

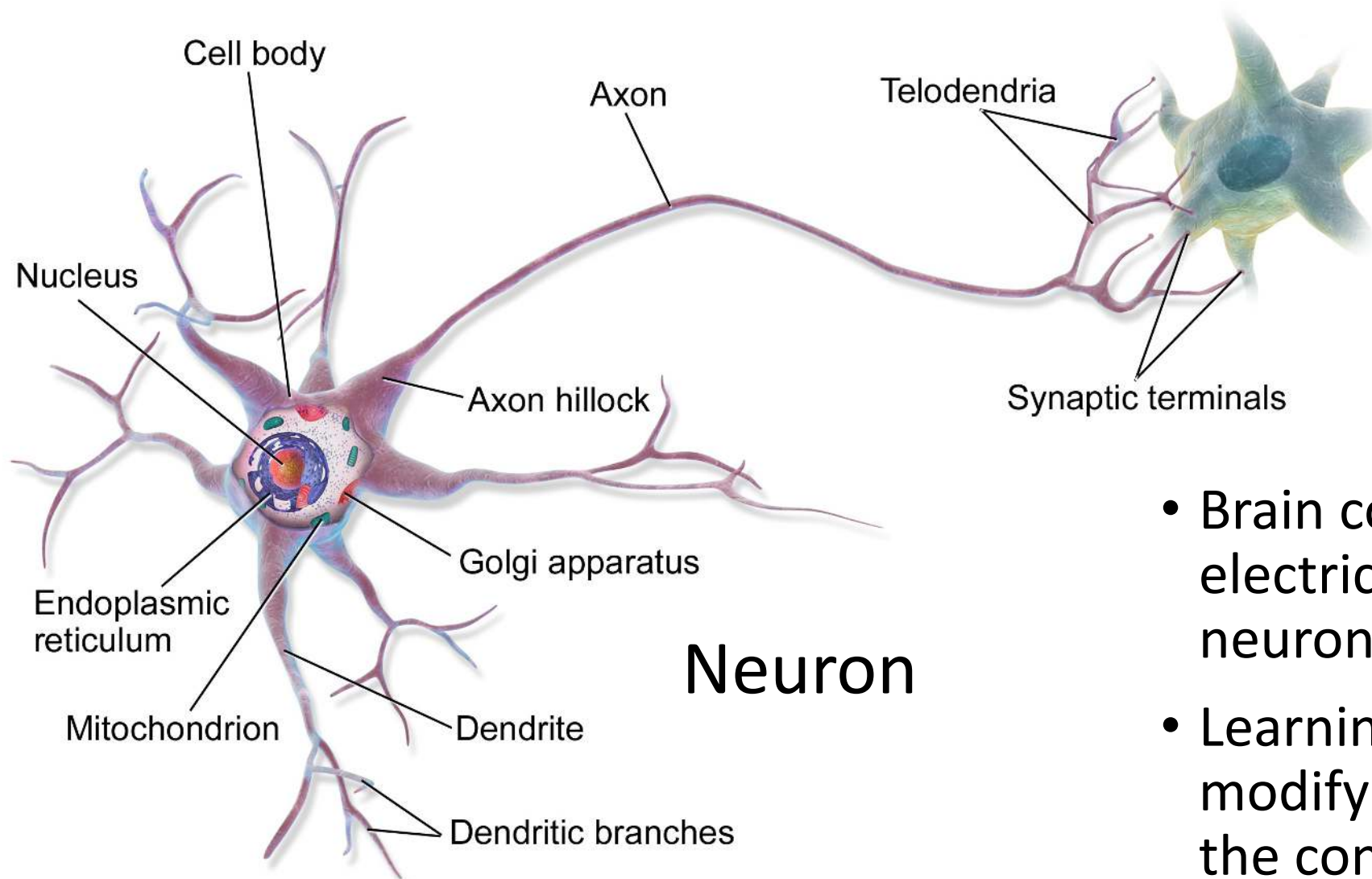
Neural Networks 1

Anders Krogh

Center for Health Data Science

University of Copenhagen

Inspiration from the brain

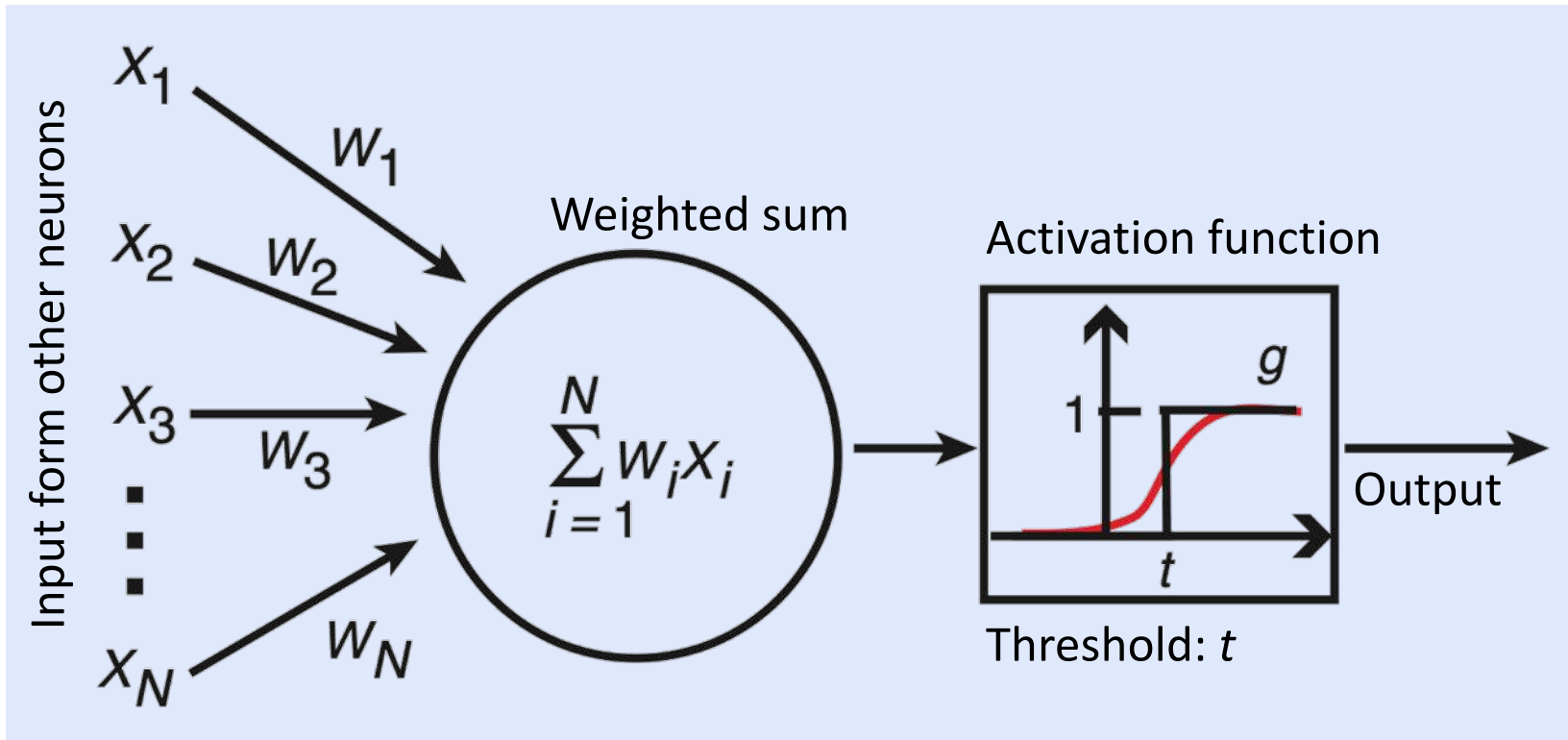


- Brain computes by sending electric signals between neurons
- Learning happens by modifying the strengths of the contacts – the synapses

A mathematical model of the neuron

McCulloch and Pitts
proposed this model in 1943

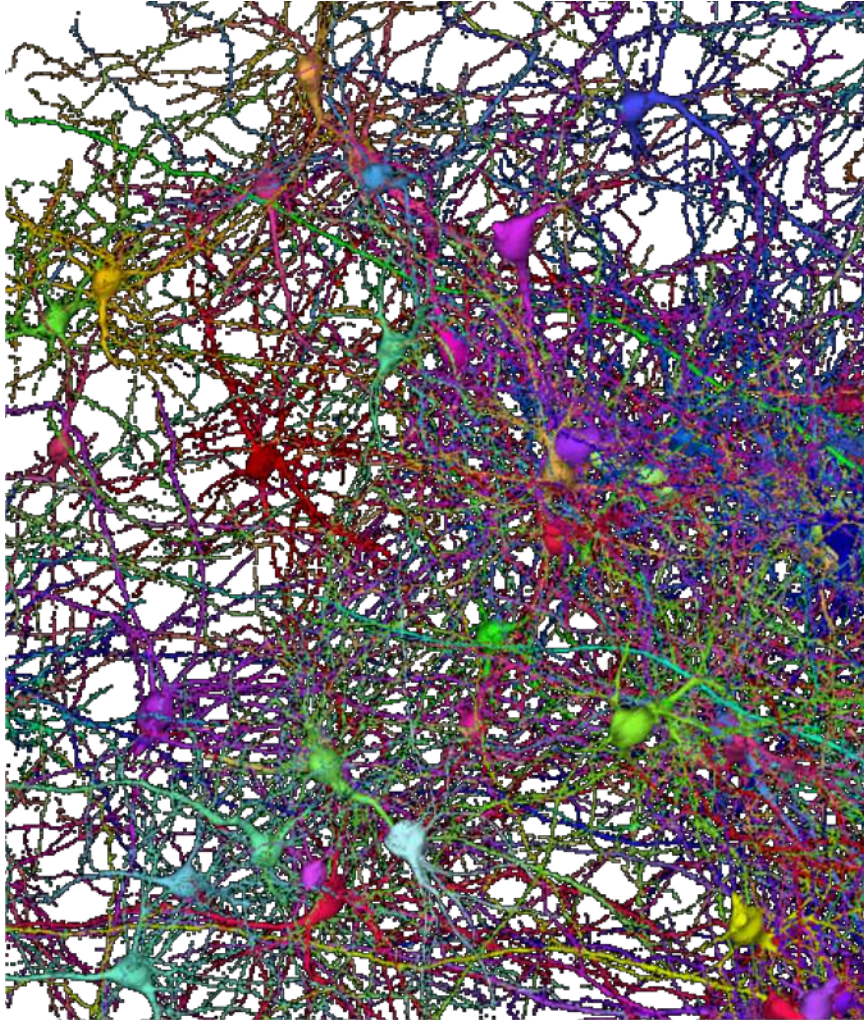
This is the basis for most artificial
neural network models



Sigmoid activation
function (red curve)

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

Many connected neurons → neural network



Screenshot from <https://h01-release.storage.googleapis.com/gallery.html>

Artificial neural network
Feed-forward NN

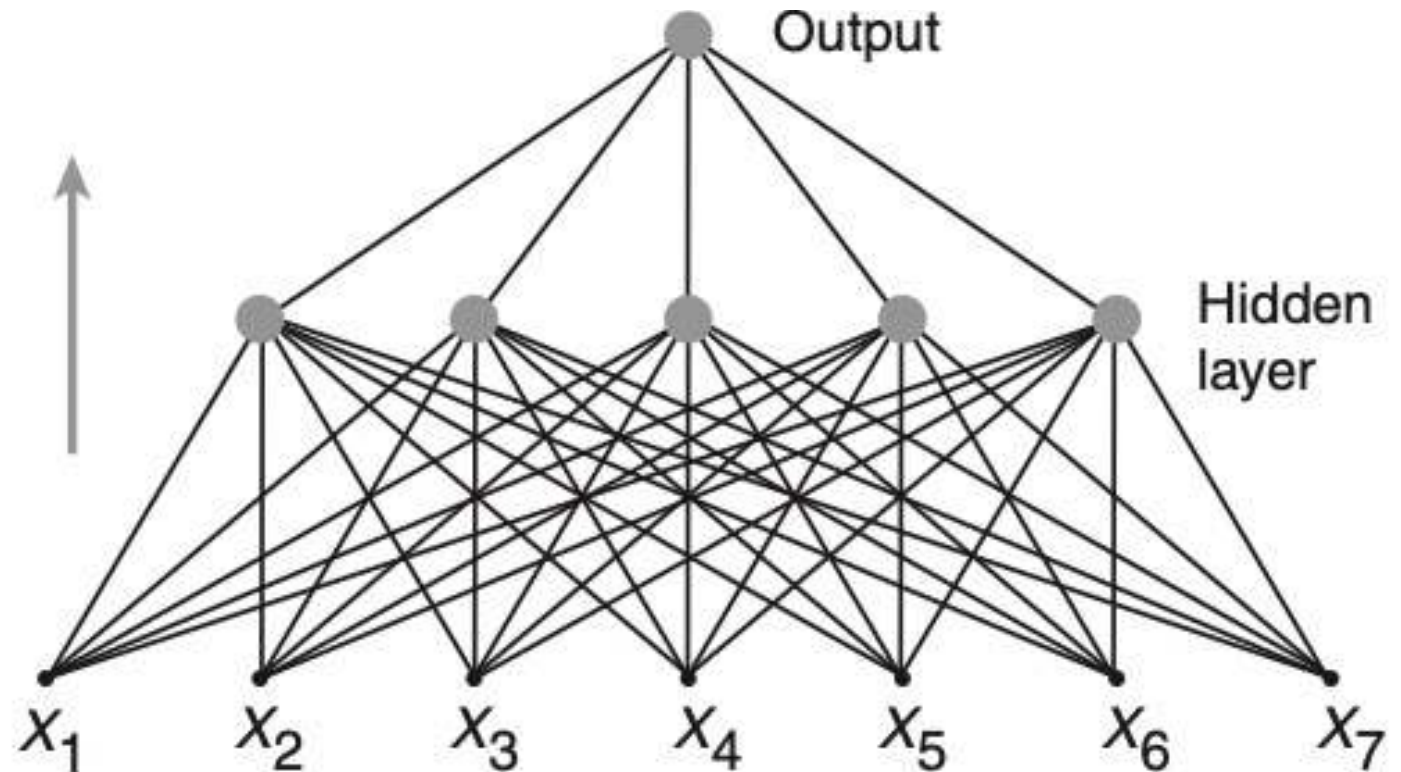
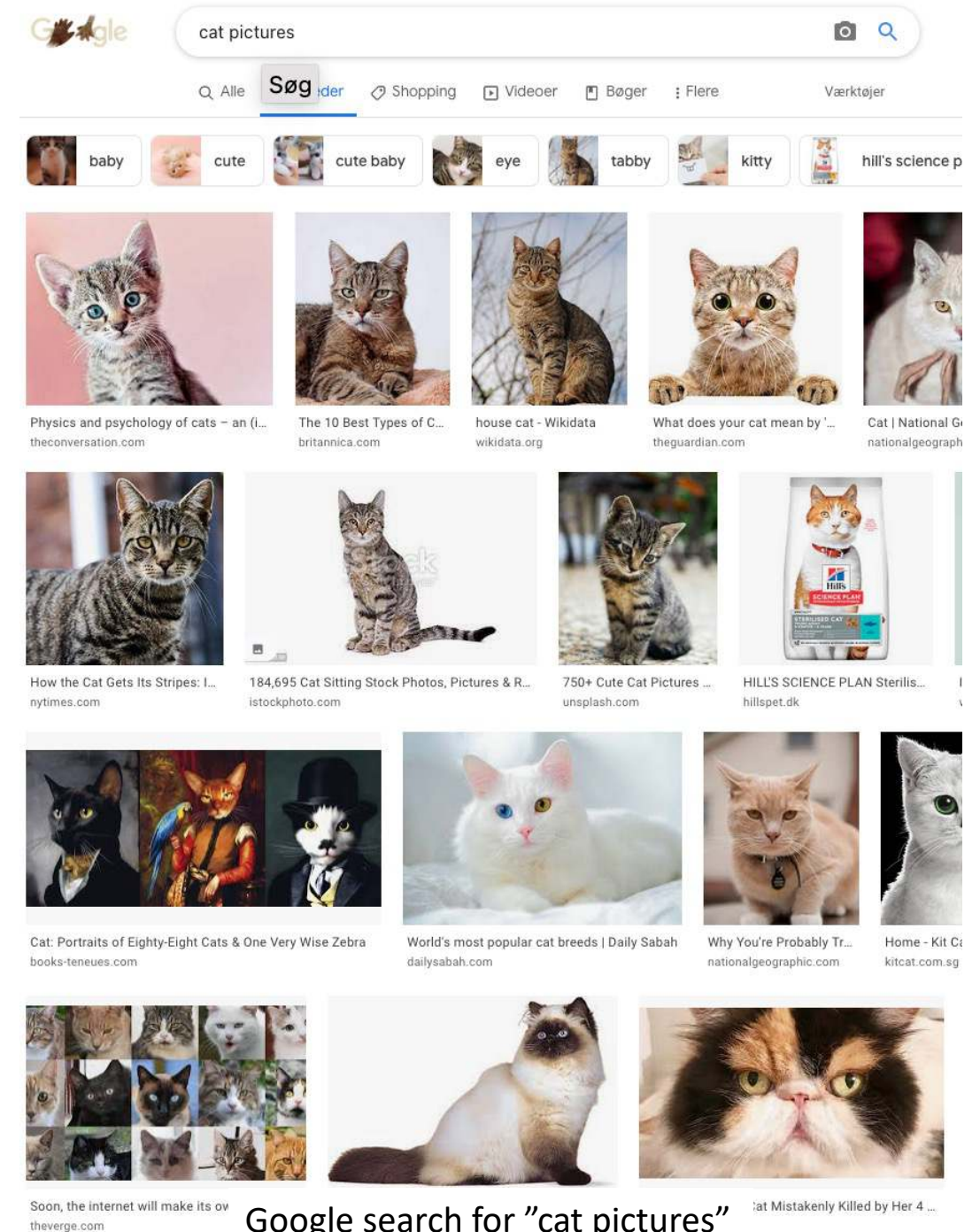


Figure from A Krogh, : What are artificial neural networks?, Nat. Biotech. 26, p. 195-197, 2008

Learning from examples

- Humans learn from examples
- By seeing enough pictures of cats, a child can learn to recognize a cat
- Artificial neural networks also learn from examples



Learning by minimizing the error

- Neural network is a function $f_w(\mathbf{x})$
- \mathbf{x} is an input vector (e.g. pixel values in cat picture)
- Output: values between zero (no cat) and one (cat in picture)
- Parametrized by the weights w (symbolizing all the weights)

Learning: Find the weights that give the desired output as close as possible

Glossary:

Error is often called **loss** or **cost**

Labels are also called **targets**

Train on a set of **labeled examples** called the **training set**.



Labels: $t=1$ (cat)



$t=0$ (not cat)

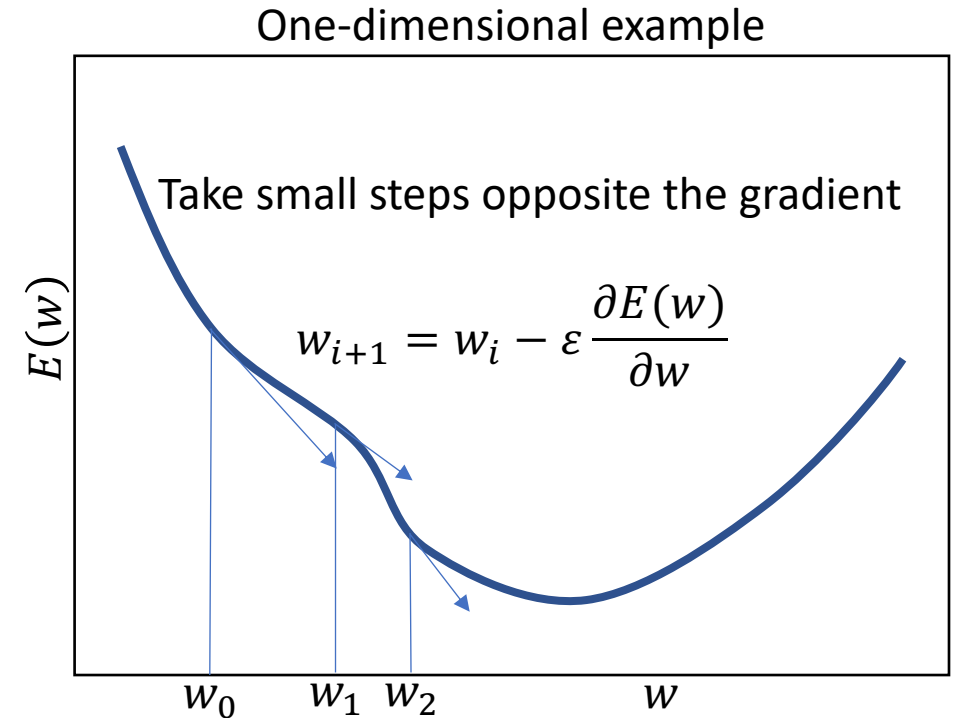
Minimize the error:

$$E(w) = \sum_i (f_w(\mathbf{x}_i) - t_i)^2$$

Sum is over training examples

Minimize the error by gradient descent

- Gradient descent is a general method for function minimization
- It is an iterative procedure: take a small step in the direction opposite to the gradient in each iteration
- The gradient:
 - The partial derivative for each weight in the network
 - A vector that points in the direction of fastest growth of the function



Gradient descent leads to the famous **Back-propagation** algorithm for neural networks

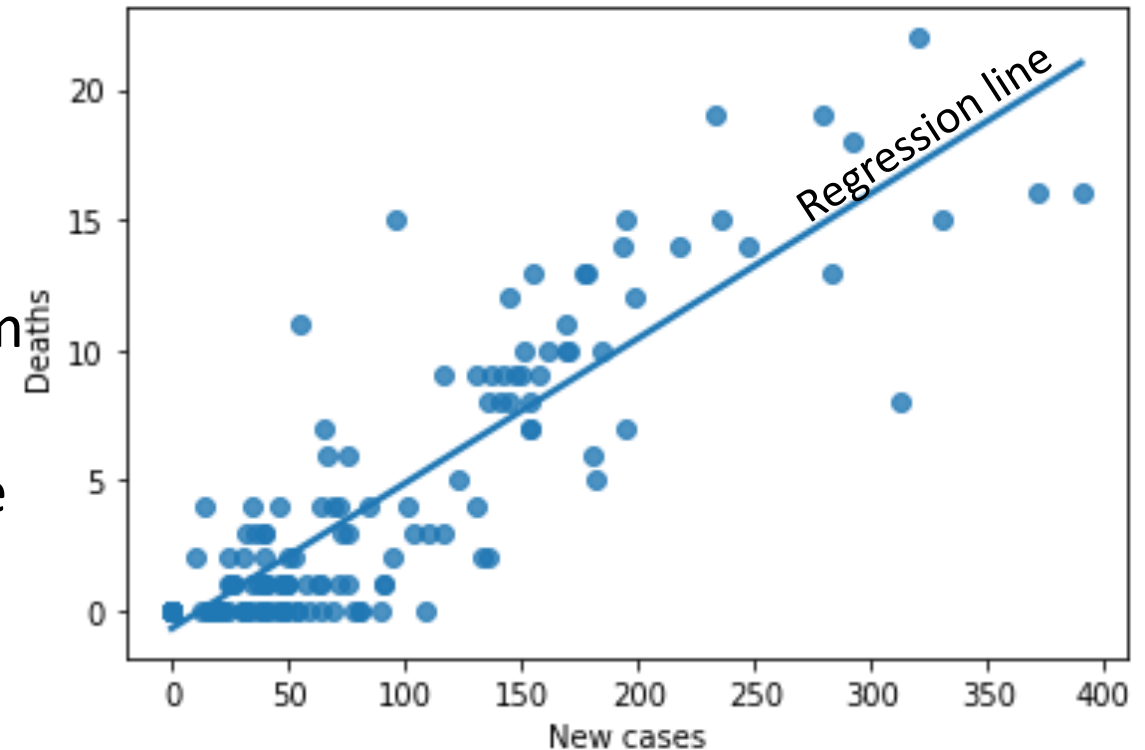
Fortunately we do not have to derive the math – modern neural network programs automatically calculate the gradients

Analogy to linear regression

Linear regression is also done by minimizing the squared error

- The error is the squared difference between the observed y for a given x and the “prediction” $y = ax + b$
- The a and b is found by minimizing the sum of the squared errors
- This can be done analytically leading to the formulas for linear regression
- It can also be done by gradient descent

Points show the number of deaths vs new Corona cases in Denmark per day from March to July 2020



There are many examples/animations of this online, e.g.:

<https://towardsdatascience.com/gradient-descent-animation-1-simple-linear-regression-e49315b24672>

Python example

- In this example, the gradient is calculated manually
- We do not have to do that again – pytorch will take care of it

Copy this Colab notebook:

<https://drive.google.com/file/d/1Oqmad5JpPI2rzzrWDrMiGPs3QinyxT8sO/view?usp=sharing>

More realistic networks

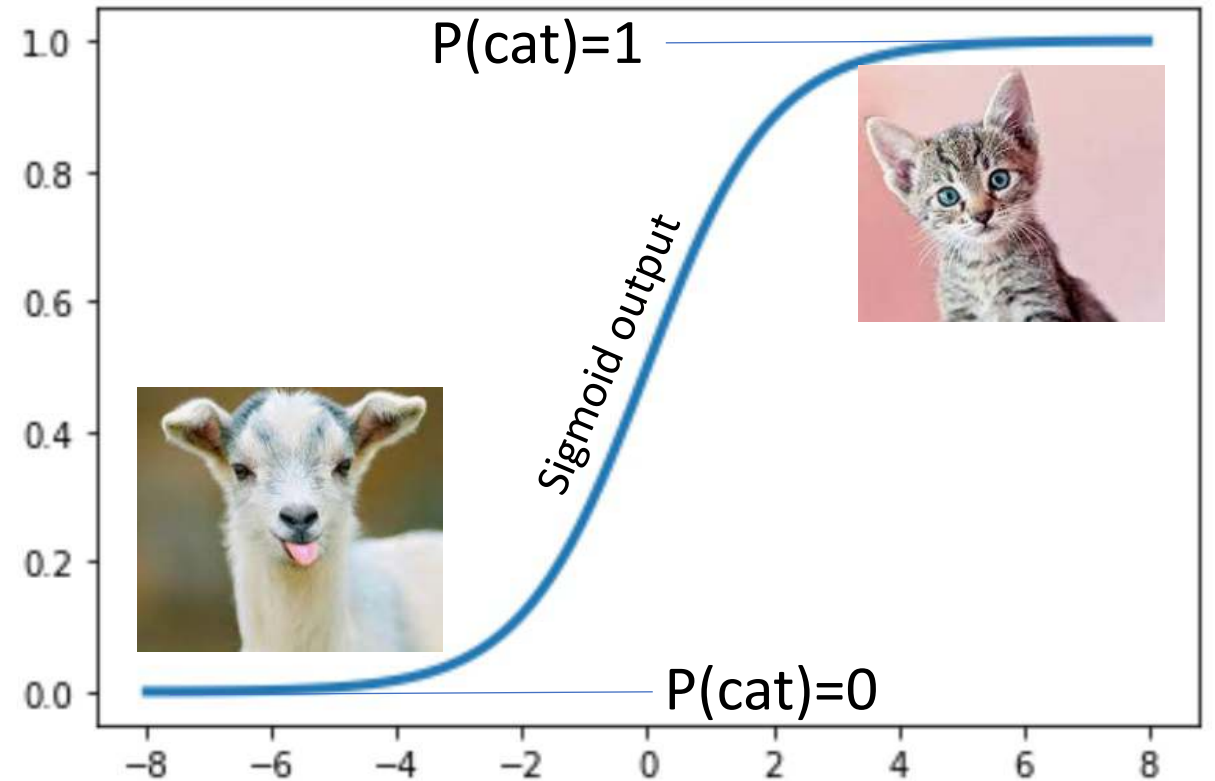
- The regression example has two “weights” a and b
- Normally the neural networks have **thousands of weights** and thresholds (some even millions)
- In the examples there were a single output unit
- Sometimes we have **several output units**
- We often discriminate between networks for
 - **Classification** with binary targets (like cat/no cat)
 - **Regression** with continuous target values (like linear regression)
- Learning follows the same principles, but the error function may change

Classification

- When there are two classes:
 - Use **probabilities**
 - Change loss function $E(w)$
- **Maximum likelihood** leads to the **binary cross entropy** loss:

$$E(w) = -\sum_i [t_i \log f_w(\mathbf{x}_i) + (1 - t_i) \log (1 - f_w(\mathbf{x}_i))]$$

- If there are no hidden units, it is the same as **logistic regression**



Stochastic gradient descent

For complex networks the loss has **multiple local minima**

Plain gradient descent does not work well

Stochastic gradient descent use “**mini batches**”

- The gradient is calculated over a random sample of a certain size – the **batch size**
- For each cycle through the training set (**epoch**), the network is updated many times instead of just one
- Because of the randomness it can better escape local minima and has turned out to be much more efficient

There are many other “tricks”. Many of these are combined in **the popular optimizer called Adam**

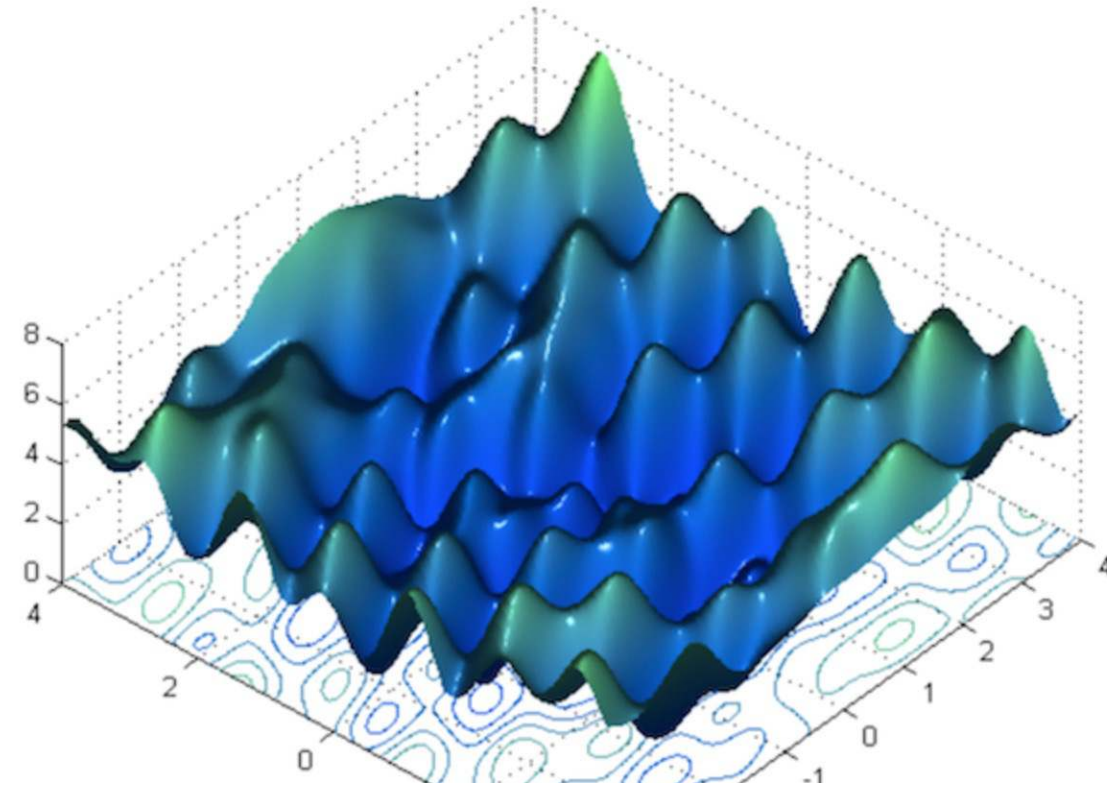


Figure copied from: <https://towardsdatascience.com/neural-network-optimization-7ca72d4db3e0>

- Pytorch is a Python package for neural networks
- It makes it easy to design and train neural networks, because of
 - Automated differentiation to calculate gradients
 - Efficient use of hardware (including GPUs)
- It uses **tensors**, which are multidimensional numerical arrays with many convenient mathematical operations (as in linear algebra)
- To start with pytorch, you need not worry about tensors

LET US TRY!