

# Foundations of Machine Learning in Python

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High-Performance Computing and Analytics Lab

Neural networks

Estimation, Overfitting and Regularization

Classification

# Neural networks

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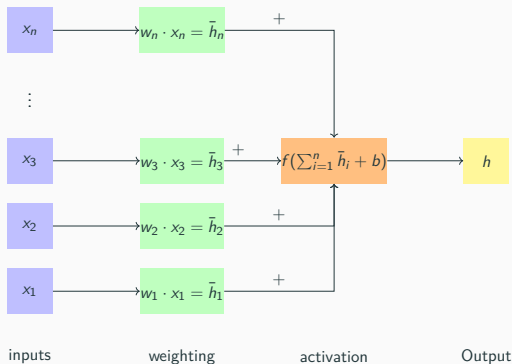
# The wonders of the human visual system



**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

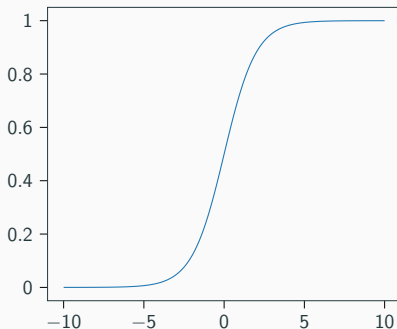
$$f(\mathbf{w}^T \mathbf{x}) = h \quad (1)$$

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

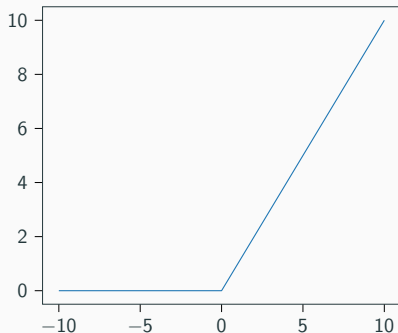
# The activation function $f$

Two popular choices for the activation function  $f$ .

Sigmoid  $\sigma(x)$

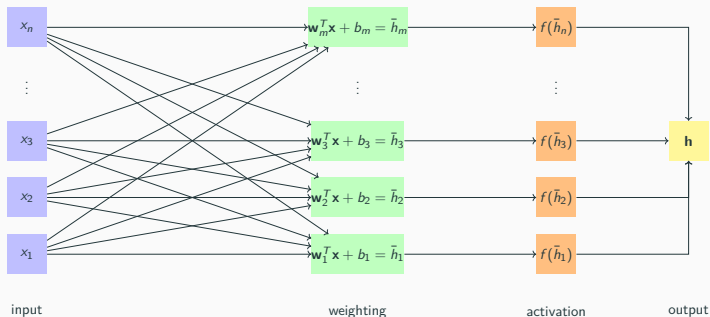


ReLU( $x$ )



# 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]

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

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

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

Good news! Jax can take care of these computations for you! You can choose to verify these equations by completing the optional deep learning project.

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## └ The gradient of a dense layer

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

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

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

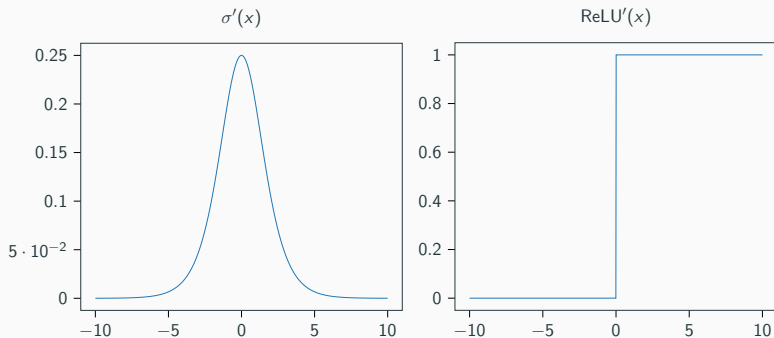
Looking at

$$\bar{\mathbf{h}} = f(\bar{\mathbf{h}}) \Rightarrow \delta \bar{\mathbf{h}} = f'(\bar{\mathbf{h}}) \odot \Delta \quad (7)$$

## Derivatives of our activation functions

$$\sigma'(x) = \sigma \cdot (1 - \sigma(x)) \quad (8)$$

$$\text{ReLU}' = H(x) \quad (9)$$



# Perceptrons can learn functions

TODO

TODO

TODO

# Estimation, Overfitting and Regularization

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TODO

# Classification

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# The cross-entropy loss

TODO

Modified National Institute of Standards and Technology database  
[**dumoulin2016guide**]