# PROBABILISTIC AND DIFFERENTIABLE PROGRAMMING

## V2: Gradient Descent

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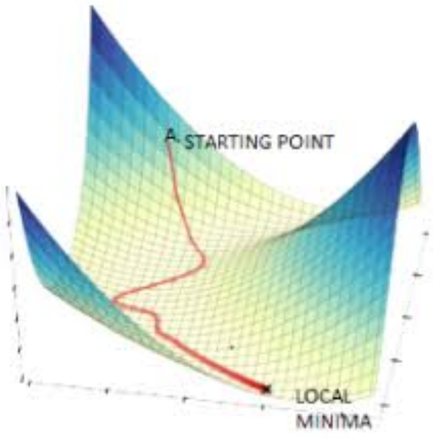
# Agenda for today's lecture

## Gradient descent (GD)

1. Differentiation

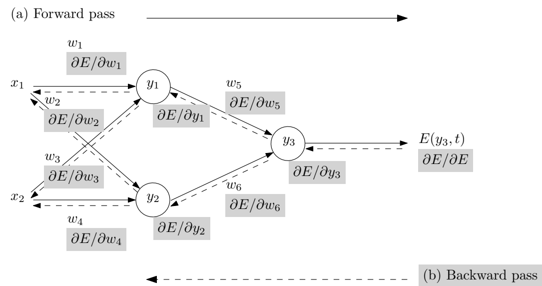
$$\frac{df}{dx}$$




2. Basic GD and variants

$$\theta_{t+1} \leftarrow \theta_t - \eta \nabla_\theta L$$

3. Backpropagation



# The big idea: follow the gradient

- Fundamentally, we're interested in machines that we train by
  - optimising parameters
- How do we select those parameters?
- In deep learning/differentiable programming we typically define an objective function to optimize
  - *minimise (in case of error or loss say)* or
  - *maximise* with respect to those parameters
- We're looking for points at which the gradient of the objective function is zero w.r.t. the parameters

# The big idea: follow the gradient

- Gradient based optimisation is a BIG field!
  - First order methods, second order methods, subgradient methods...
  - With deep learning we're primarily interested in first-order methods[1).
- Primarily using variants of gradient descent:
  - function $F(\boldsymbol{x})$ has *a (not necessarily unique or global)* minimum at a point $\boldsymbol{x} = \boldsymbol{a}$ where $\boldsymbol{a}$ is given by applying

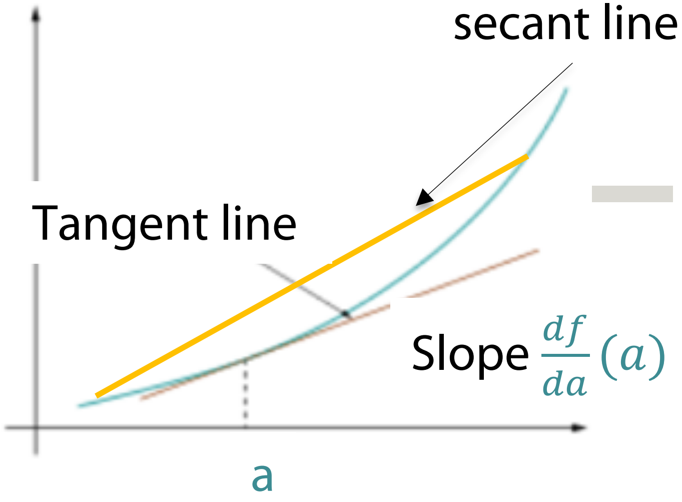
$$\boldsymbol{a}_{n+1} = \boldsymbol{a}_n - \alpha\nabla F(\boldsymbol{a}_n)$$

until convergence

1) Second order gradient optimisers are potentially better, but for systems with many variables are currently impractical as they require computing the Hessian matrix.

# DIFFERENTIATION

# Gradient in one dimension




- Gradient of a straight line is $\Delta y \,/ \Delta x$

- For arbitrary real-valued functions $f(x)$

  approximate the derivative, $\frac{df}{dx}(a)$ using the gradient of the secant line trough $(a, f(a))$ and $(a+h, f(a+h))$ for small $h$

$$f'(a) = \frac{df}{dx}(a) \approx \frac{\Delta f}{\Delta a} \approx \frac{f(a+h)-f(a)}{h}$$ (Newton's difference quotient)

$$\frac{df}{dx}(a) = \lim_{h \to 0} \frac{f(a+h)-f(a)}{h}$$ (Derivative of $f$ at $a$)

# Example: Derivative of a quadratic function

$$
\begin{aligned}
y &= x^2 \\
\frac{dy}{dx} &= \lim_{h \to 0} \frac{(x+h)^2 - x^2}{h} \\
\frac{dy}{dx} &= \lim_{h \to 0} \frac{x^2 + 2hx + h^2 - x^2}{h} \\
\frac{dy}{dx} &= \lim_{h \to 0} \frac{2hx + h^2}{h} \\
\frac{dy}{dx} &= \lim_{h \to 0} 2x + h \\
\frac{dy}{dx} &= 2x
\end{aligned}
$$

# Derivatives of „deeper“ functions

- Deep learning is all about optimising deeper functions: functions that are compositions of other functions, e.g.

$$h = (f \circ g)(x) = f(g(x))$$

- Derivative can be calculated by chain rule

**Chain rule (1-dim)**

$$\frac{dh}{dx} = \frac{df}{dg}\frac{dg}{dx} \qquad \text{for} \quad h(x) = f(g(x))$$

# Example for chain rule

$$h(x) = x^4 = (x^2)^2 \ = f\big(g(x)\big)$$
$$\frac{dh}{dx} = 2 \ \cdot x^2 \cdot 2x = 4x^3$$

You may verify this also directly

$$\frac{dh}{dx} = \lim_{h \to 0} \frac{(x+h)^4 - x^4}{h}$$
$$\frac{dh}{dx} = \lim_{h \to 0} \frac{h^4 + 4h^3x + 6h^2x^2 + 4hx^3 + x^4 \ - x^4}{h}$$
$$\frac{dh}{dx} = \lim_{h \to 0} h^3 + 4h^2x + 6hx^2 + 4x^3 \ = 4x^3$$

# Generalization: Vector functions $\boldsymbol{y}(t)$

- Split into its constituent coordinate functions:

$$\boldsymbol{y}(t) = (y_1(t), \ldots, y_n(t))$$

- Derivative is a vector (the tangent vector),

$$\boldsymbol{y}'(t) = (y_1{}'(t), \ldots, y_n{}'(t))$$

  which consists of the derivatives of the coordinate functions.

- Equivalently

$$\boldsymbol{y}'(t) = \lim_{h \to 0} \frac{\boldsymbol{y}(t+h) - \boldsymbol{y}(t)}{h}$$

  (if the limit exists)

# Differentiation with multiple variables

$$f(x,y) = x^2 + xy + y^2$$
$$\frac{\partial f}{\partial x} = 2x + y$$
$$\frac{\partial f}{\partial y} = x + 2y$$

Partial derivative of $f(x_1, \ldots x_n): \mathbb{R}^n \to \mathbb{R}$ w.r.t. $x_i$ at $\boldsymbol{a} = (a_1, \ldots, a_n)$

$$\frac{\partial f}{\partial x_i}(\boldsymbol{a}) = \lim_{h \to 0} \frac{f(a_1,\ldots,a_i+h,\ldots,a_n) - f(\boldsymbol{a})}{h}$$

Gradient of $f(x_1, \ldots x_n): \mathbb{R}^n \to \mathbb{R}$ at $\boldsymbol{a} = (a_1, \ldots, a_n)$

$$\nabla f(\boldsymbol{a}) = (\frac{\partial f}{\partial x_1}(\boldsymbol{a}), \ldots, \frac{\partial f}{\partial x_n}(\boldsymbol{a}))$$

Jacobian of $\boldsymbol{f}(x_1, \ldots x_n): \mathbb{R}^n \to \mathbb{R}^m$ at $\boldsymbol{a} = (a_1, \ldots, a_n)$

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}(\boldsymbol{a}) = \begin{pmatrix} \nabla f_1(\boldsymbol{a}) \\ \vdots \\ \nabla f_m(\boldsymbol{a}) \end{pmatrix} = \left(\frac{\partial f_i}{\partial x_j}(\boldsymbol{a})\right)_{1 \le i \le m; 1 \le j \le n} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(\boldsymbol{a}) & \cdots & \frac{\partial f_1}{\partial x_n}(\boldsymbol{a}) \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1}(\boldsymbol{a}) & \cdots & \frac{\partial f_m}{\partial x_n}(\boldsymbol{a}) \end{pmatrix}$$

# Linear algebra reminder

- Given vectors $\boldsymbol{x} = (x_1, \dots, x_n)$ and $\boldsymbol{y} = (y_1, \dots, y_n)$
- Scalar product : $\boldsymbol{x} \cdot \boldsymbol{y} = \sum_{i=1}^{n} x_i y_i$

- Jacobian is given as an $m \times n$ matrix

  $A = (a_{ij})_{1 \le i \le m, 1 \le j \le n}$ (m rows, n columns)

- An $m \times n$ matrix A defines a linear mapping

  $A\colon \mathbb{R}^n \to \mathbb{R}^m$ via

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix} \mapsto A\,x = \begin{pmatrix} \sum_{i=1}^{n} a_{1,i} x_i \\ \sum_{i=1}^{n} a_{2,i} x_i \\ \dots \\ \sum_{i=1}^{n} a_{m,i} x_i \end{pmatrix}$$

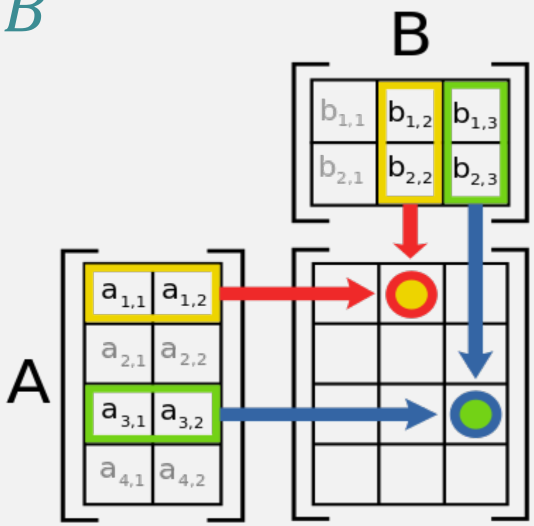
(Linearity: $A(\lambda\mathbf{x} + \mu\boldsymbol{y}) = \lambda A x + \mu A y$ where x,y vectors and $\lambda, \mu$ scalars)

# Linear algebra reminder

Matrix multiplication $C = A\,B$ for

$m \times n$ matrix $A$ and $n \times p$ matrix $B$

$$c_{i,j} = \sum_{k=1}^{n} a_{i,k} b_{k,j}$$




Transposed matrix $A^{\top}$: change columns and rows

# Gradients in Machine Learning

The kinds of functions (and programs) that are usually optimized in ML have following properties:

- They are scalar-valued
- There are multiple losses, but ultimately we can just consider optimising with respect to the sum of the losses.
- They involve multiple variables, which are often wrapped up in the form of vectors or matrices, and more generally tensors.

**How will we find the gradients of these?**

# The chain rule for vectors

Given functions $f, g$ with

- $\mathbb{R}^m \quad \xrightarrow{g} \quad \mathbb{R}^n \quad \xrightarrow{f} \quad \mathbb{R}$
- $\boldsymbol{x} \quad \mapsto \quad \boldsymbol{y} = g(\boldsymbol{x}) \mapsto \quad z = f(\boldsymbol{y})$

the chain rule gives the partial derivatives

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$$

( in short form: $\nabla_{\boldsymbol{x}} z = \left(\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}\right)^{\top} \nabla_{\boldsymbol{y}} z$

where $\left(\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}\right)$ is the n x m Jacobian matrix of g )

# Chain rule for Tensors (Informal)

- Tensors (as understood in the ML literature) generalize vectors (1D-tensors) and matrices (2D-tensors)
  - 3D-tensor: Layer of matrices
  - nD-tensor $A_{i_1 \dots i_n}$ is indexed by n-tuples $(i_1 \dots i_n)$
    - Needed e.g. to model layers of convolution matrices etc.
- Gradients of tensors by
  - flattening them into vectors
  - computing the vector-valued gradient
  - then reshaping the gradient back into a tensor.
- This is just multiplying Jacobians by gradients again

# The chain rule für tensors (formally)

- Aim: Calculate: $\nabla_{\boldsymbol{X}} z$ for scalar $z$ and tensor $\boldsymbol{X}$
  - Indices into $\boldsymbol{X}$ have multiple coordinates, but we can generalise by using a single variable $i$ to represent the complete tuple of indices.
  - For all index tuples $i$: $$(\nabla_{\boldsymbol{X}} z)_i = \frac{\partial z}{\partial X_i}$$

For $\boldsymbol{Y} = g(\boldsymbol{X})$ and $z = f(\boldsymbol{Y})$

$$\nabla_{\boldsymbol{X}} z = \sum_j (\nabla_{\boldsymbol{X}} Y_j) \frac{\partial z}{\partial Y_j}$$

# Example for tensor chain rule

- Let $\boldsymbol{D} = \boldsymbol{XW}$ where the rows of $\boldsymbol{X} \in \mathbb{R}^{n \times m}$ contains some fixed features, and $\boldsymbol{W} \in \mathbb{R}^{m \times h}$ is a matrix of weights.
- Also let $L = f(\boldsymbol{D})$ be some scalar function of $\boldsymbol{D}$ that we wish to minimise.
- What are the derivatives of $L$ with respect to the weights $\boldsymbol{W}$?

- Start by considering a specific weight $W_{uv}$
- $\frac{\partial L}{\partial W_{uv}} = \sum_{i,j} \frac{\partial L}{\partial D_{ij}} \frac{\partial D_{ij}}{\partial W_{uv}}$ (by chain rule)
- $\frac{\partial D_{ij}}{\partial W_{uv}} = 0$ if $j \neq v$ because $D_{ij}$ is the scalar product of row $i$ of $\boldsymbol{X}$ and column $j$ of $\boldsymbol{W}$.
- Therefore: $\sum_{i,j} \frac{\partial L}{\partial D_{ij}} \frac{\partial D_{ij}}{\partial W_{uv}} = \sum_i \frac{\partial L}{\partial D_{iv}} \frac{\partial D_{iv}}{\partial W_{uv}}$
- What is $\frac{\partial D_{iv}}{\partial W_{uv}}$?
  - $D_{iv} = \sum_{1 \leq k \leq m} X_{ik} W_{kv}$
  - $\frac{\partial D_{iv}}{\partial W_{uv}} = \frac{\partial}{\partial W_{uv}} \sum_{1 \leq k \leq q} X_{ik} W_{kv} = \sum_{1 \leq k \leq m} \frac{\partial}{\partial W_{uv}} X_{ik} W_{kv} = X_{iu}$

- Putting every together, we have: $\frac{\partial L}{\partial W_{uv}} = \sum_i \frac{\partial L}{\partial D_{ij}} X_{iu}$
- $= \sum_i X_{iu} \frac{\partial L}{\partial D_{ij}} = \sum_i X_{ui}^\top \frac{\partial L}{\partial D_{ij}}$

- Doing this for arbitrary $W_{iu}$ leads to
- $\frac{\partial L}{\partial \boldsymbol{W}} = \boldsymbol{X}^\top \frac{\partial L}{\partial \boldsymbol{D}}$

# VANILLA GRADIENT DESCENT, VARIANTS AND BEYOND

# Vanilla Gradient Descent (VGD)

- Given: loss function l, dataset D, and model g, parameters θ; number of passes (epochs) over the data, learning rate η
- Total loss: $L = -\sum_{(x,y)\in D} l(g(x,\theta),y)$

VGD: $\theta_{t+1} \leftarrow \theta_t - \eta\nabla_\theta L$

\+ Good statistical properties (very low variance)
\- Very data inefficient (particularly when data has many similarities)
\- Doesn’t scale to infinite data (online learning)

Problems of *GD
\- ...

# Why the hell follow the gradient?

- Make shift in parameter space $\Delta\theta = (\Delta\theta_1, \Delta\theta_2)$
- Calculus says : $\Delta L \approx \frac{\partial L}{\partial \theta_1}\Delta\theta_1 + \frac{\partial L}{\partial \theta_2}\Delta\theta_2 = \nabla \mathrm{L}\Delta\boldsymbol{\theta}$
- Loss should decrease: $\Delta L \leq 0$
- Try: $\Delta\theta = -\eta\nabla L$
- Helps, because $\Delta L \approx -\eta\, \nabla L \cdot \nabla L = -\eta \left|\left|\nabla L\right|\right|^2$

  and $\left|\left|\nabla L\right|\right|^2 \geq 0$

Linear algebra reminder:

- Norm of $v$: $\left|\left|v\right|\right| = v \cdot v$ (for scalar product $\cdot$ )

# Let's talk abut loss – only roughly for now

- Gradient descent algorithms depend on loss function $l$
- For now think of loss function l as mean squared error $l_{MSE}$
- We will see other ones and their interplay with activation functions in the next lecture

Mean squared error on one single training example

$$
\begin{array}{llcl}
l_{MSE}: & \mathbb{R}^n \times \mathbb{R}^n & \xrightarrow{\boldsymbol{l}} & \mathbb{R} \\
 & (\hat{y}, y) & \mapsto & ||\hat{y} - y||^2
\end{array}
$$

# Stochastic Gradient Descent (SGD)

- Given: loss function l, dataset D, model g, parameters θ, number of epochs, learning rate η

SGD : In each epoch do for each $(\boldsymbol{x}, y) \in D$

$$\theta_{t+1} \leftarrow \theta_t - \eta \nabla_\theta \, l(g(\boldsymbol{x}, \theta_t), y)$$

+ Faster than VGD
+ Online learning
- Poor statistical properties (high fluctuation)
- computational inefficiency

Problems of *GD

- ...

# Mini-Batch SGD (MGD)

- Given: mini-batch size m (common: 50-256), loss function l, dataset D, model g, parameters θ, number of epochs , learning rate η
- Batch loss: $L_{b(t)} = \sum_{(x,y)\in b(t)} l(g(x,\theta), y)$

  where $b(t)$ a subset of D of cardinality m.

MSGD : $\theta_{t+1} \leftarrow \theta_t - \eta \nabla_{\theta_t} L_{b(t)}$

+ reduces the parameter-updates' variance
+ stable convergencevery
+ computational efficiency

Problems of *GD

1. How to choose rate
2. No learning rate schedules
3. Trapping in local minima
4. Inefficient for sparse data set

# Problem 1: Choosing the learning rate $\eta$ [1)]

- Choice of learning rate is extremely important
- But we have to reason about the 'loss landscape'
  - Types of cost functions (see next lecture)
  - Most convergence analysis of optimisation algorithms assumes a convex loss landscape
    - Easy to reason about
    - (S)GD converges to optimal solution for a variety of $\eta$s
    - Insights into potential problems in the non-convex case
  - Deep Learning is highly non-convex
  - Many local minima; Plateaus; Saddle points; Symmetries (permutation, etc)

1) One form of hyper-parameter magic

# „Beyond“: Accelerated Gradient Methods

- Accelerated gradient methods use a *leaky* average of the gradient, rather than the instantaneous gradient estimate at each time step

- A physical analogy would be one of the momentum a ball picks up rolling down a hill...

- Helps addressing the *GD problems

# Mini-Batch SGD with Momentum (MSGDM)

- Given: momentum parameter $\beta$ (0,9 is good choice), batch size m, batch loss $L_{b(t)}$, number of epochs, learning rate η

MSGDM : update θ by accumulated velocity

$$v_{t+1} \leftarrow \beta v_t + \nabla_\theta L_{b(t)}$$
$$\theta_{t+1} \leftarrow \theta_t - \eta v_{t+1}$$

+ The momentum method allows to accumulate velocity in directions of low curvature that persist across multiple iterations
+ This leads to accelerated progress in low curvature directions compared to gradient descent

# Problem 2: Scheduling learning rates

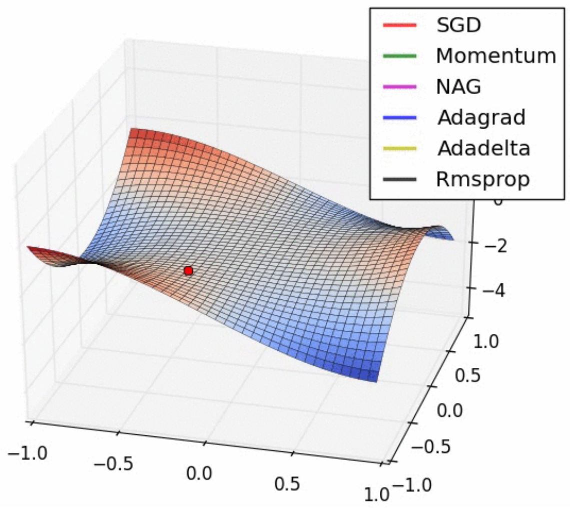
- In practice you want to decay your learning rate over time
- Smaller steps will help you get closer to the minima
- But don’t do it to early, else you might get stuck Something of an art form!
- ‘Grad Student Descent’ or GDGS (‘Gradient Descent by Grad Student‘)
- Tackling Plateaus (Common Heuristic approach)
  - if the loss hasn’t improved (within some tolerance) for *k* epochs then drop the lr by a factor of 10

# Problem 3: Stucking into local minima

- Cycle the learning rate up and down (possibly annealed), with a different lr on each batch
- See L. N. Smith. Cyclical Learning Rates for Training Neural Networks. arXiv e-prints, page https://arxiv.org/abs/1506.01186 , June 2015.

# SOTA: More advanced optimisers

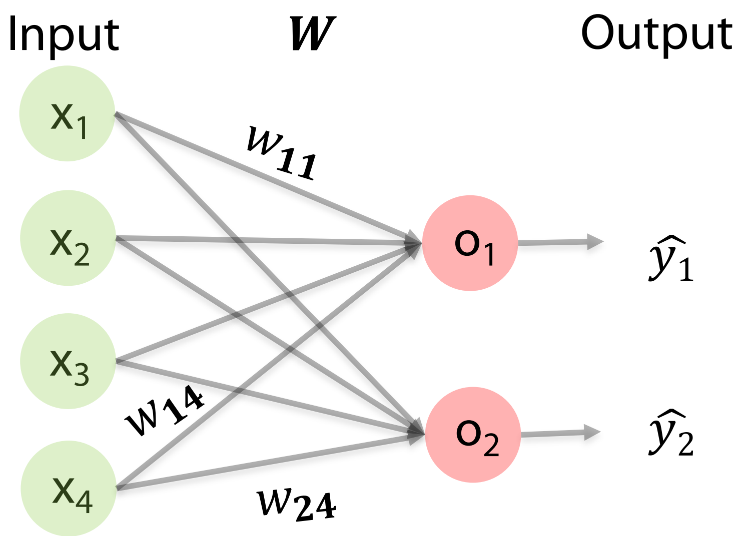
- Here only name dropping and some fancy gif from here
  - Adagrad (dynamic decrease, second moment used)
  - RMSProp (decouple learning rate from gradient)
  - Adam (BestOf(RMSProp,MSDGM) )




- J. Hare says:
  - If you're in a hurry to get results use Adam
  - If you have time (or a Grad Student at hand), then use SGD (with momentum) and work on tuning the learning rate
  - If you're implementing something from a paper, then follow what they did!

# BACKPROPAGATION

# Network view of single function[1)]




Network model

$\boldsymbol{b}$ : Bias vector $(b_1, b_2)$

$\boldsymbol{W} =$ weight matrix $(w)_{1\leq i\leq 2;1\leq j\leq 4}$ :

z: $\boldsymbol{Wx} + \boldsymbol{b}$ linear output

$\boldsymbol{\sigma}$ : activation function

$$\mathbb{R}^4 \xrightarrow{\boldsymbol{g}} \mathbb{R}^2$$

$$\boldsymbol{x} \mapsto \hat{\boldsymbol{y}} = \boldsymbol{g} = (\boldsymbol{g_1}(\boldsymbol{x}), \boldsymbol{g_2}(\boldsymbol{x}))$$

Vector-valued function in four arguments

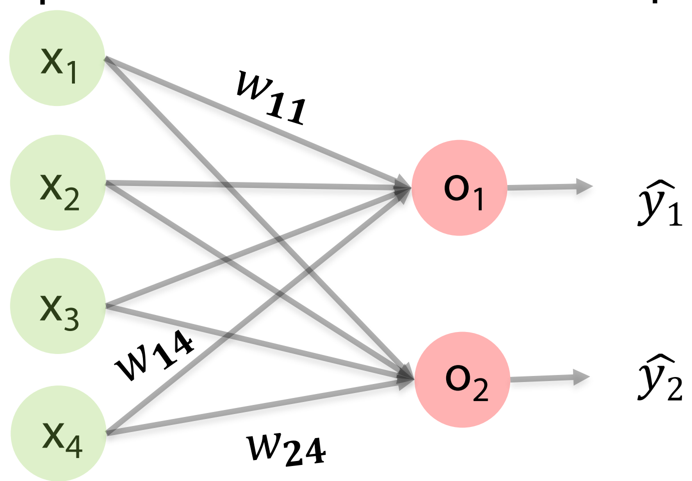
$$\hat{\boldsymbol{y}} = \boldsymbol{g}\,(\boldsymbol{x}\,; \boldsymbol{W}, \boldsymbol{b}) = \boldsymbol{\sigma}\,(\boldsymbol{Wx} + \boldsymbol{b}) = \sigma(\boldsymbol{z})$$

Decomposition into linear and activation part

1) You may find this also under the term perceptron in the literature

# Network view of single function

Input $\quad W \quad$ Output




**Example linear output**

$$\mathbf{W} = \begin{pmatrix} 1 & 2 & -1 & -2 \\ 3 & 4 & -3 & 4 \end{pmatrix} \quad \mathbf{x} = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \quad \boldsymbol{b} = \begin{pmatrix} 5 \\ 6 \end{pmatrix}$$

$$\boldsymbol{Wx} = \begin{pmatrix} 1 \cdot 1 + 2 \cdot 2 + -1 \cdot 3 - 2 \cdot 4 \\ 3 \cdot 1 + 4 \cdot 2 + -3 \cdot 3 + 4 \cdot 4 \end{pmatrix} = \begin{pmatrix} -6 \\ 18 \end{pmatrix}$$

$$\boldsymbol{Wx} + \boldsymbol{b} = \begin{pmatrix} -6 \\ 18 \end{pmatrix} + \begin{pmatrix} 5 \\ 6 \end{pmatrix} = \begin{pmatrix} -1 \\ 24 \end{pmatrix}$$

$$\mathbb{R}^4 \xrightarrow{\boldsymbol{g}} \mathbb{R}^2$$

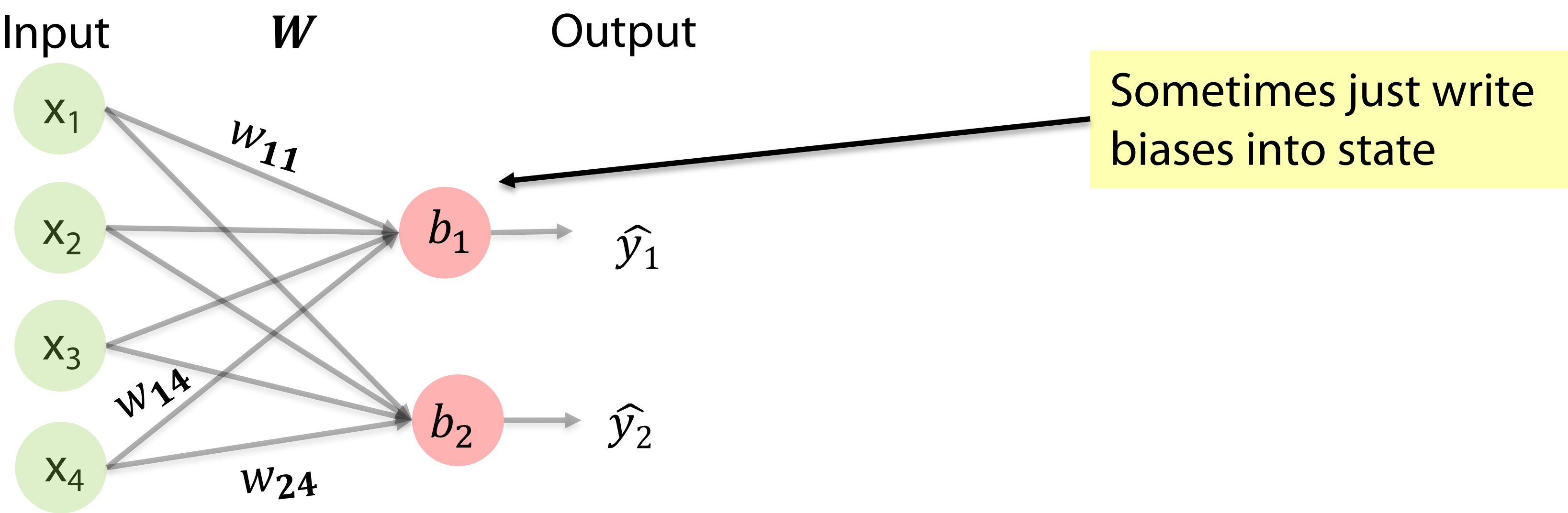
$$\boldsymbol{x} \mapsto \hat{\boldsymbol{y}} = \boldsymbol{g} = (\boldsymbol{g_1}(\boldsymbol{x}), \boldsymbol{g_2}(\boldsymbol{x}))$$

$$\hat{\boldsymbol{y}} = \boldsymbol{g}\,(\boldsymbol{x}\,; \boldsymbol{W}, \boldsymbol{b}) = \boldsymbol{\sigma}\,(\boldsymbol{Wx} + \boldsymbol{b}) = \sigma(\boldsymbol{z})$$

Vector-valued function in four arguments

Decomposition into linear and activation part

# Network view of single function




$$\mathbb{R}^4 \quad \xrightarrow{\boldsymbol{g}} \quad \mathbb{R}^2$$

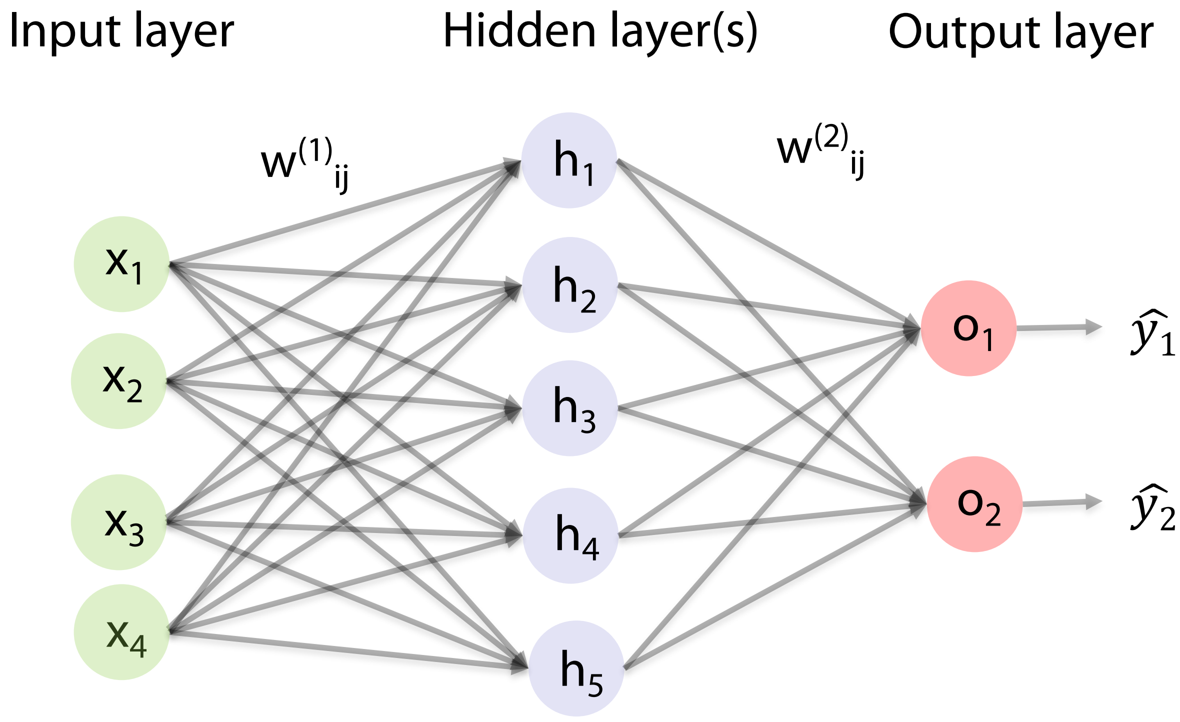
$$\boldsymbol{x} \quad \mapsto \quad \hat{\boldsymbol{y}} = \boldsymbol{g} = (\boldsymbol{g_1}(\boldsymbol{x}), \boldsymbol{g_2}(\boldsymbol{x}))$$

Vector-valued function in four arguments

$$\hat{\boldsymbol{y}} = \boldsymbol{g}\,(\boldsymbol{x}\,;\boldsymbol{W},\boldsymbol{b}) \quad = \boldsymbol{\sigma}\,(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) = \sigma(\boldsymbol{z})$$

Decomposition into linear and activation part

# Network view of composed functions[1)]




$\mathbb{R}^4 \xrightarrow{g} \mathbb{R}^5 \xrightarrow{f} \mathbb{R}^2$

$\boldsymbol{x} \mapsto \boldsymbol{h} \mapsto \hat{\boldsymbol{y}}$

| | |
|---|---|
| i: | layer i |
| $\boldsymbol{b}^i$ : | Bias in i |
| $\mathbf{W}^{(i)}$: | weight matrix in i |
| $\boldsymbol{\sigma}_i$: | activation function in i |

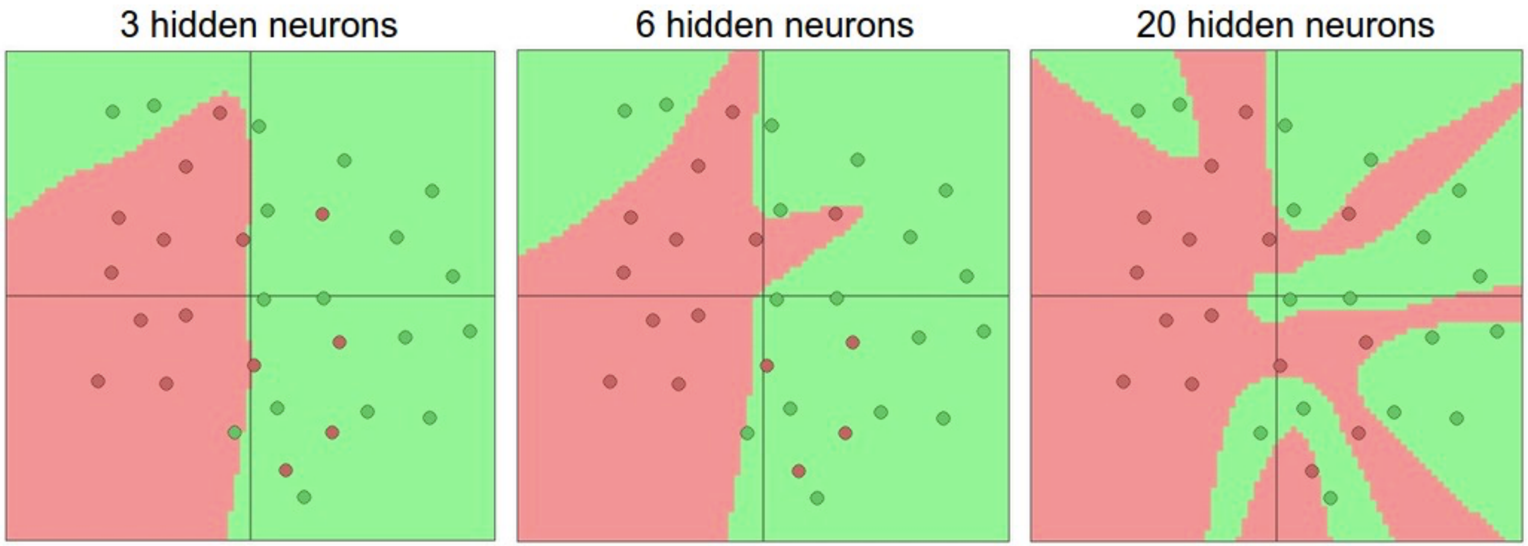
| | |
|---|---|
| $\boldsymbol{a}^i$: | $\boldsymbol{\sigma_i}(\boldsymbol{W}^{(i)}\boldsymbol{a}^{i-1} + \boldsymbol{b}_i)$ activation in i |
| $\boldsymbol{z}^i$: | $\boldsymbol{W}^{(i)}\boldsymbol{a}^{i-1} + \boldsymbol{b_i}$ linear ouptut in layer i |

$$\hat{\boldsymbol{y}} = \boldsymbol{f}\,(\boldsymbol{g}\,(\boldsymbol{x}\,;\ \boldsymbol{W}^{(1)}\ ,\boldsymbol{b}^{1}\,);\ \boldsymbol{W}^{(2)}\,,\boldsymbol{b}^{2}) \qquad = \boldsymbol{\sigma}_2\,(\boldsymbol{W}^{(2)}\,\boldsymbol{\sigma}\,1(\boldsymbol{W}^{(1)}\boldsymbol{x}\ + \boldsymbol{b}^{1}\,)\ +\ \boldsymbol{b}^{2})$$

1) You may find this also under the term multilayer perceptron in the literature

# Activation functions

Non-linearities needed to learn complex (non-linear) representations of data, otherwise the network would be just a linear function $W_1 W_2 x = Wx$



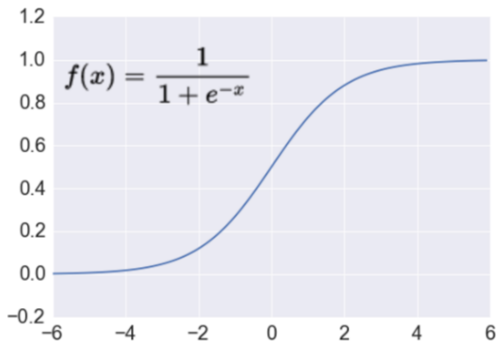

*http://cs231n.github.io/assets/nn1/layer_sizes.jpeg*

More layers and neurons can approximate more complex functions

Full list: https://en.wikipedia.org/wiki/Activation_function

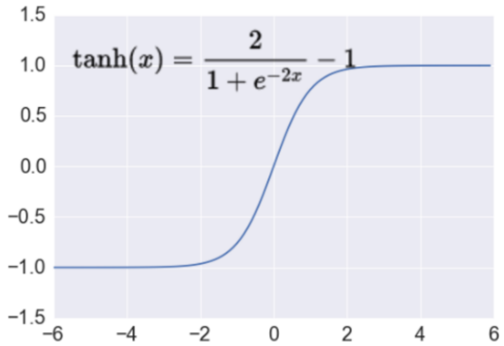
# Activation Functions

*http://adilmoujahid.com/images/activation.png*



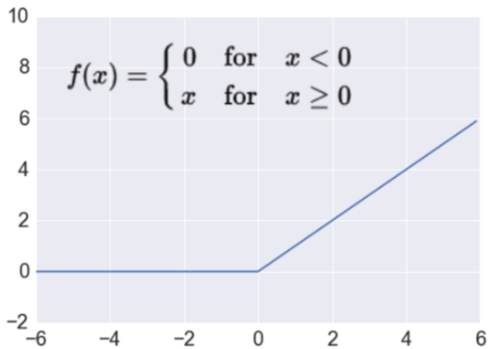

Sigmoid $\mathbb{R}^n \rightarrow [0,1]$

- Takes a real-valued number and “squashes” it into range between 0 and 1.
- Earliest used activation function (neuron)
- Leads to vanishing gradient problem




Tanh: $\mathbb{R}^n \rightarrow [-1,1]$

- Takes a real-valued number and “squashes” it into range between -1 and 1
- Same probem of vanishing gradient
- $\tanh(x) = 2sigm(2x) - 1$




Rectified Linear Unit ReLu: $\mathbb{R}^n \rightarrow \mathbb{R}^n_+$

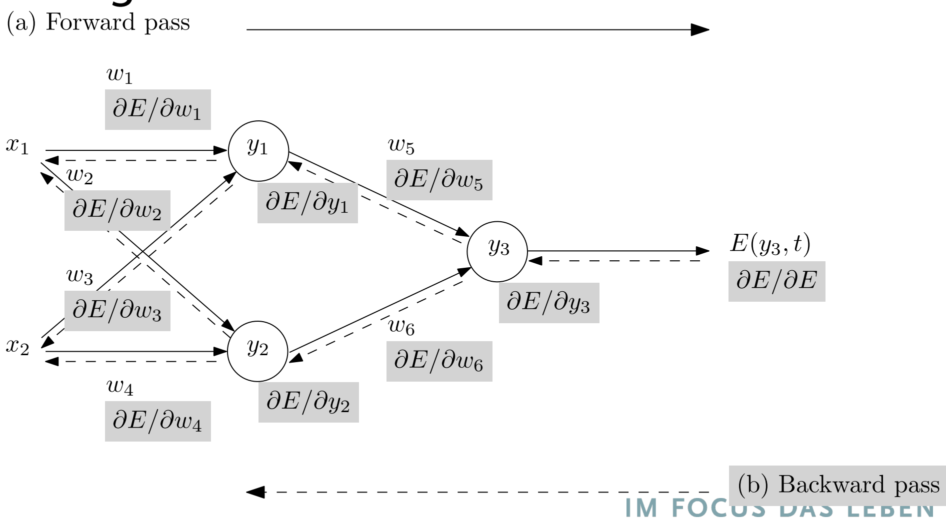
- Takes a real-valued number and thresholds it at zero
- Used in Deep Learning
- No vanishing gradient
- But: it is not differentiable (need relaxation)
- Dying ReLU

# Backprop: efficient implementation of gradient descent

Sample labeled data (**batch**) → **Forward** it through the network, get predictions → **Back-propagate** the errors → **Update** the network weights

Backpropagation idea

- Generate **error signal** that measures difference between predictions and target values
- Use error signal to change the weights and get more accurate predictions backwards
- Underlying mathematics: chain rule




**Chain rule (1-dim)**

$$\frac{dh}{dx} = \frac{df}{dg}\frac{dg}{dx}$$

( for $h(x) = f(g(x))$ )

# Computational graph perspective

**Function f**

$$f(x,y,z) = (x+y)\ \cdot z$$
$$= qz$$
$$\text{for } q = x + y$$

**Partial Derivatives**

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

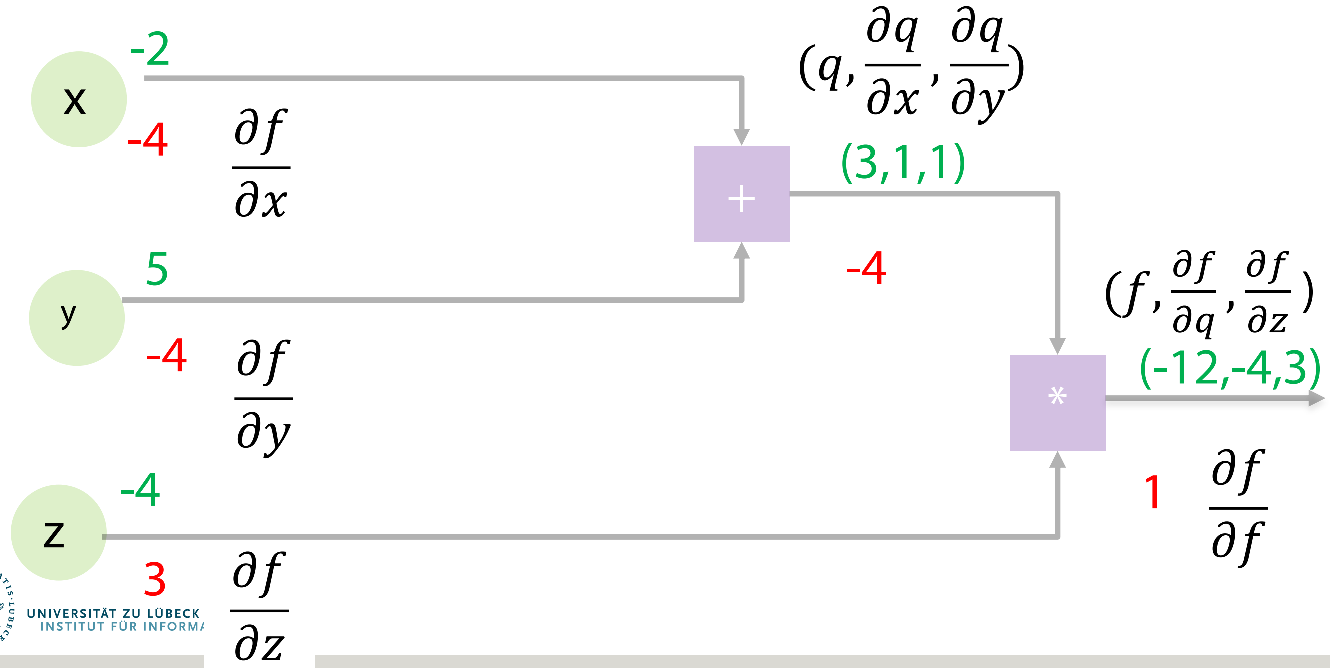
**Chain rule applied**

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x} = z$$
$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial y} = z$$

**Gradient**

$$\nabla_{x,y,z} f = (z, z, q)$$

(In particular: $(\nabla_{x,y,z} f)(-2{,}5,-4) = (-4,-4,3)$)




Forward pass: function values and local gradients

Backward: chain rule

# What this example tells us about backprop

- Every operation in the computational graph given its inputs can immediately compute two things:
  1. its output value and
  2. local gradients of its inputs

- The chain rule tells us literally that each operation should take its local gradients and multiply them by the gradient that flows backwards into it

- Backprop is an instance of 'Reverse Mode Automatic Differentiation'

# Backpropagation: requirements on cost (loss)

1. Cost $C$ (we named it $L$ before) on whole data is sum of costs on training instances
2. Cost is a function of the output $\hat{\boldsymbol{y}}$

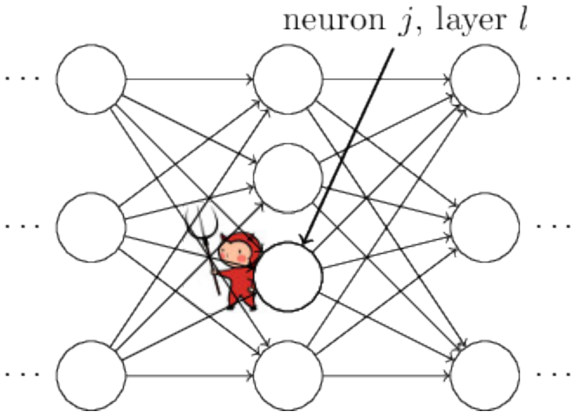
- Backpropagation in the following described for cost on single training example
- With 1. assumption backpropagation can be combined with gradiend descent.
- In the following going to use Hadamard product $\odot$

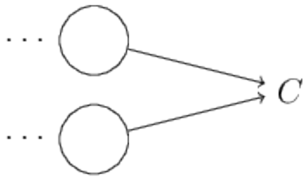
$$\begin{pmatrix} a \\ b \end{pmatrix} \odot \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} ac \\ bd \end{pmatrix}$$

# Propagation of errors

Backpropagation works on errors
(from these in the end one gets $\nabla_{\boldsymbol{W},\boldsymbol{b}}\, C$ )

$\delta_j^l \;:= \dfrac{\partial C}{\partial z_j^l}$ error in j[th] component in layer l




Demon changes $z_j^l$ to $z_j^l + \Delta z_j^l$

Resulting cost $C$ changes by $\frac{\partial C}{\partial z_j^l}\Delta z_j^l$

# Backpropagation algorithm (on single instance)

1. Input: Initialize input vector $\boldsymbol{x} = \boldsymbol{a}^0$
2. Feedforward: For i = 1,2, ... , M

$$\boldsymbol{z^i} = \boldsymbol{W}^{(i)}\boldsymbol{a^{i-1}} + \boldsymbol{b_i} \text{ and } \boldsymbol{a^i} = \boldsymbol{\sigma_i}(\boldsymbol{z^i})$$

3. Compute error on last layer

$$\boldsymbol{\delta}^M = \nabla_{\hat{\boldsymbol{y}}} C \odot \sigma'(\boldsymbol{z}^M) \qquad \text{(BP1)}$$

4. Backpropagate error: For i = M-1, M-2, ...,

$$\boldsymbol{\delta}^i = (\boldsymbol{w^{i+1}})^\top \boldsymbol{\delta}^{i+1} \odot \sigma'(\boldsymbol{z}^i) \qquad \text{(BP2)}$$

5. Compute gradients

$$\frac{\partial C}{\partial w^i_{jk}} = a_k^{i-1}\delta_j^i \quad \text{and} \quad \frac{\partial C}{\partial b^i_j} = \delta^i_j \qquad \text{(BP3/4)}$$

# Proof of (BP1) in backprop

- $\delta_j^M = \frac{\partial C}{\partial z_j^M}$ (by definition)
- $\delta_j^M = \sum_k \frac{\partial C}{\partial a_k^M} \frac{\partial a_k^M}{\partial z_j^M}$ (chain rule;

  k over all components in output)
- $\delta_j^M = \frac{\partial C}{\partial a_j^M} \frac{\partial a_j^M}{\partial z_j^M}$ ($\frac{\partial a_k^M}{\partial z_j^M}$ vanishes if $k \neq j$)
- $\delta_j^M = \frac{\partial C}{\partial a_j^M} \sigma'(z_j^M)$ ($a_j^M = \sigma(z_j^M)$)

# Backpropagation algorithm (within MSGD)

1. Input: mini-batch of m training examples x
2. For each training example set corresponding activation $\boldsymbol{a}^{\boldsymbol{x},\boldsymbol{1}}$ and do the following
   1) Feedforward: For i = 1,2, ... , M

      $$\boldsymbol{z}^{\boldsymbol{x},\boldsymbol{i}} = \boldsymbol{W}^{(\boldsymbol{i})}\boldsymbol{a}^{\boldsymbol{x},\boldsymbol{i}-\boldsymbol{1}} + \boldsymbol{b}_{\boldsymbol{i}} \text{ and } \boldsymbol{a}^{\boldsymbol{x},\boldsymbol{i}} = \boldsymbol{\sigma}_{\boldsymbol{i}}(\boldsymbol{z}^{\boldsymbol{x},\boldsymbol{i}})$$

   2) Compute error on last layer

      $$\boldsymbol{\delta}^{\boldsymbol{x},M} = \nabla_{\hat{\boldsymbol{y}}} C_x \odot \sigma'(\boldsymbol{z}^{\boldsymbol{x},M})$$

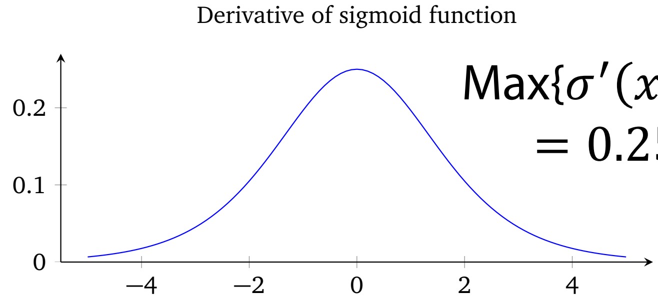
   3) Backpropagate error: For i = M-1, M-2, ...,

      $$\boldsymbol{\delta}^{i} = (\boldsymbol{w}^{\boldsymbol{i}+\boldsymbol{1}})^{\top}\boldsymbol{\delta}^{\boldsymbol{x},i+1} \odot \sigma'(\boldsymbol{z}^{\boldsymbol{x},i})$$

3. Gradient descent:

$$\boldsymbol{w}^{i} = \boldsymbol{w}^{i} - \frac{\eta}{m}\sum_x \boldsymbol{\delta}^{\boldsymbol{x},i}\left(\boldsymbol{a}^{\boldsymbol{x},i-1}\right)^{\top} \text{ and } \boldsymbol{b}^{i} = \boldsymbol{b}^{i} - \frac{\eta}{m}\sum_x \boldsymbol{\delta}^{\boldsymbol{x},i}$$

# Problem: Vanishing gradient for sigmoid $\sigma$

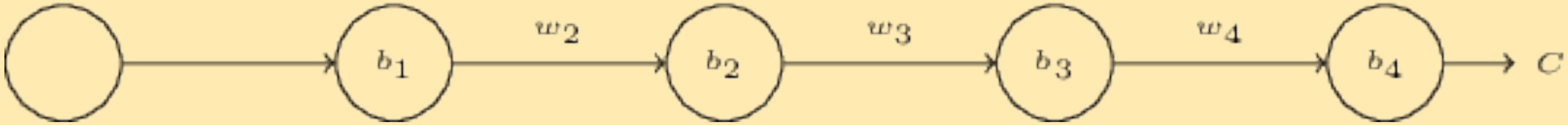



- Gradient of sigmoid:
  $\sigma'(x) = \sigma(x)(1 - \sigma(x))$

$\text{Max}\{\sigma'(x)\} = 0.25$

## Gradients in linear network of depth 4

$$\frac{\partial C}{\partial b_1} = \sigma'(z_1) \times \underbrace{w_2 \times \sigma'(z_2)}_{\leq\, 0{,}25} \times \underbrace{w_3 \times \sigma'(z_3)}_{\leq\, 0{,}25} \times \underbrace{w_4 \times \sigma'(z_4)}_{\leq\, 0{,}25} \times \frac{\partial C}{\partial a_4}$$

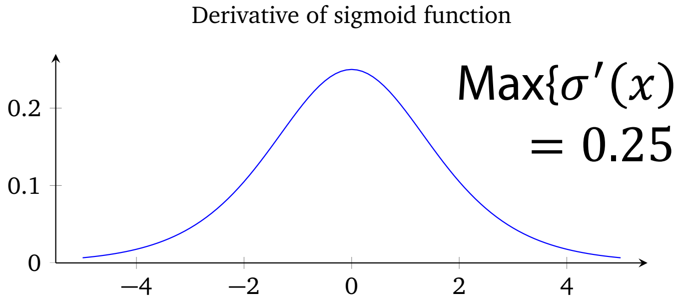



- Assume $|w_i| \leq 1$ (e.g. $w_i \sim N(0,1)$ )
- Then: $||w_i\sigma'(z_i)| \leq 0{,}25$
- Exponential decrease from later derivatives to earlier ones due to chain rule

Gradient vanishes moving backwards

# Problem: Vanishing gradient with large input

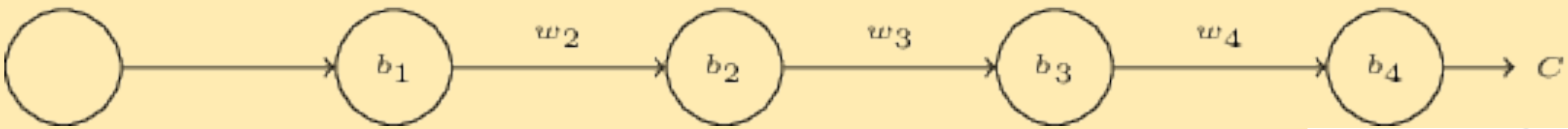
- Gradient of sigmoid:
  $\sigma'(x) = \sigma(x)(1 - \sigma(x))$



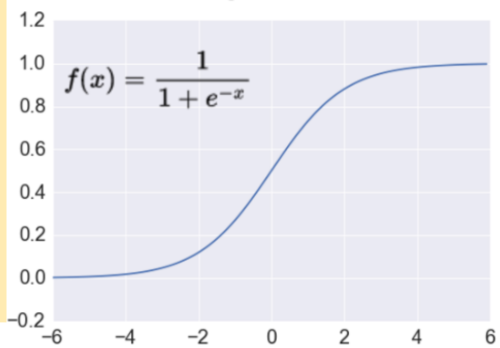

Max$\{\sigma'(x)\}$ $= 0.25$

## Gradients in linear network of depth 4

$$\frac{\partial C}{\partial b_1} = \sigma'(z_1) \times w_2 \times \sigma'(z_2) \times w_3 \times \sigma'(z_3) \times w_4 \times \sigma'(z_4) \times \frac{\partial C}{\partial a_4}$$




- If $|x|$ very large , then $\sigma(x)$ or (1-- $\sigma(x)$) becomes zero
- So $\sigma'(x)$ becomes zero




**Gradient vanishes for large inputs to activation functions**

# NEARLY THE END

# Take Home Message

Follow the gradient – with care

Uhhh, a lecture with a hoepfully useful

# APPENDIX

# Color Convention in this Course

- Formulae, when occurring inline
- Newly introduced terminology and definitions
- Important results (observations, theorems) as well as emphasizing some aspects
- Examples are given with standard orange with possibly light orange frame
- Comments and notes in nearly opaque post-it
- Algorithms
- Reminders (in the grey fog of your memory)

# Todays lecture is based on the following

- Jonathon Hare: Lectures 2,3,4,6 of course „COMP6248 Differentiable Programming (and some Deep Learning“)
  http://comp6248.ecs.soton.ac.uk/

- Nielsen: Neural Networks and Deep Learning.
  http://neuralnetworksanddeeplearning.com/, chapters 1,2

- https://medium.com/@ramrajchandradevan/the-evolution-of-gradient-descend-optimization-algorithm-4106a6702d39

- I. Lorentzou: Introduction to Deep Learning, link