

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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“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

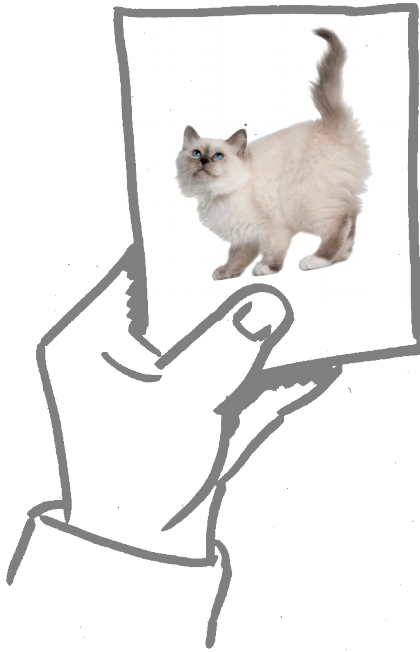
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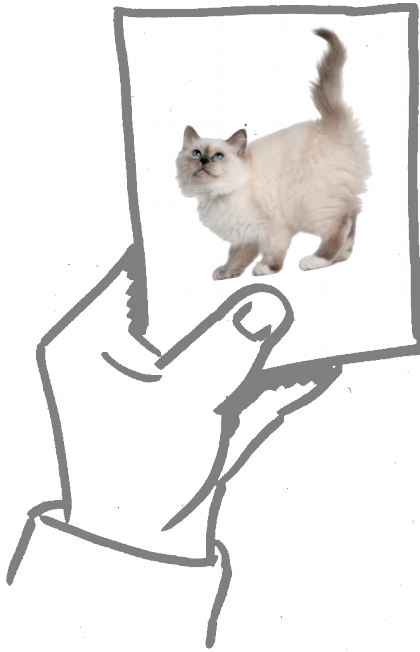
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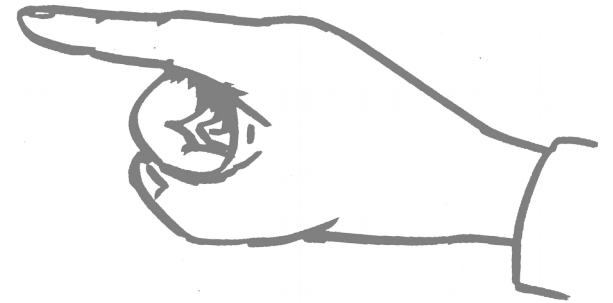
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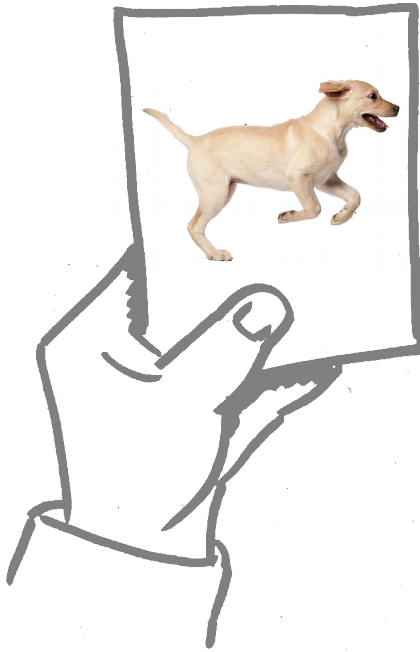
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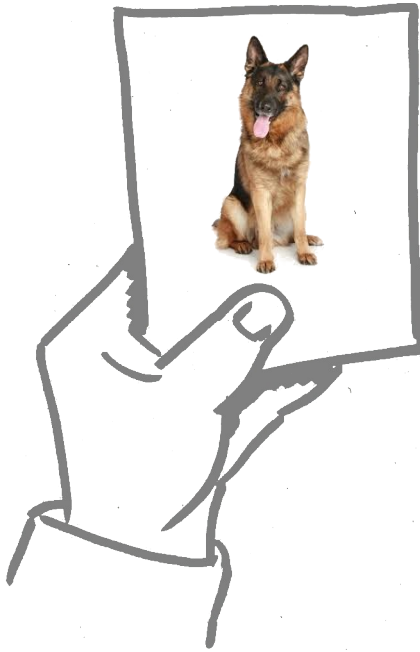
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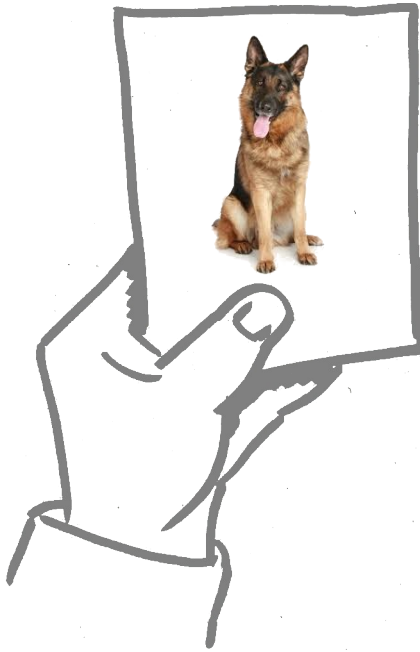
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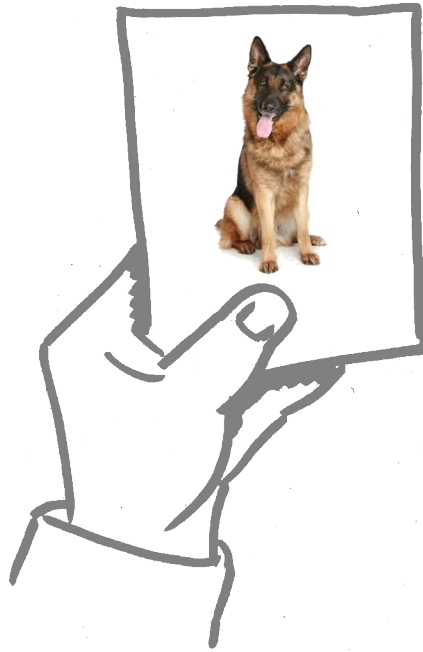
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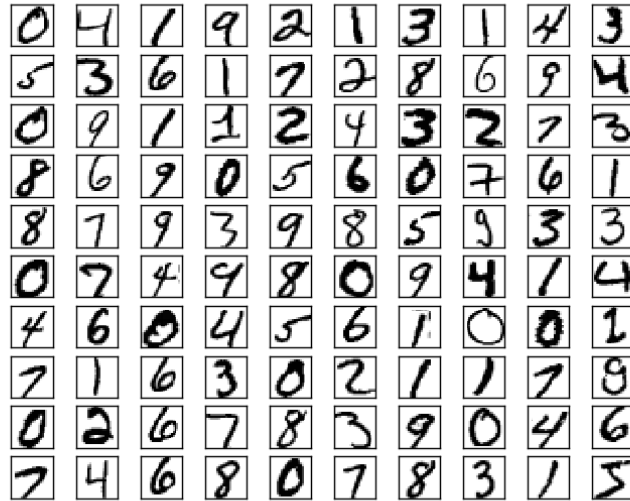
dog

Generalization to unseen picture

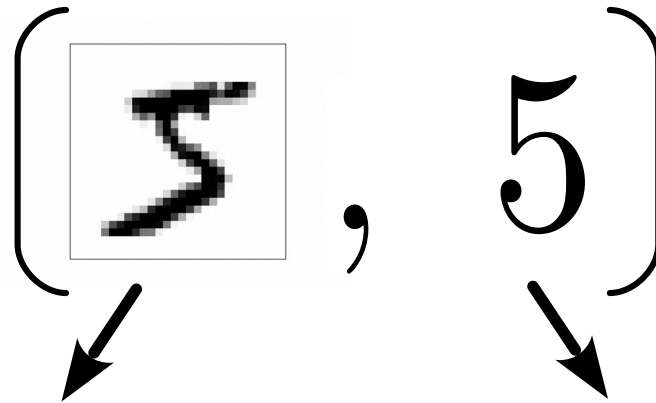
Let us play with digits...

... the MNIST database

Classification of
handwritten
digits



70'000
input/output
pairs



How to use
them?

Input x

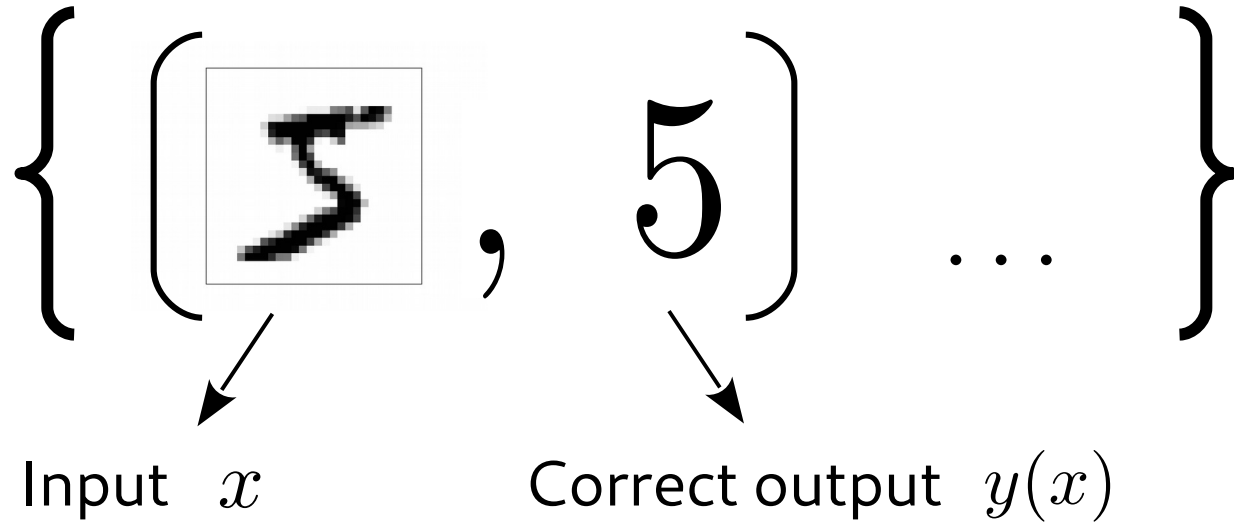
Correct output $y(x)$

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

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

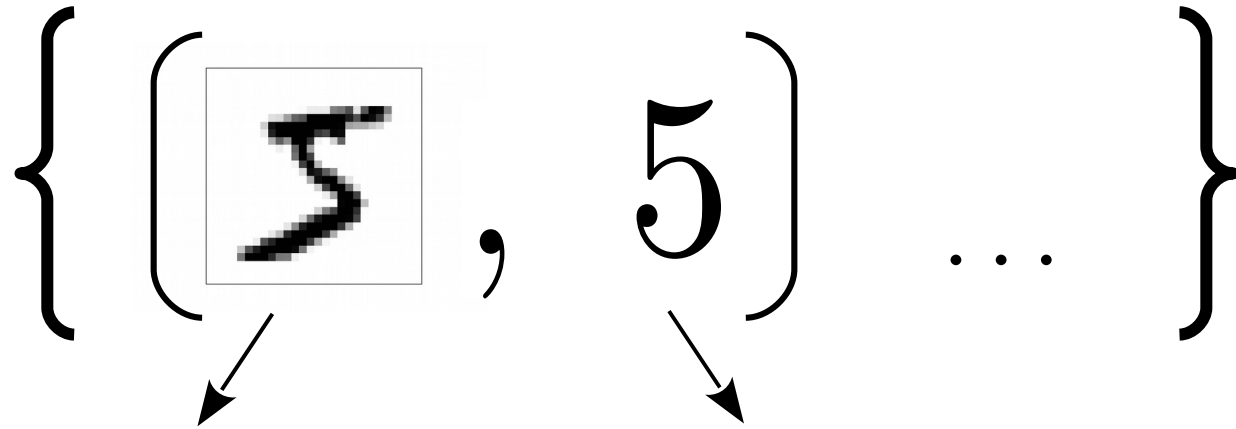
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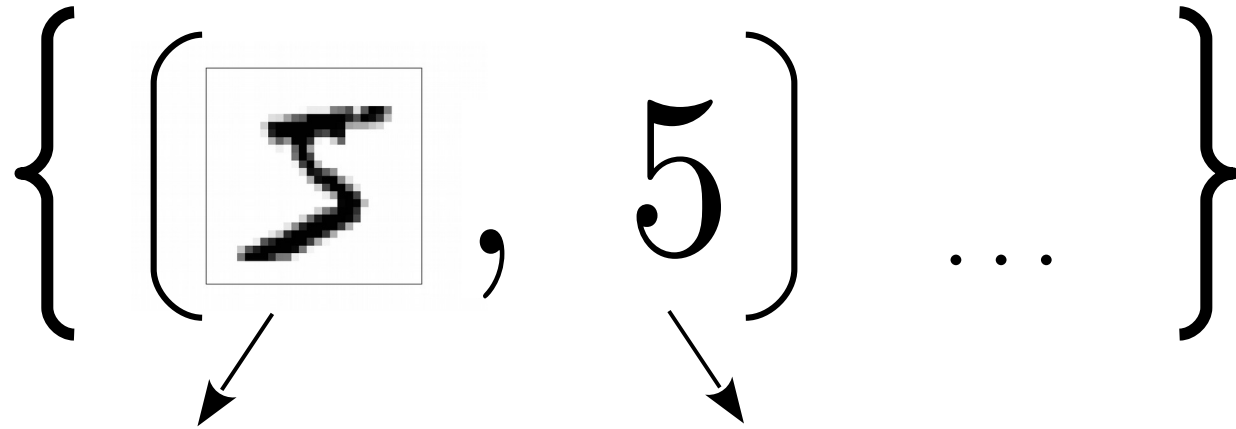
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$$f_{\bar{w}, \bar{b}} : [0, 1]^{784} \rightarrow \{0, 1 \dots 9\}$$

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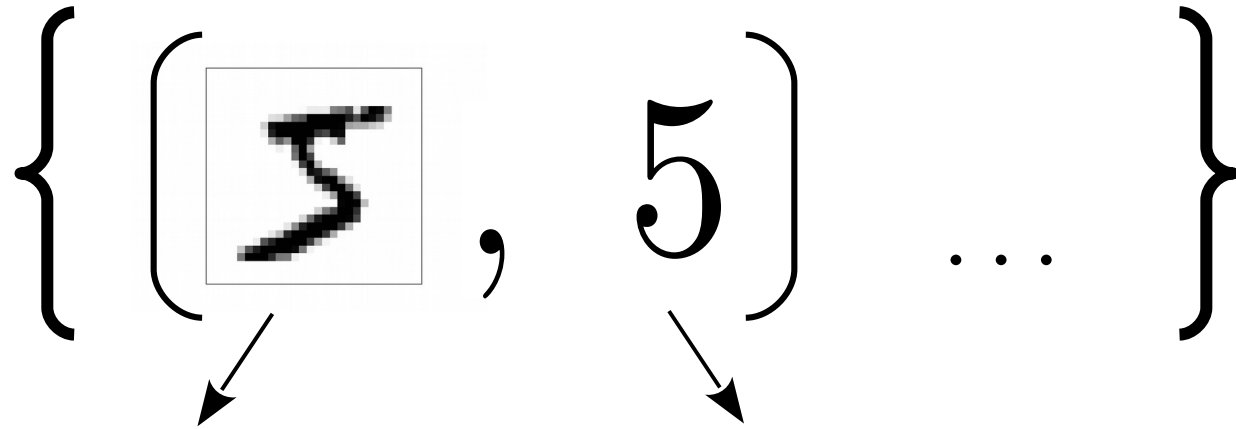


A parametrized function...

How to **construct** it?

Let us play with digits...

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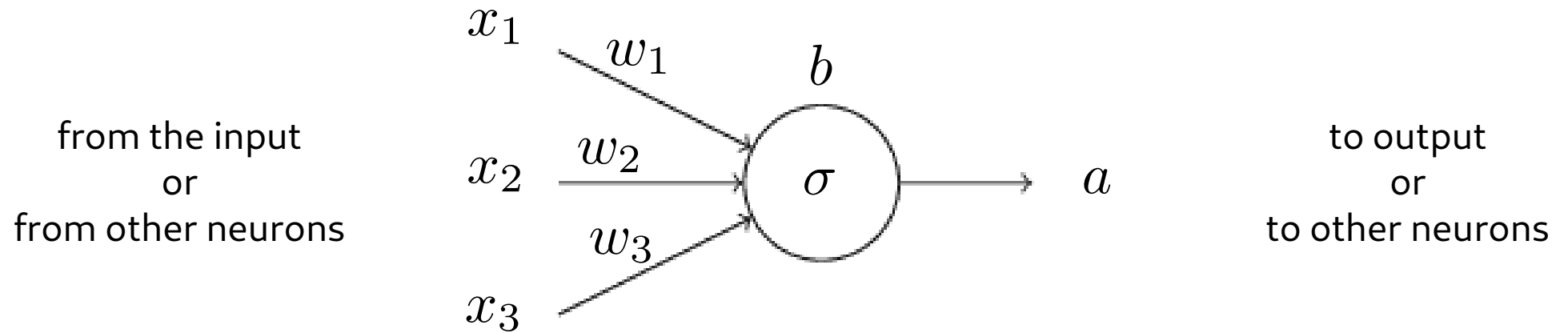
A parametrized function...

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Feed-Forward Neural Networks

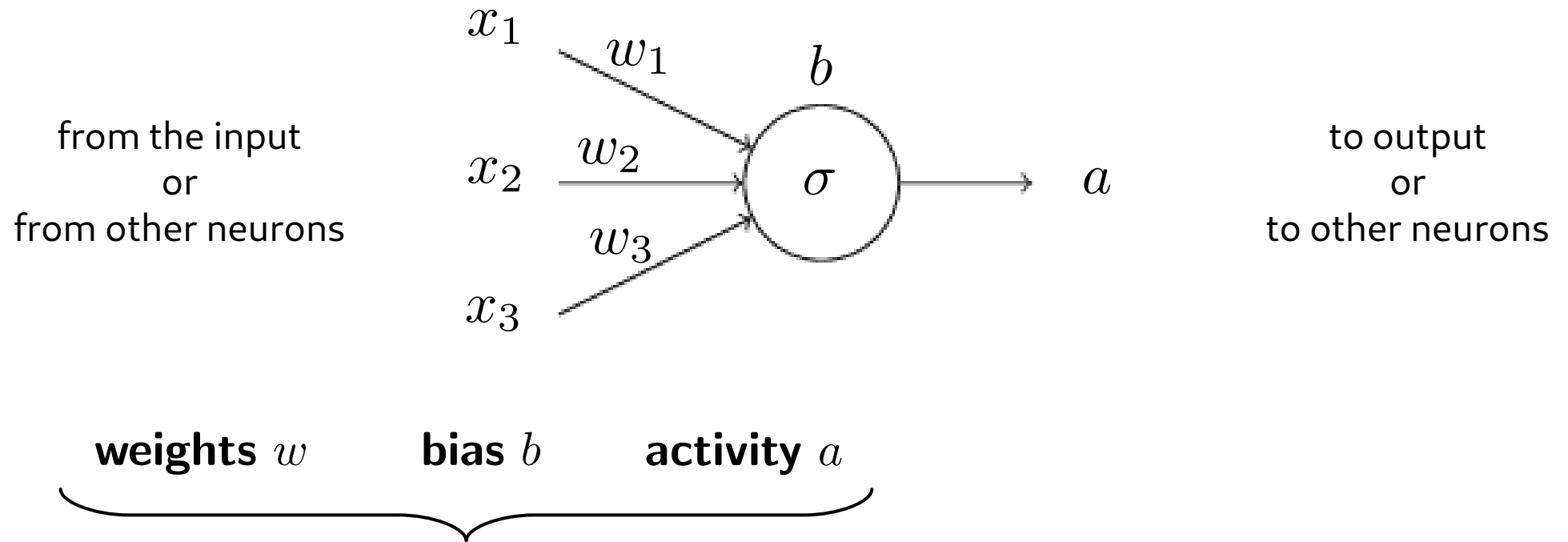
Feed-Forward Neural Networks...

...the ingredients



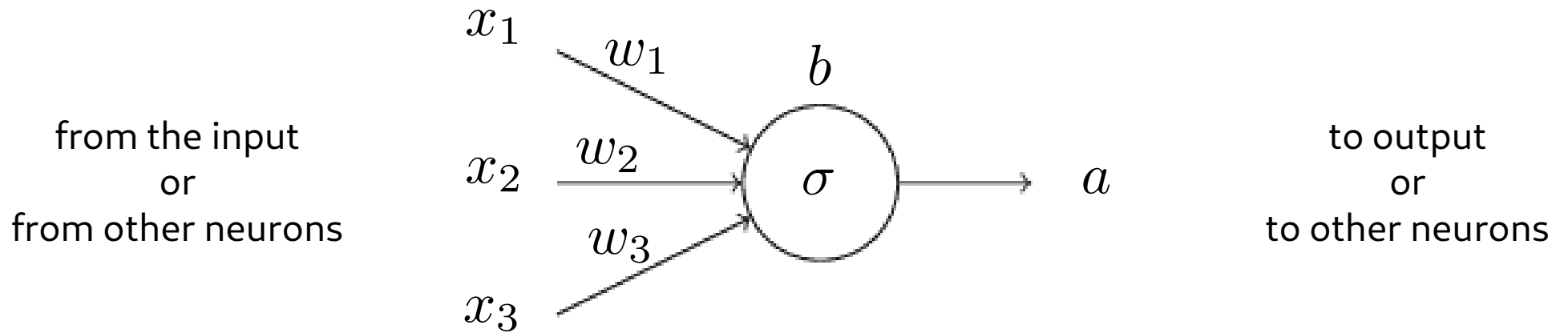
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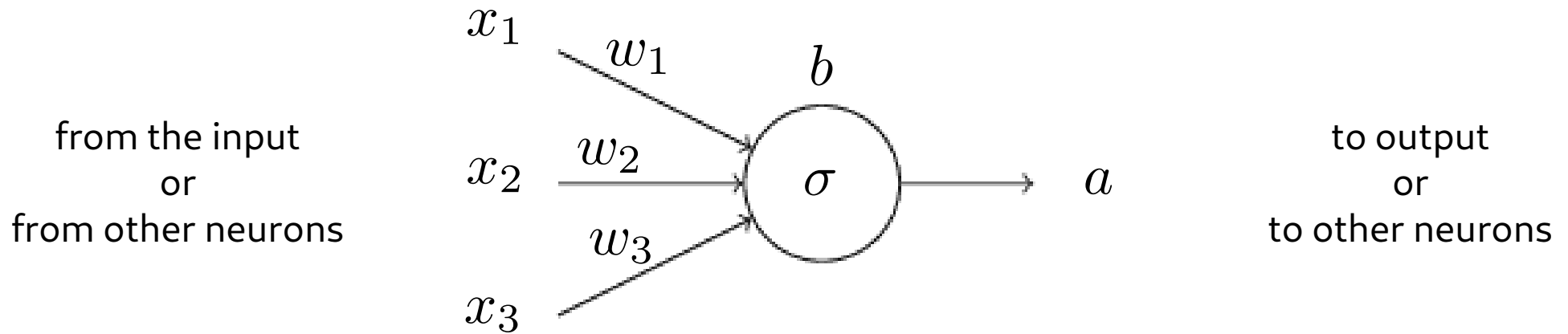
weights w **bias** b **activity** a

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

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

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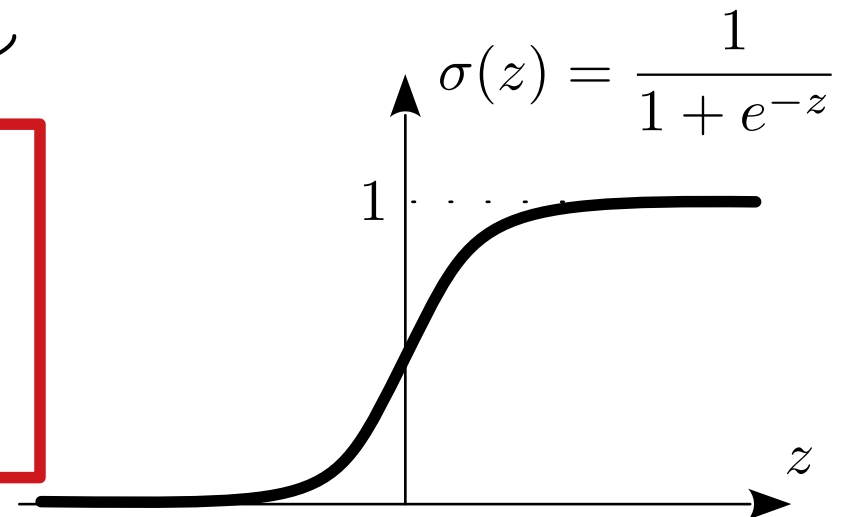
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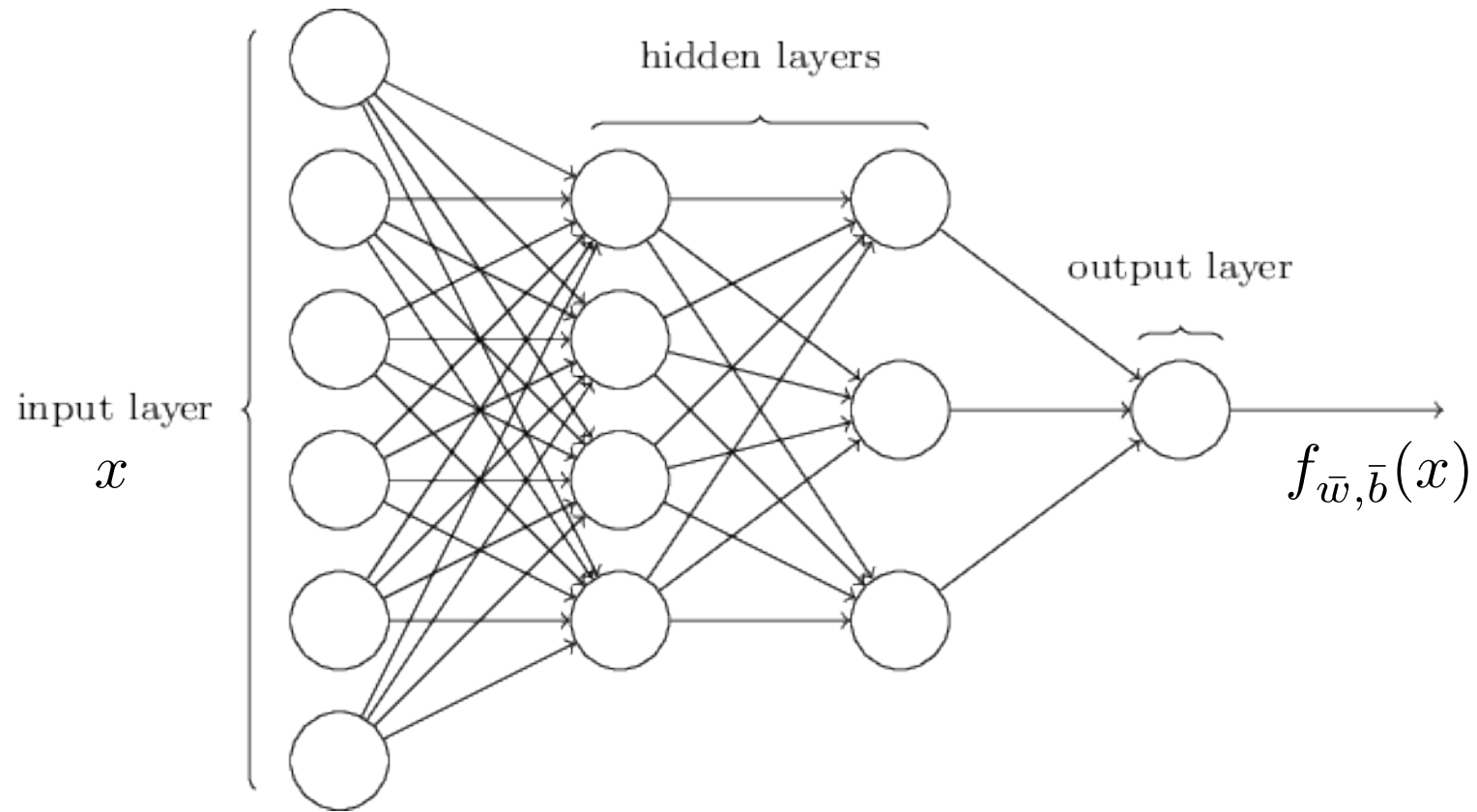
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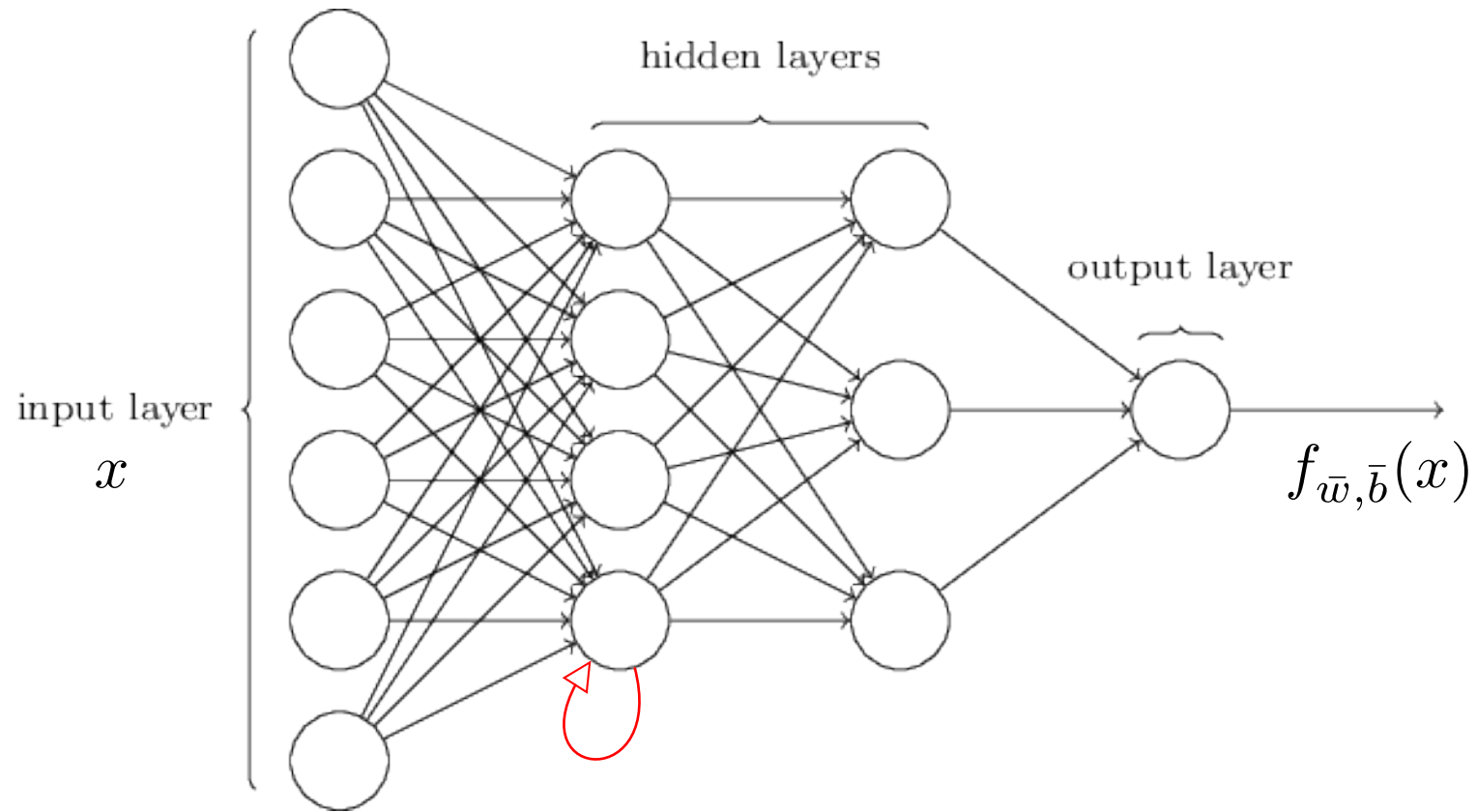
Feed-Forward Neural Networks...

...the **architecture**



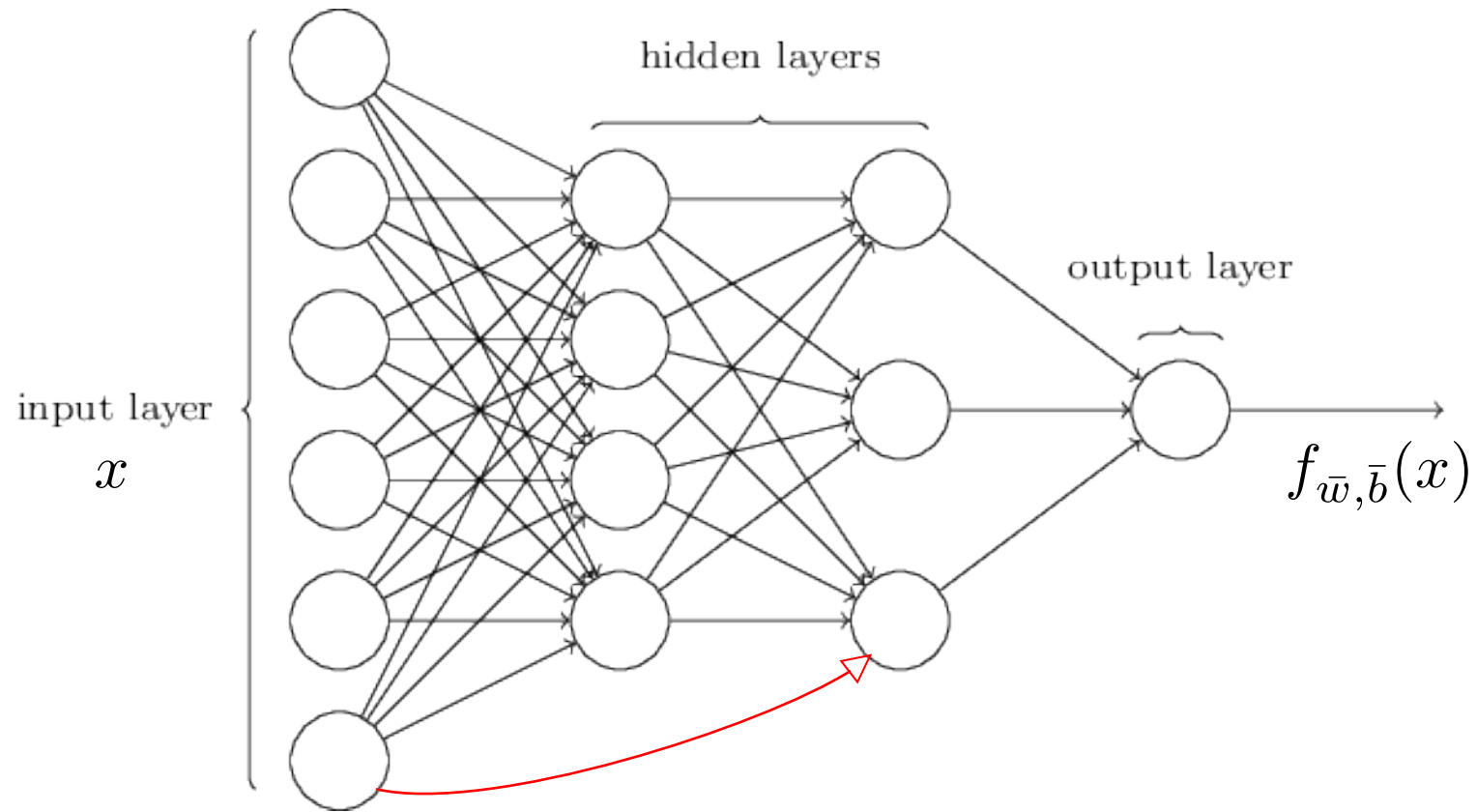
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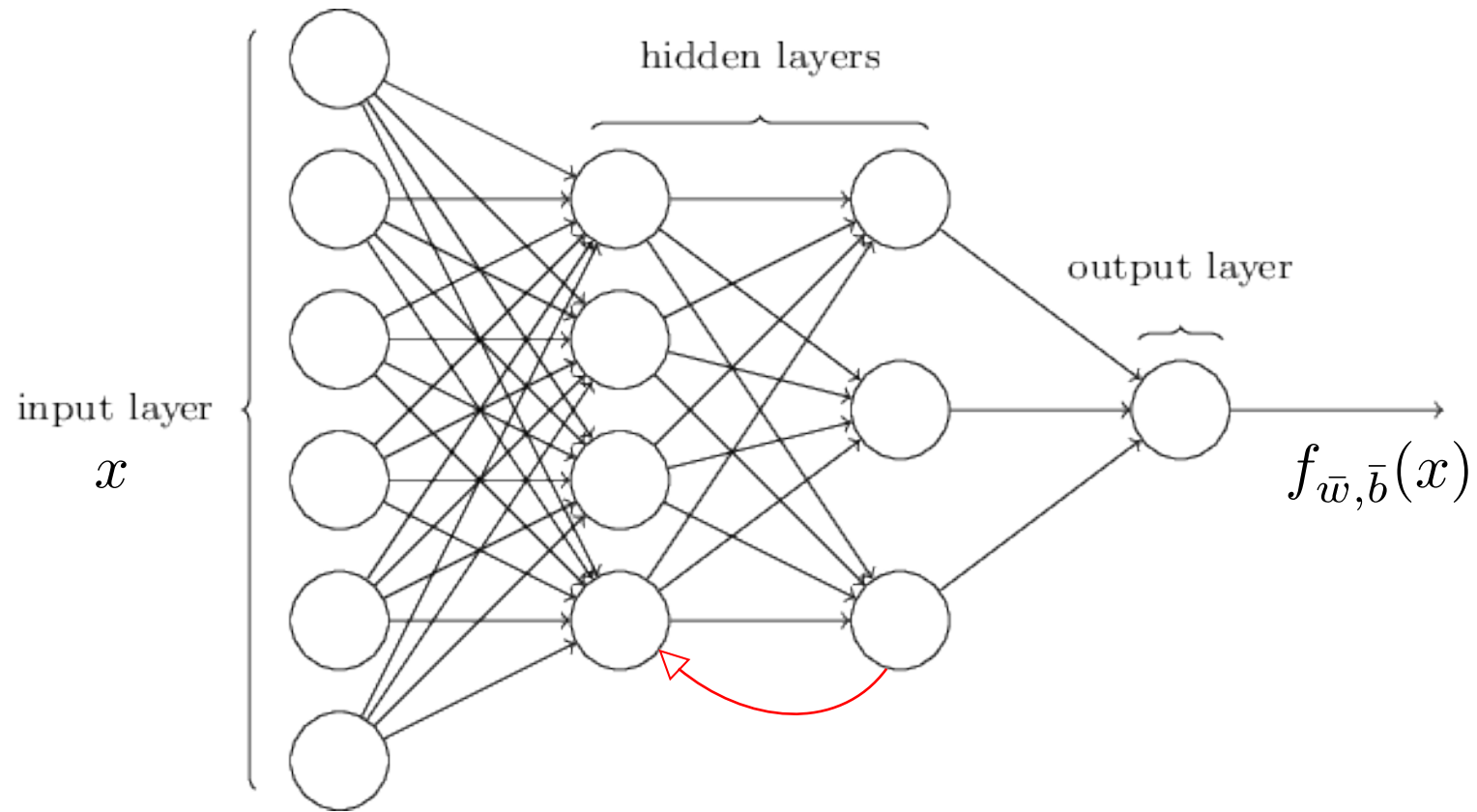
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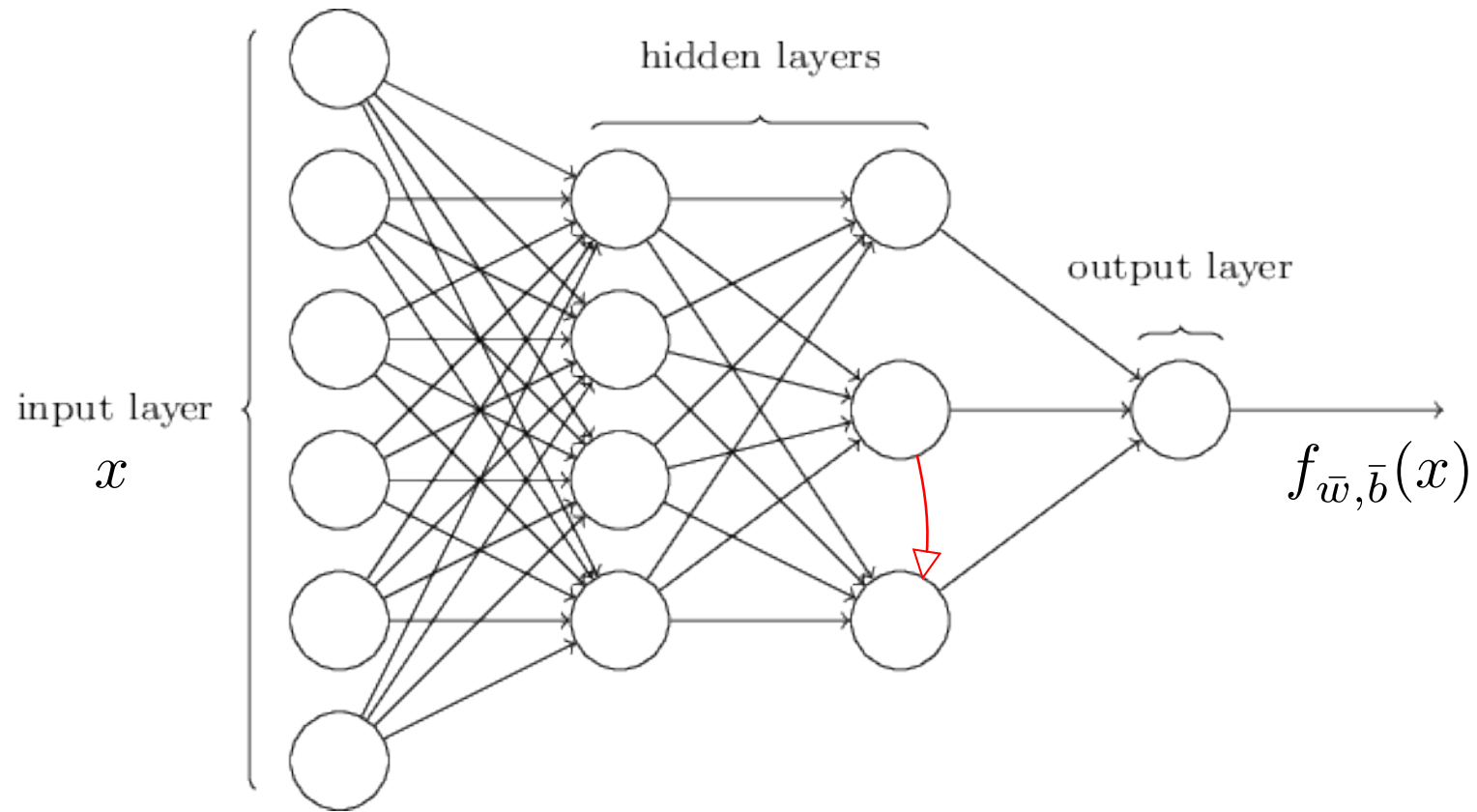
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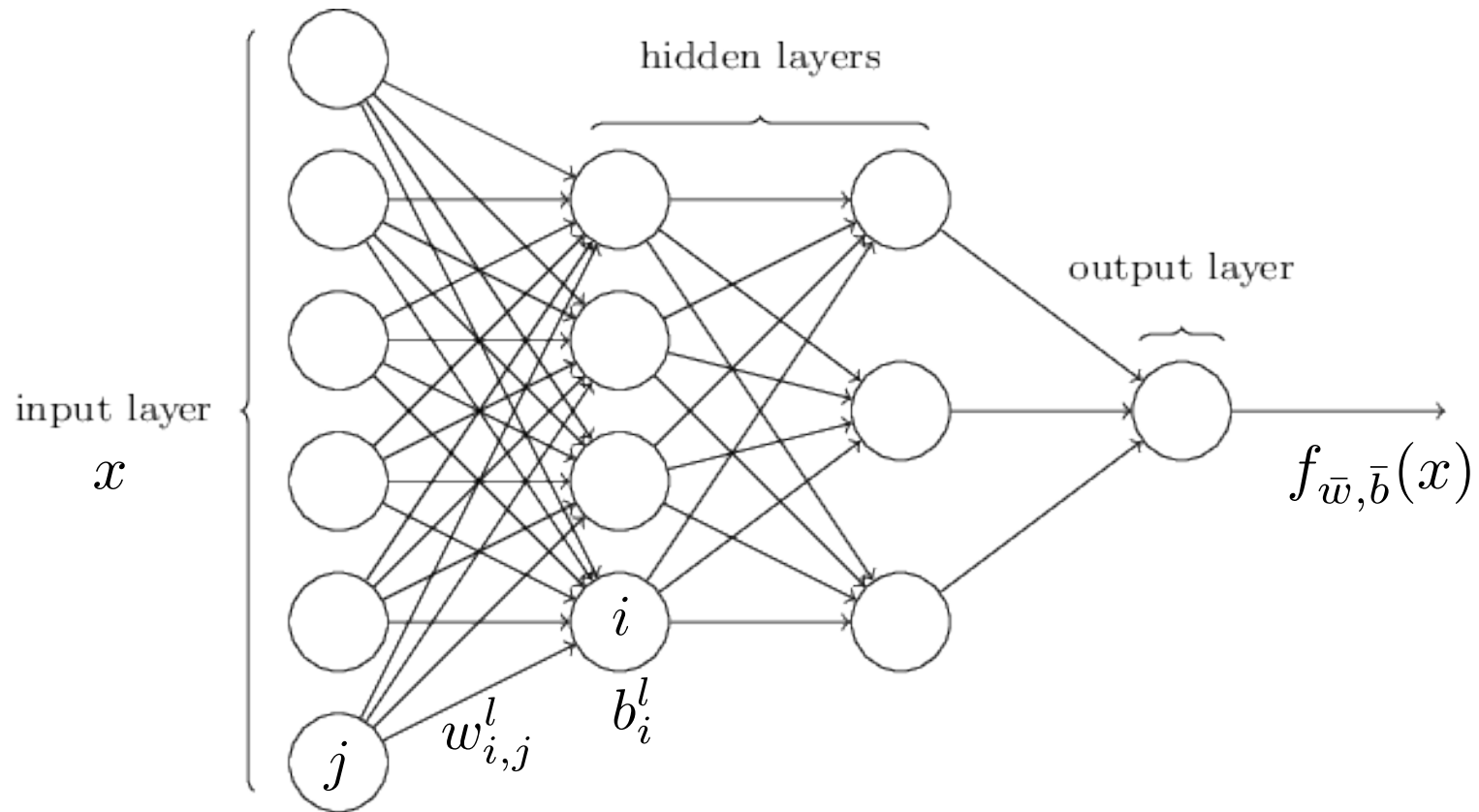
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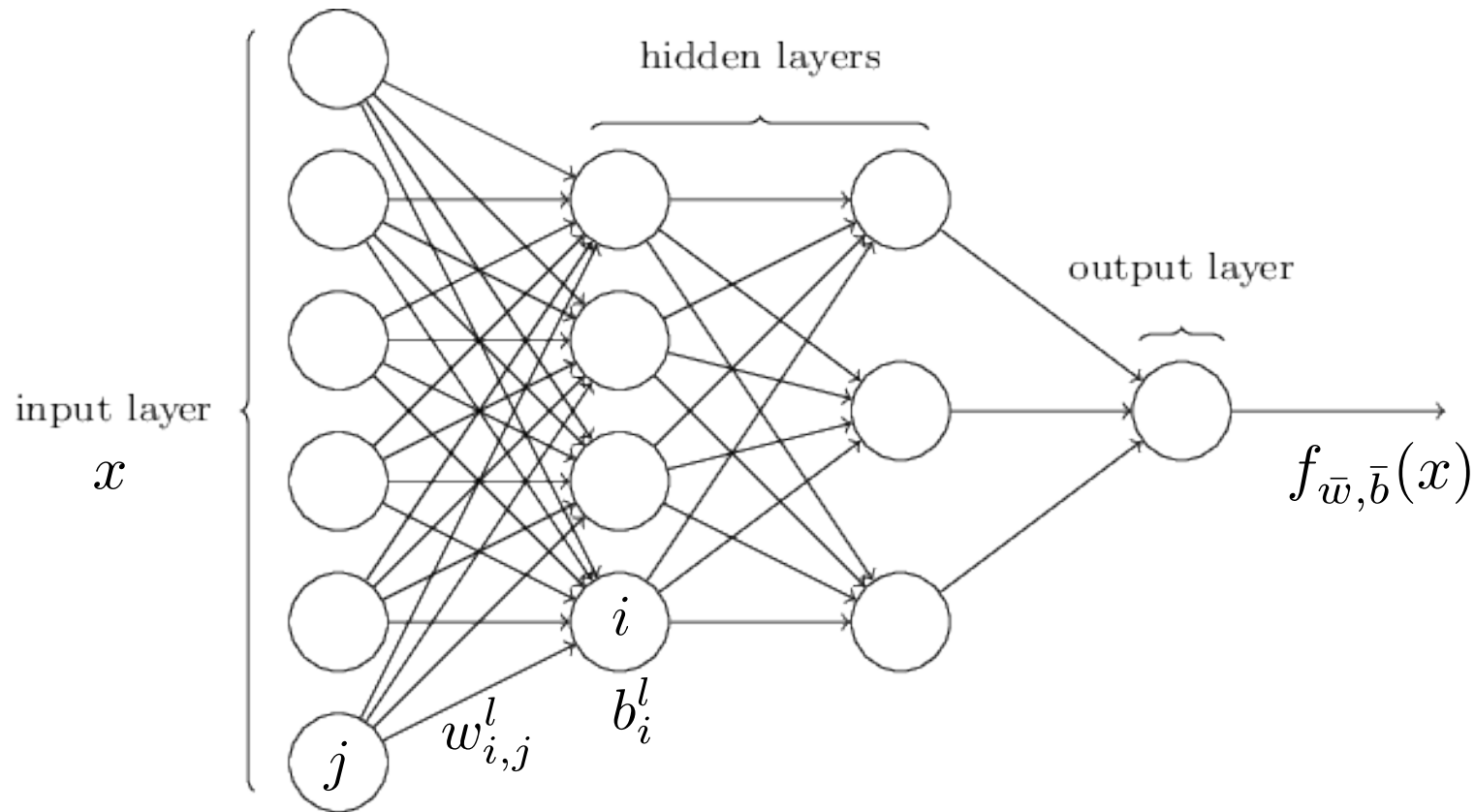


one **weight** per arrow
one **bias** per neuron

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

Feed-Forward Neural Networks...

...the **architecture**



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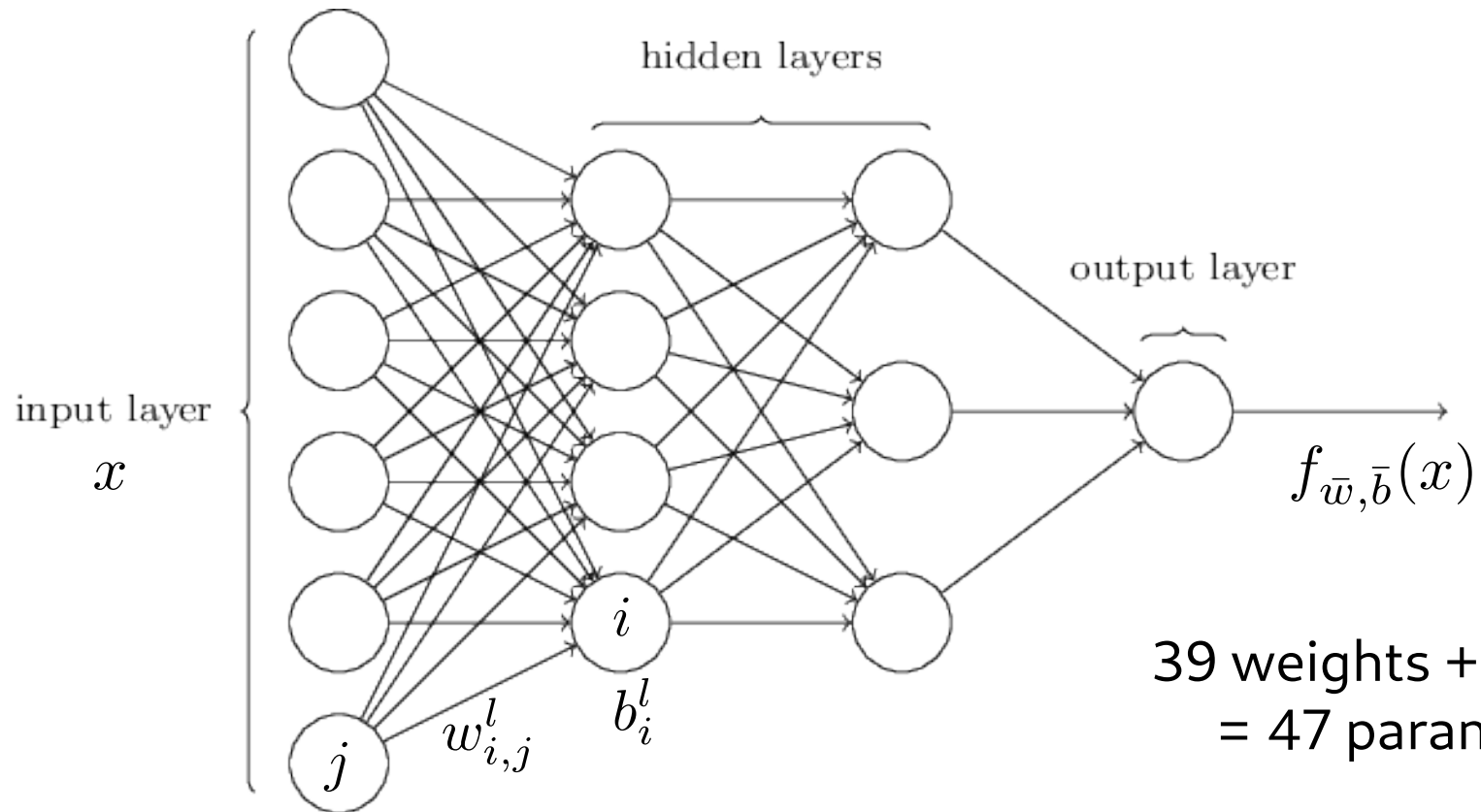
$$w_{i,j}^l \quad b_i^l$$

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

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

Feed-Forward Neural Networks...

...the **architecture**



39 weights + 8 biases
= 47 parameters

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

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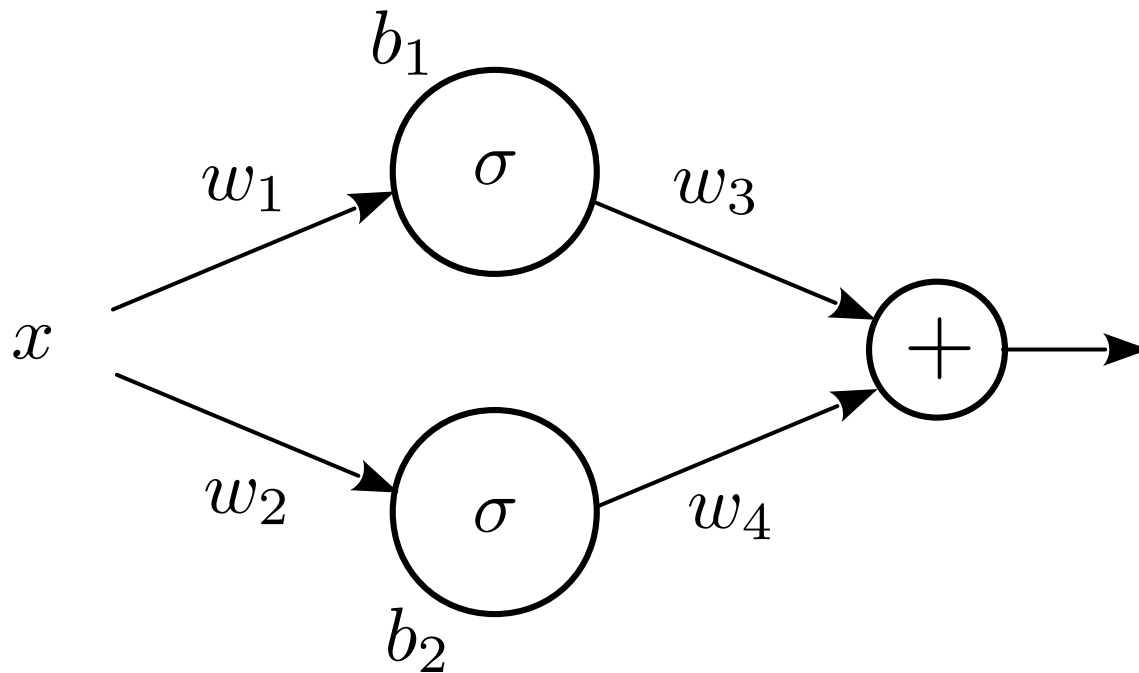
...universal function approximators

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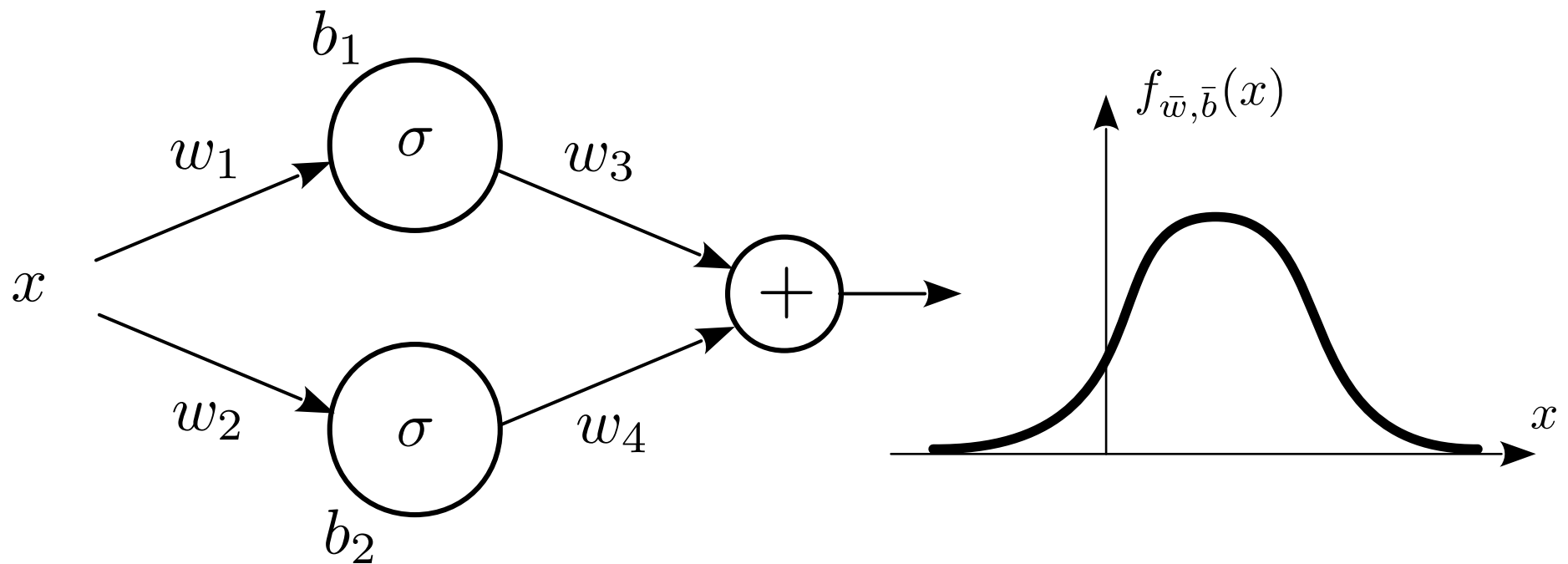


$$f_{\bar{w}, \bar{b}}(x) = w_3 \sigma(b_1 + w_1 x) \\ + w_4 \sigma(b_2 + w_2 x)$$

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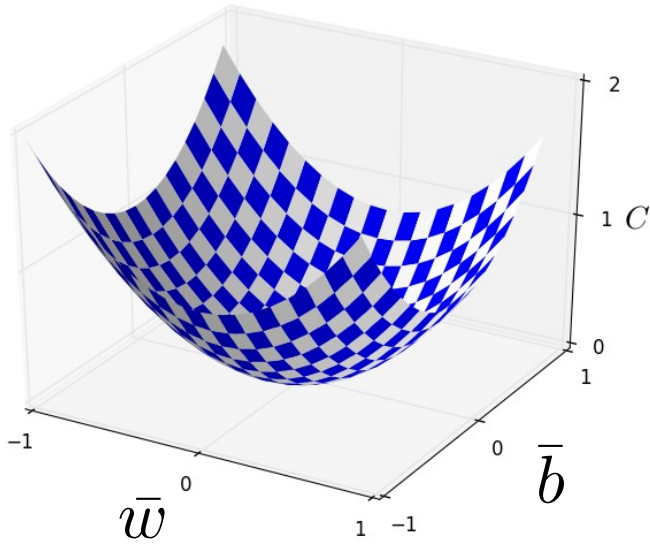


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Learning through gradient descent

Minimize a **cost function**:

$$C(\bar{w}, \bar{b}) = \left\langle \frac{1}{2} \|\text{output} - \text{desired one}\|^2 \right\rangle_{\text{training data}}$$



Learning through gradient descent

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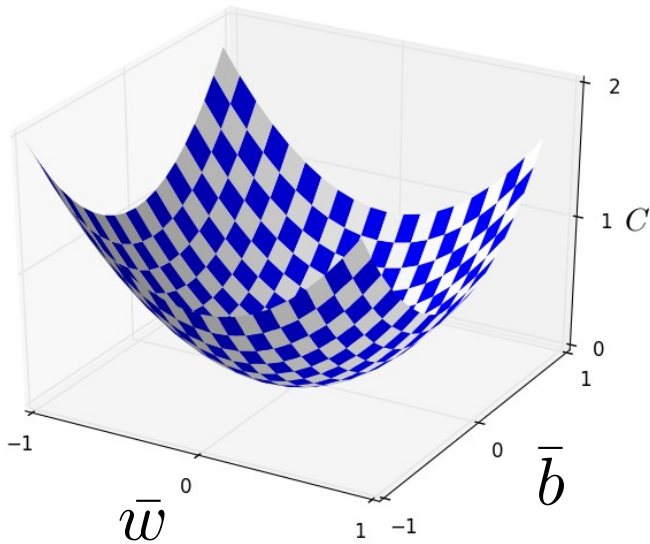
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$$= \frac{1}{N} \sum_x C_x(\bar{w}, \bar{b})$$

$$= \frac{1}{2N} \sum_x \sum_i (a_i^L(x) - y_i(x))^2$$

training
data

neurons
in layer L
(output)



Learning through gradient descent

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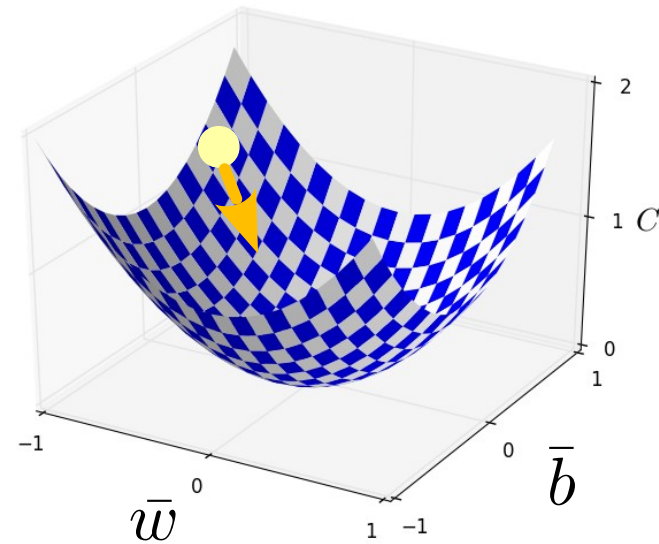
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Gradient descent update rules:

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

η

learning rate

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

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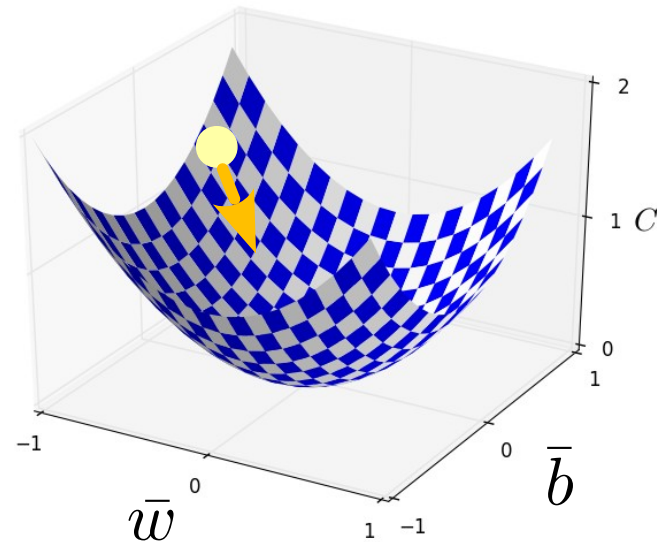
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$$\frac{\partial C}{\partial w_{i,j}^l}, \frac{\partial C}{\partial b_i^l} = ?$$

The backpropagation algorithm

The **error**:

How much does the cost change as
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Small if the parameters are close to **optimal**.

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chain rule

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

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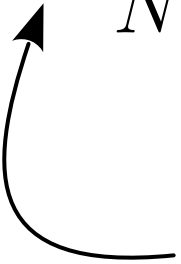
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The backpropagation algorithm

Start from the **output** layer...

$$\delta_i^L = \frac{\partial C}{\partial z_i^L} = \frac{1}{N} \sum_x \left(a_i^L(x) - y_i(x) \right) \sigma'(z_i^L)$$

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

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

$$\delta_j^{l-1} = \frac{\partial C}{\partial z_j^{l-1}} = \sum_i \frac{\partial C}{\partial z_i^l} \frac{\partial z_i^l}{\partial z_j^{l-1}} = \sum_i \delta_i^l w_{ij}^l \sigma'(z_j^{l-1})$$

The mini-batch update

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

$$w \leftarrow w - \eta \overline{\nabla_w C_m}$$

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Divide the training dataset into M **batches** of size S: $N = M \times S$

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

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Average **within** mini-batches first...

$$\overline{C}_m = \frac{1}{S} \sum_{\substack{\text{mini-batch} \\ m}} C_x$$

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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)