Neural networks I: Perceptron

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Outline

- Representation learning
- Introduction to neural networks
- Perceptron
- Multilayer perceptron

Representation learning

“yes”

“no”

Example: Text representation

- How to represent the main idea of a text?
- Simple option: “bag of words”
  - Vector representing word frequencies
  - Values within the vector represent word count
  - Discards word order and context


intelligence
can
human
system
artificial
machine
used
systems
machines
humans
will
people
become
consider
reward
world
society
already
phase
like
way
intelligent
training
work
time
companies
Artificial
better
right
ways
many
individuals
instances
people
new
just
animals
cancer
tools
Google
capable
beings
create
learning
Intelligence
labour
attention
keep
might
whether
complex
input
mechanisms
majority
economy
consequences
examples
workforce
technology
Goostman
Silicon
families
self-driving
progress
adversaries
bring
aversion
weapons
Robot
happen
raters
trucks
well
created
frontier
video
software
Tech
service
building
robots
cognitive
wealth
point
advanced
opportunity
physical
suffering
example
happens
hourly
economic
think
games
bots
comes
ethical
genetic
performs
three
make
becomes
next
lives
jobs
faster
Musk
fooled
form
revenues
algorithms
company
negative
patterns
look
fair
Eugene
hand
bias
use
now
day
wrong
may
act
rely
still
using
often
headlines
learning
control
risk
even
end
see
one
question
Valley
similar
relationships
means
Alphabet
fewer
according
biggest
Elon


dive
species
operators
Marine
coral
site
diving
Reef
fish
sharks
sea
Bay
reef
Park
experience
diver
Island
Shoals
Rowley
Australia
Ningaloo
sites
trips
Port
Hole
underwater
Eric
Peninsula
Rock
might
you're
one
Flinders
Tasmania's
Australia's
says
can
dragon
Phillip
Cod
Lord
Fish
Rapid
waters
cage
located
check
world
day
website
Howe
Moreton
continental
adventure
rockcod
creatures
National
marine
Epinephelus
includes
encounter
Neptune
Several
southern
whales
Australian
South
Queensland
green
deep
just
north
Cape
found
depth
jetty
leafy
supports
qualified
Tasman
ocean
include
World
Rocks
close
turtles
rising
surface
moray
NSW
QLD
cave
around
much
way
find
temperate
November
home
information
option
often
new
two
runs
Dive
also
Heads
sizable
giant
West
Jetty
novice
Cave
eels
see
water
live-aboard
Heritage-listed
Islands
list
will

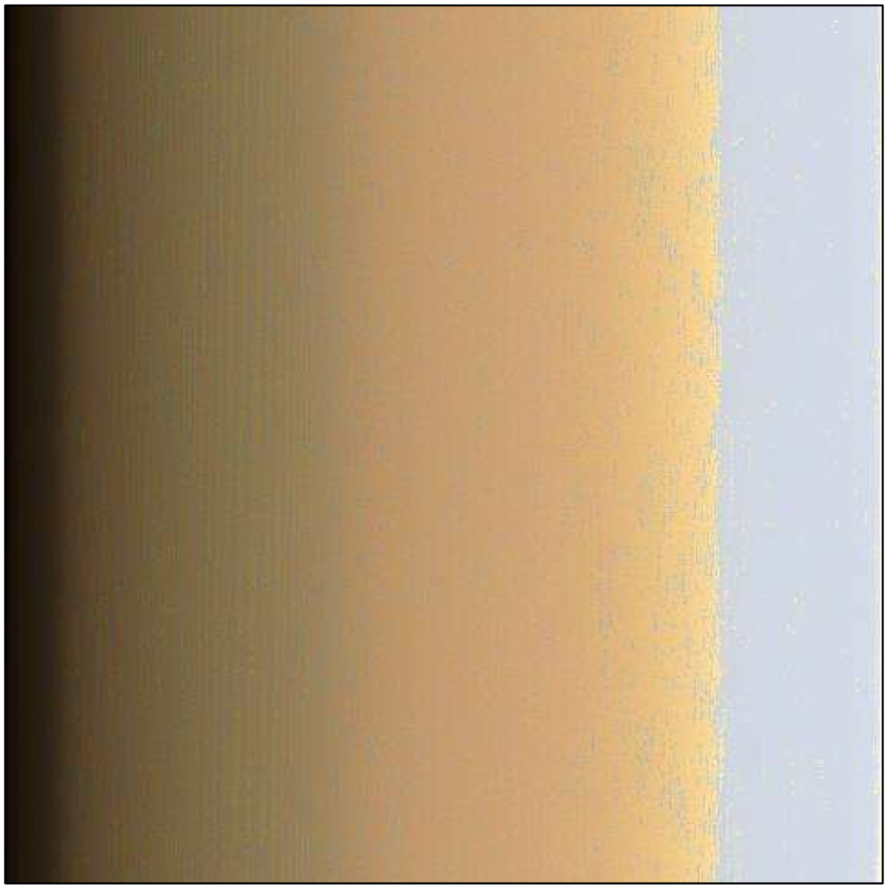
Example: Text representation

- “Bag of words” works quite well for many tasks
- Problems?
  - Missing context, order, understanding of synonyms and phrases
  - Curse of dimensionality -- “words” space is very high-dimensional (~170,000 words in English)

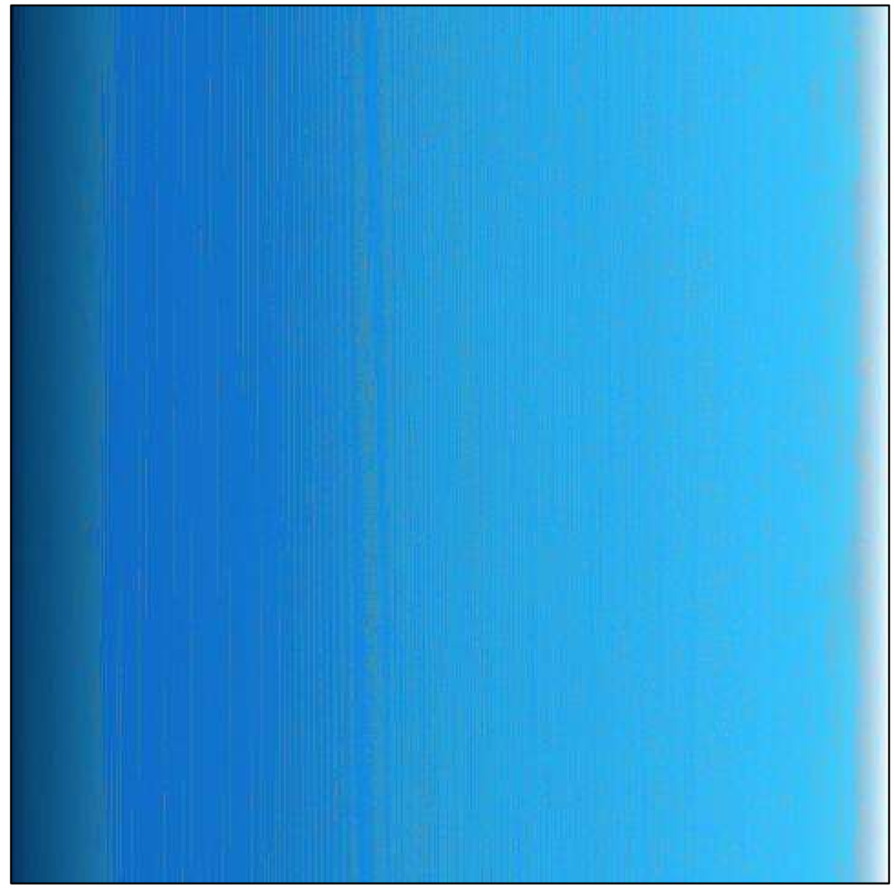
Example: Image representation

- How to represent the main idea of an image?
- Images are made up of pixel values, each pixel has an RGB value
- How much information can you get from “bags of pixels”?

Pixels



A



B

Example: Image representation

- Pixel-level representations can work for constrained tasks
- But more complex visual tasks require more complex features (shapes, objects)
  - How to define these?
- Curse of dimensionality – raw pixel space is very high-dimensional (~700,000 dimensions in the example images)

Representation learning in NNs

- Representation learning is a common application for neural networks
- Networks learn a feature hierarchy – from simple combinations of the input to more complex features (sometimes called **embeddings**)
- Embeddings are:
  - Low-dimensional representations of the input
  - Often useful for a range of tasks (not just the task on which the network was originally trained)

Introduction to neural networks

Convolutional neural network

"AlexNet": Krizhevsky, Sutskever, & Hinton (2012)

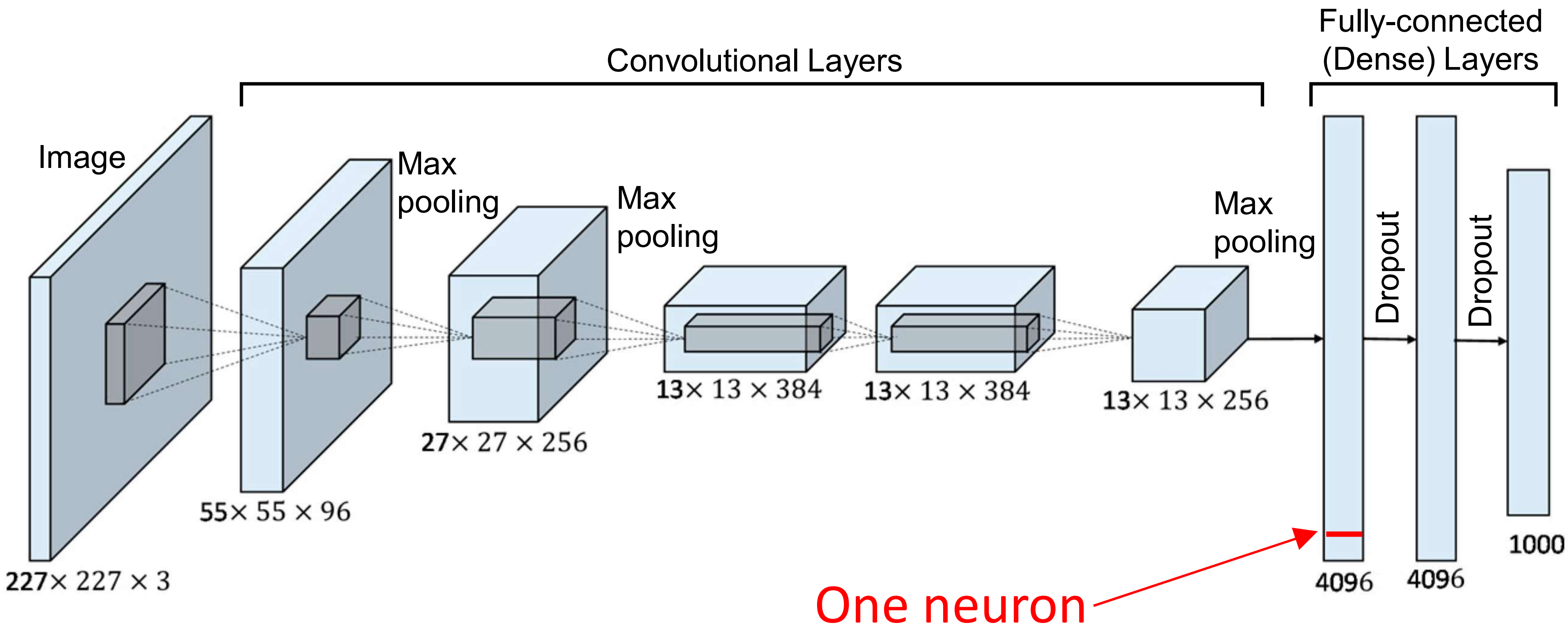


Image: Han, Zhong, Cao, & Zhang (2017)

Biological basis

- Hebbian learning (Hebb, 1949) – model for how neural connections change during learning
- "neurons wire together if they fire together" (Löwel & Singer, 1992)
- Over time, more weight on features associated with a target (like a class label), low weight on features not associated with the target

Biological neuron

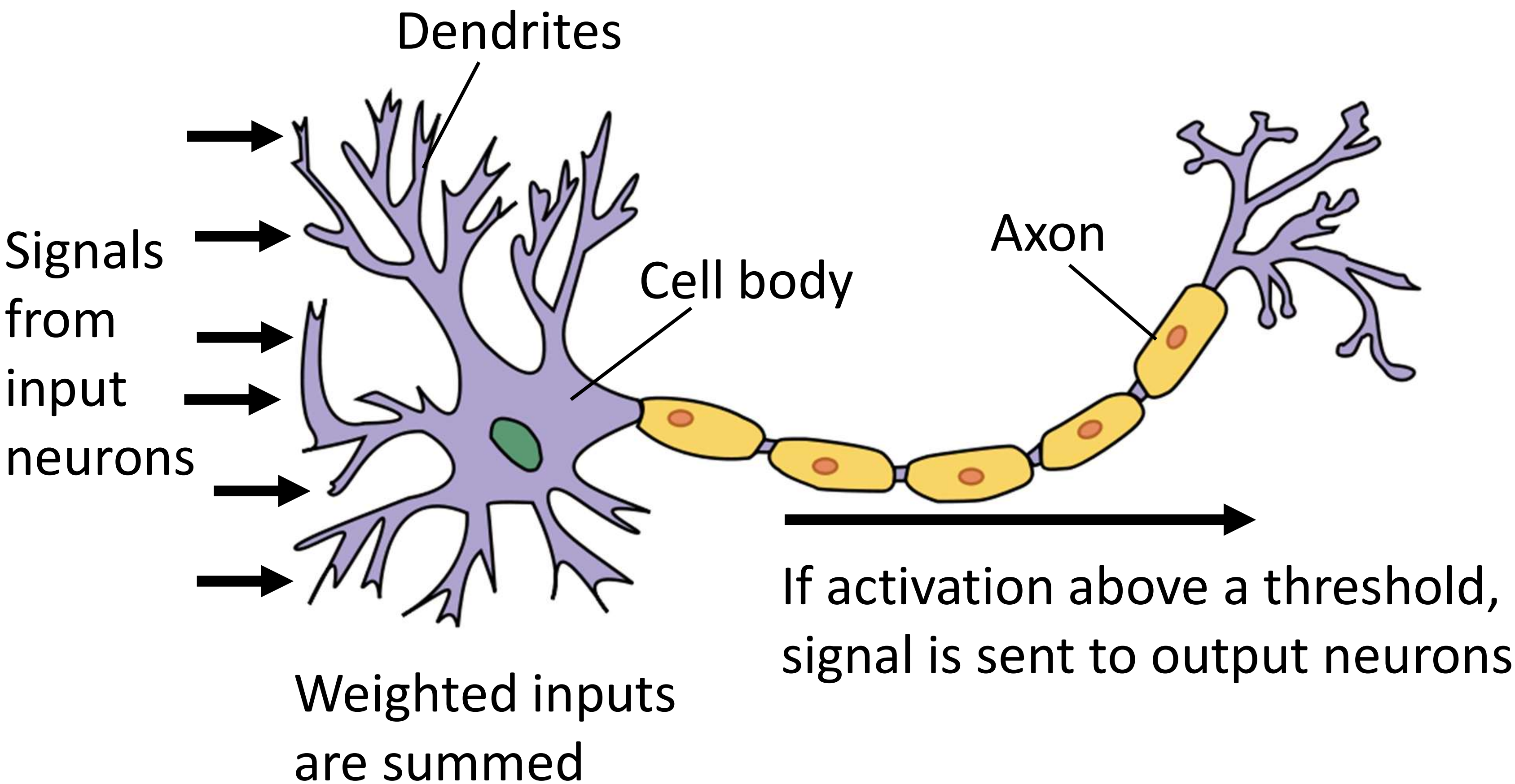
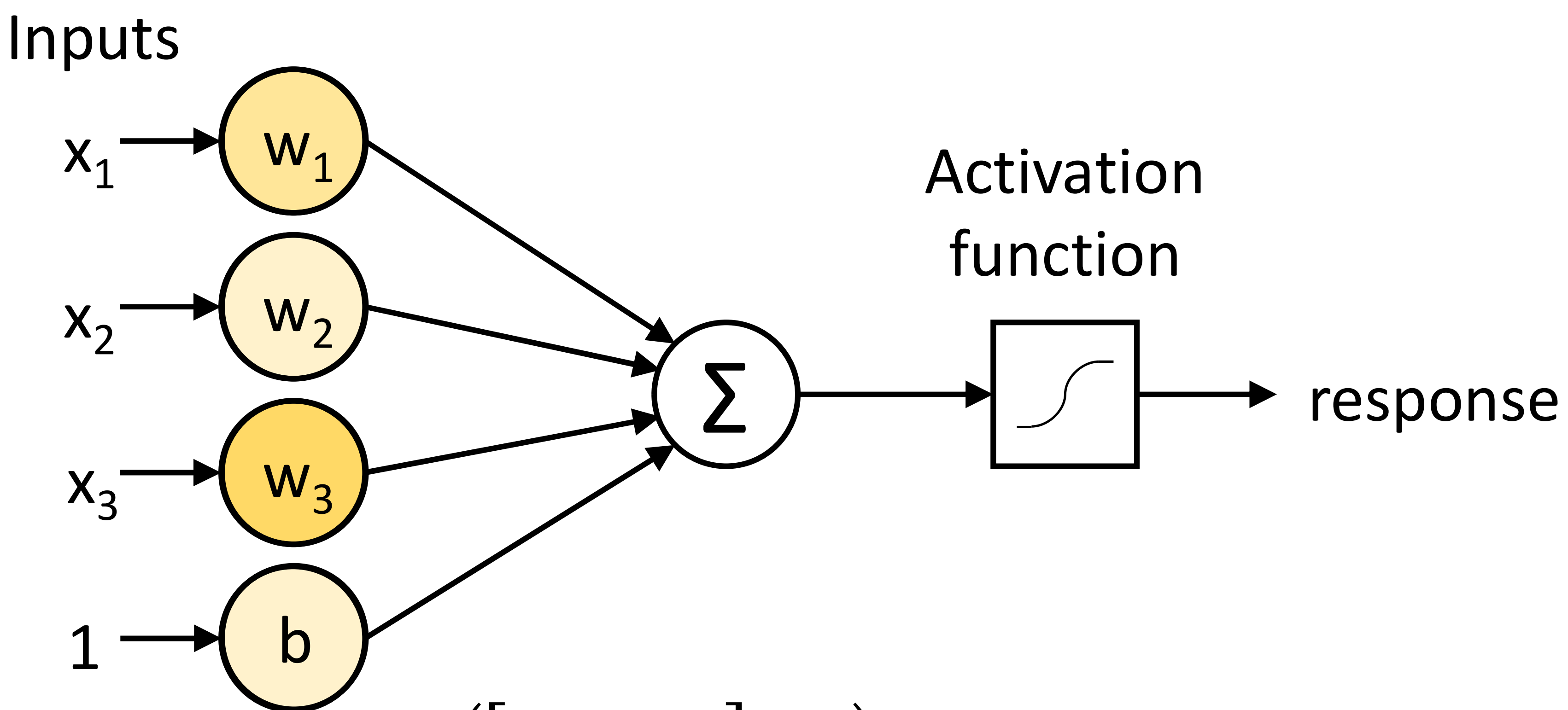


Image: *Anatomy and Physiology*, US National Cancer Institute SEER Program

Artificial neuron



$$y_i = f\left(\left[\sum_j w_j x_{ij}\right] + b\right) = f(\mathbf{w} \cdot \mathbf{x_i} + b)$$

Artificial neuron

- The basic unit of a neural network is the neuron, which is defined as follows:
  - input = a vector $\mathbf{x_i}$ ($\langle x_{i1}, x_{i2}, \ldots x_{in} \rangle \in \mathbb{R}^n$)
  - output = a scalar $y_i \in \mathbb{R}^n$
  - hyper-parameter: an activation function f
  - parameters: a vector of weights $\mathbf{w}$ ($\langle w_1, w_2, \ldots w_n \rangle \in \mathbb{R}^n$) plus a bias term b ($b \equiv w_0$)
- Mathematically:

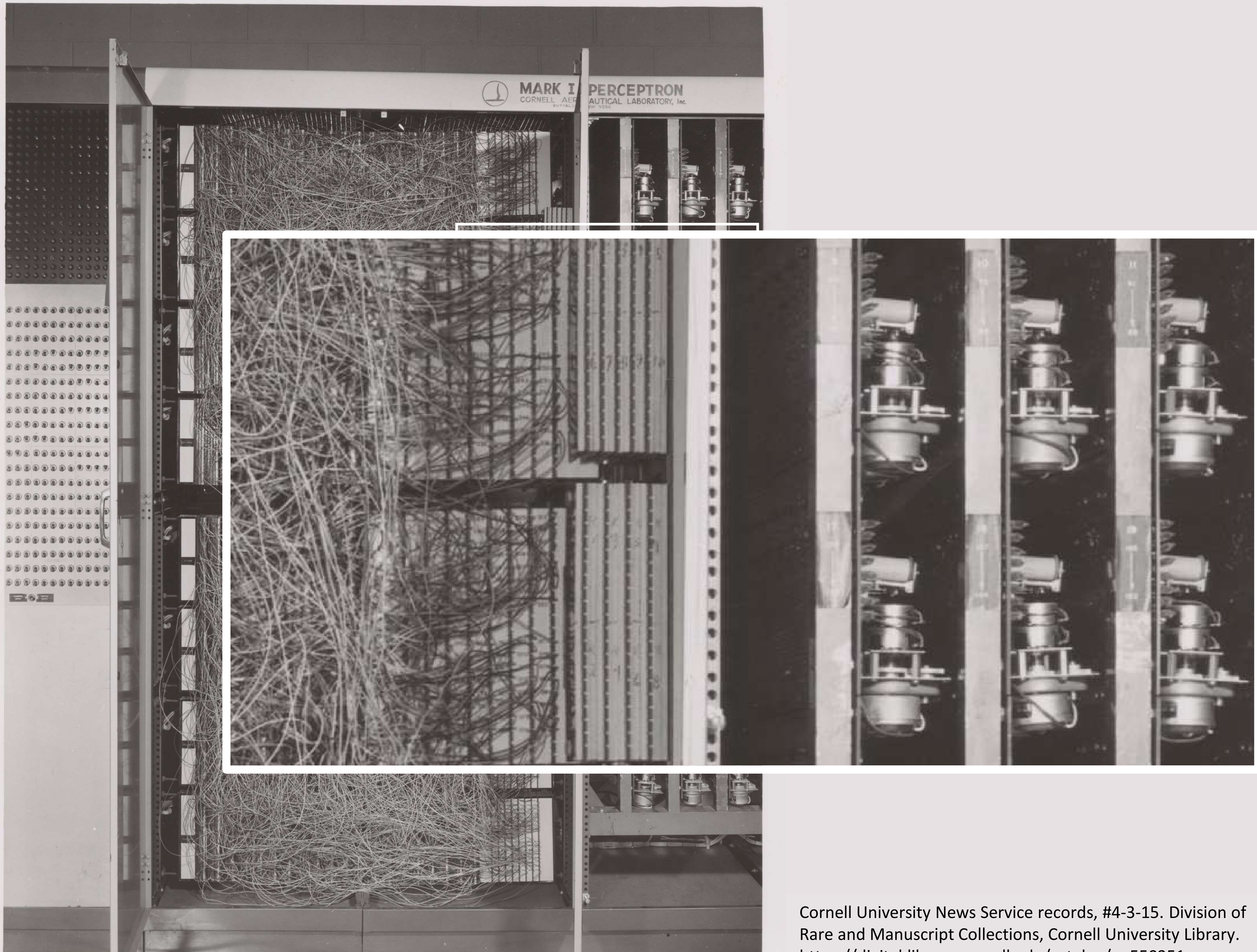
$$y_i = f\left(\left[\sum_j w_j x_{ij}\right] + b\right) = f(\mathbf{w} \cdot \mathbf{x_i} + b)$$

Perceptron

Perceptron

- Perceptron = a neural network with just a single neuron
- A perceptron is a binary linear classifier, which can be written as

$$f(\mathbf{w} \cdot \mathbf{x_i} + b) = \begin{cases} 1 & if\ \mathbf{w} \cdot \mathbf{x_i} + b \geq 0 \\ 0 & otherwise \end{cases}$$



Cornell University News Service records, #4-3-15. Division of Rare and Manuscript Collections, Cornell University Library. https://digital.library.cornell.edu/catalog/ss:550351

Training a perceptron

- Training a perceptron entails finding the weights $\mathbf{w}$ which minimize errors on the training data
- The classic way to train a perceptron is by iterating over examples in a training dataset. Each iteration over the whole dataset is called an **epoch**.
- Perceptron algorithm
  - For training examples, compute y based on current weights
  - Update weights based on the difference between predicted y and true label

Training a perceptron

Initialize weight vector $\mathbf{w}$ to random values

repeat

  for each training instance $(\mathbf{x_i}, y_i)$ **do**

    compute $\hat{y_i} = f(\mathbf{w} \cdot \mathbf{x_i} + b)$

    for each weight w_j **do**

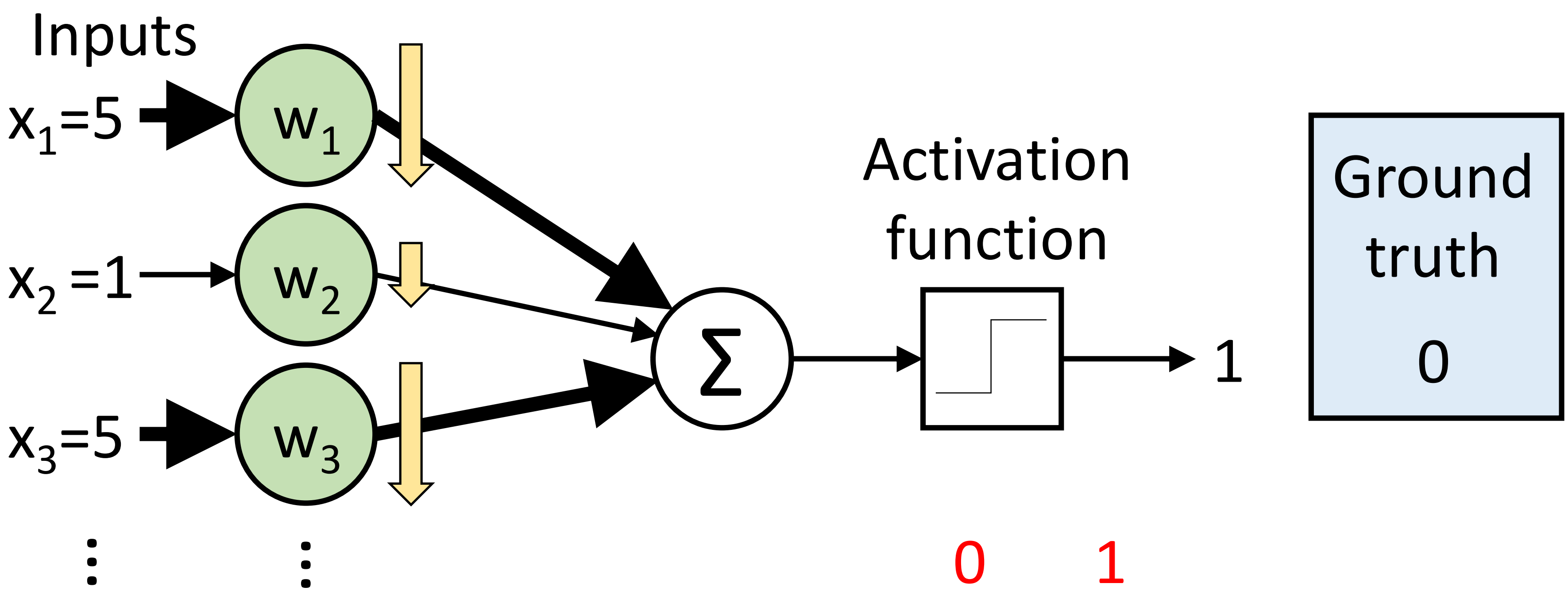
      update $w_j \leftarrow w_j + \underline{\lambda(y_i - \hat{y_i})}x_{ij}$

    end for

  end for

until stopping condition is met

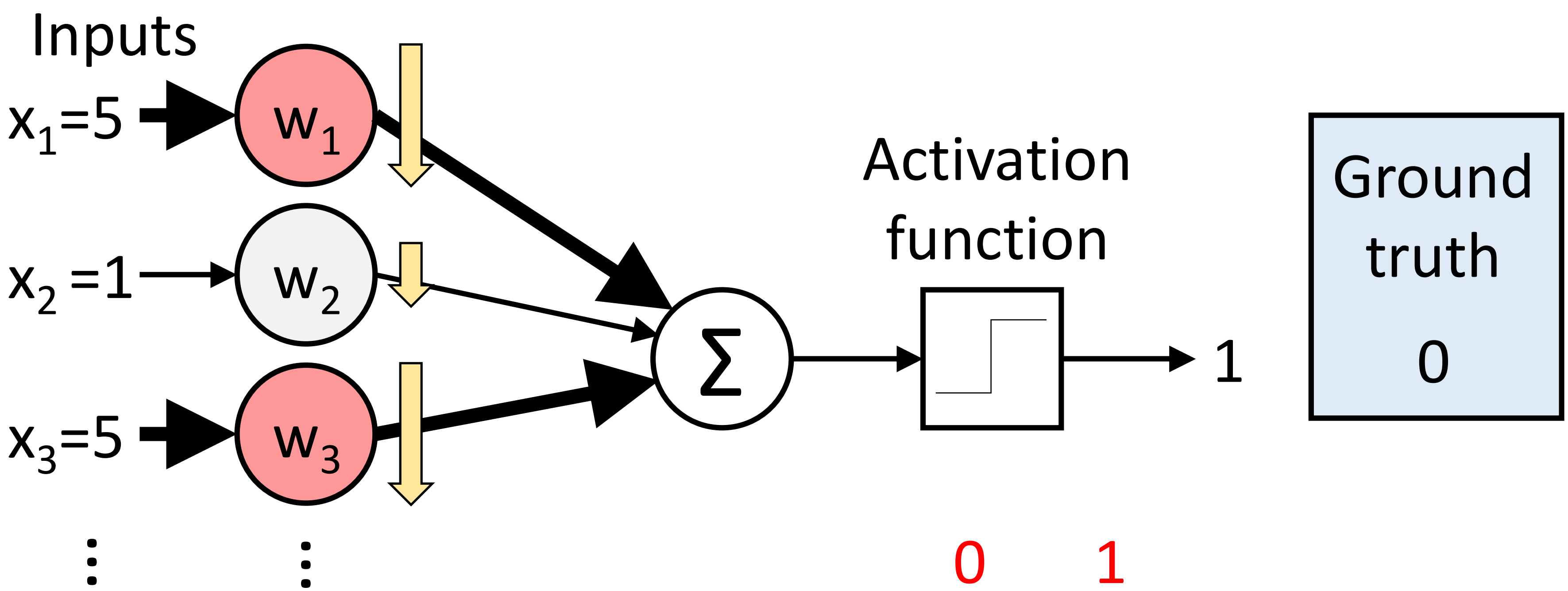
Weight update



$$w_j = w_j + \lambda(\overset{0}{y_i} - \overset{1}{\widehat{y_i}})x_{ij}$$

Learning rate

Weight update



$$\overset{0}{}\quad\overset{1}{}$$

$$w_j = w_j + \lambda(y_i - \hat{y_i})x_{ij}$$

Learning rate

Numeric example

Training instances

$\langle x_{i1}, x_{i2} \rangle$	y_i
1,1	1
1,2	1
0,0	0
-1,0	0

$\langle b, w_1, w_2 \rangle$ = 0, 0, 0

Epoch 1:

$\langle x_{i1}, x_{i2} \rangle$	$b + w_1 \cdot x_{i1} + w_2 \cdot x_{i2}$	$\hat{y}_i$	y_i
1,1	0 + 0 + 0 = 0	1	1

Learning rate

λ = 1

$$f(\mathbf{w} \cdot \mathbf{x_i} + b) = \begin{cases} 1 & if\ \mathbf{w} \cdot \mathbf{x_i} + b \geq 0 \\ 0 & otherwise \end{cases}$$

Numeric example

Training instances

$\langle x_{i1}, x_{i2} \rangle$	y_i
1,1	1
1,2	1
0,0	0
-1,0	0

$\langle b, w_1, w_2 \rangle$ = -1, 0, 0

Epoch 2:

$\langle x_{i1}, x_{i2} \rangle$	$b + w_1 \cdot x_{i1} + w_2 \cdot x_{i2}$	$\hat{y}_i$	y_i
1,1	-1 + 0 + 0 = -1	0	1

Learning rate

λ = 1

$$f(\mathbf{w} \cdot \mathbf{x_i} + b) = \begin{cases} 1 & if\ \mathbf{w} \cdot \mathbf{x_i} + b \geq 0 \\ 0 & otherwise \end{cases}$$

Numeric example

Training instances

$\langle x_{i1}, x_{i2} \rangle$	y_i
1,1	1
1,2	1
0,0	0
-1,0	0

$\langle b, w_1, w_2 \rangle$ = -1, 1, 1

Epoch 3:

$\langle x_{i1}, x_{i2} \rangle$	$b + w_1 \cdot x_{i1} + w_2 \cdot x_{i2}$	$\hat{y}_i$	y_i
1,1	-1 + 1 + 1 = 1	1	1

Learning rate

λ = 1

Convergence – there were no updates in this epoch, so end training

$$f(\mathbf{w} \cdot \mathbf{x_i} + b) = \begin{cases} 1 & if\ \mathbf{w} \cdot \mathbf{x_i} + b \geq 0 \\ 0 & otherwise \end{cases}$$

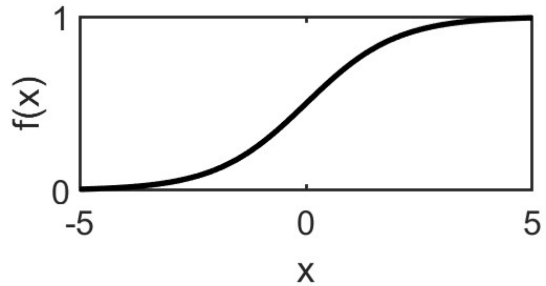
Activation function

- What does it do?
- In a perceptron
  - Maps the linear response to the range we want (class labels 0 or 1)
- In a multilayer perceptron / neural network:
  - Adds a non-linearity after each linear operation
  - More about this later!

Activation function

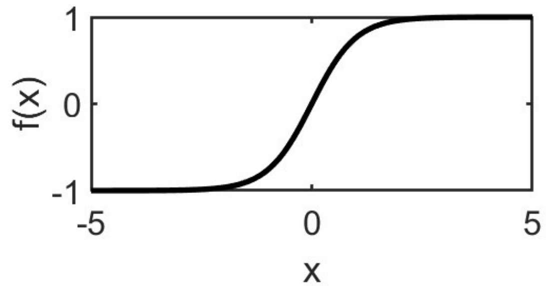
- Common choices:
- (logistic) sigmoid (σ):

$$f(x) = \frac{1}{1 + e^{-x}}$$



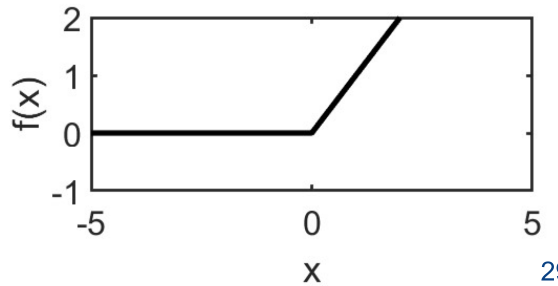
- hyperbolic tan (tanh):

$$f(x) = \frac{e^{2x} - 1}{e^{2x} + 1}$$



- rectified linear unit (ReLU):

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



Perceptron properties

- The perceptron algorithm is guaranteed to converge for linearly-separable data, but the convergence point (class boundary) will depend on:
  - The initial values of the weights and bias
  - The learning rate
- Not guaranteed to maximise the margin between classes
- Not guaranteed to converge over non-linearly-separable data

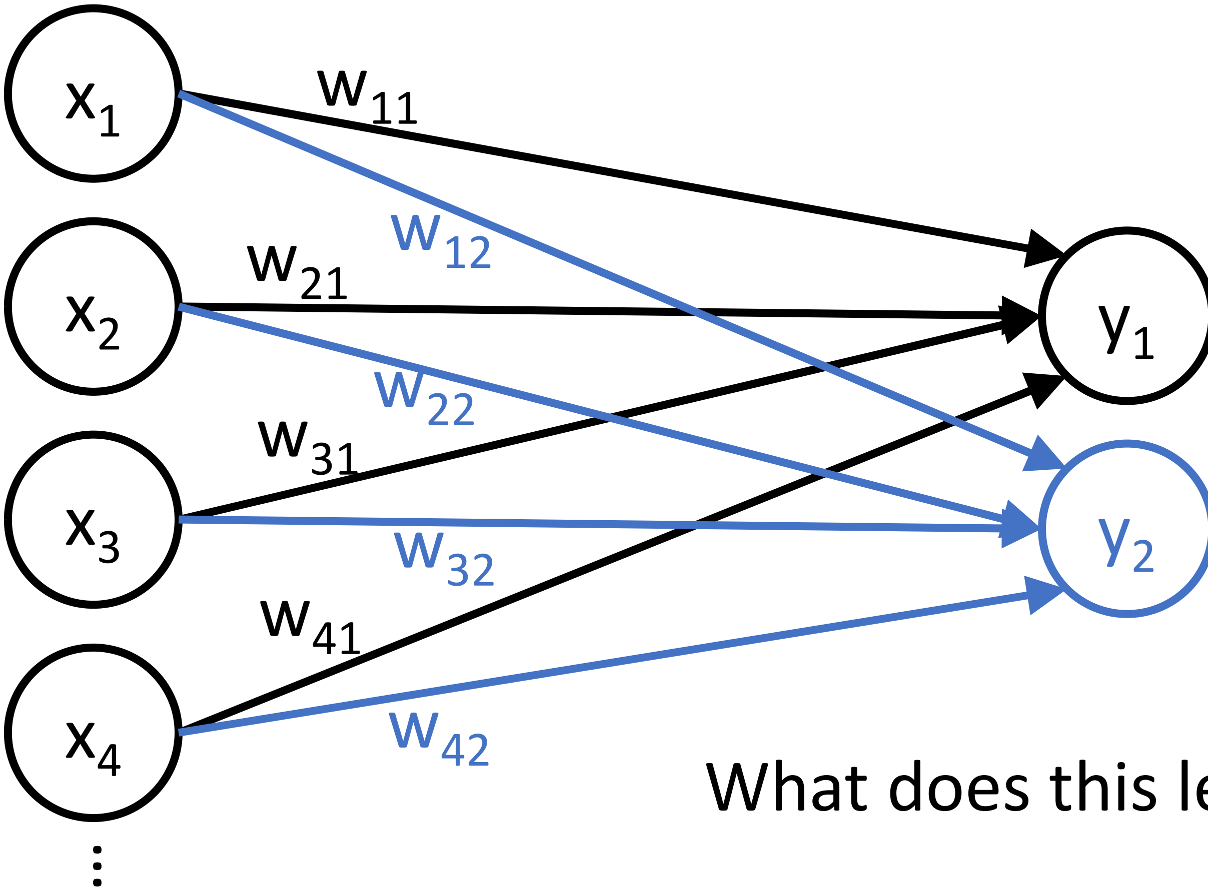
Perceptron properties

- A perceptron with a sigmoid activation function (plus a binary step to convert the output to 0 or 1) is equivalent to logistic regression:

$$y_i = \frac{1}{1 + e^{-(\mathbf{w} \cdot \mathbf{x_i} + b)}}$$

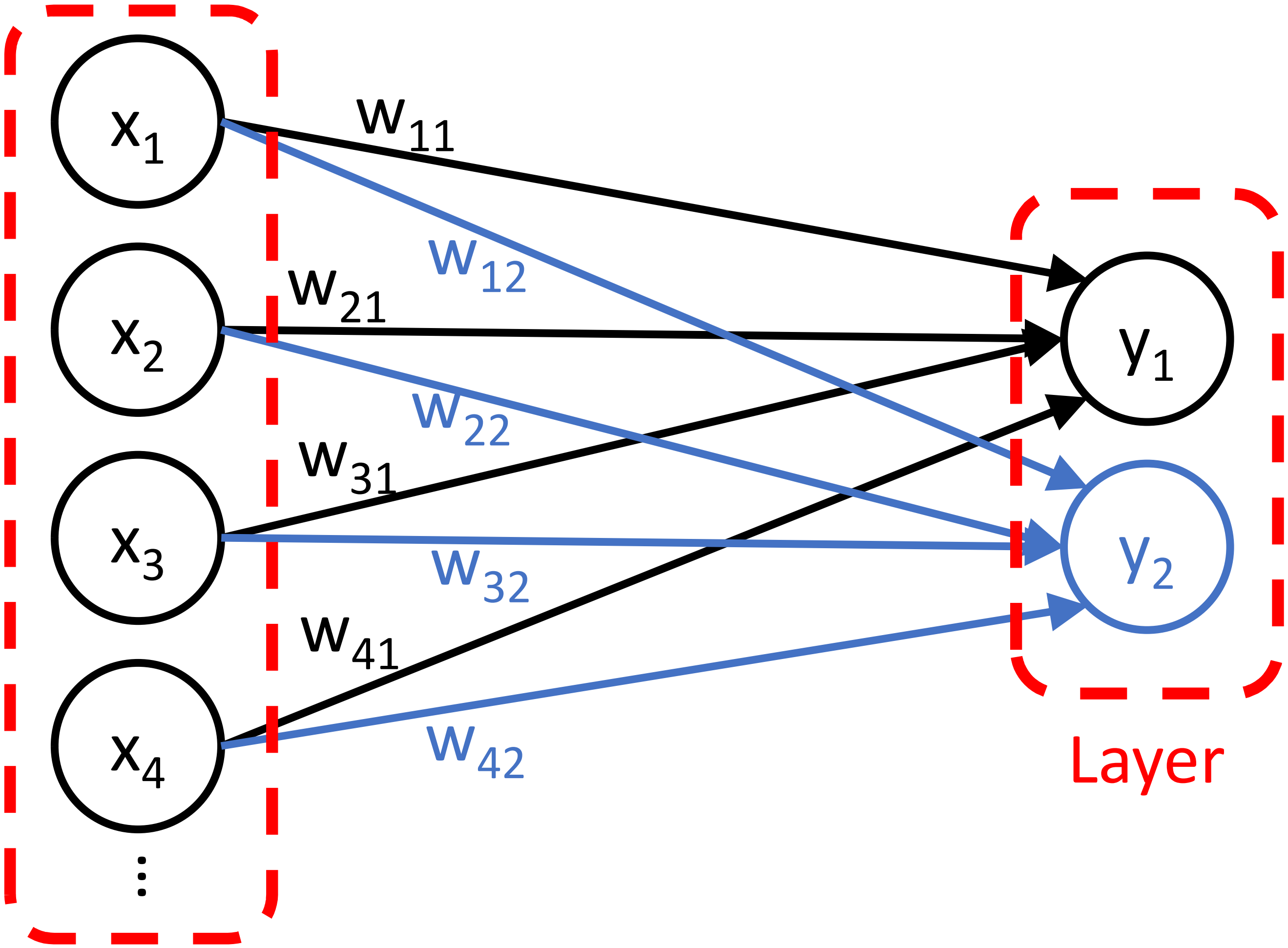
Multilayer perceptron

Extension 1: Multiple outputs

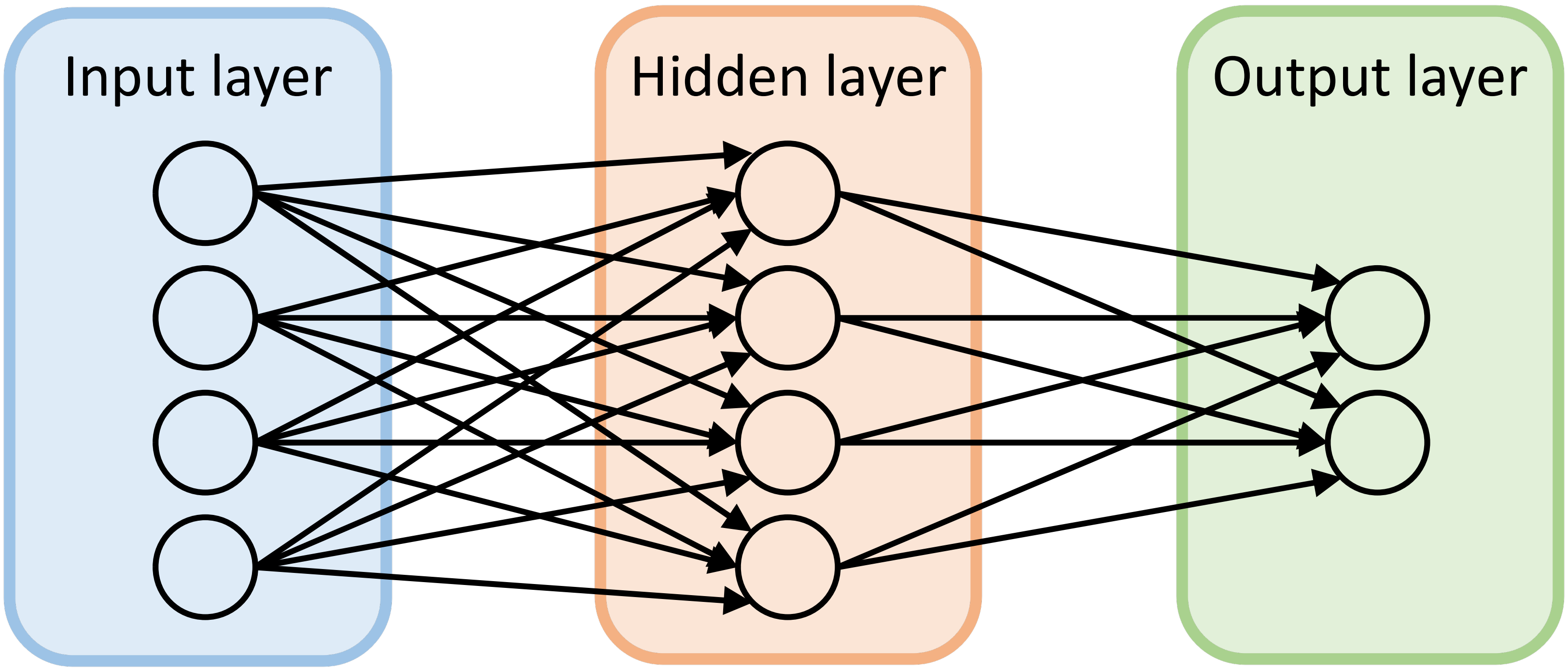


What does this learn?

Extension 1: Multiple outputs



Extension 2: Multiple layers



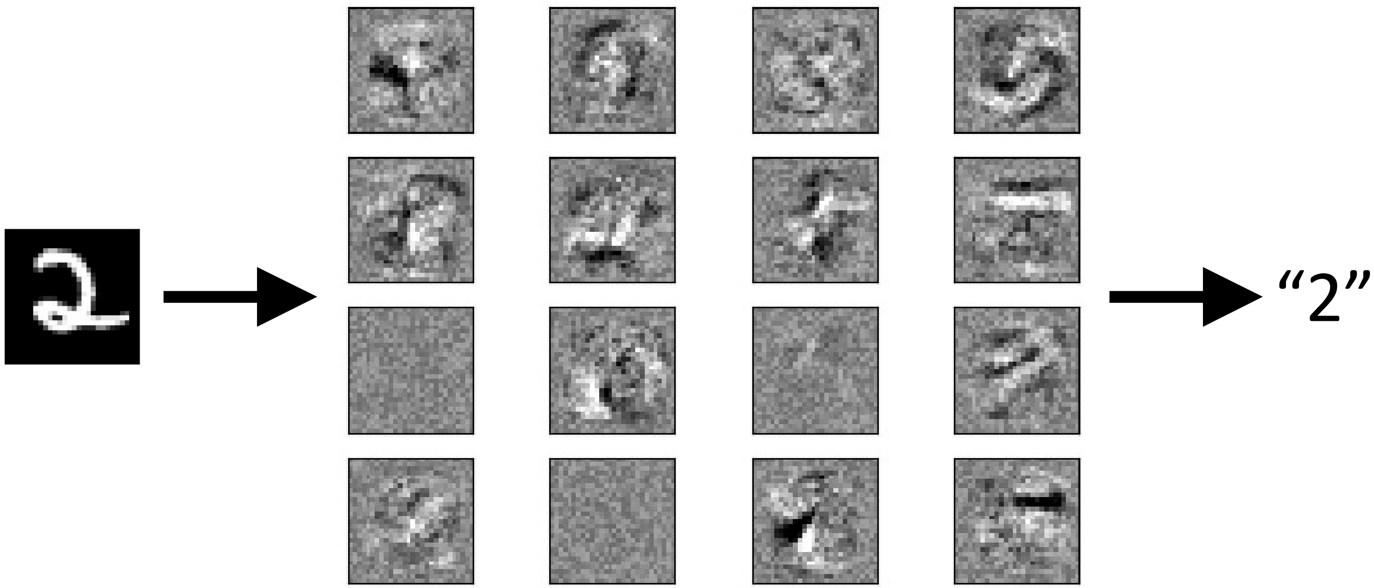
What does this learn?

Multilayer perceptron

- Layer = a group of neurons working in parallel on the same input
- Multilayer perception (MLP):
  - An **input layer**
  - At least one **hidden layer**. Each hidden layer receives the previous layer's output as its input
  - An **output layer** which receives input from a hidden layer and outputs the class label

Hidden layer

- What does it learn?
  - Representation learning – hidden layers learn some features that are useful for the output layer



https://scikit-learn.org/stable/auto_examples/neural_networks/plot_mnist_filters.html

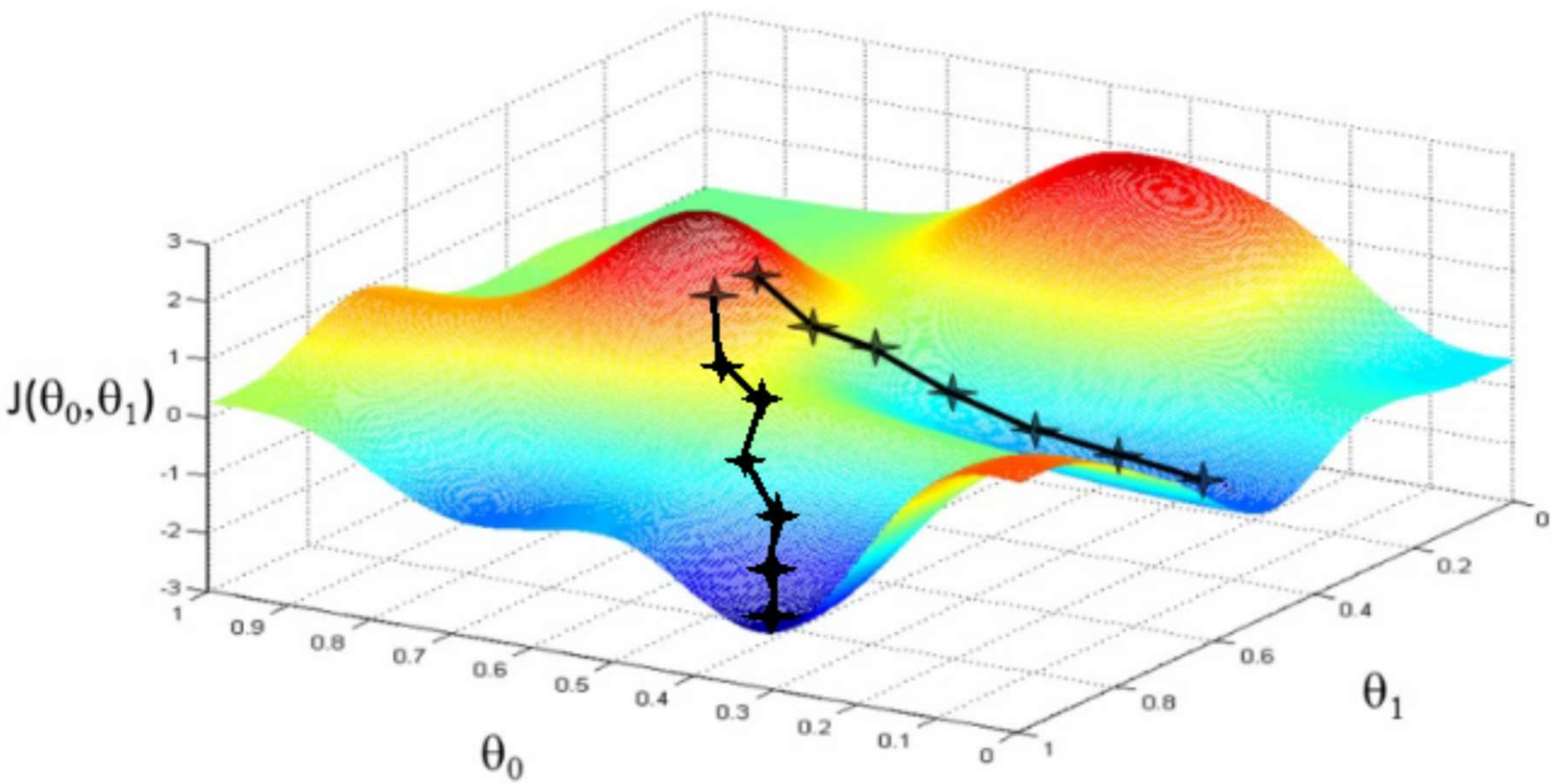
Hidden layer

- How many neurons?
  - Given that we don’t know exactly what features this layer should learn, how to pick the right number of neurons?
  - In theory, depends on factors like complexity of decision boundary
  - In practice, often just pick an arbitrary value in between the input and output size

Hidden layer

- How does it learn?
  - There's not just one "correct" output for the neurons in a hidden layer, like there is for the output layer
  - How can the hidden layer(s) be trained?
- Solution: backpropagation
  - **Stochastic** gradient descent
  - Find parameters (weights+biases) to minimize loss on the training dataset

Gradient descent



Backpropagation

- Form of gradient descent – iterative process for finding the weight parameters that minimize error
- Just like single perceptron training, requires a learning rate (hyperparameter)
- Idea: look at the derivative of error and update weights in the direction that would reduce error
  - Compute errors at the output layer w.r.t. each weight using partial differentiation
  - Propagate errors back to each of the earlier layers
  - Chain rule used to efficiently compute derivatives

Output layer

- Structure depends on task
- Common options:
  - Binary classification – 1 output neuron with step activation function
  - N-way classification – N output neurons and softmax activation function
  - Regression – 1 output neuron with identity activation function

Neural network/MLP properties

- Universal approximation theorem: a feed-forward neural network with a single hidden layer (with finite neurons) is able to approximate any continuous function on $\mathbb{R}^n$
- Means the network can learn any (linear or non-linear) basis function dynamically, unlike many other methods (e.g., SVM where kernel is a hyperparameter)
- Note that this requires non-linearities

Non-linearities

- With a non-linear activation function:
  $f(\mathbf{w_{L2}} \cdot f(\mathbf{w_{L1}} \cdot f(\mathbf{w_{L0}} \cdot \mathbf{x_i} + \mathbf{b_{L0}}) + \mathbf{b_{L1}}) + \mathbf{b_{L2}})$

- Without non-linearity:
  $$\mathbf{w_{L2}} \cdot (\mathbf{w_{L1}} \cdot (\mathbf{w_{L0}} \cdot \mathbf{x_i} + \mathbf{b_{L0}}) + \mathbf{b_{L1}}) + \mathbf{b_{L2}}$$
  $$= \mathbf{w}_\alpha \cdot \mathbf{x_i} + \mathbf{b_\alpha}$$
  - Multiple layers don't accomplish anything – the same computations could have been done in one layer

Neural network/ MLP properties

- True or false?

- Since NNs are universal approximators, they are guaranteed to generalise better than any other machine learning method.

- Since NNs learn their own representations in hidden layers, they don't require any feature engineering.

Neural network/ MLP properties

- MLP advantages
  - Can be adapted to many types of problems (classification, regression)
  - Universal approximator – can model arbitrary basis functions
  - Representation learning in hidden layers
- MLP disadvantages
  - Very high number of parameters – slow to train, prone to overfitting, high memory requirements
  - Stochastic gradient descent – not guaranteed to converge to the same solution every time