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

What is this about?

Classification tasks

"is this a cat or a dog?"

What is this about?

Classification tasks

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

What is this about?

Classification tasks

"is this a cat or a dog?"
"what digit is this?"

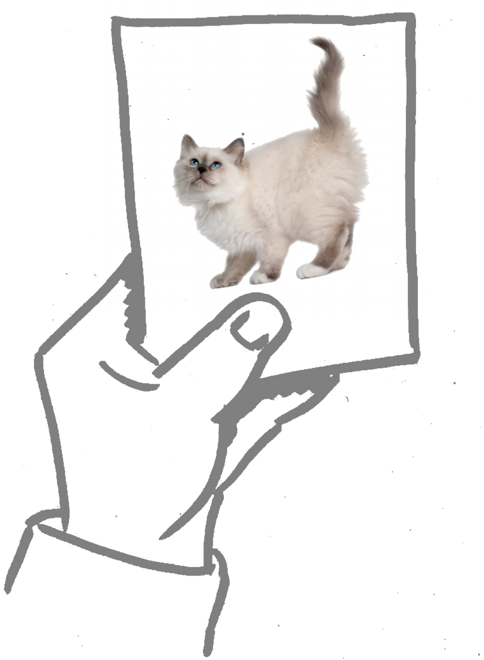
Supervised Learning: by examples, with a teacher

What is this about?

Classification tasks

"is this a cat or a dog?"
"what digit is this?"

Supervised Learning: by examples, with a teacher



`cat`

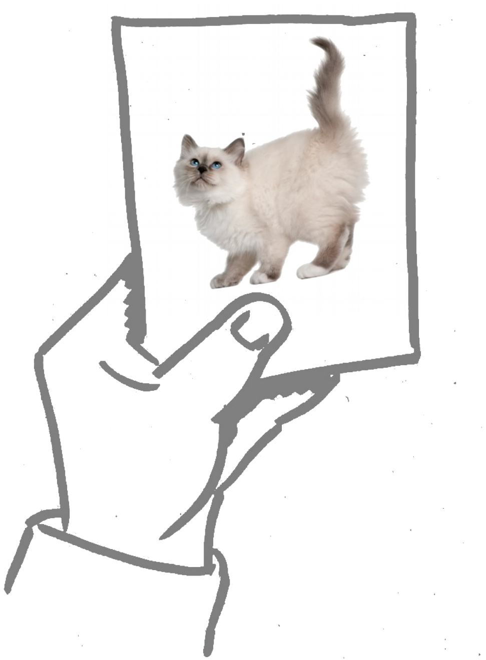
`dog`

What is this about?

Classification tasks

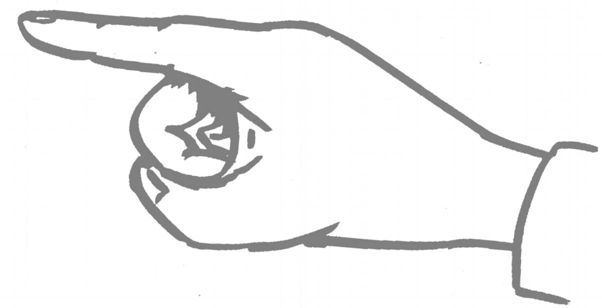
"is this a cat or a dog?"
"what digit is this?"

Supervised Learning: by examples, with a teacher



cat

dog

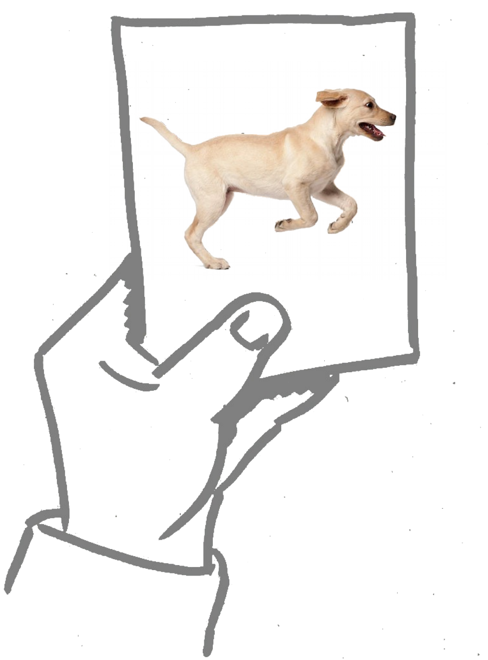


What is this about?

Classification tasks

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

Supervised Learning: by examples, with a teacher



`cat`

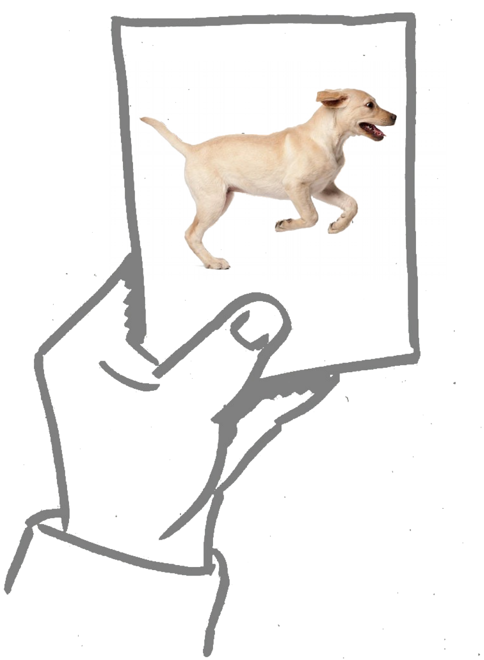
`dog`

What is this about?

Classification tasks

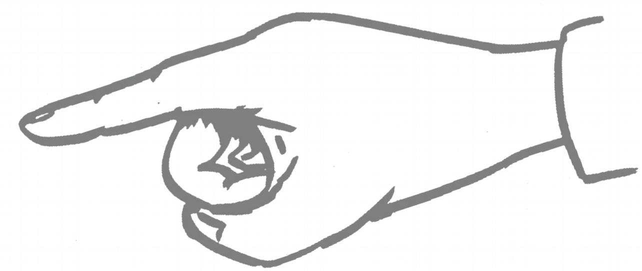
"is this a cat or a dog?"
"what digit is this?"

Supervised Learning: by examples, with a teacher



cat

dog

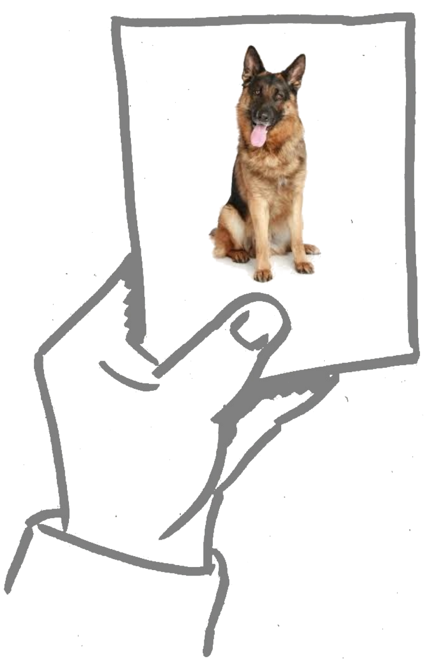


What is this about?

Classification tasks

"is this a cat or a dog?"
"what digit is this?"

Supervised Learning: by examples, with a teacher



`cat`

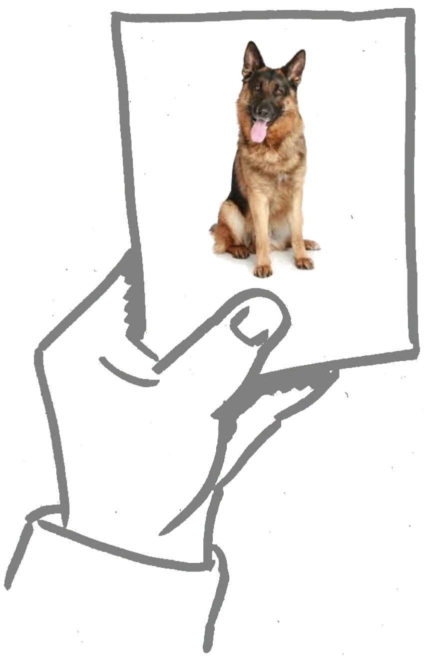
`dog`

What is this about?

Classification tasks

"is this a cat or a dog?"
"what digit is this?"

Supervised Learning: by examples, with a teacher



`cat`

??

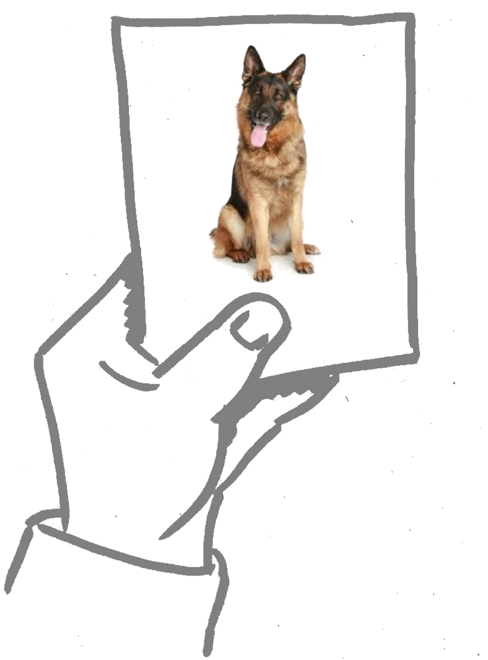
`dog`

What is this about?

Classification tasks

"is this a cat or a dog?"
"what digit is this?"

Supervised Learning: by examples, with a teacher



cat

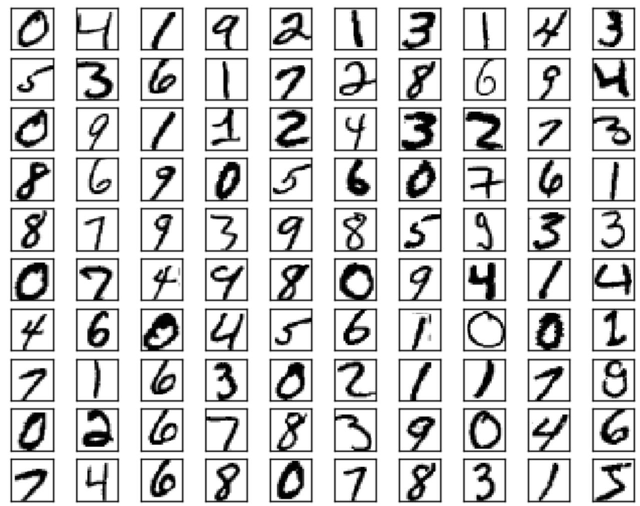
??

dog

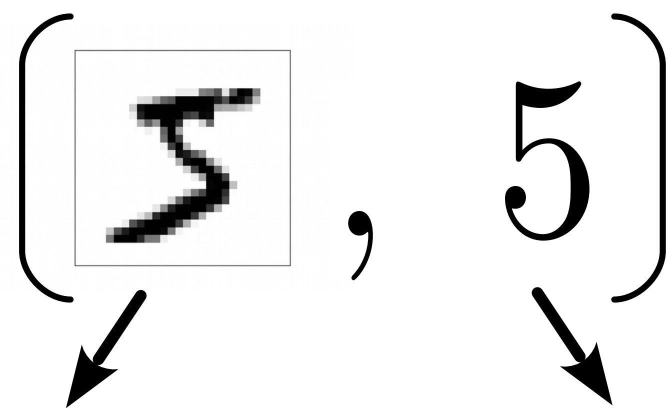
Generalization to unseen picture

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

Classification of handwritten digits



70’000 input/output pairs



How to use them?

Input x

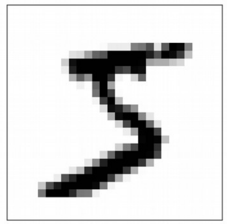
$28 \times 28,\ [0,\ 1]^{784}$

Correct output $y(x)$

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

Let us play with digits...

... the MNIST database



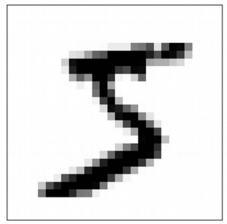
$$\left\{ \left(x , \; 5 \right) \; \ldots \right\}$$

Input x

Correct output $y(x)$

Let us play with digits...

... the MNIST database

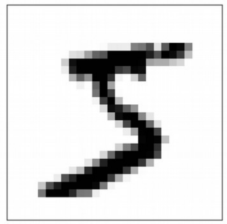
$\Big\{ \Big($  $,\ 5 \Big) \ \ldots \Big\}$

Input x Correct output $y(x)$

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

Let us play with digits...

... the MNIST database

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

Input x Correct output $y(x)$

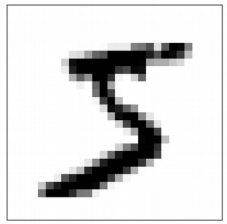
$$f_{\bar{w},\bar{b}} : [0,1]^{784} \to \{0,\, 1 \dots 9\}$$

A parametrized function...

How to **construct** it?

Let us play with digits...

... the MNIST database

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

Input x Correct output $y(x)$

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

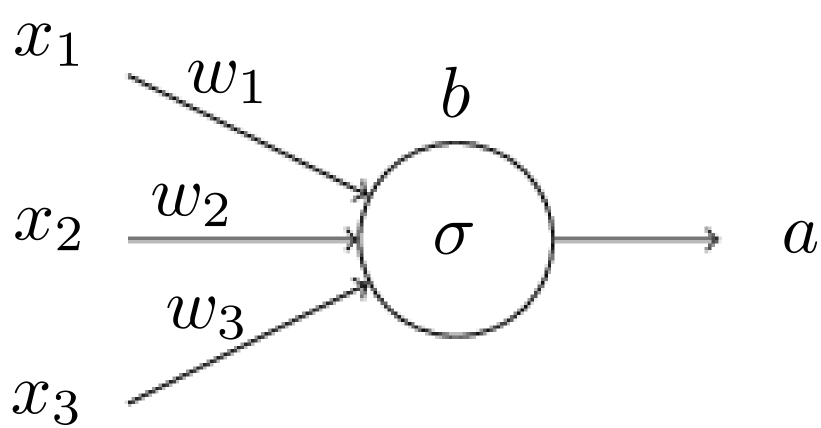
A parametrized function...

How to **construct** it?

Feed-Forward Neural Networks

Feed-Forward Neural Networks…
…the ingredients

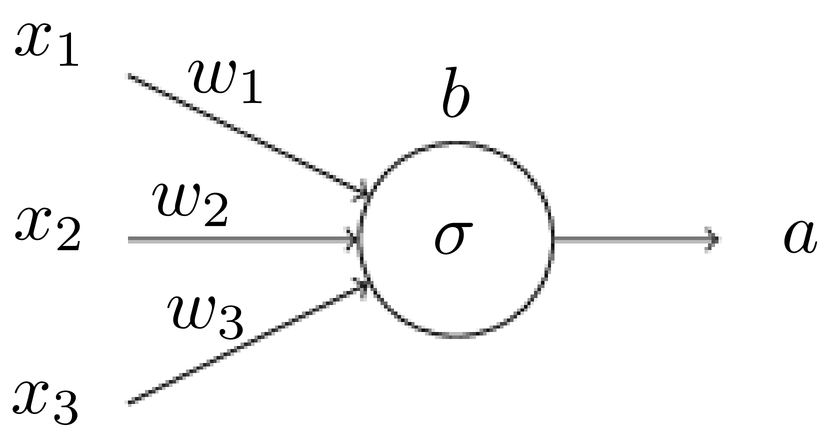
from the input
or
from other neurons



to output
or
to other neurons

Feed-Forward Neural Networks…
…the ingredients

from the input
or
from other neurons

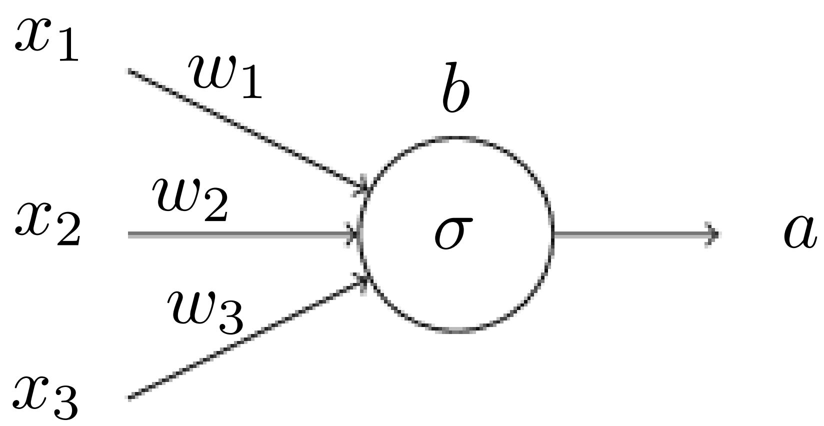


to output
or
to other neurons

$$\underbrace{\textbf{weights } w \qquad \textbf{bias } b \qquad \textbf{activity } a}$$

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

from the input
or
from other neurons



to output
or
to other neurons

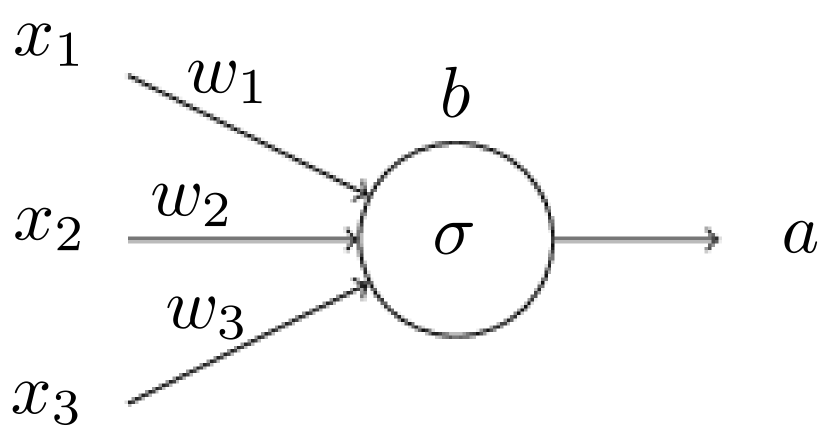
weights w **bias** b **activity** a

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



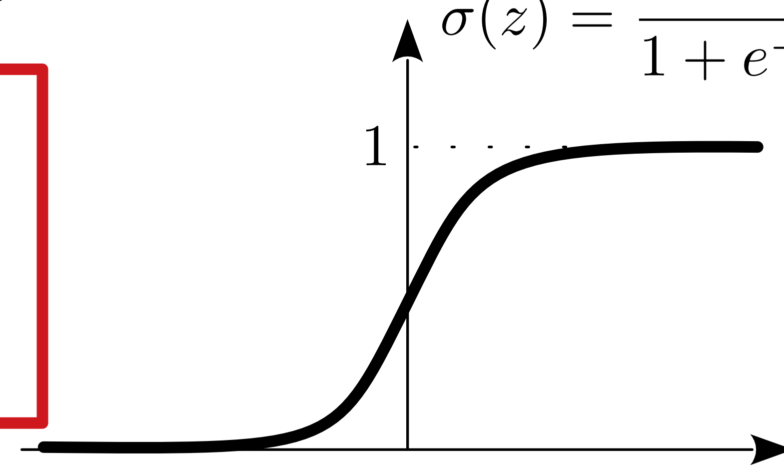
to output
or
to other neurons

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

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

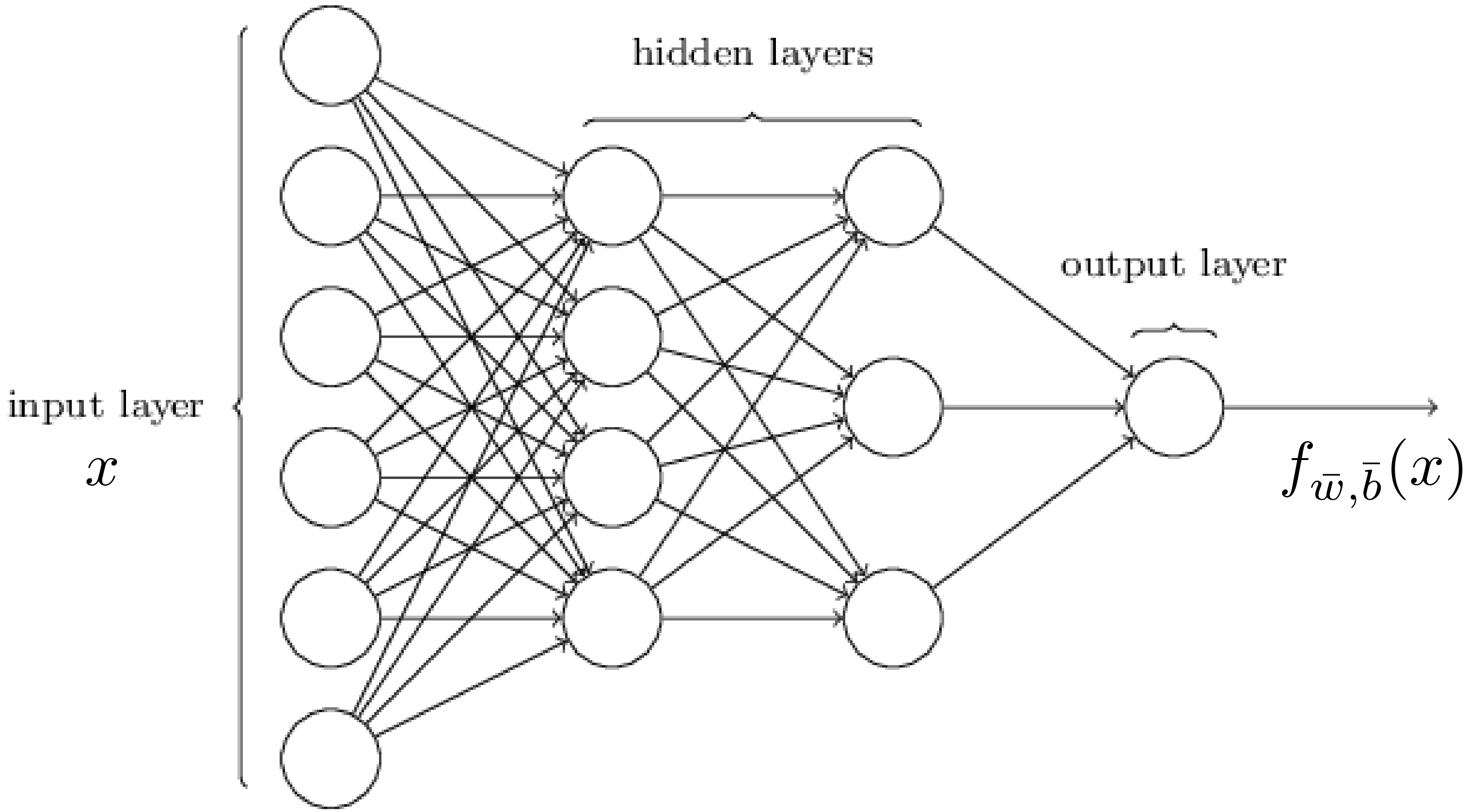
activation function σ, $\quad a = \sigma(z)$

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

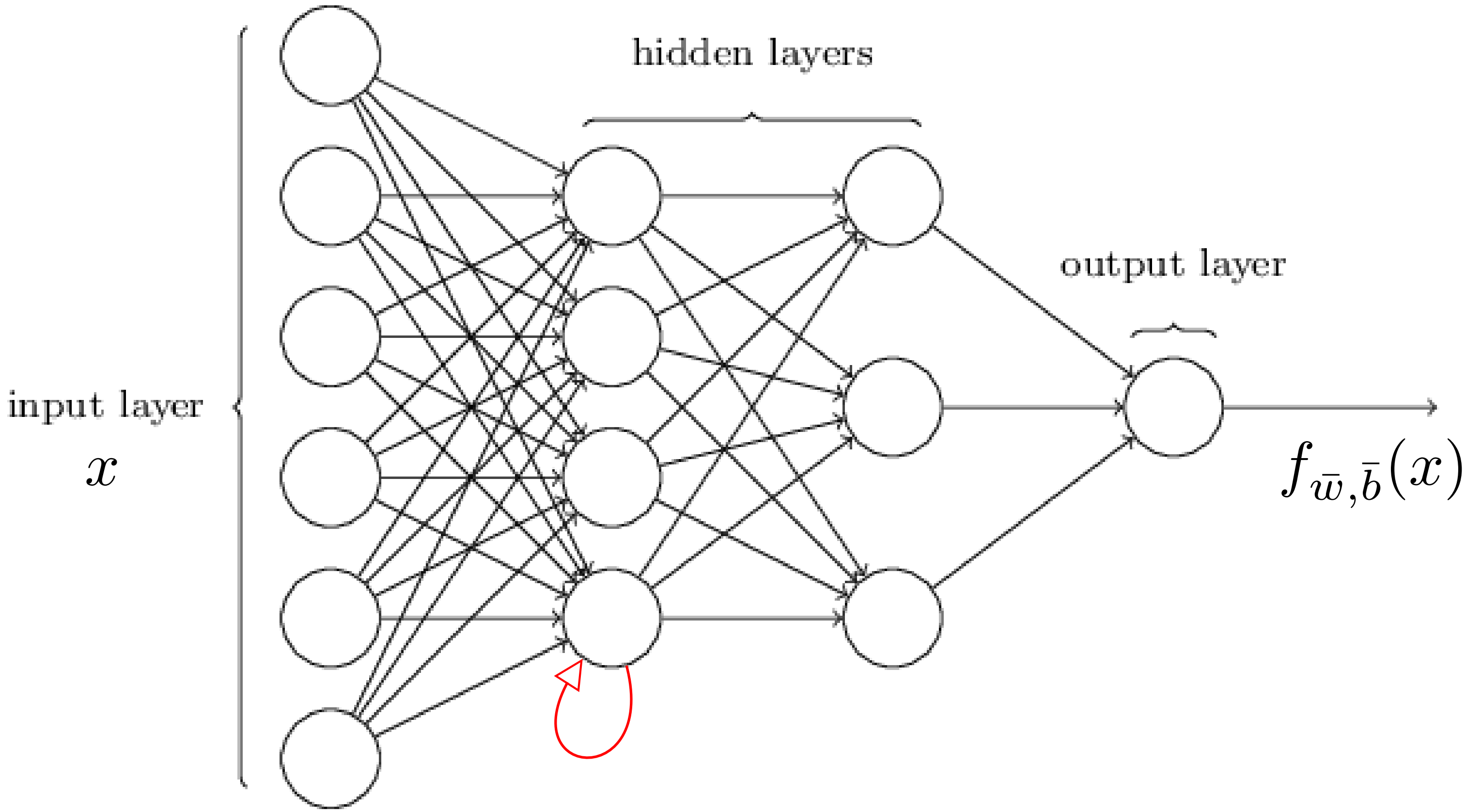


Feed-Forward Neural Networks...

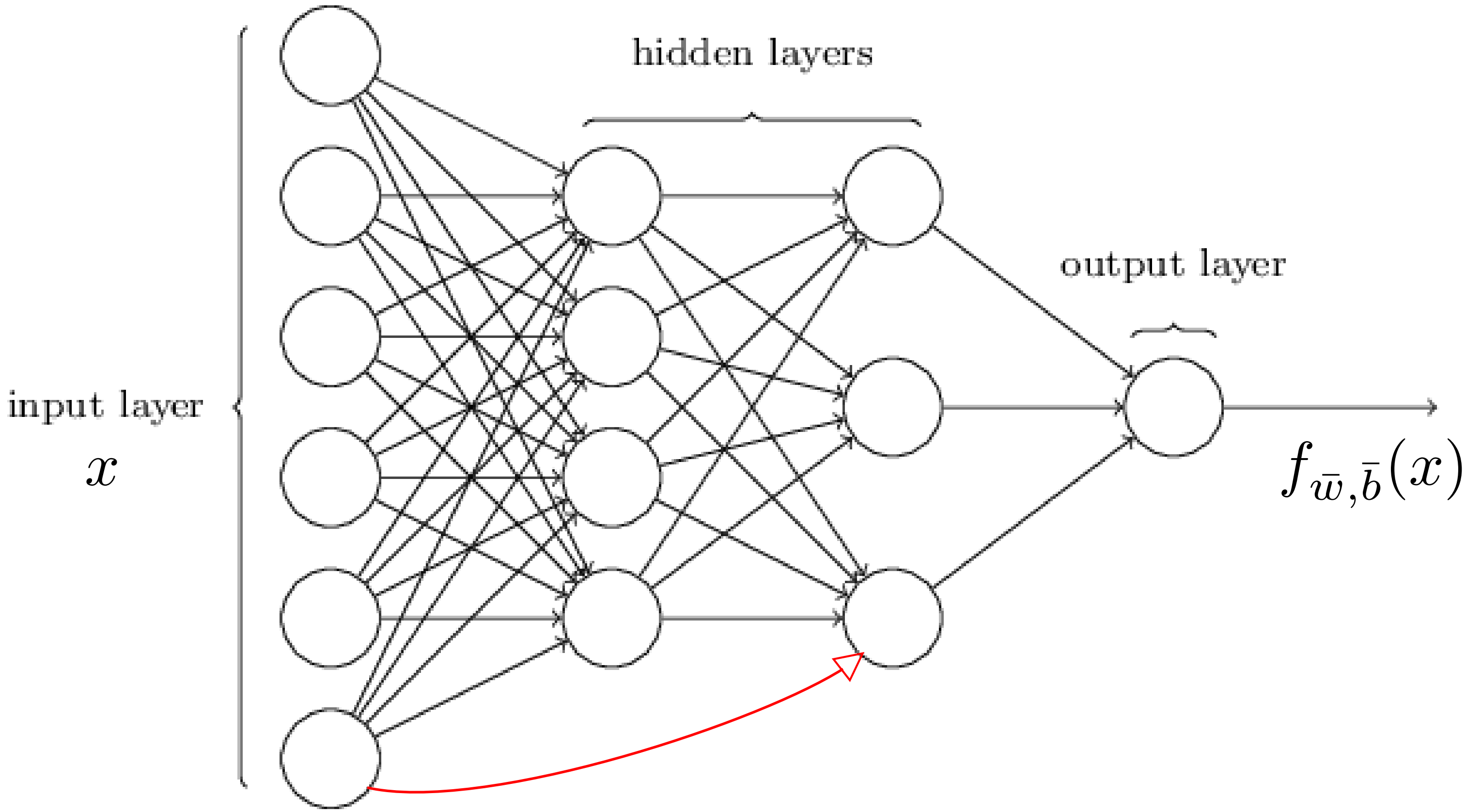
...the architecture



Feed-Forward Neural Networks...
...the architecture

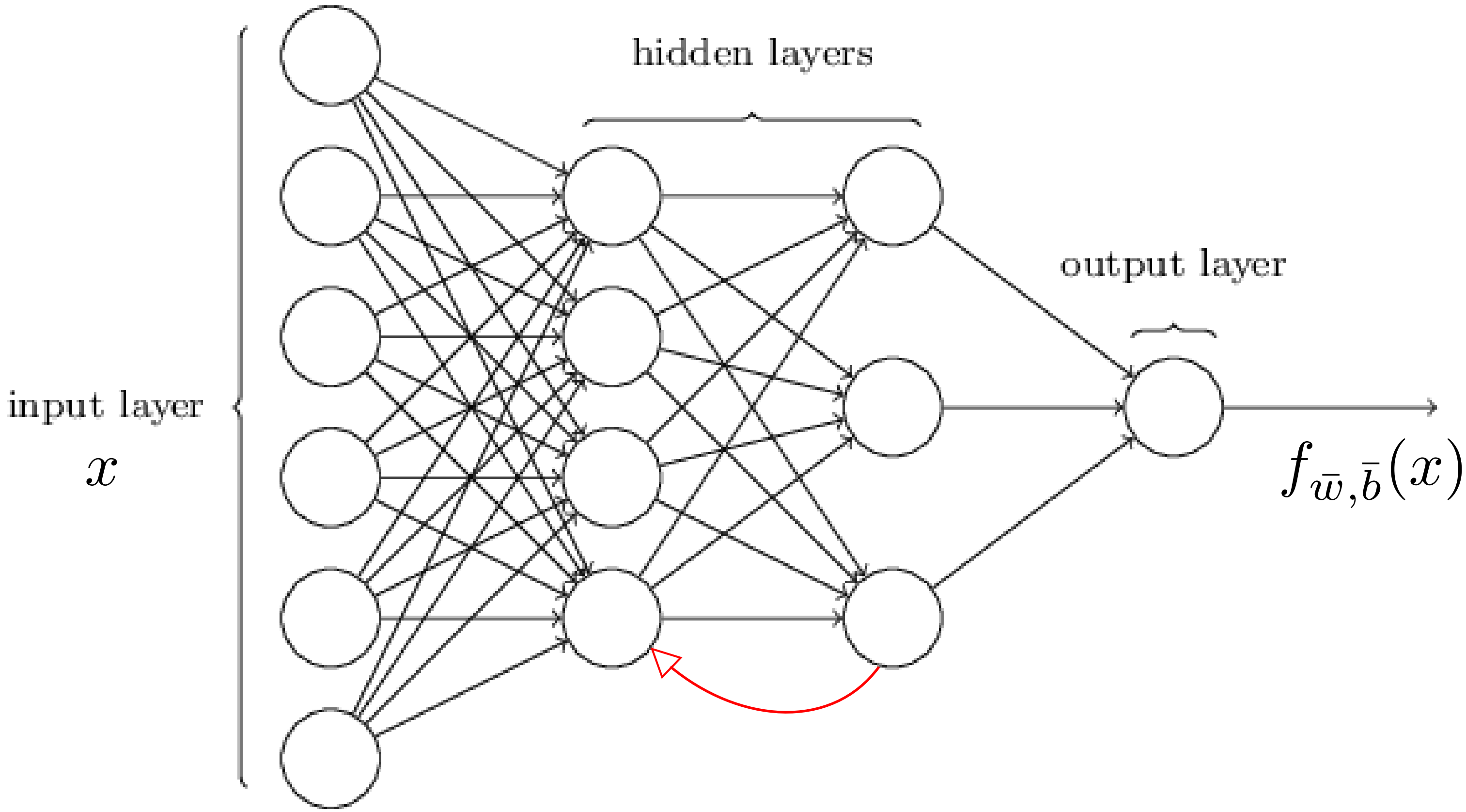


Feed-Forward Neural Networks...
...the architecture



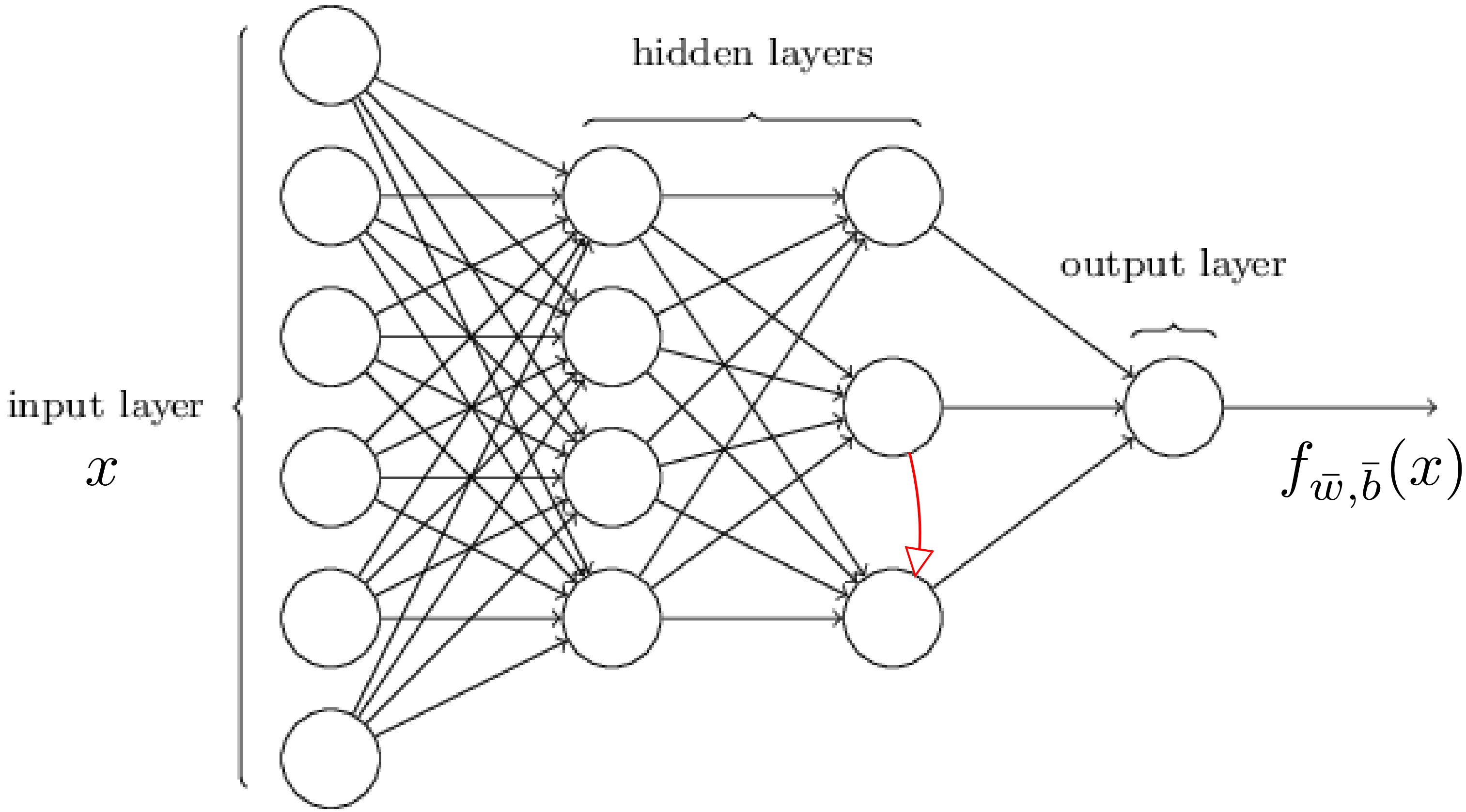
Feed-Forward Neural Networks…

…the architecture

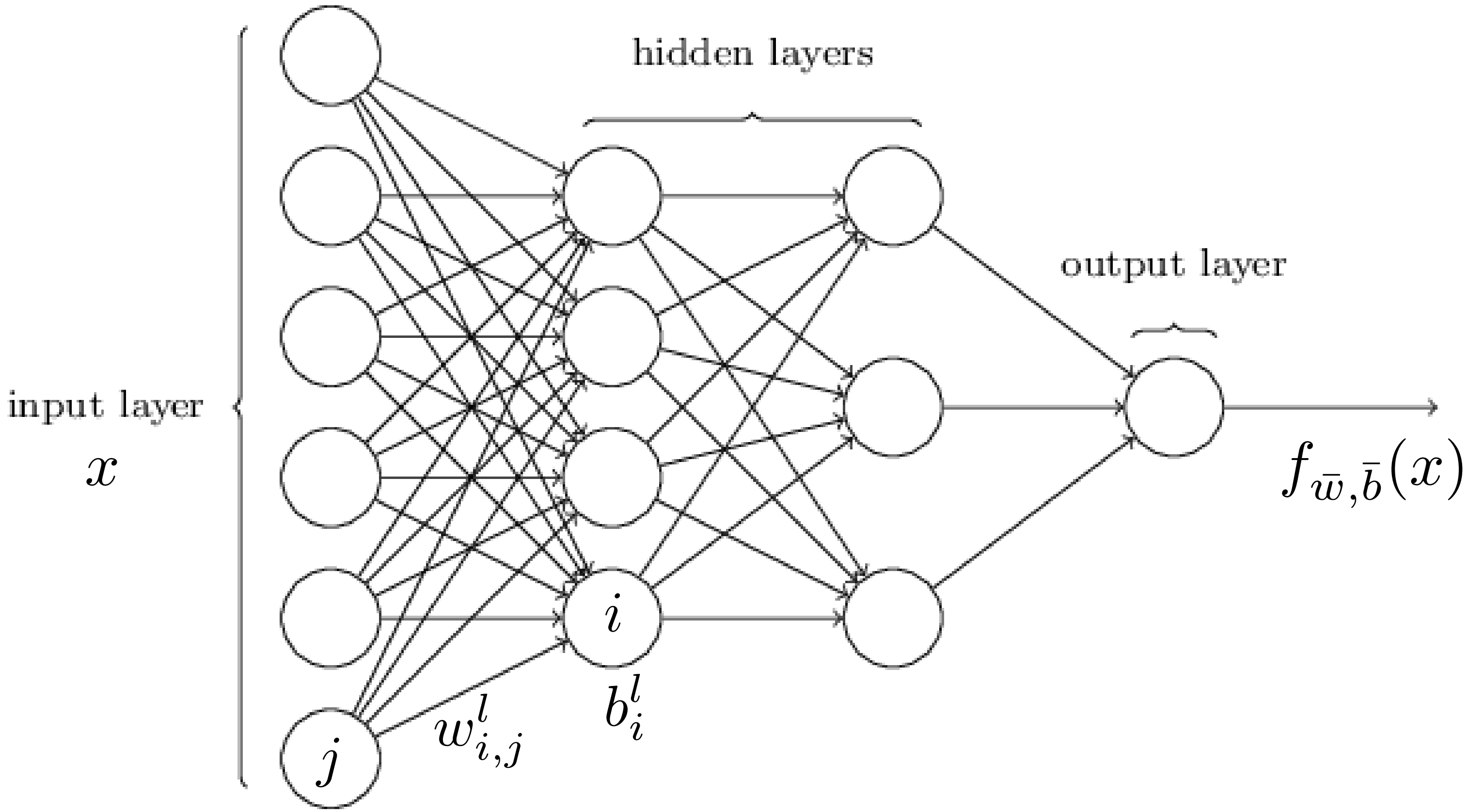


Feed-Forward Neural Networks...

...the architecture



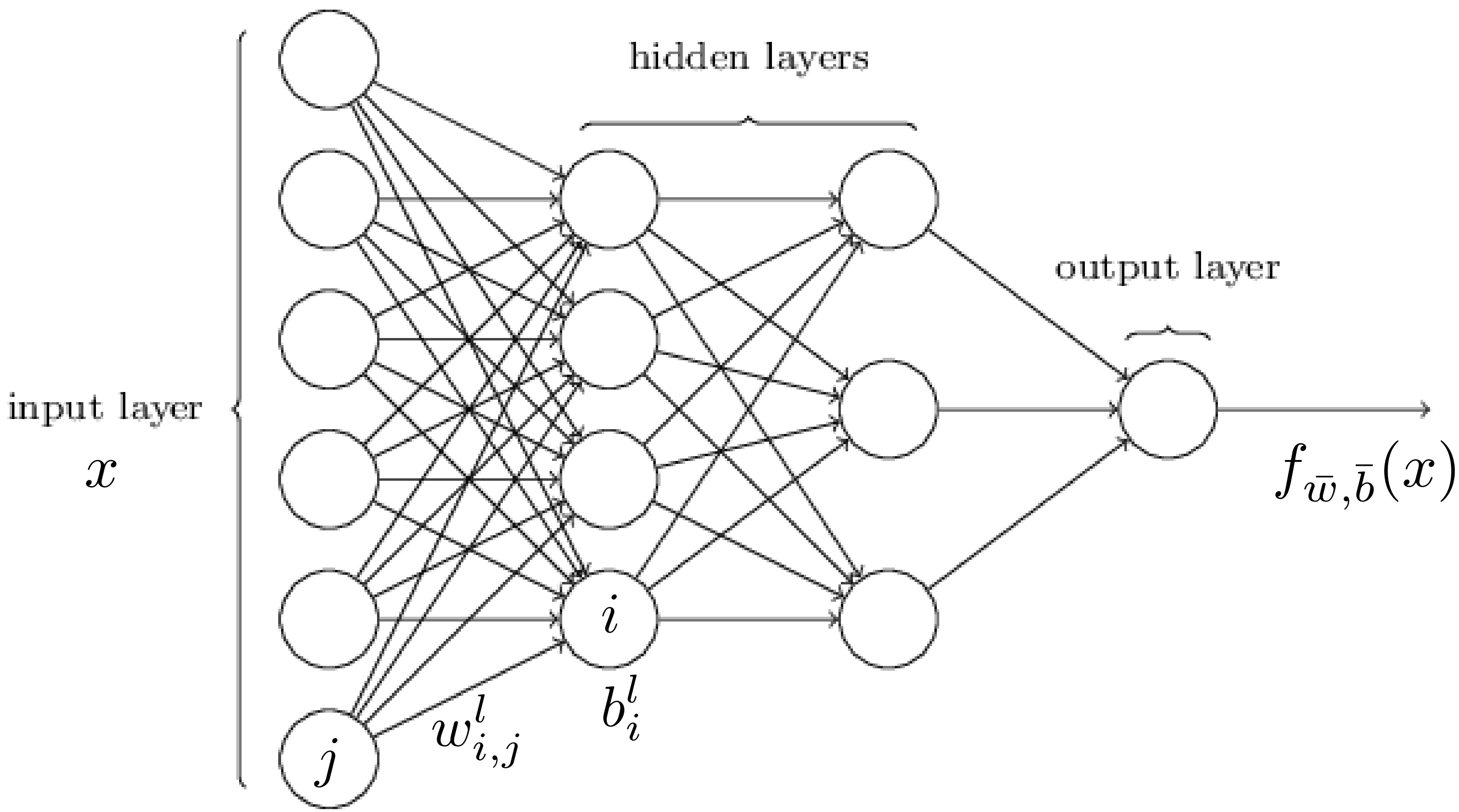
Feed-Forward Neural Networks...
...the architecture



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

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

Feed-Forward Neural Networks...
...the architecture



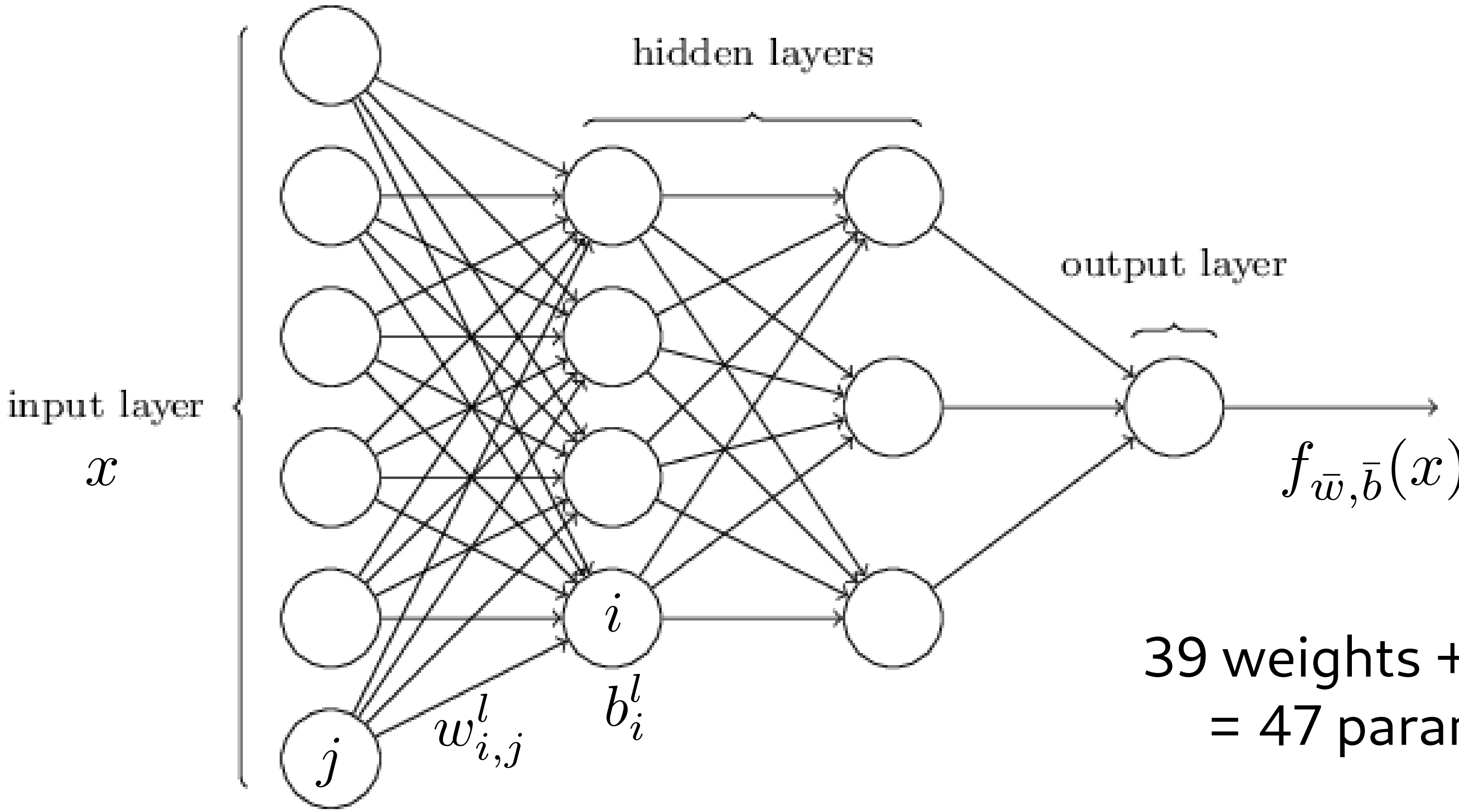
one **weight** per arrow
one **bias** per neuron

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

$$a^l_i = \sigma\left(z^l_i\right)$$

$$= \sigma\left(b^l_i + \sum_j w^l_{i,j} a^{l-1}_j\right)$$

Feed-Forward Neural Networks...
...the architecture



39 weights + 8 biases
= 47 parameters

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

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

$$a^l_i = \sigma\left(z^l_i\right)$$

$$= \sigma\left(b^l_i + \sum_j w^l_{i,j} a^{l-1}_j\right)$$

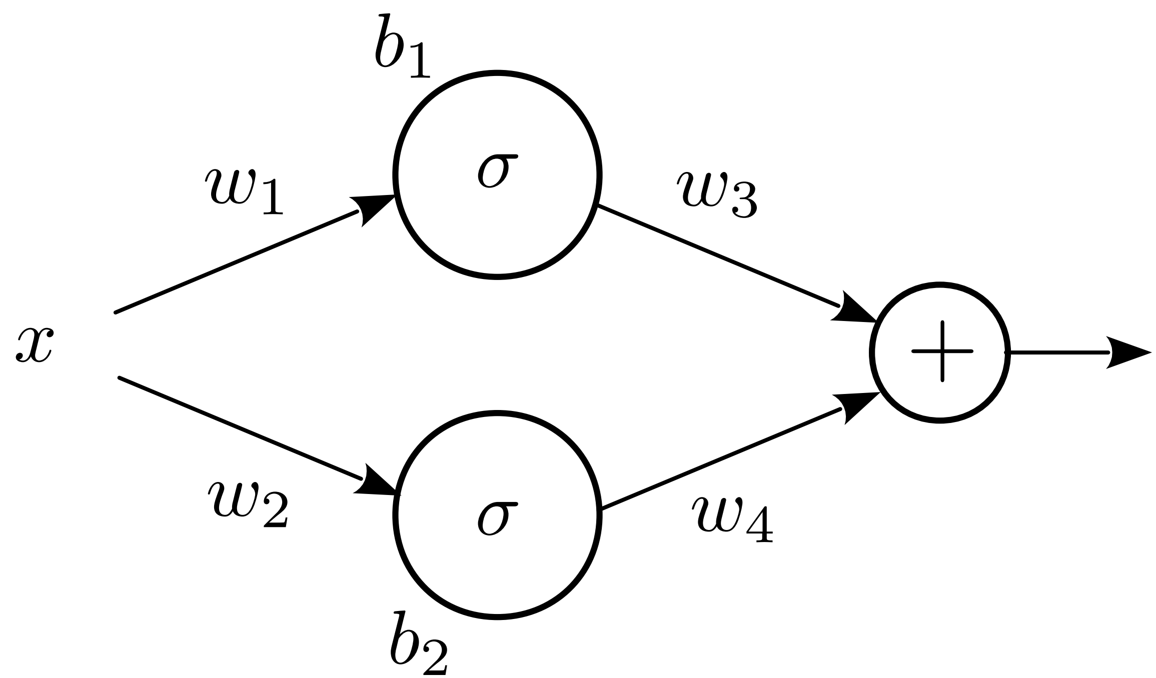
Feed-Forward Neural Networks…

…universal function approximators

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

Feed-Forward Neural Networks…
…universal function approximators

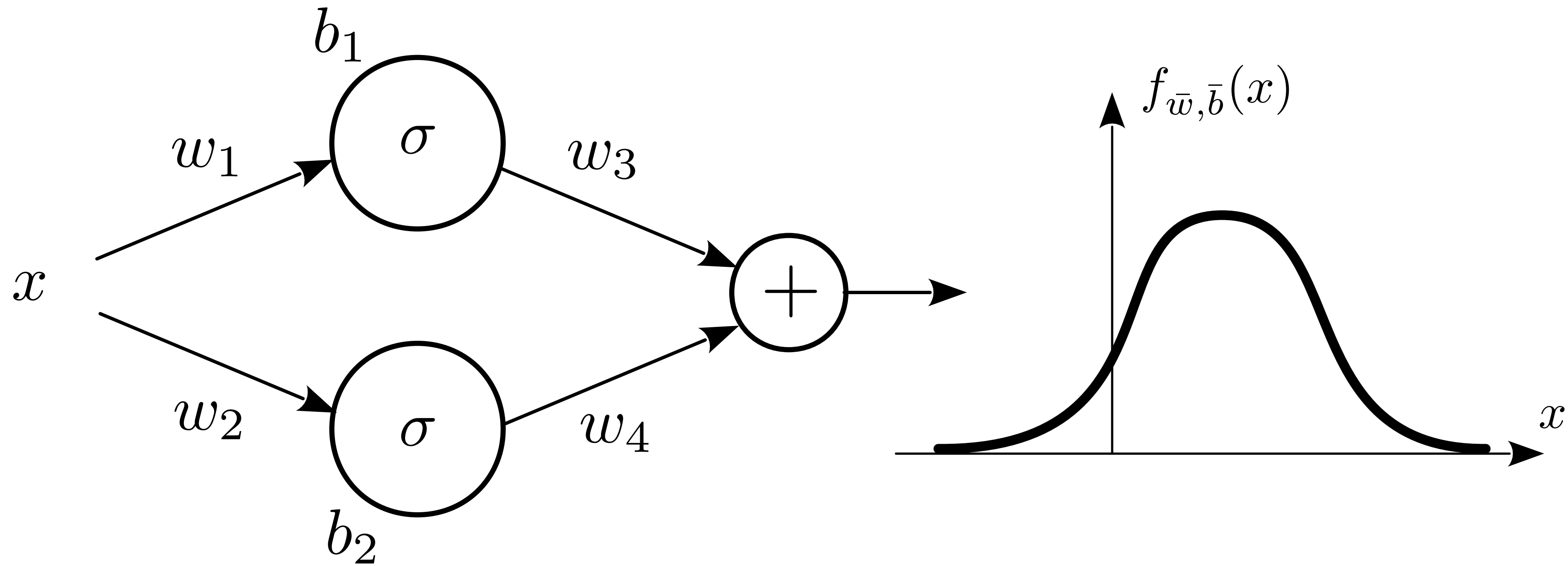
[Cybenko, G. (1989) *Approximations by superpositions of sigmoidal functions*]



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

Feed-Forward Neural Networks…
…universal function approximators

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

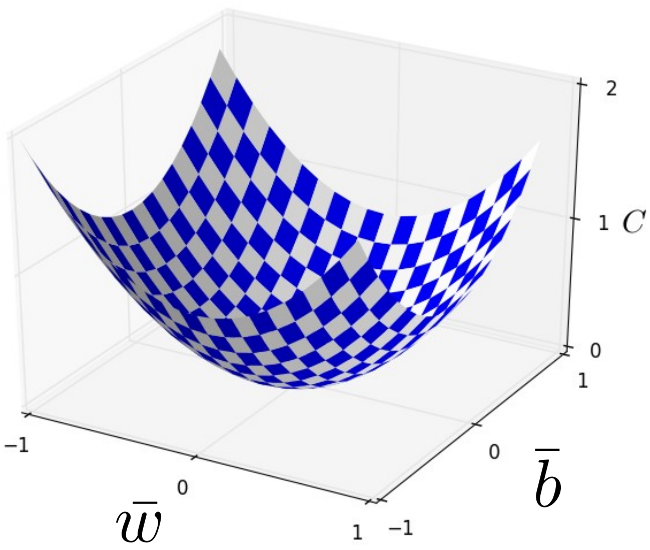


$$f_{\bar{w},\bar{b}}(x) = w_3\,\sigma\big(b_1 + w_1 x\big) + w_4\,\sigma\big(b_2 + w_2 x\big)$$

Learning through gradient descent

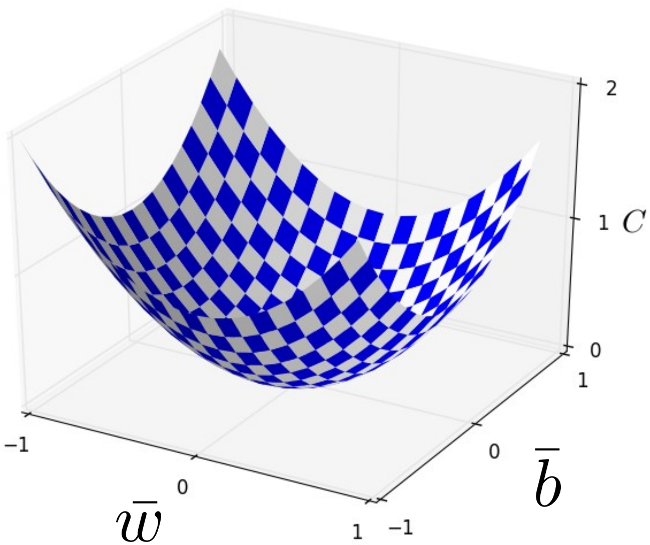
Minimize a **cost function**:

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



Learning through gradient descent

Minimize a **cost function**:



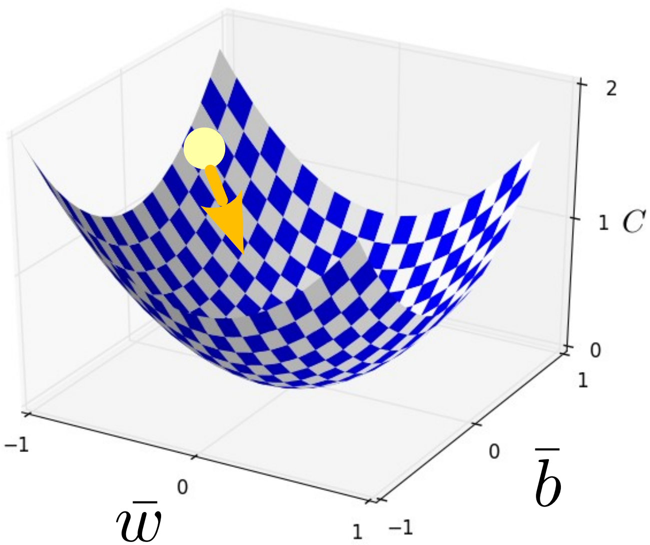
$$C(\bar{w},\bar{b}) = \left\langle \frac{1}{2}\left\|\text{output} - \text{desired one}\right\|^2 \right\rangle_{\text{training data}}$$

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

$$= \frac{1}{2N}\underbrace{\sum_x}_{\text{training data}}\underbrace{\sum_i}_{\text{neurons in layer } L \text{ (output)}}\left(a_i^L(x) - y_i(x)\right)^2$$

Learning through gradient descent

Minimize a **cost function:**



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

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

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

training data

neurons in layer L (output)

Gradient descent update rules:

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

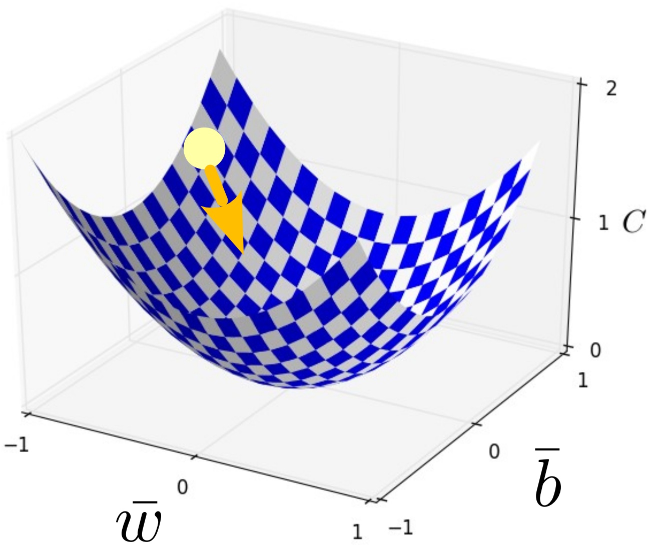
$$b_i^l \leftarrow b_i^l - \eta\,\frac{\partial C}{\partial b_i^l}$$

η

learning rate

Learning through gradient descent

Minimize a **cost function:**



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

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

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

training data

neurons in layer L (output)

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

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

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?

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?

$$\delta_i^l \equiv \frac{\Delta C}{\Delta z_i^l} \rightarrow \frac{\partial C}{\partial z_i^l}$$

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?

$$\delta_i^l \equiv \frac{\Delta C}{\Delta z_i^l} \rightarrow \frac{\partial C}{\partial z_i^l}$$

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

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?

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

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

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

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?

$$\delta_i^l \equiv \frac{\Delta C}{\Delta z_i^l} \rightarrow \frac{\partial C}{\partial z_i^l}$$

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

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

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

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?

$$\delta_i^l \equiv \frac{\Delta C}{\Delta z_i^l} \rightarrow \frac{\partial C}{\partial z_i^l}$$

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

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

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

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?

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

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

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

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

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

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?

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

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

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

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

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

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?

$$\delta_i^l \equiv \frac{\Delta C}{\Delta z_i^l} \rightarrow \frac{\partial C}{\partial z_i^l}$$

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

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

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

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

The backpropagation algorithm

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

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

The backpropagation algorithm

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

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

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

The backpropagation algorithm

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

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

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

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

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

The backpropagation algorithm

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

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

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

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

$$\delta_j^{l-1} = \frac{\partial C}{\partial z_j^{l-1}} = \sum_i \frac{\partial C}{\partial z_i^l}\, \frac{\partial z_i^l}{\partial z_j^{l-1}}$$

chain rule $\quad \mathrm{z}_i^l = b_i^l + \sum_j w_{i,j}^l \sigma(z_j^{l-1})$

The backpropagation algorithm

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

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

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

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

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

chain rule $\quad \mathrm{z}_i^l = b_i^l + \sum_j w_{i,j}^l \sigma(z_j^{l-1})$

The mini-batch update

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

The mini-batch update

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

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

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

The mini-batch update

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

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

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

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

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

The mini-batch update

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

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

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

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

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

The mini-batch update

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

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

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

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

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

... 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)

The mini-batch update

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

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

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

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

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

... 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)

Stochastic Gradient Descent (SGD)