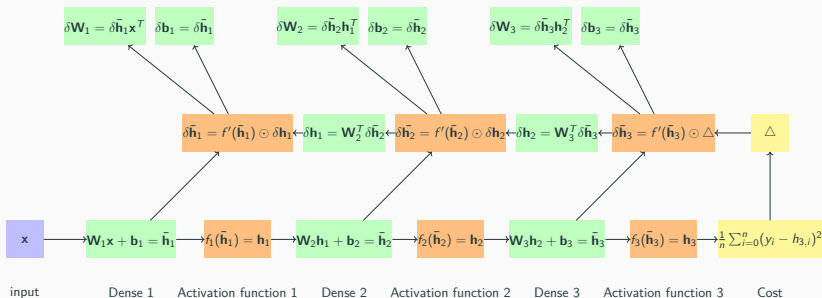
Classification with neural networks

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]

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

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└ Classification with neural networks

└ The cross-entropy loss

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

$$C_{ce}(\mathbf{y}, \mathbf{a}) = - \sum_k^n (y_k \ln a_k) + (1 - y_k) \ln(1 - a_k). \quad (18)$$

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

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

TODO: find the proof.

The MNIST-Dataset



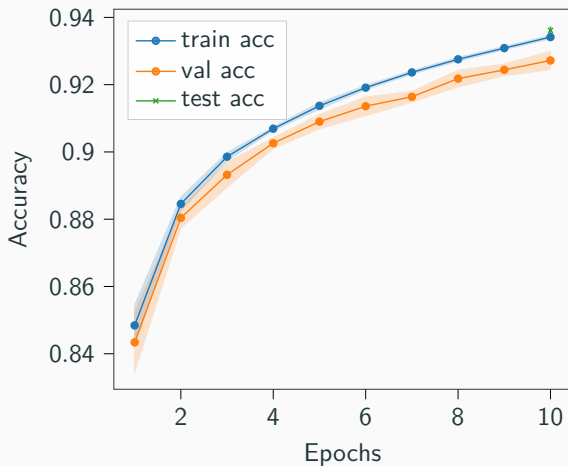
Figure: The MNIST-dataset contains 70k images of handwritten digits.

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.

MNIST-Classification

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



Conclusion

- 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

- [Bis06] Christopher M Bishop. *Pattern recognition and machine learning*. springer, 2006.
- [Gre+16] 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.

- [Nie15] Michael A Nielsen. *Neural networks and deep learning*. Vol. 25. Determination press San Francisco, CA, USA, 2015.