Machine Learning for Physics and Astronomy

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Natuur- en Sterrenkunde BSc (Joint Degree), Honours Track

Lecture 3, 21/09/2021

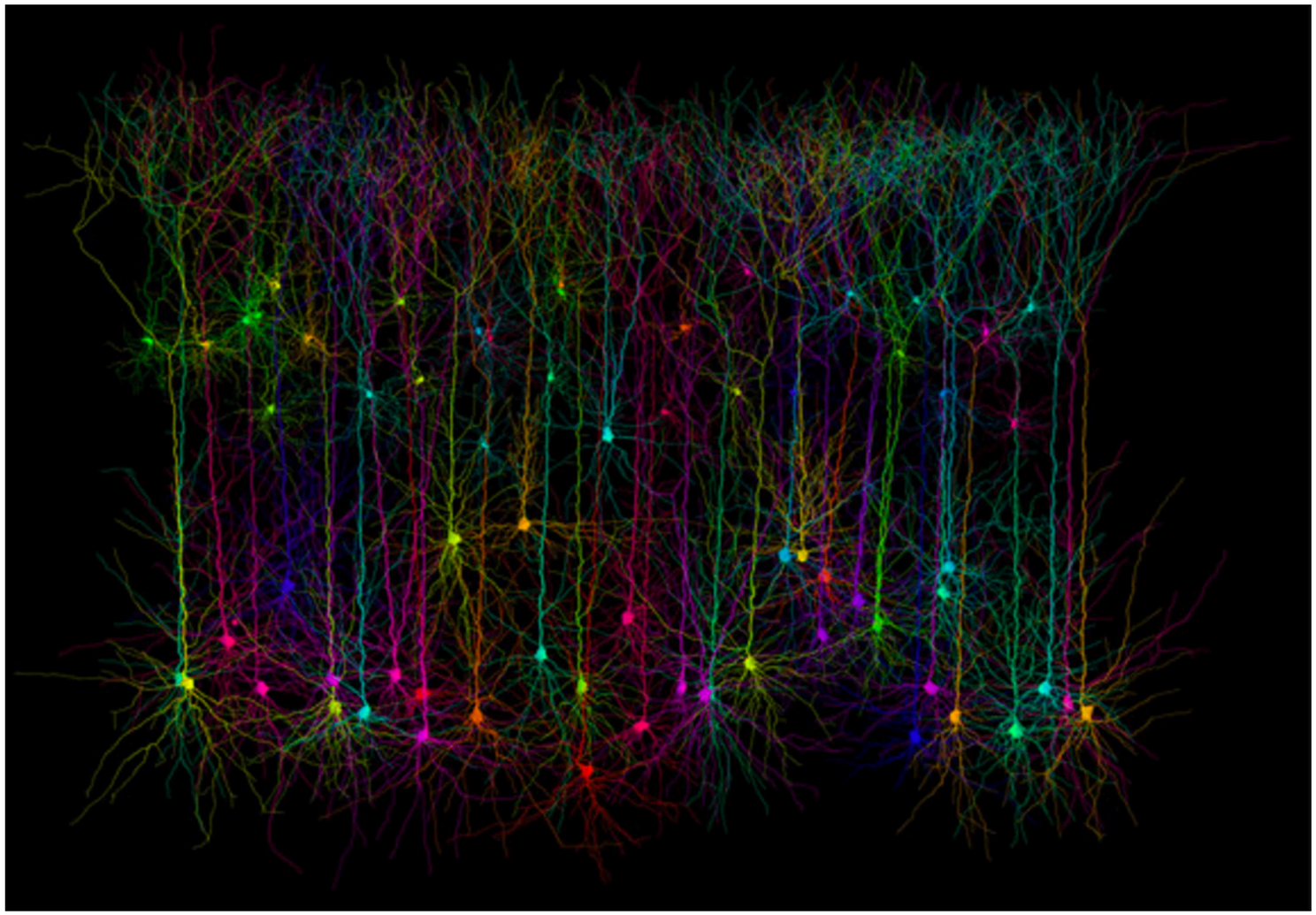
Today's lecture

- Neural Networks and perceptrons
- Deep Learning
- Supervised NN learning: backpropagation
- Optimal training and hyperoptimisation

Neural Networks and Deep Learning

Artificial Neural Networks

Inspired by **biological brain models**, **Artificial Neural Networks** (ANNs) are mathematical algorithms designed to excel where domains as their evolution-driven counterparts outperforms traditional algorithms in tasks such as **pattern recognition, forecasting, classification**, ...



what makes our brain so powerful?

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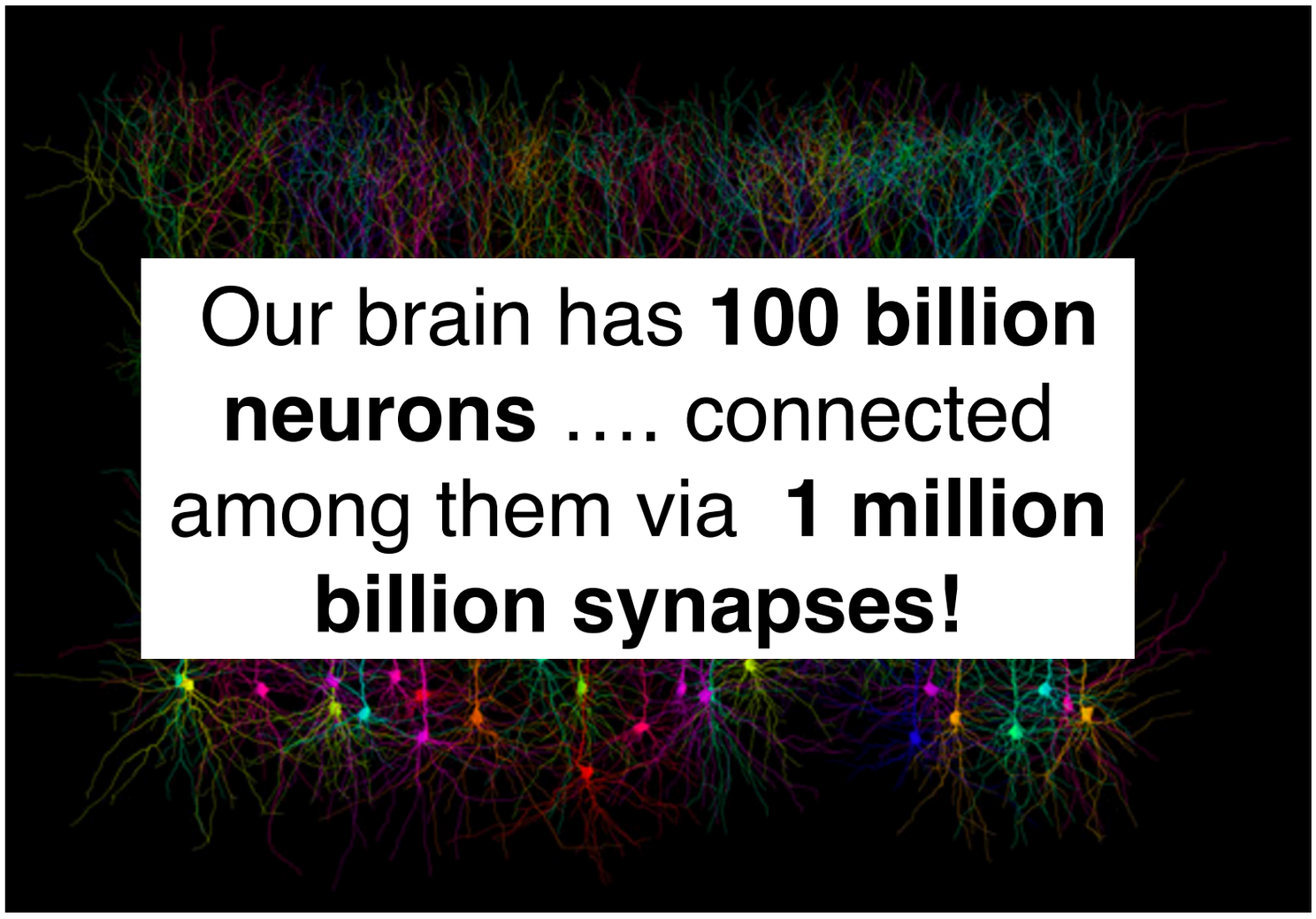

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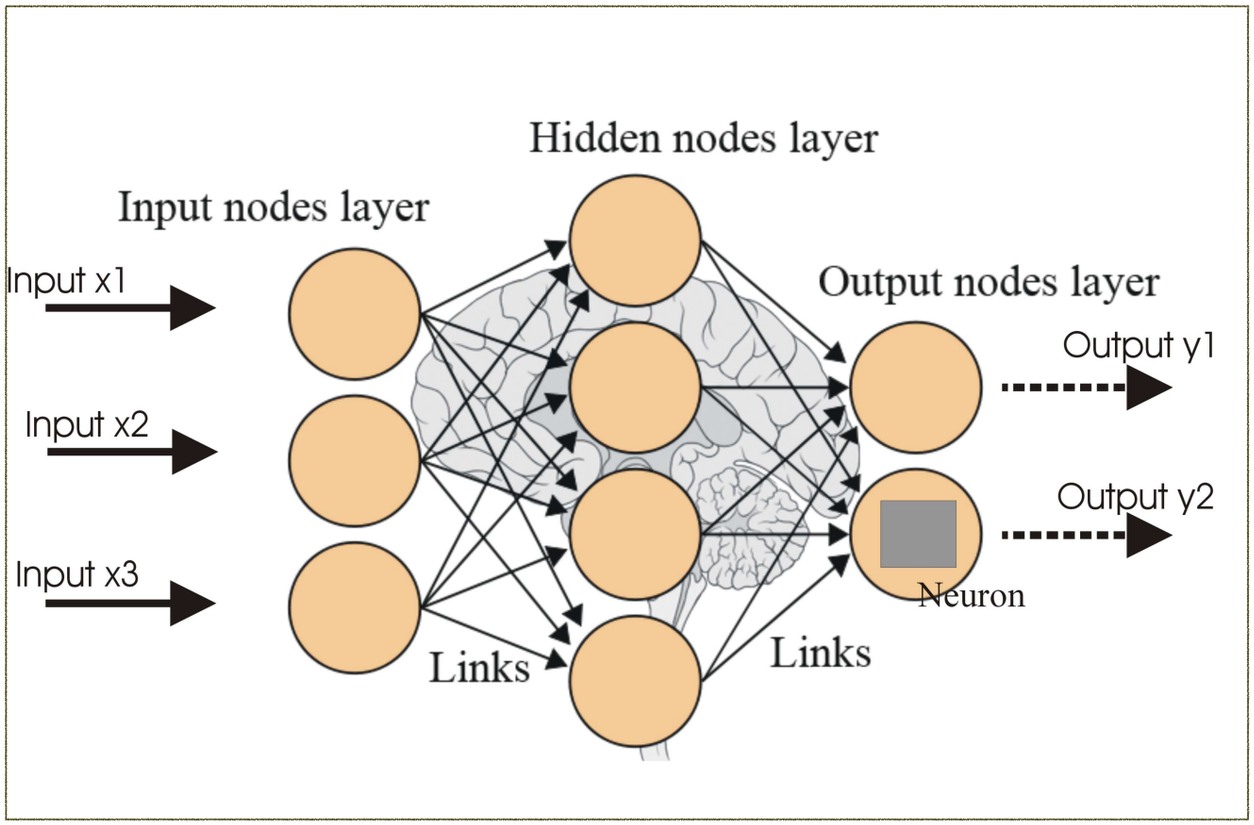

in ML context, ANN provide a flexible, powerful non-linear model for many problems

Neural Networks

Neural Nets can be defined as **neural-inspired nonlinear models** for supervised learning

- The basic unit of a NN is the **neuron,** a transformation of a set of *d* input features into a scalar output

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_d) \rightarrow a(\boldsymbol{x})$$

mapping

neuron inputs

neuron output (activation state)

key feature: mapping is (highly) non-linear

Q: why a non-linear mapping could be so important for neural networks?

(what happens when combining linear transformations?)

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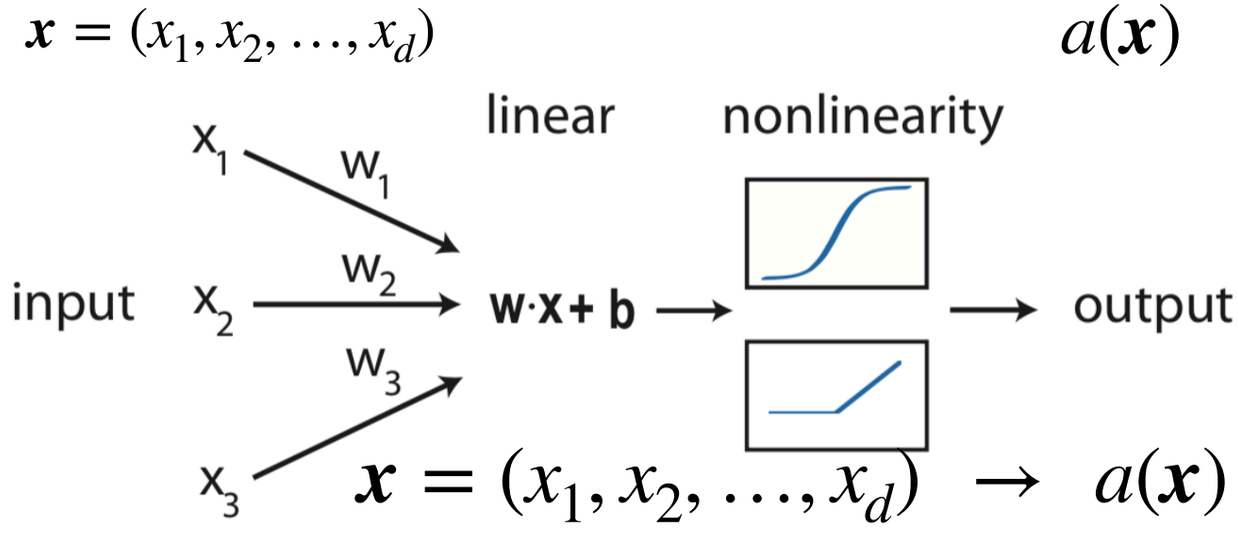
biology analog: input are electric pulses, output the activation state of the neuron



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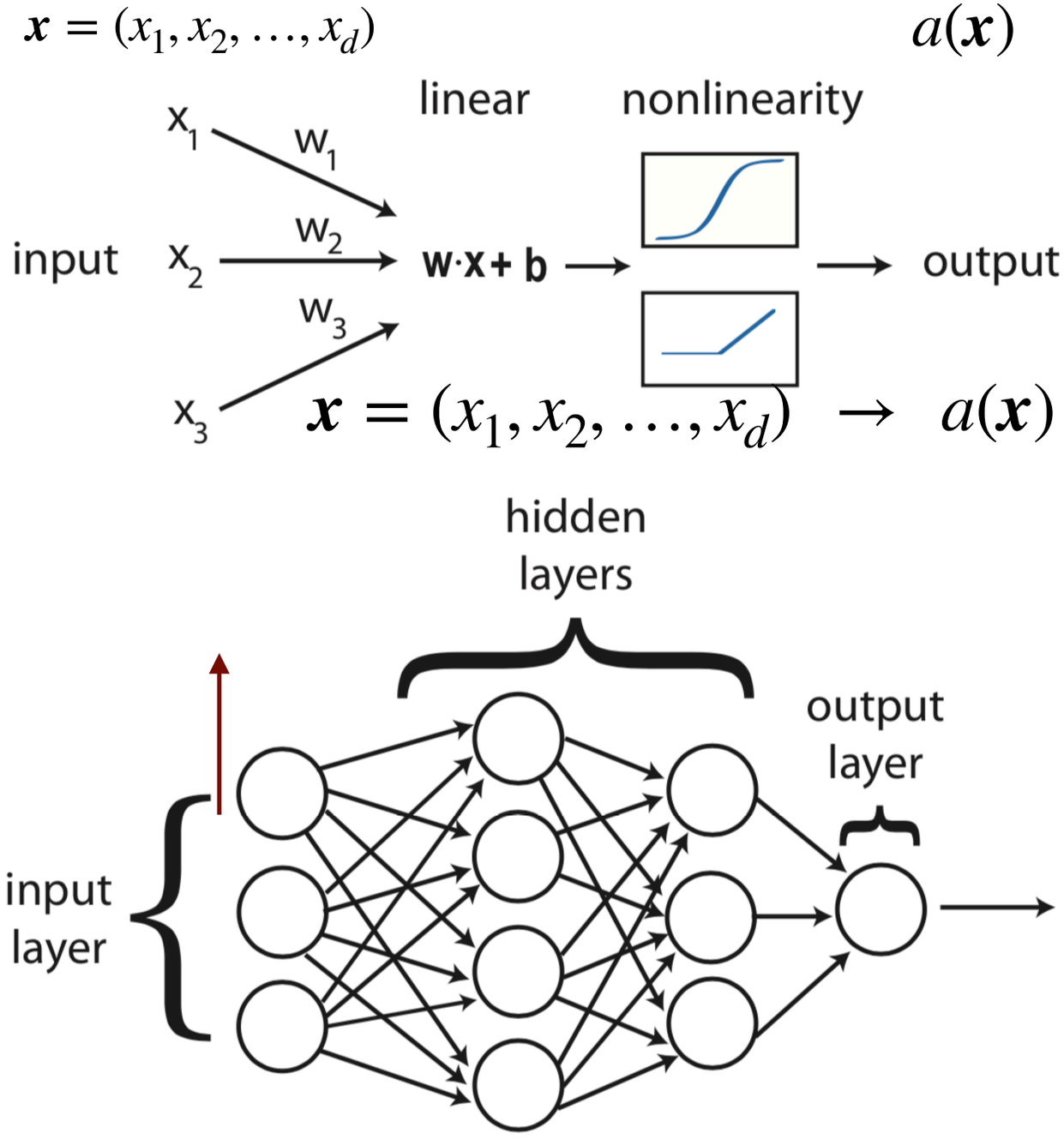
neuron inputs — *neuron output (activation state)*



- These neutrons are arranged in **layers**, which in turn are stacked on each other. The intermediate layers are called **hidden layers**

- Here we will focus on **feed-forward NNs,** where the output of the neurons of the previous layer becomes the input of the neurons in the subsequent layer

Neural Networks

Neural Nets can be defined as **neural-inspired nonlinear models** for supervised learning

the neural network output has two components

a **linear operation**, weighting the various inputs

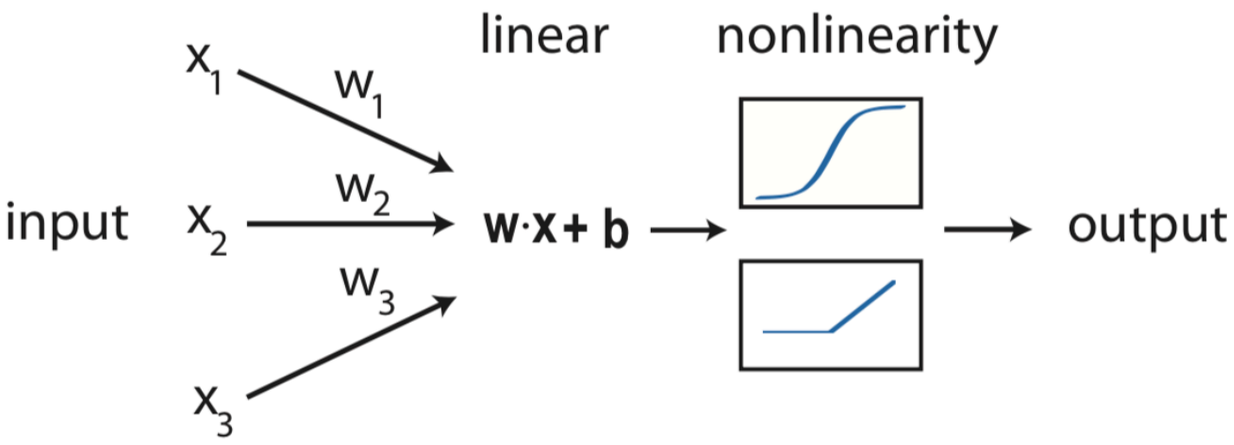
$$z^{(i)} = \boldsymbol{x}^T \cdot \boldsymbol{\theta}^{(i)} + \boldsymbol{\theta}_0^{(i)}$$

neuron inputs — *i-th neuron parameters* — *i-th neuron bias*

a **non-linear transformation**

$$a^{(i)}(\boldsymbol{x}) = \sigma_i(z^{(i)})$$

i-th neuron activation state — *i-th neuron activation function (non-linear)*



the parameters of NNs are often called ``weights" and ``thresholds"

the choice of non-linear activation function affects the **computational and training properties** of the neural nets, since they modify the output gradients required for GD training

NN nonlinearly only via activation functions!

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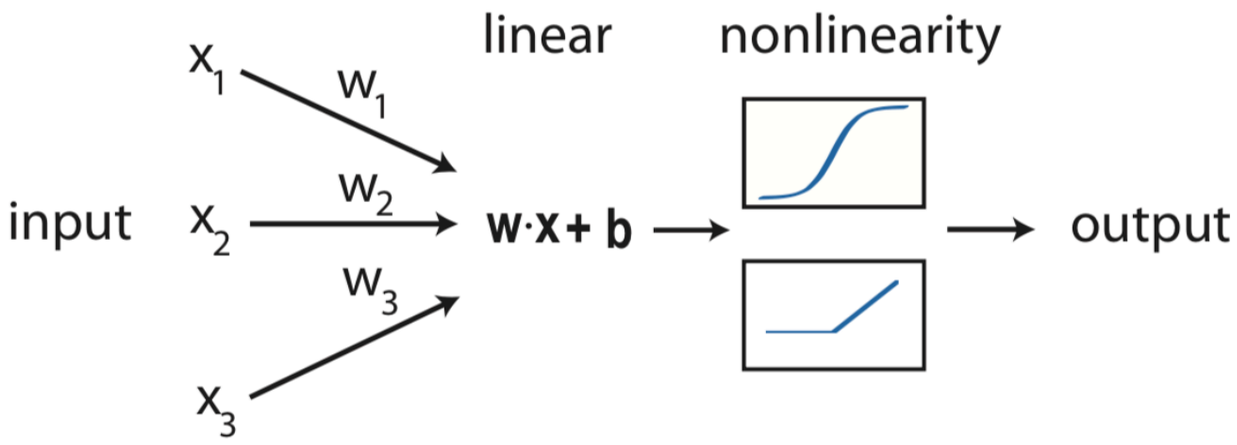

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What do you think that ``neural network training" means at this point?

Neural Networks

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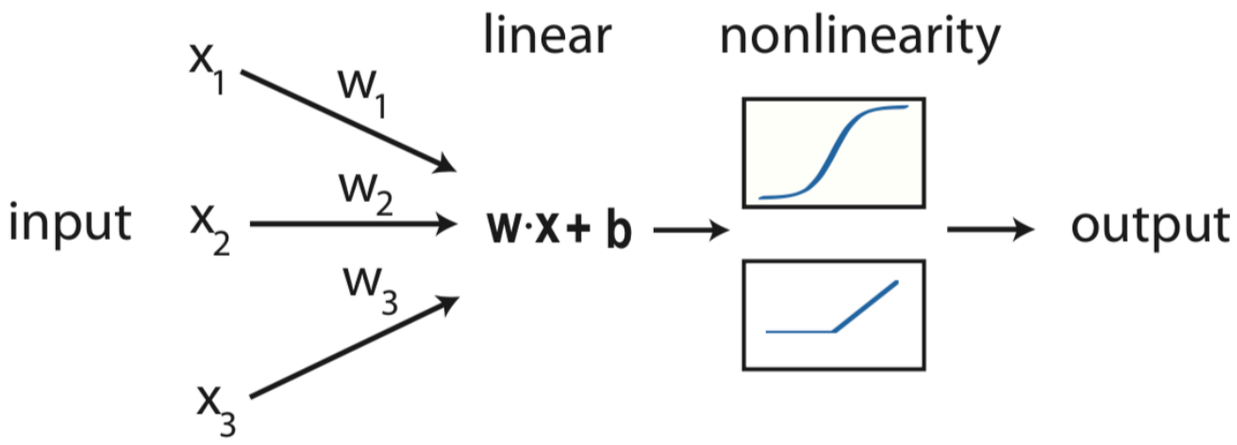

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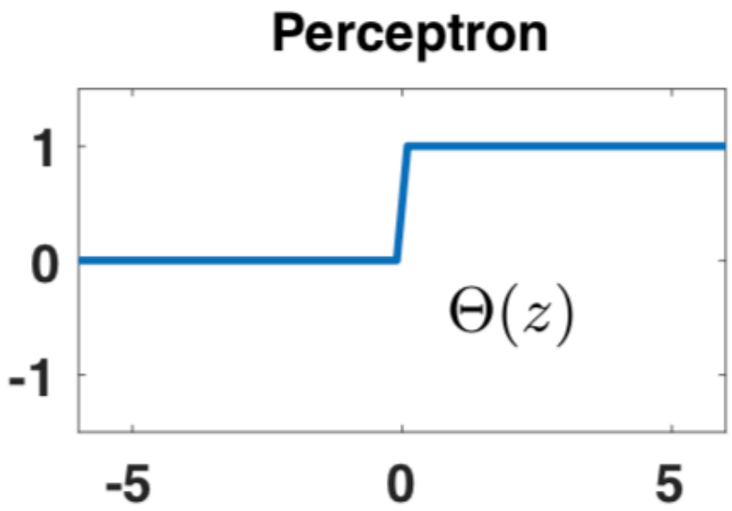
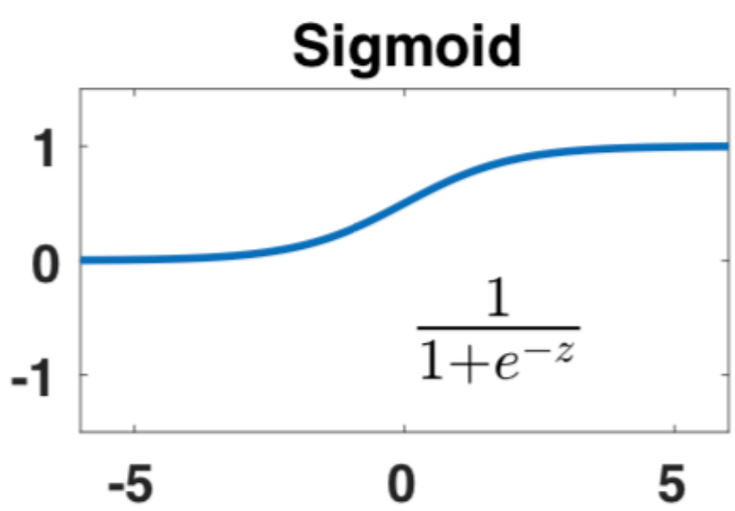
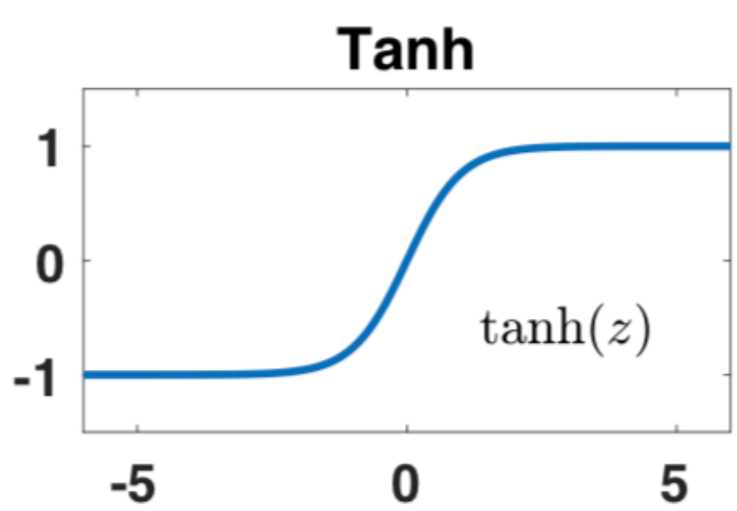
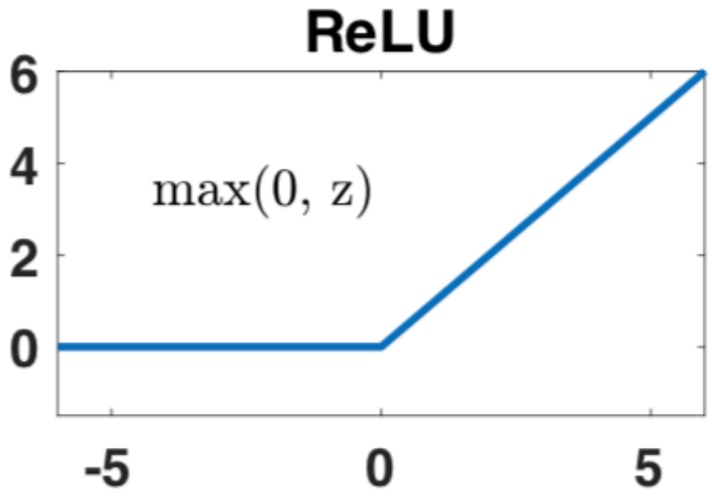
Neural Network **training** or **learning** means adjusting the model parameters (weights and biases) to **optimise** some figure of merit (cost function)

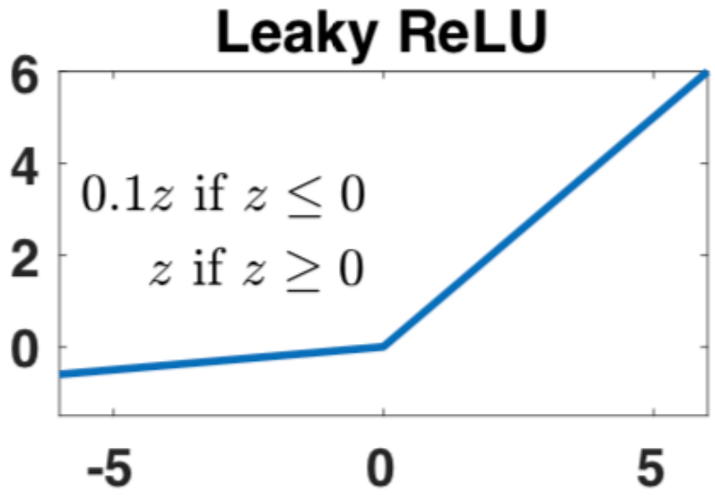
Activation functions

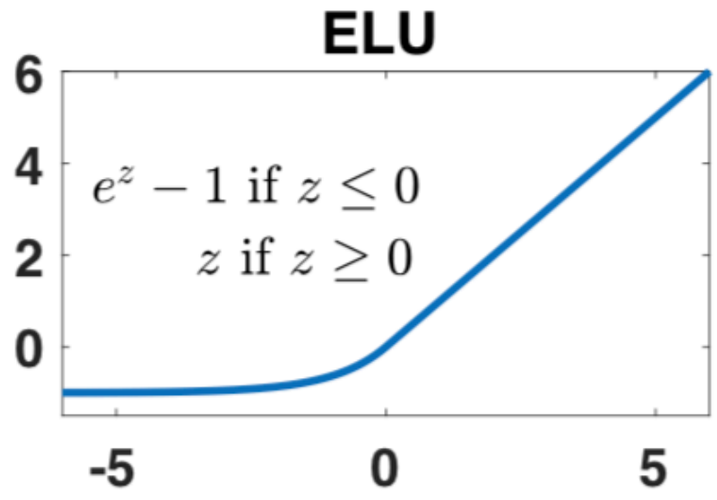








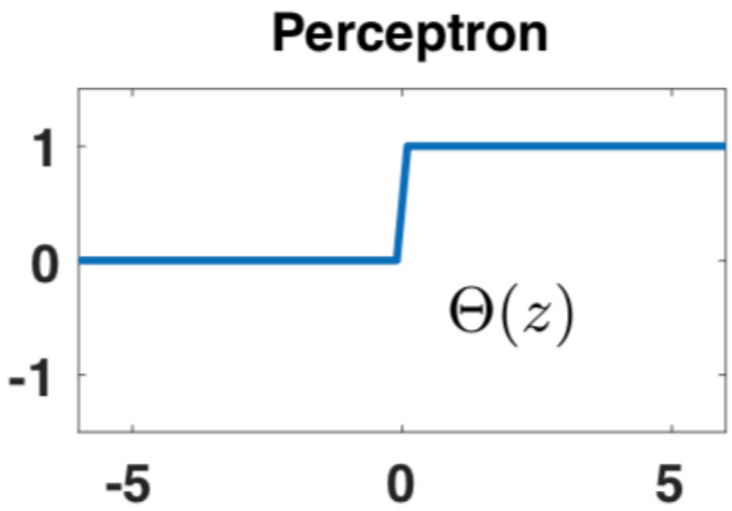


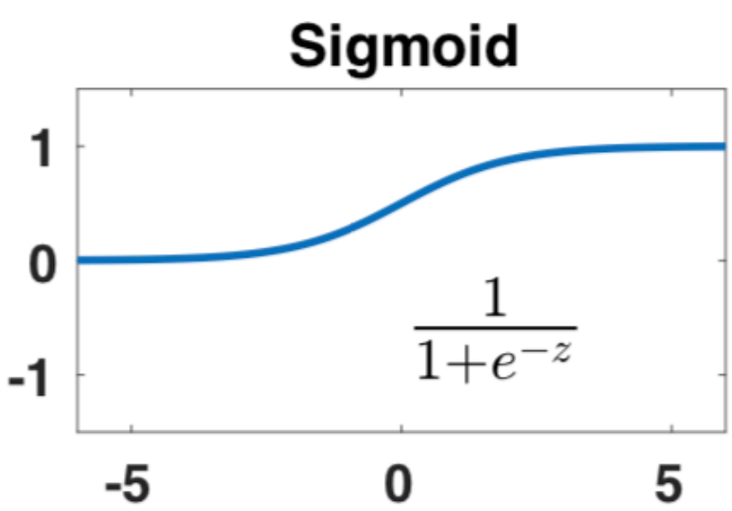


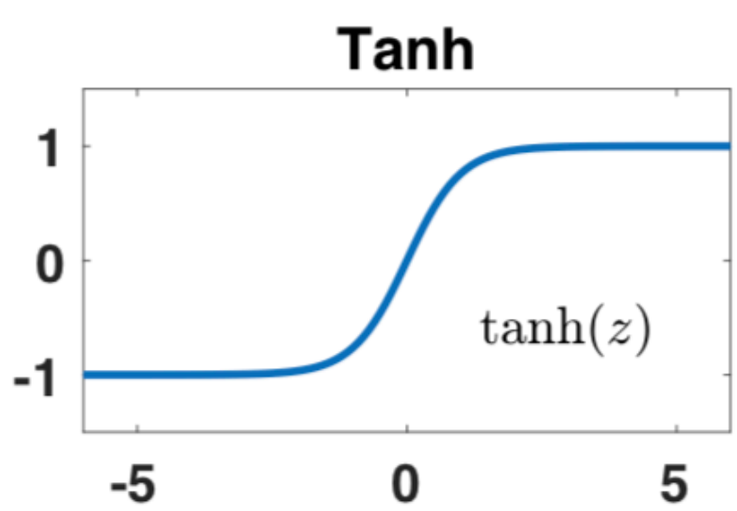
what is the main difference between these various activation functions?

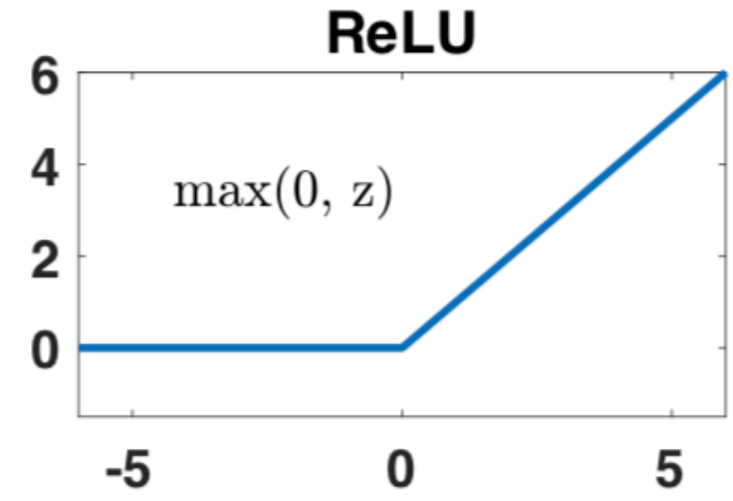
and how it could affect NN training?

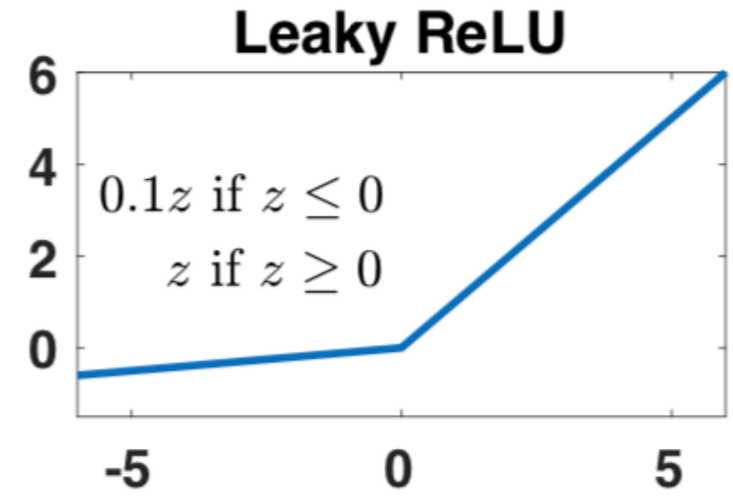
Activation functions

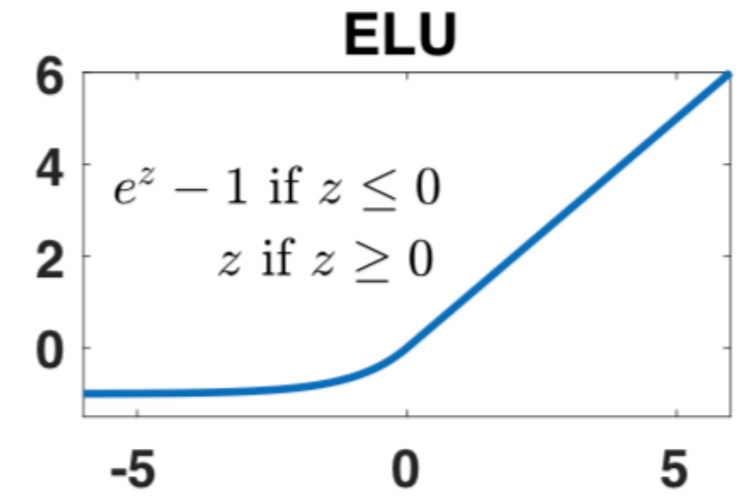












- Activation functions can be classified between those that **saturate at large inputs** (*e.g.* sigmoid) and those that **do not saturate at large inputs** (*e.g.* Rectified Linear Units ReLU)

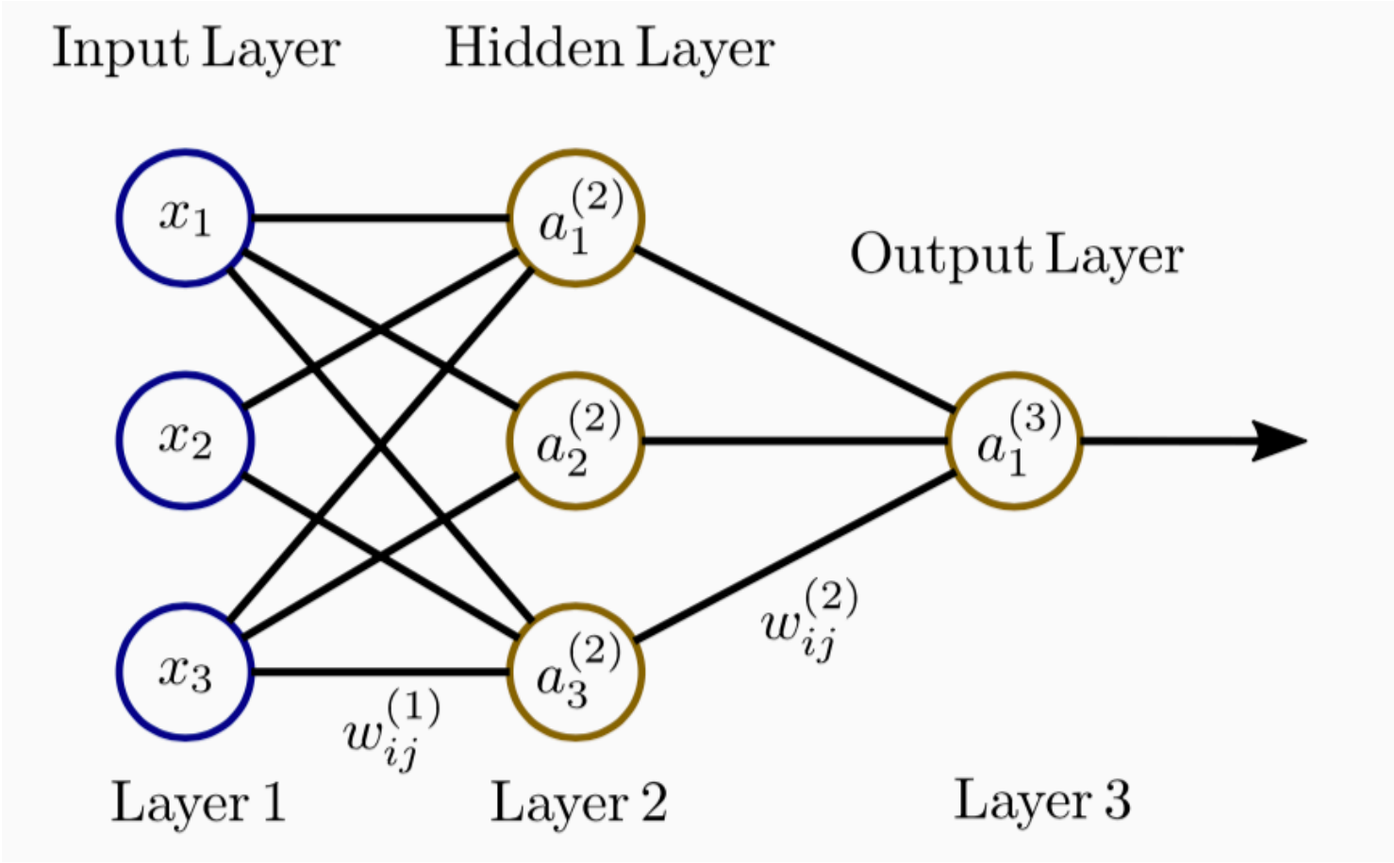
- The choice of non-linearities has important implications for **GD NN training methods:**

sigmoid $\longrightarrow \left.\frac{d\sigma}{dz}\right|_{z\gg 1} = 0$ ***ReLU*** $\longrightarrow \left.\frac{d\sigma}{dz}\right|_{z\gg 1} \neq 0$

vanishing gradients are problematic for deep networks: loss of sensitivity

A simple network

to realise that NNs are nothing mysterious but just a **complex non-linear mapping** between inputs and outputs, consider the explicit calculation of the output of a simple network



can we evaluate analytically $a_1^{(3)}$ as function of x_1, x_2, x_3?

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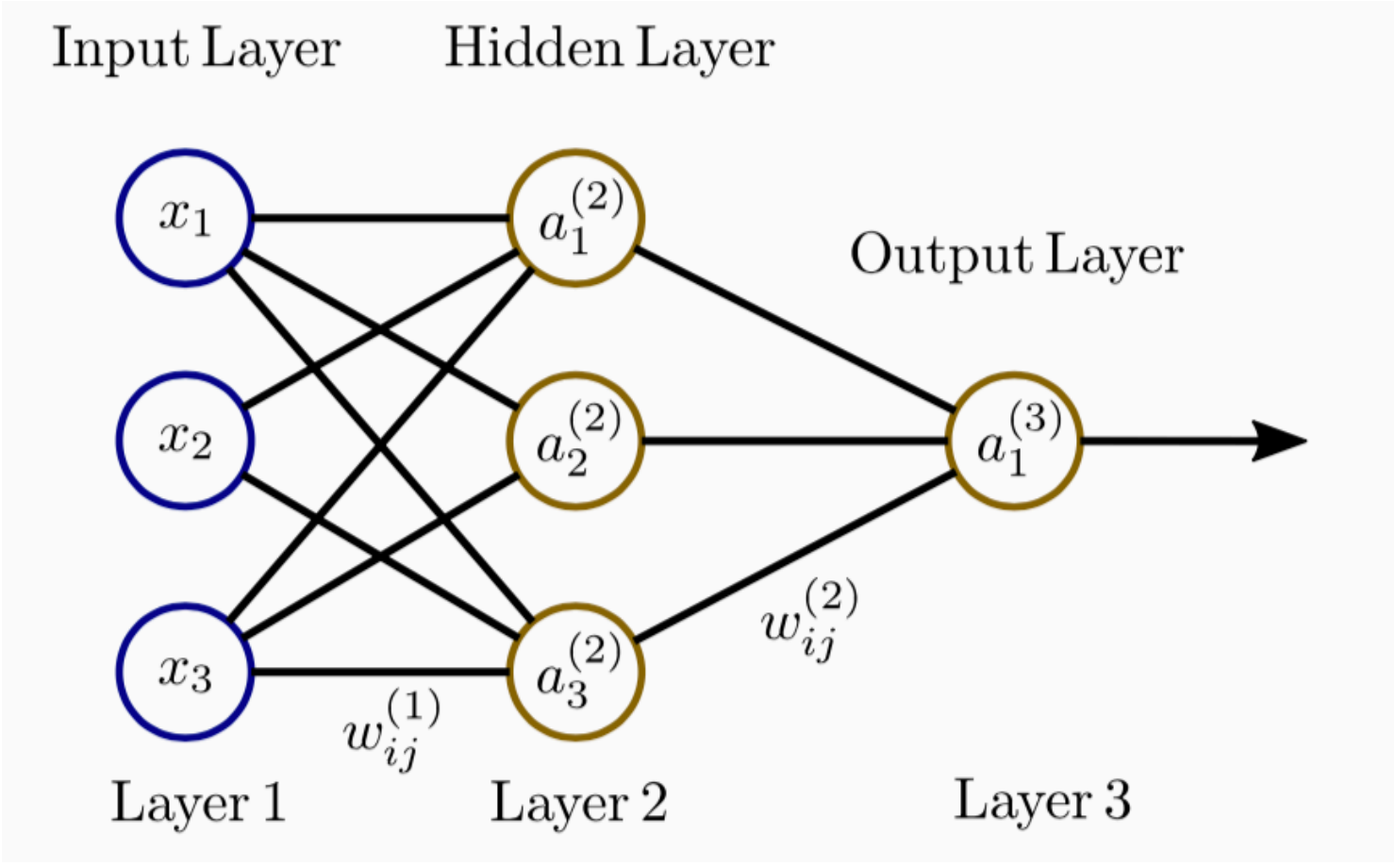

using the three inputs (Layer 1), compute activation states of neurons in Layer 2

$$a_1^{(2)} = \sigma\left(x_1\theta_{11}^{(1)} + x_2\theta_{12}^{(1)} + x_3\theta_{13}^{(1)} + \theta_{10}^{(1)}\right)$$

$$a_2^{(2)} = \sigma\left(x_1\theta_{21}^{(1)} + x_2\theta_{22}^{(1)} + x_3\theta_{23}^{(1)} + \theta_{20}^{(1)}\right)$$

$$a_2^{(3)} = \sigma\left(x_1\theta_{31}^{(1)} + x_2\theta_{32}^{(1)} + x_3\theta_{33}^{(1)} + \theta_{30}^{(1)}\right)$$

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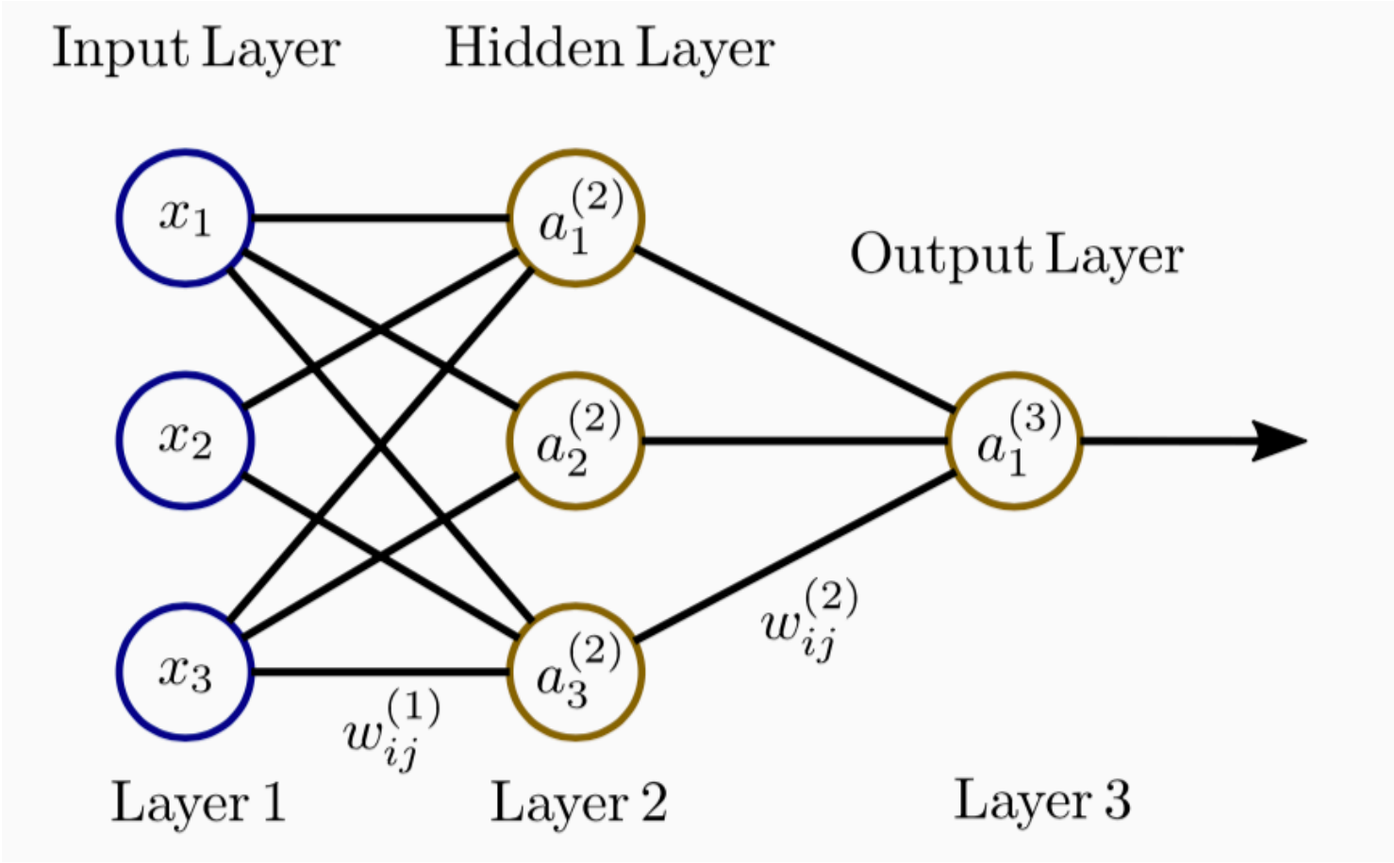


using the activation states of neurons in Layer 2, compute activation state of output neuron

$$a_1^{(3)} = \sigma\left(a_1^{(2)}\theta_{11}^{(2)} + a_2^{(2)}\theta_{12}^{(2)} + a_3^{(2)}\theta_{13}^{(2)} + \theta_{10}^{(2)}\right)$$

NN output is **analytical function** of the inputs and the model parameters

A simple network

to realise that NNs are nothing mysterious but just a **complex non-linear mapping** between inputs and outputs, consider the explicit calculation of the output of a simple network

$$a_1^{(3)} = \sigma\Bigg(\sigma\left(x_1\theta_{11}^{(1)} + x_2\theta_{12}^{(1)} + x_3\theta_{13}^{(1)} + \theta_{10}^{(1)}\right)\theta_{11}^{(2)} +$$

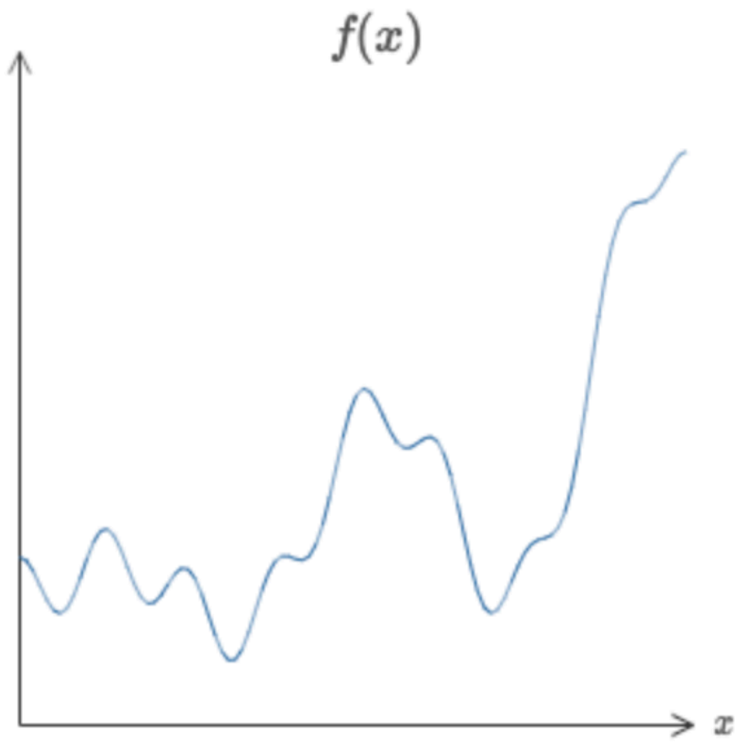
$$\sigma\left(x_1\theta_{21}^{(1)} + x_2\theta_{22}^{(1)} + x_3\theta_{23}^{(1)} + \theta_{20}^{(1)}\right)\theta_{12}^{(2)} +$$

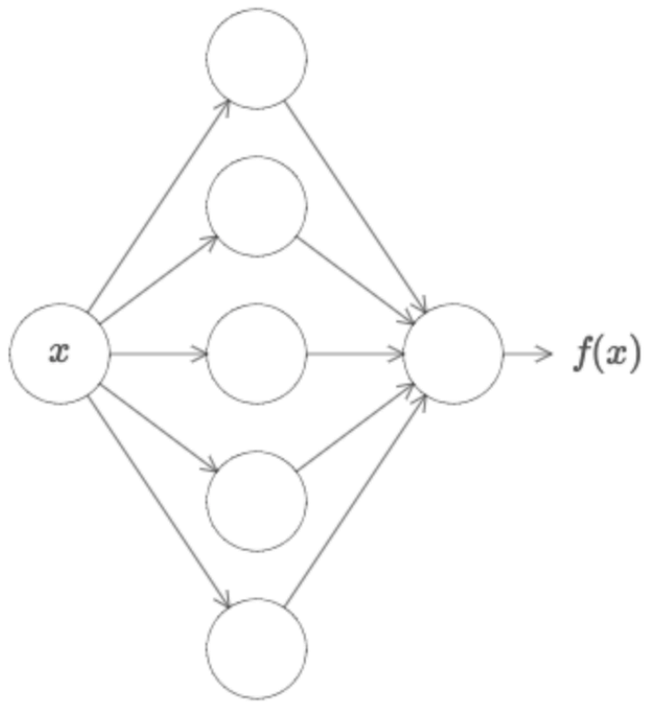
$$\sigma\left(x_1\theta_{31}^{(1)} + x_2\theta_{32}^{(1)} + x_3\theta_{33}^{(1)} + \theta_{30}^{(1)}\right)\theta_{13}^{(2)} + \theta_{10}^{(2)}\Bigg)$$

substitute the activation function *e.g.* for the sigmoid and you have the **analytic output** of a simple NN

The Universal Approximation Theorem

theorem: a neural network with a single hidden layer and enough neurones can **approximate any continuous, multi-input/multi-output function** with arbitrary accuracy





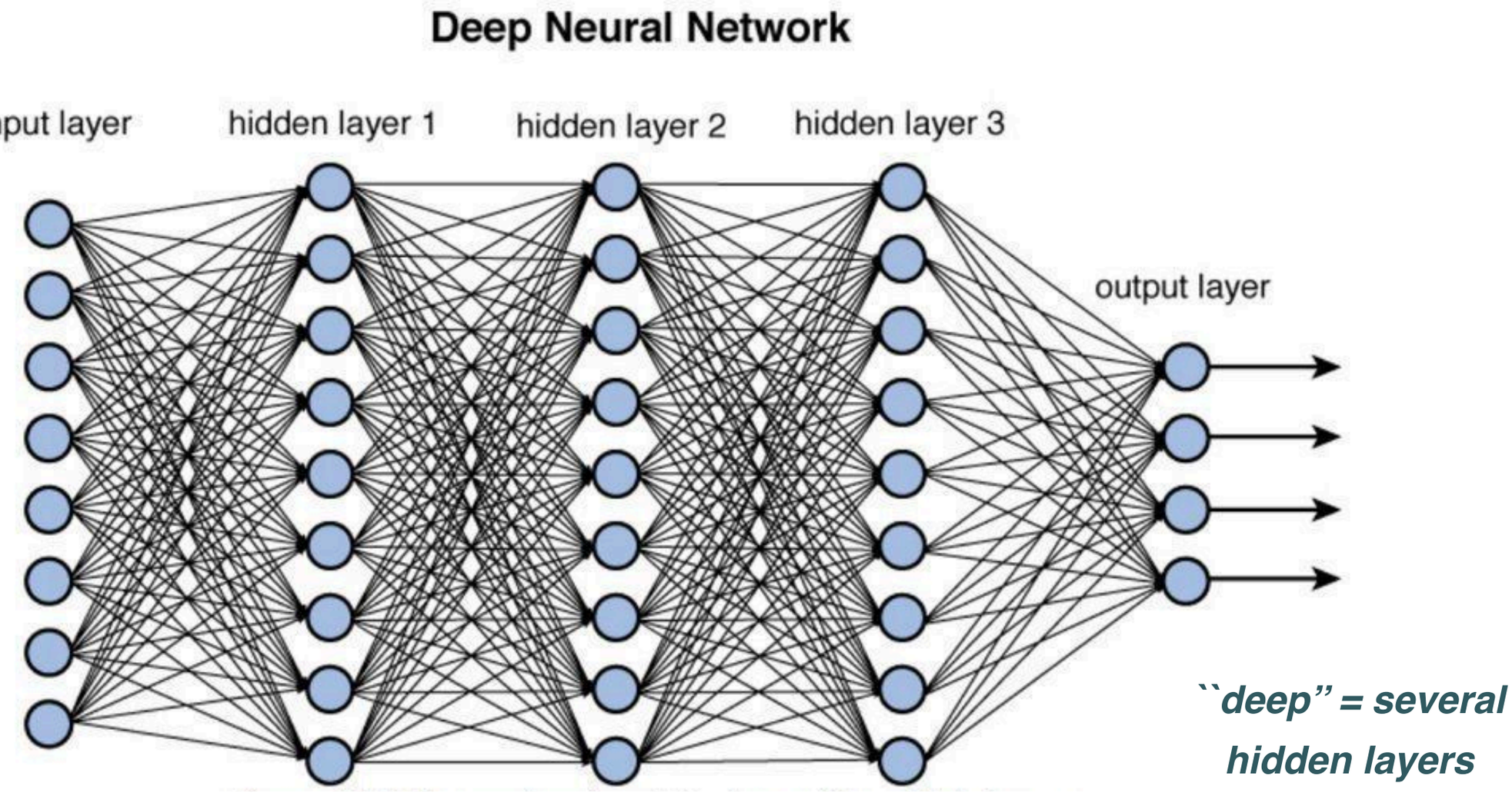
neural networks exhibit *universality properties:* no matter what function we want to compute, we know (theorem!) that there is a neural network which can carry out this task

See M. Nielsen, *Neural Networks and Deep Learning*: http://neuralnetworksanddeeplearning.com/chap4.html

Deep Networks

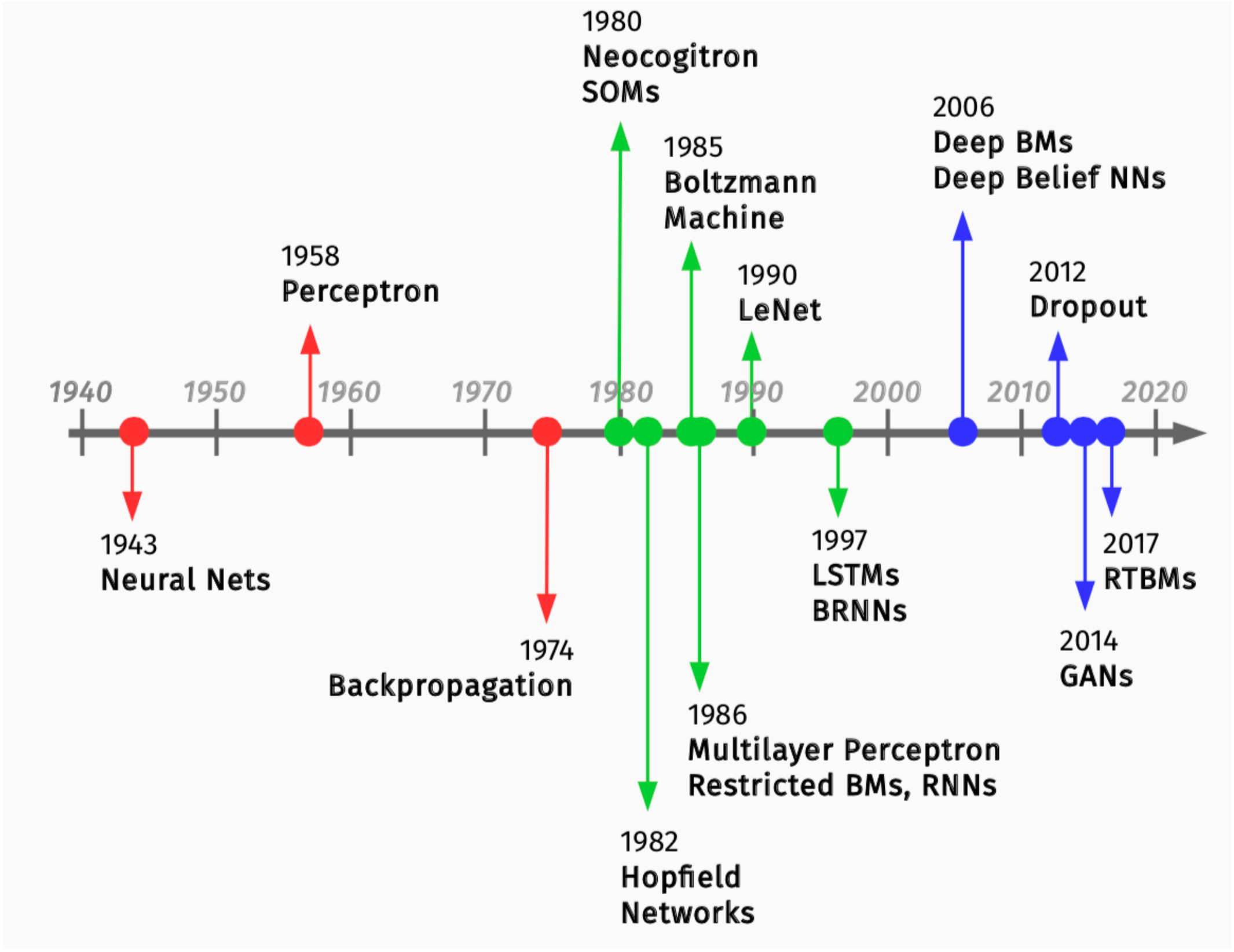
A neural network can thus be thought of a **complicated non-linear mapping** between the inputs and the outputs that depends on the parameters (weights and bias) of each neuron

We can make a NN **deep** by adding hidden layers, which greatly expands their **representational power**, also known as **expressivity**



``deep'' = several hidden layers

A timeline of neural networks



NN training

As standard in **Supervised Learning**, the first step to train a NN is to specify a **cost function**

$$\left(\boldsymbol{x}_i, y_i\right) \ , \quad i = 1,\ldots,n \longrightarrow \hat{y}_i\left(\boldsymbol{\theta}\right) \ , \quad i = 1,\ldots,n$$

for each of the n data points … *… the output of the NN provides the model prediction*

the loss function depends on whether the NN should provide **continuous or categorical** (discrete) predictions. For continuous data we can have the **mean square error**

$$E(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_i\left(\boldsymbol{\theta}\right)\right)^2$$

for categorical data we use the **cross-entropy**, which for binary (true/false) classification is

$$E(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i \ln \hat{y}_i(\boldsymbol{\theta}) + (1 - y_i)\ln(1 - \hat{y}_i(\boldsymbol{\theta}))\right)$$

where the true labels satisfy $y_i \in \{0,1\}$

NN training are based on a specific version of GD methods: **backpropagation**

Backpropagation

For deep NNs the brute-force evaluation of the **gradients of the cost function** is impractical

GD method:

$$\mathbf{v}_t = \eta_t \nabla_\theta E(\boldsymbol{\theta}_t)\,, \qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_t$$

learning rate

gradient of cost function

*update of model parameters between iterations **t** and **t+1***

Why? What prevents us from using simple GD to train NNs?

Backpropagation

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*update of model parameters between iterations **t** and **t+1***

instead one uses **backpropagation**, which cleverly exploits the **layered structure** of NNs

we will use the following notation:

- A neural network with ***L* layers**, labelled as *l=1,…,L*
- $\omega_{jk}^{(l)}$**: weights** connecting *k*-th neuron in the *(l-1)*-th layer to *j*-th neutron in the *l*-th layer
- $b_j^{(l)}$ **: bias** of the *j*-th neuron in the *l*-th layer
- $a_j^{(l)}$**: activation state** of the *j*-th neuron in the *l*-th layer

Backpropagation

feed-forward NNs: the activation state of the *j*-th neuron in the *l*-th layer is a (nonlinear) function of the activation states of all the neutrons in the *(l-1)*-th layer

$$a_j^{(l)} = \sigma\left(\sum_{k=1}^{n_{l-1}} \omega_{jk}^{(l)} a_k^{(l-1)} + b_j^{(l)}\right) \equiv \sigma(z_j^{(l)}), \quad j = 1,\ldots,n_l$$

the cost function of the NN therefore depends on:

- $a_j^{(L)}$: **activation states** of the neurons on the **output layer *L*** (directly)
- $a_j^{(l)}$: **activation states** of the neurons on the hidden layers ***l* <*L*** (indirectly)

we define the **error** associated to the *j*-th neuron in the output layer and hidden layers as

$$\Delta_j^{(L)} \equiv \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(L)}} \qquad \Delta_j^{(l)} \equiv \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(l)}} = \frac{\partial E(\boldsymbol{\theta})}{\partial a_j^{(l)}} \frac{da_j^{(l)}}{dz_j^{(l)}}$$

here assume that output layer is linear: ensures that model predictions are unbounded

Backpropagation

$$\Delta_j^{(L)} = \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(L)}} \qquad \Delta_j^{(l)} = \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(l)}} = \frac{\partial E(\boldsymbol{\theta})}{\partial a_j^{(l)}} \sigma'\left(z_j^{(l)}\right)$$

to derive the backpropagation equations, we will use the chain rule & NN layer structure

$$\Delta_j^{(l)} = \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(l)}} = \sum_{k=1}^{n_{l+1}} \frac{\partial E(\boldsymbol{\theta})}{\partial z_k^{(l+1)}} \frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}} = \sum_{k=1}^{n_{l+1}} \Delta_k^{(l+1)} \frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}}$$

where here we exploit the **NN layered structure:** activation states of neurons in *(l+1)*-th layer depends only on activation states of neurons in *l*-th layer

$$\Delta_j^{(l)} = \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(l)}} = \sum_{k=1}^{n_{l+1}} \Delta_k^{(l+1)} \frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}} = \left(\sum_{k}^{n_{l+1}} \Delta_k^{(l+1)} \omega_{kj}^{(l+1)} \right) \sigma'\left(z_j^{(l)}\right)$$

Backpropagation

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where here we exploit the **NN layered structure:** activation states of neurons in *(l+1)*-th layer depends only on activation states of neurons in *l*-th layer

$$\Delta_j^{(l)} = \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(l)}} = \sum_{k=1}^{n_{l+1}} \Delta_k^{(l+1)} \frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}} = \left(\sum_{k}^{n_{l+1}} \Delta_k^{(l+1)} \omega_{kj}^{(l+1)} \right) \sigma'\left(z_j^{(l)}\right)$$

$$z_k^{(l+1)} = \sum_{k'=1}^{n_l} \omega_{jk'}^{(l+1)} a_{k'}^{(l)} + b_j^{(l+1)} = \sum_{k'=1}^{n_l} \omega_{jk'} \sigma(z_{k'}^{l}) + b_j^{(l+1)}$$

Backpropagation

$$\Delta_j^{(L)} = \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(L)}} \qquad \Delta_j^{(l)} = \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(l)}} = \frac{\partial E(\boldsymbol{\theta})}{\partial a_j^{(l)}} \sigma'\left(z_j^{(l)}\right)$$

to derive the backpropagation equations, we will use the chain rule & NN layer structure

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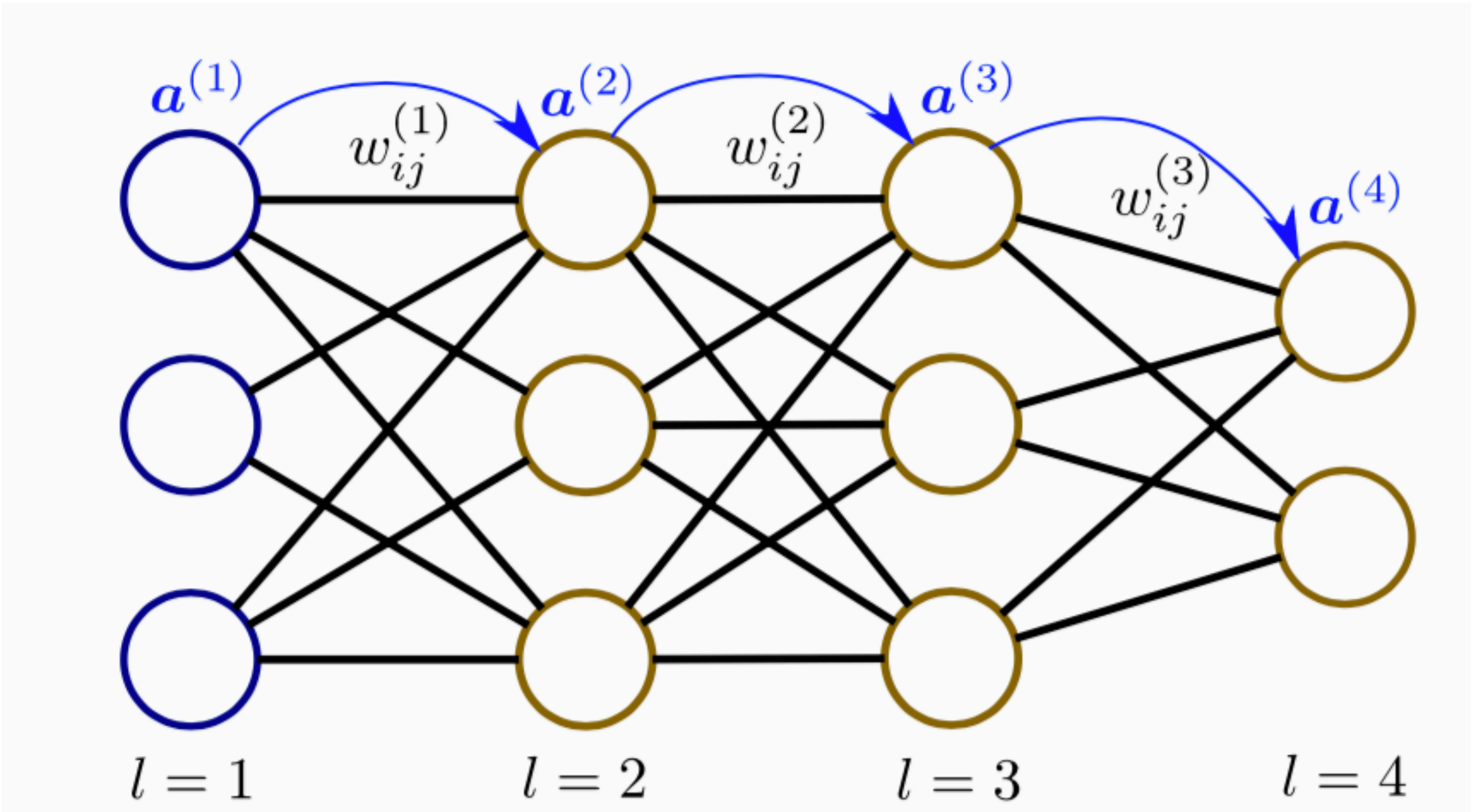
$$\frac{\partial E}{\partial \omega_{jk}^{(l)}} = \frac{\partial E}{\partial z_j^{(l)}} \frac{\partial z_j^{(l)}}{\partial \omega_{jk}^{(l)}} = \Delta_j^{(l)} a_k^{(l-1)}$$

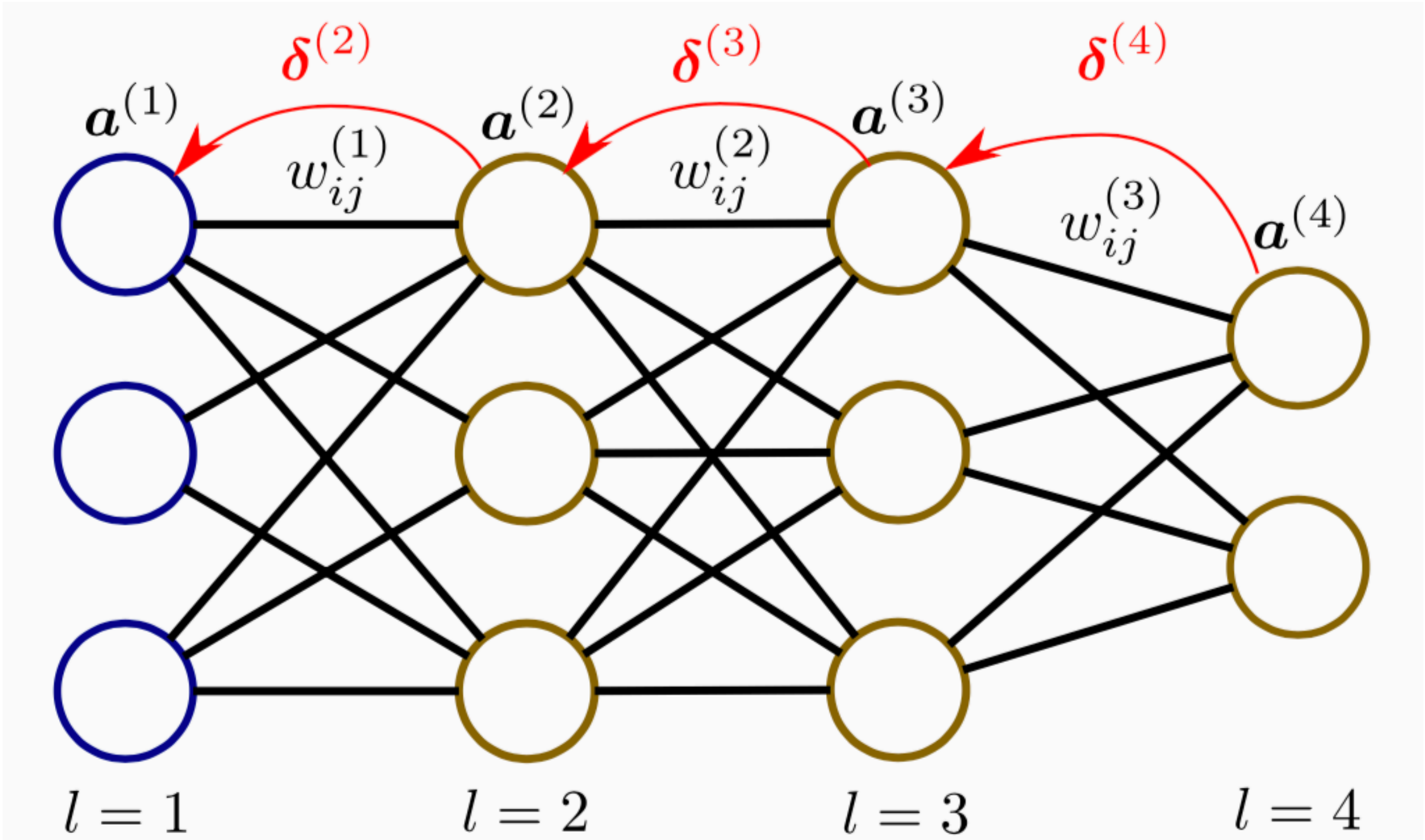
Backpropagation

first evaluate the activation states of all neurons using **forward propagation …**



Backpropagation

then **backpropagate** to evaluate the **errors Δ** and thus the gradients over model parameters



Backpropagation

we now have all the ingredients to deploy the **backpropagation algorithm for NN training**

- ***(1)*** Evaluate activation state of neurons in input layer $a_j^{(1)}, \quad j = 1,\ldots,n_1$

- ***(2)*** **Feed-forward:** evaluate activation states for each subsequent layer

$$a_j^{(l)} = \sigma\left(\sum_{k=1}^{n_l} \omega_{jk}^{(l)} a_k^{(l-1)} + b_j^{(l)}\right) \equiv \sigma(z_j^{(l)}) \quad , l = 2,\ldots,L$$

- ***(3)*** With this information evaluate error on network's output layer

$$\Delta_j^{(L)} = \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(L)}}$$

here enters dependence on cost function

- ***(4)*** **Backpropagate** this error to evaluate the errors on all hidden layers

$$\Delta_j^{(l)} = \left(\sum_{k}^{n_{l+1}} \Delta_k^{(l+1)} \omega_{kj}^{(l+1)}\right) \sigma'\left(z_j^{(l)}\right)$$

error in j-th neuron in (l)-th layer

error in k-th neuron in (l+1)-th layer

Backpropagation

we now have all the ingredients to deploy the **backpropagation algorithm for NN training**

- ***(5)*** Evaluate **gradients of the model parameters** associated to the gradient of cost function

$$\frac{\partial E}{\partial \omega_{jk}^{(l)}} = \Delta_j^{(l)} a_k^{(l-1)} \qquad \frac{\partial E}{\partial b_j^{(l)}} = \Delta_j^{(l)}$$

extremely efficient way of calculating the gradients of the model parameters, requiring only a **single forward and backward pass** of the neural network

$$\Delta_j^{(L)} = \frac{\partial E(\boldsymbol{\theta})}{\partial z_j^{(L)}}$$

at most j numerical derivatives need to be evaluated, even in NNs with millions of parameters

Backpropagation

we now have all the ingredients to deploy the **backpropagation algorithm for NN training**

- ***(5)*** Evaluate **gradients of the model parameters** associated to the gradient of cost function

$$\frac{\partial E}{\partial \omega_{jk}^{(l)}} = \Delta_j^{(l)} a_k^{(l-1)} \qquad \frac{\partial E}{\partial b_j^{(l)}} = \Delta_j^{(l)}$$

extremely efficient way of calculating the gradients of the model parameters, requiring only a **single forward and backward pass** of the neural network

with this info one can carry out with Gradient Descent and **update the model parameters**

$$\mathbf{v}_t = \eta_t \nabla_\theta E(\boldsymbol{\theta}_t)\,, \qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_t$$

note that even with BP training of large (deep) networks can be **computationally intensive!**

Note that we are hiding under the carpet an important problem: what happens if the NN output enters the cost function in a non-trivial manner? Where is this issue relevant in BP?

Backpropagation

we now have all the ingredients to deploy the **backpropagation algorithm for NN training**

- ***(5)*** Evaluate **gradients of the model parameters** associated to the gradient of cost function

$$\frac{\partial E}{\partial \omega_{jk}^{(l)}} = \Delta_j^{(l)} a_k^{(l-1)} \qquad \frac{\partial E}{\partial b_j^{(l)}} = \Delta_j^{(l)}$$

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note that even with BP training of large (deep) networks can be **computationally intensive!**

Further complication if cost function **depends non-trivially on NN output**

$$E(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left(\mathscr{F}_i^{(\mathrm{dat})} - \mathscr{F}_i^{(\mathrm{model})}(\hat{\boldsymbol{y}};\boldsymbol{\theta})\right)^2$$

e.g. model requires integral of NN output

NN initialisation

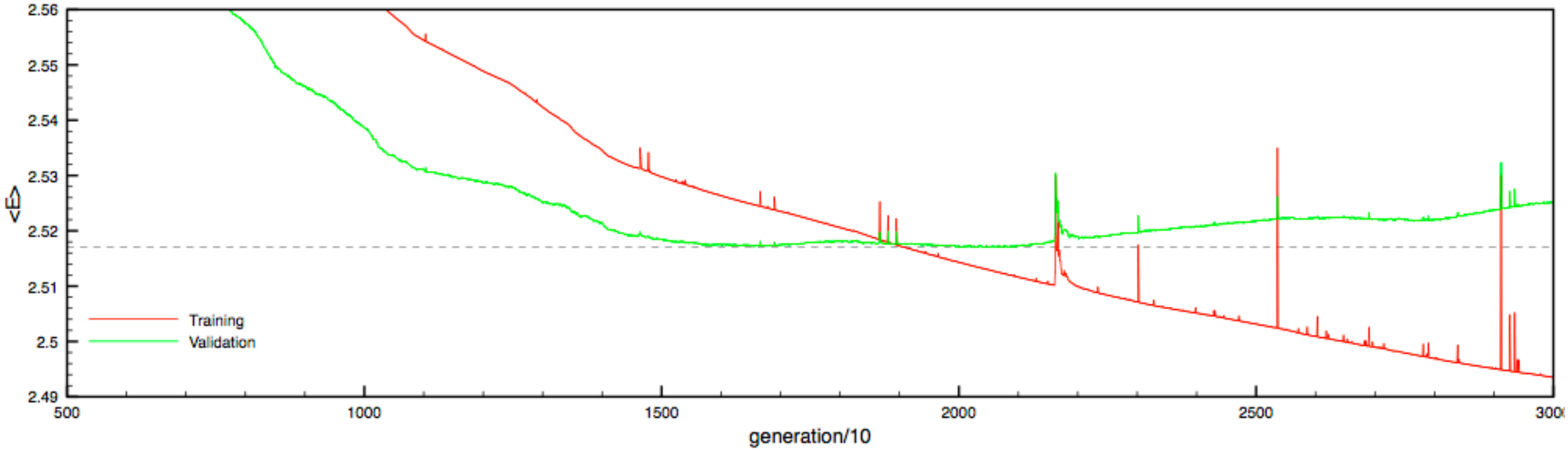
A further subtlety concerning NN training is that sometimes **a clever initialisation of the model parameters** helps in the learning process

- **zero:** all weights set to zero (initial complexity equivalent to single neuron)
- **random:** breaks parameter symmetry
- **glorot/xavier:** weights distributed randomly with Gaussian with variance based on in/out size of the neutron
- **he:** random initialisation avoiding the saturation region of the activation function

in many cases trial-and-error required to assess what works best

NN regularisation: cross-validation

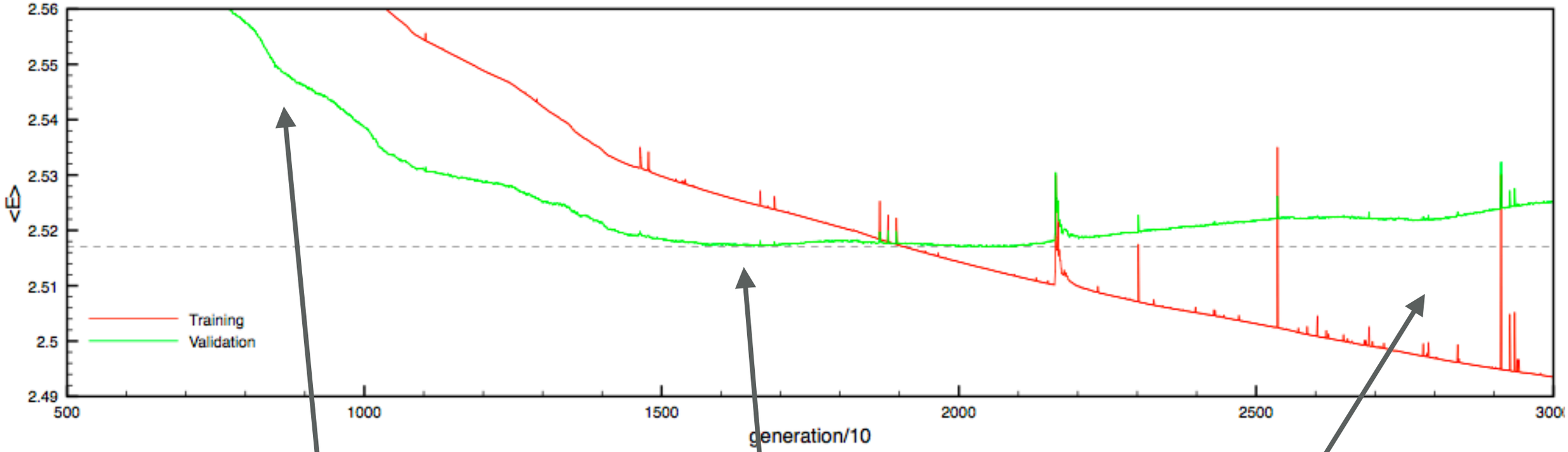
Neural networks provide extremely flexible models to describe complex datasets, but one should **avoid overfitting**, else the model will be **unable to generalise**



what is the optimal training length for this model?

NN regularisation: cross-validation

Neural networks provide extremely flexible models to describe complex datasets, but one should **avoid overfitting**, else the model will be **unable to generalise**



underlearning

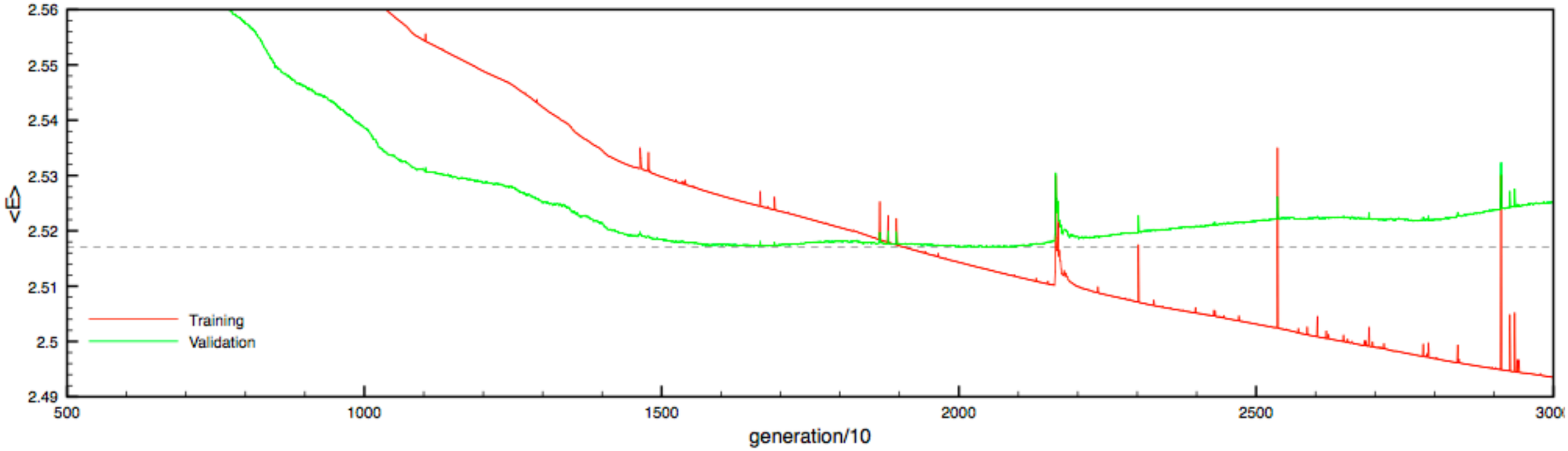
Optimal stopping

overfitting

recall the bias/variance tradeoff!

NN regularisation: cross-validation

Neural networks provide extremely flexible models to describe complex datasets, but one should **avoid overfitting**, else the model will be **unable to generalise**



Cross-validation look-back stopping: train the NN for a large fixed number of iterations. Then look back and determine the point at the training where the out-of-sample error was the smallest. Take as best-fit NN parameters those corresponding to that point of the training

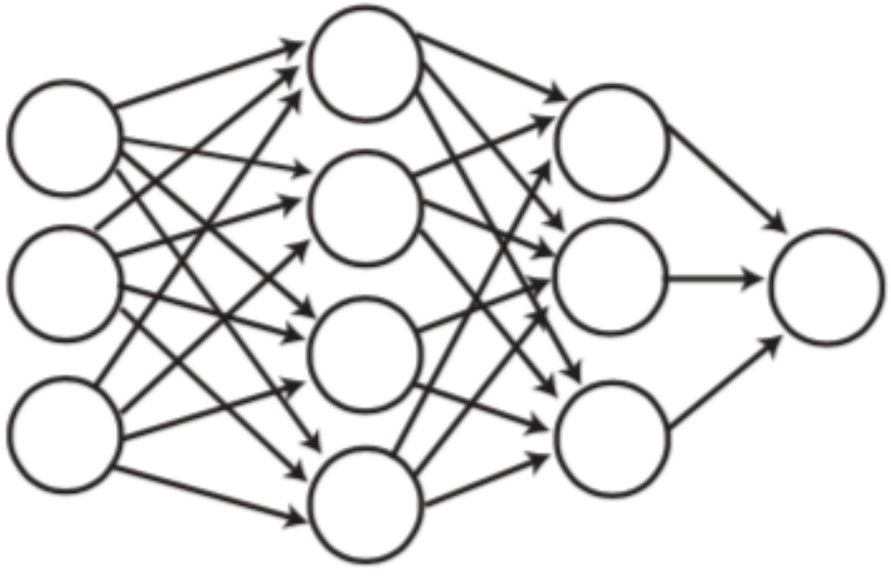
NN regularisation: Dropout

- Dropout is one of the standard **regularisation procedures** that aim to avoid overfitting when training deep NNs

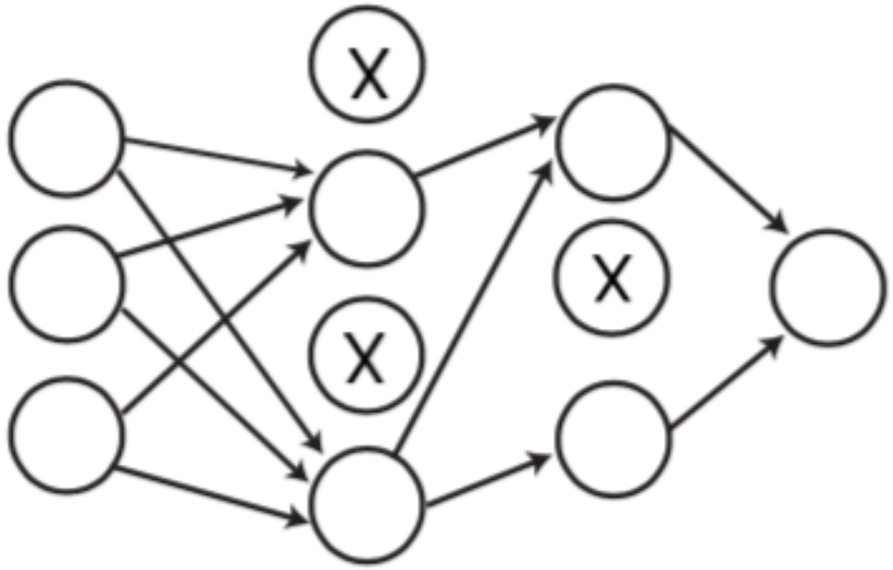
- During the training procedure, neurons are randomly "**dropped out**" of the neural network with some probability *p* giving rise to a thinned network, and the GD gradients are computed only there

- Dropout prevents overfitting by **reducing correlations among neurons** and reducing the variance

Standard Neural Net



After applying Dropout



effective reduction of model complexity!

Hyperoptimisation

In most Machine Learning applications, the model has several parameters which are typically **adjusted by hand** (trial and error) rather than algorithmically:

- Network architecture: number of layers of neurons per layer, activation functions, …
- Choice of minimiser (which of the GD variants?)
- Learning rate, momentum, memory, size of mini-batches, ….
- Regulariation parameters, stopping, dropout rate, patience, …

one can avoid the need of subjective choice by means of **an hyperoptimisation procedure**, where all model and training/stopping parameters are determined algorithmically

Such hyperoptimisation requires introducing a **reward function** to grade the model. Note that this is different from the **cost function:** the latter is optimised separately model by model (e.g. for each NN architecture) while the former compares between all optimised models

e.g. cost function $C = E_{\text{tr}}$ $R = E_{\text{val}}$ ***reward function***

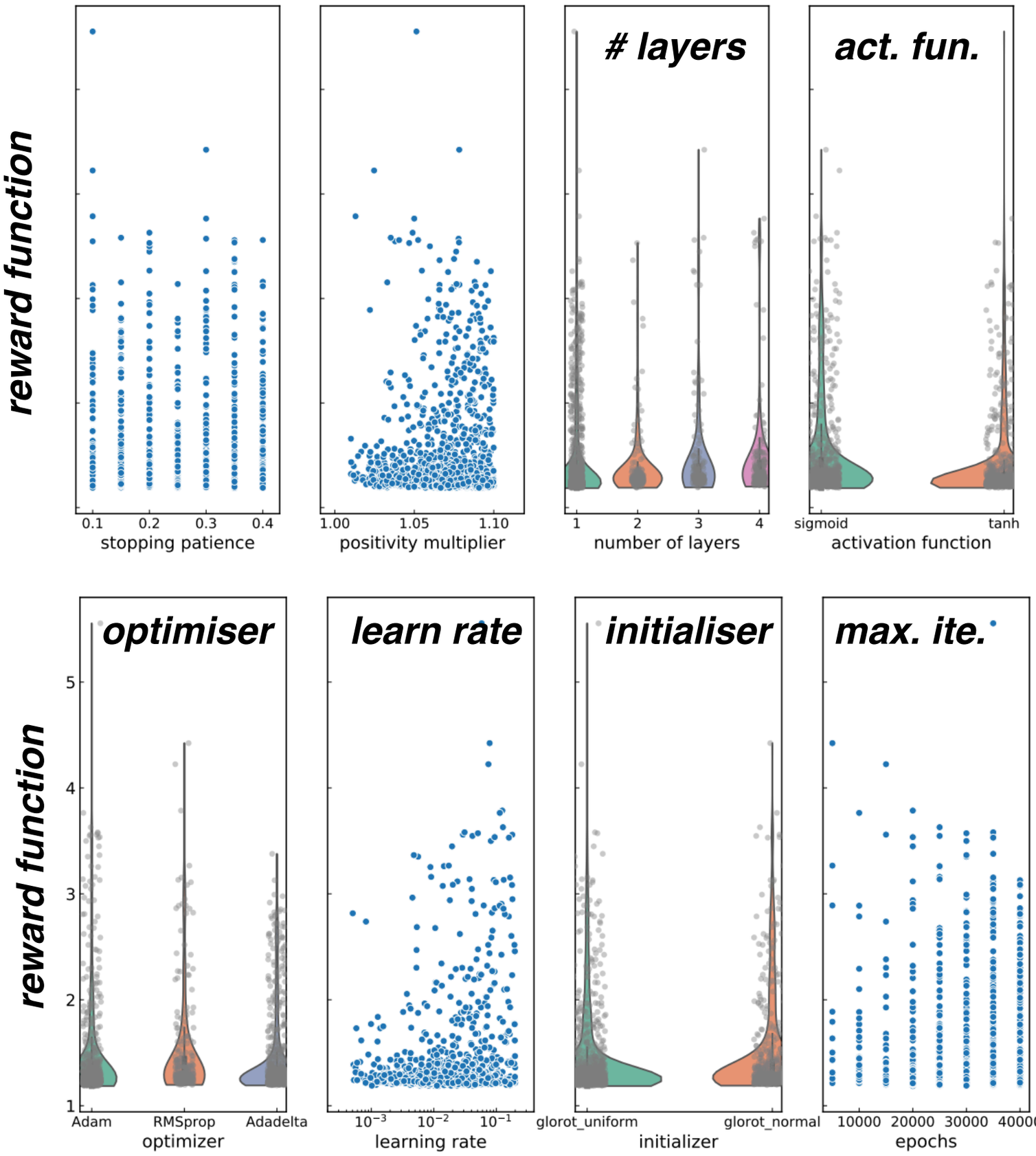
Hyperoptimisation

- In a hyperparameter scan one can compare the performance of **hundreds or thousands** of parameter combinations

- Some choices are **discrete** (type of minimiser, # of layers) others are **continuous** (learning rate)

- One can also **visualise** which choices are more crucial and which ones less important

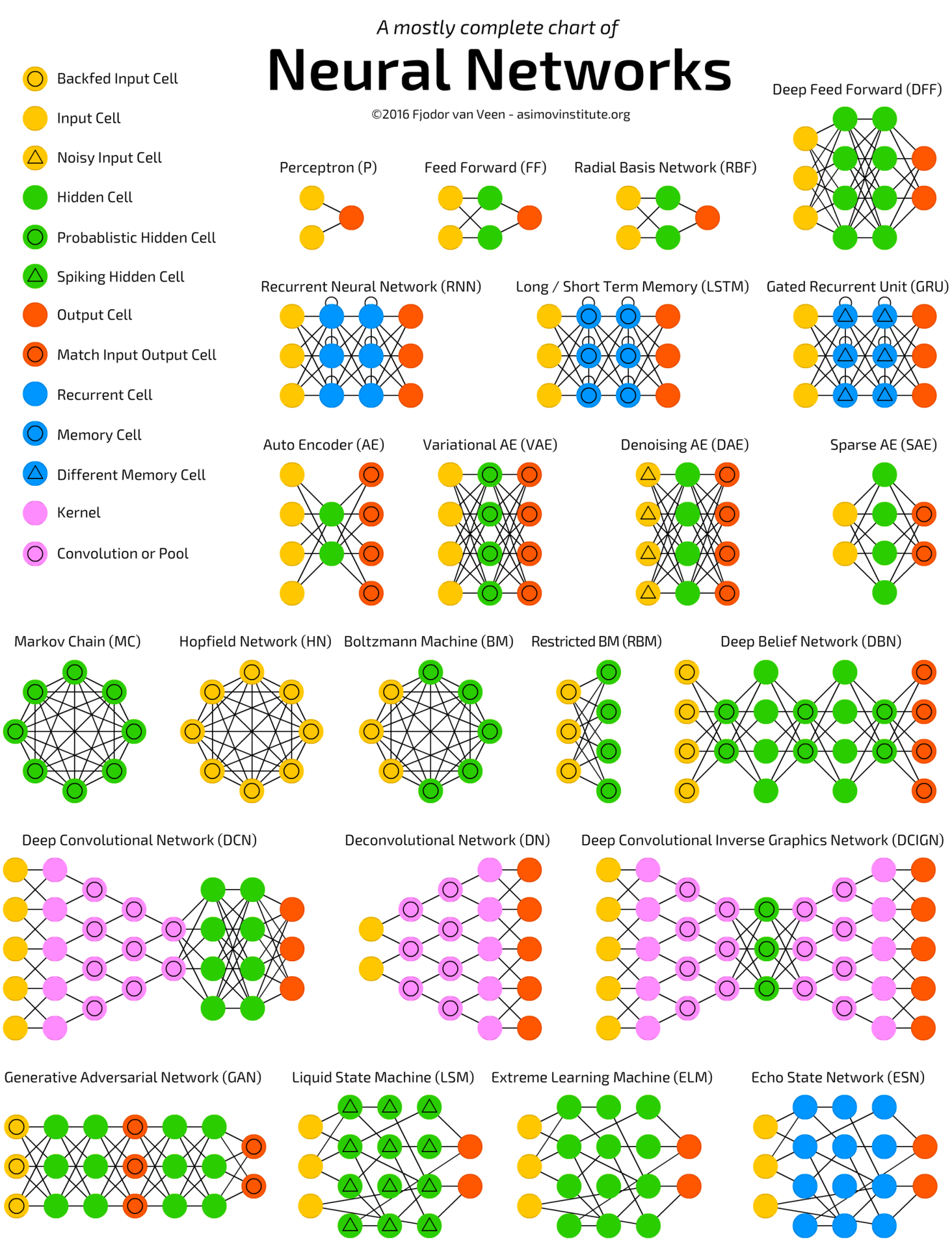
- The violin plots are the **KDE-reconstructed probability distributions** for the hyper-parameters



- A **large variety of neural network architectures** have been proposed: we will only study some of them in this course

- They differ in: number of layers and neurons, role of the neurons, connections between neurons and layers, ….

- Each architecture in general has associated **different training and regularisation strategies**: no fit-for-all methods available!

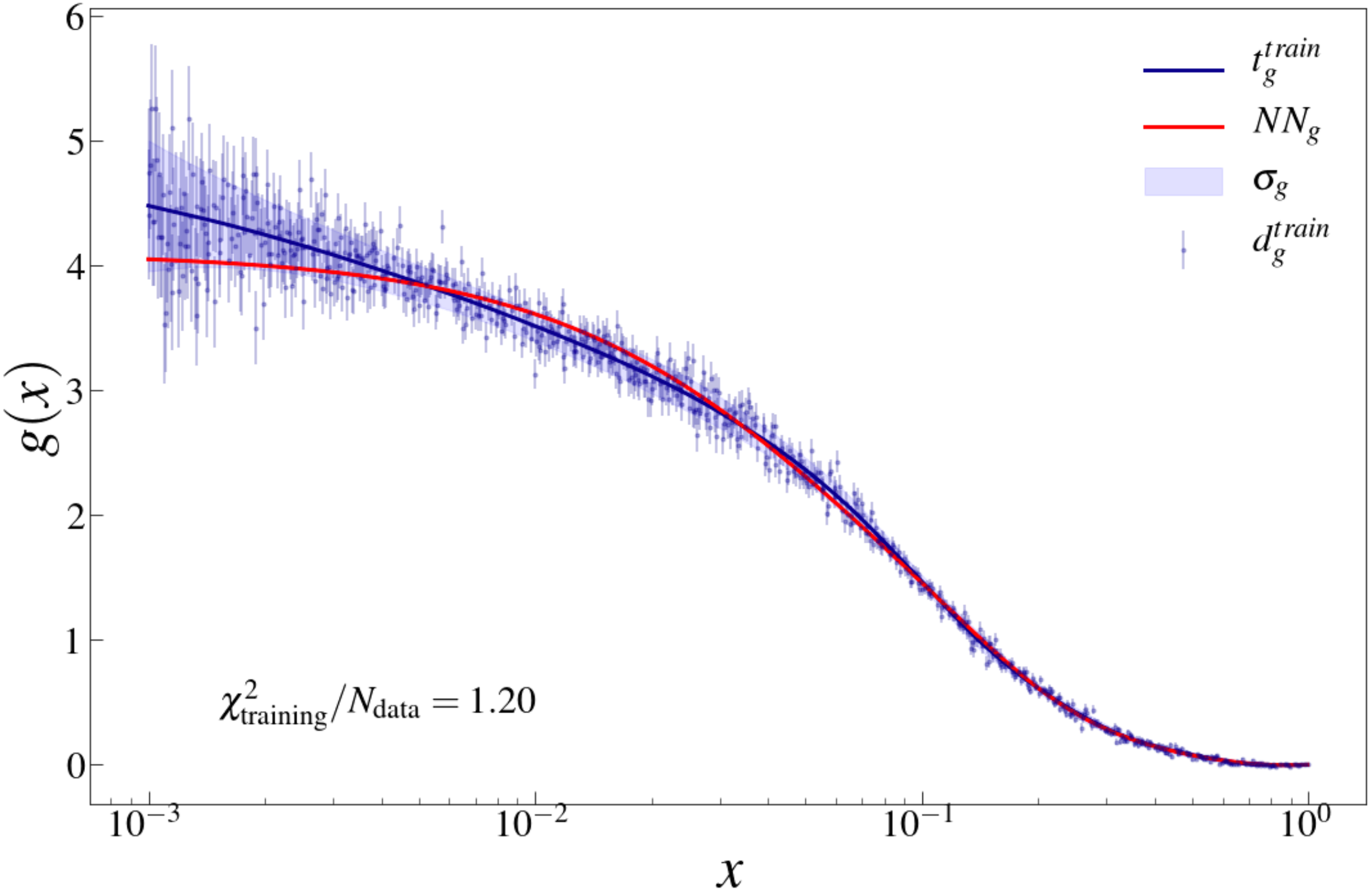


Tutorial 3: NN training with TensorFlow

- ☑ Introduction to **non-linear regression problems** using neural networks.
- ☑ You will learn how to **build and train neural networks** with TensorFlow, a powerful machine learning library.
- ☑ The goal will be to extract a certain physical property of protons, the distribution of momentum carried by their gluons, **from simulated pseudo-data** based on some known underlying truth
- ☑ The neural nets should then aim to l**earn this known underlying truth** from the data
- ☑ **Assess/avoid overfitting** and how to **estimate the model uncertainties**, e.g. What happens when different sets of NN parameters give an equally good description of the *experiment* data?

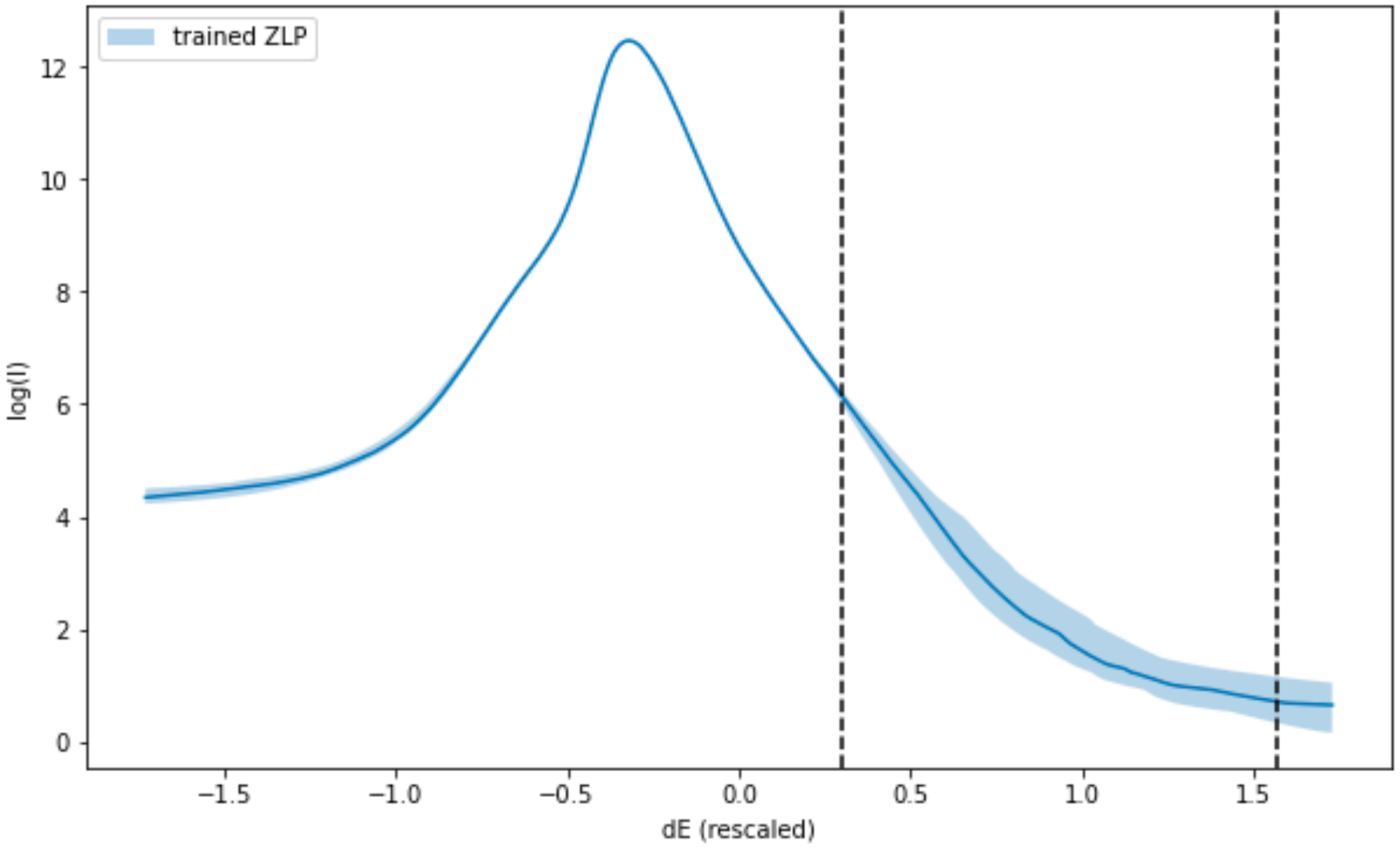
NB this procedure is known as ``closure test'', since by construction the ``truth'' underlying law is know (not the case in realistic applications)

Tutorial 3: NN training with TensorFlow



your first ever neural network training!

Tutorial 3(extra): NN training with PyTorch



☑ In the repo you will also find a notebook for NN regression now in the **PyTorch** framework.

☑ Here the goal is to model the dominant source of background, known as the **Zero-Loss-Peak** which arise in **Electron Energy Loss Spectroscopy** measurements

☑ If you are particularly brave, try to replace PyTorch by TensorFlow and check results are unchanged!

Summary and outlook

- Neural network are at the core of modern machine learning methods

- Today we discussed one of the most representative architectures, **deep feed-forward neural networks**

- Training of models with a very large number of free parameters can be efficiently carried out with **stochastic gradient descent combined with backpropagation**

- Crucial is to **avoid overfitting,** which will reduce the productivity performance of your NN model

- We will see many more NN architectures in the rest of this course!