

A decorative graphic consisting of a grid of colored squares. The top row has a large blue square on the left and a smaller light green square on the right. The middle row has a teal square on the left and a light yellow square on the right. The bottom row has a pink square on the left, an orange square in the middle, and a yellow square on the right. The text is overlaid on these squares.

# neural networks

statistics and data analysis (chapter 10)

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## wrap up: Bayesian evidence

- probability  $p(H|I)$  of a hypothesis  $H$  being true, given information  $I$
- require
  - sum-rule:  $p(H|I) + p(\bar{H}|I) = 1$
  - product-rule:  $p(X, Y|I) = p(X|Y, I)p(Y|I)$

- Bayes' law:

$$p(X|Y, I) = p(Y|X, I) \times \frac{p(X|I)}{p(Y|I)} \quad (1)$$

with the hypothesis  $X$  and the data  $Y$ . identify:

- $p(X|Y, I)$  posterior
  - $p(Y|X, I)$  likelihood
  - $p(X|I)$  prior
  - $p(Y|I)$  evidence
- $I$  is the model family,  $X$  one specific model characterised by a parameter value

# Bayesian evidence for comparing models

- look at Bayes' law

$$p(X|Y, I) = p(Y|X, I) \times \frac{p(X|I)}{p(Y|I)} \quad (2)$$

with

- $Y$  data
  - $X$  model: model choice in a model family
  - $I$  model family, with  $Y$  as one element
- evidence:

$$p(Y|I) = \sum_X p(Y|I, X)p(X|I) \quad \text{or} \quad p(Y|I) = \int_{\Omega} d\theta p(y|\theta, I)p(\theta, I) \quad (3)$$

for a continuous parameter space

- need prior  $p(\theta, I)$ , from theory or previous experiments, look for consistency between experiment and prior
- compare two models by evidence ratio: complexity vs. ability to fit

# Bayesian evidence: Jeffrey's scale

- Neyman-Pearson-lemma: likelihood ratio is the best way of comparing hypotheses
- in this context, the likelihood ratio is called Bayes-ratio
- let's write down the **Bayes-ratio** between two competing models  $I_1$  and  $I_2$

$$B = \frac{p(Y|I_1)}{p(Y|I_2)} \quad (4)$$

- the Bayes-ratio can be expressed by marginalisation over all possible parameter choices  $\theta$

$$p(Y|I_i) = \int d\mu p(D|\theta)p(\theta|I_i) \quad (5)$$

- simple models are preferred, because they've more "likelihood within the prior"
- Jeffreys scale for  $B$  for making decisions concerning  $I_1$  vs.  $I_2$
- scale for the degree of confidence in a model is arbitrary

# prosecutor's fallacy

- Roman law: everybody is innocent until proven guilty, degree of evidence must support the hypothesis of being guilty beyond a reasonable doubt: if the prosecutor fails in proving the guilt, one reverts to the null-hypothesis innocence
- prosecutor's fallacy: neglecting the prior if evidence is used in court
- $E$  is some evidence,  $I$  is the state of an accused being innocent:
  - $p(E|I)$  probability of damning evidence if the person is innocent
  - $p(I|E)$  probability of being innocent despite the evidence
- $p(E|I) \neq p(I|E)$  for conditional probabilities, but rather

$$p(I|E) = p(E|I) \times \frac{p(I)}{p(E)} \quad (6)$$

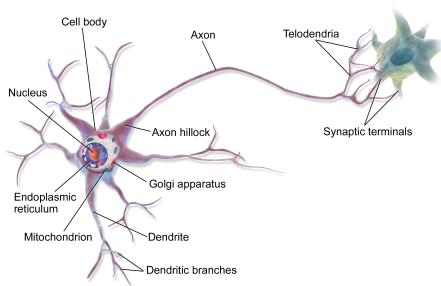
probability  $p(E)$  of observing the evidence, and  $p(I)$  being innocent

- $p(E|I)$  is tiny, but that does not mean that  $p(I|E)$  is tiny as well!
- $p(E) = p(E|I)p(I) + p(E|\bar{I})(1 - p(I))$ , with the wrong identification of an innocent person  $p(E|I)$  and the identification of a guilty person  $p(E|\bar{I})$

# neural networks: idea

- up to now we
  - fitted physical models to data (regression) and
  - selected models based on simplicity and evidence
- this was motivated by a fundamental understanding of the laws of Nature
- but there might be applications where we may admit unphysical and complex models
  - effective description of data without underlying principles
  - difficult to understand classification tasks
- construct mathematical models with a high degree of complexity and flexibility
  - adjust all degree of freedom with known data
  - system might be able to abstract and perform well on similar data
  - without understanding the details

# Ramon y Cajal: discovery of neurons



neuron (source: wikipedia)

- nerve cell is linked by synapses to other cells and form a network
- signal transmission is electrical (inside cells) and chemical (between cells)
- nice thought: evolution can't construct for a purpose, rather it uses methods which can adapt to model a certain behaviour

# neurons in different animals

compare the number of neurons in different animals:

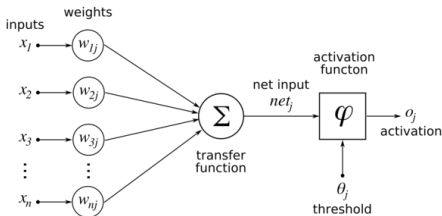
- sponge: 0
- jellyfish:  $5 \times 10^3$
- fruit fly:  $2.5 \times 10^5$
- frog:  $1.6 \times 10^7$
- hamster:  $9 \times 10^7$
- cat:  $8 \times 10^8$
- human:  $8 \times 10^{10}$
- elephant:  $2.7 \times 10^{11}$

**please check out**

[https://en.wikipedia.org/wiki/List\\_of\\_animals\\_by\\_number\\_of\\_neurons](https://en.wikipedia.org/wiki/List_of_animals_by_number_of_neurons)



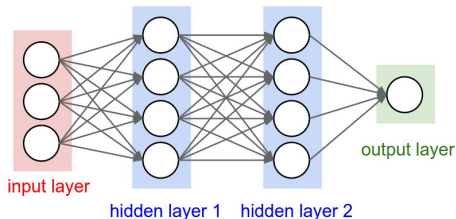
# working principle of a neuron



**artificial neuron (source: wikipedia)**

- a neuron collects inputs  $x_i$  and computes a weighted sum  $\sum_i w_i x_i$
- and compares the sum to a threshold  $\theta$ : if  $\sum_i w_i x_i > \theta$ , it produces an output or an activation
- output is given by  $\phi(\sum_i w_i x_i - \theta)$  with an activation function  $\phi$

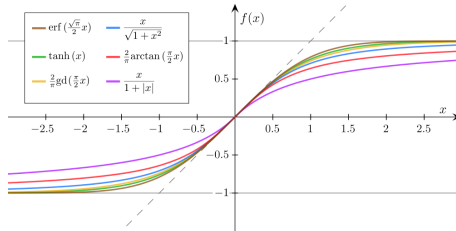
# neural networks



**network composed of artificial neurons**

- neural networks are networks of many neurons
- neurons are arranged in layers
- representation theorem by Kolmogorov (different Kolmogorov): 2 layered networks can do every job, but there's no statement about how many nodes are needed
- if the information flux is from an input layer through hidden layers to an output layer, one refers to it as a feed-forward network

# response functions



activation functions (source: wikipedia)

- many choices of the response function  $\phi$  are possible
- usually one selects a monotonic, differentiable function, which asymptotes to constants
- the precise functional form usually does not matter a lot

# classification by a neuron

- a neuron computes  $\sum_i w_i x_i$  from the inputs and compares to the threshold  $\theta$
- think of  $w_i$  and  $x_i$  as a vectors: defines plane

$$w_i x_i - \theta = w_i x_i - w_i y_i \quad (7)$$

with a normal vector  $w_i$  and a point  $y_i$  inside the plane

- $w_i x_i > \theta$  means that  $x_i$  lies above the plane,  $w_i x_i < \theta$  below
- neuron defines a plane and quantifies if  $x_i$  lies above or below it
- response  $\phi(w_i x_i - \theta)$  quantifies by how much
- application to a classification problem: find the best  $w_i$  and  $\theta$ !

# training as a fitting process

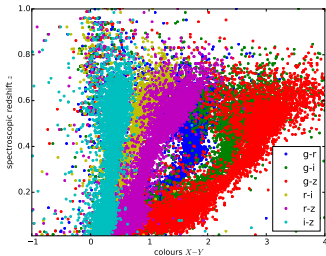
- adjust the every neuron's weights  $w_i$  and thresholds  $\theta$  by requiring a minimised error on a training data set where the output is known
- technically, define the error as the difference between required and computed output,

$$\Delta^2(\{w_i, \theta\}) = \sum_{\text{data}} \Delta_i^2 \quad (8)$$

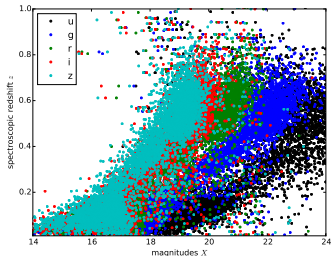
summed over all the training data

- $\Delta^2$  is a function of all weights and thresholds
- backpropagation: weights are adjusted according to a gradient descent rule

## example: estimating redshifts of galaxies



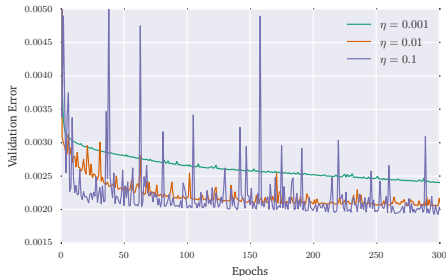
colours of galaxies in SDSS



magnitudes of galaxies in SDSS

- regression problem: estimation of the redshift based on colour or magnitude of a galaxy
- complicated relation, strong noise

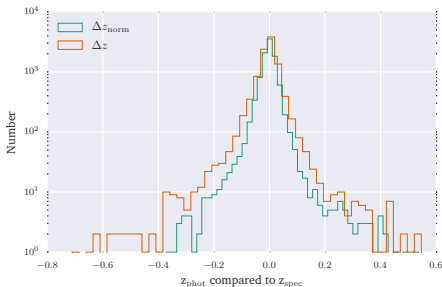
# example: estimating redshifts of galaxies



**error of the neural network on a verification sample (credit: L. Kiehl)**

- use colours and magnitudes as input, estimate redshift
- compare estimated redshift to spectroscopic redshift

# example: estimating redshifts of galaxies



**distribution of the difference between estimated and true redshift (credit: L. Kiehl)**

- distribution of the error shows a good accuracy of estimation



## example: trying different networks

- finding the right solution involves a lot of skill and trial'n'error
- number of neurons and layers should be varied
- activation function, learning rate

**please check out**

<https://playground.tensorflow.org>

# summary

- Bayesian evidence
  - test which model is preferred by data
  - complexity vs. simplicity, quantified by Bayes-evidence
  - very old idea, Occam's razor (scholastic era)
- neural networks
  - regression or classification with a very flexible but unphysical model
  - based on biological systems
  - difficult to understand what it actually does, but very powerful
  - new development: deep networks, with  $O(100)$  layers