UNIVERSITAT JAUME•I

MACHINE LEARNING

University Master's Degree in Intelligent Systems

artificial neural networks

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fuel of the future

The Economist, May 6th 2017

https://www.economist.com/briefing/2017/05/06/data-is-giving-rise-to-a-new-economy.

"AN OIL refinery... Data centres... the two have much in common. For one thing, both are stuffed with pipes. In refineries these collect petrol, propane and other components of crude oil ... In big data centres ... tens of thousands of computers ... extract value —patterns, predictions and other insights— from raw digital information."

deep learning

massive raw data
(big data, raw material)

$\downarrow$

```
010010110101001010101001010001001100010011
100100100100110101101001001001110010101000
110010000011010101110100100110010001010001
111011001001110011001100100010010110010001
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001001101001010100010000100011111000101010
101010101001001110001000011110010101010101
```

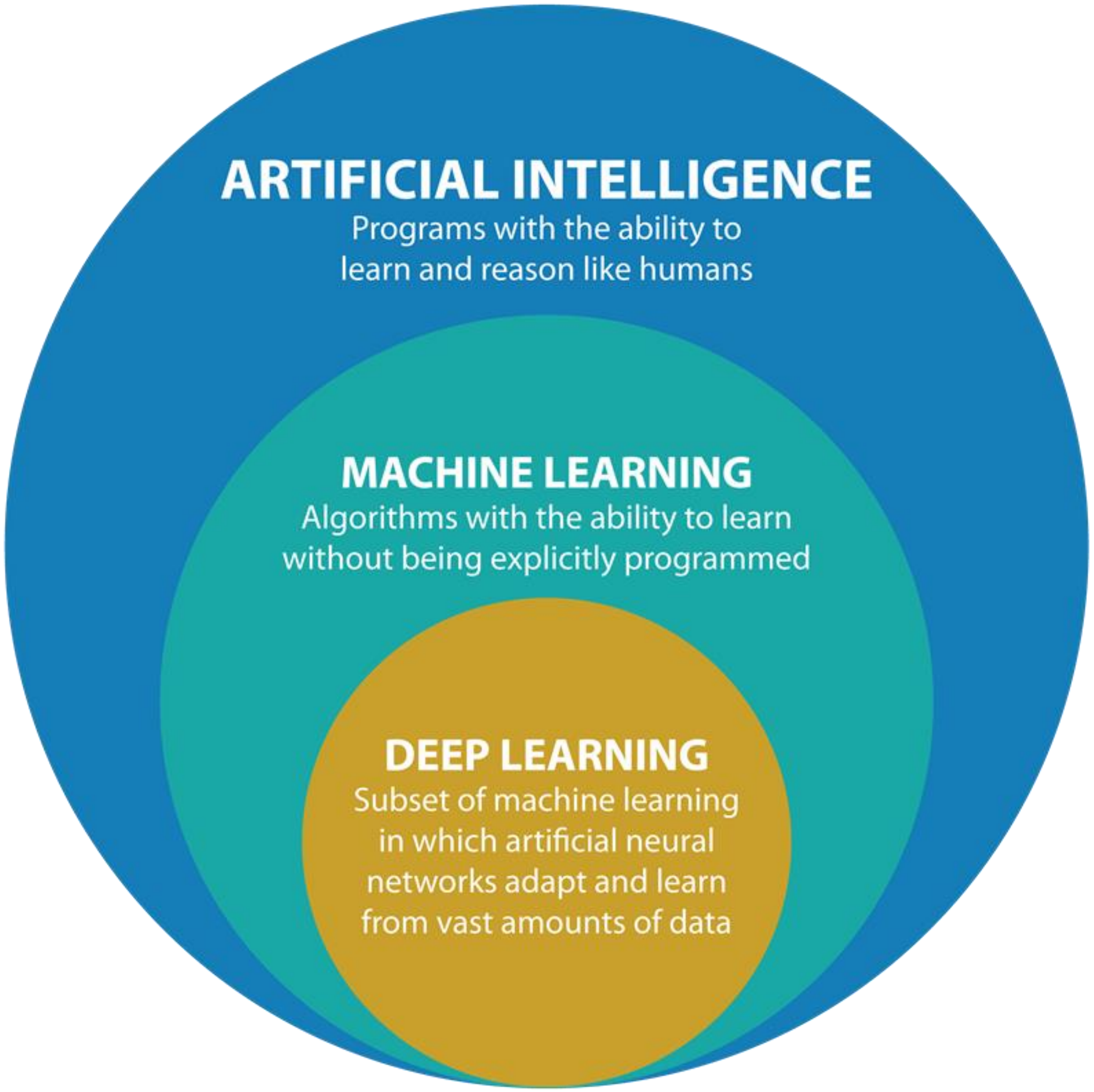
$\rightarrow$ deep learning (refinery, distillery) $\rightarrow$ $f_\theta(x)$

$\downarrow$

concepts, patterns, predictions, manifolds, etc.
(product with practical value)

deep learning

some context


ARTIFICIAL INTELLIGENCE
Programs with the ability to learn and reason like humans
MACHINE LEARNING
Algorithms with the ability to learn without being explicitly programmed
DEEP LEARNING
Subset of machine learning in which artificial neural networks adapt and learn from vast amounts of data

Fuente: *ARGILITY. https://www.argility.com/argility-ecosystem-solutions/industry-4-0/machine-learning-deep-learning/.*

deep learning

artificial neural networks outperform humans

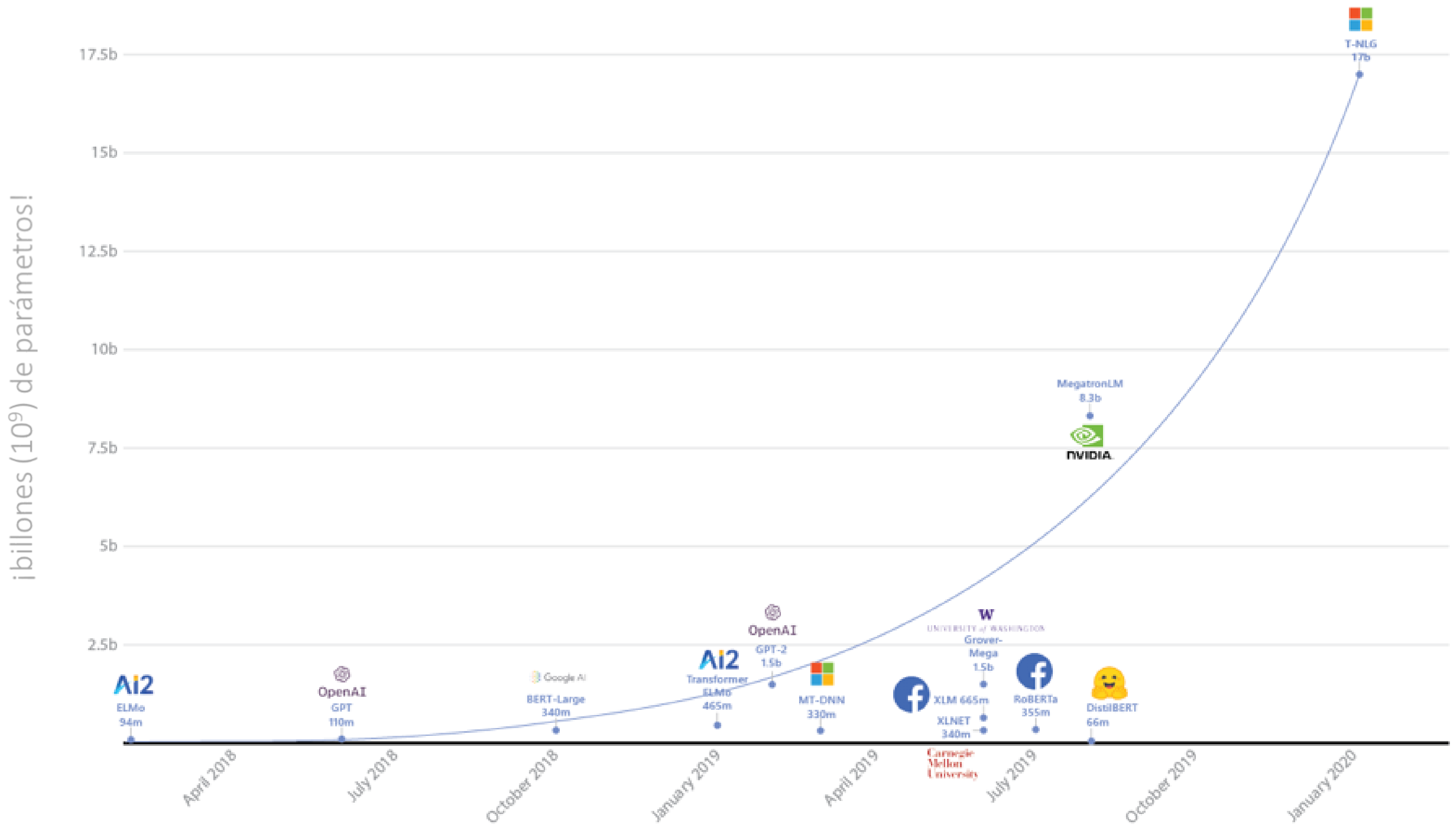
- object and image recognition (ILSVRC, ¿aceptas el reto?)
- imitation of art styles (DeepArt.io, transferencia de estilo)
- medical diagnosis (DL 95% - senior doctors 87% in the diagnosis of malignant melanomas -distinguishing them from benign moles-)
- computer gaming (modelos que aprenden, AlphaGo vs. Lee Sedol)
- lipreading (LipNet 95% - humanos 52% according to grammar
  "command(4) + color(4) + preposition(4) + letter(25) + digit(10) + adverb(4)")
- big data analytics (demografía a partir de Google Street View).
  "Using deep learning ..., we determined the make, model, and year of all motor vehicles encountered .... Data from this census of motor vehicles, which enumerated 22M automobiles in total (8% of all automobiles in the US), was used to accurately estimate income, race, education, and voting patterns ..." (Gebru et al. 2017)

Ver más en Roman Steinberg (2017), 6 areas where artificial neural networks outperform humans, VentureBeat (ir).

deep learning

natural language generation models

OpenAI
GPT-3
175 billion
parameters

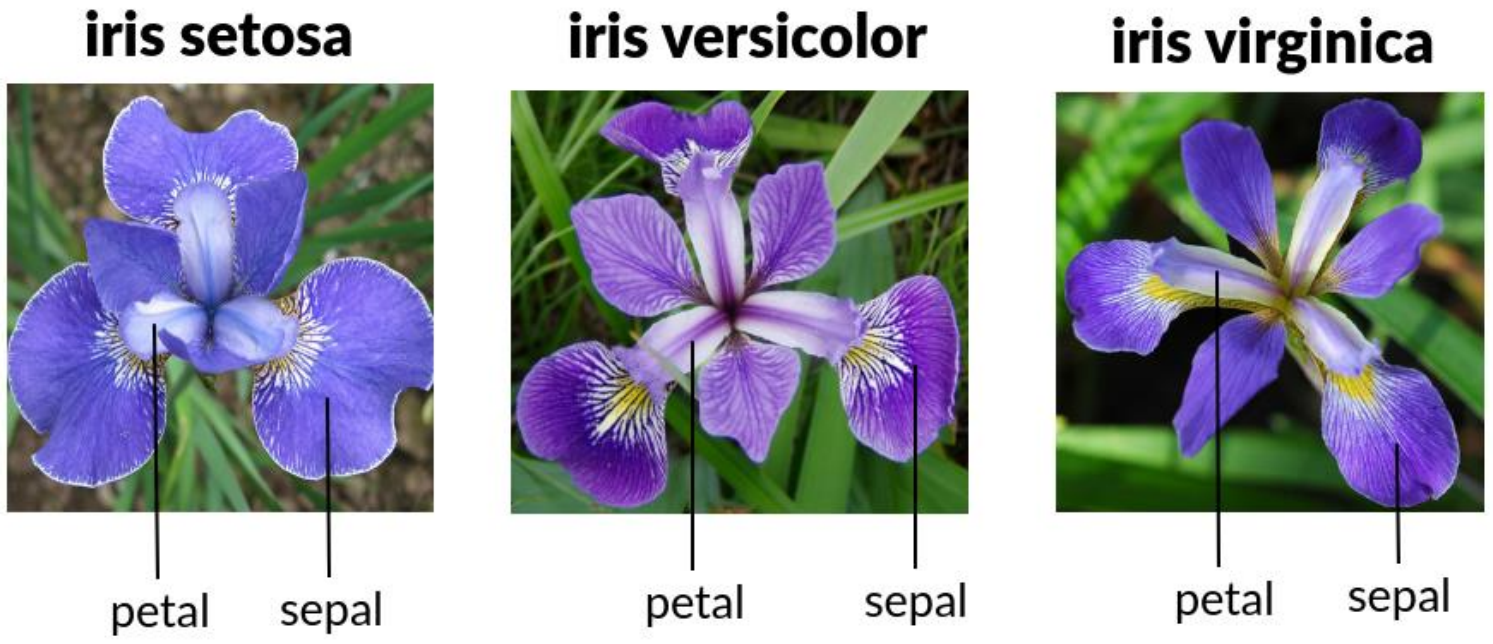


applications to summarize texts, generate responses (chatbots), write stories, etc.

news

IRIS Data Set

classes



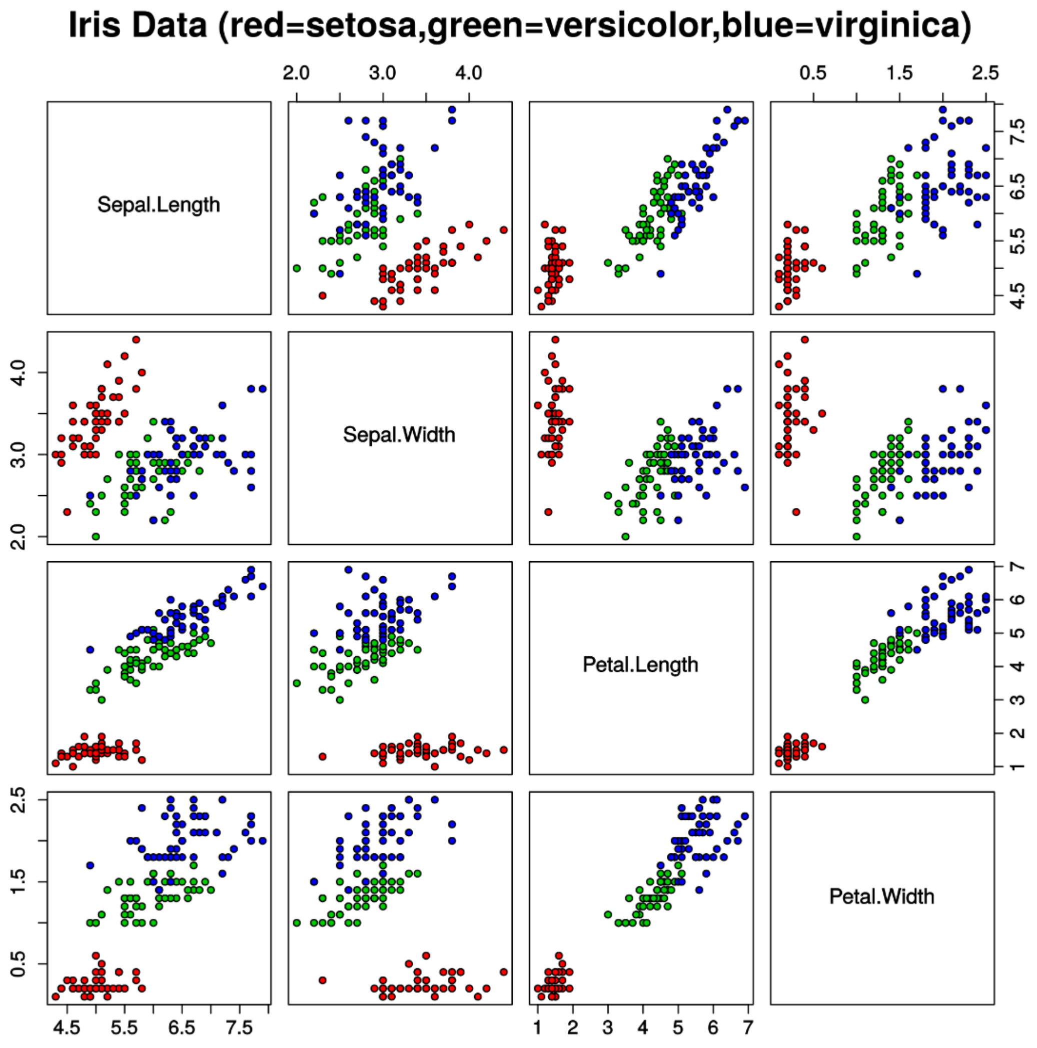
IRIS Data Set

description

- most popular database in machine learning
- 150 examples distributed among 3 classes :
  - Iris Versicolor (50)
  - Iris Setosa (50)
  - Iris Virginica (50)
- examples described by 4 measurements (in cm):
  - sepal length
  - sepal width
  - petal length
  - petal width

IRIS Data Set

distributions by classes in 2D subspaces



https://upload.wikimedia.org/wikipedia/commons/thumb/5/56/Iris_dataset_scatterplot.svg/2000px-Iris_dataset_scatterplot.svg.png

IRIS Data Set

original paper

Fisher, R.A. (1936). The use of multiple measurements in taxonomic problems. Annual Eugenics, 7, Part II, 179-188 (acceder).

linear model

a fully connected neural network f is a composition of nonlinear transformations of linear models (linear combinations of features)

$$f(x|w_k, \dots w_2, w_1) = g^*\left(w_k^t g_{k-1}\left(\cdots g_2\left(w_2^t g_1(w_1^t x)\right)\right)\right)$$

being…

- x, the input vector to the network
- k, the number of layers (or transformations)
- w_i, weight matrix of the layer i, $1 \leq i \leq k$
- g_i, nonlinear activation function of the layer i (they are generally the same)
- g^*, output layer activation function (can be the identity function)
- f, network function composed from chains of linear and nonlinear functions

linear model

a fully connected neural network f is a composition of nonlinear transformations of linear models (linear combinations of features)

$$f(x|w_k, \ldots w_2, w_1) = g^*\left(w_k^t g_{k-1}\left(\cdots g_2\left(w_2^t g_1(\underbrace{w_1^t x}_{\text{linear model}})\right)\right)\right)$$

being...

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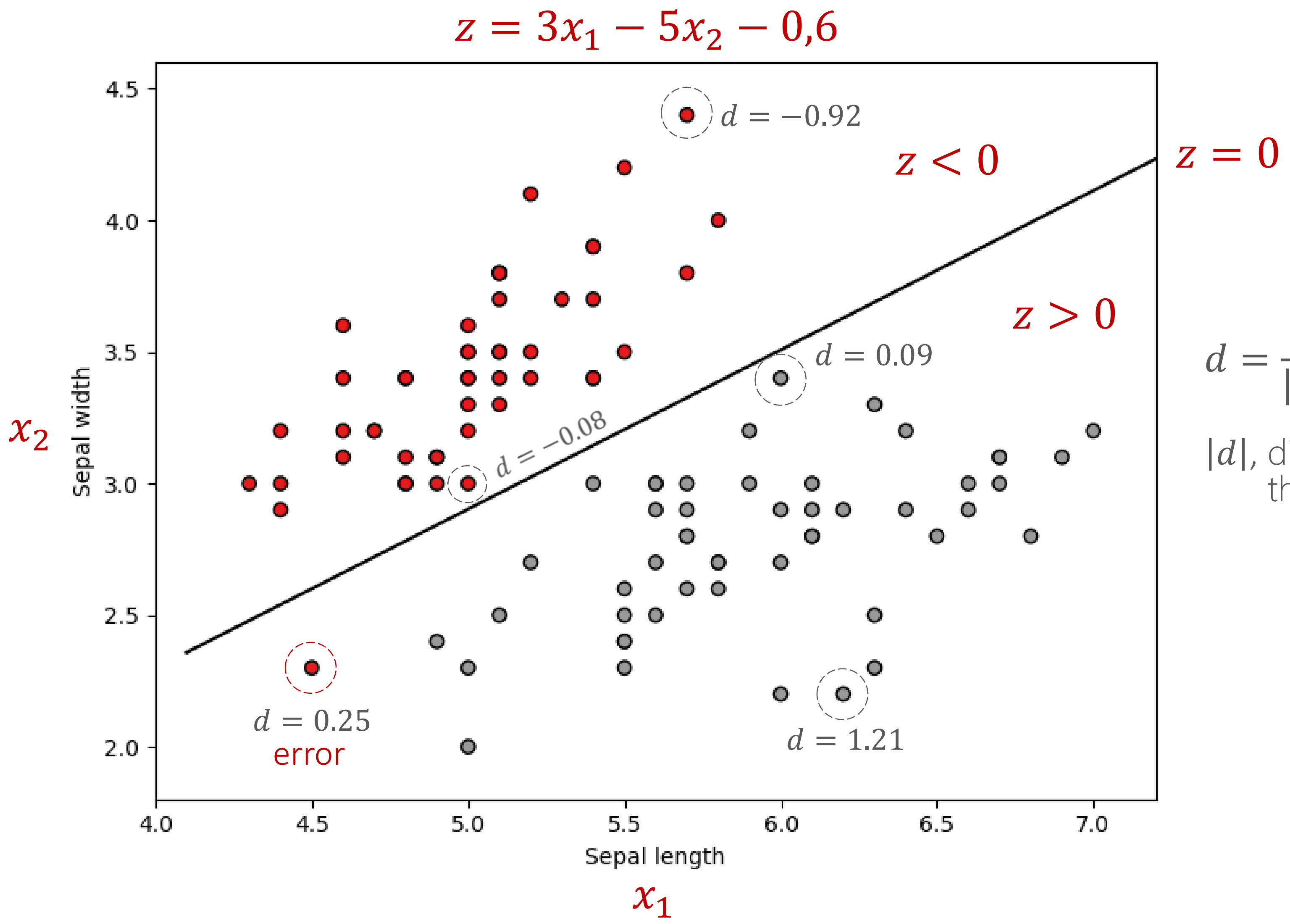
- f, network function composed from chains of linear and nonlinear functions

linear model

classes Setosa (red) and Versicolor (gray)



$$d = \frac{z}{\|w\|_2}$$

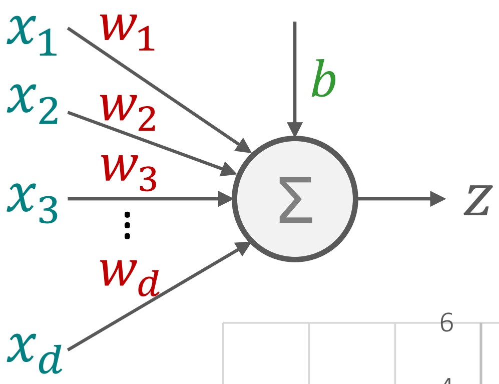
$|d|$, distance to the plane

linear model

affine/linear transformation

$$z = w^T x + b$$

$$z = \sum_{i=1}^{d} w_i x_i + b$$



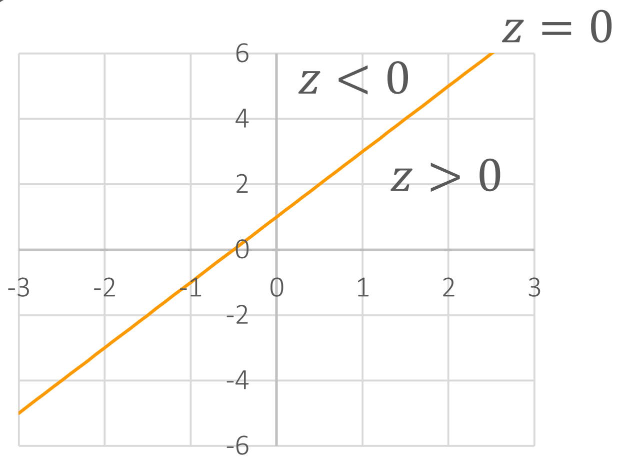
where:

w, weight vector

x, input data vector

b, scalar; bias, threshold

z, scalar; affine transformation output



$z = 2x_1 - x_2 + 1$

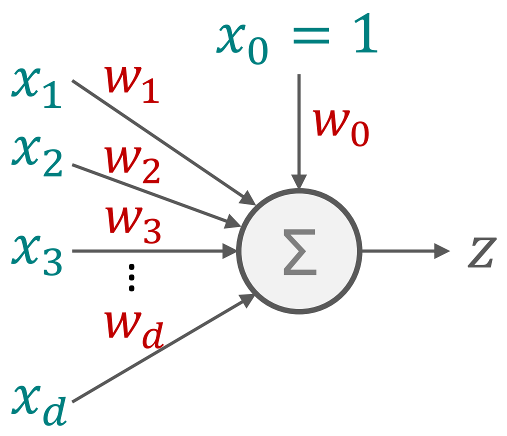
linear division of space

linear model

affine/linear transformation: compact notation

$$z = w^T x$$

$$z = \sum_{i=0}^{d} w_i x_i$$



where:

w, weight vector (w_0, bias)

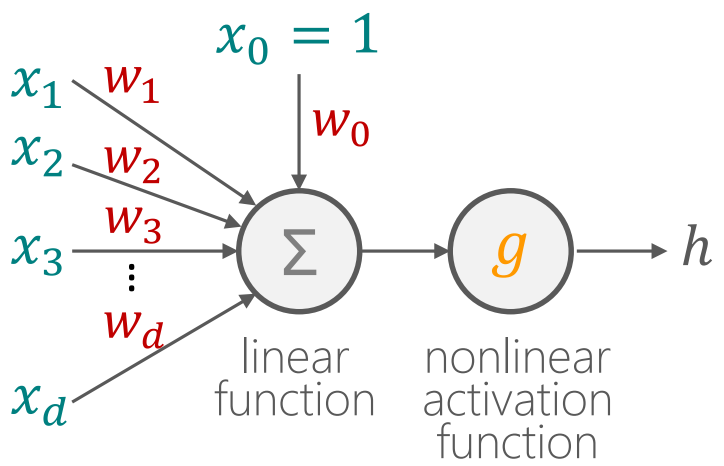
x, input data vector

z, scalar; affine transformation output

linear model

activation function

$$h = g(z) = g(w^T x)$$



where:

z, scalar; affine transformation output

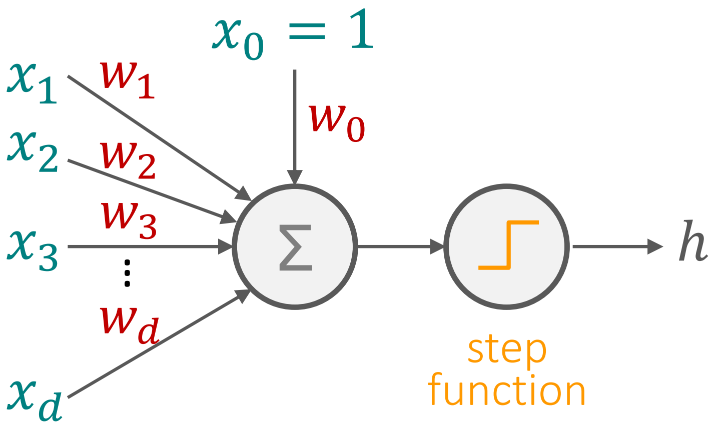
g, nonlinear activation function

h, scalar; nonlinear function output

linear model

Perceptron (Frank Rosenblatt, 1958)

$$h = g(z) = g(w^T x)$$

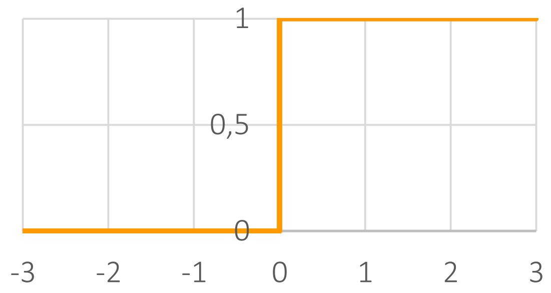


where:

z, affine transformation output

g, step function (derivative 0 at all points)

$h \in \{0,1\}$

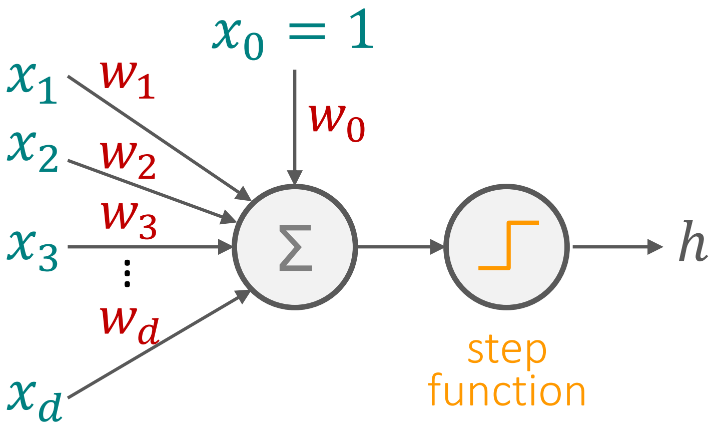


$$g(z) = \begin{cases} 1, \text{si } z \geq 0 \\ 0, \text{si } z < 0 \end{cases}$$

linear model

Perceptron (Frank Rosenblatt, 1958)

$$h = g(z) = g(w^T x)$$



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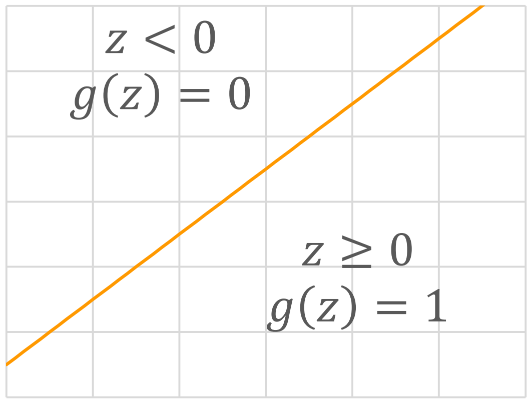
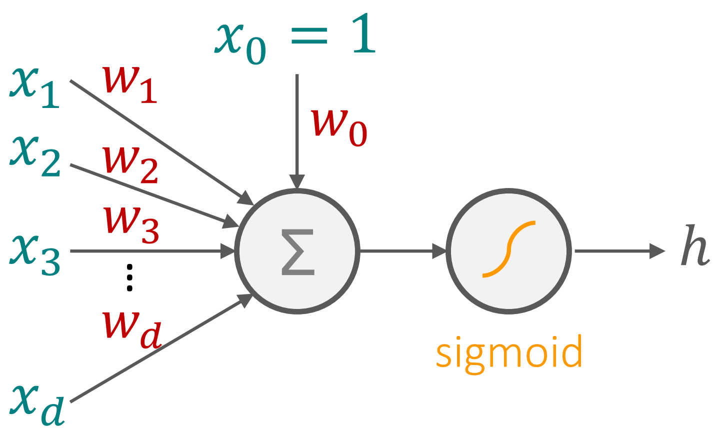


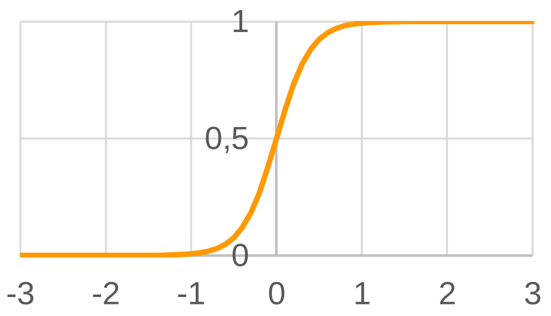
$z = 2x_1 - x_2 + 1$

linear model

logistic regression: a linear decision boundary

$$h = g(z) = g(w^T x)$$





where:

z, affine transformation output

g, sigmoid function (derivative ≠ 0 at all points)

$h \in (0,1)$

$h = Pr(y = 1|x, w)$

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

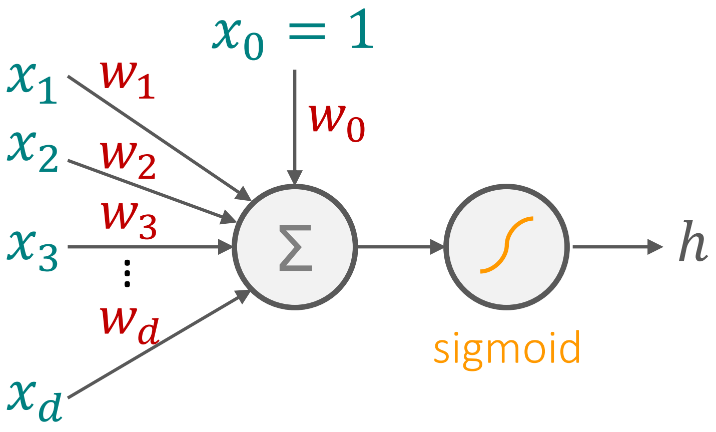
Why is logistic regression a linear classifier? (link)

logistic regression

linear model

logistic regression: a linear decision boundary

$$h = g(z) = g(w^T x)$$



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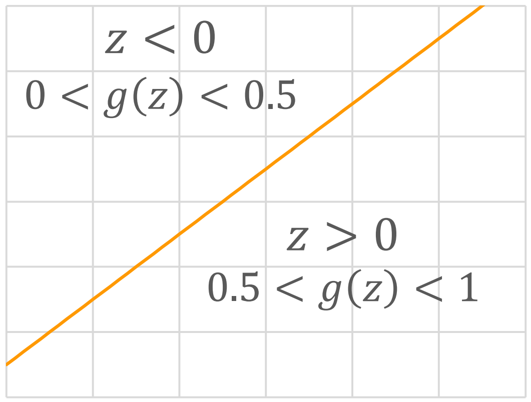
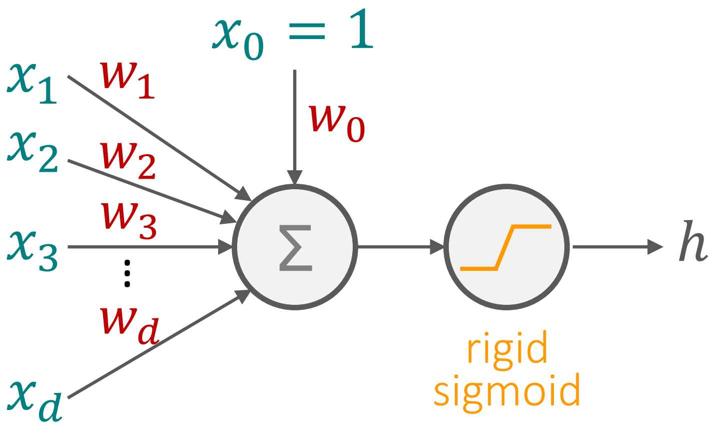


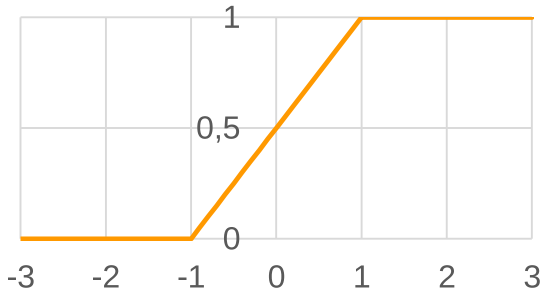
$z = 2x_1 - x_2 + 1$

linear model

approximate (or rigid) logistic regression

$$h = g(z) = g(w^T x)$$





$$g(z) = max\left(0, min\left(1, \frac{x+1}{2}\right)\right)$$

where:

z, affine transformation output

g, rigid sigmoid function

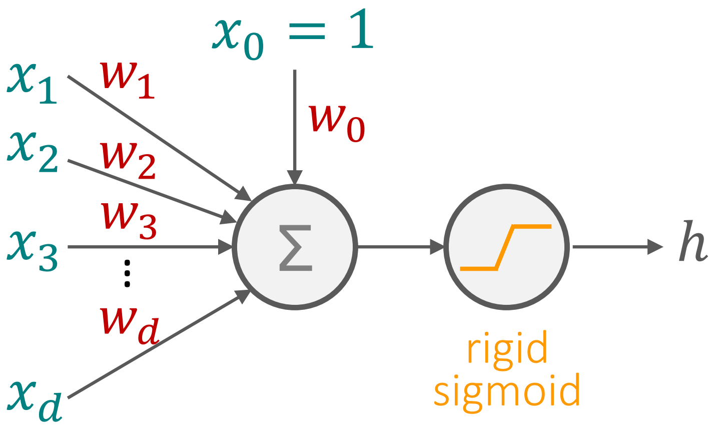
$h \in (0,1)$

$h = Pr(y = 1|x, w)$

linear model

approximate (or rigid) logistic regression

$$h = g(z) = g(w^T x)$$



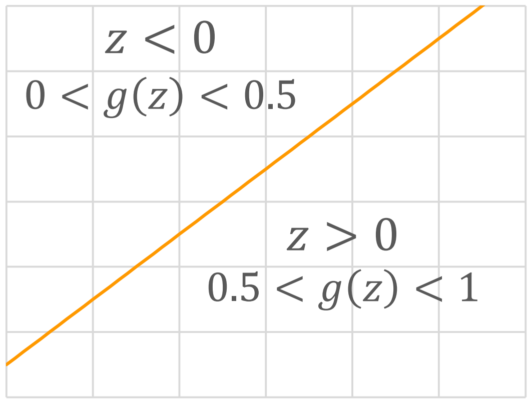
where:

z, affine transformation output

g, rigid sigmoid function

$h \in (0,1)$

$h = Pr(y = 1|x, w)$



$z = 2x_1 - x_2 + 1$

linear model

approximate perceptron on Setosa and Versicolor classes

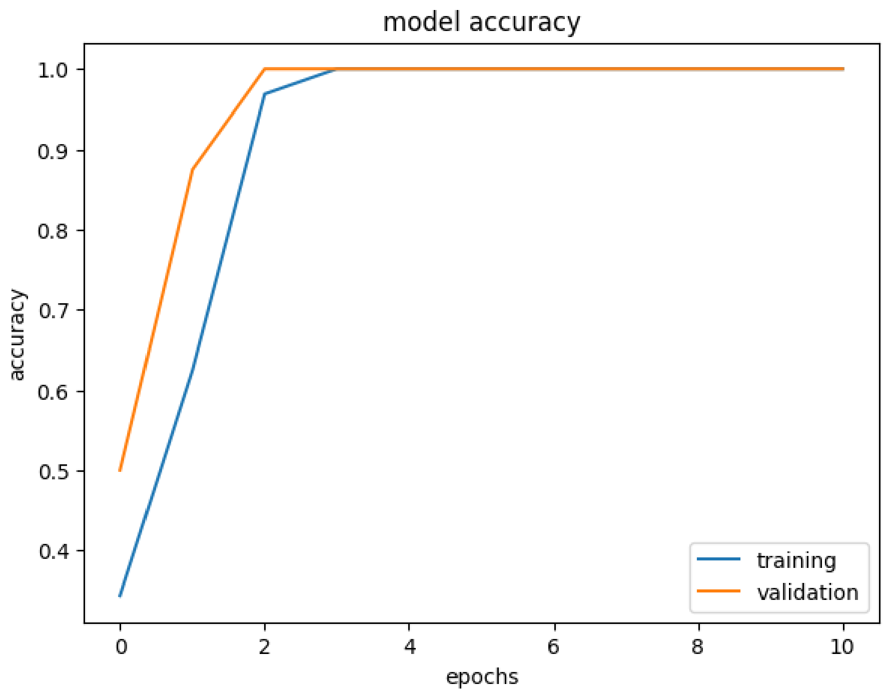
script simplificado usando numpy, sklearn y keras:

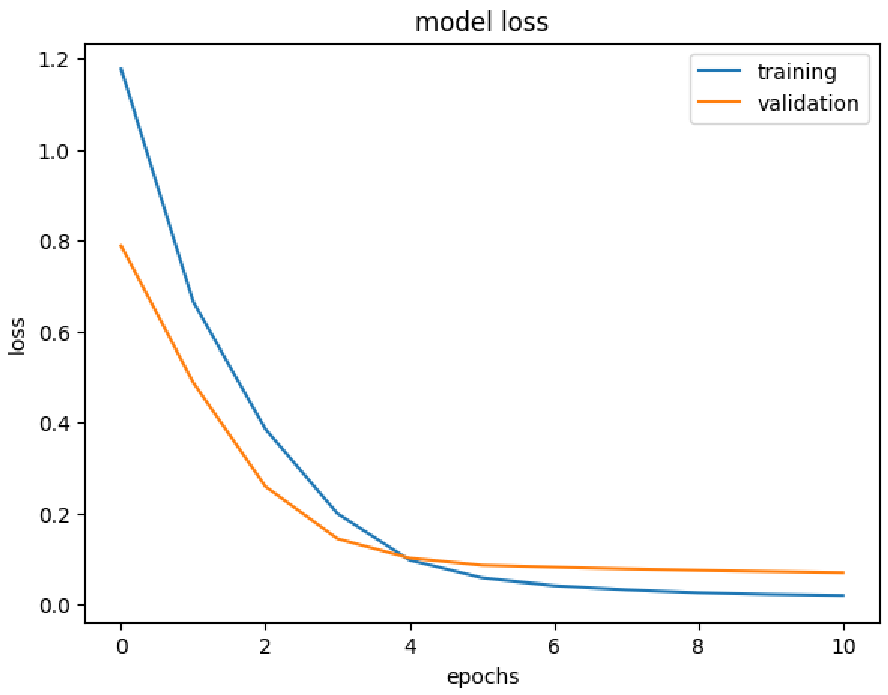
```
iris = sklearn.datasets.load_iris()
X = iris.data[:, :2]  # first two features (sepal width, sepal length)
y = iris.target
X = (X-numpy.mean(X, axis=0))/numpy.std(X, axis=0)  # data standardization

model = keras.models.Sequential()
model.add(keras.layers.Dense(1, input_shape=(2,),
          activation=keras.activations.hard_sigmoid))

opt = keras.optimizers.SGD(learning_rate = 0.1, momentum=0.9)
model.compile(loss='binary_crossentropy', optimizer=opt, metrics=['accuracy'])
history = model.fit(X, y, epochs=10, batch_size=10, verbose=1,
          validation_split=0.2)
```

See: Understanding binary cross-entropy / log loss: a visual explanation (link). Published in Towards Data Science.

linear model

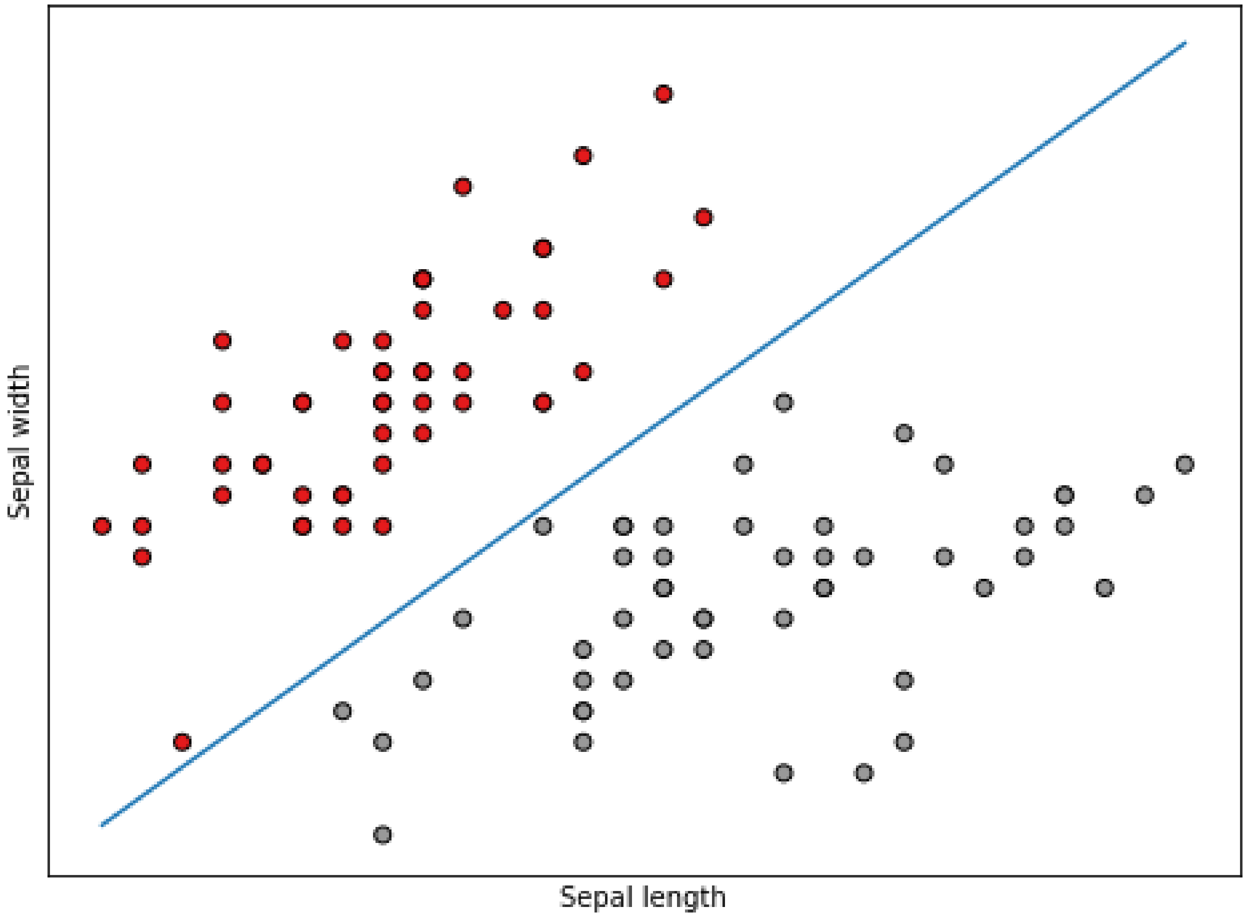
approximate perceptron on Setosa and Versicolor classes





linear model

approximate perceptron on Setosa and Versicolor classes

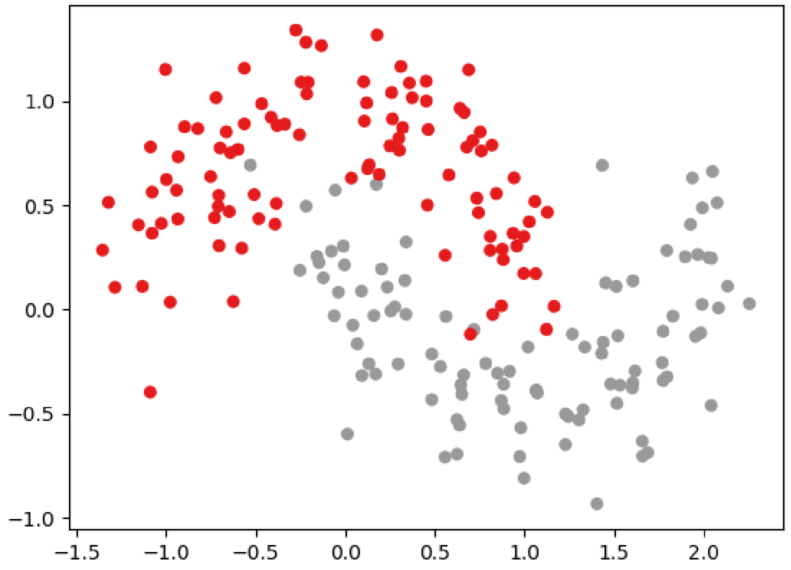


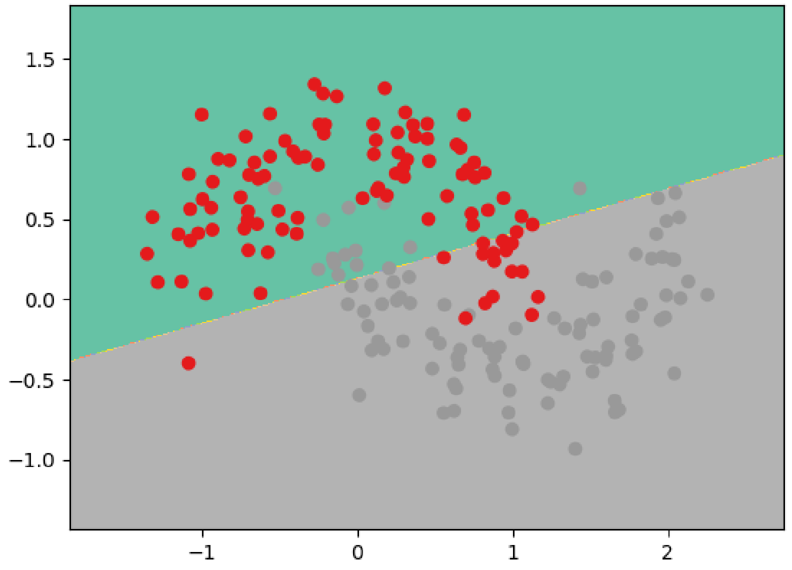
linear model

limitations

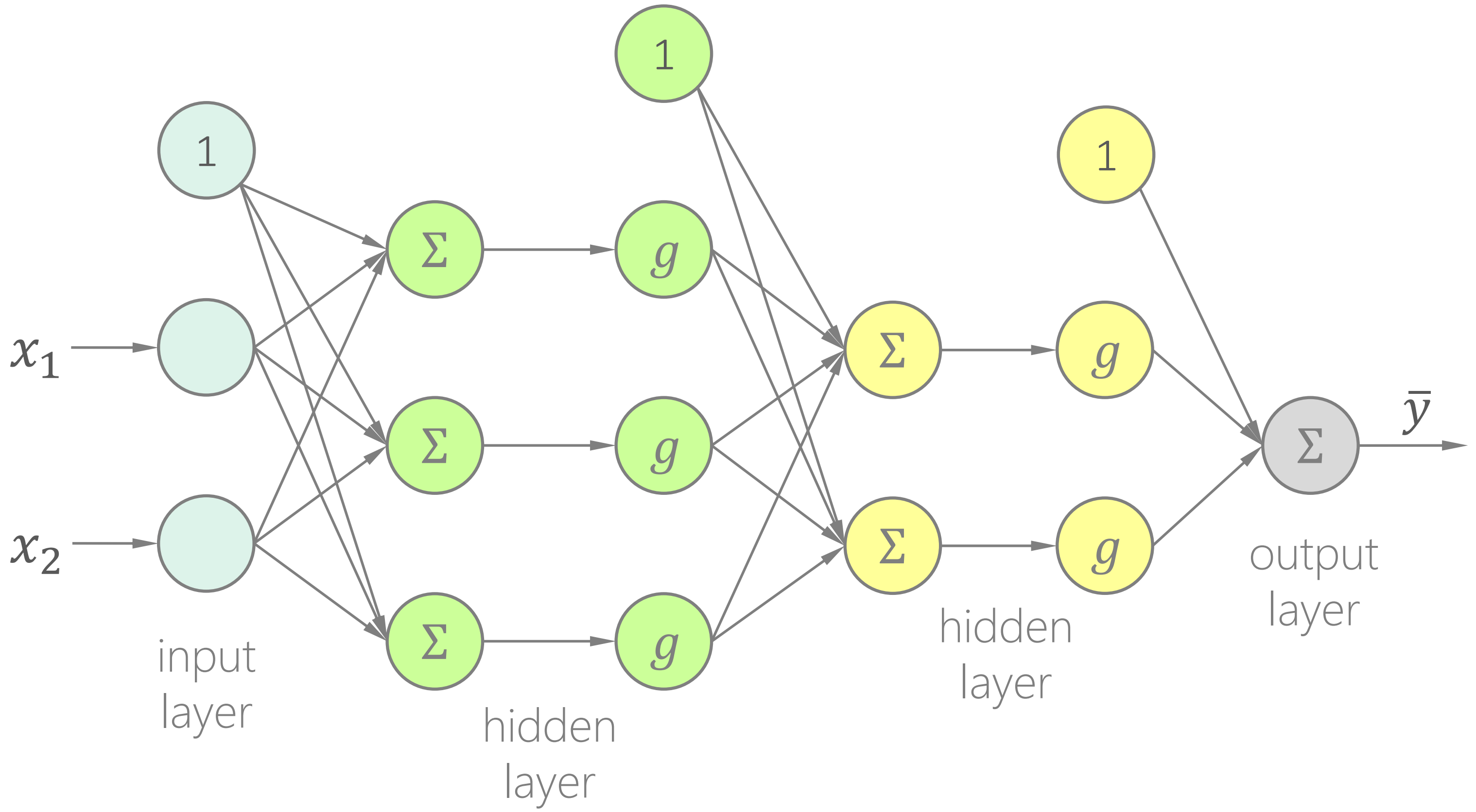
linear classifier

logistic regression => “sigmoid” activation function



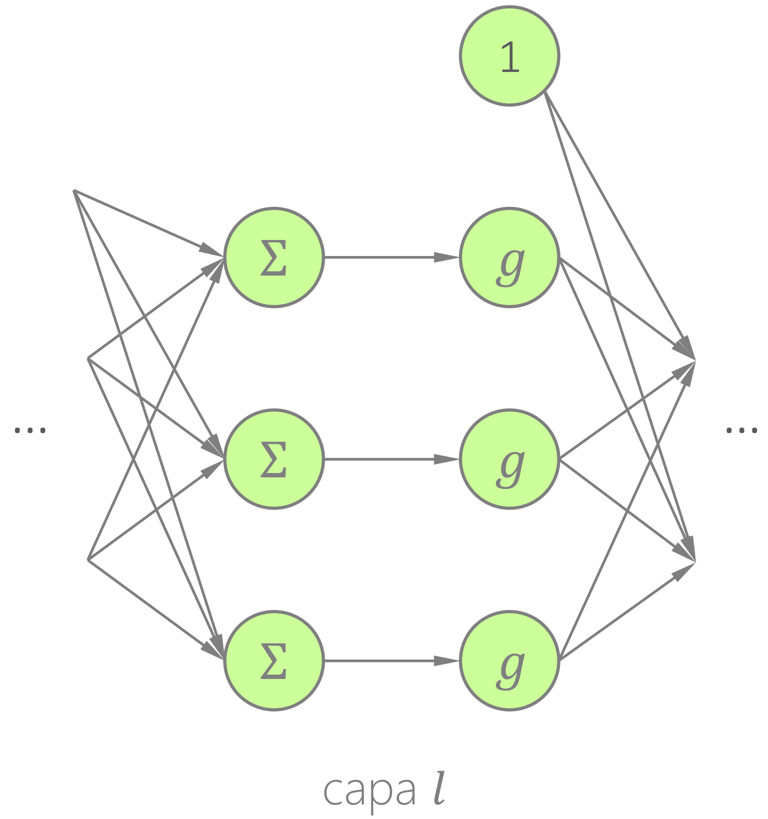


fully connected multilayer networks



g: función de activación (e.g. sigmoid, tanh, softmax, relu, …)

fully connected multilayer networks



- cada capa consiste en:
  función lineal + activación no lineal
- función de transformación en capa l:

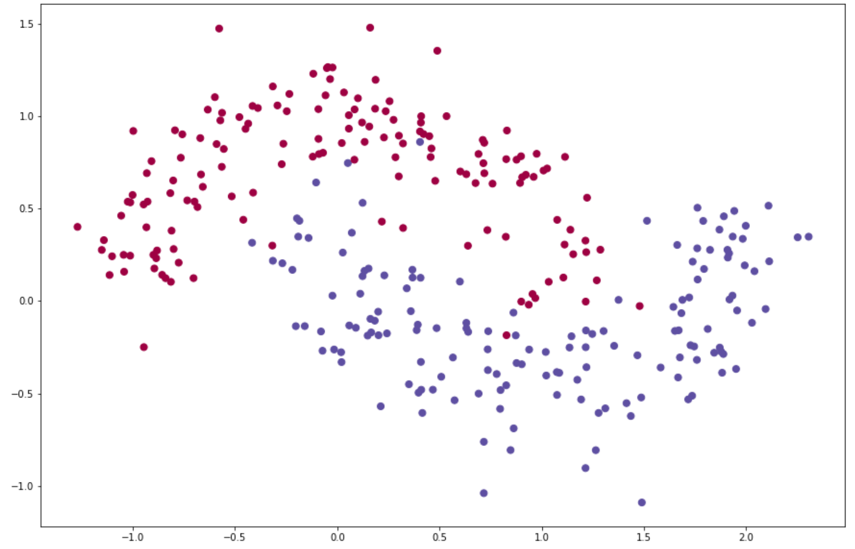
  $z_l = W^l \cdot I_l$
  $I_{l+1} = g(z_l)$
- sea H_l el número de unidades de la capa l; el tamaño de W^l sería …

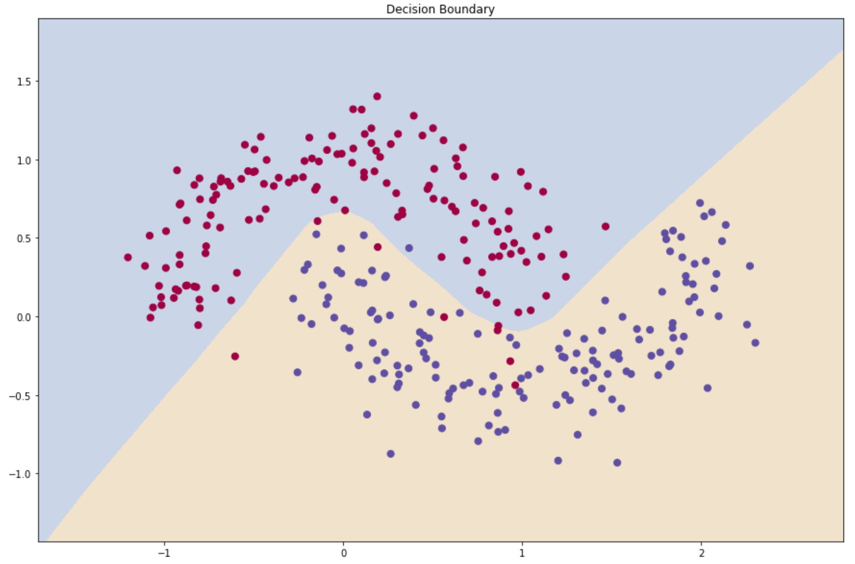
  $H_l \times H_{l-1}$
- I_l es de tamaño $H_{l-1} \times 1$

fully connected multilayer networks

multilayer network

3 layers of 12+6+1 units, "relu" and "sigmoid" activation functions

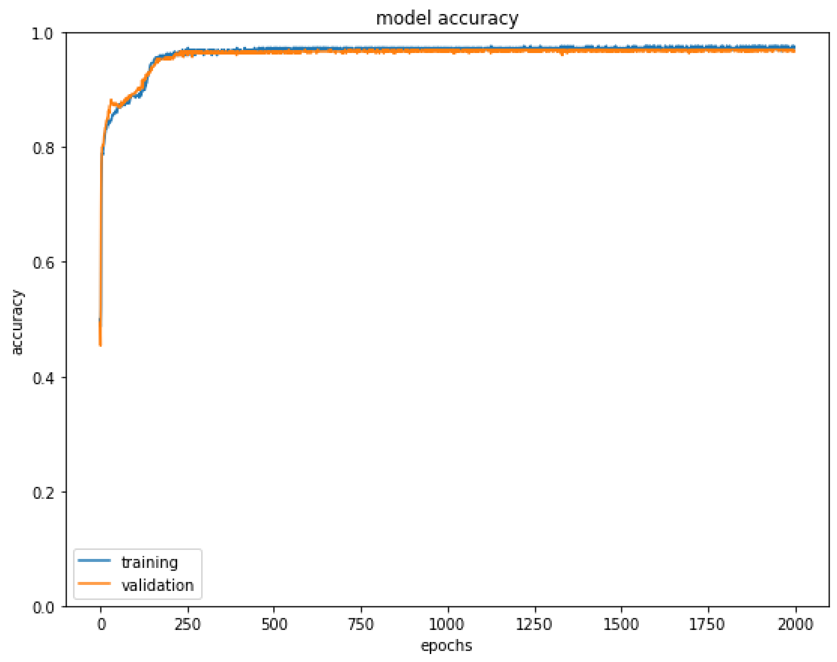


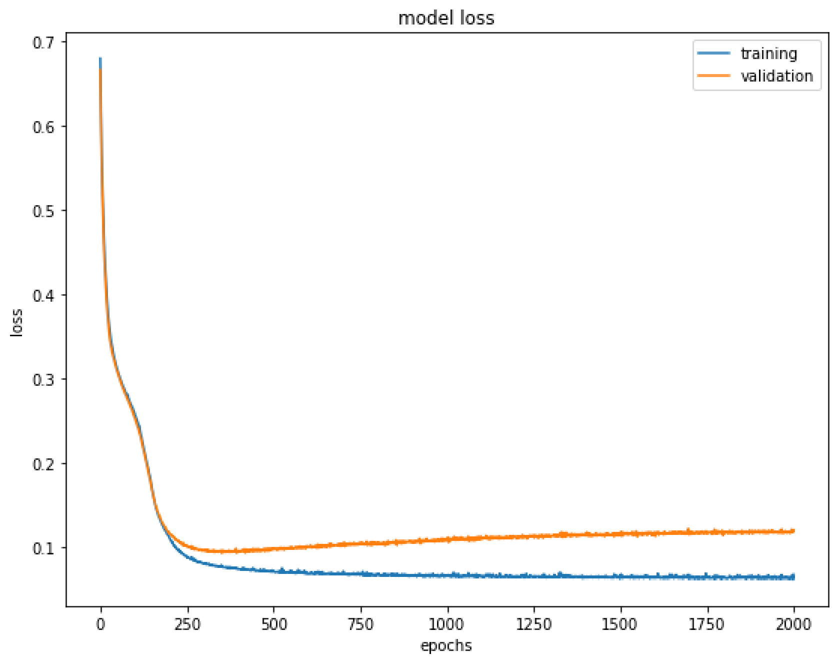


fully connected multilayer networks

multilayer network

3 layers of 12+6+1 units, "relu" and "sigmoid" activation functions





backpropagation

learning goal

progressive adjustment (iterative optimization) of weights that minimize the error/loss of the network on a representative set of training samples.

potentially, a network with sufficient learning capacity could achieve zero error on the training set; however, it is not usually a desirable goal (overfitting risk).

backpropagation

training a neural network (mini-batches)

backpropagation

```
initialize network weights w(0) with small arbitrary values
for epoch = 1...K, do
   for batch = 1...N/batch_size, do
      batch <- randomly choose batch_size instances
      X, y <- preprocess(batch)
      z <- network(X) (forward execution)
      ℓ <- loss(z, y)
      g <- gradients(ℓ, w)  (backward execution)
      w(t+1) <- w(t) - γ · g  (weight optimization/fitting)
   end for
end for
```

backpropagation

fundamentals: chain rule

some examples of composite of two (differentiable) functions $f(g(x))$:

- $f(g(x)) = (2x+1)^3$
- $f(g(x)) = \sin(x^2)$
- $f(g(x)) = \sin(x)^2$

their derivative functions $f' = f'(g(x)) \cdot g'(x)$, or $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial x}$

- $\frac{\partial f}{\partial x} = 3(2x+1)^2 \cdot 2$
- $\frac{\partial f}{\partial x} = \cos(x^2) \cdot 2x$
- $\frac{\partial f}{\partial x} = 2 \cdot \sin(x) \cdot \cos(x)$

backpropagation

fundamentals: gradient descent

gradient descent (steepest descent) is an iterative optimization algorithm for finding a local minimum of a differentiable function.

strategy

- starting from an initial value of the parameter
- move "downhill" along the surface of the function, in the direction of the negative gradient, looking for a parameter value that minimizes it
- stop when the minimum of the function is reached

https://www.jeremyjordan.me/gradient-descent/
https://youtu.be/CsKCT5ezVdI

backpropagation

fundamentals: gradient descent

goal

to find $\theta = \theta^*$ such that $L(\theta^*)$ is the minimum value of L

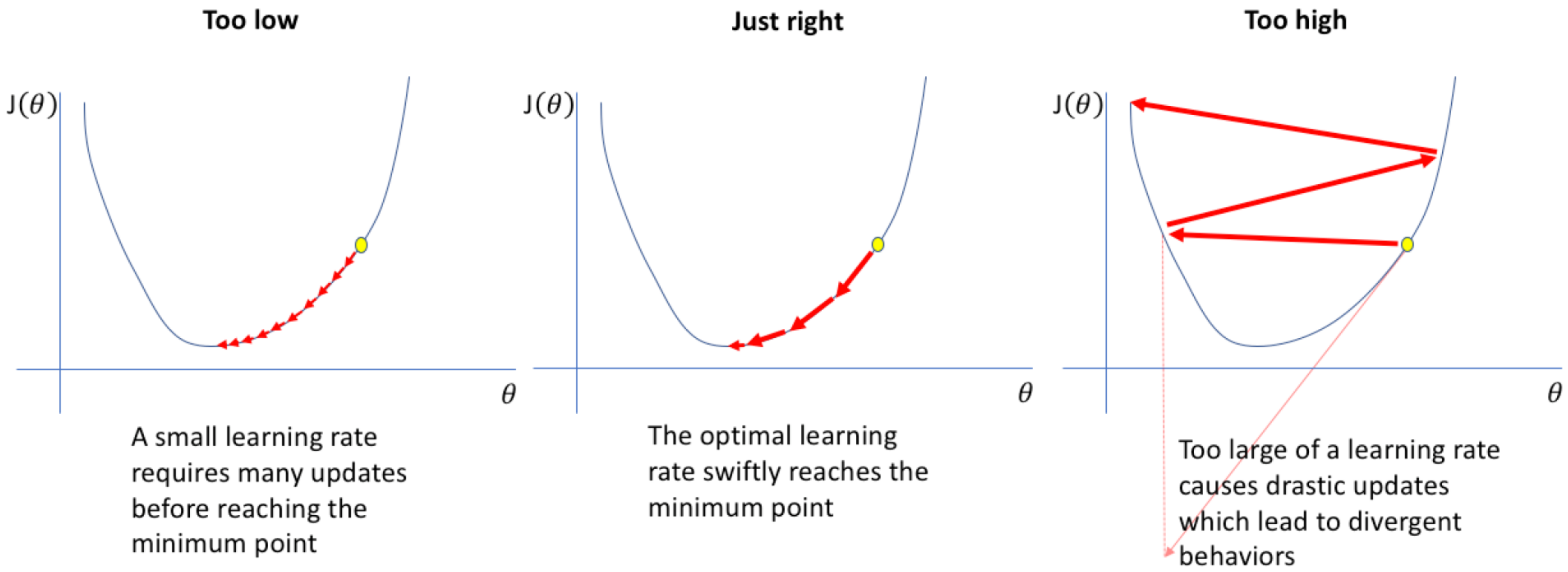
method

- let $L(\theta)$ be a function defined by the parameter θ
- initialization : $\theta_0 = \theta_{inicial}$
- updating: $\theta_{i+1} = \theta_i - \gamma \frac{\partial L}{\partial \theta}(\theta_i)$,
  - $\gamma \ll 1$ is the learning rate; it determines the magnitude of change
- repeat as long as $L(\theta_{i+1}) < L(\theta_i)$
- solution: $\theta^* = \theta_i$

backpropagation

fundamentals: gradient descent

effect of the learning coefficient γ



A small learning rate requires many updates before reaching the minimum point

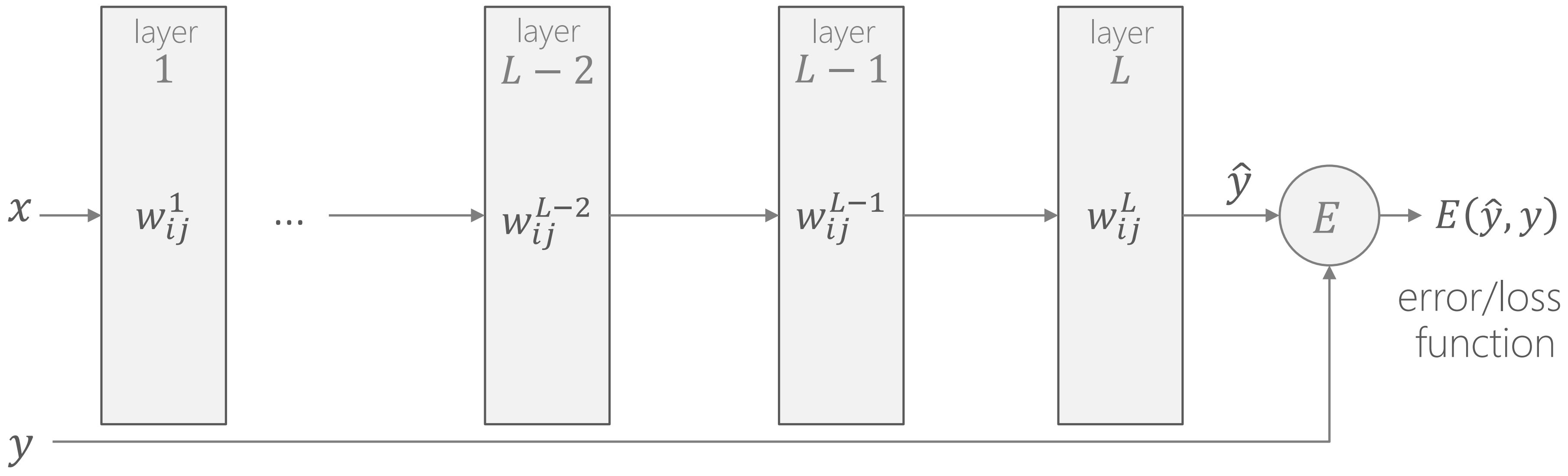
The optimal learning rate swiftly reaches the minimum point

Too large of a learning rate causes drastic updates which lead to divergent behaviors

source: https://www.jeremyjordan.me/nn-learning-rate/

backpropagation

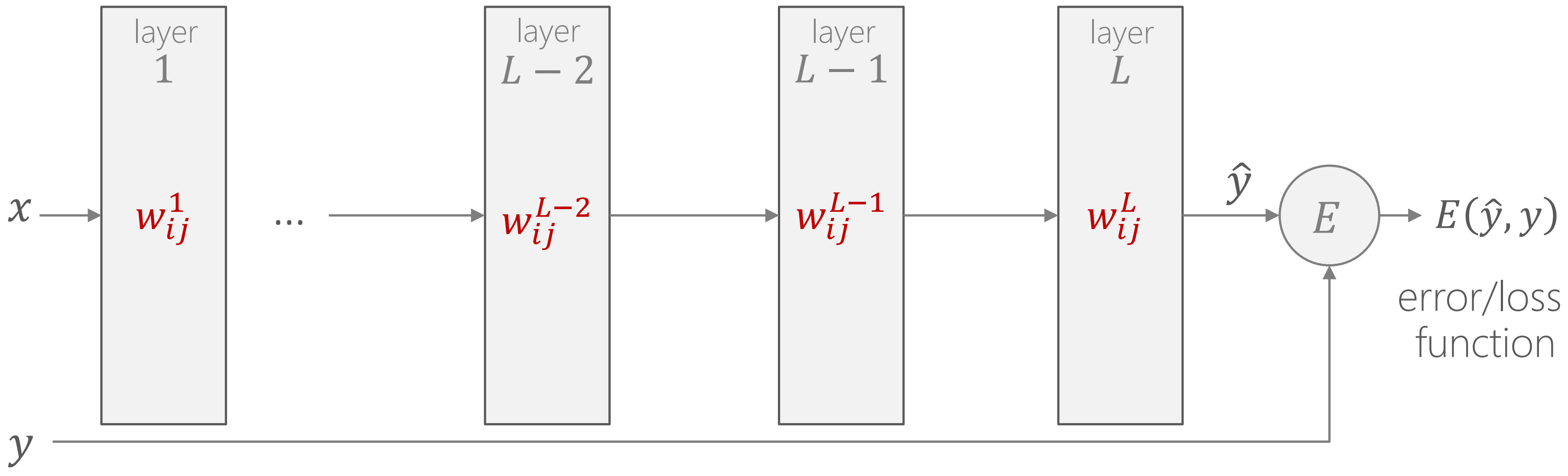
solution scheme



backpropagation

solution scheme

goal: $\frac{\partial E}{\partial w_{ij}^{l}}$ for all w_{ij}^{l}



backpropagation

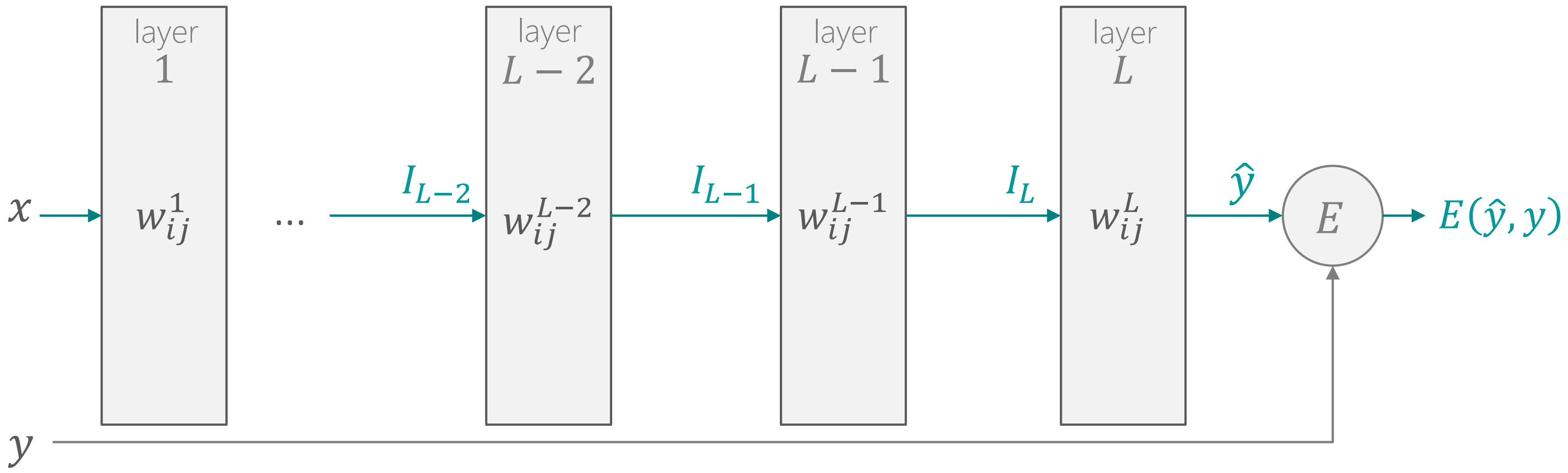
solution scheme

1. initialize weights, choose learning coefficient, choose stop criterion
2. create an arbitrary batch (X, y) --> (subset of instances, expected output).
3. forward execution: walk X through the network and get output z.
4. compute loss(y, z)
5. backward execution (**backpropagation**)
   - compute sensitivity coefficient $\delta_L = f(\delta_{L+1})$ from input to layer L
   - compute gradients $\frac{\partial E}{\partial w_{ij}^{L-1}} = f(\delta_L)$
6. weight optimization
7. check stopping criteria; if it is fulfilled, then finish; otherwise, go to step 2.

backpropagation

solution scheme

forward execution

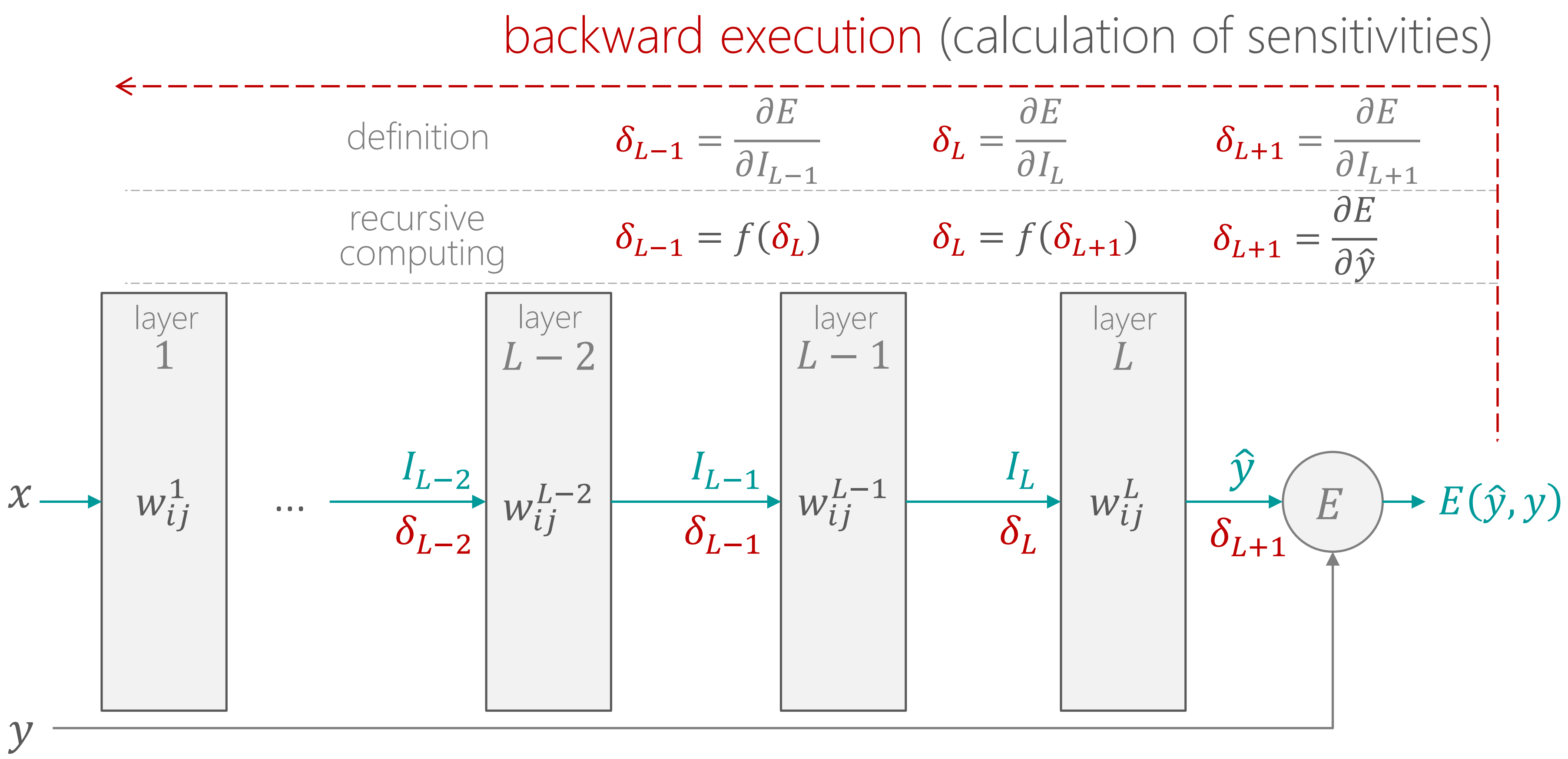


the following pieces of information are calculated:

- input I_l to each layer l (matches the output of the layer $l-1$),
- actual network output $\hat{y}$
- value of the error or loss function $E(\hat{y}, y)$

backpropagation

solution scheme


backward execution (calculation of sensitivities)
definition
$\delta_{L-1} = \frac{\partial E}{\partial I_{L-1}}$
$\delta_L = \frac{\partial E}{\partial I_L}$
$\delta_{L+1} = \frac{\partial E}{\partial I_{L+1}}$
recursive computing
$\delta_{L-1} = f(\delta_L)$
$\delta_L = f(\delta_{L+1})$
$\delta_{L+1} = \frac{\partial E}{\partial \hat{y}}$
layer 1
layer $L-2$
layer $L-1$
layer L
x
w_{ij}^1
…
I_{L-2}
δ_{L-2}
w_{ij}^{L-2}
I_{L-1}
δ_{L-1}
w_{ij}^{L-1}
I_L
δ_L
w_{ij}^L
$\hat{y}$
δ_{L+1}
E
$E(\hat{y}, y)$
y

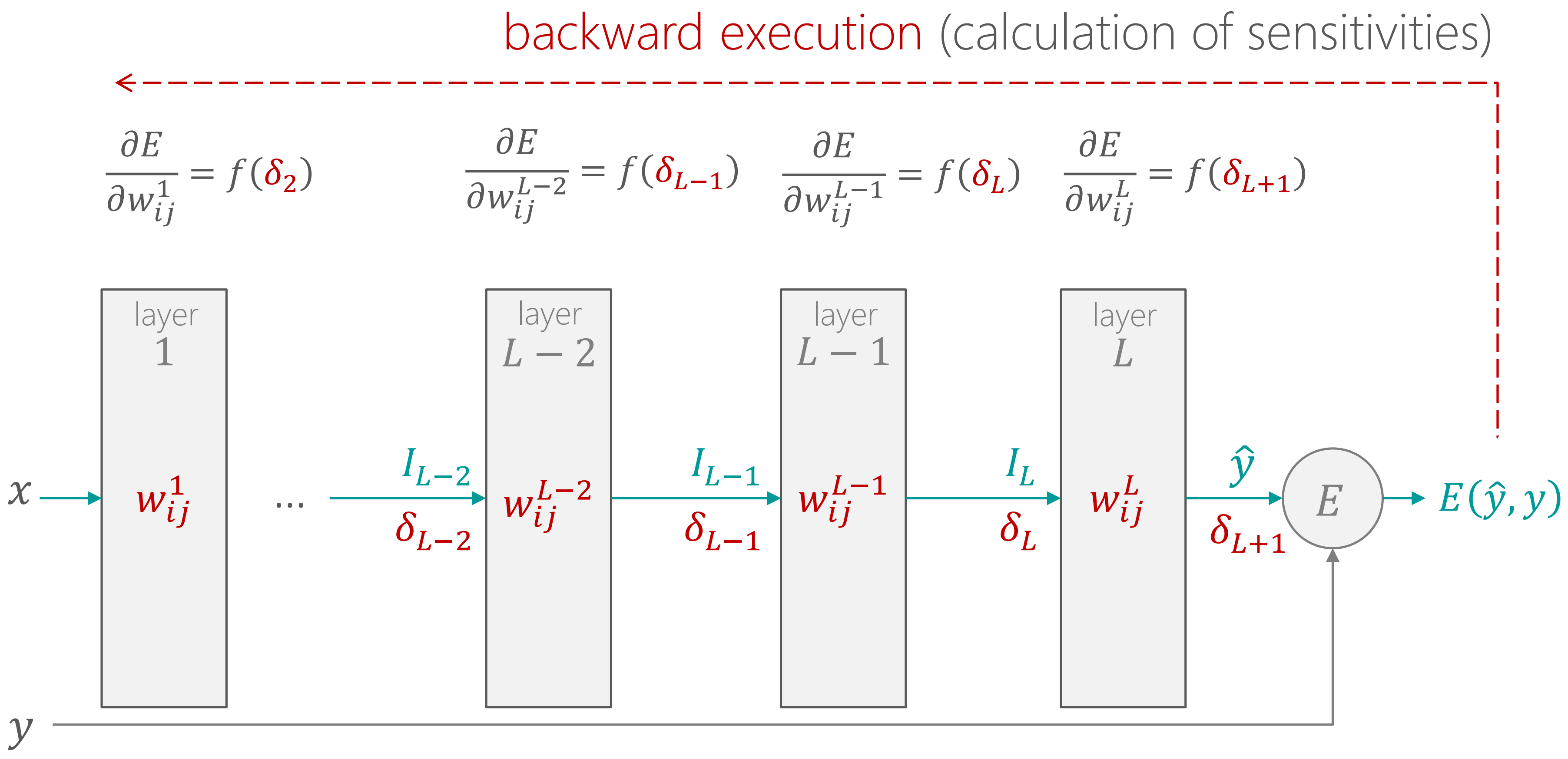
δ_l measures the sensitivity of E to changes in I_l

δ_l is computed recursively from δ_{l+1}

δ_l allows efficient computation of $\frac{\partial E}{\partial w_{ij}^{l-1}}$

backpropagation

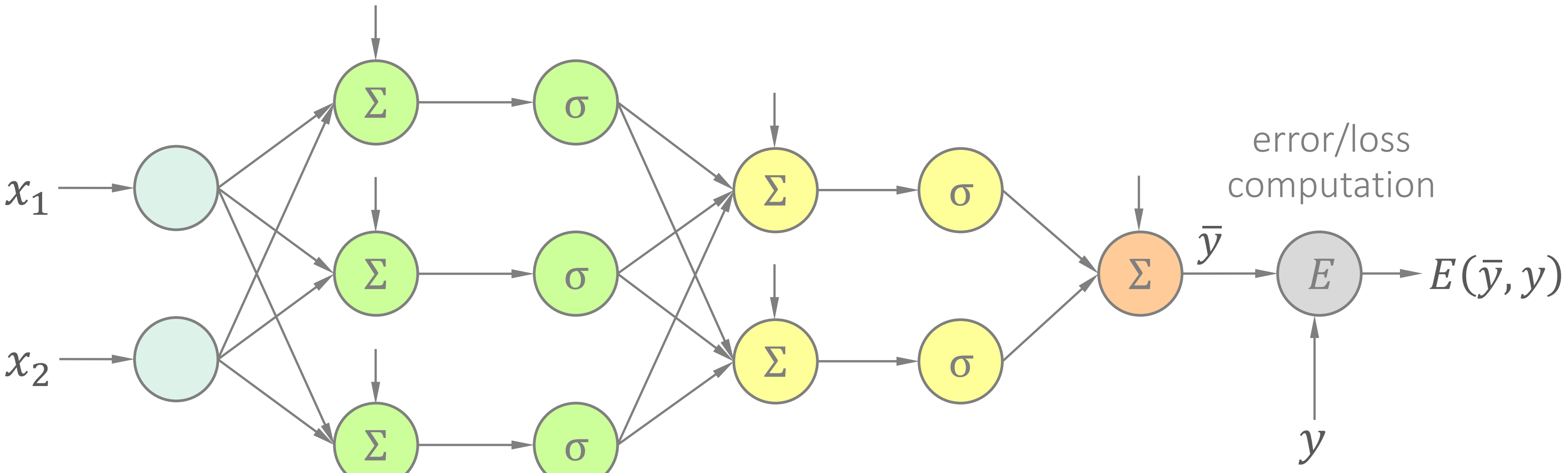
solution scheme



backward execution (calculation of sensitivities)
$\frac{\partial E}{\partial w_{ij}^{1}} = f(\delta_2)$
$\frac{\partial E}{\partial w_{ij}^{L-2}} = f(\delta_{L-1})$
$\frac{\partial E}{\partial w_{ij}^{L-1}} = f(\delta_L)$
$\frac{\partial E}{\partial w_{ij}^{L}} = f(\delta_{L+1})$
layer 1
layer $L-2$
layer $L-1$
layer L
x
w_{ij}^{1}
…
I_{L-2}
δ_{L-2}
w_{ij}^{L-2}
I_{L-1}
δ_{L-1}
w_{ij}^{L-1}
I_L
δ_L
w_{ij}^{L}
$\hat{y}$
δ_{L+1}
E
$E(\hat{y}, y)$
y

backpropagation

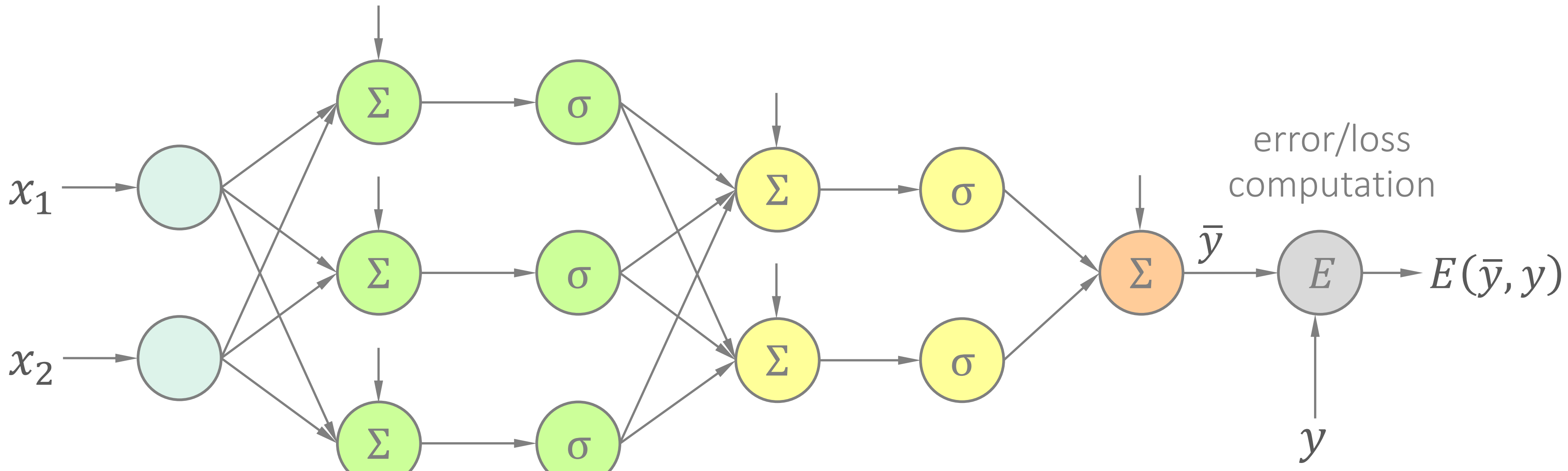
case study: fully connected network with 3 layers



σ: activation function (e.g. sigmoid, tanh, relu, etc.)

backpropagation

case study: fully connected network with 3 layers

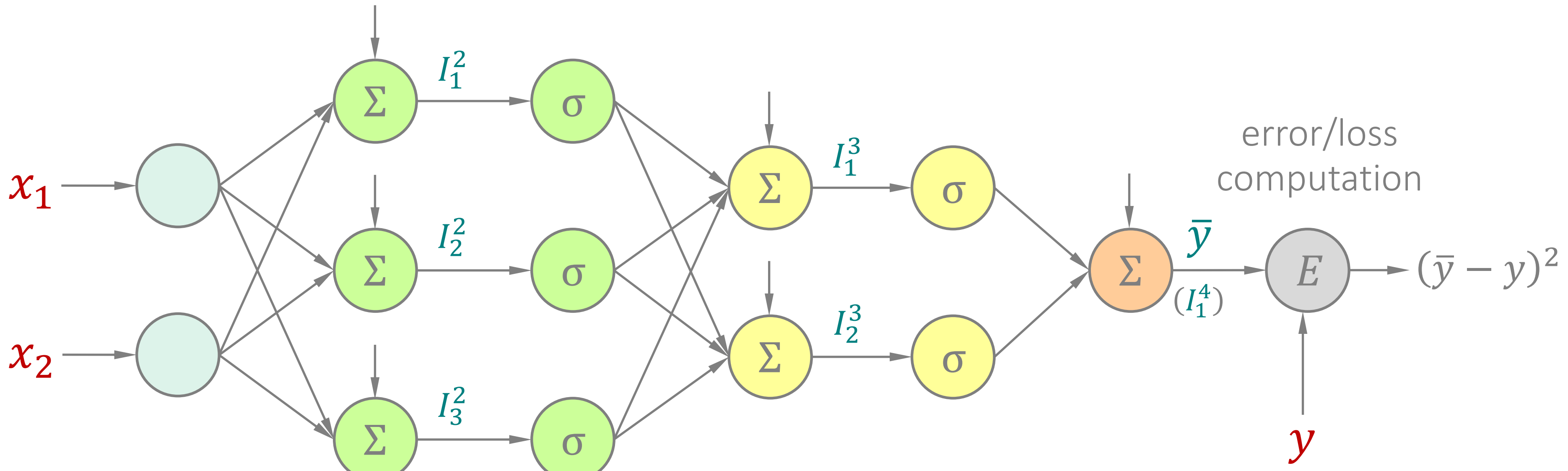


2 x 3 + 3	+	3 x 2 + 2	+	2 x 1 + 1	=
9	+	8	+	3	=
20 trainable parameters/weights					

backpropagation

case study: fully connected network with 3 layers

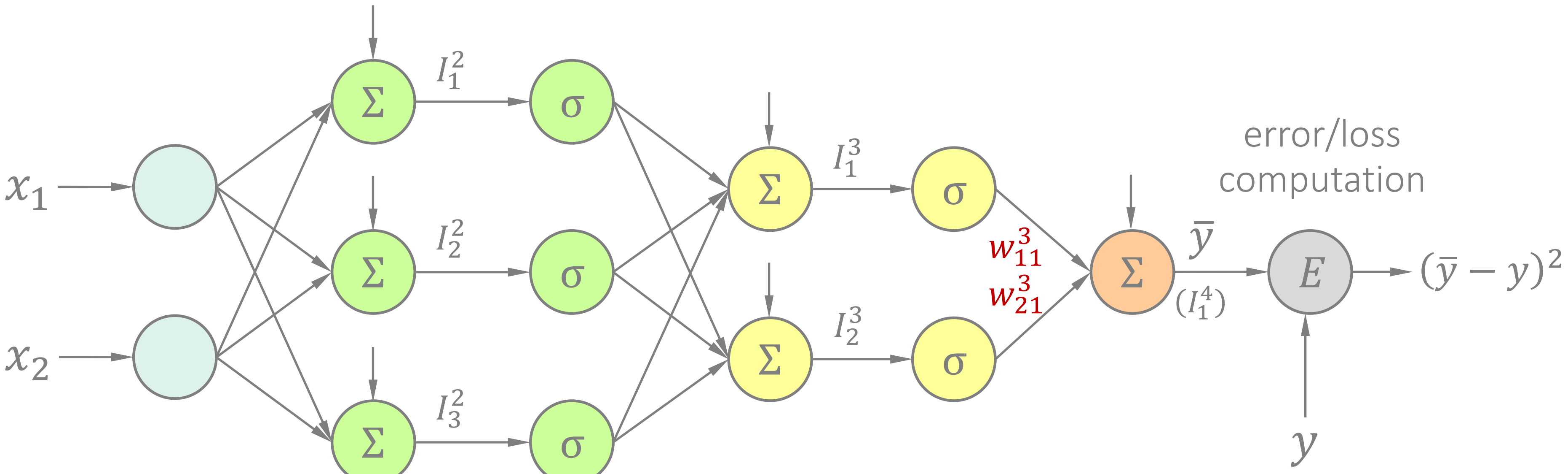
forward execution: introduce (x, y) and compute I_i^l and $\bar{y}$



backpropagation

case study: fully connected network with 3 layers

backward execution: compute gradients $\frac{\partial E}{\partial w_{ij}^{l}}$

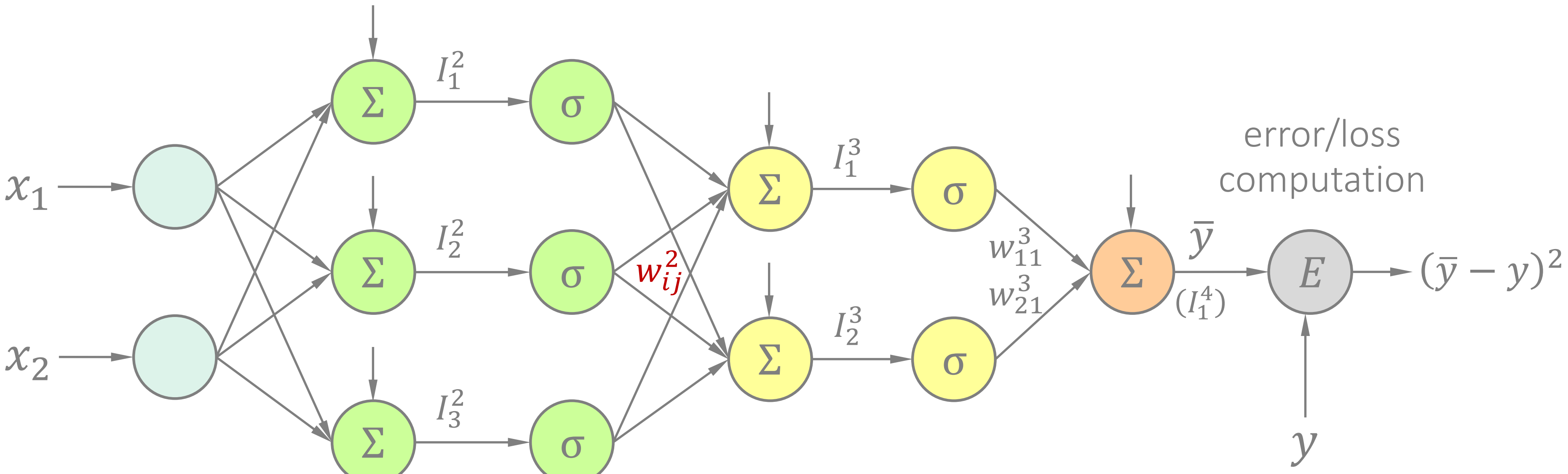


$$\frac{\partial E}{\partial w_{ij}^{3}} = \frac{\partial I_1^4}{\partial w_{ij}^{3}} \cdot \delta_1^4 = \sigma\left(I_i^3\right) \cdot 2(\bar{y} - y)$$

backpropagation

case study: fully connected network with 3 layers

backward execution: compute gradients $\frac{\partial E}{\partial w_{ij}^{l}}$

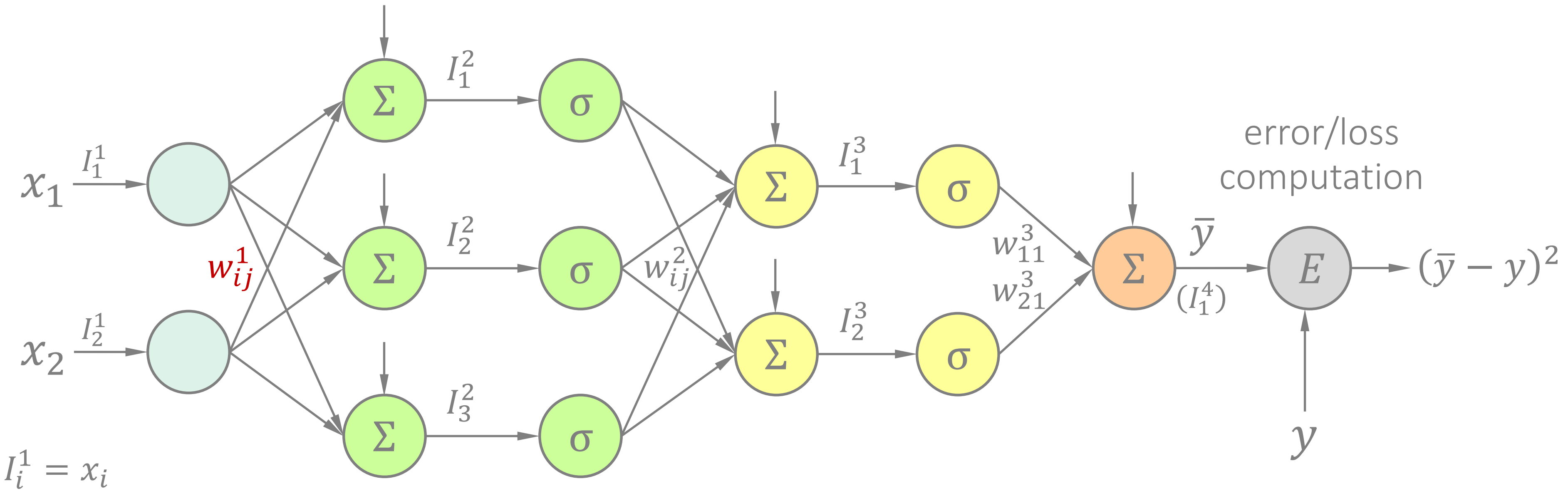


$$\frac{\partial E}{\partial w_{ij}^2} = \frac{\partial I_j^3}{\partial w_{ij}^2} \cdot \delta_j^3 = \sigma\left(I_i^2\right) \cdot \sigma'\left(I_j^3\right) \cdot w_{j1}^3 \cdot \delta_1^4$$

backpropagation

case study: fully connected network with 3 layers

backward execution: compute gradients $\frac{\partial E}{\partial w_{ij}^{l}}$



$$\frac{\partial E}{\partial w_{ij}^1} = \frac{\partial I_j^2}{\partial w_{ij}^1} \cdot \delta_j^2 = \sigma\left(I_i^1\right) \cdot \sigma'\left(I_j^2\right) \sum_{k=1}^{2} w_{jk}^2 \cdot \delta_k^3$$

case study

fully connected neural network for the MNIST digits task

implementation in Keras

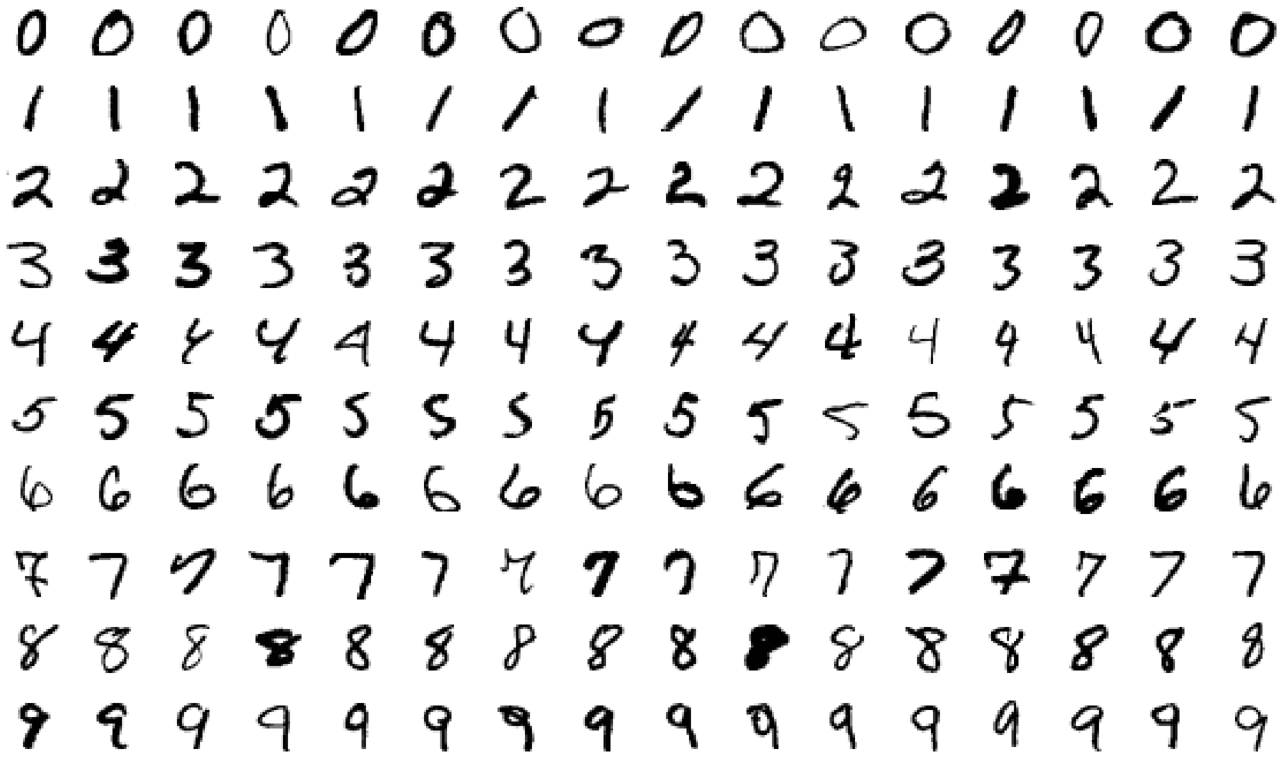
- deep learning framework: Python library for creating neural networks
- high-level interface based on Tensorflow, Theano, or the Microsoft Cognitive Toolkit
- it allows defining and assembling pieces in neural networks such as layers, objective functions, activation, optimizers, etc.

case study

fully connected neural network for the MNIST digits task

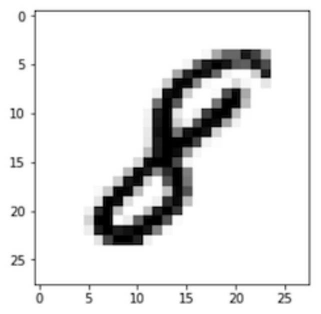
MNIST (Modified National Institute of Standards and Technology database)

handwritten digits image collection (official website)



Source: Wikipedia (+)

- 60,000 training images
- 10,000 test images
- 10 classes
- image size: 28x28
- grey images



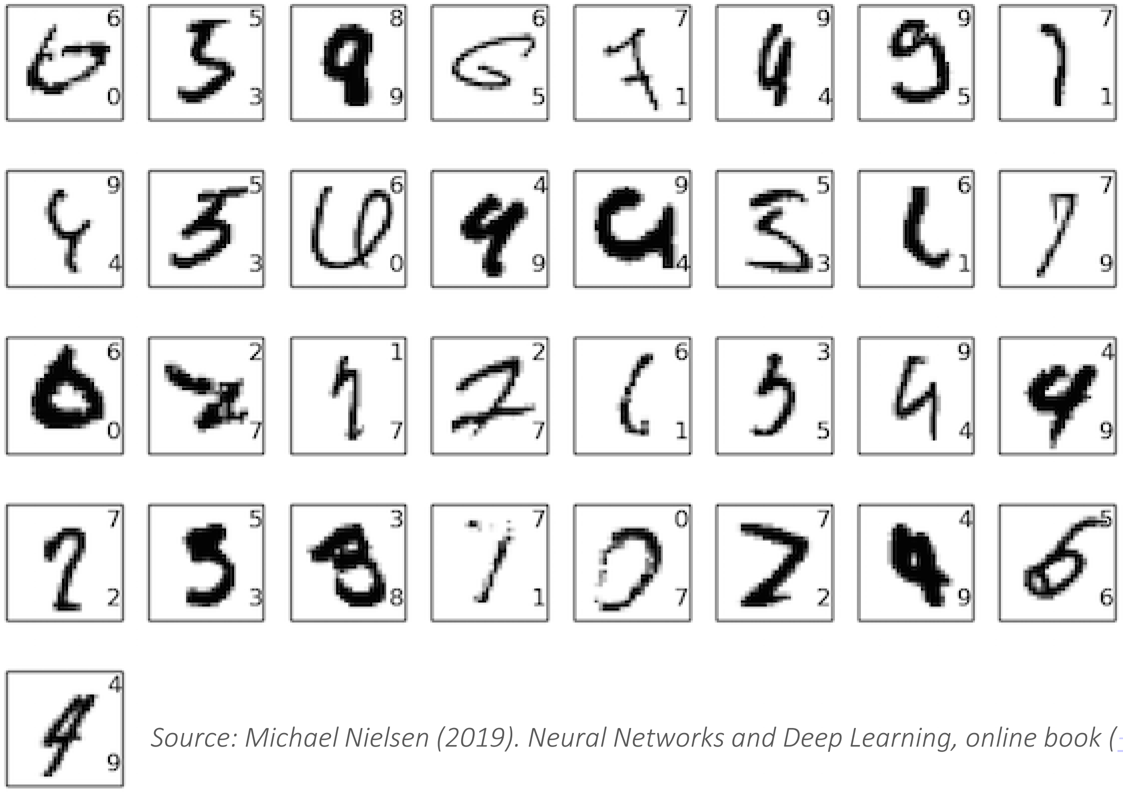
Source: Medium (+)

case study

fully connected neural network for the MNIST digits task

MNIST (Modified National Institute of Standards and Technology database)

- relatively simple task
- although it includes complex cases that are difficult to read (noise)



33 test errors with CNN

- 33 errors + 9,967 hits
- true class at top right
- estimated class at bottom right
- error rate = 0.33%

Source: Michael Nielsen (2019). Neural Networks and Deep Learning, online book (+).

case study

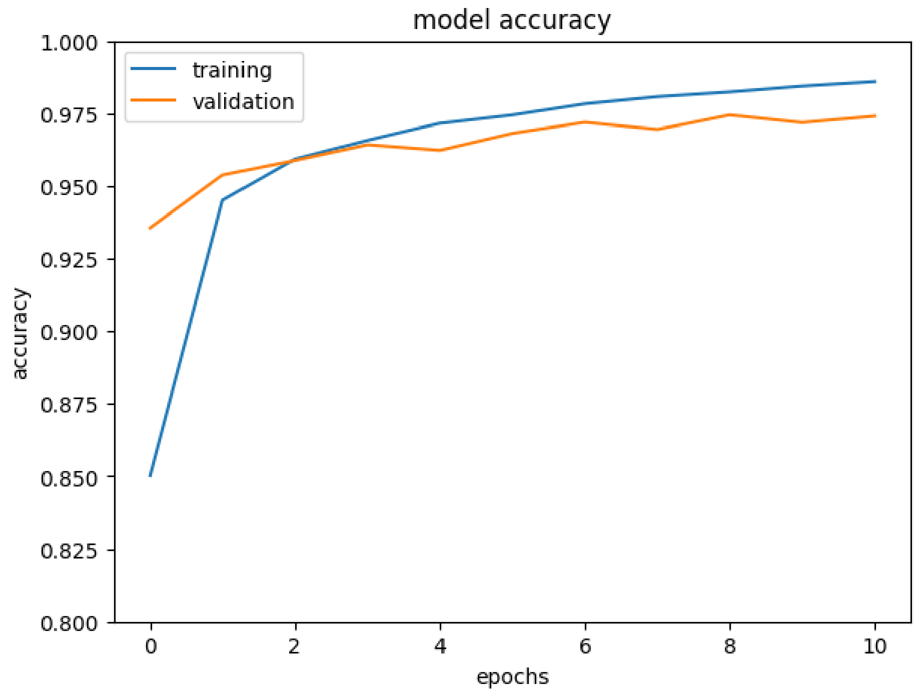
fully connected neural network for the MNIST digits task

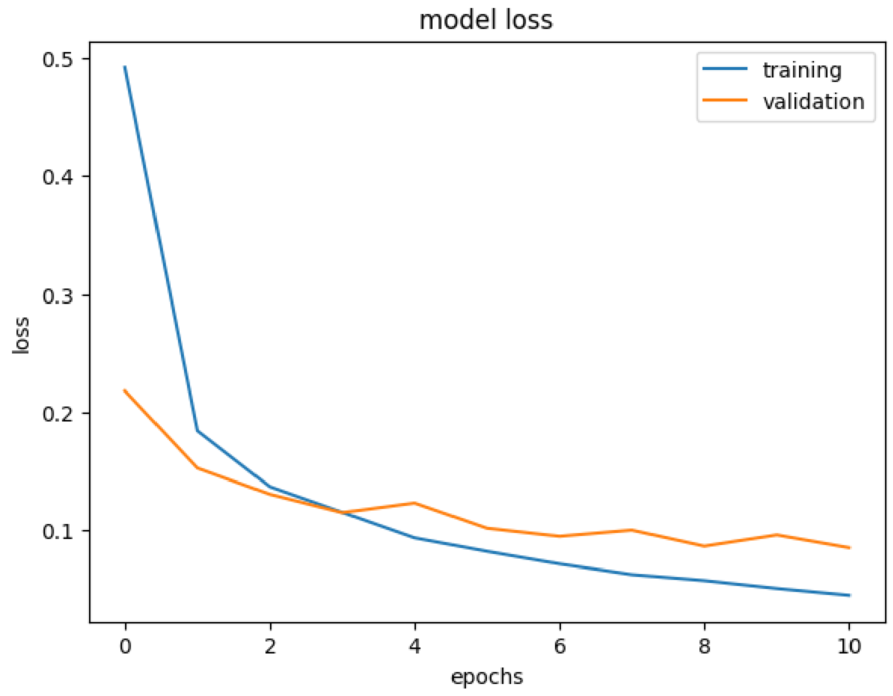
simplified script

```
(x_train, y_train), (x_test, y_test) = mnist.load_data()
x_train = x_train.reshape(60000, 784).astype('float32')/255
x_val = x_test.reshape(10000, 784).astype('float32')/255
y_train = keras.utils.to_categorical(y_train, num_classes)
y_val = keras.utils.to_categorical(y_test, num_classes)

model = Sequential()
model.add(Dense(64, activation='relu', input_shape=(784,)))
model.add(Dense(64, activation='relu'))
model.add(Dense(64, activation='relu'))
model.add(Dense(64, activation='softmax'))

sgd=SGD(lr=0.01, decay=1e-6, momentum=0.9)
model.compile(loss='categorical_crossentropy', optimizer=sgd, metrics=['accuracy'])
history = model.fit( x_train, y_train, batch_size=100, epochs=10, validation_data=(x_val, y_val))
```

case study

fully connected neural network for the MNIST digits task





case study

fully connected neural network for the MNIST task

How many parameters does this fully connected network have?

case study

fully connected neural network for the MNIST task

layers	input	hidden 1	hidden 2	hidden 3	output	TOTAL
units	784	64	64	64	10	202
weights		50,176	4,096	4,096	640	59,008
bias		64	64	64	10	202
TOTAL		50,240	4,160	4,160	650	59,210

case study

fully connected neural network for the MNIST task

hyperparameters

```
(x_train, y_train), (x_test, y_test) = mnist.load_data()
x_train = x_train.reshape(60000, 784).astype('float32')/255
x_test = x_test.reshape(10000, 784).astype('float32')/255
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model.add(Dense(64, activation='relu'))
model.add(Dense(10, activation='softmax'))

sgd=SGD(lr=0.01, momentum=0.9)
model.compile(loss='categorical_crossentropy', optimizer=sgd, metrics=['accuracy’])
history = model.fit(  x_train, y_train, batch_size=100, epochs=10, validation_data=(x_val, y_val))
```

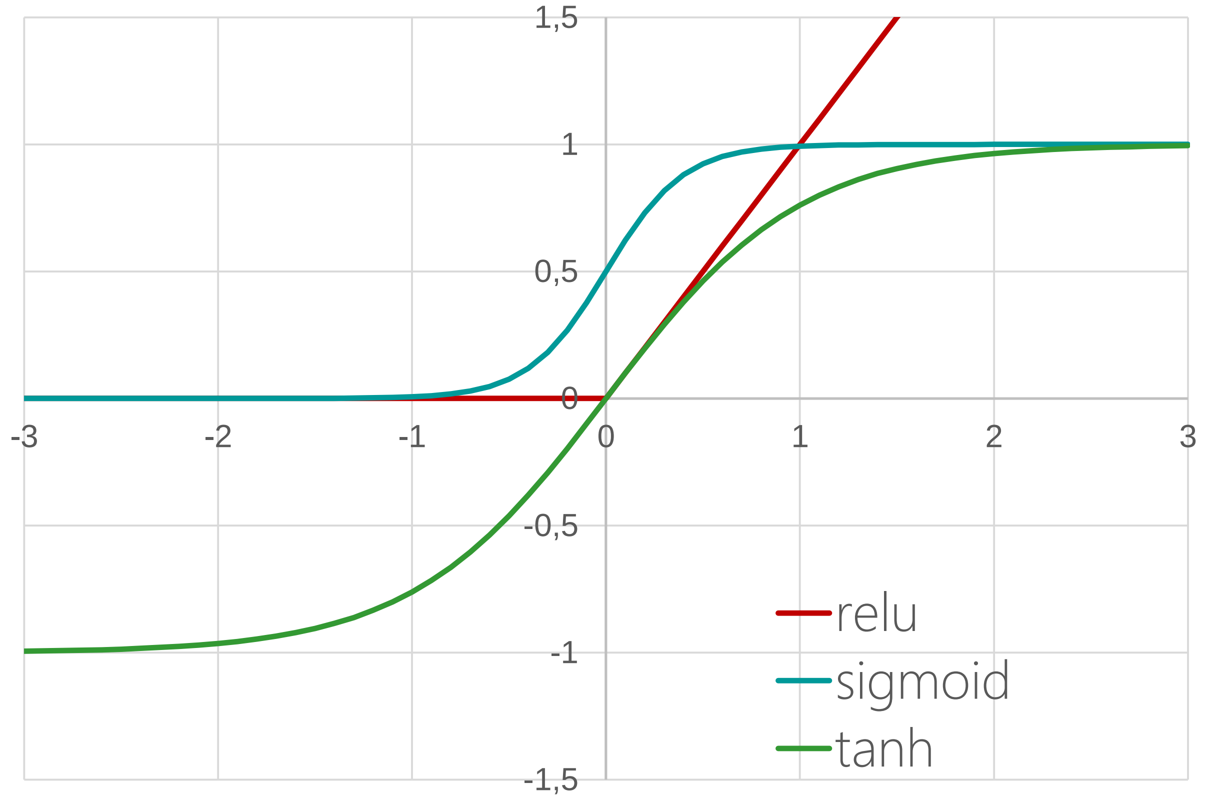
case study

fully connected neural network for the MNIST task

activation	'relu'	• Rectified Linear Unit (ReLU) • a piecewise linear activation function (hidden u)
activation	'softmax'	• output layer activation function • probability distribution over K outputs
loss	'categorical_crossentropy'	• one-hot vector + softmax + cross entropy • loss function • measures discrepancy between two distributions
optimizer	'sgd'	• stochastic gradient descent • basic optimization method
batch_size	100	• mini-batch based training • stochastic method (random subsets) • weights update after each batch
epochs	5	• learning loop over all training samples

activation function

relu, sigmoid, tanh



relu

$$g(z) = max\{0, z\}$$

sigmoid

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

tanh

$$g(z) = 2\sigma(2z) - 1$$

activation function

softmax (normalized exponential function)

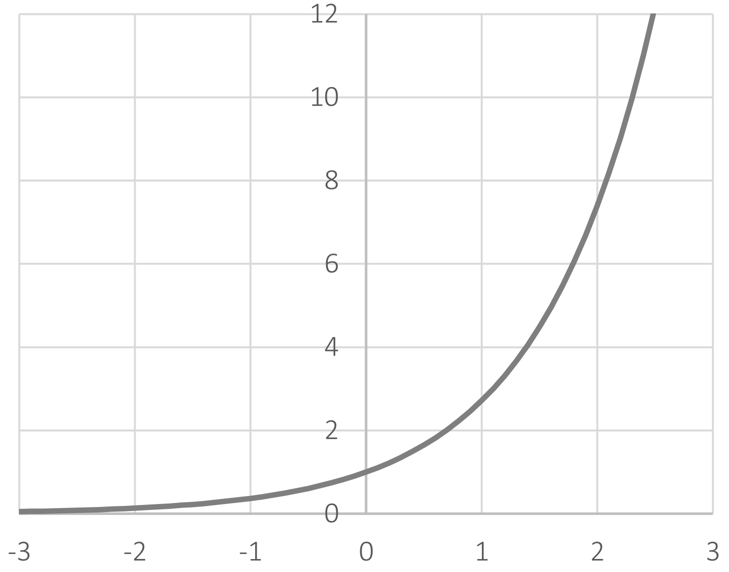
given a vector $z \in \mathbb{R}^K$

softmax projects a vector of real data onto a “probability distribution”

$$s: \mathbb{R}^K \to [0,1]^K, \quad \sum_i s(z)_i = 1$$

formulation:

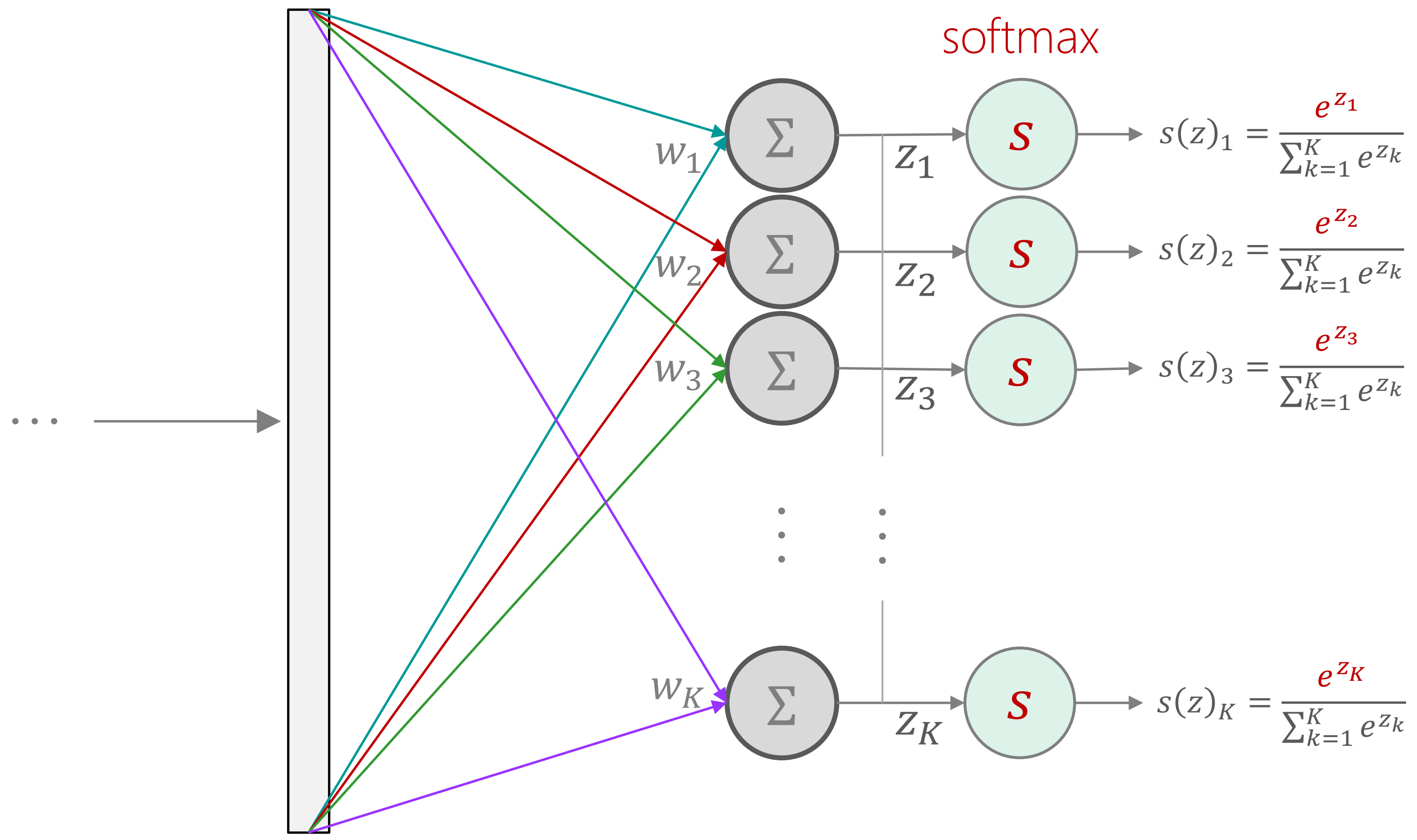
$$s(z)_i = \frac{e^{z_i}}{\sum_{k=1}^{K} e^{z_k}}$$



e^x

activation function

softmax (normalized exponential function)



softmax
w_1
w_2
w_3
w_K
Σ
z_1
z_2
z_3
z_K
s
$s(z)_1 = \frac{e^{z_1}}{\sum_{k=1}^{K} e^{z_k}}$
$s(z)_2 = \frac{e^{z_2}}{\sum_{k=1}^{K} e^{z_k}}$
$s(z)_3 = \frac{e^{z_3}}{\sum_{k=1}^{K} e^{z_k}}$
$s(z)_K = \frac{e^{z_K}}{\sum_{k=1}^{K} e^{z_k}}$

activation function

softmax (normalized exponential function)

softmax is increasing: if $z_i < z_j$, then $s(z_i) < s(z_j)$

example

z_i	e^{z_i}	$s(z)_i$
-1	0,37	0,01
0	1,00	0,02
1	2,72	0,04
2	7,39	0,11
4	54,60	0,83
	66,07	1,00

penalizes non-maximum activation values

reinforces the highest activation value

activation function

softmax (normalized exponential function)

softmax saturates if $min_i z_i \ll max_i z_i$

example

z_i	e^{z_i}	$s(z)_i$
-1	0,37	0,00
0	1,00	0,00
1	2,72	0,00
2	7,39	0,00
8	2.980,96	1,00
	2.992,43	1,00

$\leftarrow$ the winner takes it all

loss function

operating principle

given

- y, expectation (ground truth)
- $\hat{y}$, prediction, estimation

a los/cost/error function $L(y, \hat{y})$

- measures the distance, difference, or discrepancy between y e $\hat{y}$
- when y e $\hat{y}$ are very different, then L is large (high loss)
- when y e $\hat{y}$ are very similar, then L is small (low loss)
- when y e $\hat{y}$ are equal, then $L = 0$

learning objective

- find parameters of the model that minimize L over the validation set (part of the training data, not the test data!)

loss function

one-hot encoding (output encoding)

categorical/nominal variable: takes symbolic values, not numeric ones.

examples:

- pet: "dog", "cat", "bird"
- model: "sedan", "minivan", "bus", "truck"
- dígitos: '0', '1', '2', …'9'

limitation: do not support numerical comparisons/operations

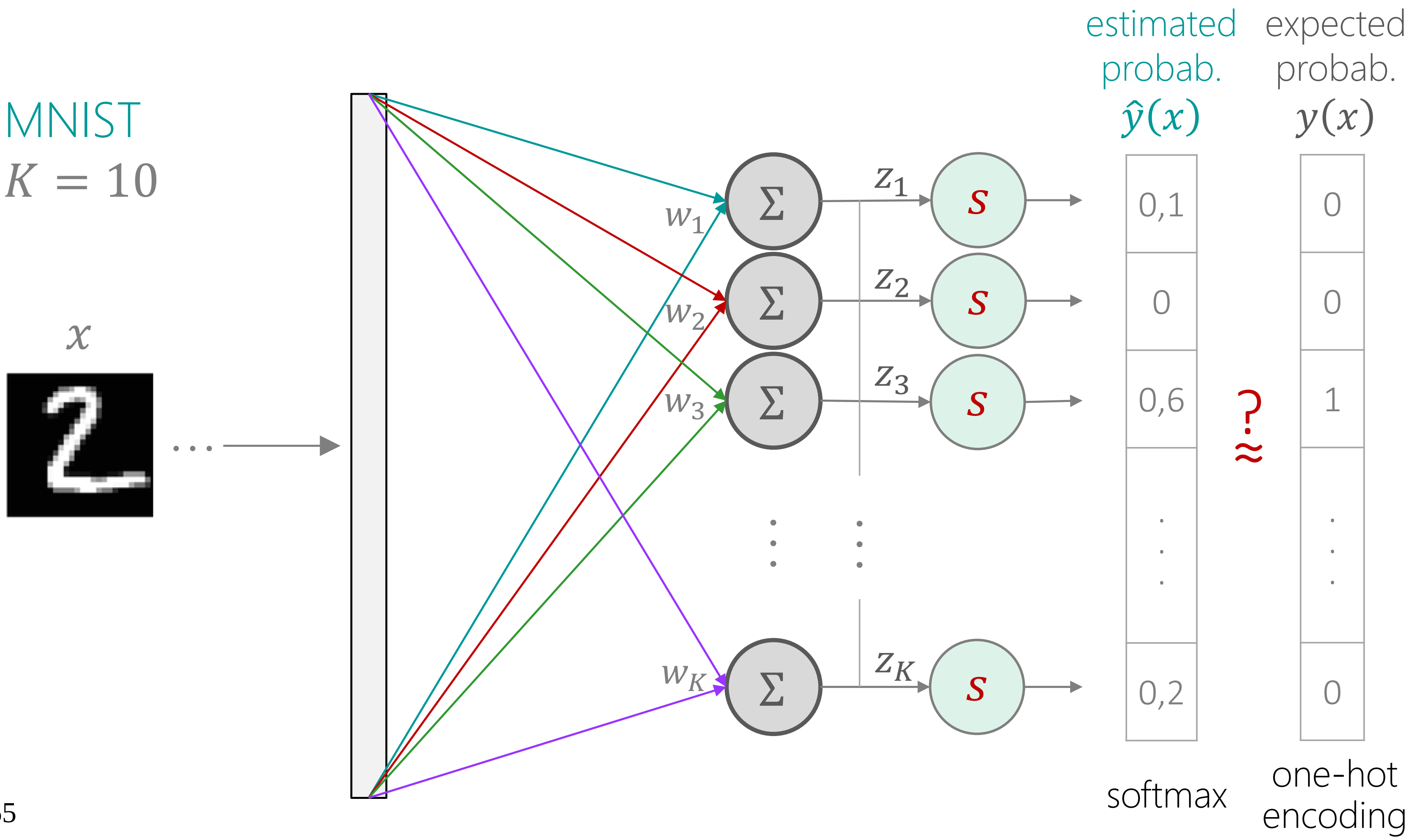
one-hot encoding:

	sedan	minivan	bus	truck
x_{sed}	1	0	0	0
x_{min}	0	1	0	0
x_{bus}	0	0	1	0
x_{tru}	0	0	0	1

loss function

how to measure the difference between two distributions?

MNIST
$K = 10$



loss function

categorical cross entropy

given two probability distributions:

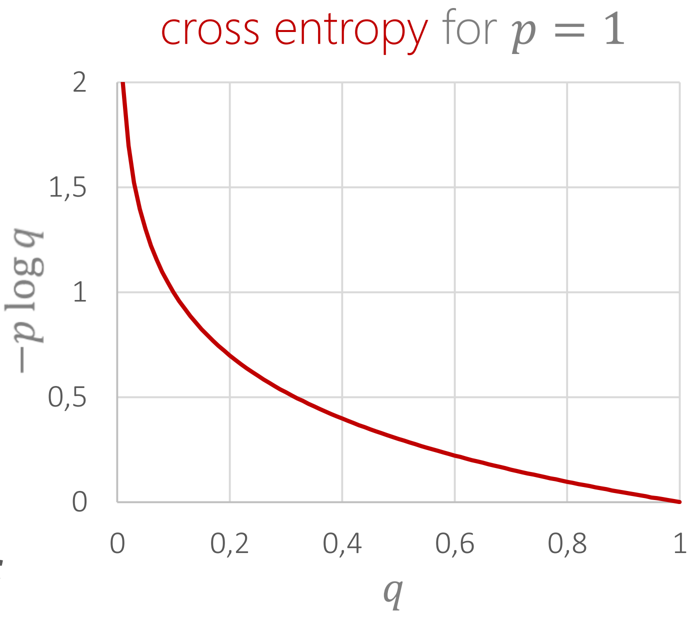
- y (e.g. expected, ground truth)
- $\hat{y}$ (e.g. predicted, observed)

cross entropy (single sample):

$$E(y, \hat{y}) = -\sum_i y_i \log \widehat{y_i} = -\log \widehat{y_c}$$

effect:

- $\widehat{y_c}$ is the model's prediction for the correct class c
- if y and $\hat{y}$ are similar, then $E(y, \hat{y})$ is small
- if y and $\hat{y}$ are different, then $E(y, \hat{y})$ is large



loss function

categorical cross entropy

two opposite scenarios

favorable scenario

y	$\hat{y}$	$-y_i \log \hat{y}_i$
0	0,05	0,00
0	0,05	0,00
1	0,80	0,10
0	0,05	0,00
0	0,05	0,00
	loss	0,10

<u>un</u>favorable scenario

y	$\hat{y}$	$-y_i \log \hat{y}_i$
0	0,20	0,00
0	0,20	0,00
1	0,20	0,70
0	0,20	0,00
0	0,20	0,00
	loss	0,70

only the $\hat{y}_i$ associated with $y_i = 1$ contributes (-$\log 1$ is the smallest loss)

loss function

can we pay more attention to minority classes?

what if classes are imbalanced?

- many more loss terms from the majority class than from the rest
- all the loss terms matter (wheigh) the same
- the majority class examples dominate the loss function
- the majority class examples dominate gradient propagation
- more model weight updates to favor the majority class
- the model will be more confident in predicting the majority class
- little emphasis on minority classes
- summary: biased classifier learning

loss function
balanced cross entropy

given two probability distributions and…

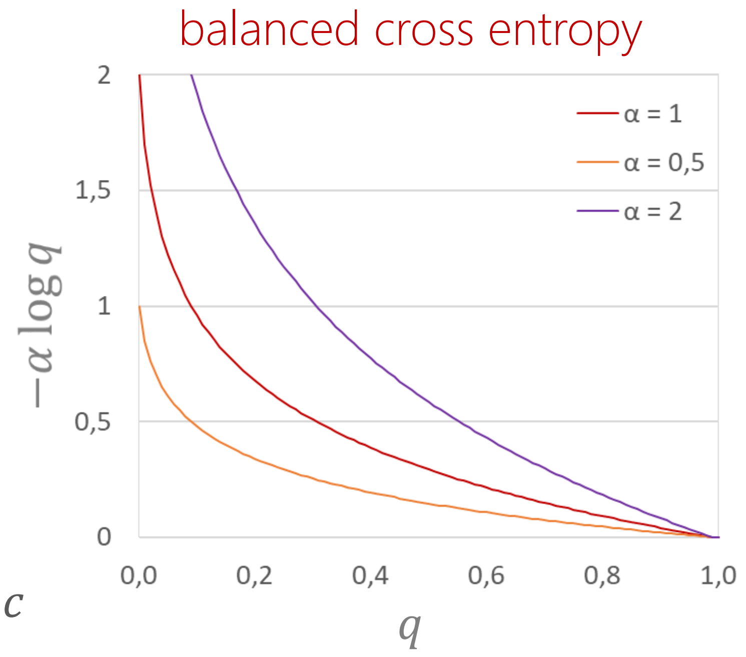
- y (e.g. expected, ground truth)
- $\hat{y}$ (e.g. predicted, observed)

balanced cross entropy (single sample):

$$E(y, \hat{y}) = -\alpha_c \log \hat{y_c}$$

comments:

- $\hat{y_c}$ is the model's prediction for the correct class c
- α_c is a class weight related to class c
- α_c is inversely proportional to the frequency of class c



loss function

balanced cross entropy

how to compute class weights?

- by hyperparameter tuning
- by compute_class_weight from sklearn.utils

$$\propto_i = \frac{n}{k \cdot n_i}$$

where:

- n is the total number of training simples
- n_i is the number of training samples of class i
- k is the number of classes

loss function

paying more attention to hard-to-classify examples

how to improve predictions on hard examples

- hard examples = samples classified with less confidence
- strategy: guide learning to focus more on hard examples
- side effect: natural mitigation of biases from imbalanced classes
  - examples from the majority class are usually easy to predict
  - examples from the minority class are usually hard to predict
  - examples from the majority class dominate loss & gradients

loss function

focal cross entropy

given two probability distributions

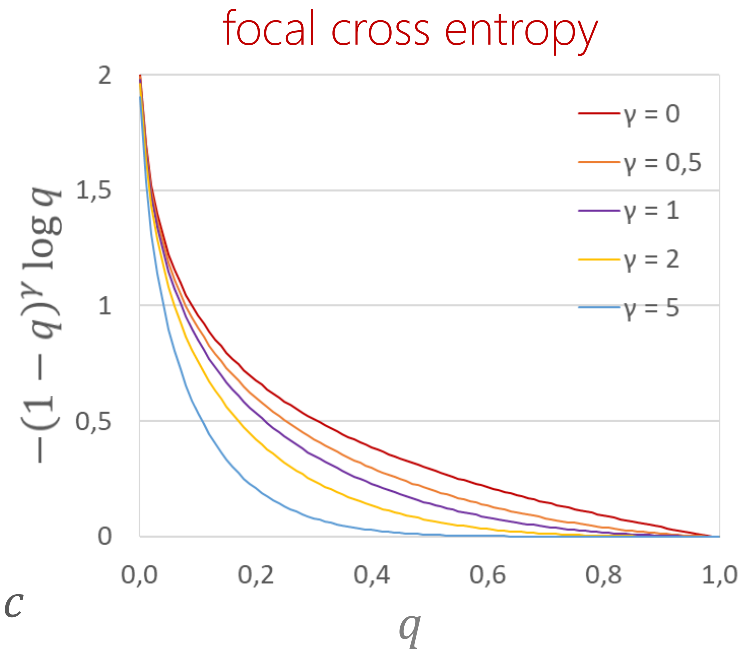
- y (e.g. expected, ground truth)
- $\hat{y}$ (e.g. predicted, observed)

focal cross entropy (for a single sample):

$$E(y, \hat{y}) = -(1 - \widehat{y_c})^{\gamma} \log \widehat{y_c}$$

where:

- $\widehat{y_c}$ is the model's prediction for the correct class c
- γ: focal factor (hyperparameter)
- γ reduces the contribution of easy examples to the total loss
- typical values for γ range from 1 to 5



loss function

focal cross entropy

how focal loss works?

- when a sample is misclassified (hard examples)…
  - $\hat{y_c}$ is small => the modulating factor $(1 - \hat{y_c})^\gamma$ is close to 1
  - the loss term keeps unaffected (it behaves as in cross entropy loss)
- when a sample is correctly classified (easy examples)…
  - $\hat{y_c}$ is close to 1 => the modulating factor $(1 - \hat{y_c})^\gamma$ is close to 0
  - the loss term is down weighted, reducing its impact on the loss function
- γ adjusts the rate at which easy examples are down-weighted
- $\gamma = 0$ reduces focal loss to standard cross entropy
- higher values of γ encourage the model to focus on harder examples

loss function

focal cross entropy

α-balanced focal loss (single sample):

$$E(y, \hat{y}) = -\alpha_c (1 - \widehat{y_c})^{\gamma} \log \widehat{y_c}$$

comments:

- typical implementation of focal loss
- it usually leads to better results than the unbalanced version.

optimization problem

MNIST dataset

given 60.000 training digit images, with their classes annotated as one-hot vectors…

$$T = \{(x_i, y_i)\}_{i=\overline{1,60.000}} \text{ such that } x_i \in [0,1]^{784},\ \ y_i \in \{0,1\}^{10}$$

goal: to find optimal values for the 2.913.920 model parameters

$$W^* = \arg\min_W L(W), \quad W \in \mathbb{R}^{2.913.920}$$

with $L(W)$ being the loss function defined as follows:

$$L(W) = \frac{1}{60.000} \sum_{i=1}^{60.000} E(y_i, \hat{y}_i) = -\frac{1}{60.000} \sum_{i=1}^{60.000} \sum_{j=1}^{10} y_{ij} \log \hat{y}_{ij}$$

optimizer

sgd + momentum + weight decay

stochastic gradient descent (sgd):

$$\theta_{t+1} = \theta_t - \gamma \frac{\partial L}{\partial \theta}(\theta_t)$$

sgd + momentum + weight decay (γ denotes the learning rate):

$$\theta_{t+1} = \theta_t + v_t$$

$$v_t = momentum \cdot v_{t-1} - \gamma \frac{\partial L}{\partial \theta}(\theta_t)$$

$$\gamma = \gamma \cdot \frac{1}{1 + decay \cdot iteración}$$

hyperparameters
overview

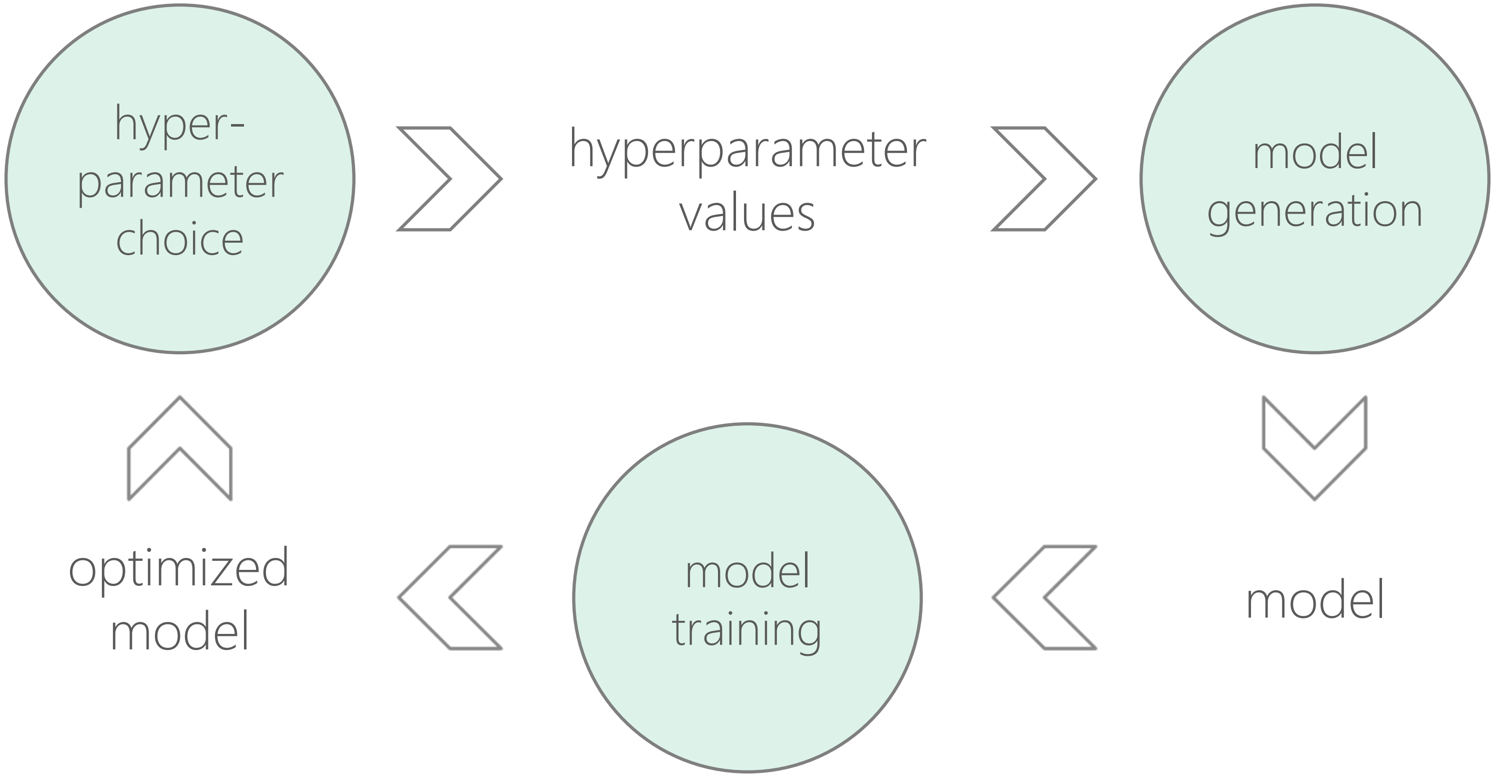
hyperparameters are parameters needed to generate the model or to define the training process

hyperparameters determine the structure or configuration of the model or characteristics of the learning process; their values are chosen before each training session.

their optimal values depend on the complexity of the task, the nature of the data (dimensionality, distribution, quantity, etc.), and the interdependence with other hyperparameters.

hyperparameters

overview



hyperparameters

fully connected neural network for the MNIST task

hyperparameters of the network architecture defined for MNIST:

- 4 trainable layers
- layer 1: 1024 units, ReLU activation
- layer 1: 1024 units, ReLU activation
- layer 1: 1024 units, ReLU activation
- layer 4: softmax activation

hyperparameters

fully connected neural network for the MNIST task

hyperparameters of the learning process defined for MNIST:

- optimizer: SGD(lr=0.01, decay=1e-6, momentum=0.9)
- loss = 'categorical_crossentropy'
- batch_size = 100
- epochs = 5

summary

- a machine learning algorithm optimizes models from data
- a linear model solves only tasks with linear boundaries
- Perceptron is a linear model of binary classification
- a fully connected multilayer network is composed of a sequence of fully connected layers.
- each unit consists of a linear function + nonlinear activation
- a multilayer network could learn any decision boundary
- backpropagation is an algorithm for training feedforward networks in supervised learning; includes calculation of gradients, not how to use them.