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data science

CAIDAS

Chapter 2

Neural Network Basics

The slides are mostly from the Stanford University course cs231n (F. Li, http://cs231n.stanford.edu).

Content of this Chapter

1. Classification
2. Neural Networks
3. Gradient Descent
    1. Backpropagation
    2. Optimisation Algorithms

2.1 Classification

- What is classification?
- What are some popular classifiers?
- What are their (dis-)advantages?

Classification

- General Task:
  - Given a set of objects and their labels (classes)…
  - … train a classifier to predict the label for a previously unseen object

- Example: Text Classification (20 Newsgroups)
  - Given the text of a document (20 different forums)
  - Predict which forum it came from

20 Newsgroups Text Classification

- 20 Newsgroups is a dataset of online discussion
  - 18,828 documents total
  - 20 forums, some closely related (pc.hardware vs mac.hardware), some highly unrelated (misc.forsale vs religion.christian)
- Popular evaluation set in Natural Language Processing

- Not completely solved (Error rate ~ 11.4%)

Felix Wu, Tianyi Zhang, Amauri Holanda de Souza Jr.,
Christopher Fifty, Tao Yu, & Kilian Q. Weinberger. (2019).
Simplifying Graph Convolutional Networks

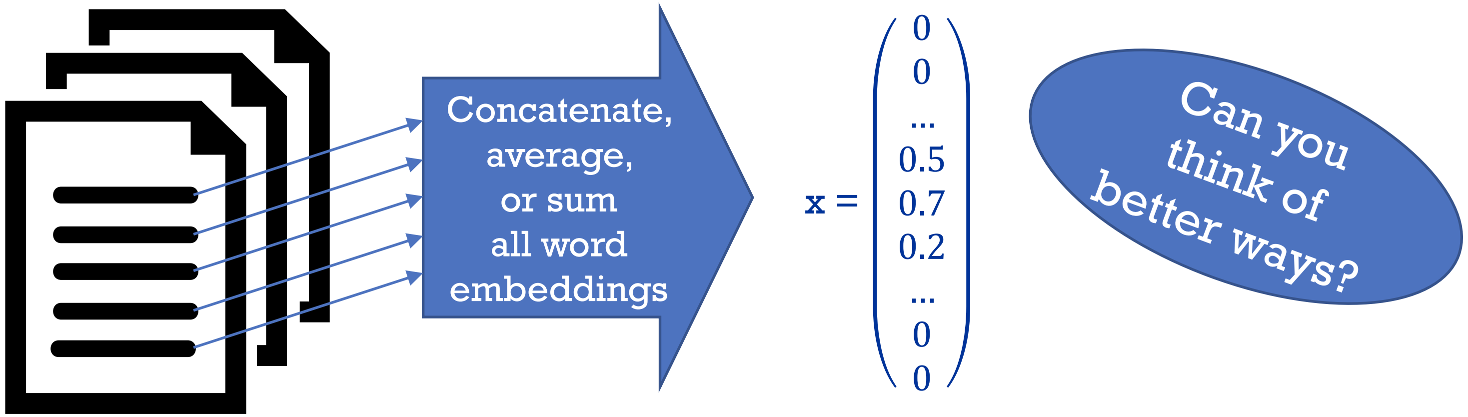
Classification

Known from Data Mining

- Many classification methods exist
  - **Linear Classifiers**
  - Support Vector Machines
  - Decision Trees/Random Forests
  - **Perceptrons**
  - **(Deep) Neural Networks**

Linear Text Classification

- Represent the document as a vector x of (for now) fixed length



- Determine unnormalised probabilities using **weights** and a **bias**
  - **Weights**: Which influence does each embedding dim. have on the classification?
  - **Bias**: Roughly: Which class is more likely a priori?

Linear Text Classification

- Determine unnormalised probabilities by multiplying with a weight matrix W of dim. 20×300 (classes $\times$ embedding length) and adding a bias b of dim. 1×20

$$y = Wx + b = [0.1, 0.3, 0.2, \mathbf{0.8}, 0{,}5, 0.7, 0.5, 0.01, 0.7, \ldots]$$

„Probability“ for class	0	1	2	3	4	5	6	7	8

→ Our Goal:

Find values for W and b that provide a good classification!

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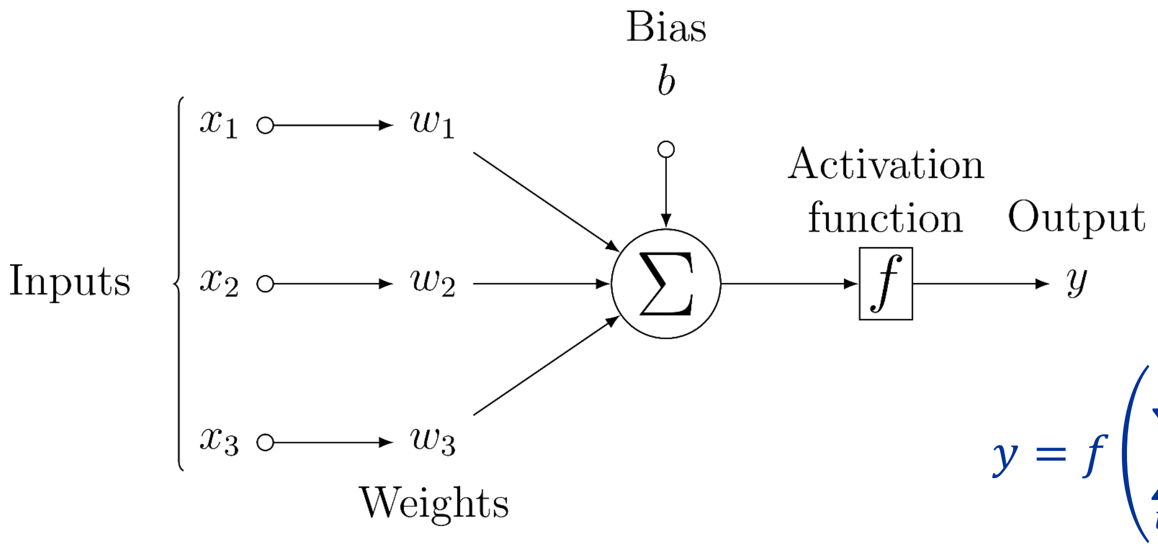
Perceptron — a simple Classifier

- Inspired by the human brain
- Models one „brain cell“/**neuron**
- Based on its inputs, the neuron can either „fire“ or not

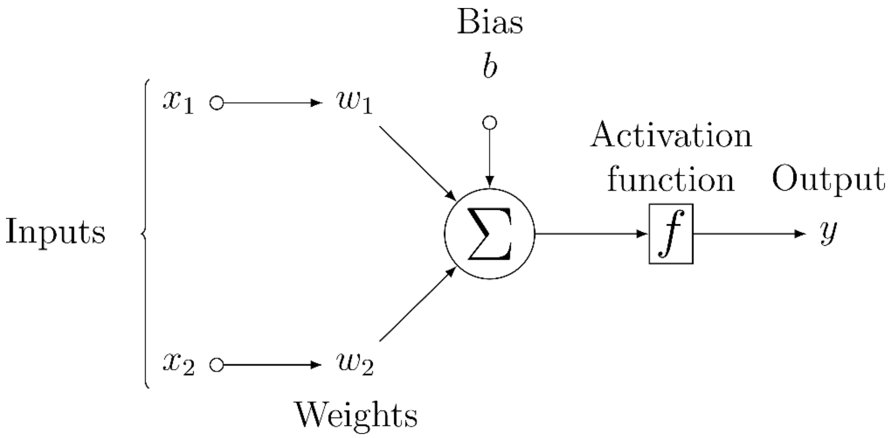
→ „Firing“ is interpreted as a positive classification



$$y = f\left(\sum_{i=1}^{3} w_i x_i + b\right) = f(w^T x + b)$$

Rosenblatt, Frank (1958), The Perceptron: A Probabilistic Model for Information Storage and Organization in the Brain, Cornell Aeronautical Laboratory, Psychological Review, v65, No. 6, pp. 386–408. doi:10.1037/h0042519

Perceptron for the „or"-function



x_1	x_2	x_1 OR x_2
0	0	0
1	0	1
0	1	1
1	1	1

- Parameter Settings:
  - $w_1 = 1, w_2 = 1$
  - $b = -1$
  - $f(x) = \sigma(x)$
  - Activation:
    Neuron „fires" iff $y \geq 0.5$

Example:

Let $x_1 = 1$ and $x_2 = 0 \rightarrow x_1\ OR\ x_2 = 1$

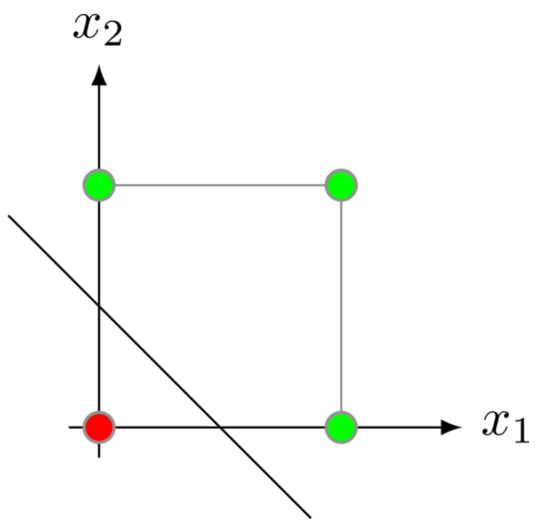
$$
\begin{aligned}
y &= \sigma(w_1 \cdot x_1 + w_2 \cdot x_2 + b) \\
&= \sigma(1 \cdot 1 + 1 \cdot 0 + (-1)) \\
&= \sigma(0) = 0.5
\end{aligned}
$$

→ Neuron fires!

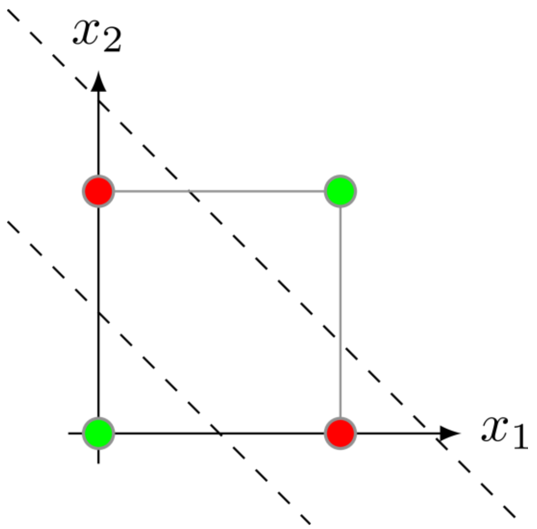
Perceptron for the „xor“-Function?

- No such perceptron exists!
- A perceptron can only model linear dependencies

x_1	x_2	x_1 XOR x_2
0	0	0
1	0	1
0	1	1
1	1	0



OR
Linearly separable



XOR
Not linearly separable!

Perceptron as a Linear Classifier

- A perceptron is an example of a linear classifier
- An SVM is another example

- These classifiers have some limitations:
  They can only learn linear functions

- Many important functions are not linear!
  → For example XOR

Limitations of Linear Classification

- Many functions can not be learned by linear classifiers ☹

→We need to modify the model to make it more expressive!

→For SVMs, use **kernels**

See Data Science / Data Mining

→For other linear classifiers, use multiple layers!

Deep Neural Networks. This is what we do here!

2.2 Neural Networks

- What is a neural network?
- What can we do with it?
- How do we use it for classification?

What is a neural network?

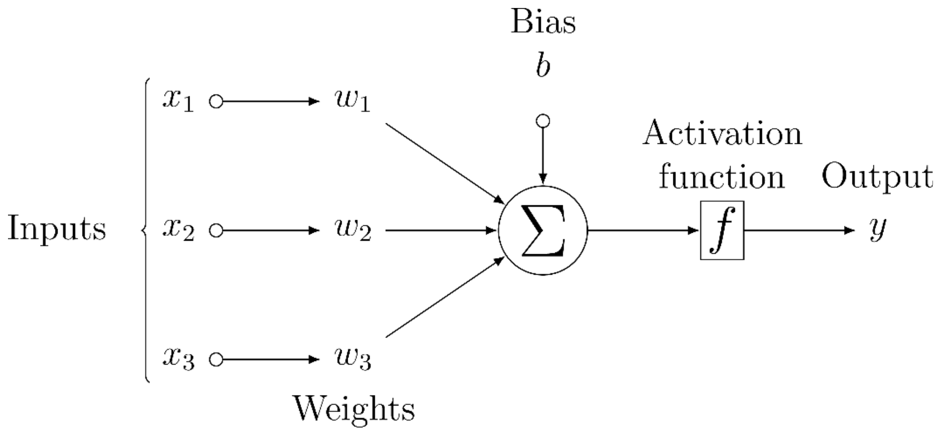
Rough and simple definition:
A simple (fully connected feed-forward) neural network is

- a bunch of linear classifiers
- with non-linear activation functions
- chained together

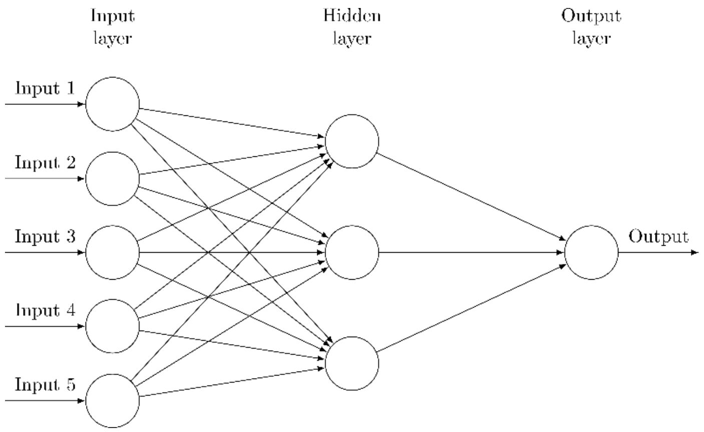
Neural Network

- „Model for the human brain“
- Classifier based on neurons (perceptrons) structured in **layers**

- Remember: A single neuron/perceptron is a linear classifier

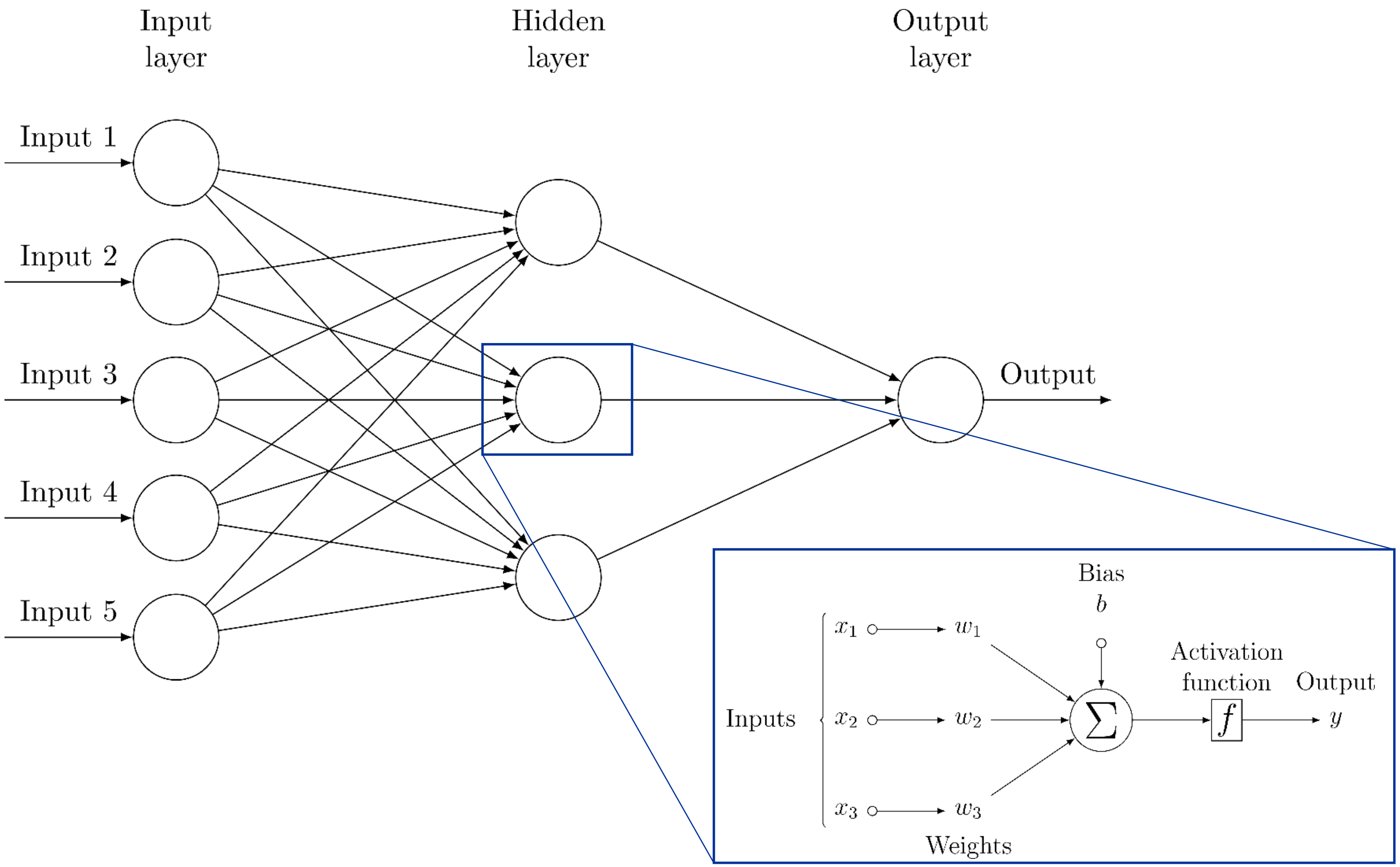


Single Neuron



Neural Network

Neural Networks



Neural Networks – Forward Pass

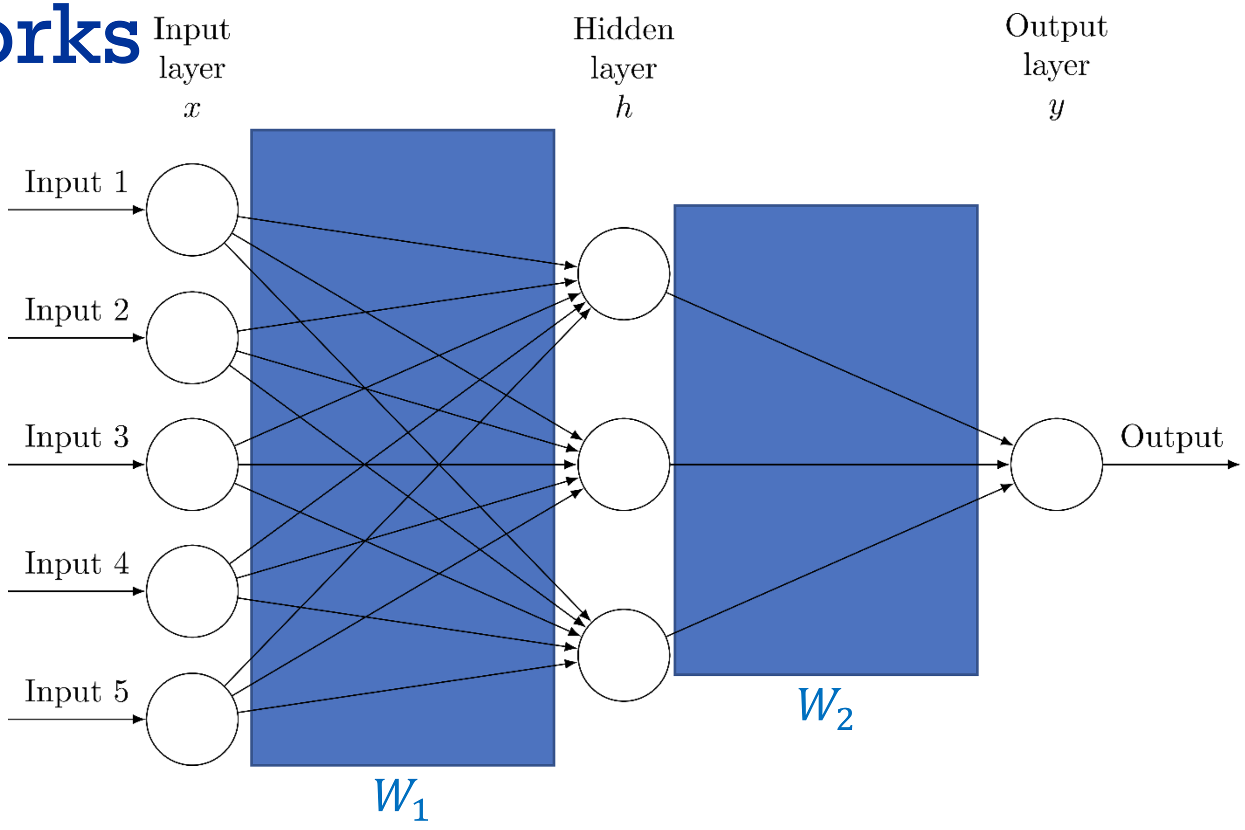
- Given
  - A neural network with a fixed set of weights
  - An input sample to be classified

- How to get the classification?

→A layer is „applied“ by multiplying its weight matrix with its input vector

→See next slide for an example

Neural Networks



$$h = f(W_1 x + b_1)$$
$$y = f(W_2 h + b_2)$$

Linear classifiers!

Neural Networks as Chained Linear Classifiers

- Remember:
  - A linear classifier provides class scores by calculating $y = f(Wx + b)$
  - A neural network is a chain of linear classifiers with activation functions *f*

→A neural network is some function like this:

Linear classifier

$$y = f(W_3\, f(W_2 f(W_1 x + b_1) + b_2) + b_3)$$

→ We can chain this as deep as we want

Activation Functions

- After each layer, an **activation function** is used
- An activation function can be **any function**
- However, **non-linearity** is required for a more expressive model

- Why do we need this?
  →Remember: Linear classifiers can separate data linearly
  →A neural network with a linear activation function (e.g. $f(q) = q$) is still a linear classifier (we could reduce all the weight matrices back into one)
  →Non-linear activation functions enable us to learn non-linear relations!

Using Linear Activation Functions

- Using a linear activation function can be reduced to a new linear classifier
- For example, setting $f(q) = q$:

$$
\begin{aligned}
y &= f(W_3 f(W_2 f(W_1 x + b_1) + b_2) + b_3) \\
&= W_3(W_2(W_1 x + b_1) + b_2) + b_3) \\
&= W_3(W_2 W_1 x + W_2 b_1 + b_2) + b_3) \\
&= W_3 W_2 W_1 x + \underbrace{W_3 W_2 b_1 + W_3 b_2 + b_3}_{\text{constant term}} \\
&= \boldsymbol{W} x + \boldsymbol{b}
\end{aligned}
$$

Neural Networks as Chained Linear Classifiers

Using some common non-linear activation functions for f, our network:

$$y = f(W_3 f(W_2 f(W_1 x + b_1) + b_2) + b_3)$$

becomes:

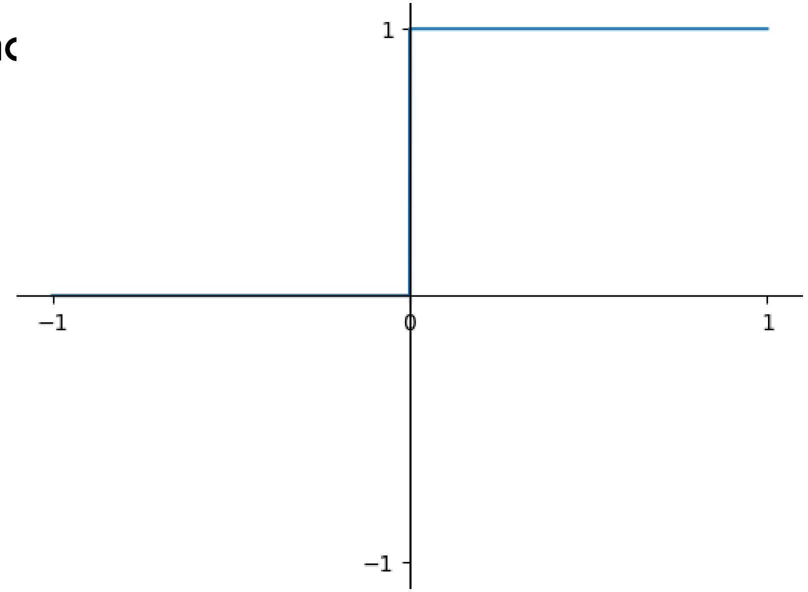
$$y = softmax(W_3 \tanh(W_2 \tanh(W_1 x + b_1) + b_2) + b_3)$$

Activation function

Activation Functions

- Initial approaches were inspired by natural scienc

$$\text{heaviside}(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0 \end{cases}$$

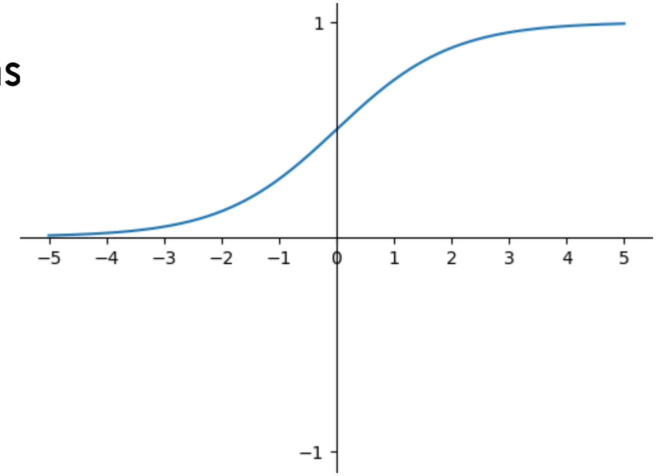


- Its derivative posed some problems however
  - Not defined at 0
  - 0 everywhere else

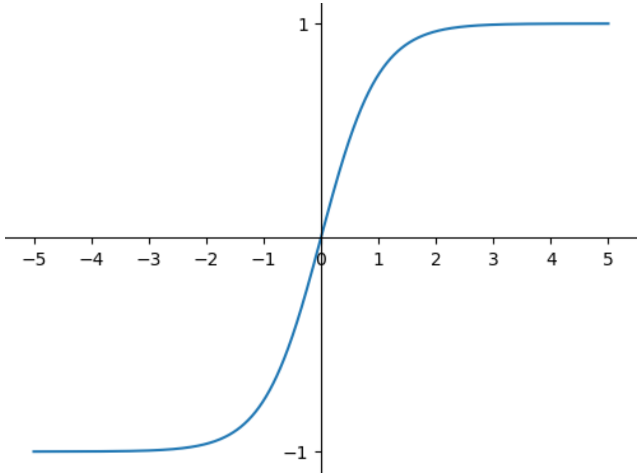
Activation Functions

- Better functions emerged to solve these problems

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



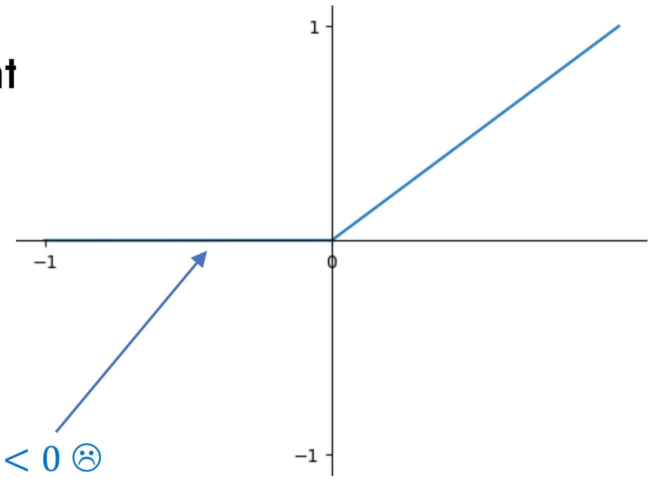
tanh



Activation Functions

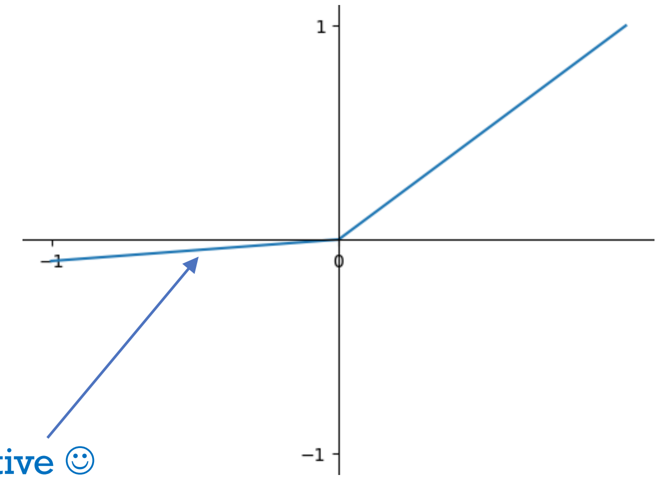
- ReLU proved to be best, resulting in more variant

$$\mathrm{ReLU}(x) = \begin{cases} 0, & x < 0 \\ x, & x \geq 0 \end{cases}$$



Derivative is zero for $x < 0$ ☹

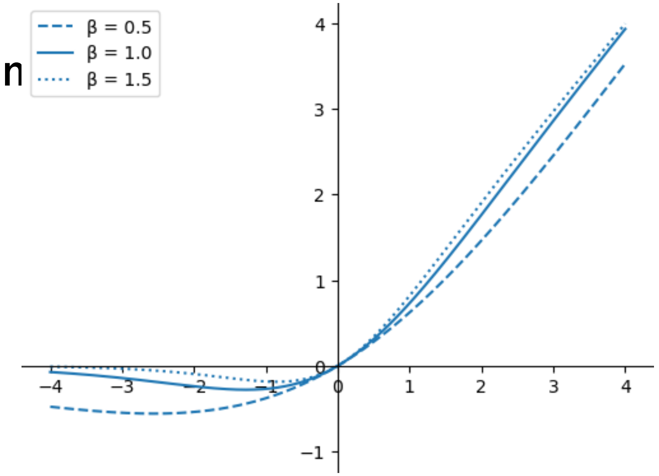
$$\mathrm{LeakyReLU}(x) = \begin{cases} \alpha x, & x < 0 \\ x, & x \geq 0 \end{cases}$$



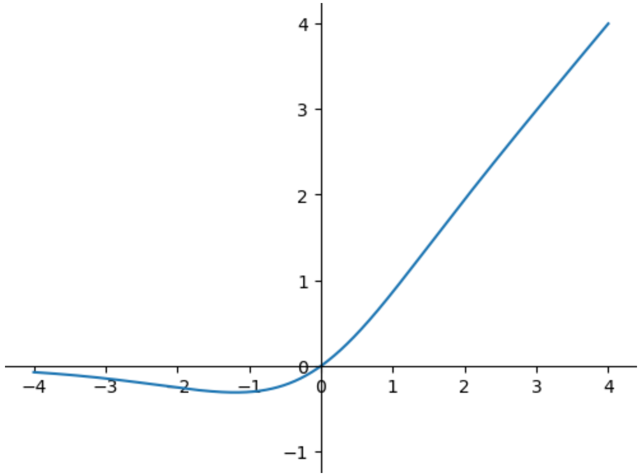
No „dead“ derivative ☺

Even More Activation Functions

- A great deal of research has gone into further in



$$^{1}\text{swish}(x) = x \cdot \frac{1}{1 + e^{-\beta x}}$$



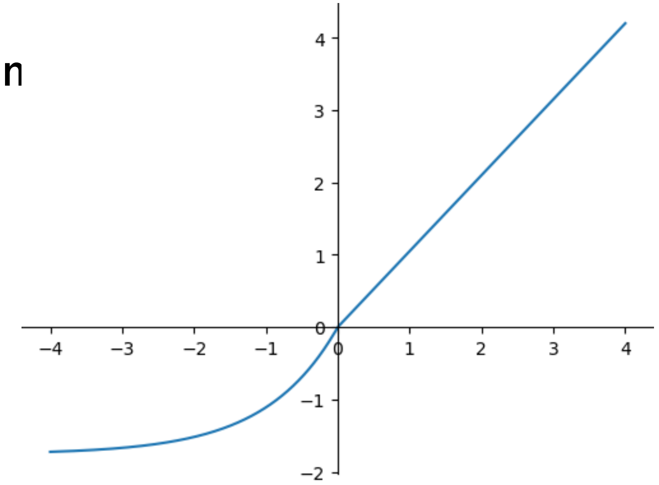
$$^{2}\text{mish}(x) = x \cdot \tanh(\ln(1 + e^{x}))$$

[1] Prajit Ramachandran, Barret Zoph, and Quoc V. Le. (2017). *Searching for Activation Functions.*
[2] Diganta Misra. (2019). *Mish: A Self Regularized Non-Monotonic Neural Activation Function.*

Even More Activation Functions

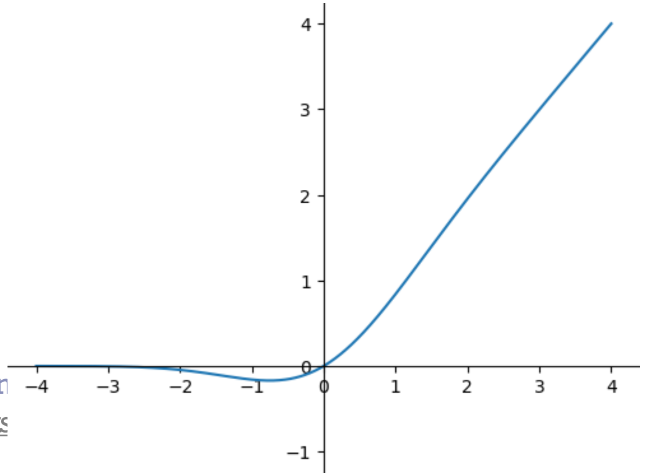
- A great deal of research has gone into further in

$$^{1}\mathrm{selu}(x) = \lambda \begin{cases} x, & x > 0 \\ \alpha e^{-x} - \alpha, & x \leq 0 \end{cases}$$



$$^{2}\mathrm{gelu}(x) = 0.5x\left(1 + \tanh\left(\sqrt{\frac{2}{\pi}} \cdot \left(x + \alpha x^{3}\right)\right)\right)$$

Mostly used in modern NLP



[1] Günter Klambauer, Thomas Unterthiner, Andreas Mayr, ar Sepp Hochreiter. (2017). *Self-Normalizing Neural Networks*
[2] Dan Hendrycks, and Kevin Gimpel. (2016). *Gaussian Error Linear Units (GELUs).*

Neural Networks – Optimisation

- So far, we assumed given weights for our networks
- In practice, we have given **data** and need to **find the weights**

→We need a method to do that!

- Roadmap:
  - Rate the current weights
  - Change the weights to get a better rating

Neural Networks – Loss Function

- Recall Word2Vec:
  - Given a **corpus** of contexts („training examples")…
  - … determine the **quality** of the network's current weights

- Generally: Rate the current weights W (more generally parameters θ) by a **loss function**

> A loss function $L_\theta(x, l)$ quantifies how unhappy you would be if you used θ to make a prediction on x when the correct output is l. It is the object we want to minimize.
>
> https://web.stanford.edu/class/cs221/lectures/learning1.pdf

Neural Networks – Loss Function

- A loss function quantifies the error a classifier makes with its current weights

- Common loss function for classification:
  Cross-Entropy Loss
  - Given
    - the **true label** l of a sample (that is, a 1-hot vector with a **1** at the position of the correct class)
    - The label y_θ(x) **predicted by the neural network for the input x** as a vector of probabilities
  - The cross-entropy loss for parameters θ for one sample x is defined as

$$L_\theta(l, x) = -\sum_i l[i] \cdot \log y_\theta(x)[i]$$

All trainable weights   All possible classes

Cross-Entropy Loss

$$L_\theta(l, x) = -\sum_i l[i] \cdot \log y_\theta(x)[i]$$

- L gets smaller the closer y_θ is to l

→Minimising L leads to better predictions!

→This is done by changing θ in a way that minimises the loss

Neural Networks – Optimisation

- For shallow networks, finding good weights is easy
- But shallow networks are not very powerful*
- For deep networks, the influence of early layers on the classification is not obvious

- Early attempts at using deep networks failed, because
  - No good optimisation algorithm was known
  - Computational power did not suffice

- Very important step in 1975: Backpropagation!

* In theory, a network with one hidden layer and a finite number of neurons can learn any continuous function in a compact subset of $\mathbb{R}^n$ *(Universal approximation theorem)*. However, there is no guarantee that we can find such a network with our optimisation algorithms. In practice, deeper networks work better.

2.3 Backpropagation & Gradient Descent

- How do we optimise the weights in a neural network?

Optimisation

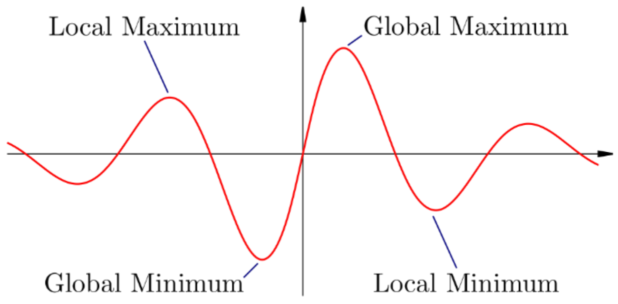
- The big goal in neural network optimisation:
  - Given a neural network, find the weights that provide the best classification by minimising the loss

- General Problem:
  - Given any function, find the input that minimises/maximises this function
  - Methods exist for this kind of problem!
    → Map the optimisation goal to this problem
    → Minimise the objective/loss function by finding the best set of parameters („inputs“)

How can we do this?

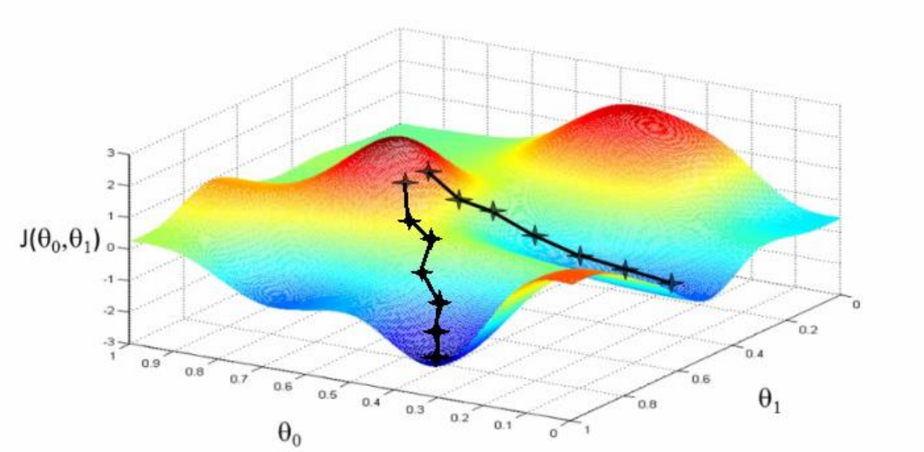
Optimisation Idea (Known From School)

- Set the first derivative of the function to 0
- Solve for the input analytically
  → $x_{candidate}$
- Is the second derivative at $x_{candidate} \neq 0$?
  → local minimum or local maximum
  → check if minimum/maximum is global
- Check the function value at the found inputs
  → get input that obtains the lowest/highest value



- This is not feasible for neural networks
  - Too many parameters and inputs to solve analytically
- But calculating the derivative is possible
  → Gradient Descent

Gradient Descent – The Analogy



http://blog.datumbox.com/wp-content/uploads/2013/10/gradient-descent.png

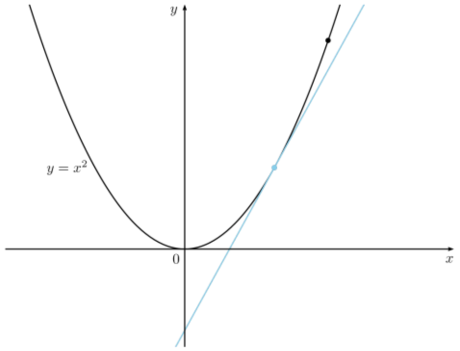
https://raftrek.com/wp-content/uploads/2015/10/Hiking-down-mountain-ridge.jpg

Gradient Descent – The Basics

Gradient Descent

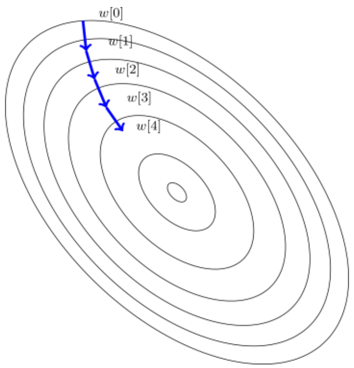
Gradient

= The vector of all partial derivatives of a function



Descent

= Finding a way towards the minimum of the function



Gradient Descent – The Gradient

- Any neural network is just an arbitrarily complex function
- More precisely:
  Any neural network is just an arbitrarily complex chain of simple functions!

- Simple functions are easy to derive
- Chains of simple functions are also easy to derive by using the **chain rule**

Gradient Descent – Deriving very simple functions

- Some basics rules (you **really** know these from school):

  - Multiplying with a constant c

$$f(x) = c \cdot x \quad \rightarrow \quad \frac{df}{dx} = c$$

  - Adding a constant c

$$f(x) = x + c \quad \rightarrow \quad \frac{df}{dx} = 1$$

  - Exponentiating with a constant c

$$f(x) = x^c \rightarrow \quad \frac{df}{dx} = c \cdot x^{c-1}$$

Gradient Descent – Deriving simple functions

- All these functions had only one parameter
- Neural networks have thousands or even millions!

→Partial derivatives (you may know these from school)

- Keep all variables except one (e.g. x) constant
- Derive by x
- Repeat for all other input variables

- The **Gradient** ∇ is the vector of all partial derivatives

Gradient Descent – Deriving simple functions

- An example:

$$f(x) = c \cdot x \quad \rightarrow \quad \frac{df}{dx} = c$$

$$f(x, y) = xy$$

$$\rightarrow \frac{\partial f}{\partial x} = y$$

y is treated as a constant

$$\rightarrow \frac{\partial f}{\partial y} = x$$

x is treated as a constant

- Remember: The Gradient is the vector of all partial derivatives:

$$\nabla f = \left[\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right] = [y, x]$$

Gradient Descent – Deriving simple functions

- Another example:

$$g(x, y) = x + y$$

$$\rightarrow \frac{\partial g}{\partial x} = 1$$ y is treated as a constant

$$\rightarrow \frac{\partial g}{\partial y} = 1$$ x is treated as a constant

$$\rightarrow \nabla g = [1, 1]$$

Gradient Descent – Backpropagation

- We need to derive more complex functions...
- … but these are just chained simple functions!

→Use **Backpropagation**…

→… which is just recursive application of the **chain rule**

Gradient Descent – Backpropagation

- A slightly more complex function:

$$f(x, y, z) = (x + y)z$$

- This is a chain of two functions:

$$q(x, y) = x + y, \qquad p(q, z) = qz$$

- We already know:

$$\frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1; \qquad \frac{\partial p}{\partial q} = z, \frac{\partial p}{\partial z} = q$$

- The chain rule tells us:

$$f(x, y, z) = p(q(x, y), z)$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x} = z \cdot 1$$

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial y} = z \cdot 1 \qquad \frac{\partial f}{\partial z} = (x + y)$$

Gradient Descent – Backpropagation

- The chain rule in general:

If $f(x) = p\big(q(x)\big)$ then $\frac{df}{dx} = \frac{df}{dq}\frac{dq}{dx}$

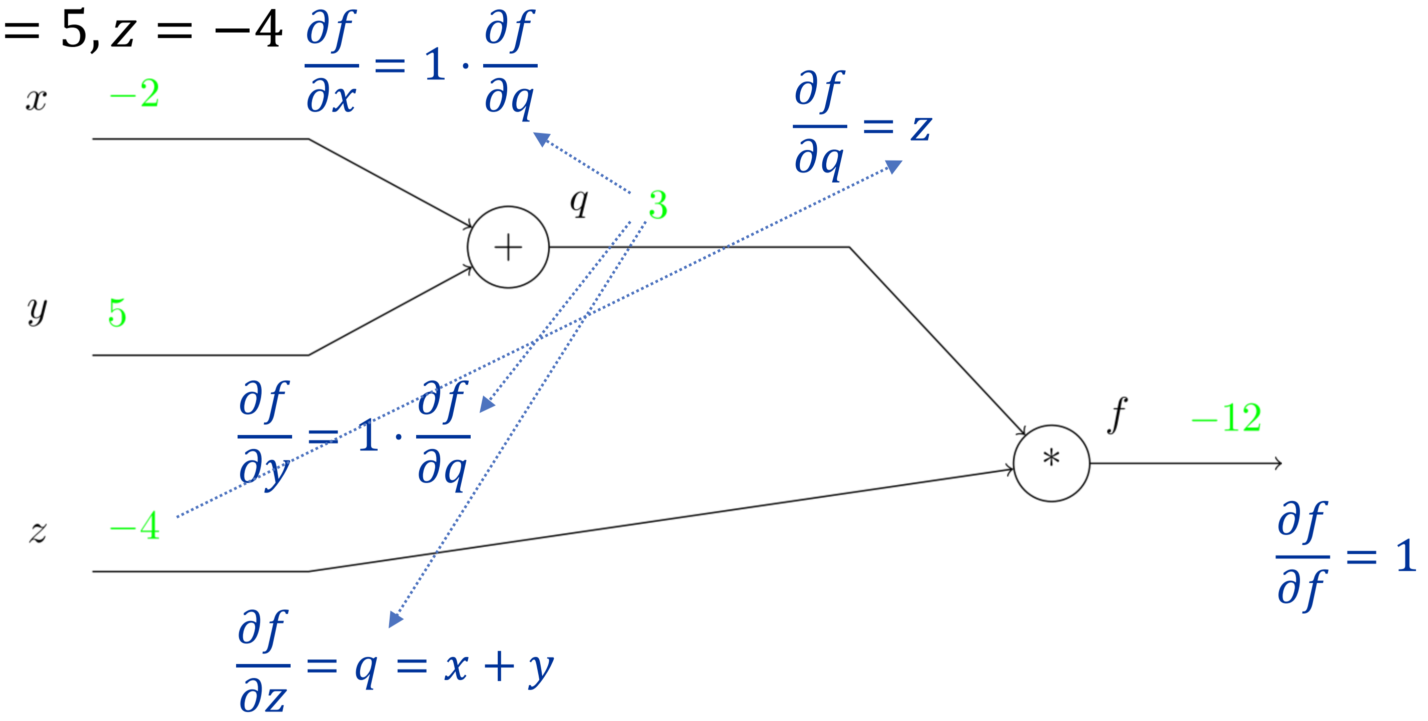
- This is the same thing as before, just the general notation

Gradient Descent – Backpropagation

- A nice visualisation: Circuit Diagrams

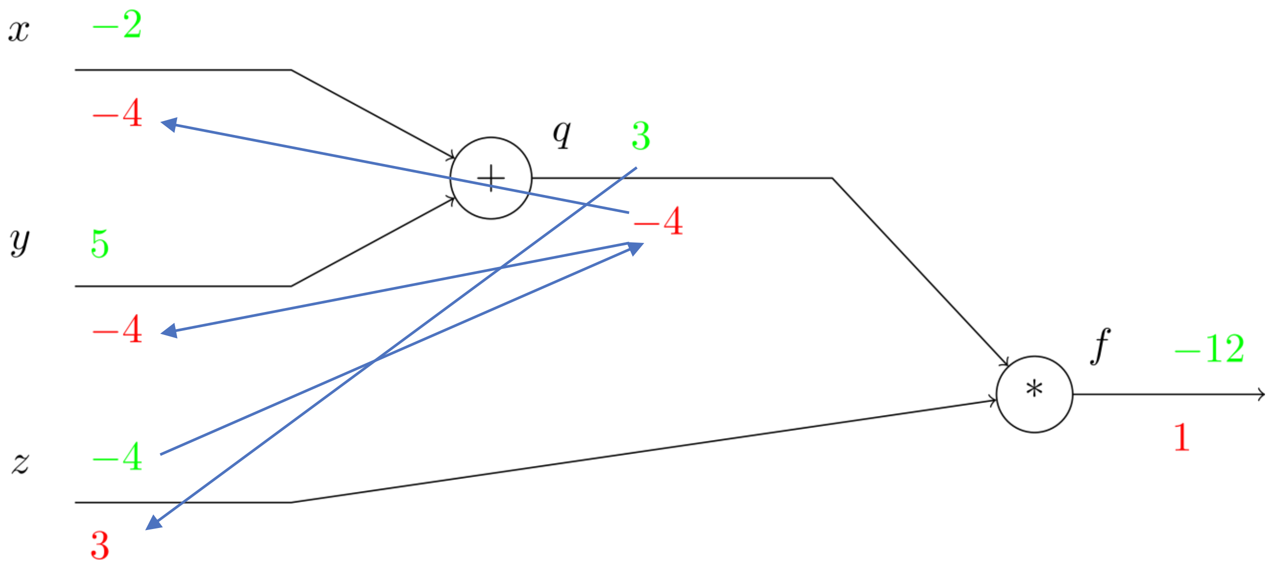
$$f(x, y, z) = (x + y)z$$

- Example: $x = -2, y = 5, z = -4$



Gradient Descent - Backpropagation

- Some gates have „intuitive“ gradient properties:
  - * „switches“ the inputs
  - + just „passes through“
  - More of those in homework ☺

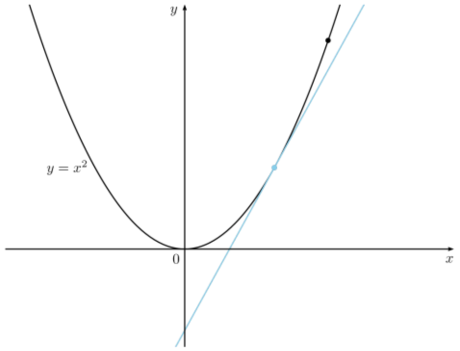


Gradient Descent – The Basics

Gradient Descent

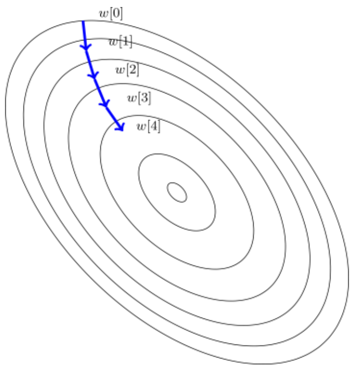
Gradient ✓

= The Vector of all partial derivatives of a function



Descent

= Finding a way towards the minimum of the function



Gradient Descent

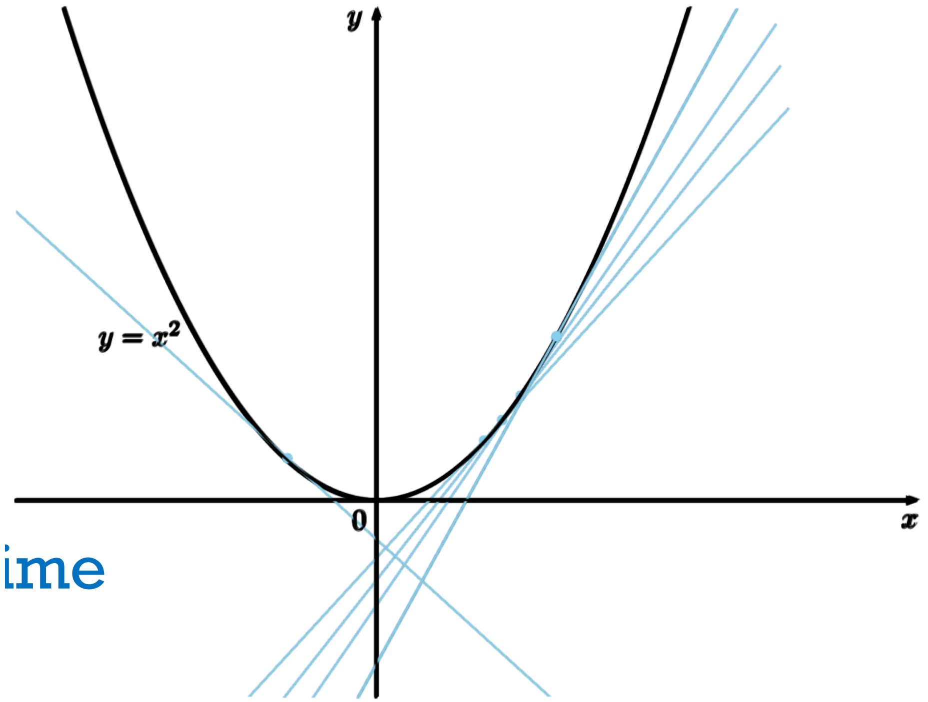
- We know how to get the gradient!
- But what to do with it?

- Take a step along the inverse direction of the gradient!
- How far to go?

Gradient says to decrease

Let's take big steps!

Too far! ime

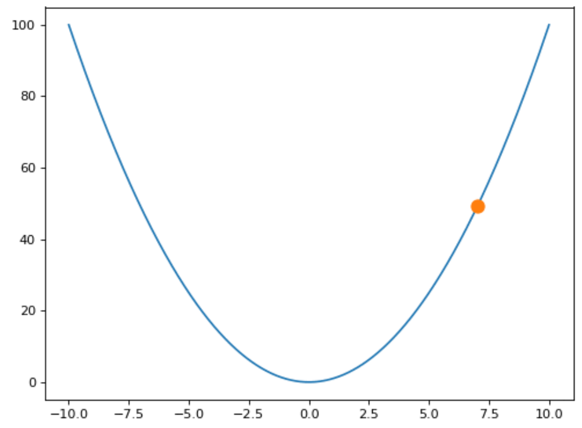


Gradient Descent – The Learning Rate

- Size of the steps = **Learning Rate**
- Second component of (Stochastic) Gradient Descent

- Simplest form of update for an input x:
  Vanilla Gradient Descent

$$x \mathrel{+}= -learningrate \cdot \frac{df}{dx}(x)$$



- Drawbacks:
  - Somewhat unintuitive parameter learning rate (how to set this?)
  - Very dependent on the learning rate
  - Rather slow convergence in practice

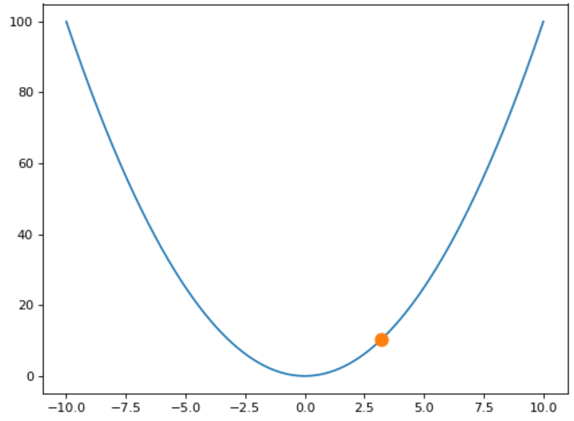
Gradient Descent – Improvements

- Momentum
  - Keep part of the velocity v from the last step!
    - So far: A hiker takes steps towards the steepest descent
    - Now: A ball rolls down the hill

$$v = \underbrace{mu \cdot v}_{\text{Momentum}} \underbrace{- learningrate \cdot \frac{df}{dx}(x)}_{\text{SGD}}$$

$$x += v$$

v: current speed of the ball
mu: how much of he speed to keep



Gradient Descent – Improvements

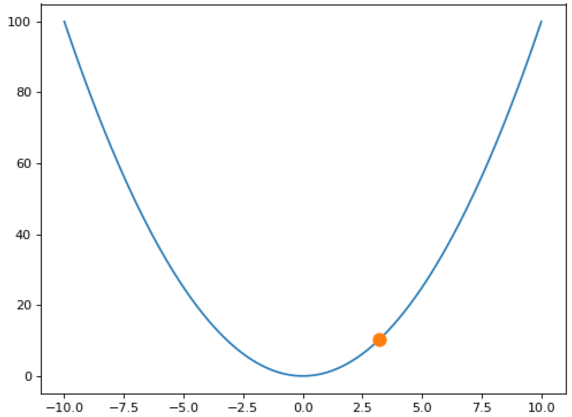
- Nesterov Momentum
  - Momentum tends to overshoot the minimum → Prevent that!
  - Use a lookahead: Take the gradient at the position that would be reached by the next step with the current velocity

Momentum:

$$v = mu \cdot v \; - learningrate \cdot \frac{df}{dx}(x)$$

$$xahead = x + mu \cdot v$$
$$v = mu \cdot v \; - learningrate \cdot \frac{df}{dx}(xahead)$$
$$x \mathrel{+}= v$$

v: current speed of the ball
mu: how much of he speed to keep



Gradient Descent – Improvements

- All methods so far are very dependent on the learning rate
- Can we get away without tuning the learning rate?

→ Yes! Some methods adapt it themselves*

* Not completely, but mostly

Gradient Descent – Improvements

- Adagrad
  - Introduces a **cache** variable that modifies the effective learning rate **per parameter**

$$cache \mathrel{+}= \frac{df}{dx}(\mathrm{x})^2$$

$$x \mathrel{+}= -\frac{learningrate}{\sqrt{cache} + \epsilon} \cdot \frac{df}{dx}(x)$$

- (Relatively) **decreases** learning rate for parameters that have **large** updates
- (Relatively) **increases** learning rate for parameters that have **small** updates

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Gradient Descent – Improvements

- RMSProp
  - Adagrad usually decreases the learning rate too aggressively. Fix that!

$$cache = decayrate \cdot cache + (1 - decayrate) \cdot \frac{df}{dx}(\mathrm{x})^2$$

Same as Adagrad

$$x \mathrel{+}= -\frac{learningrate}{\sqrt{cache} + \epsilon} \cdot \frac{df}{dx}(x)$$

- Still tunes the learning rate per parameter…
- … but does not decrease it monotonically

Gradient Descent – Improvements

- Adam
  - „RMSProp with Momentum“

Basically the velocity from Momentum

$$m = \beta_1 \cdot m + (1 - \beta_1) \cdot \frac{df}{dx}(x)$$

Basically the cache from RMSProp

$$v = \beta_2 \cdot v + (1 - \beta_2) \cdot \frac{df}{dx}(\mathrm{x})^2$$

$$x \mathrel{+}= -\frac{learningrate}{\sqrt{v} + \epsilon} \cdot m$$

- Usually works well
- Also try Nesterov Momentum!

Gradient Descent – Even More Improvements

- RAdam[1]
  - „Rectified Adam“ → Introduces a rectifier term

$$m = \beta_1 \cdot m + (1-\beta_1) \cdot \frac{df}{dx}(x)$$

$$v = \beta_2 \cdot v + (1-\beta_2) \cdot \frac{df}{dx}(\mathrm{x})^2$$

$$\boxed{\begin{gathered} \rho = \rho_\infty - \frac{2t\beta_2}{1-\beta_2}, \qquad \rho_\infty = \frac{2}{\beta_2} - 1 \\ r = \frac{(\rho-4)(\rho-2)\rho_\infty}{(\rho_\infty-4)(\rho_\infty-2)\rho} \end{gathered}}$$

$$x \mathrel{+}= -\frac{learningrate}{\sqrt{v}+\epsilon} \cdot m \cdot \boxed{\sqrt{r}}$$

- Rectifies the variance of the adaptive learning rate
  → can be dramatically large in the early stage of training

[1] Liyuan Liu, Haoming Jiang, Pengcheng He, Weizhu Chen, Xiaodong Liu, Jianfeng Gao, and Jiawei Han. (2019). *On the Variance of the Adaptive Learning Rate and Beyond.*

Gradient Descent – Even More Improvements

- Ranger
  - Combines RAdam and Lookahead[1]

Algorithm 1 Lookahead Optimizer:

Require: Initial parameters ϕ_0, objective function L
Require: Synchronization period k, slow weights step size α, optimizer A
  for $t = 1, 2, \ldots$ **do**
    Synchronize parameters $\theta_{t,0} \leftarrow \phi_{t-1}$
    for $i = 1, 2, \ldots, k$ **do**
      sample minibatch of data $d \sim \mathcal{D}$
      $\theta_{t,i} \leftarrow \theta_{t,i-1} + A(L, \theta_{t,i-1}, d)$
    end for
    Perform outer update $\phi_t \leftarrow \phi_{t-1} + \alpha(\theta_{t,k} - \phi_{t-1})$
  end for
  return parameters ϕ

A here is RAdam

- RAdam stabilizes training at the early stage…
- … Lookahead stabilizes it during the rest

[1] Michael R. Zhang, James Lucas, Geoffrey Hinton, and Jimmy Ba. (2019). Lookahead Optimizer: k steps forward, 1 step back.

Gradient Descent

- Improving optimisers is becoming a new field of research
- **Research goal:** Find an optimiser that
  - **converges fast:** use as few optimisation steps as possible to find a minimum
  - **generalises well:** do not step into bad local minima
  - **is easy to use:** no large hyperparameter search to get good performance
- Currently, Adam is the state-of-the-art optimiser [1]
  - it usually converges fast, but
  - it shows bad generalisation performance on some tasks [2]
- New methods are getting more theoretically grounded and show empirical improvements w.r.t. Adam, e.g. MADGRAD [3]
- Time will show the applicability of optimisers in ML fields

[1] Choi, D., Shallue, C. J., Nado, Z., Lee, J., Maddison, C. J., & Dahl, G. E. (2019). On empirical comparisons of optimizers for deep learning. *arXiv preprint arXiv:1910.05446*.
[2] Wilson, A. C., Roelofs, R., Stern, M., Srebro, N., & Recht, B. (2017). The marginal value of adaptive gradient methods in machine learning. *arXiv preprint arXiv:1705.08292*.
[3] Defazio, A., & Jelassi, S. (2021). Adaptivity without Compromise: A Momentumized, Adaptive, Dual Averaged Gradient Method for Stochastic Optimization. *arXiv preprint arXiv:2101.11075*.