An introduction to Deep Learning

More at neuralnetworksanddeeplearning.com

Winter School on Quantitative Biology
Learning and Artificial Intelligence

ICTP – November 2018

What is this about?

Classification tasks

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Classification tasks

"is this a cat or a dog?"

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“is this a cat or a dog?”
“what digit is this?”

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Supervised Learning: by examples, with a teacher

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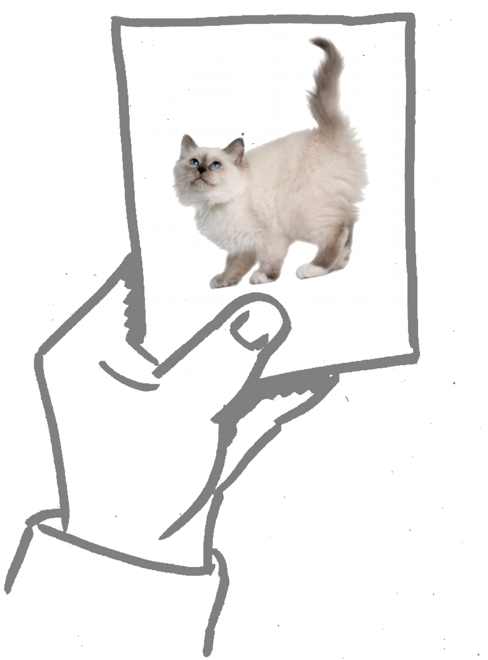

`cat`

`dog`

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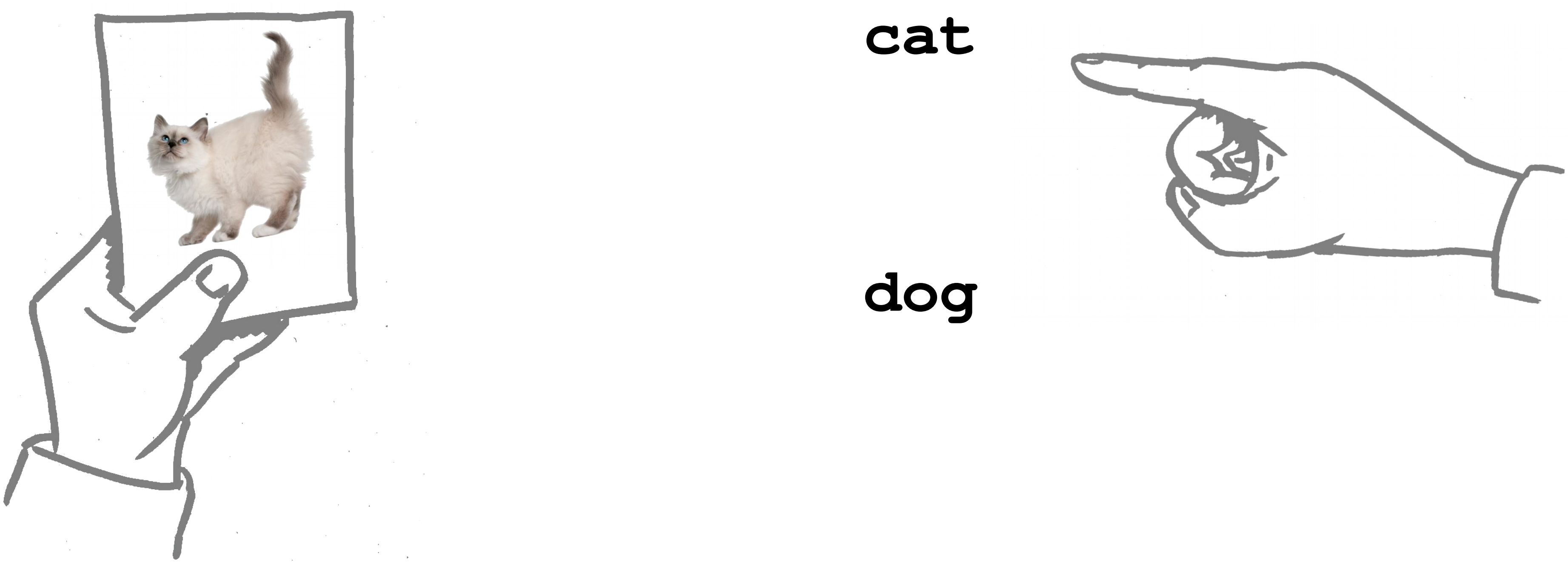

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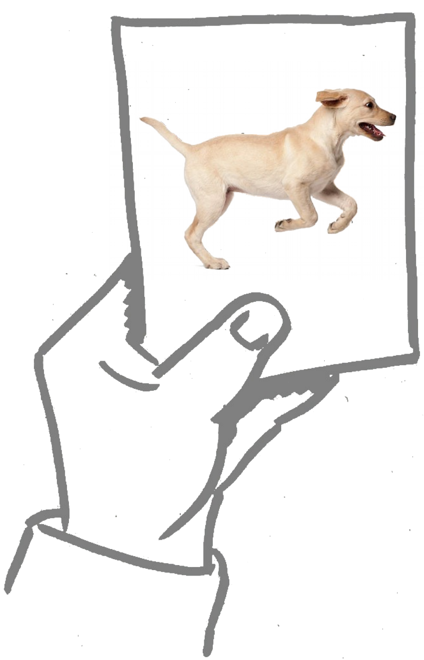

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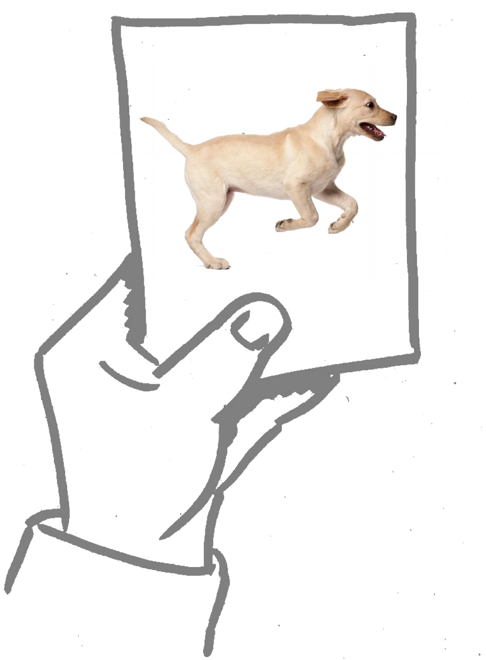

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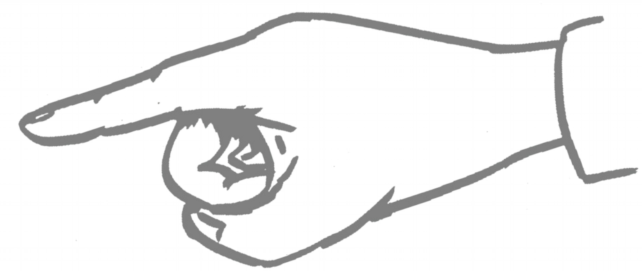

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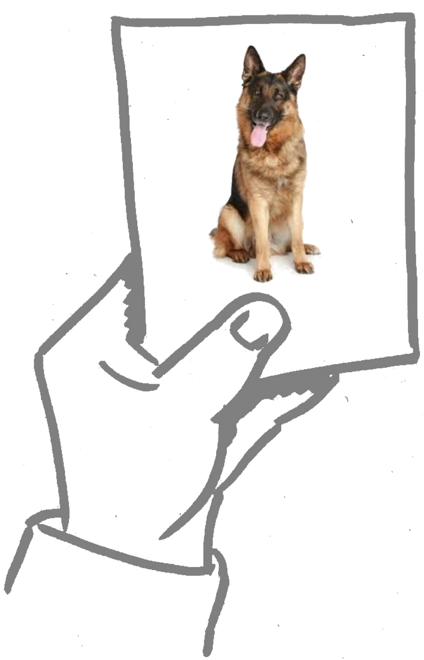

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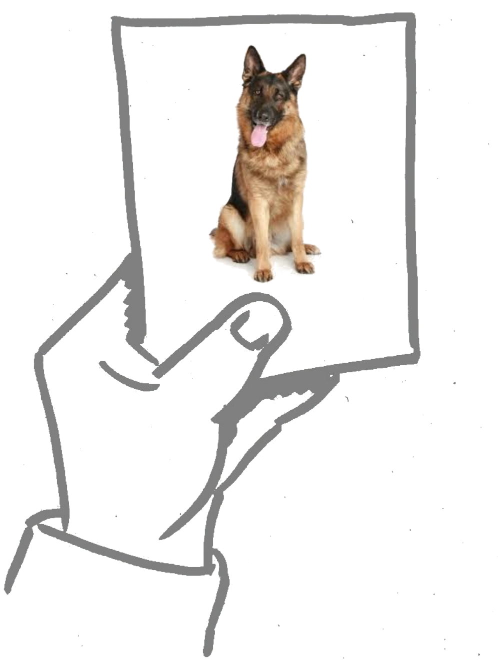

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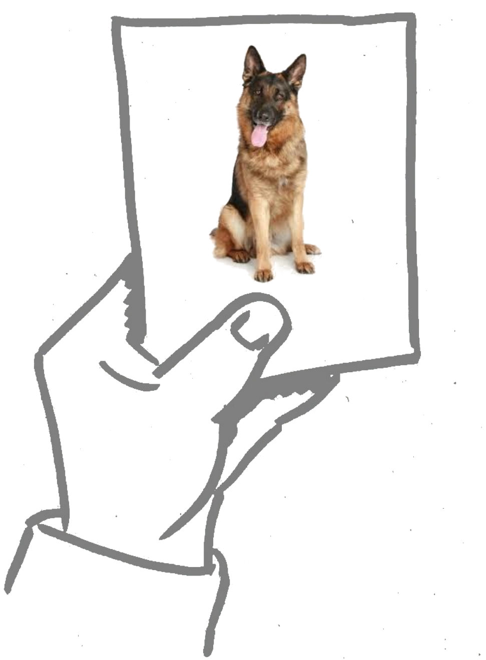


`cat`

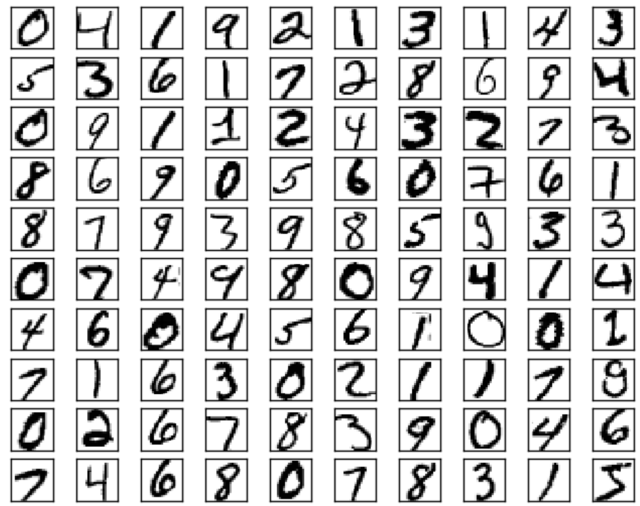
??

`dog`

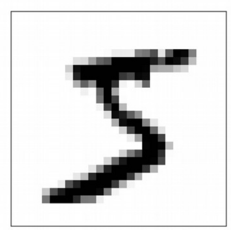
Generalization to unseen picture

Let us play with digits...
... the MNIST database

Classification of handwritten digits



70’000 input/output pairs

$\Big($  $, \; 5 \Big)$

How to use them?

Input x

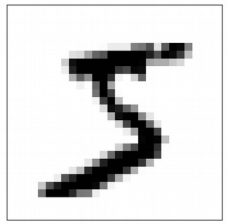
$28 \times 28, \;\; [0,\, 1]^{784}$

Correct output $y(x)$

$\{0, 1 \ldots 9\}$

Let us play with digits...

... the MNIST database

$\Big\{ \Big($  $, \; 5 \Big) \quad \ldots \quad \Big\}$

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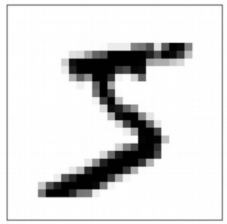
$\Big\{ \Big($  $, \quad 5 \Big) \quad \ldots \quad \Big\}$

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$$f_{\bar{w},\bar{b}} : [0,1]^{784} \to \{0, 1 \ldots 9\}$$

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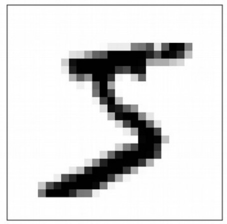
$\Big\{\Big($  $, \; 5 \Big) \; \ldots \Big\}$

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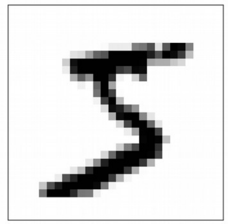
A parametrized function...

How to **construct** it?

Let us play with digits...

... the MNIST database

$\Big\{ \Big($  $, \; 5 \Big) \; \ldots \Big\}$

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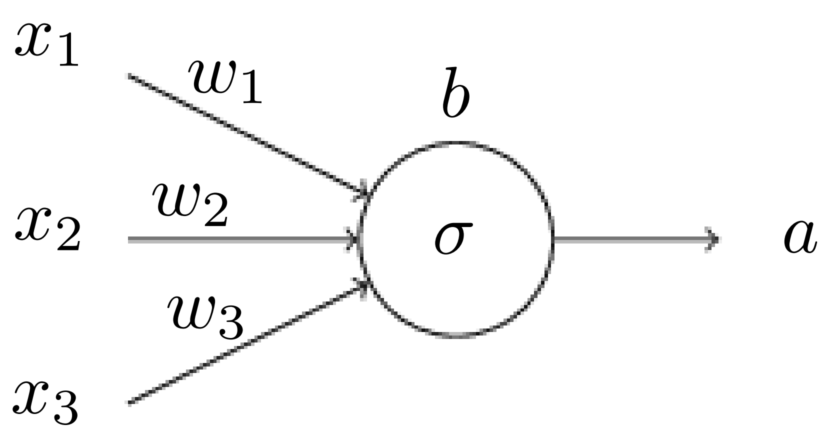
A parametrized function...

How to **construct** it?

Feed-Forward Neural Networks

Feed-Forward Neural Networks...
...the ingredients

from the input
or
from other neurons



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Feed-Forward Neural Networks...
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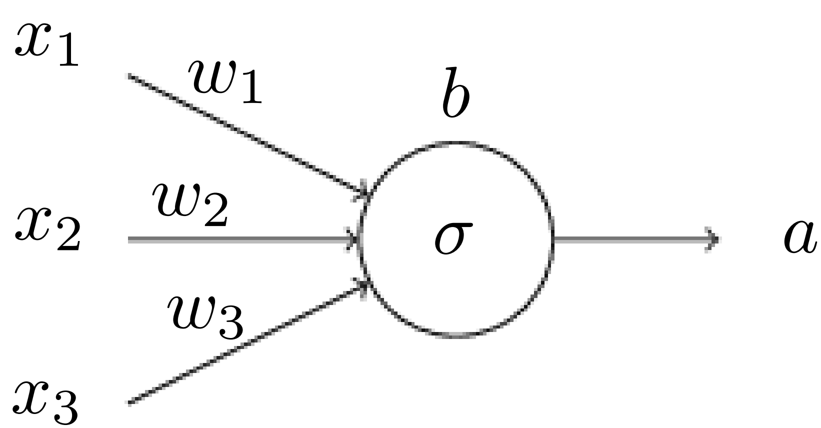

to output
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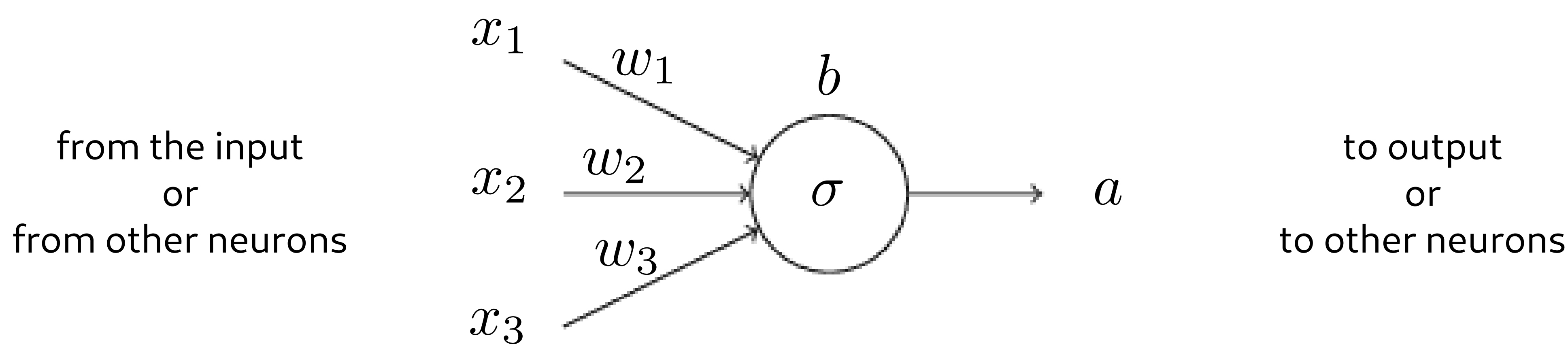
weights w **bias** b **activity** a

Feed-Forward Neural Networks...
...the ingredients



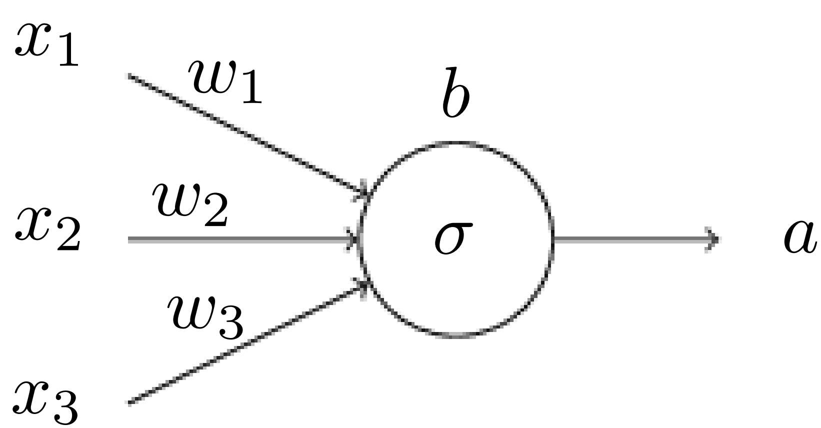
weights w **bias** b **activity** a

weighed input $z = b + \sum_i w_i \, x_i$

activation function σ, $\quad a = \sigma(z)$

Feed-Forward Neural Networks...
...the ingredients

from the input
or
from other neurons



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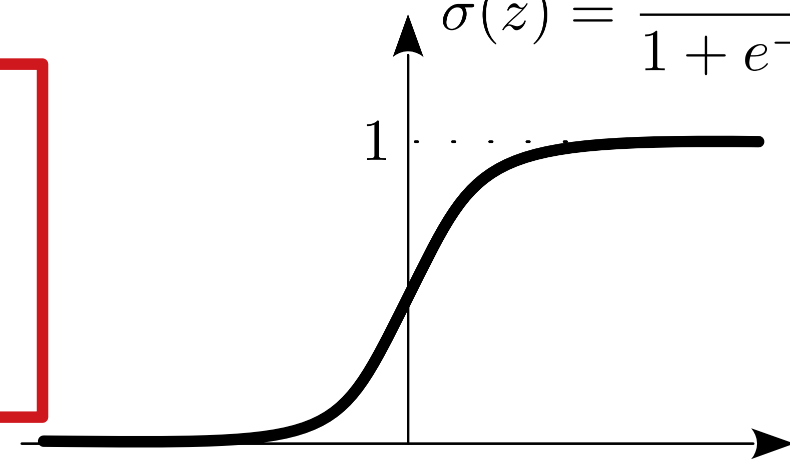
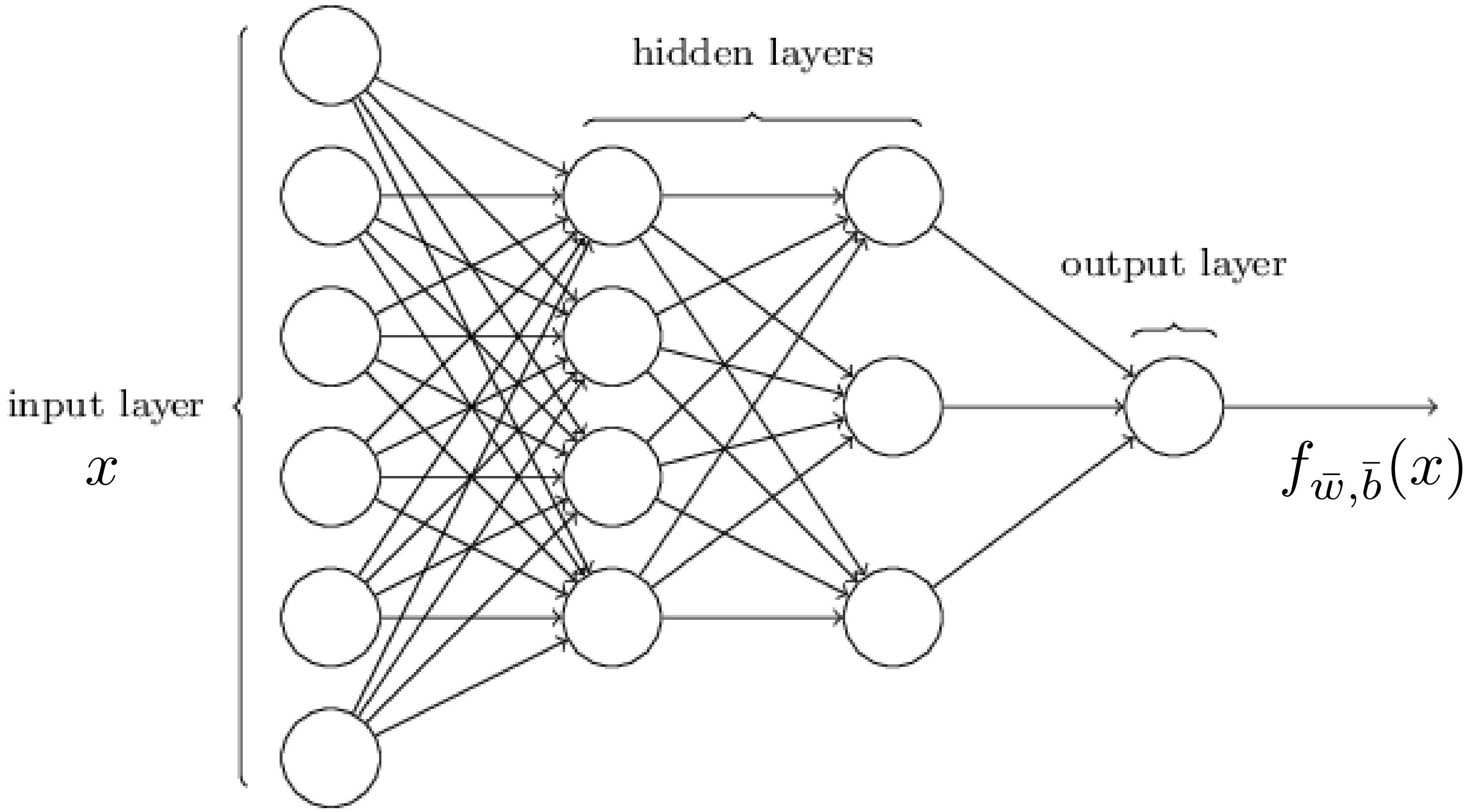
$$\sigma(z) = \frac{1}{1+e^{-z}}$$



Feed-Forward Neural Networks…
…the architecture



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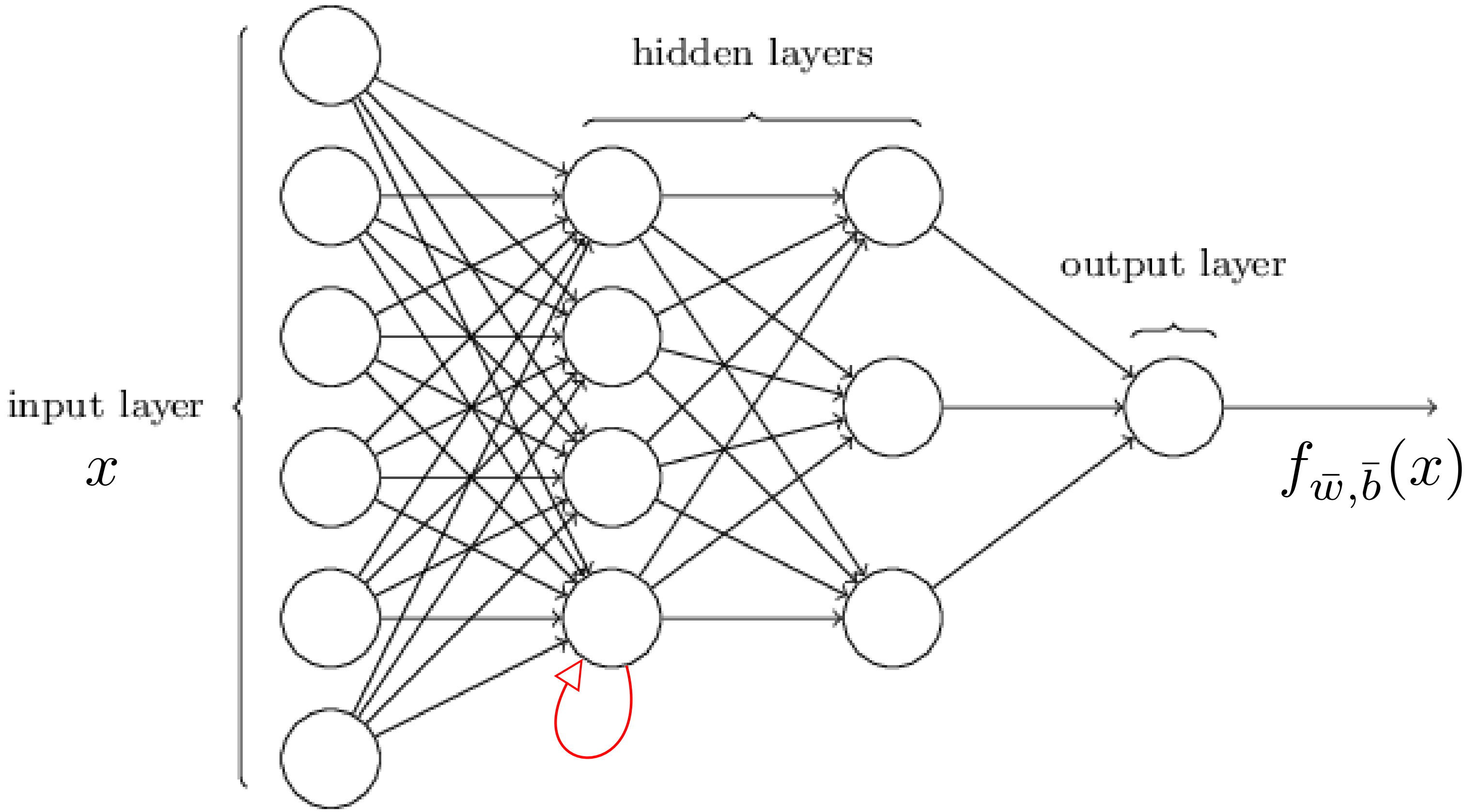

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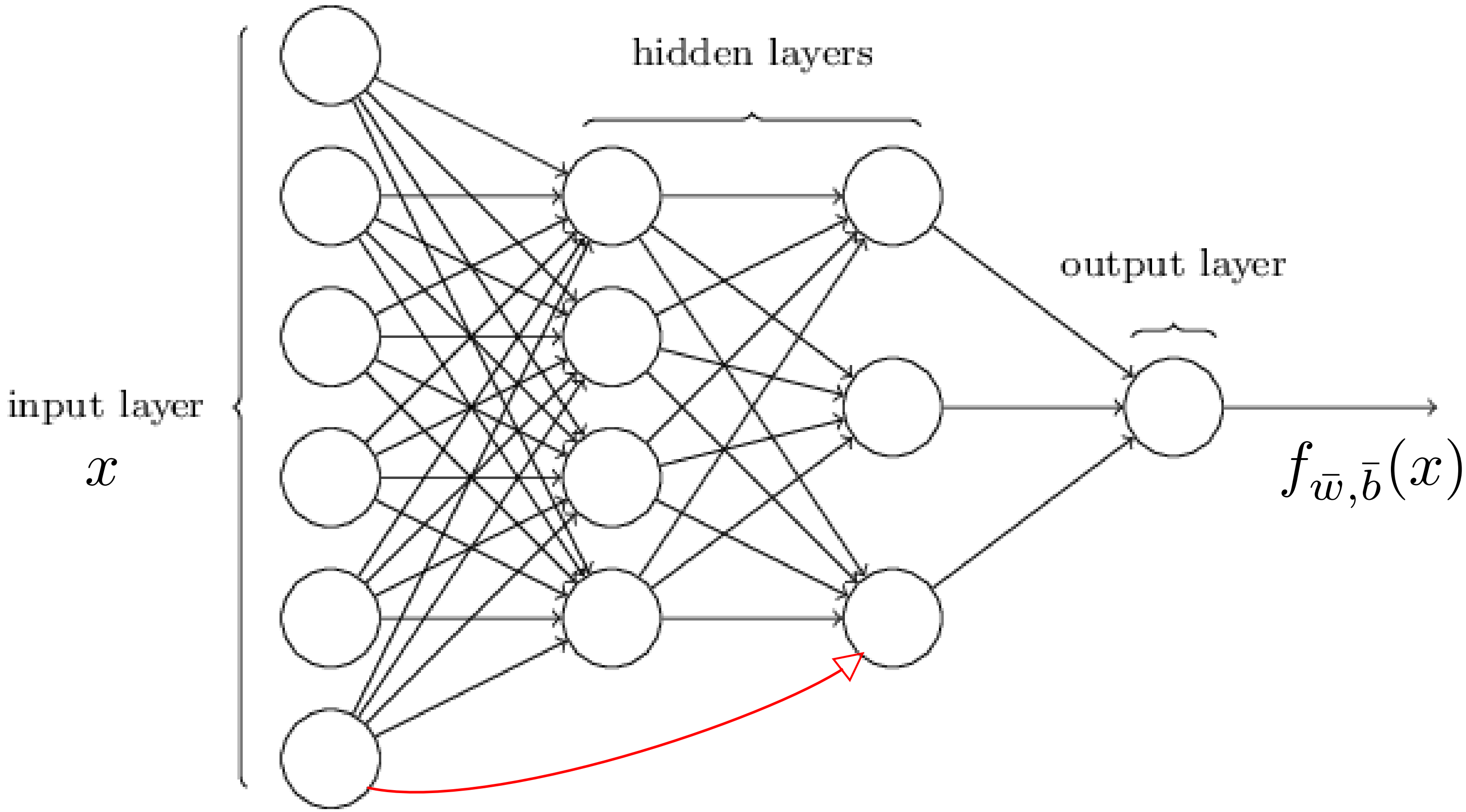

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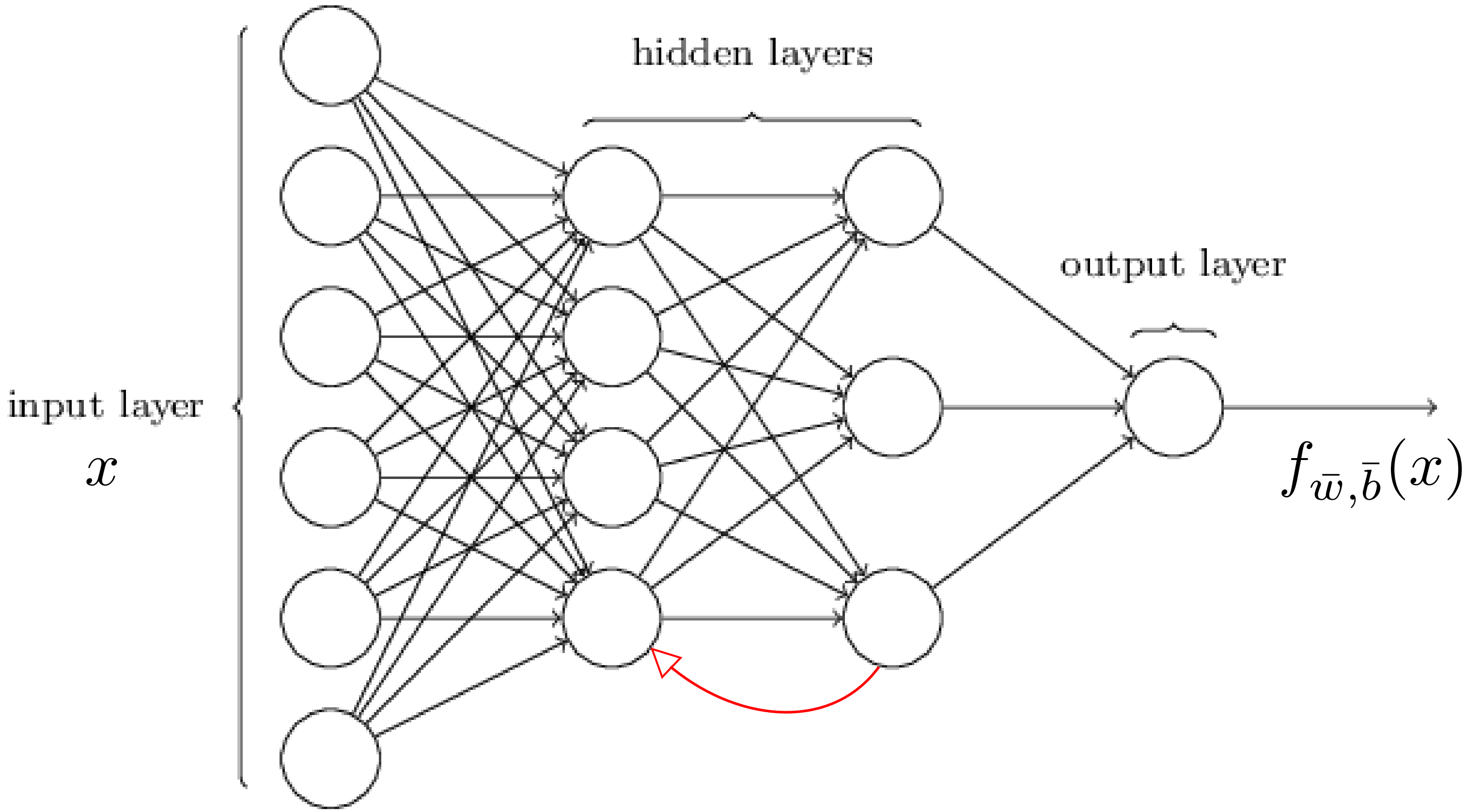

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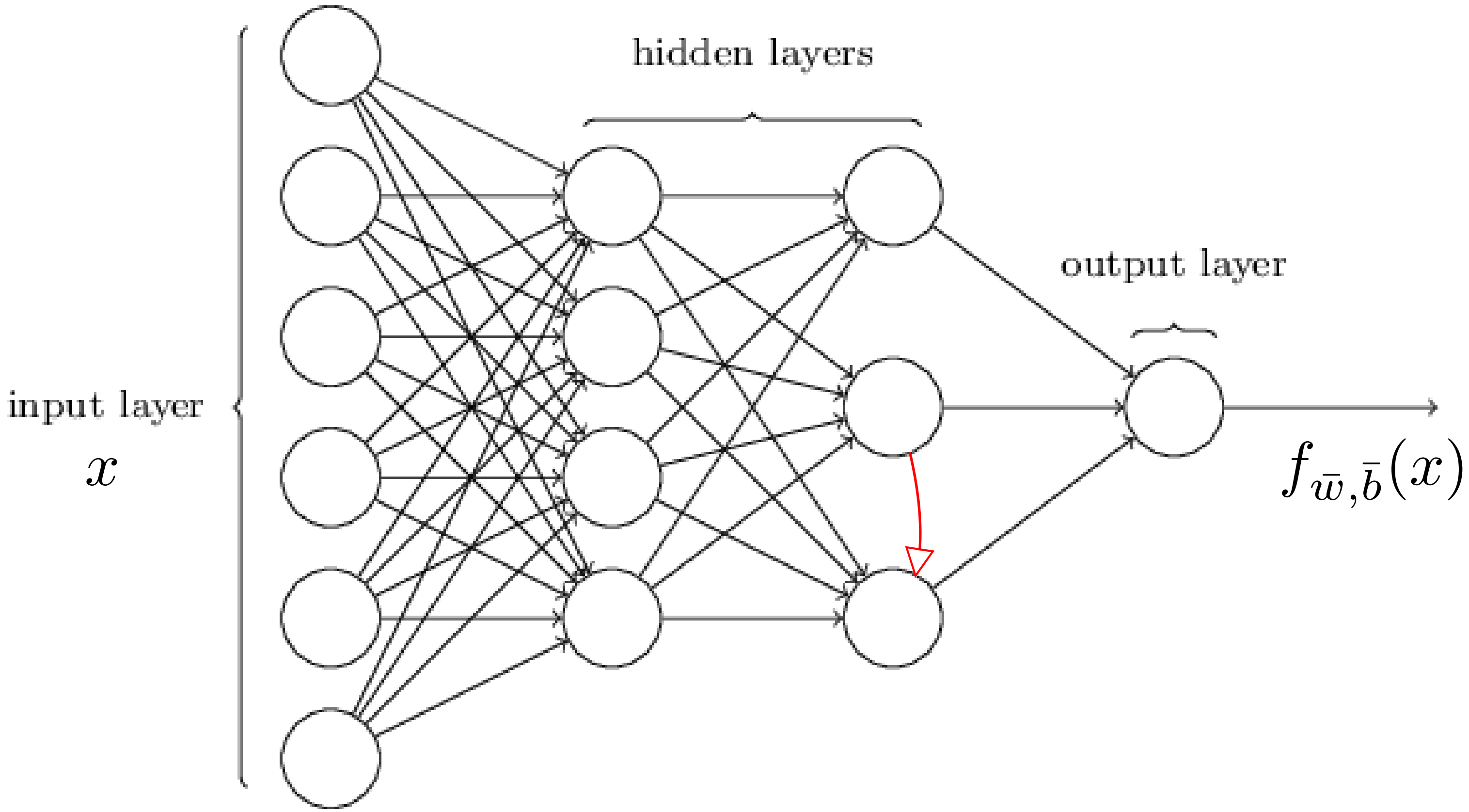

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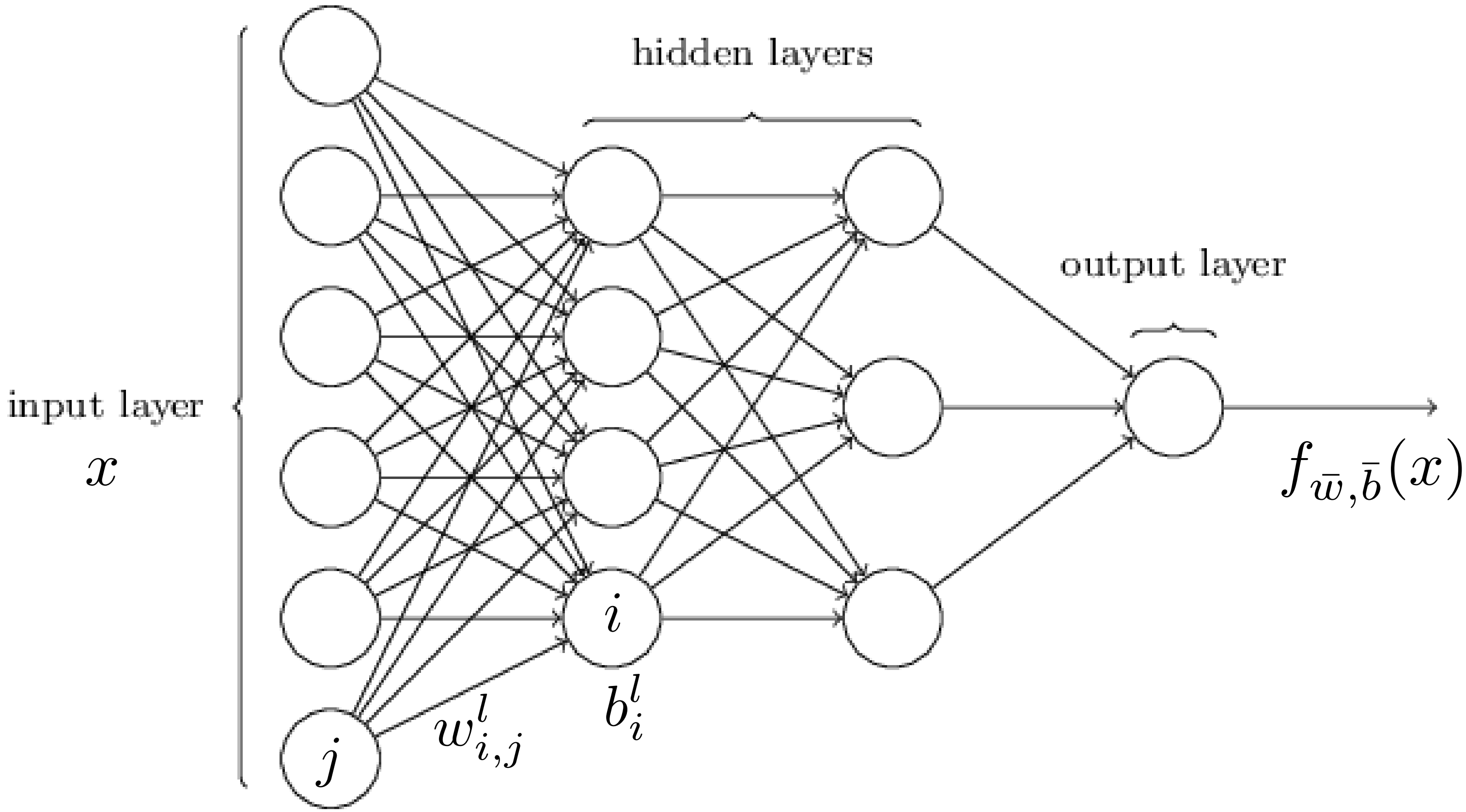
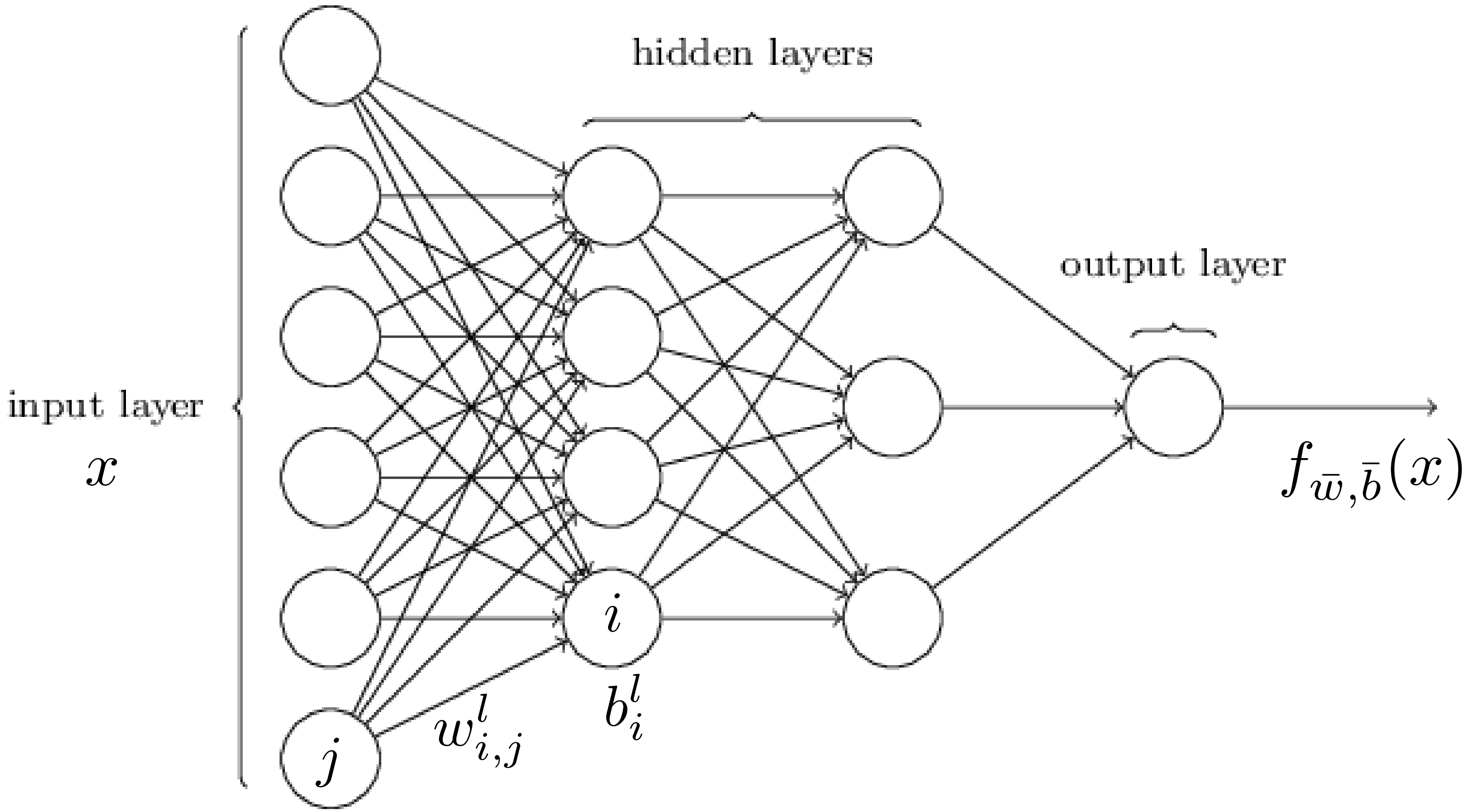


one **weight** per arrow
one **bias** per neuron

$$w^l_{i,j} \qquad b^l_i$$

Feed-Forward Neural Networks…
…the architecture



one **weight** per arrow
one **bias** per neuron

$w_{i,j}^l \qquad b_i^l$

$$a_i^l = \sigma\left(z_i^l\right)$$

$$= \sigma\left(b_i^l + \sum_j w_{i,j}^l a_j^{l-1}\right)$$

Feed-Forward Neural Networks...
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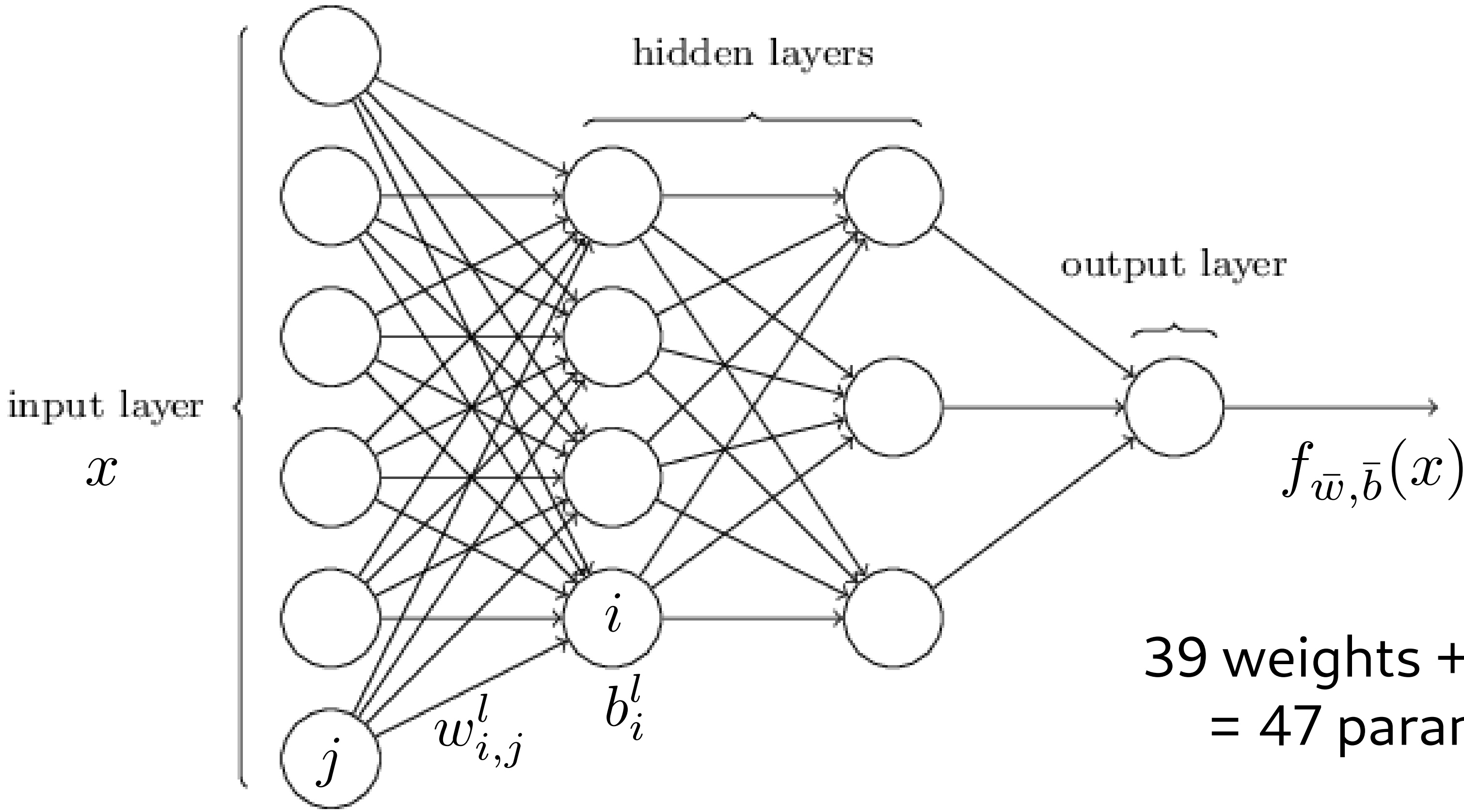

39 weights + 8 biases
= 47 parameters

one **weight** per arrow
one **bias** per neuron

$w_{i,j}^{l}$ $\quad$ b_i^l

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Feed-Forward Neural Networks…

…universal function approximators

[Cybenko, G. (1989) *Approximations by superpositions of sigmoidal functions*]

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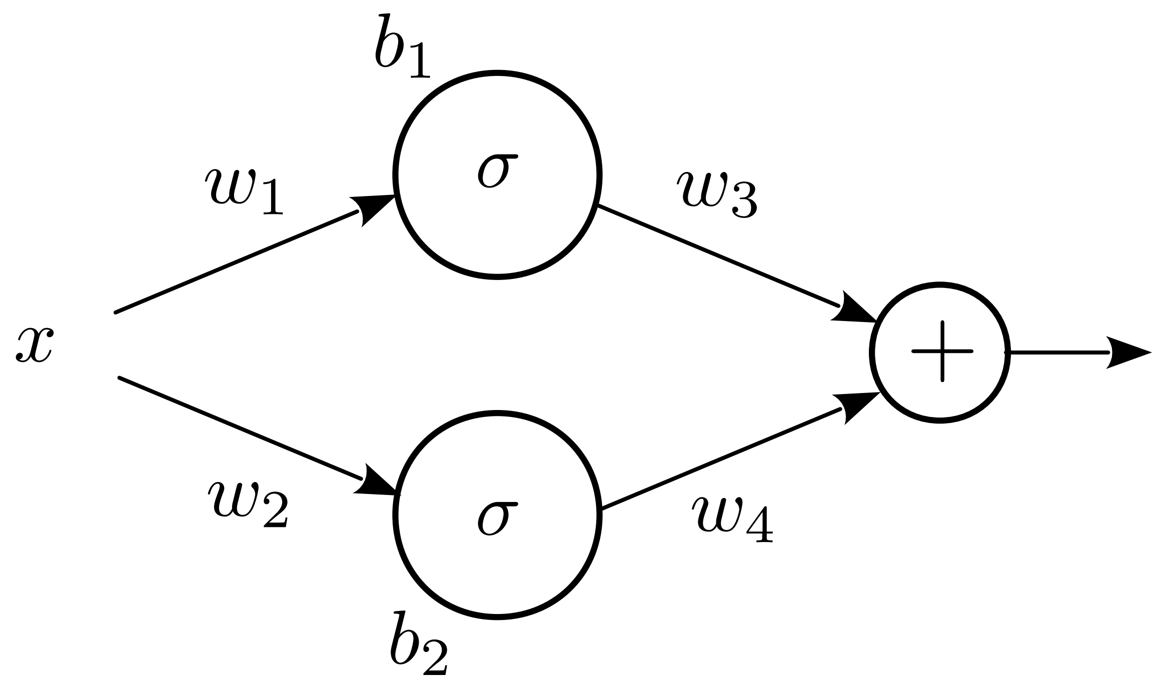

$$f_{\bar{w},\bar{b}}(x) = w_3\,\sigma\big(b_1 + w_1 x\big) + w_4\,\sigma\big(b_2 + w_2 x\big)$$

Feed-Forward Neural Networks...
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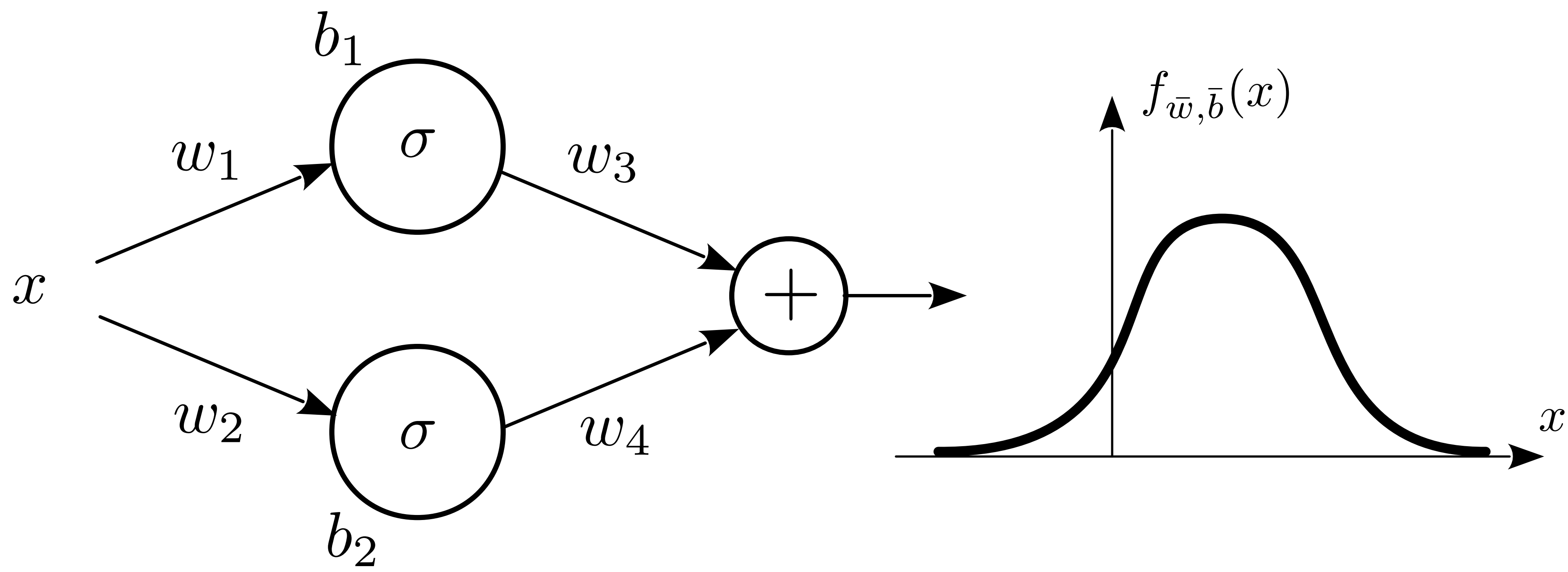

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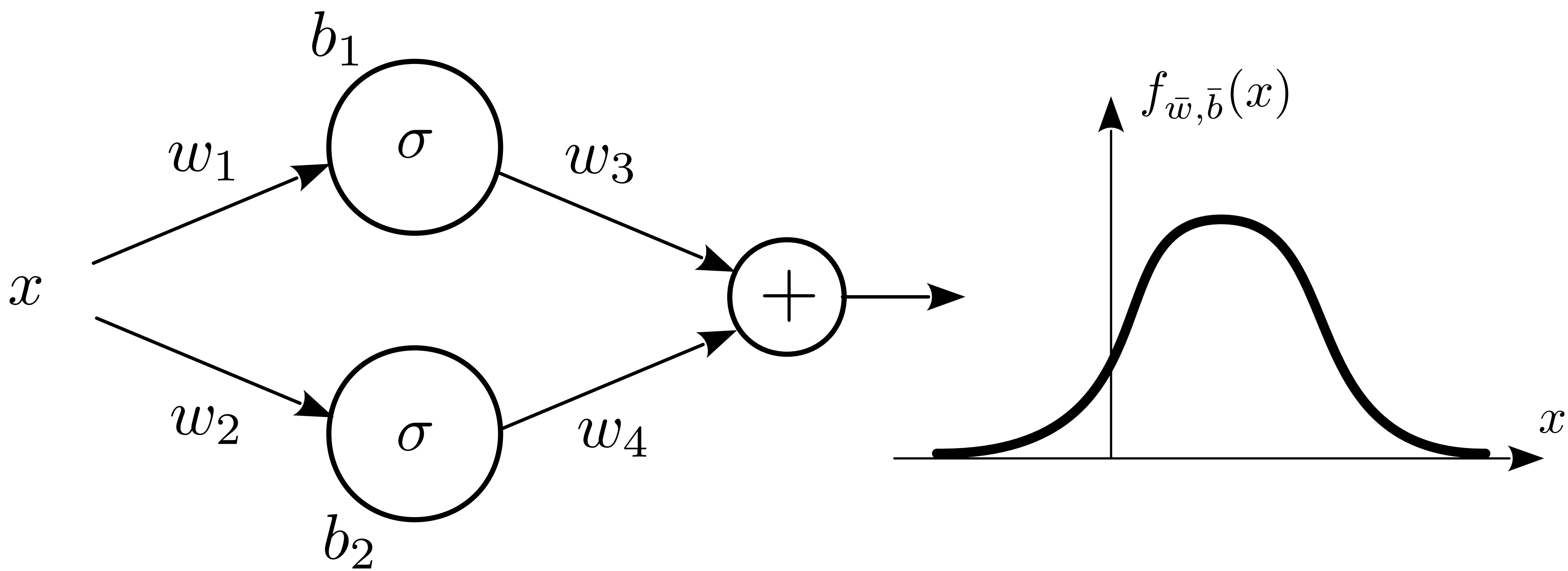

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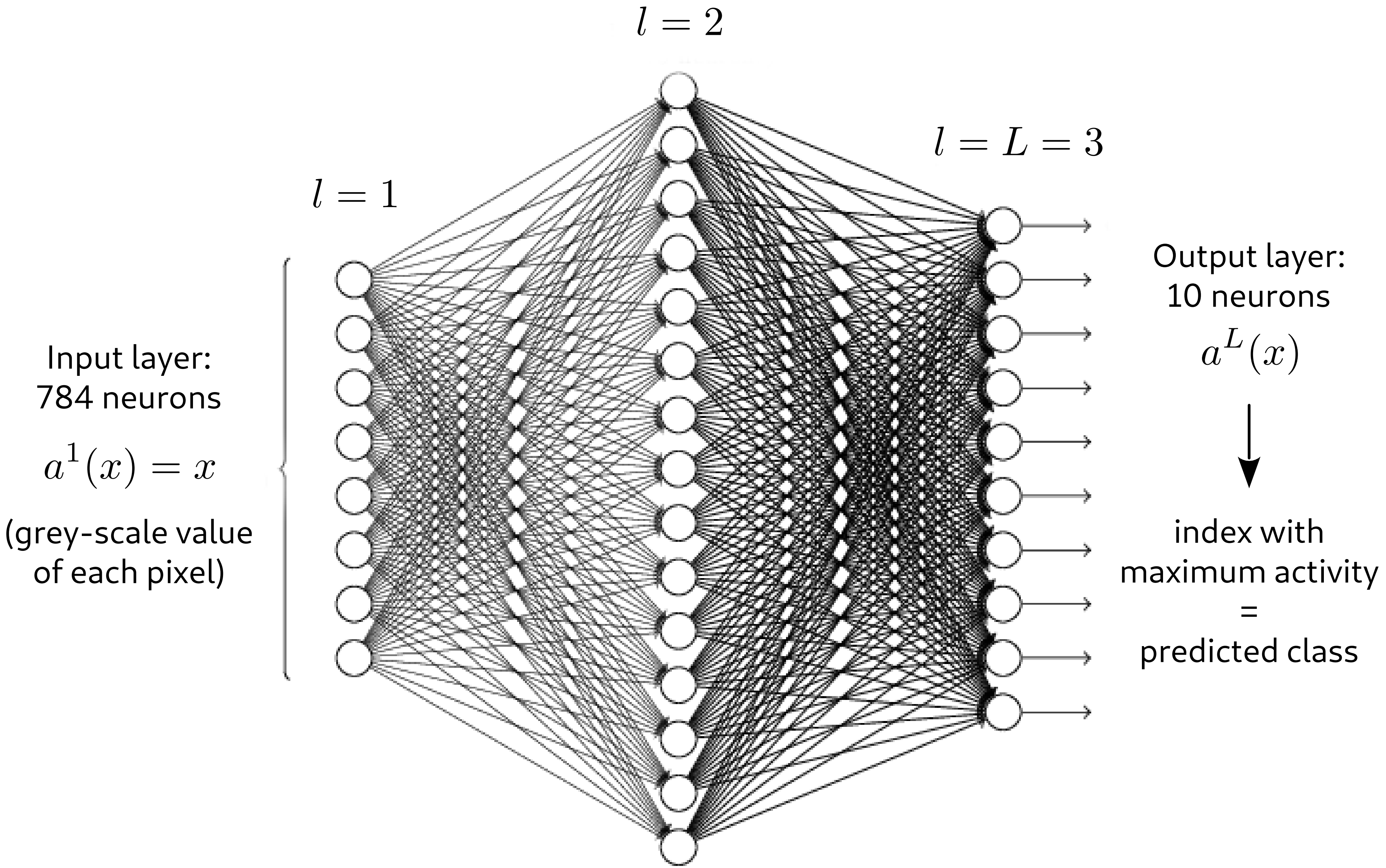
Open Firefox: **www.geogebra.org**

Network for MNIST handwritten digit classification



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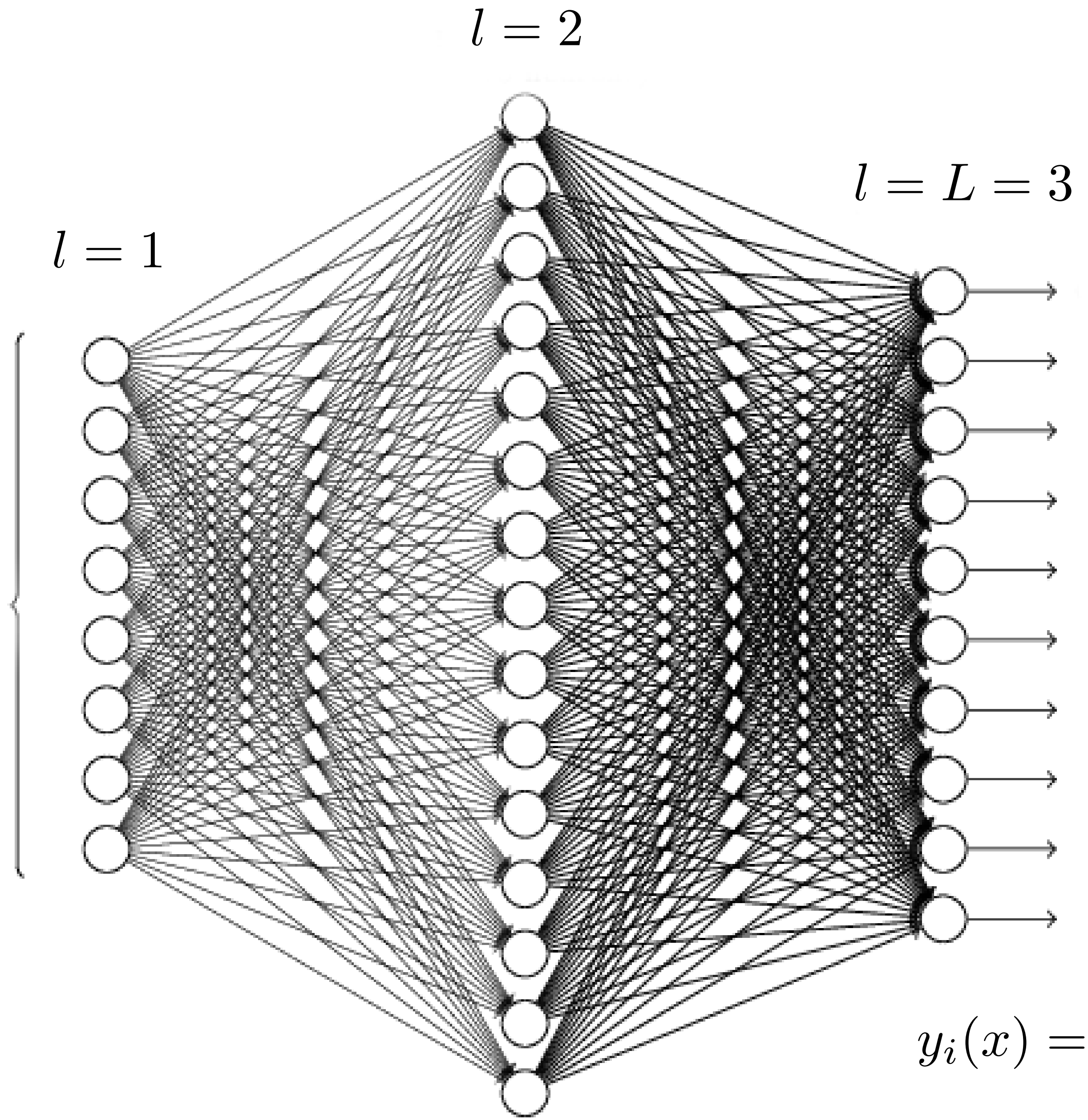


Input layer:
784 neurons

$$a^1(x) = x$$

(grey-scale value
of each pixel)

Output layer:
10 neurons

$$a^L(x)$$

$\downarrow$

index with
maximum activity
=
predicted class

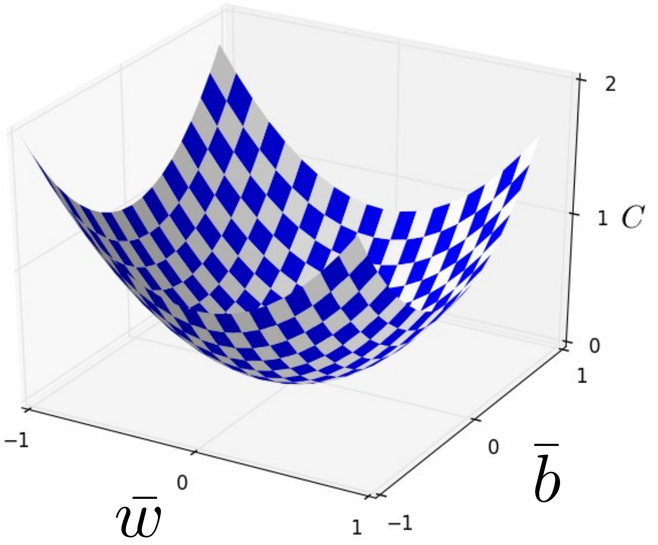
$$y_i(x) = \begin{cases} 1 & i = \text{digit} \\ 0 & \text{otherwise} \end{cases}$$

Learning through gradient descent

Minimize a **cost** (or **loss**) **function**:

$$C(\bar{w},\bar{b}) = \Big\langle C_x(\bar{w},\bar{b}) \Big\rangle_{\substack{\text{training}\\ \text{data } x}} = \frac{1}{N}\sum_{x} C_x(\bar{w},\,\bar{b})$$

training data



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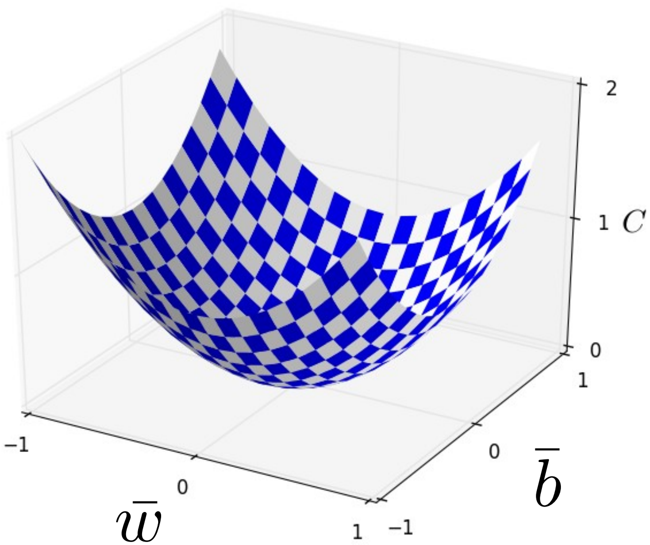

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training data

A possible choice: **quadratic** cost

$$C_x = \frac{1}{2}\sum_i \left(a_i^L(x) - y_i(x)\right)^2$$

neurons
in layer L
(output)

Learning through gradient descent

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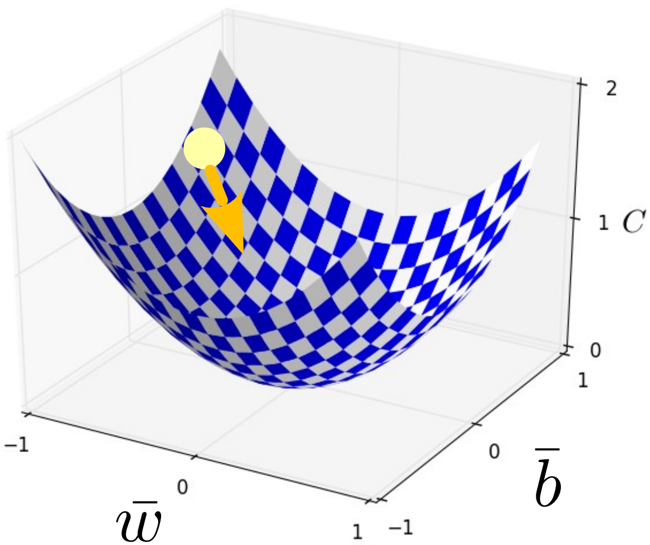

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Gradient descent update rules:

$$w_{i,j}^l \leftarrow w_{i,j}^l - \eta\,\frac{\partial C}{\partial w_{i,j}^l}$$

$$b_i^l \leftarrow b_i^l - \eta\,\frac{\partial C}{\partial b_i^l}$$

η

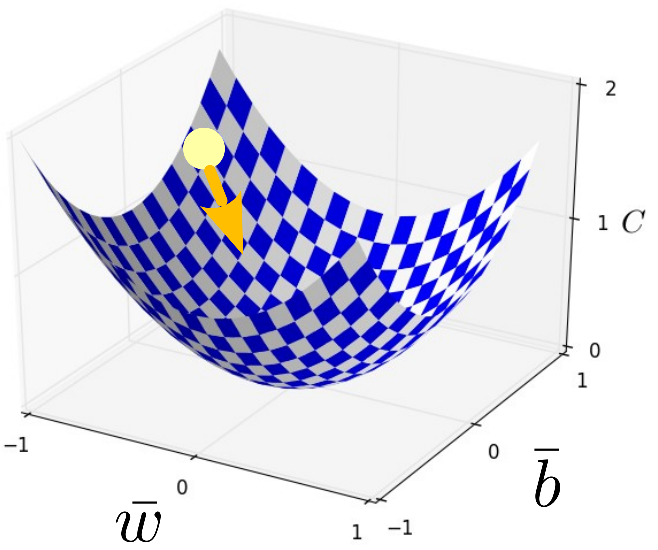
learning rate

Learning through gradient descent

Minimize a **cost** (or **loss**) **function**:

$$C(\bar{w}, \bar{b}) = \Big\langle C_x(\bar{w}, \bar{b}) \Big\rangle_{\substack{\text{training}\\ \text{data } x}} = \frac{1}{N} \sum_x C_x(\bar{w},\, \bar{b})$$

training data



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neurons in layer L (output)

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η

learning rate

$$\frac{\partial C}{\partial w_{i,j}^l}, \ \frac{\partial C}{\partial b_i^l} = \ ?$$

The backpropagation algorithm

The **error**:

How much does the cost change as an effect of a change in the input of a given neuron in a given layer?

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How much does the cost change as an effect of a change in the input of a given neuron in a given layer?

$$\delta_i^l \equiv \frac{\Delta C_x}{\Delta z_i^l} \to \frac{\partial C_x}{\partial z_i^l}$$

The backpropagation algorithm

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Small if the parameters are close to **optimal**.

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$$\frac{\partial C_x}{\partial w_{ij}^l}$$

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$$\frac{\partial C_x}{\partial w_{ij}^l} = \frac{\partial C}{\partial z_i^l}\,\frac{\partial z_i^l}{\partial w_{ij}^l}$$

chain rule $z_i^l = b_i^l + \sum_j w_{i,j}^l \, a_j^{l-1}$

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$$\frac{\partial C_x}{\partial b_i^l}$$

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$$\frac{\partial C_x}{\partial b_i^l} = \frac{\partial C}{\partial z_i^l} \frac{\partial z_i^l}{\partial b_i^l} = \delta_i^l$$

The backpropagation algorithm

From the activity of the **output** layer...

$$\delta_i^L = \frac{\partial C_x}{\partial z_i^L}$$

The backpropagation algorithm

From the activity of the **output** layer...

$$\delta_i^L = \frac{\partial C_x}{\partial z_i^L} = \overbrace{\Big(a_i^L(x) - y_i(x)\Big)}^{\text{predicted – desired}} \sigma'\big(z_i^L\big)$$

$$C_x = \sum_{\substack{j \\ \text{layer } L}} \frac{1}{2}\big(a_j^L(x) - y_j(x)\big)^2 \qquad C = \frac{1}{N}\sum_x C_x$$

The backpropagation algorithm

From the activity of the **output** layer...

$$\delta_i^L = \frac{\partial C_x}{\partial z_i^L} = \overbrace{\left(a_i^L(x) - y_i(x)\right)}^{\text{predicted – desired}} \sigma'\left(z_i^L\right)$$

$$C_x = \sum_{\substack{j \\ \text{layer } L}} \frac{1}{2}\left(a_j^L(x) - y_j(x)\right)^2 \qquad C = \frac{1}{N}\sum_x C_x$$

... and **back-propagate** to the previous layers

$$\color{red}{\delta_j^{l-1}} = \frac{\partial C_x}{\partial z_j^{l-1}}$$

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chain rule $\quad z_i^l = b_i^l + \sum_j w_{i,j}^l \, a_j^{l-1}$

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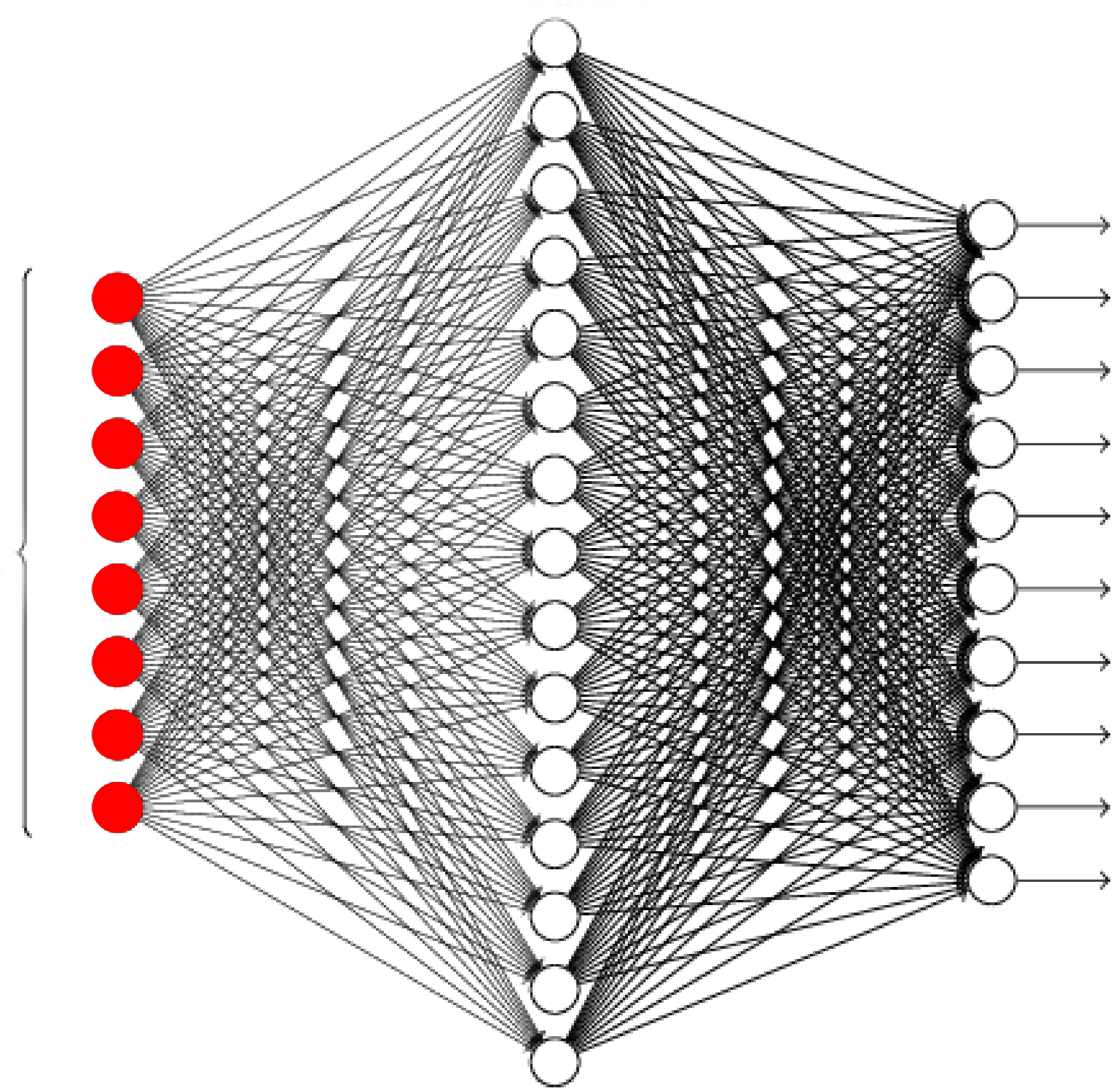
The backpropagation algorithm

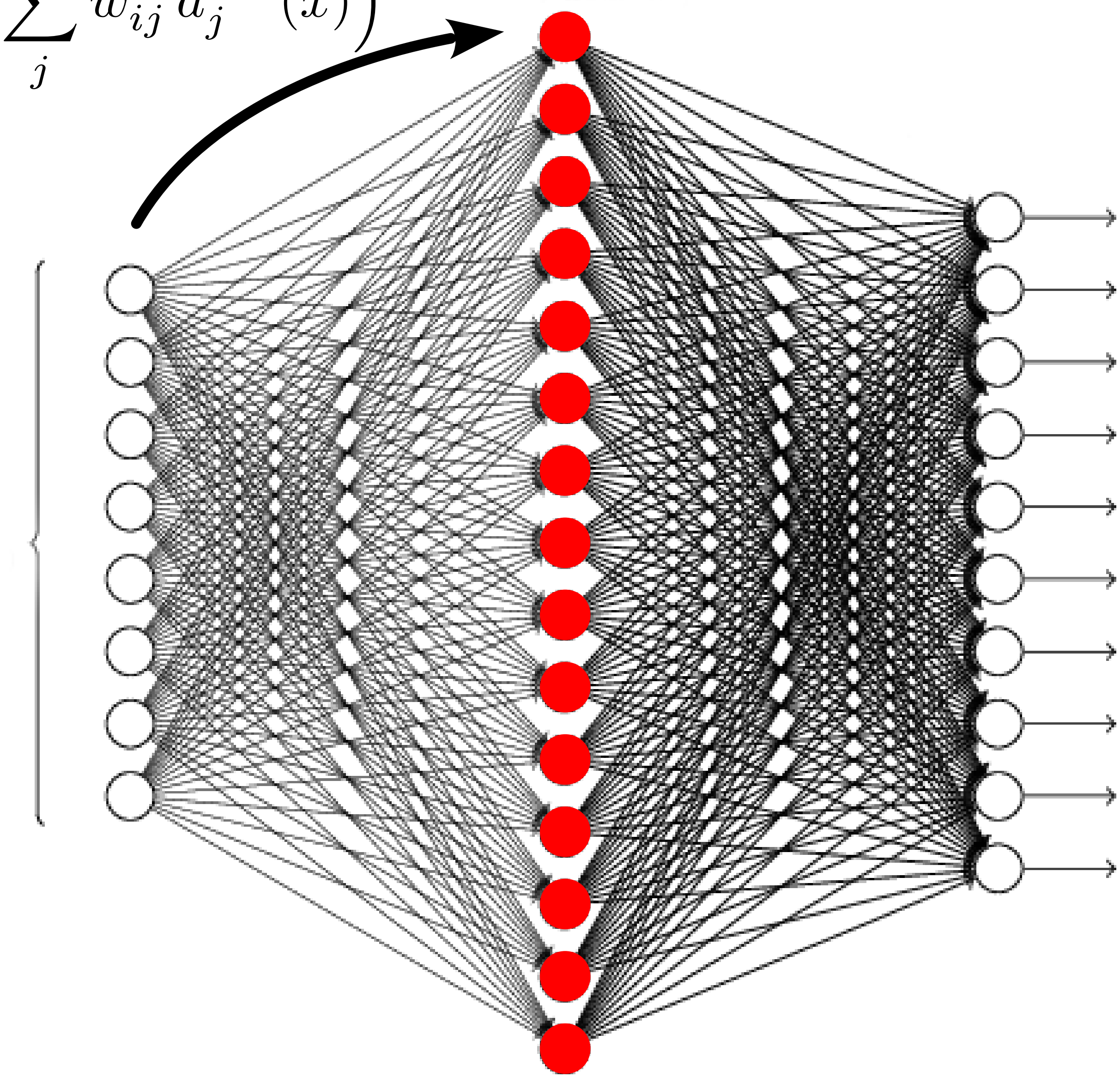
For every input x $\boxed{\text{1. } \textbf{Feed-forward}}$



The backpropagation algorithm

For every input x $\boxed{\text{1. } \textbf{Feed-forward}}$

$$a_i^l(x) = \sigma\left(b_i^l + \sum_j w_{ij}^l \, a_j^{l-1}(x)\right)$$



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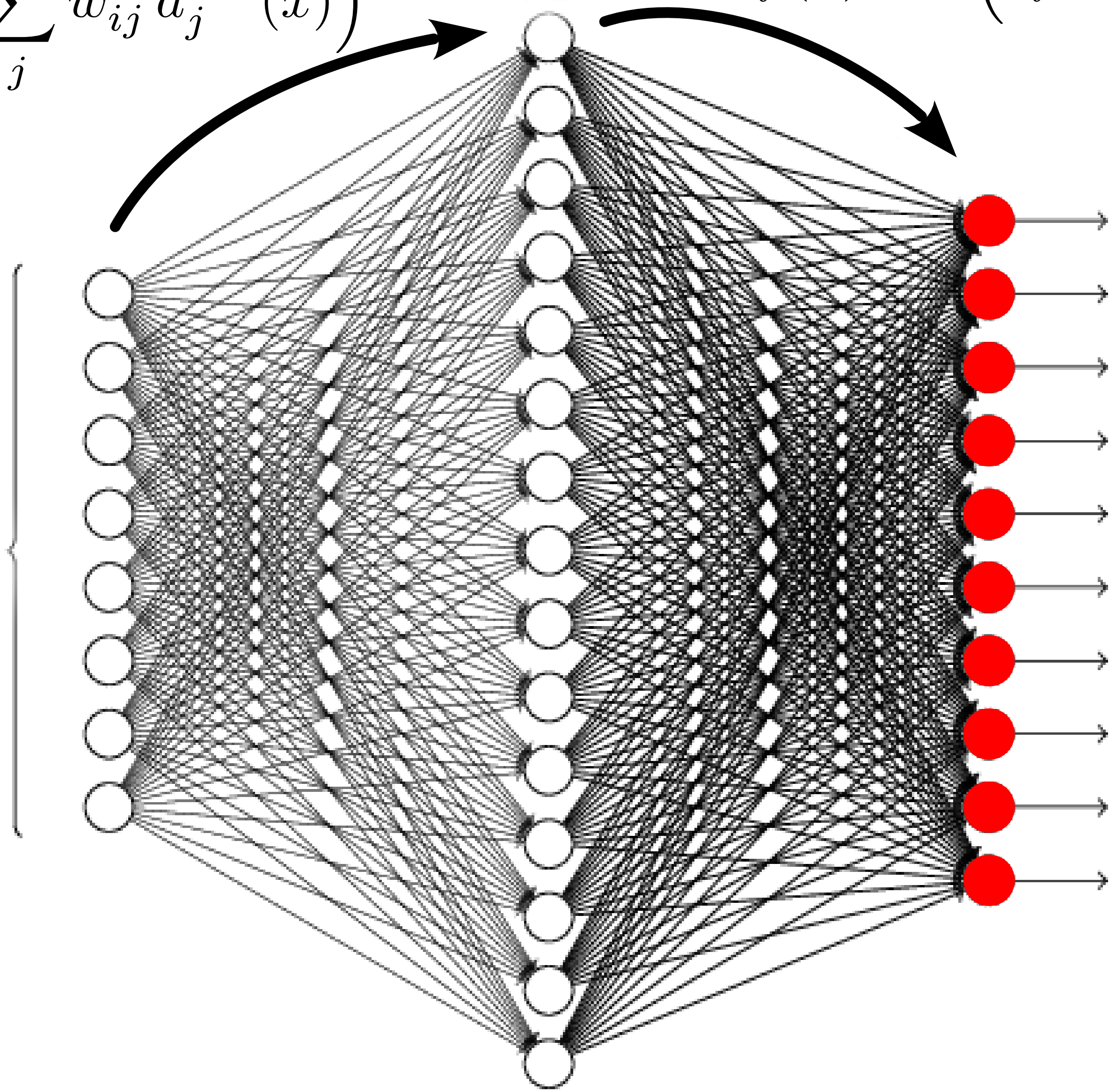
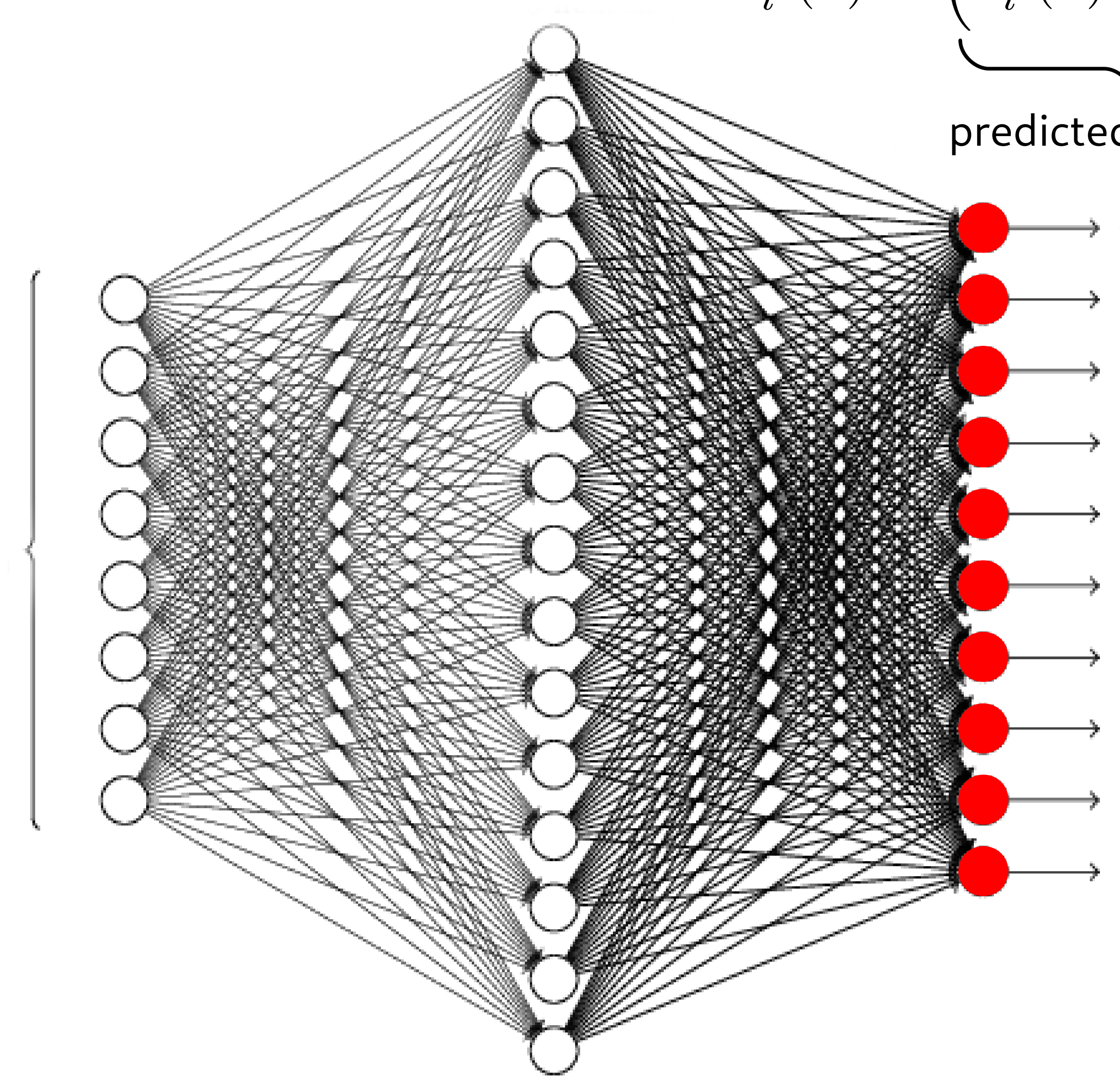


The backpropagation algorithm

For every input x

$\boxed{\text{2. Calculate the \textbf{error} at \textbf{output}}}$

$$\delta_i^L(x) = \underbrace{\left(a_i^L(x) - y_i(x)\right)}_{\text{predicted – desired}} \sigma'\left(z_i^L\right)$$

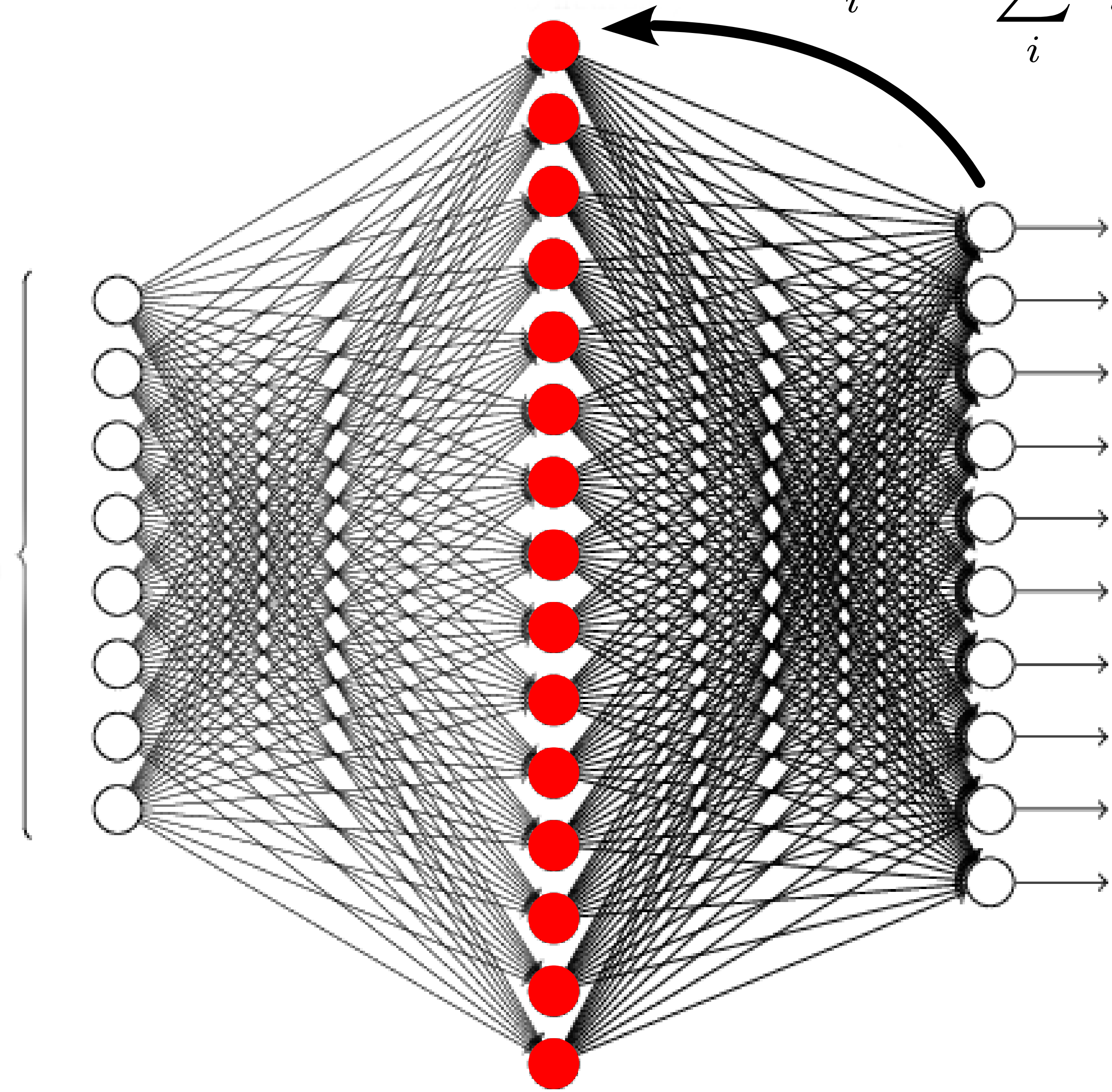


The backpropagation algorithm

For every input x

$\boxed{\text{3. \textbf{Back-propagate} the error}}$

$$\delta_i^{l-1} = \sum_i \delta_i^l \, w_{ij}^l \, \sigma'(z_j^{l-1})$$



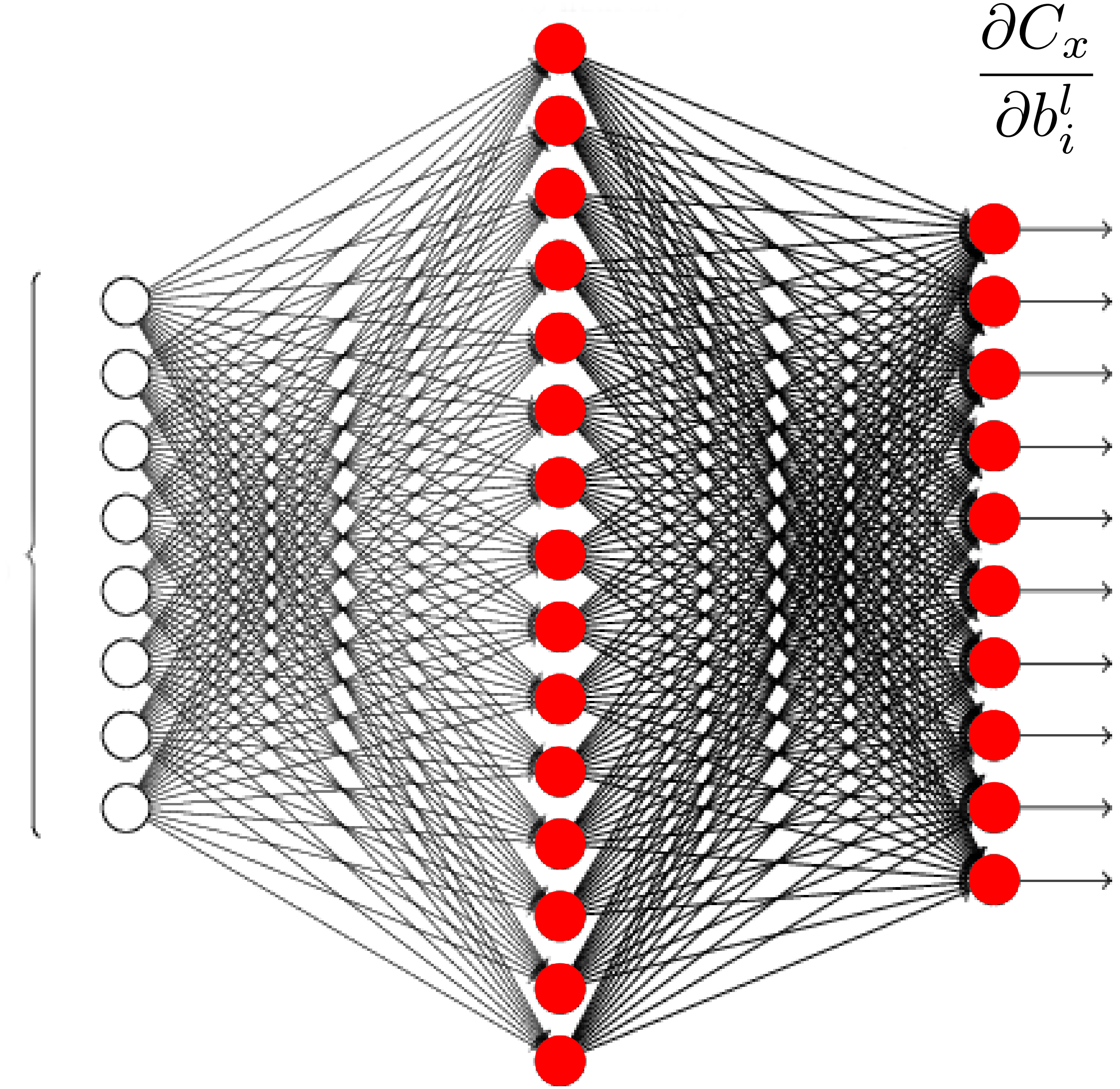
The backpropagation algorithm

For every input x

$\boxed{\text{4. Calculate the } \textbf{derivatives}}$

$$\frac{\partial C_x}{\partial w_{ij}^l} = \delta_i^l \, a_j^{l-1}$$

$$\frac{\partial C_x}{\partial b_i^l} = \delta_i^l$$



The mini-batch update

$$C = \frac{1}{N}\sum_x C_x \qquad \Rightarrow \qquad \nabla C = \frac{1}{N}\sum_x \nabla C_x$$

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{training data} = { {mini-batch 1}, {mini-batch 2}, ... {mini-batch M} }

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... and use the **mini-batch estimate** of the gradient for gradient descent

$$w \leftarrow w - \eta\,\overline{\nabla_w C}_m \qquad b \leftarrow b - \eta\,\overline{\nabla_b C}_m$$

(then **iterate** over all mini-batches)

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Stochastic Gradient Descent (SGD)