TECHNISCHE UNIVERSITÄT
CHEMNITZ

Neurocomputing

Multi-layer Perceptron

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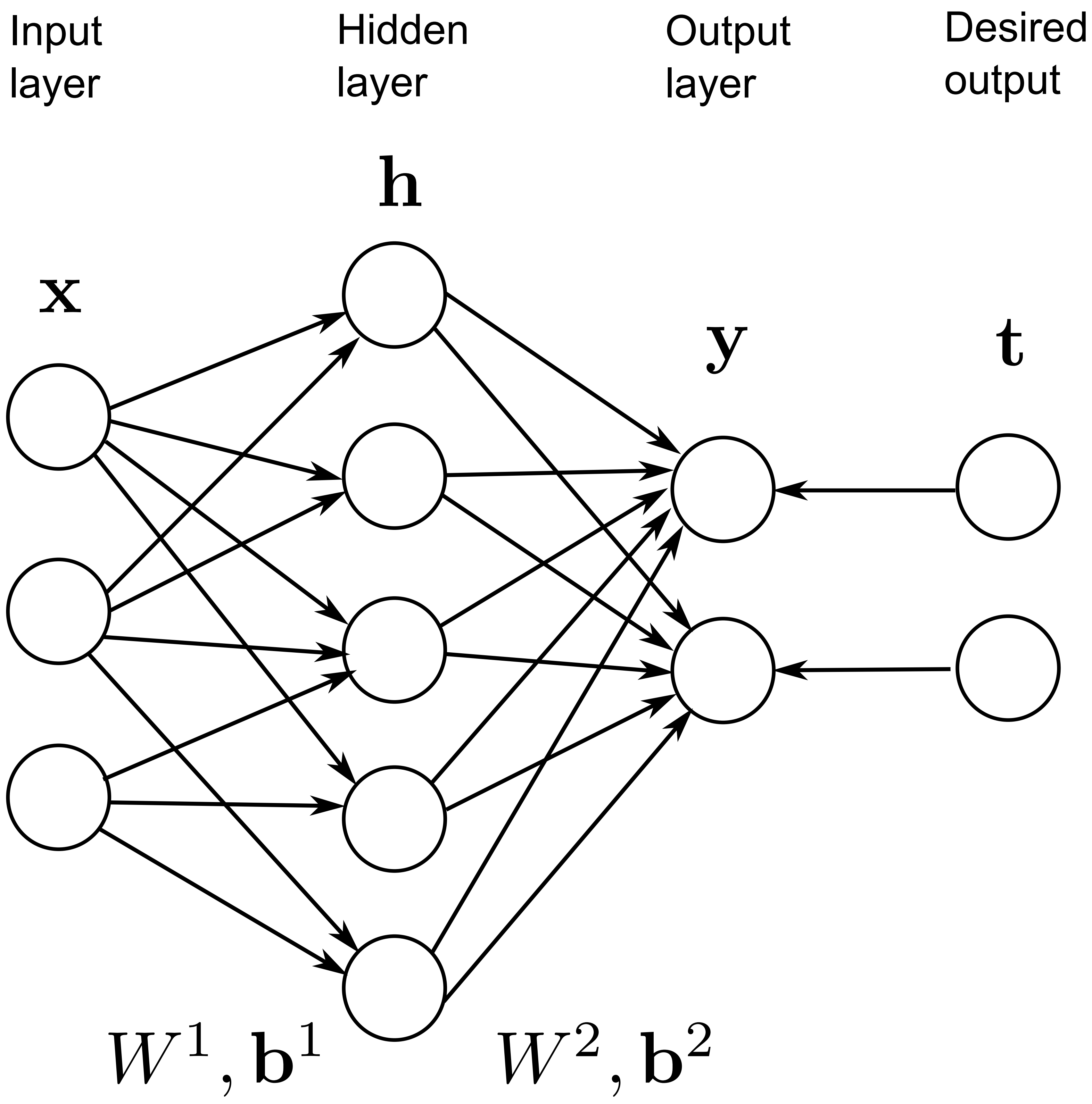
https://tu-chemnitz.de/informatik/KI/edu/neurocomputing

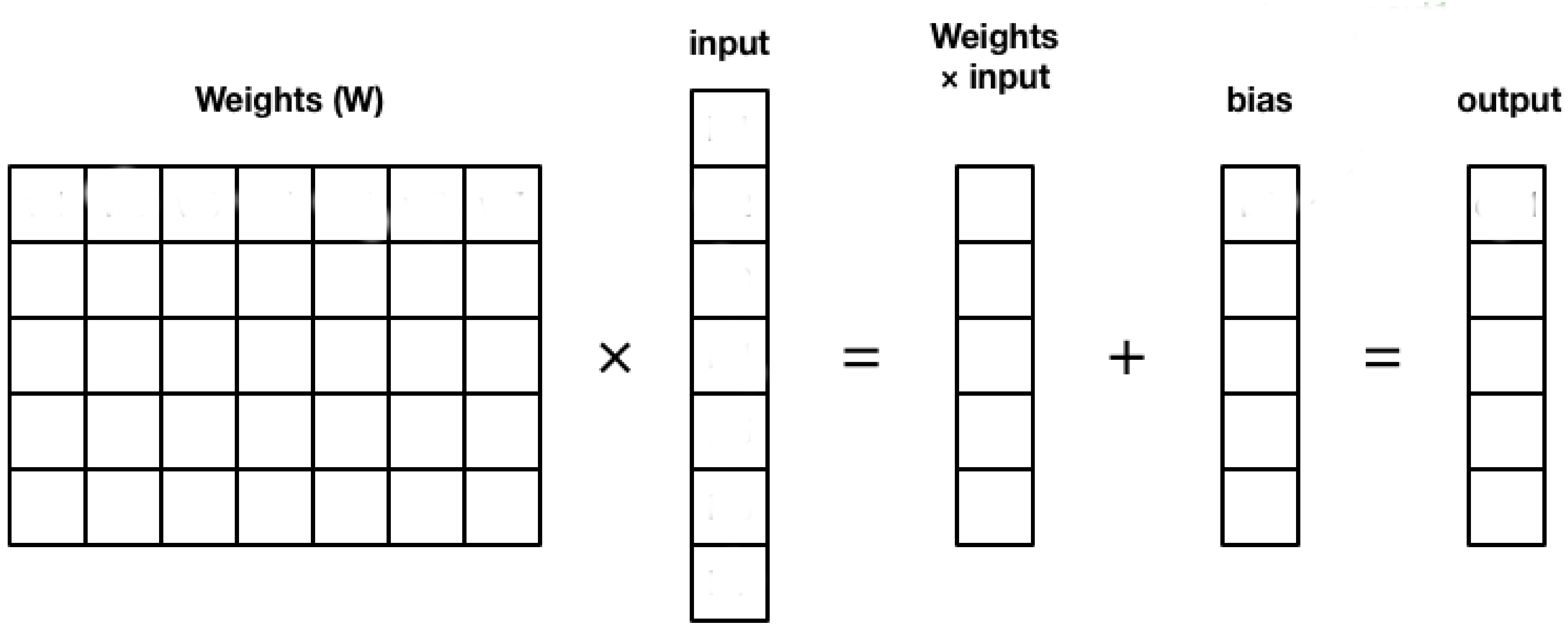
1 - Multi-layer perceptron

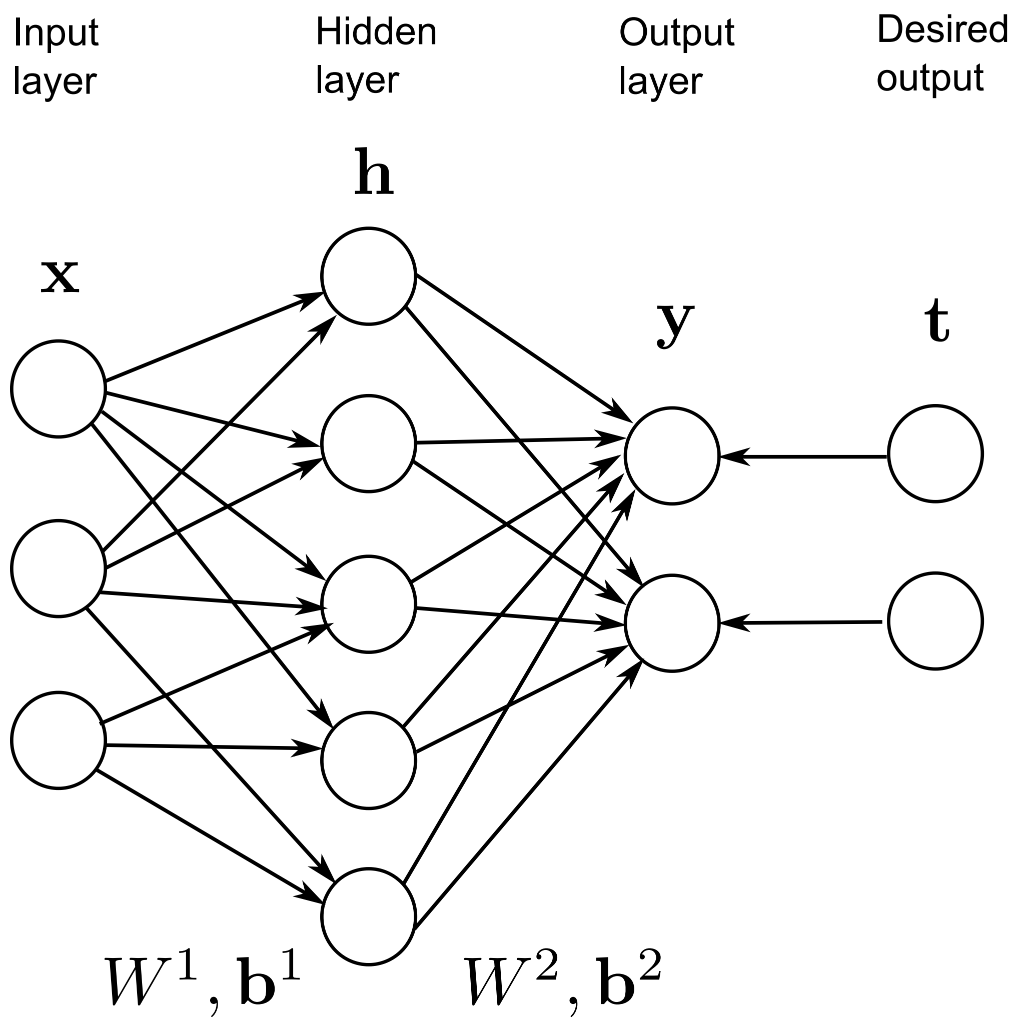
Multi-layer perceptron



- A **Multi-Layer Perceptron** (MLP) or **feedforward neural network** is composed of:
  - an input layer for the input vector $\mathbf{x}$
  - one or several hidden layers allowing to project non-linearly the input into a space of higher dimensions $\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3, \ldots$.
  - an output layer for the output $\mathbf{y}$.
- If there is a single hidden layer $\mathbf{h}$, it corresponds to the feature space.
- Each layer takes inputs from the previous layer.
- If the hidden layer is adequately chosen, the output neurons can learn to replicate the desired output $\mathbf{t}$.

Fully-connected layer





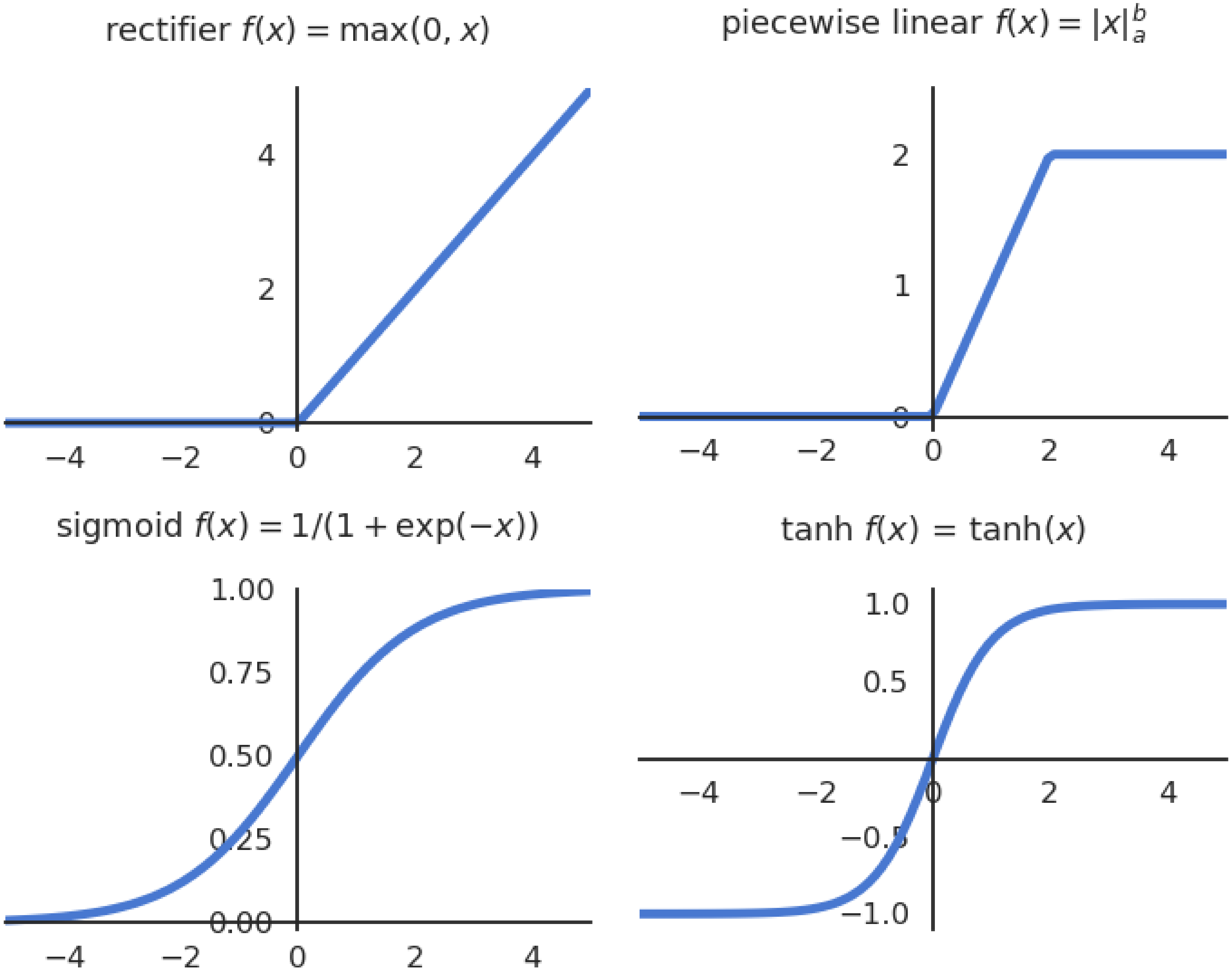
- The operation performed by each layer can be written in the form of a **matrix-vector** multiplication:

$$\mathbf{h} = f(\mathbf{net_h}) = f(W^1 \, \mathbf{x} + \mathbf{b}^1)$$

$$\mathbf{y} = f(\mathbf{net_y}) = f(W^2 \, \mathbf{h} + \mathbf{b}^2)$$

- **Fully-connected layers** (FC) transform an input vector $\mathbf{x}$ into a new vector $\mathbf{h}$ by multiplying it by a **weight matrix** W and adding a **bias vector** $\mathbf{b}$.
- A non-linear **activation function** transforms each element of the net activation.

Activation functions



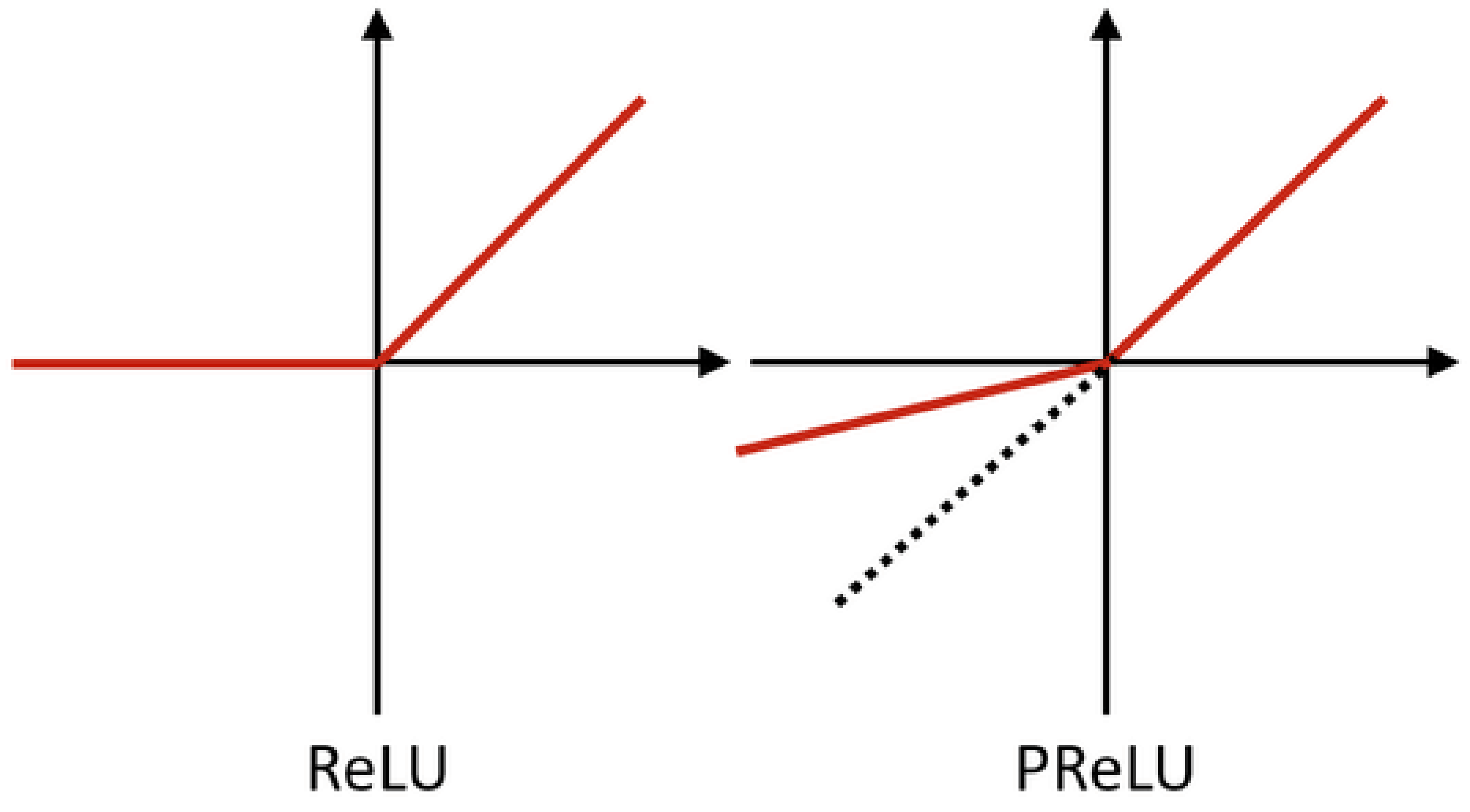
rectifier $f(x) = \max(0, x)$

piecewise linear $f(x) = |x|_a^b$

sigmoid $f(x) = 1/(1 + \exp(-x))$

tanh $f(x) = \tanh(x)$

Modern activation functions



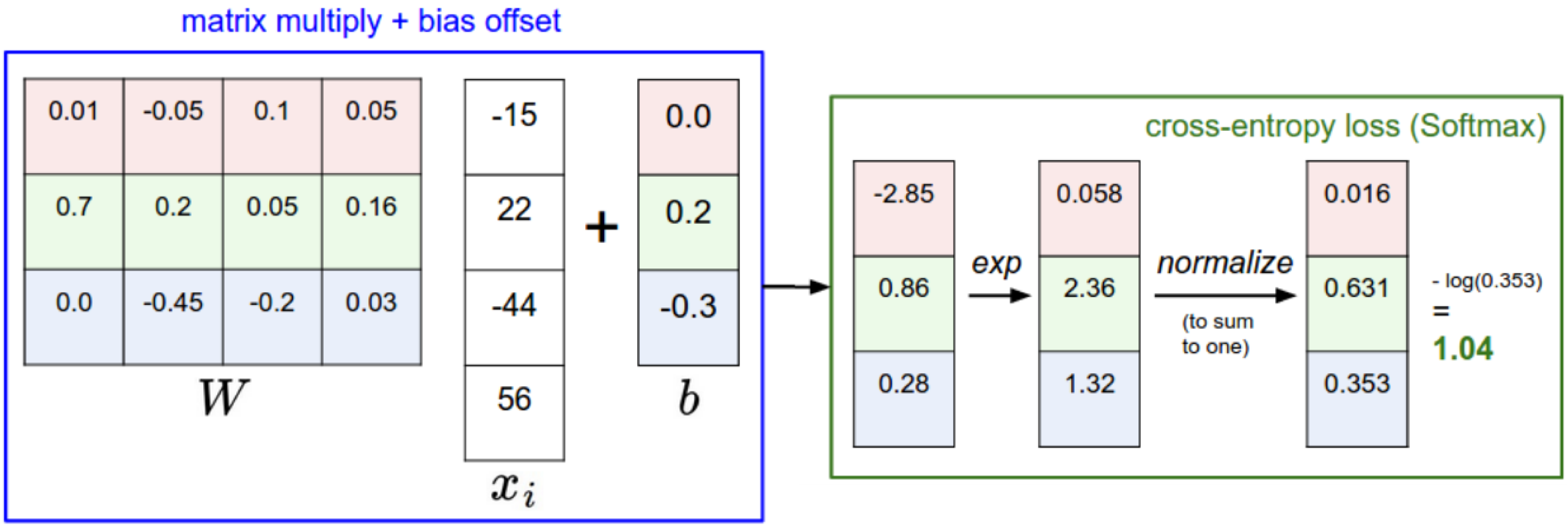
- Rectified linear function - ReLU (output is continuous and positive).

$$f(x) = \max(0, x) = \begin{cases} x & \text{if} \quad x \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$

- Parametric Rectifier Linear Unit - PReLU (output is continuous).

$$f(x) = \begin{cases} x & \text{if} \quad x \geq 0 \\ \alpha\, x & \text{otherwise.} \end{cases}$$

Softmax activation function



matrix multiply + bias offset

0.01	-0.05	0.1	0.05
0.7	0.2	0.05	0.16
0.0	-0.45	-0.2	0.03

W

-15
22
-44
56

x_i

+

0.0
0.2
-0.3

b

cross-entropy loss (Softmax)

-2.85
0.86
0.28

exp

0.058
2.36
1.32

normalize

(to sum to one)

0.016
0.631
0.353

- log(0.353) = 1.04

Source http://cs231n.github.io/linear-classify

- For classification problems, the **softmax** activation function can be used in the output layer to make sure that the sum of the outputs $\mathbf{y} = \{y_j\}$ over all output neurons is one.

$$y_j = P(\text{class} = \text{j}) = \frac{\exp(\text{net}_j)}{\sum_k \exp(\text{net}_k)}$$

- The higher the net activation net_j, the higher the probability that the example belongs to class j.
- Softmax is not *per se* a transfer function (not local to each neuron), but the idea is similar.

Why non-linear activation functions?

- Why not use the linear function $f(x) = x$ in the hidden layer?

$$\mathbf{h} = W^1 \, \mathbf{x} + \mathbf{b}^1$$

$$\mathbf{y} = W^2 \, \mathbf{h} + \mathbf{b}^2$$

- The equivalent function would be linear…

$$\begin{aligned}
\mathbf{y} &= W^2 \, (W^1 \, \mathbf{x} + \mathbf{b}^1) + \mathbf{b}^2 \\
&= (W^2 \, W^1) \, \mathbf{x} + (W^2 \, \mathbf{b}^1 + \mathbf{b}^2) \\
&= W \, \mathbf{x} + \mathbf{b}
\end{aligned}$$

- Remember Cover's theorem:

> A complex pattern-classification problem, cast in a high dimensional space **non-linearly**, is more likely to be linearly separable than in a low-dimensional space, provided that the space is not densely populated.

- In practice it does not matter how non-linear the function is (e.g PReLU is almost linear), but there must be at least one non-linearity.

Training a MLP : loss functions

- We have a training set composed of N input/output pairs $(\mathbf{x}_i, \mathbf{t}_i)_{i=1..N}$.
- **Optimization problem:**
  - What are the free parameters θ (weights W^1, W^2 and biases $\mathbf{b}^1, \mathbf{b}^2$) making the prediction $\mathbf{y}$ as close as possible from the desired output $\mathbf{t}$?
- We define a **loss function** $\mathcal{L}(\theta)$ of the free parameters which should be minimized:
  - For **regression** problems, we take the **mean square error** (mse):

$$\mathcal{L}_\text{reg}(\theta) = \mathbb{E}_{\mathbf{x}, \mathbf{t} \in \mathcal{D}} [||\mathbf{t} - \mathbf{y}||^2]$$

  - For **classification** problems, we take the **cross-entropy** or **negative log-likelihood** on a softmax output layer:

$$\mathcal{L}_\text{class}(\theta) = \mathbb{E}_{\mathbf{x}, \mathbf{t} \sim \mathcal{D}} [- \langle \mathbf{t} \cdot \log \mathbf{y} \rangle]$$

Training a MLP : optimizer

- To minimize the chosen loss function, we are going to use **stochastic gradient descent** iteratively until the network converges:

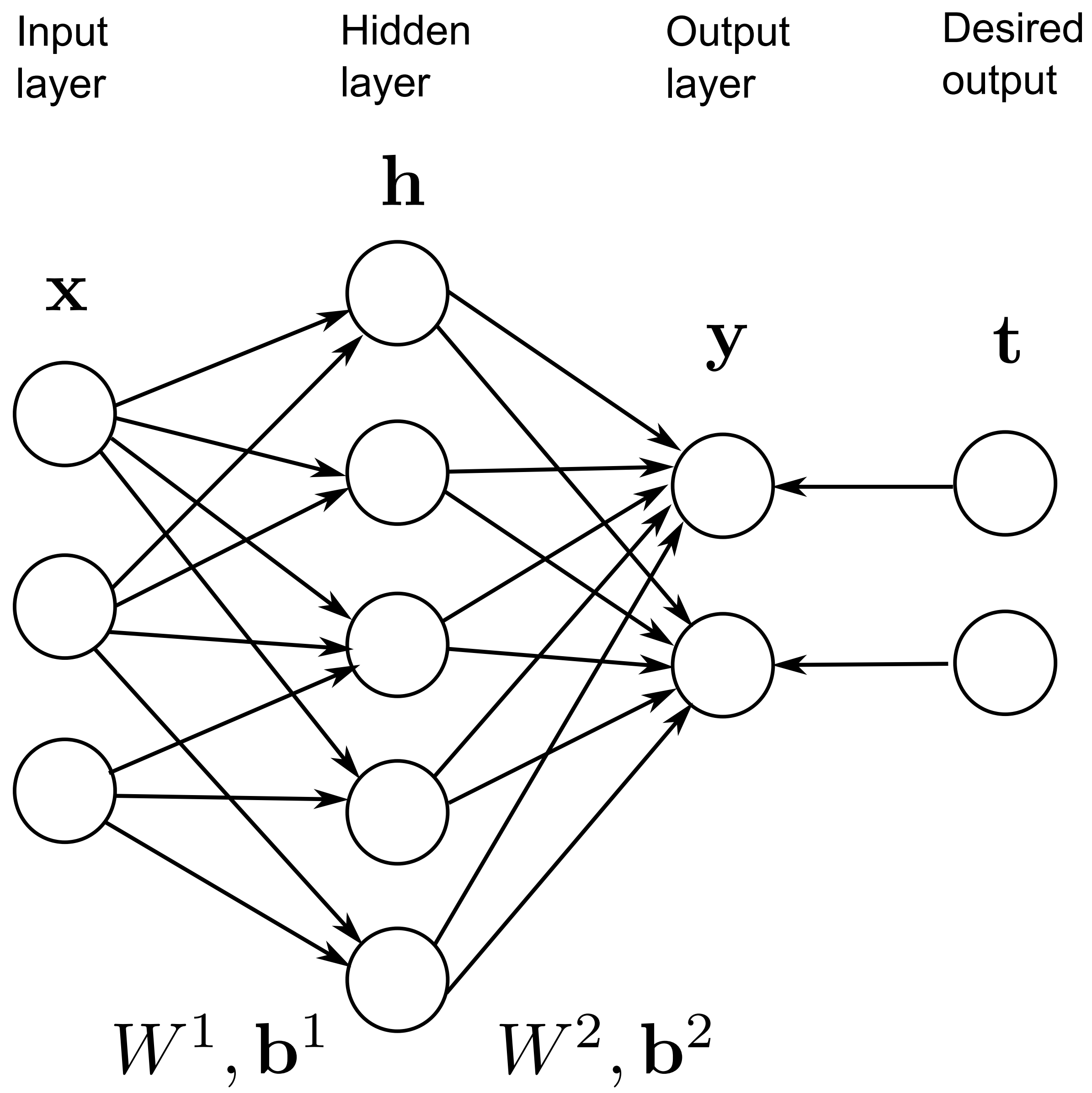
$$\begin{cases} \Delta W^1 = - \eta \, \nabla_{W^1} \, \mathcal{L}(\theta) \\ \\ \Delta \mathbf{b}^1 = - \eta \, \nabla_{\mathbf{b}^1} \, \mathcal{L}(\theta) \\ \\ \Delta W^2 = - \eta \, \nabla_{W^2} \, \mathcal{L}(\theta) \\ \\ \Delta \mathbf{b}^2 = - \eta \, \nabla_{\mathbf{b}^2} \, \mathcal{L}(\theta) \end{cases}$$

- We will see later that other optimizers than SGD can be used.
- The question is now how to compute efficiently these **gradients** w.r.t all the weights and biases.
- The algorithm to achieve this is called **backpropagation**, which is simply a smart implementation of the chain rule.

Rumelhart, Hinton, Williams (1986). “Learning representations by back-propagating errors”. Nature.

2 - Backpropagation

Backpropagation on a shallow network



$$\mathbf{h} = f(\mathbf{net_h}) = f(W^1 \, \mathbf{x} + \mathbf{b}^1)$$

$$\mathbf{y} = f(\mathbf{net_y}) = f(W^2 \, \mathbf{h} + \mathbf{b}^2)$$

- The chain rule gives us for the parameters of the output layer:

$$\frac{\partial \mathcal{L}(\theta)}{\partial W^2} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{y}} \times \frac{\partial \mathbf{y}}{\partial \mathbf{net_y}} \times \frac{\partial \mathbf{net_y}}{\partial W^2}$$

$$\frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{b}^2} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{y}} \times \frac{\partial \mathbf{y}}{\partial \mathbf{net_y}} \times \frac{\partial \mathbf{net_y}}{\partial \mathbf{b}^2}$$

- and for the hidden layer:

$$\frac{\partial \mathcal{L}(\theta)}{\partial W^1} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{y}} \times \frac{\partial \mathbf{y}}{\partial \mathbf{net_y}} \times \frac{\partial \mathbf{net_y}}{\partial \mathbf{h}} \times \frac{\partial \mathbf{h}}{\partial \mathbf{net_h}} \times \frac{\partial \mathbf{net_h}}{\partial W^1}$$

$$\frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{b}^1} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{y}} \times \frac{\partial \mathbf{y}}{\partial \mathbf{net_y}} \times \frac{\partial \mathbf{net_y}}{\partial \mathbf{h}} \times \frac{\partial \mathbf{h}}{\partial \mathbf{net_h}} \times \frac{\partial \mathbf{net_h}}{\partial \mathbf{b}^1}$$

- If we can compute all these partial derivatives / gradients individually, the problem is solved.

Gradient of the loss function

- We have already seen for the linear algorithms that the derivative of the loss function w.r.t the net activation of the output $\mathbf{net_y}$ is proportional to the **prediction error** $\mathbf{t} - \mathbf{y}$:
  - mse for regression:

$$\delta_{\mathbf{y}} = - \frac{\partial l_\text{reg}(\theta)}{\partial \mathbf{net_y}} = - \frac{\partial l_\text{reg}(\theta)}{\partial \mathbf{y}} \times \frac{\partial \mathbf{y}}{\partial \mathbf{net_y}} = 2 \, (\mathbf{t} - \mathbf{y}) \, f'(\mathbf{net_y})$$

  - cross-entropy using a softmax output layer:

$$\delta_{\mathbf{y}} = - \frac{\partial l_\text{class}(\theta)}{\partial \mathbf{net_y}} = (\mathbf{t} - \mathbf{y})$$

- $\delta_{\mathbf{y}} = - \dfrac{\partial l(\theta)}{\partial \mathbf{net_y}}$ is called the output error.
- The output error is going to appear in all partial derivatives, i.e. in all learning rules.
- The backpropagation algorithm is sometimes called **backpropagation of the error**.

Gradient in the output layer

- We now have everything we need to train the output layer:

$$\frac{\partial l(\theta)}{\partial W^2} = \frac{\partial l(\theta)}{\partial \mathbf{net_y}} \times \frac{\partial \mathbf{net_y}}{\partial W^2} = - \delta_{\mathbf{y}} \times \frac{\partial \mathbf{net_y}}{\partial W^2}$$

$$\frac{\partial l(\theta)}{\partial \mathbf{b}^2} = \frac{\partial l(\theta)}{\partial \mathbf{net_y}} \times \frac{\partial \mathbf{net_y}}{\partial \mathbf{b}^2} = - \delta_{\mathbf{y}} \times \frac{\partial \mathbf{net_y}}{\partial \mathbf{b}^2}$$

- As $\mathbf{net_y} = W^2 \, \mathbf{h} + \mathbf{b}^2$, we get for the cross-entropy loss:

$$\frac{\partial l(\theta)}{\partial W^2} = - \delta_{\mathbf{y}} \times \mathbf{h}^T$$

$$\frac{\partial l(\theta)}{\partial \mathbf{b}^2} = - \delta_{\mathbf{y}}$$

i.e. exactly the same delta learning rule as a softmax linear classifier or multiple linear regression using the vector $\mathbf{h}$ as an input.

$$\begin{cases} \Delta W^2 = \eta \, \delta_{\mathbf{y}} \times \mathbf{h}^T = \eta \, (\mathbf{t} - \mathbf{y}) \times \mathbf{h}^T \\ \\ \Delta \mathbf{b}^2 = \eta \, \delta_{\mathbf{y}} = \eta \, (\mathbf{t} - \mathbf{y}) \end{cases}$$

Gradient in the hidden layer

- Let's note $\delta_{\mathbf{h}}$ the **hidden error**, i.e. minus the gradient of the loss function w.r.t the net activation of the hidden layer:

$$\delta_{\mathbf{h}} = - \frac{\partial l(\theta)}{\partial \mathbf{net_h}} = - \frac{\partial l(\theta)}{\partial \mathbf{net_y}} \times \frac{\partial \mathbf{net_y}}{\partial \mathbf{h}} \times \frac{\partial \mathbf{h}}{\partial \mathbf{net_h}} = \delta_{\mathbf{y}} \times \frac{\partial \mathbf{net_y}}{\partial \mathbf{h}} \times \frac{\partial \mathbf{h}}{\partial \mathbf{net_h}}$$

- Using this hidden error, we can compute the gradients w.r.t W^1 and $\mathbf{b}^1$:

$$\frac{\partial l(\theta)}{\partial W^1} = \frac{\partial l(\theta)}{\partial \mathbf{net_h}} \times \frac{\partial \mathbf{net_h}}{\partial W^1} = - \delta_{\mathbf{h}} \times \frac{\partial \mathbf{net_h}}{\partial W^1}$$

$$\frac{\partial l(\theta)}{\partial \mathbf{b}^1} = \frac{\partial l(\theta)}{\partial \mathbf{net_h}} \times \frac{\partial \mathbf{net_h}}{\partial \mathbf{b}^1} = - \delta_{\mathbf{h}} \times \frac{\partial \mathbf{net_h}}{\partial \mathbf{b}^1}$$

- As $\mathbf{net_h} = W^1 \, \mathbf{x} + \mathbf{b}^1$, we get:

$$\frac{\partial l(\theta)}{\partial W^1} = - \delta_{\mathbf{h}} \times \mathbf{x}^T$$

$$\frac{\partial l(\theta)}{\partial \mathbf{b}^1} = - \delta_{\mathbf{h}}$$

Gradient in the hidden layer

$$\frac{\partial l(\theta)}{\partial W^1} = - \delta_{\mathbf{h}} \times \mathbf{x}^T$$

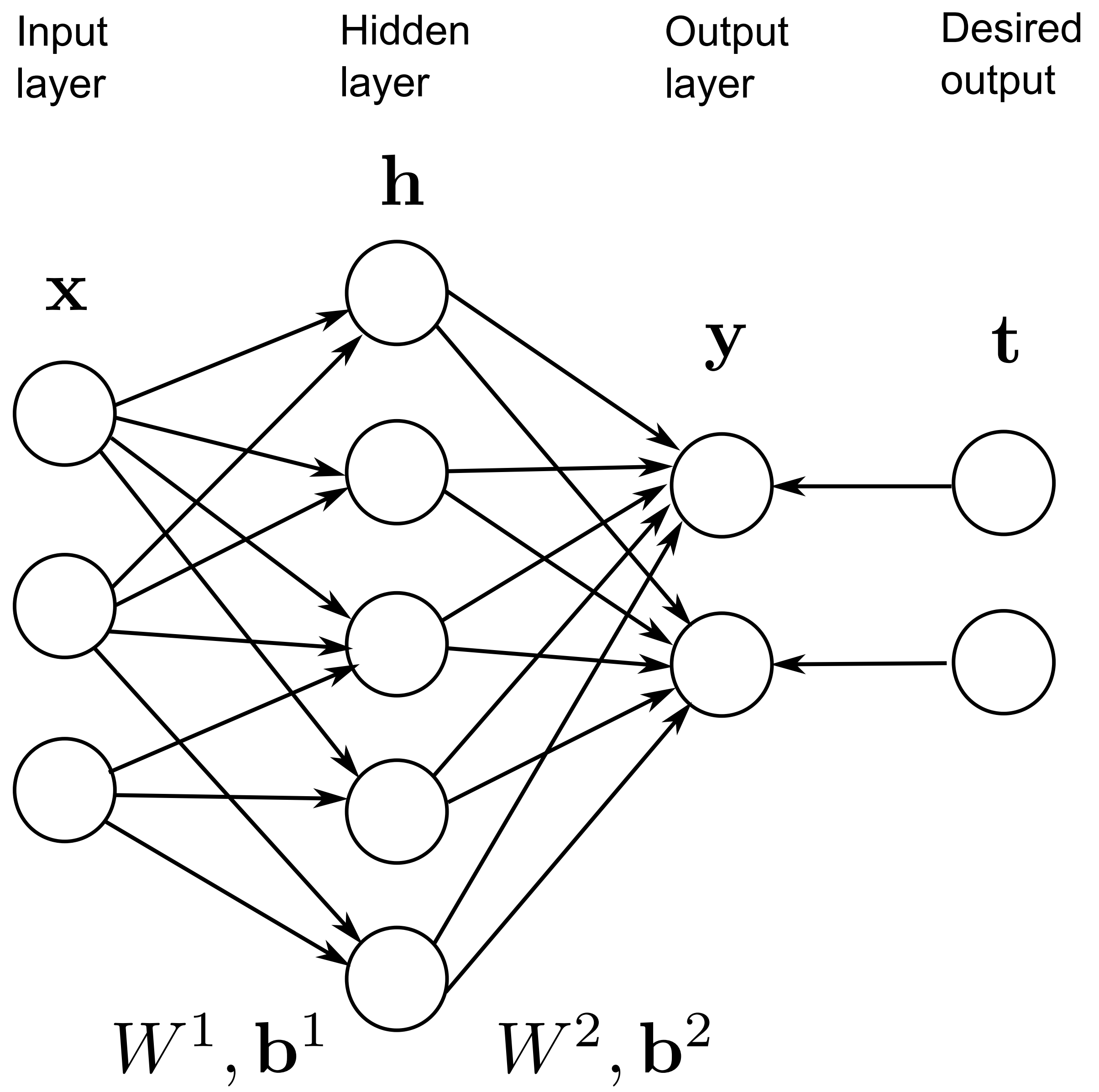
$$\frac{\partial l(\theta)}{\partial \mathbf{b}^1} = - \delta_{\mathbf{h}}$$

- If we know the **hidden error** $\delta_{\mathbf{h}}$, the update rules for the input weights W^1 and $\mathbf{b}^1$ also take the form of the delta learning rule:

$$\begin{cases} \Delta W^1 = \eta \, \delta_{\mathbf{h}} \times \mathbf{x}^T \\ \\ \Delta \mathbf{b}^1 = \eta \, \delta_{\mathbf{h}} \end{cases}$$

- This is the classical form eta * error * input.
- All we need to know is the **backpropagated error** $\delta_{\mathbf{h}}$ and we can apply the delta learning rule!

Backpropagated error



- The backpropagated error $\delta_{\mathbf{h}}$ is a vector assigning an error to each of the hidden neurons:

$$\delta_{\mathbf{h}} = - \frac{\partial l(\theta)}{\partial \mathbf{net_h}} = \delta_{\mathbf{y}} \times \frac{\partial \mathbf{net_y}}{\partial \mathbf{h}} \times \frac{\partial \mathbf{h}}{\partial \mathbf{net_h}}$$

- As :

$$\mathbf{net_y} = W^2 \, \mathbf{h} + \mathbf{b}^2$$

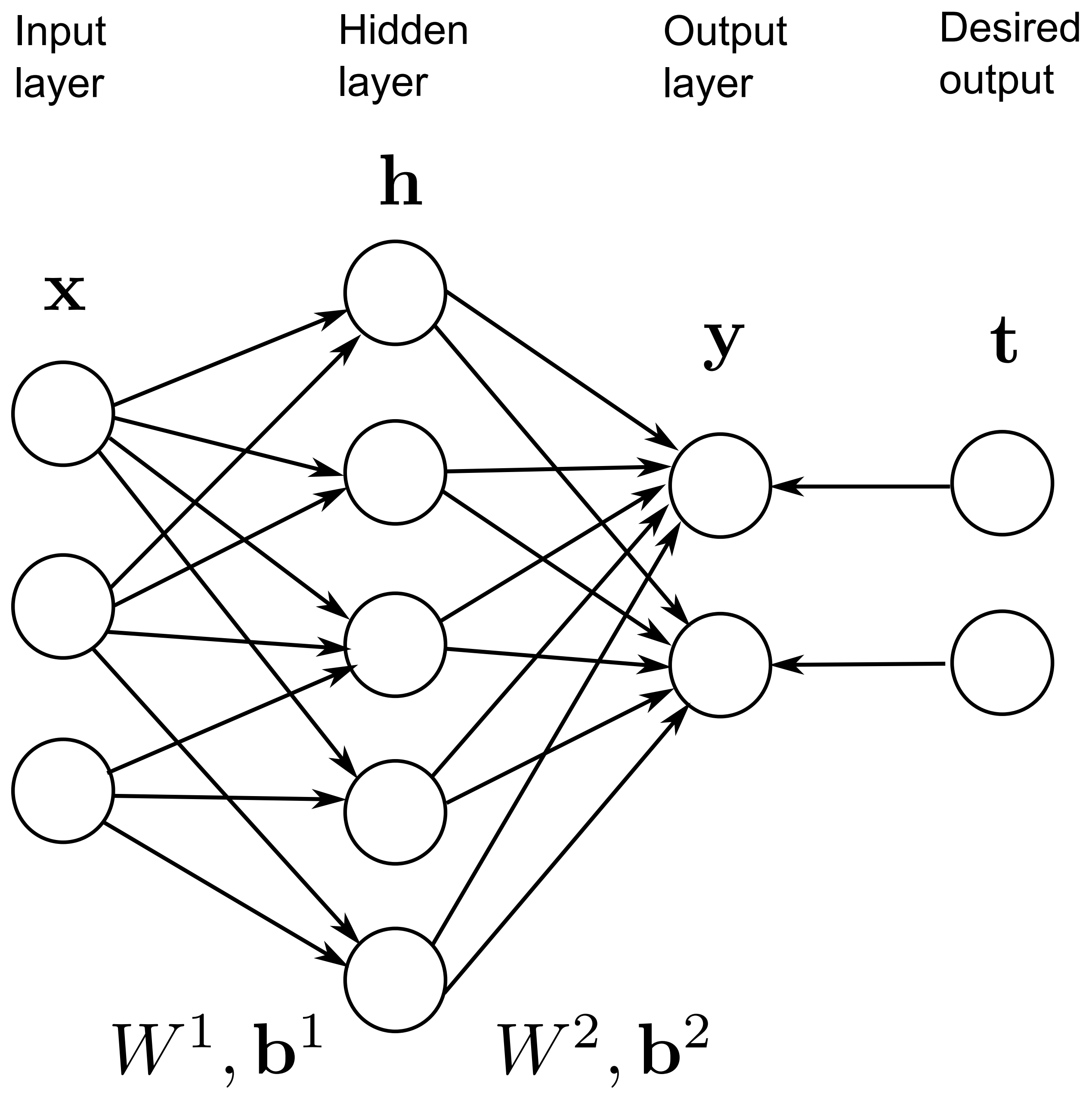
$$\mathbf{h} = f(\mathbf{net_h})$$

we obtain:

$$\delta_{\mathbf{h}} = f'(\mathbf{net_h}) \, (W^2)^T \times \delta_{\mathbf{y}}$$

- If $\mathbf{h}$ and $\delta_{\mathbf{h}}$ have K elements and $\mathbf{y}$ and $\delta_{\mathbf{y}}$ have C elements, the matrix W^2 is $C \times K$ as $W^2 \times \mathbf{h}$ must be a vector with C elements.
- $(W^2)^T \times \delta_{\mathbf{y}}$ is therefore a vector with K elements, which is then multiplied element-wise with the derivative of the transfer function to obtain $\delta_{\mathbf{h}}$.

Backpropagation for a shallow MLP



- For a shallow MLP with one hidden layer:

$$\mathbf{h} = f(\mathbf{net_h}) = f(W^1 \, \mathbf{x} + \mathbf{b}^1)$$

$$\mathbf{y} = f(\mathbf{net_y}) = f(W^2 \, \mathbf{h} + \mathbf{b}^2)$$

the output error:

$$\delta_{\mathbf{y}} = - \frac{\partial l(\theta)}{\partial \mathbf{net_y}} = (\mathbf{t} - \mathbf{y})$$

is **backpropagated** to the hidden layer:

$$\delta_{\mathbf{h}} = f'(\mathbf{net_h}) \, (W^2)^T \times \delta_{\mathbf{y}}$$

what allows to apply the delta learning rule to all parameters:

$$\begin{cases} \Delta W^2 = \eta \, \delta_{\mathbf{y}} \times \mathbf{h}^T \\ \Delta \mathbf{b}^2 = \eta \, \delta_{\mathbf{y}} \\ \Delta W^1 = \eta \, \delta_{\mathbf{h}} \times \mathbf{x}^T \\ \Delta \mathbf{b}^1 = \eta \, \delta_{\mathbf{h}} \end{cases}$$

Derivative of the activation functions

- Threshold and sign functions are not differentiable, we simply consider the derivative is 1.

$$f(x) = \begin{cases} 1 \quad \text{if} \quad x \geq 0 \\ 0 \text{ or } 1 \quad \text{otherwise.} \end{cases} \qquad \rightarrow \qquad f'(x) = 1$$

- The logistic or sigmoid function has the nice property that its derivative can be expressed as a function of itself:

$$f(x) = \frac{1}{1 + \exp(-x)} \qquad \rightarrow \qquad f'(x) = f(x) \, (1 - f(x))$$

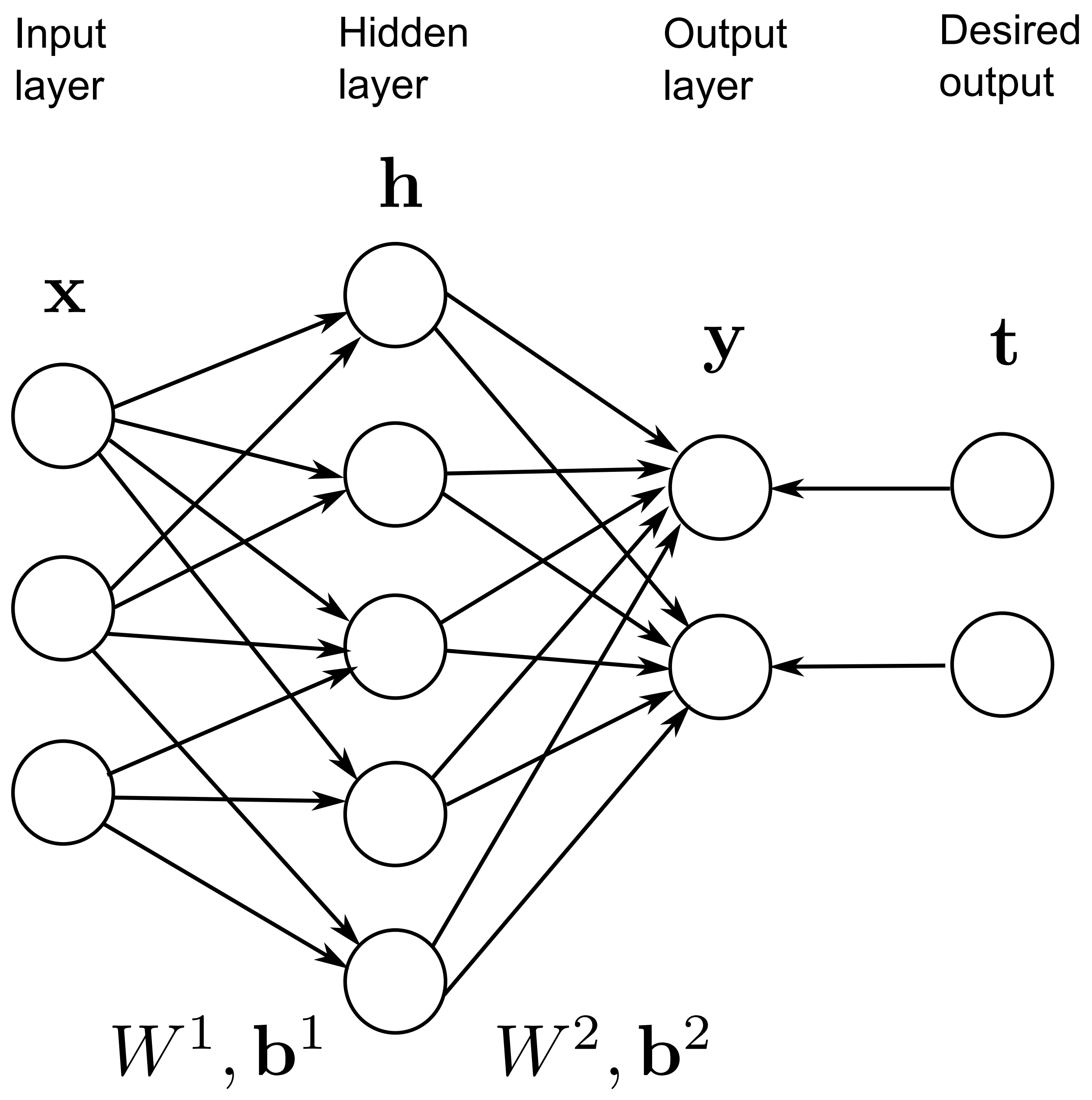
- The hyperbolic tangent function too:

$$f(x) = \tanh(x) \qquad \rightarrow \qquad f'(x) = 1 - f(x)^2$$

- ReLU is even simpler:

$$f(x) = \max(0, x) = \begin{cases} x \quad \text{if} \quad x \geq 0 \\ 0 \quad \text{otherwise.} \end{cases} \qquad \rightarrow \qquad f'(x) = \begin{cases} 1 \quad \text{if} \quad x \geq 0 \\ 0 \quad \text{otherwise.} \end{cases}$$

What is backpropagated?



- Let’s have a closer look at what is backpropagated using single neurons and weights.
- The output neuron y_k computes:

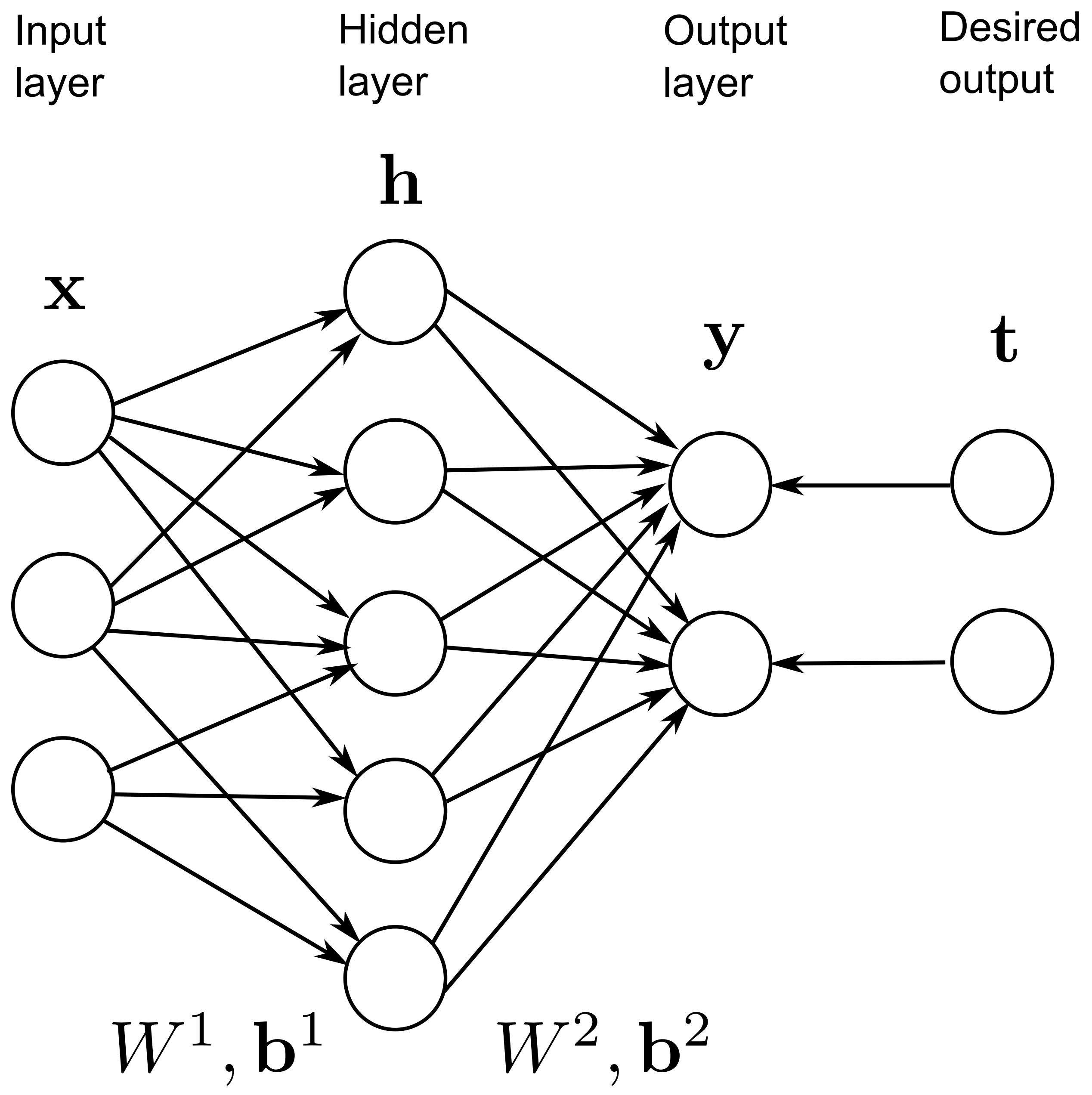
$$y_k = f(\sum_{j=1}^K W^2_{jk} \, h_j + b^2_k)$$

- All output weights W^2_{jk} are updated proportionally to the output error of the neuron y_k:

$$\Delta W^2_{jk} = \eta \, \delta_{y_k} \, h_j = \eta \, (t_k - y_k) \, h_j$$

- This is possible because we know the output error directly from the data t_k.

What is backpropagated?



- The hidden neuron h_j computes:

$$h_j = f(\sum_{i=1}^d W^1_{ij} \, x_i + b^1_j)$$

- We want to learn the hidden weights W^1_{ij} using the delta learning rule:

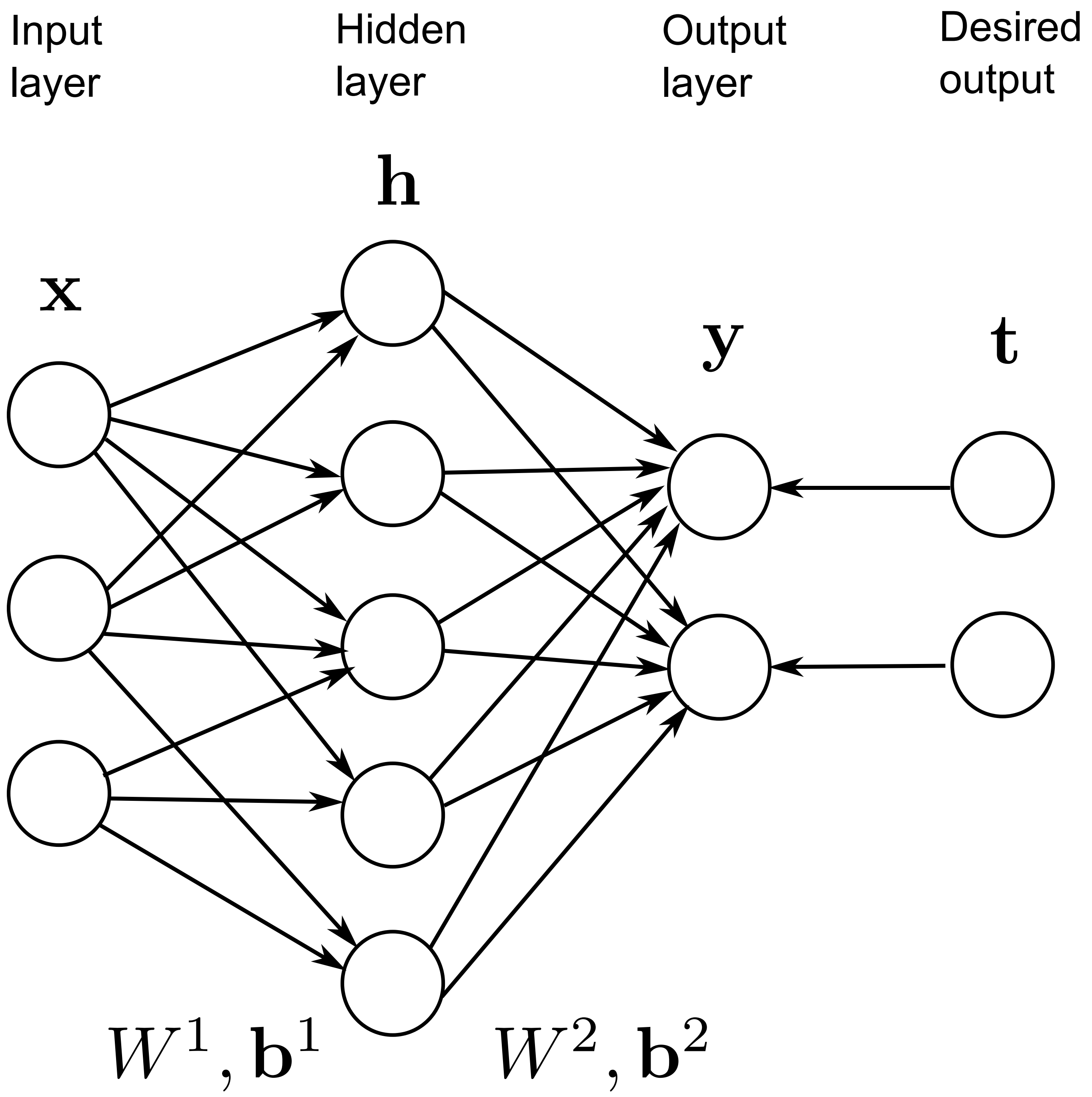
$$\Delta W^1_{ij} = \eta \, \delta_{h_j} \, x_i$$

but we do not know the ground truth of the hidden neuron in the data:

$$\delta_{h_j} = (? - h_j)$$

- We need to **estimate** the backpropagated error using the output error.

What is backpropagated?



$$\delta_{\mathbf{h}} = f'(\mathbf{net_h}) \, (W^2)^T \times \delta_{\mathbf{y}}$$

- If we omit the derivative of the transfer function, the backpropagated error for the hidden neuron h_j is:

$$\delta_{h_j} = - \sum_{k=1}^C W^2_{jk} \, \delta_{y_k}$$

- The backpropagated error is an **average** of the output errors δ_{y_k}, weighted by the output weights between the hidden neuron h_j and the output neurons y_k.

- The backpropagated error is the **contribution** of each hidden neuron h_j to the output error:
  - If there is no output error, there is no hidden error.
  - If a hidden neuron sends **strong weights** $|W^2_{jk}|$ to an output neuron y_k with a strong prediction error δ_{y_k}, this means that it participates strongly to the output error and should learn from it.
  - If the weight $|W^2_{jk}|$ is small, it means that the hidden neuron does not take part in the output error.

MLP: the universal approximation theorem

Universal approximation theorem

Cybenko, 1989

Let $\varphi()$ be a nonconstant, bounded, and monotonically-increasing continuous function. Let I_{m_0} denote the m_0-dimensional unit hypercube $[0, 1]^{m_0}$. The space of continuous functions on I_{m_0} is denoted by $C(I_{m_0})$. Then, given any function $f \in C(I_{m_0})$ and $\epsilon > 0$, there exists an integer m_1 and sets of real constants α_i, b_i and $w_{ij} \in \Re$, where $i = 1, ..., m_1$ and $j = 1, ..., m_0$ such that we may define:

$$F(\mathbf{x}) = \sum_{i=1}^{m_1} \alpha_i \cdot \varphi \left(\sum_{j=1}^{m_0} w_{ij} \cdot x_j + b_i \right)$$

as an approximate realization of the function f; that is,

$$|F(\mathbf{x}) - f(\mathbf{x})| < \epsilon$$

for all $x \in I_m$.

- This theorem shows that for **any** input/output mapping function f in supervised learning, there exists a MLP with m_1 neurons in the hidden layer which is able to approximate it with a desired precision!

Properties of MLP

- The universal approximation theorem only proves the existence of a shallow MLP with m_1 neurons in the hidden layer that can approximate any function, but it does not tell how to find this number.
- A rule of thumb to find this number is that the generalization error is empirically close to:

$$\epsilon = \frac{\text{VC}_{\text{dim}}(\text{MLP})}{N}$$

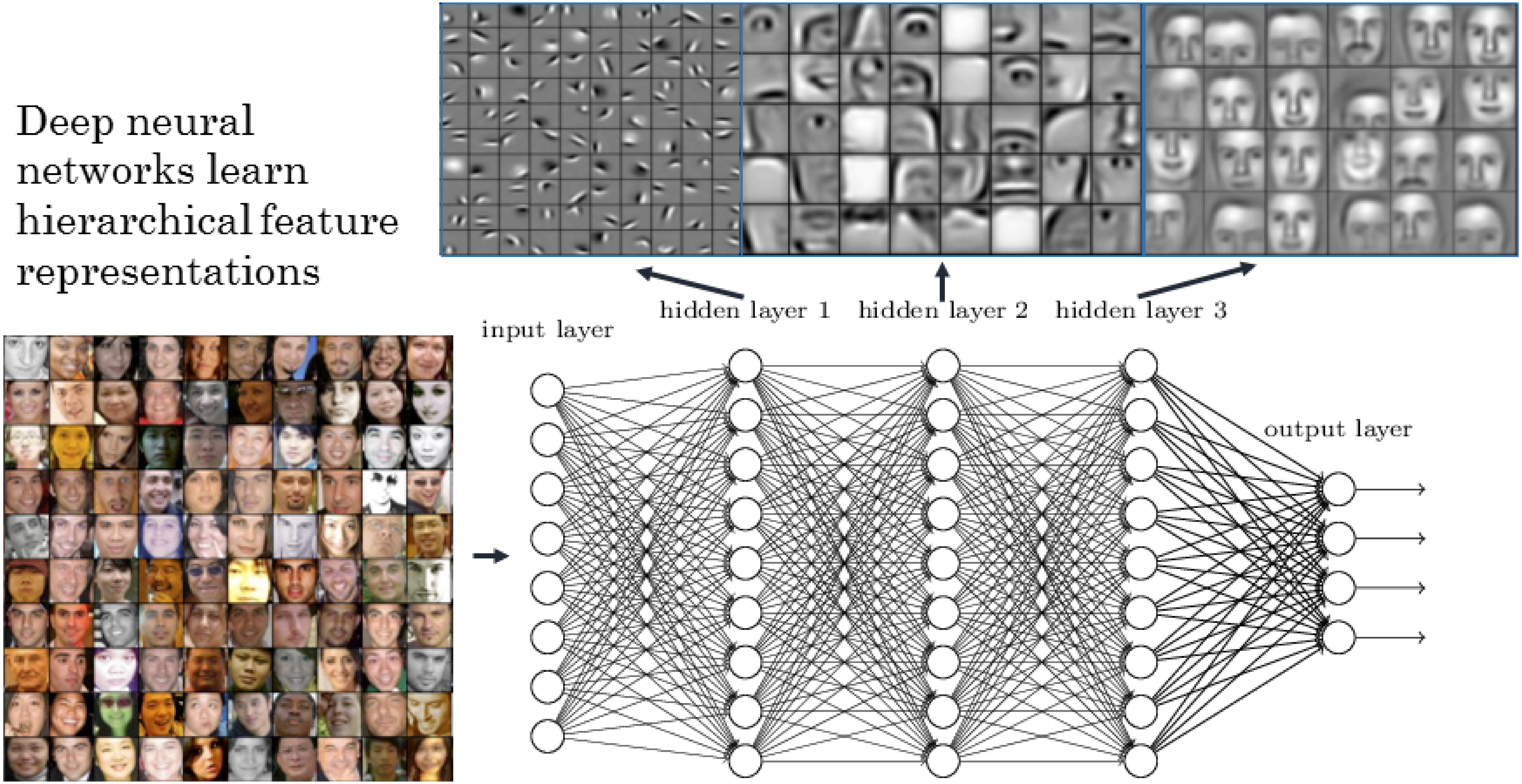
where $\text{VC}_{\text{dim}}(\text{MLP})$ is the total number of weights and biases in the model, and N the number of training samples.

- The more neurons in the hidden layer, the better the training error, but the worse the generalization error (overfitting).
- The optimal number should be found with cross-validation methods.
- For most functions, the optimal number m_1 is high and becomes quickly computationally untractable. We need to go deep!

3 - Deep neural networks

Deep Neural Network

- A MLP with more than one hidden layer is a **deep neural network**.



Deep neural networks learn hierarchical feature representations

Backpropagation for deep neural networks

- Backpropagation still works if we have many hidden layers $\mathbf{h}_1, \dots, \mathbf{h}_n$:

$$\begin{tikzcd}
x \arrow[r] & h_1 \arrow[r] & \dots \arrow[r] & h_n \arrow[r] & y \arrow[r] & l \\
& w_1 \arrow[u] & \dots & w_n \arrow[u] & &
\end{tikzcd}$$

- If each layer is differentiable, i.e. one can compute its gradient $\frac{\partial \mathbf{h}_k}{\partial \mathbf{h}_{k-1}}$, we can chain **backwards** each partial derivatives to know how to update each layer:

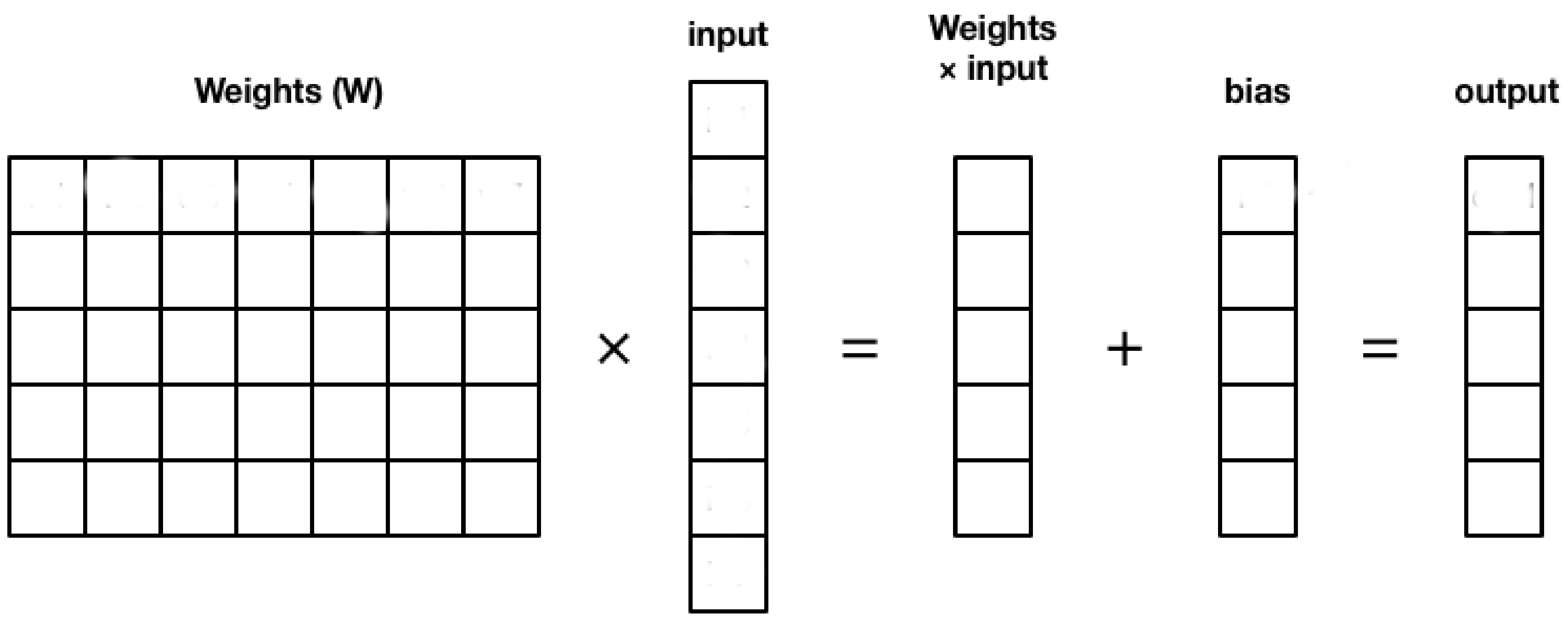
$$\begin{tikzcd}
\frac{\partial l}{\partial x} & \frac{\partial l}{\partial h_1} \arrow[l, "\frac{\partial h_1}{\partial x}"'] \arrow[d, "\frac{\partial h_1}{\partial w_1}"'] & \dots \arrow[l, "\frac{\partial h_2}{\partial h_1}"'] & \frac{\partial l}{\partial h_n} \arrow[l, "\frac{\partial h_n}{\partial h_{n-1}}"'] \arrow[d, "\frac{\partial h_n}{\partial w_n}"'] & \frac{\partial l}{\partial y} \arrow[l, "\frac{\partial y}{\partial h_n}"'] \\
& \frac{\partial l}{\partial w_1} & \dots & \frac{\partial l}{\partial w_n} &
\end{tikzcd}$$

- **Backpropagation** is simply an efficient implementation of the chain rule: the partial derivatives are iteratively reused in the backwards phase.

Source: David Silver, Tutorial: Deep Reinforcement Learning

Gradient of a fully connected layer

- A fully connected layer transforms an input vector $\mathbf{h}_{k-1}$ into an output vector $\mathbf{h}_k$ using a weight matrix W^k, a bias vector $\mathbf{b}^k$ and a non-linear activation function f:



$$\mathbf{h}_k = f(\textbf{net}_{\mathbf{h}^k}) = f(W^k \, \mathbf{h}_{k-1} + \mathbf{b}^k)$$

- The gradient of its output w.r.t the input $\mathbf{h}_{k-1}$ is (using the chain rule):

$$\frac{\partial \mathbf{h}_k}{\partial \mathbf{h}_{k-1}} = f'(\textbf{net}_{\mathbf{h}^k}) \, W^k$$

- The gradients of its output w.r.t the free parameters W^k and $\mathbf{b}_k$ are:

$$\frac{\partial \mathbf{h}_k}{\partial W^k} = f'(\textbf{net}_{\mathbf{h}^k}) \, \mathbf{h}_{k-1}$$

$$\frac{\partial \mathbf{h}_k}{\partial \mathbf{b}_k} = f'(\textbf{net}_{\mathbf{h}^k})$$

Gradient of a fully connected layer

$$\begin{tikzcd}
\frac{\partial l}{\partial x} & \frac{\partial l}{\partial h_1} \arrow[l, "\frac{\partial h_1}{\partial x}"'] \arrow[d, "\frac{\partial h_1}{\partial w_1}"'] & \cdots \arrow[l, "\frac{\partial h_2}{\partial h_1}"'] & \frac{\partial l}{\partial h_n} \arrow[l, "\frac{\partial h_n}{\partial h_{n-1}}"'] \arrow[d, "\frac{\partial h_n}{\partial w_n}"'] & \frac{\partial l}{\partial y} \arrow[l, "\frac{\partial y}{\partial h_n}"'] \\
 & \frac{\partial l}{\partial w_1} & \cdots & \frac{\partial l}{\partial w_n} &
\end{tikzcd}$$

- A fully connected layer $\mathbf{h}_k = f(W^k \, \mathbf{h}_{k-1} + \mathbf{b}^k)$ receives the gradient of the loss function w.r.t. its output $\mathbf{h}_k$ from the layer above:

$$\frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_k}$$

- It adds to this gradient its own contribution and transmits it to the previous layer:

$$\frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_{k-1}} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_k} \times \frac{\partial \mathbf{h}_k}{\partial \mathbf{h}_{k-1}} = f'(\mathbf{net}_{\mathbf{h}^k}) \, (W^k)^T \times \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_k}$$

- It then updates its parameters W^k and $\mathbf{b}_k$ with:

$$\begin{cases} \dfrac{\partial \mathcal{L}(\theta)}{\partial W^k} = \dfrac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_k} \times \dfrac{\partial \mathbf{h}_k}{\partial W^k} = f'(\mathbf{net}_{\mathbf{h}^k}) \, \dfrac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_k} \times \mathbf{h}_{k-1}^T \\ \\ \dfrac{\partial \mathcal{L}(\theta)}{\partial \mathbf{b}_k} = \dfrac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_k} \times \dfrac{\partial \mathbf{h}_k}{\partial \mathbf{b}_k} = f'(\mathbf{net}_{\mathbf{h}^k}) \, \dfrac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_k} \end{cases}$$

Training a deep neural network with backpropagation

- A **feedforward** neural network is an acyclic graph of differentiable and parameterized layers.

$$\mathbf{x} \rightarrow \mathbf{h}_1 \rightarrow \mathbf{h}_2 \rightarrow \ldots \rightarrow \mathbf{h}_n \rightarrow \mathbf{y}$$

- The **backpropagation** algorithm is used to assign the gradient of the loss function $\mathcal{L}(\theta)$ to each layer using backward chaining:

$$\frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_{k-1}} = \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_k} \times \frac{\partial \mathbf{h}_k}{\partial \mathbf{h}_{k-1}}$$

$$\begin{tikzcd}
\frac{\partial l}{\partial x} & \frac{\partial l}{\partial h_1} \arrow[l, "\frac{\partial h_1}{\partial x}"'] \arrow[d, "\frac{\partial h_1}{\partial w_1}"'] & \ldots \arrow[l, "\frac{\partial h_2}{\partial h_1}"'] & \frac{\partial l}{\partial h_n} \arrow[l, "\frac{\partial h_n}{\partial h_{n-1}}"'] \arrow[d, "\frac{\partial h_n}{\partial w_n}"'] & \frac{\partial l}{\partial y} \arrow[l, "\frac{\partial y}{\partial h_n}"'] \\
 & \frac{\partial l}{\partial w_1} & \ldots & \frac{\partial l}{\partial w_n} &
\end{tikzcd}$$

- **Stochastic gradient descent** is then used to update the parameters of each layer:

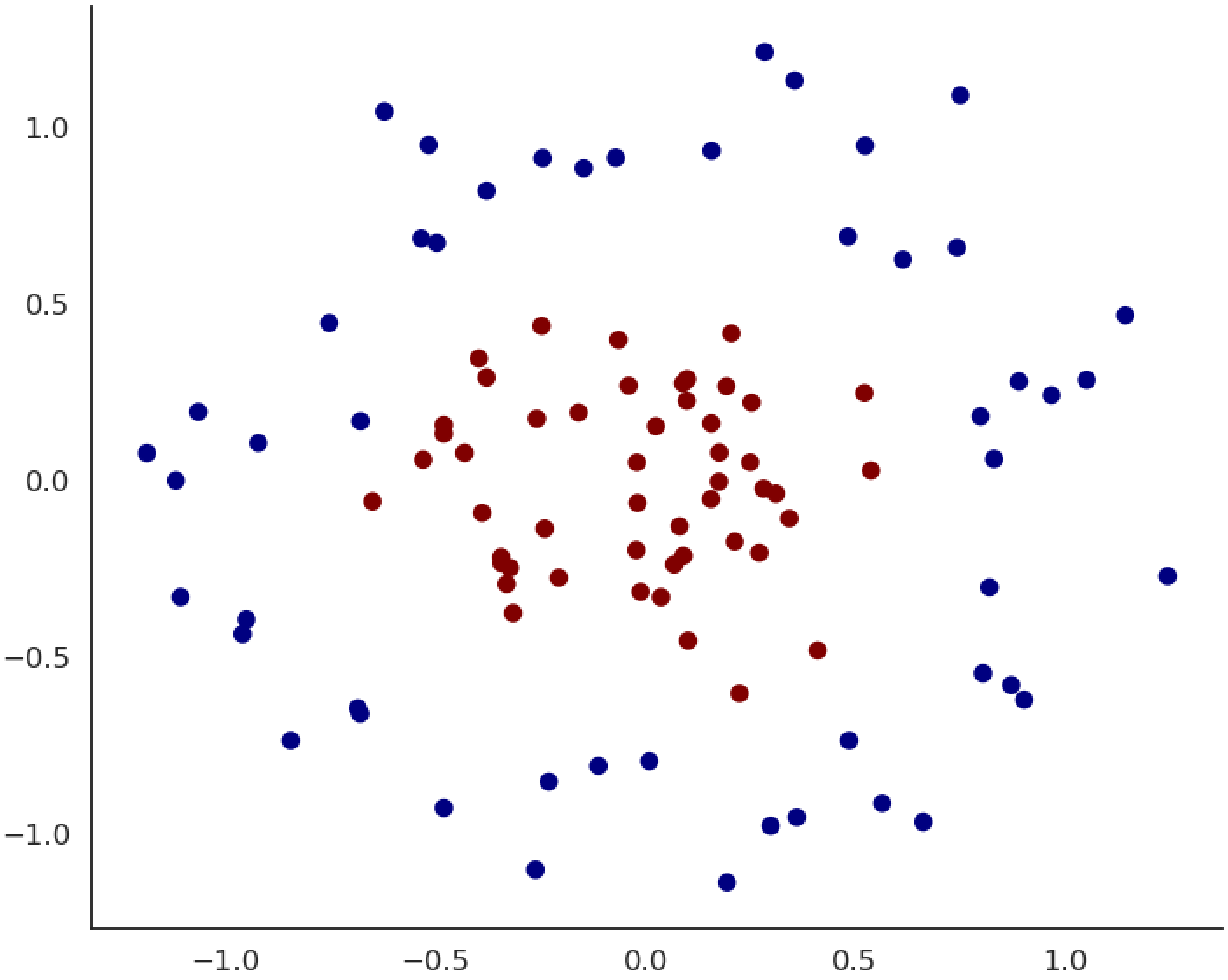
$$\Delta W^k = -\eta \, \frac{\partial \mathcal{L}(\theta)}{\partial W^k} = -\eta \, \frac{\partial \mathcal{L}(\theta)}{\partial \mathbf{h}_k} \times \frac{\partial \mathbf{h}_k}{\partial W^k}$$

Rumelhart, Hinton, Williams (1986). “Learning representations by back-propagating errors”. Nature.

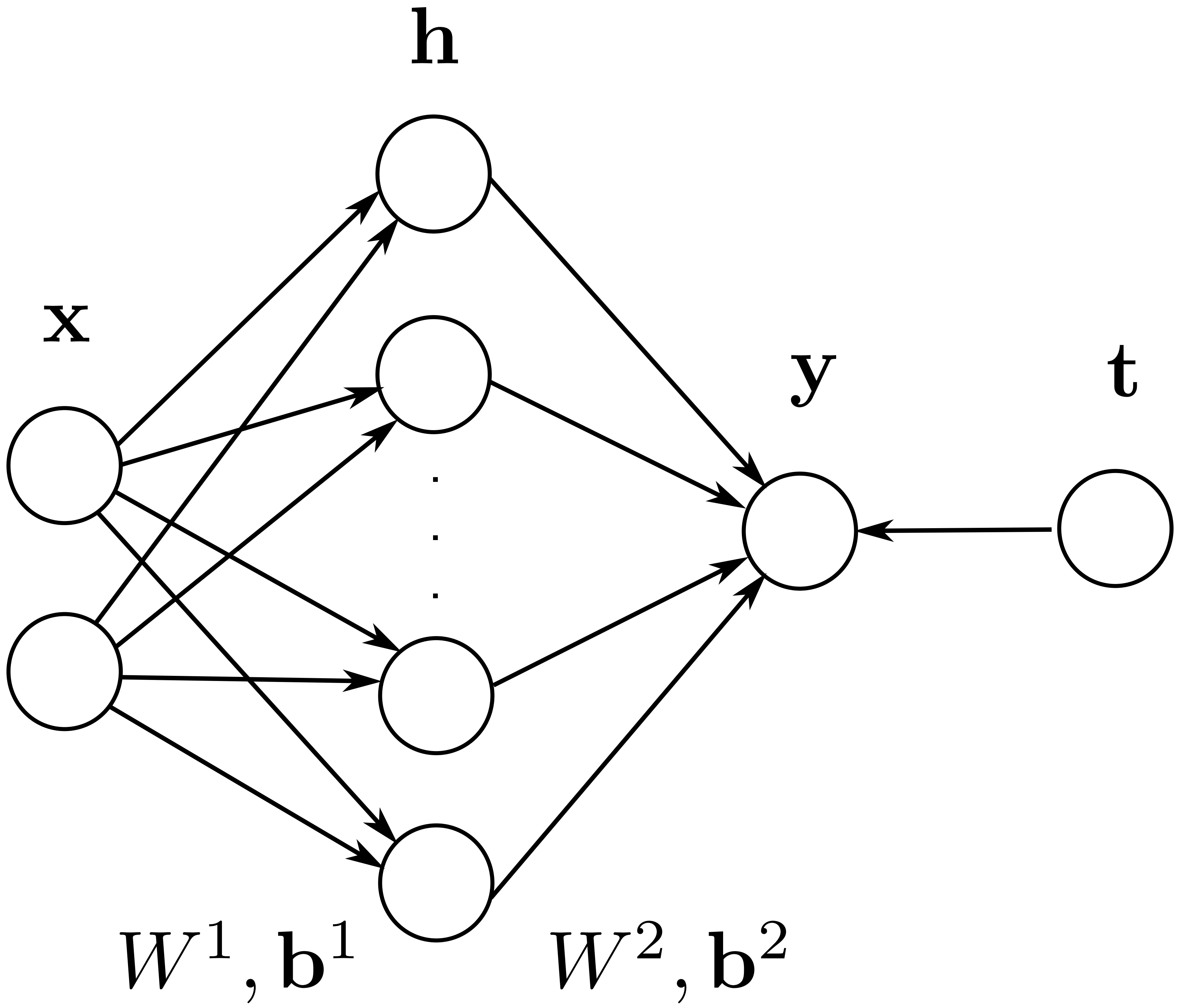
4 - Example

MLP example

- Let’s try to solve this **non-linear** binary classification problem:

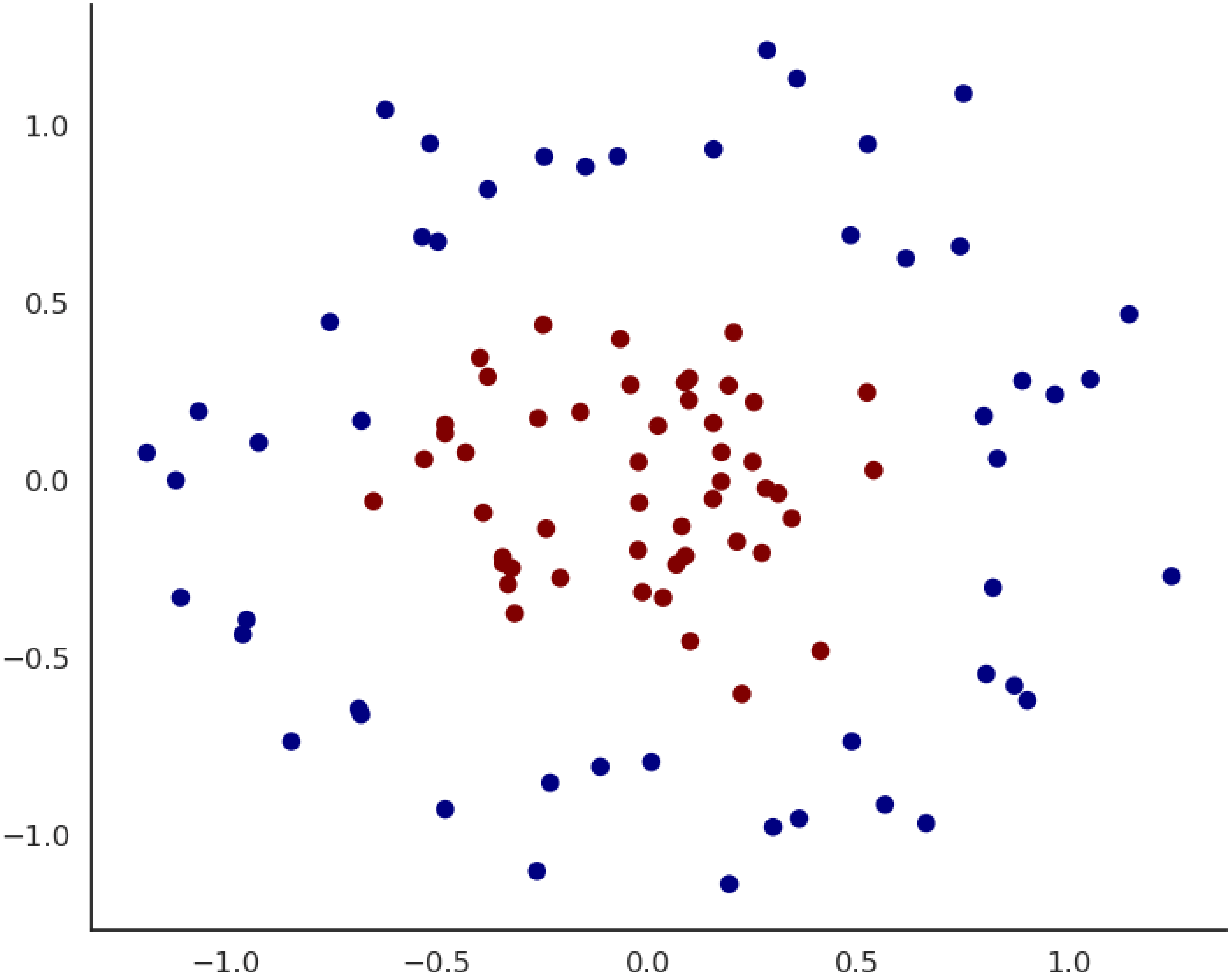


MLP example



- We can create a shallow MLP with:
  - Two input neurons x_1, x_2 for the two input variables.
  - Enough hidden neurons (e.g. 20), with a sigmoid or ReLU activation function.
  - One output neuron with the logistic activation function.
  - The cross-entropy (negative log-likelihood) loss function.
- We train it on the input data using the backpropagation algorithm and the SGD optimizer.

MLP example



- Experiment live on https://playground.tensorflow.org/!

Automatic differentiation Deep Learning frameworks

Current:

- **Tensorflow** https://www.tensorflow.org/ released by Google in 2015 is one of the two standard DL frameworks.
- **Keras** https://keras.io/ is a high-level Python API over tensorflow (but also theano, CNTK and MxNet) written by Francois Chollet.
- **PyTorch** http://pytorch.org by Facebook is the other standard framework.

Historical:

- **Theano** http://deeplearning.net/software/theano/ released by U Toronto in 2010 is the predecessor of tensorflow. Now abandoned.
- **Caffe** http://caffe.berkeleyvision.org/ by U Berkeley was long the standard library for convolutional networks.
- **CNTK** https://github.com/Microsoft/CNTK (Microsoft Cognitive Toolkit) is a **free** library by Microsoft!
- **MxNet** https://github.com/apache/incubator-mxnet from Apache became the DL framework at Amazon.

Example of a shallow neural network with keras

- Let's implement the previous MLP using keras.
- We first need to generate the data using `scikit-learn`:

```python
import sklearn.datasets
X, t = sklearn.datasets.make_circles(n_samples=100, shuffle=True, noise=0.15, factor=0.3)
```

- We then import `tensorflow`:

```python
import tensorflow as tf
```

- The neural network is called a `Sequential` model in keras:

```python
model = tf.keras.Sequential()
```

Example of a shallow neural network with keras

- Creating a NN is simply **stacking** layers in the model. The input layer is just a placeholder for the data:

```
model.add( tf.keras.layers.Input(shape=(2, )) )
```

- The hidden layer has 20 neurons, the ReLU activation and takes input from the previous layer:

```
model.add(
    tf.keras.layers.Dense(
        20, # Number of hidden neurons
        activation='relu' # Activation function
    )
)
```

- The output layer has 1 neuron with the logistic/sigmoid activation function:

```
model.add(
    tf.keras.layers.Dense(
        1, # Number of output neurons
        activation='sigmoid' # Soft classification
    )
)
```

Example of a shallow neural network with keras

- We now choose an optimizer (SGD) with a learning rate $\eta = 0.001$:

```
optimizer = tf.keras.optimizers.SGD(lr=0.001)
```

- We choose a loss function (binary cross-entropy, aka negative log-likelihood):

```
loss = tf.keras.losses.binary_crossentropy
```

- We compile the model (important!) and tell it to track the accuracy of the model:

```
model.compile(
    loss=loss,
    optimizer=optimizer,
    metrics=tf.keras.metrics.categorical_accuracy
)
```

Example of a shallow neural network with keras

- Et voilà! The network has been created.

```
print(model.summary())
```

```
Model: "sequential_1"
_________________________________________________________________
Layer (type)                 Output Shape              Param #   
=================================================================
dense (Dense)                (None, 20)                60        
_________________________________________________________________
dense_1 (Dense)              (None, 1)                 21        
=================================================================
Total params: 81
Trainable params: 81
Non-trainable params: 0
_________________________________________________________________
None
```

Example of a shallow neural network with keras

- We now train the model on the data for 100 epochs using a batch size of 10 and wait for it to finish:

```
model.fit(X, t, batch_size=10, nb_epoch=100)
```

- With keras (and the other automatic differentiation frameworks), you only need to define the structure of the network.
- The rest (backpropagation, SGD) is done automatically.
- To make predictions on new data, just do:

```
model.predict(X_test)
```