

The building blocks of deep learning models - part 1

A light overview

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Deep learning: the building blocks

1. Function approximation
2. The neural network model:
 - a. the “neuron”
 - b. the network
3. Activation functions

This session

4. Cost functions
5. Gradient descent (and solvers/optimizers)
6. Forward propagation and the backward propagation algorithm

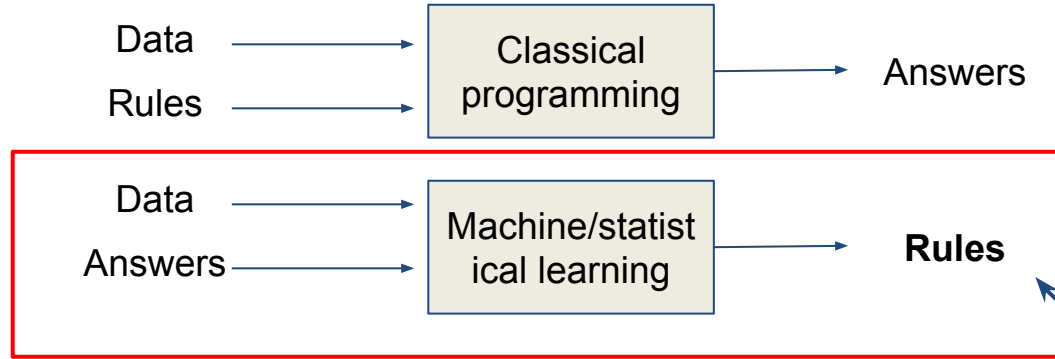
**Through the
logistic
regression
example**



Function approximation



Function approximation?

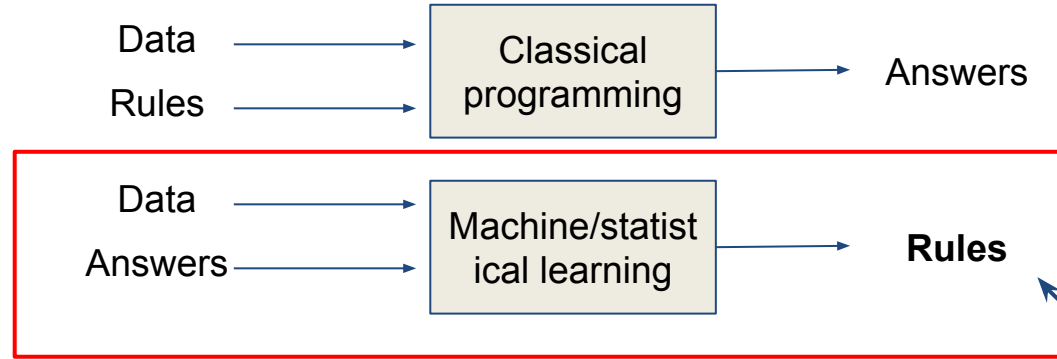


- **unknown function** that maps input data to output results (answers):

» $y = f(x) \leftarrow$ [mapping function]



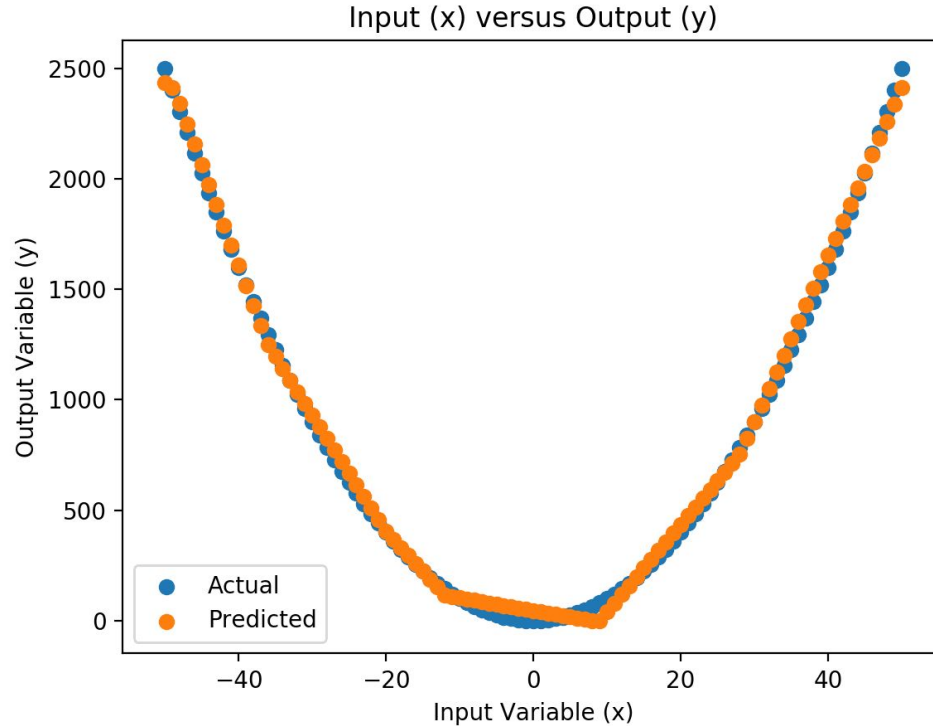
Function approximation?



- **unknown function** that maps input data to output results (answers):
 » $y = f(x) \leftarrow$ [mapping function]
- learn this function \rightarrow **function approximation**
- $f(x)$ can be **nonlinear** and quite **complex**



Function approximation - intuition



- (known) **quadratic function** (blue line)
- approximated with a **neural network model** [2 hidden layers with 10 nodes each] (orange line)



The universal approximation theorem

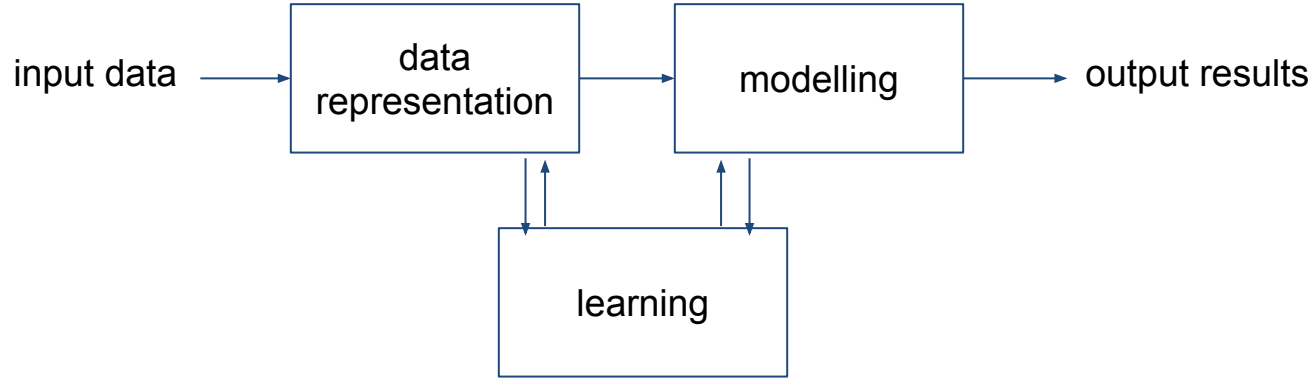
neural networks can approximate **any function**: “no matter what the function, there is guaranteed to be a neural network so that for every possible input, x , the value $f(x)$ (or some close approximation) is output from the network”

- naming a piece of music based on a short sample of the piece
- predicting a future phenotype (e.g. disease risk) from genomic data
- translating an Italian text into English (many possible functions, since there are often many acceptable translations of a given text)

powerful learning algorithms + universality → success of DL!



Function approximation



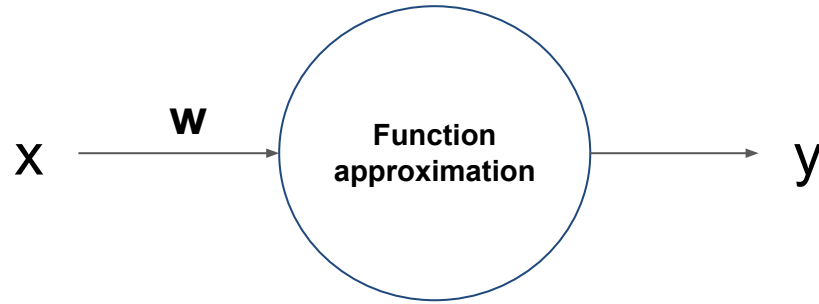
- NNs are ~~good~~ excellent at finding functions that accurately map x to y
- deep neural networks (NNs) are powerful **function approximators**
 - » $y = f(x)$
- **complex highly non-linear functions can lead to problems with generalization!**



The neural network model



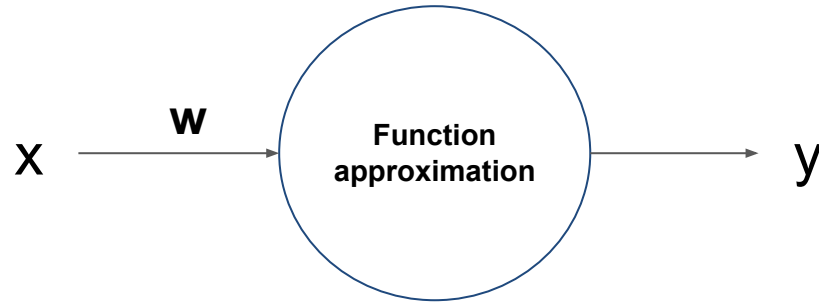
Neural network, the basic unit: the “neuron”



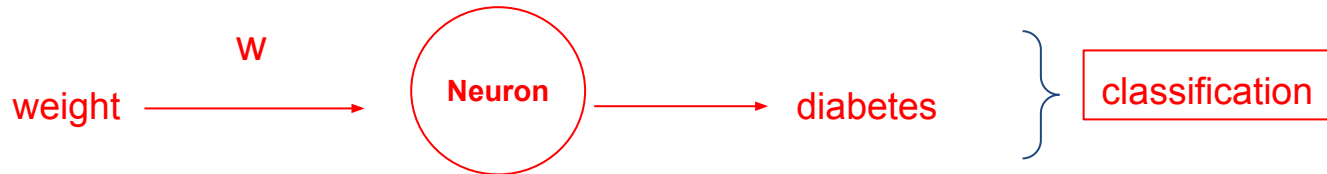
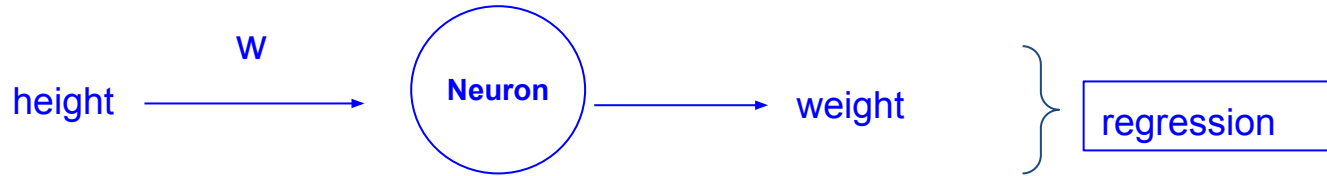
- Mc Culloch & Pitts (1943)
- **perceptron** (“neuron”):
 - dendrites
 - neuron
 - axon



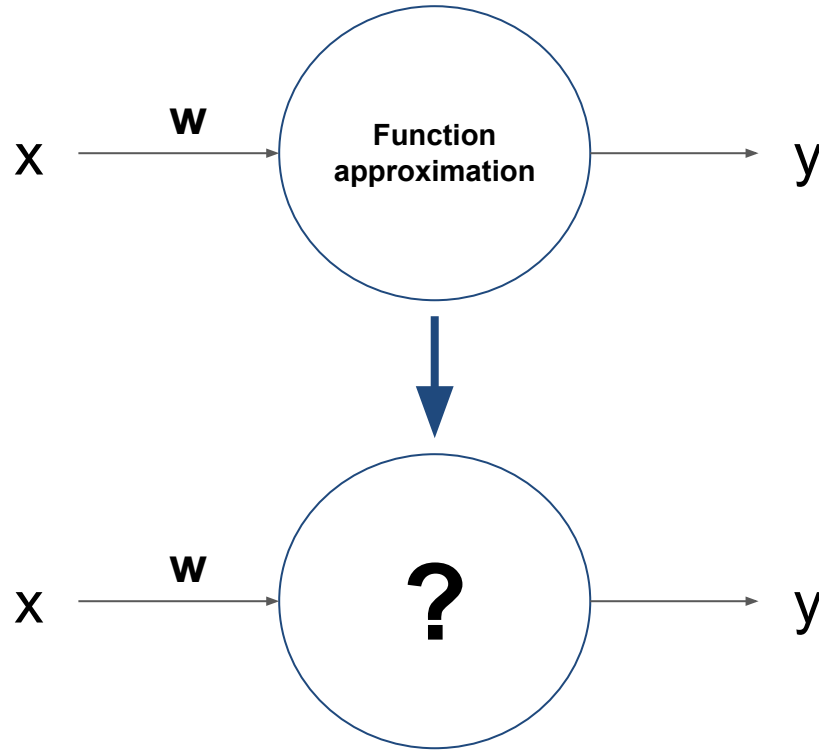
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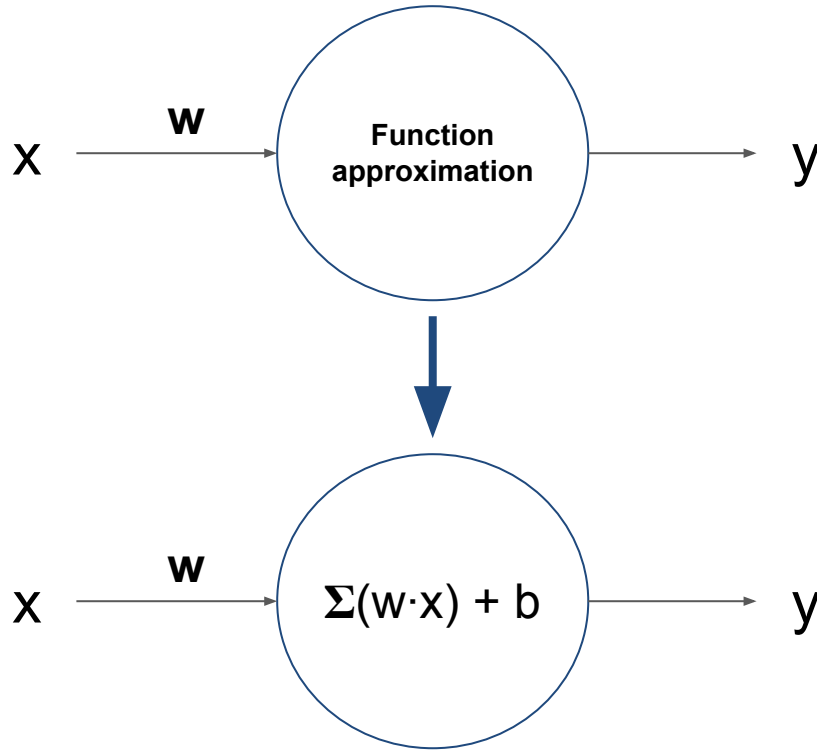
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- **learning the weights**

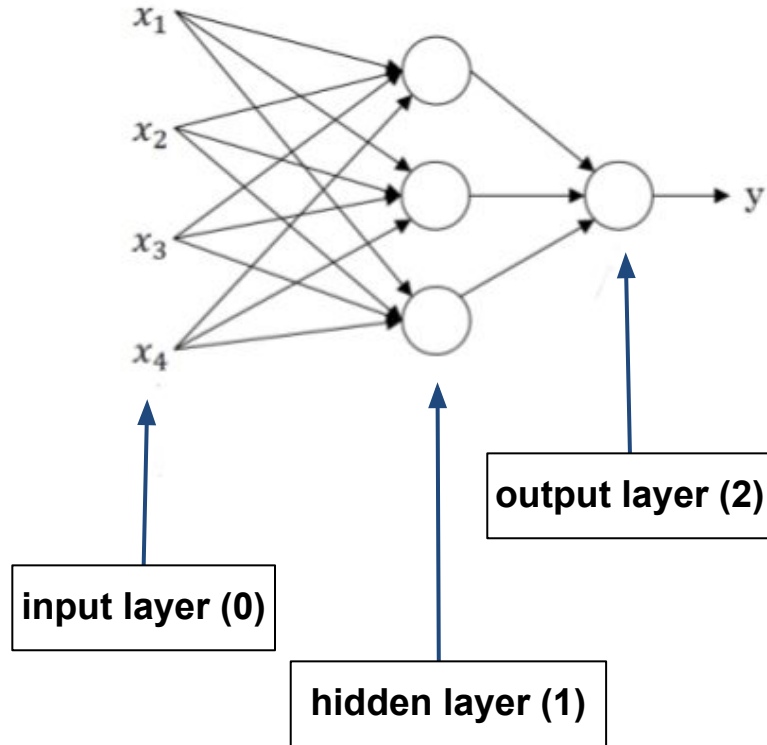
- e.g. linear combination of weights*features + bias
- fancy way to perform linear regression
- solved through NN rather than OLS or ML



Anatomy of a neural network



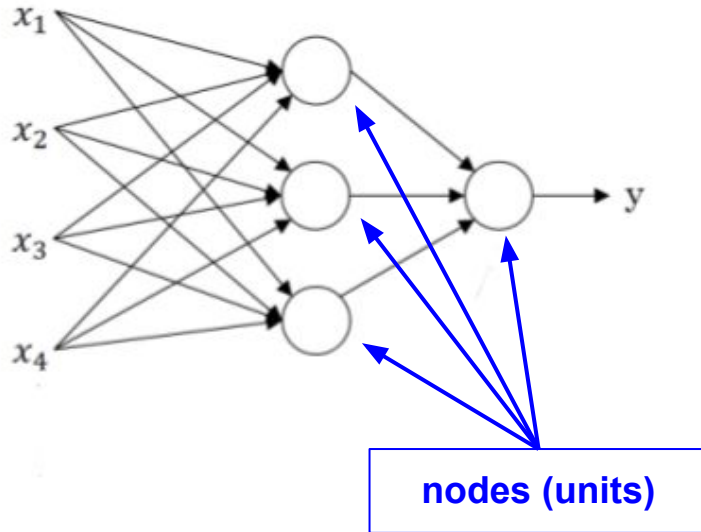
Fully connected (dense) neural network



- two-layer NN (not strictly “deep”):
 - input layer: [0]
 - hidden layer: [1]
 - output layer: [2]



Fully connected (dense) neural network

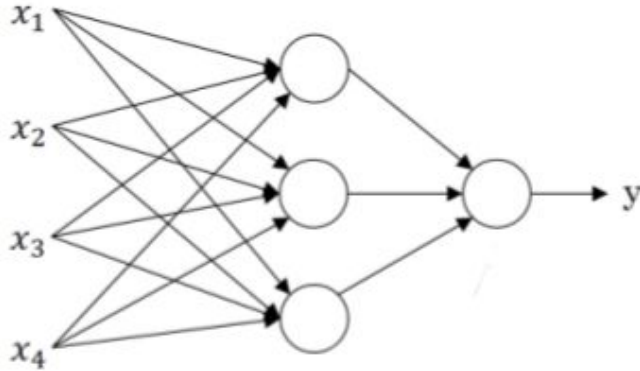


IMPORTANT!

- each hidden unit takes in input all x features
- replicates the predictive model as many times as there are units ("neurons")
- if the approximated function is linear regression, each unit will fit a different linear regression model
 - e.g.: 3 units \rightarrow 3 regression models



Fully connected (dense) neural network

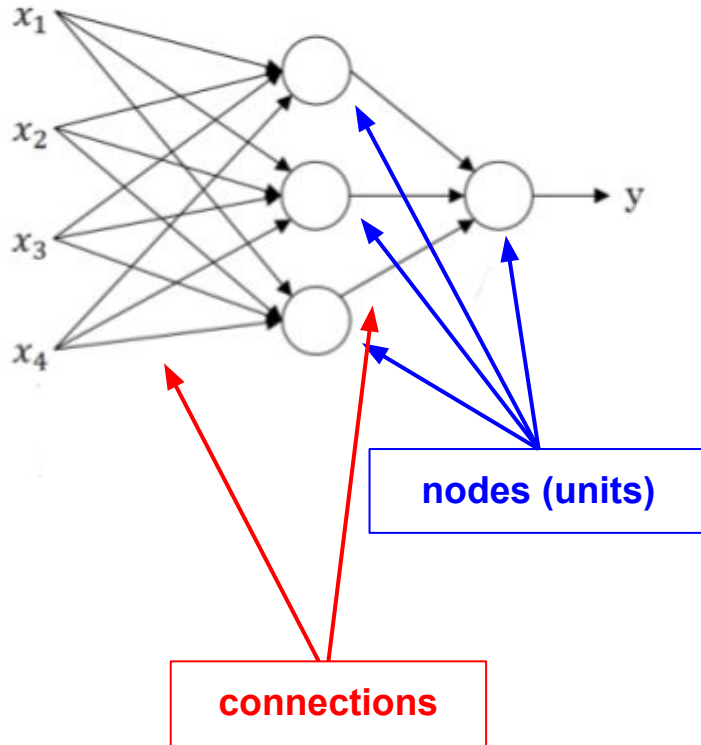


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Fully connected (dense) neural network



- **two-layer NN** (not strictly “deep”):
 - input layer: [0]
 - hidden layer: [1]
 - output layer: [2]
- all features connected to all “neurons” in the hidden layer
- the NN will decide which variables to use (and how) in each node (by **learning the weights**)

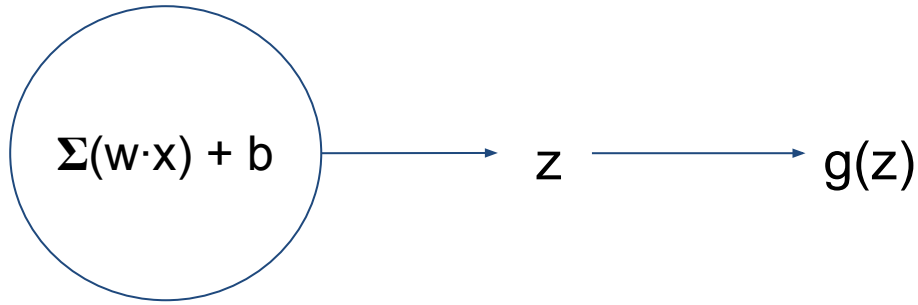


Activation functions



Activation functions: what?

“neuron” (unit)

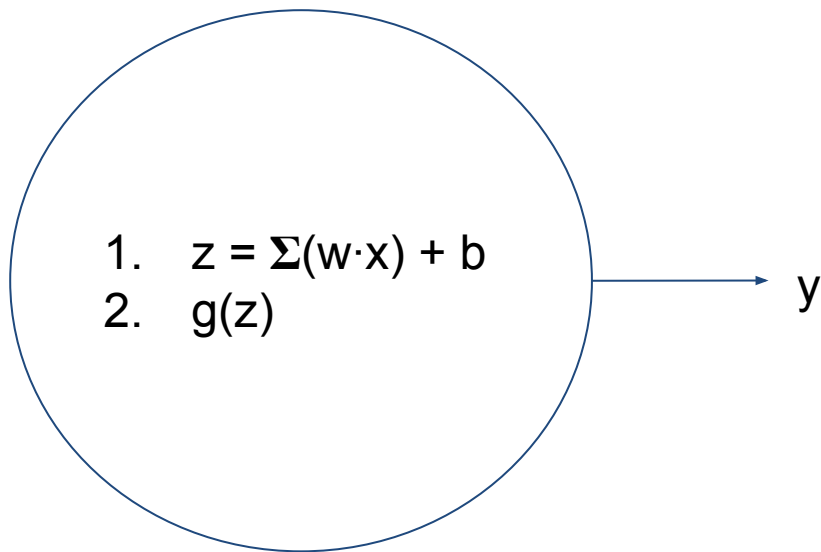


- $g(z)$: **activation function**



Activation functions: what?

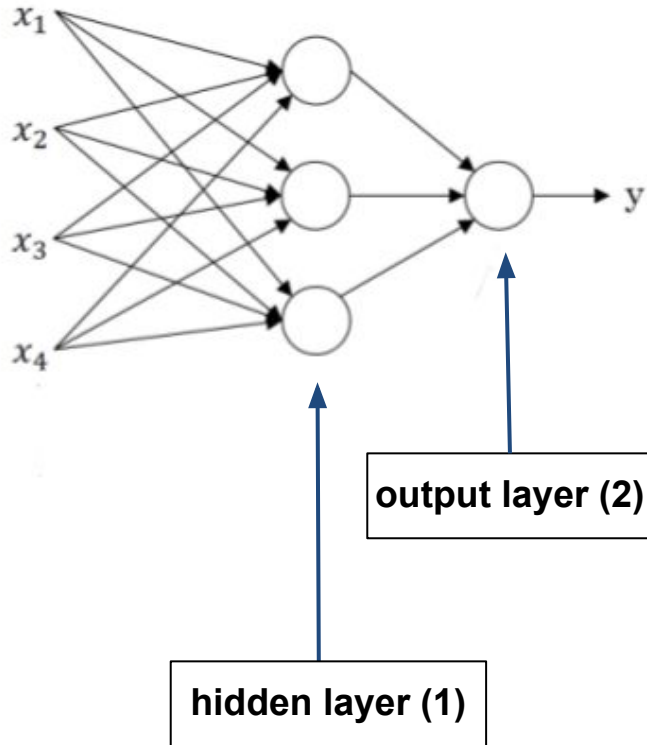
“neuron” (unit)



- $g(z)$: **activation function**
- the unit actually processes both the combination of weights and features and the activation function
- the output can be i) the final prediction, or ii) the intermediate output of a hidden layer



Activation functions: when and where?



- **when:** each time a unit is activated: input data (initial features, intermediate output) is processed and output is transferred to the next layer (or final output) through an activation function
- **where:** hidden layers and output layer

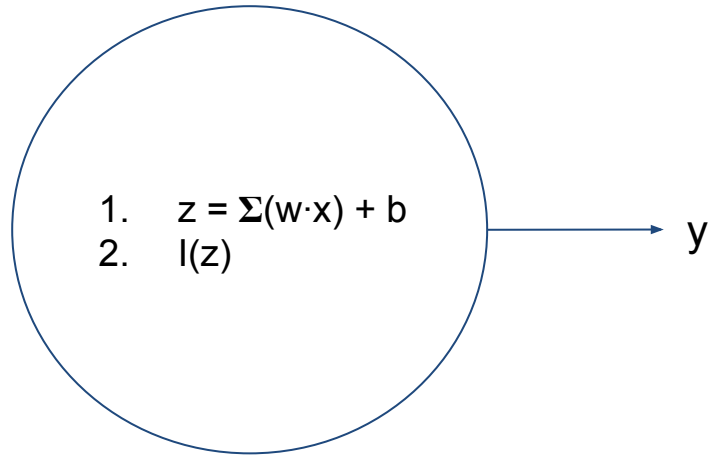


Activation functions: which one?

- Identity function
- Logistic function
- Hyperbolic tangent function
- ReLU (Rectified Linear Unit) function
- Softmax function



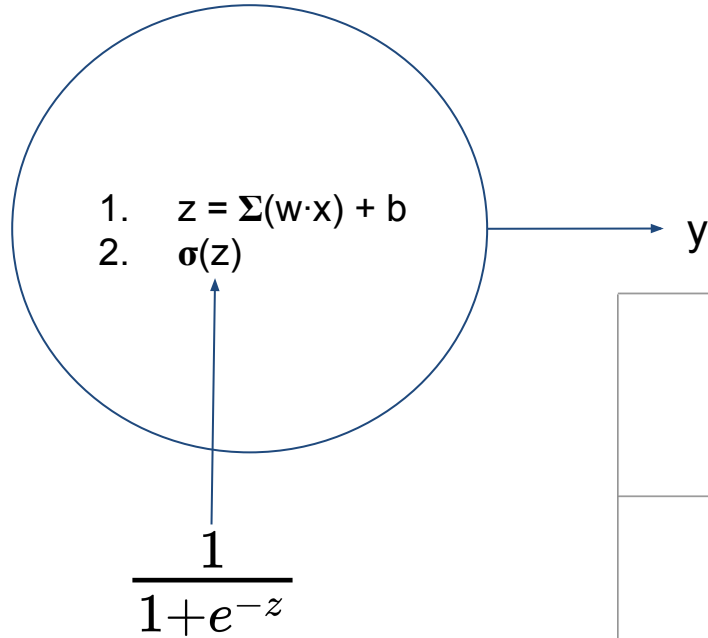
Activation functions: identity function



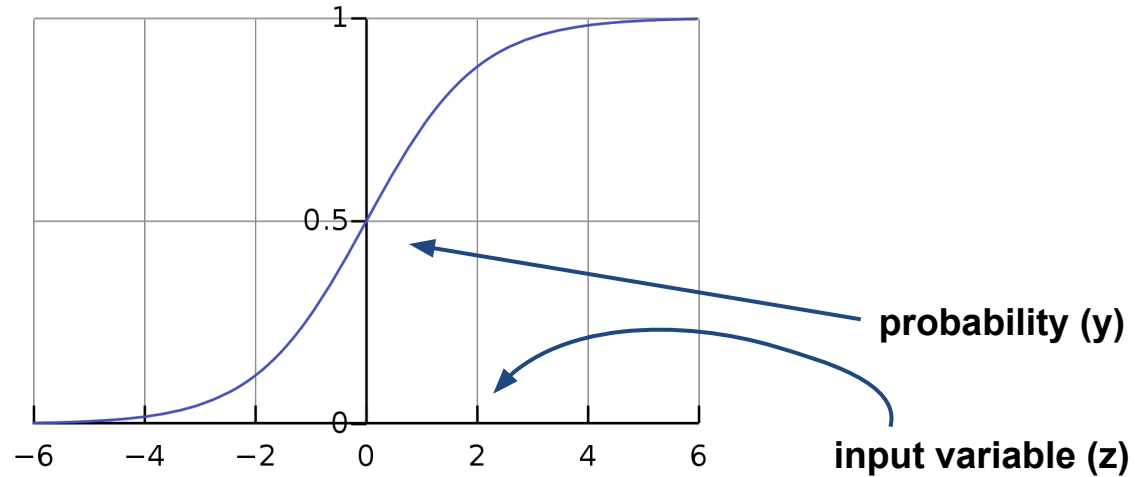
- identity function: a.k.a. **linear activation** function
- returns the value z that comes from the combination of input features and learned weights
- **never used**, except for the output layer in regression problems



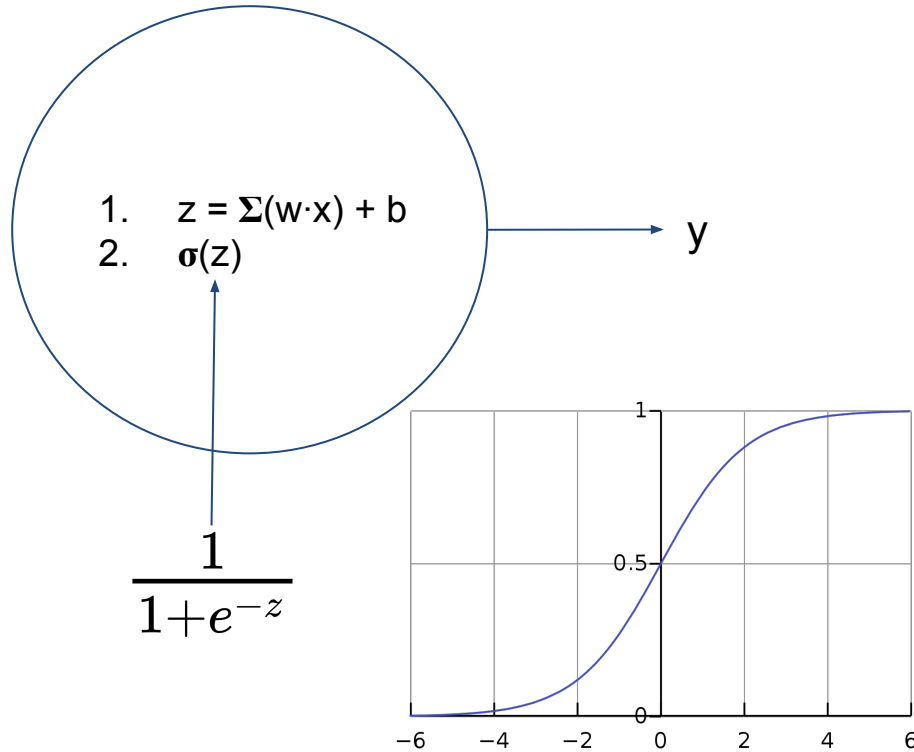
Activation functions: logistic function



- logistic (**sigmoid**) function
- converts real input in $[-\infty, +\infty]$ to output in the range $[0, 1]$



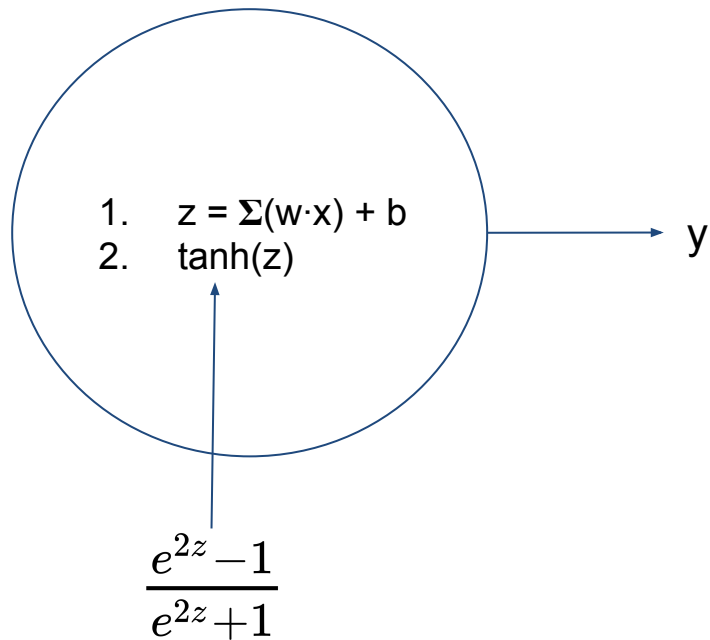
Activation functions: logistic function



- historically very popular
- now less popular \rightarrow problems with gradient descent (solution of the model)
- when z is very large or very small derivatives are close to 0 \rightarrow **slow descent**
- still used for the output layer in binary classification problems (and also for specialised hidden layers/units)



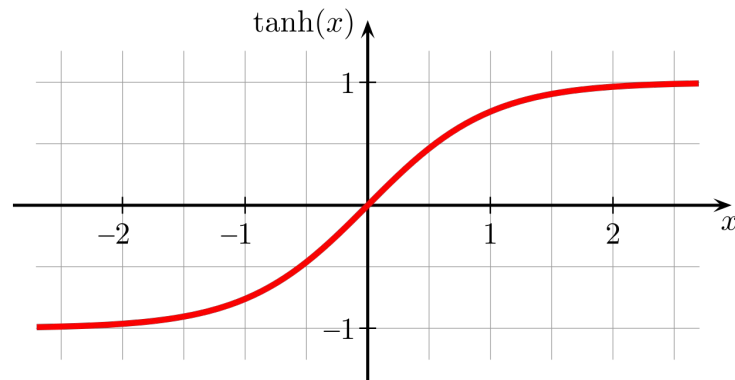
Activation functions: tanh



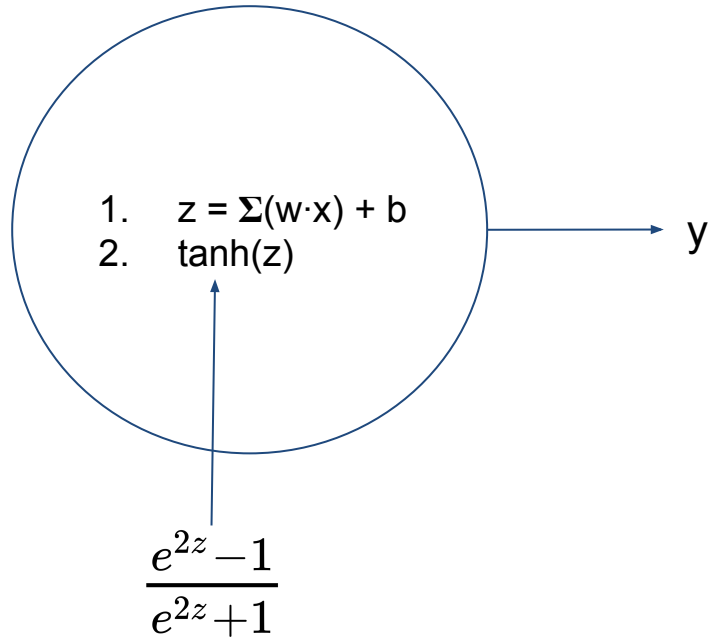
- hyperbolic tangent function
- rescaling of the logistic function:

$$\tanh = 2\sigma(2z) - 1 \text{ [proof [here](#)]}$$

- output in **[-1,+1]**, **mean 0**, ~ “centering of the data”



Activation functions: tanh



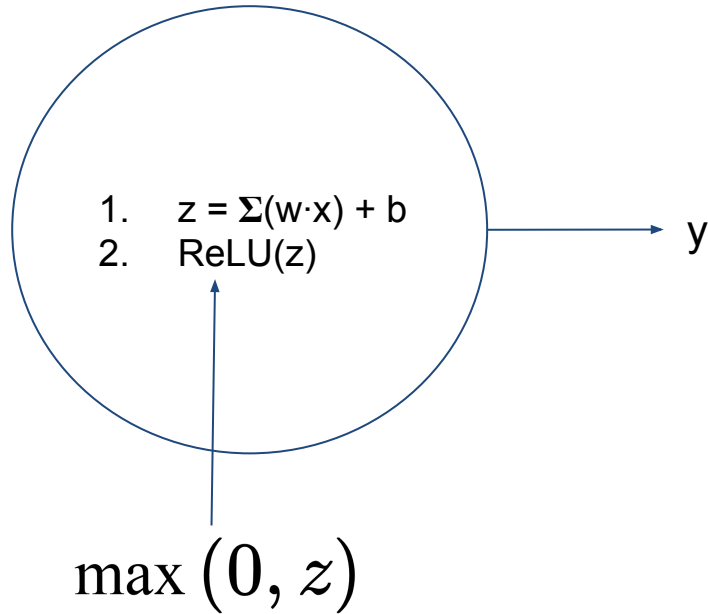
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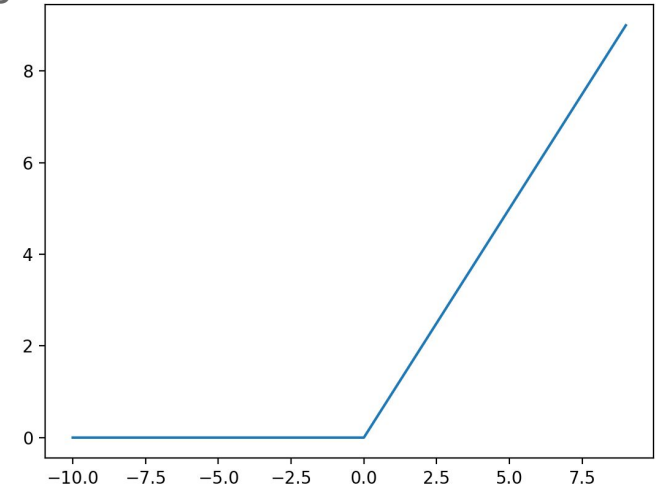
- output in **[-1,+1]**, **mean 0**, ~ “centering of the data”
- more efficient learning in the intermediate hidden layers
- still suffers from similar limitations as $\sigma(z)$ when z is very large or small
- used in specialized layers/units (e.g. RNN)



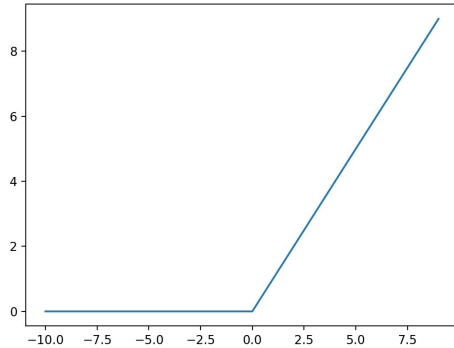
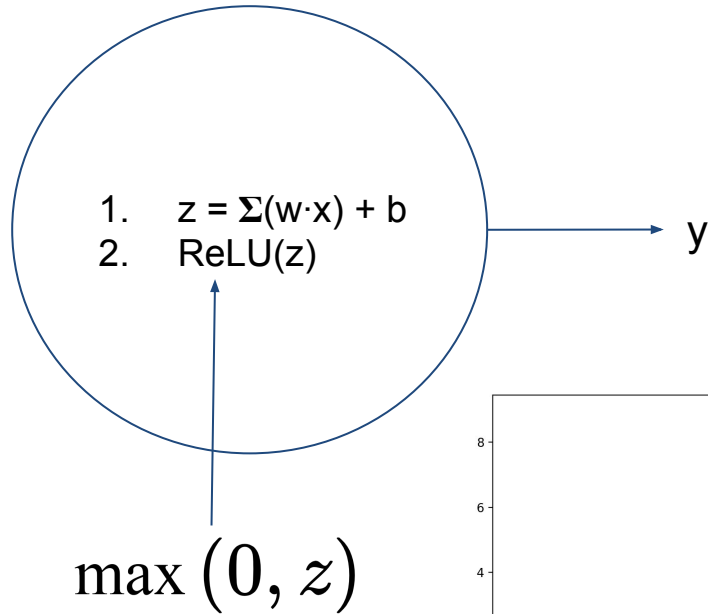
Activation functions: ReLU



- derivative is 0 for $z < 0$, 1 for $z > 0$
- most common activation function (default choice in many cases)
- much faster and efficient learning of DL models



Activation functions: ReLU



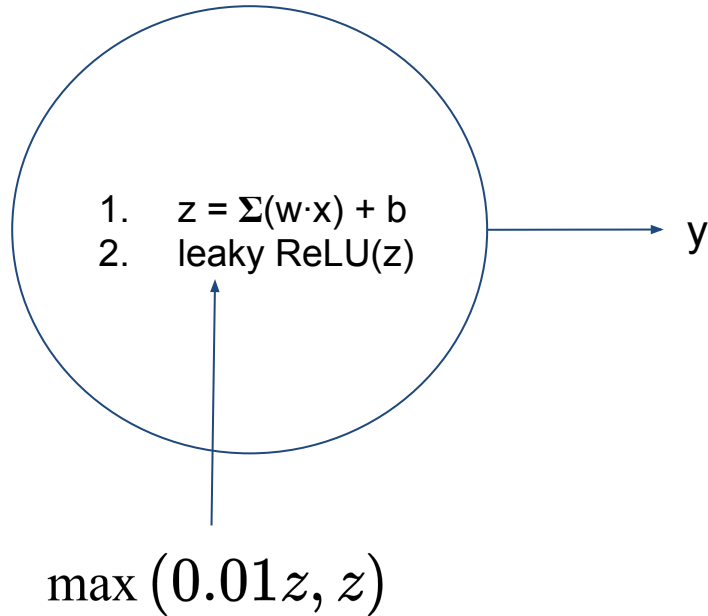
Pros of ReLU activation:

- easy to compute
- sparse representation: many output values will be exactly 0 (unlike sigmoid and tanh, which tends asymptotically to 0)
- reduces vanishing gradients \rightarrow faster learning (training of multi-layered NNs)

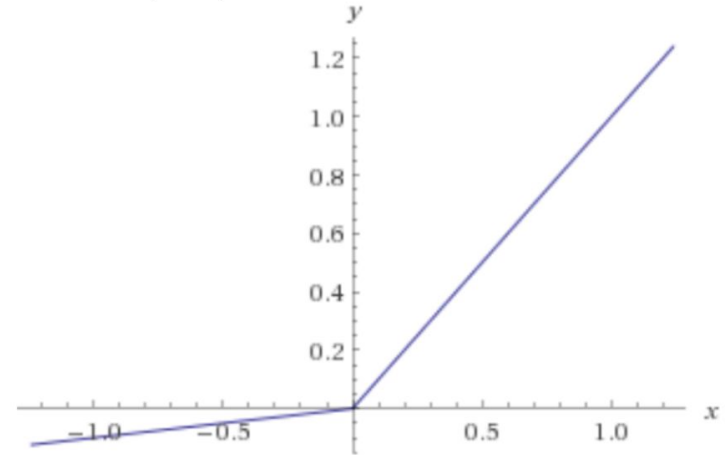
\rightarrow ReLU is one of the ingredients that made deep learning possible



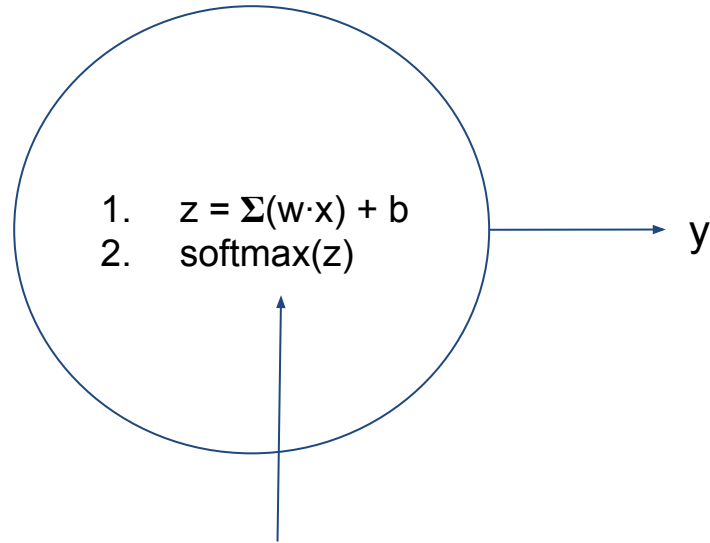
Activation functions: leaky ReLU



- uses a slight slope for $z < 0$
- can help when there are too many flat neurons (0 slopes, “dying neurons”), e.g.:
 - large negative bias
 - learning rate is too large



Activation functions: softmax



$$\text{softmax}(z_i) = \frac{\exp(x_i)}{\sum_{j=1}^k \exp(x_j)}$$

- returns a probability distribution over the target classes in a **multiclass classification** problem
- k classes
- negative inputs converted to non-negative values (exponential function)
- each output will be in the interval $[0,1]$
- same denominator \rightarrow normalization (sum to 1)
- Softmax is used in the output layer of multinomial classification problems
- Softmax is differentiable \rightarrow backpropagation for optimization of the weights (parameters of the deep learning model)



Activation functions: why not linear?

- the linear (identity) activation function is never used: why?



Activation functions: why not linear?

- the linear (identity) activation function is never used: why?
- has to do with **function approximation**: NNs (deep learning) are excellent at finding complex non-linear relationships in the data (e.g. between features and target variables)
- with the identity activation function, the intermediate output of each layer will just be a linear combination of the input, and so no matter how many hidden layers you have, the final output $\hat{\mathbf{y}}$ will be a **linear combination** of the initial features \mathbf{X}
- deep learning would then just be a very expensive way of doing linear regression!

$$\begin{cases} y_1 = w_1 x + b_1 \\ y_2 = w_2 y_1 + b_2 \end{cases} \rightarrow y_2 = w_2(w_1 x + b_1) + b_2 = \underbrace{(w_2 w_1)}_{\mathbf{w}'} x + \underbrace{(w_2 b_1 + b_2)}_{\mathbf{b}'}$$

