### Deep Feedforward Networks

Master-Seminar: Introduction to Deep Learning

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### Overview

- 1. Basics of artificial neural networks
  - Historical notes
- 2. Architecture design
  - Output units
  - · Hidden units
- 3. Gradient-based learning
  - · Back-propagation
  - Other differentiation algorithms
- 4. Application
  - · Odd/Even
  - · "multiple of"

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Basics of Artificial Neural Networks

### Deep feedforward networks?

### What are deep feedforward networks?

- · the basic deep learning model
- alternative terms: feedforward neural networks, multilayer perceptrons (MLPs)

### What is a network?

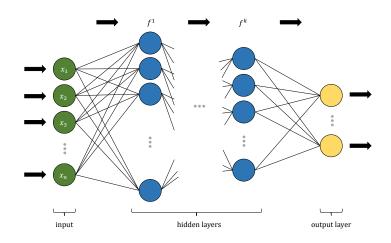
· composing together many different functions

$$f(\mathbf{x}) = f^{(3)}(f^{(2)}(f^{(1)}(\mathbf{x})))$$

 $f^{(1)}$  would be the first layer,  $f^{(2)}$  the second layer, and so on ...

- · length of the chain: depth of the network
- input: x
   output layer: last layer
   hidden layers: layers in between

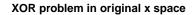
### Graphical representation of a neural network

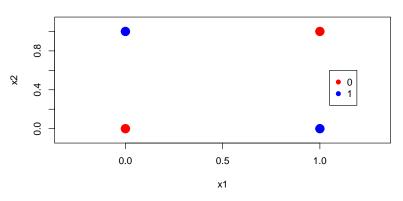


### Function approximation

- $\cdot$  given: noisy example x, corresponding label y
- The goal of the neural network is to approximate a function  $f^*(x)$   $(y \approx f^*(x))$ .
- Find optimal parameters  $m{ heta}$  so that a function f maps  $(x, m{ heta})$  on y.

### Example: XOR





### How to overcome the limitations of a linear model?

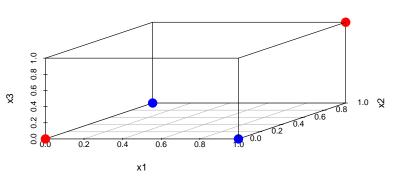
Transform the input x by a nonlinear transformation  $\phi$ . Possible solutions for  $\phi$ :

- · kernel trick, Support Vector Machine
- $\cdot$  manually engineer  $\phi$
- learn  $\phi$

### Example: XOR

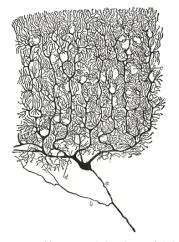
Adding a third input  $x_3 = x_1 \cdot x_2$ :

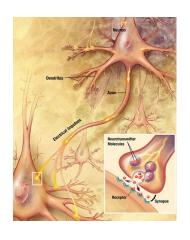
### XOR problem in new space



### Why neural?

### Human brain: around 85 billion neurons



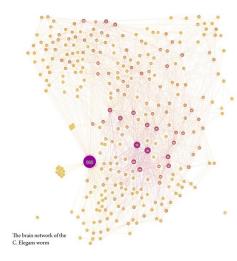


left: https://commons.wikimedia.org/wiki/File:Purkinje\_cell\_by\_Cajal.png

right: https://commons.wikimedia.org/wiki/File:Chemical\_synapse\_schema\_cropped.jpg

### Why neural?

### C. elegans: worm with around 300 neurons



### Why neural?

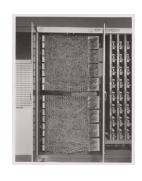
- · More precise: artificial neural networks (ANN)
- architecture is inspired by biological neural networks
- · but: not an exact model of the function of a brain
- · development of ANN shaped by maths / computer science

**Historical Notes** 

Basics of Artificial Neural Networks

### Historical notes

- 1943: McCulloch / Pitts create first computational model for neural networks
- · late 1940s: Hebbian learning
- 1951: Minsky develops SNARC, possibly the first ANN
- 1958: Rosenblatt creates the Mark I perceptron



https://upload.wikimedia.org/wikipedia/en/5/52/Mark\_I\_perceptron.jpeg

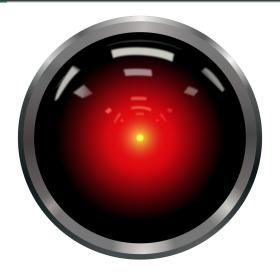
### Historical notes

- 1969: Minsky/Papert "Perceptrons: An Introduction to Computational Geometry"
- limited processing power of computers at the time
- 1986: Rumelhart, Hinton and Williams on MLP and back-propagation
- · Schmidhuber: "Deep learning since 1991"

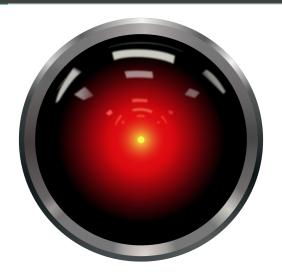
### New developments

- since 2000s: many breakthroughs because of increasing processing power and massive data availability
- · Google Translate
- Voice recognition in smartphones
- Amazon Echo / Alexa speech recognition
- DeepMind's AlphaGo
- · Self-driving cars

### What will come next?



### What will come next?



 $\verb|https://commons.wikimedia.org/wiki/File:HAL9000\_Better\_Reflection.svg|$ 

### Lip-reading

### Robotics

## Al Has Beaten Humans at Lip-reading

A pair of new studies show that a machine can understand what you're saying without hearing a sound.

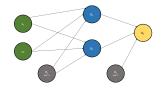
by Jamie Condliffe November 21, 2016



https://www.technologyreview.com/s/602949/ai-has-beaten-humans-at-lip-reading/

Architecture Design

### Architecture design



What is the structure of the neural network?

- How many units?
- · Which units?
- How do you connect these units?

### Chain structure

**Typical design approach**: multiple layers that consist of multiple units are linked in a chain structure.

First layer is a function of the inputs:

$$\boldsymbol{h}^{(1)} = g^{(1)} \left( \boldsymbol{W}^{(1)T} \boldsymbol{x} + \boldsymbol{b}^{(1)} \right)$$

Second layer is a function of the first layer's output:

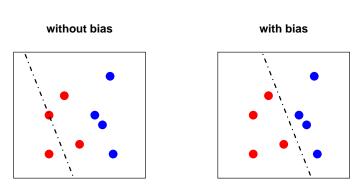
$$\boldsymbol{h}^{(2)} = g^{(2)} \left( \boldsymbol{W}^{(2)T} \boldsymbol{h}^{(1)} + \boldsymbol{b}^{(2)} \right)$$

...

 $g^{()}$  is called activation function.

### Bias

Bias puts the decision boundary at the correct position in the learned space.



### Depth and width

### Depth of the network

number of layers of the network

### Width of a layer

number of units in a layer

Deeper networks often work with thiner layers which means less parameters.

Ideal architecture has to be found via experimentation.

### Universal approximation theorem

Cybenko (1989) Approximation by Superpositions of a Sigmoidal Function.

Hornik (1991) Approximation capabilities of multilayer feedforward networks.

### Universal approximation theorem

"In the mathematical theory of artificial neural networks, the universal approximation theorem states that a feed-forward network with a single hidden layer containing a finite number of neurons (i.e., a multilayer perceptron), can approximate continuous functions on compact subsets of  $\mathbb{R}^n$ , under mild assumptions on the activation function. The theorem thus states that simple neural networks can represent a wide variety of interesting functions when given appropriate parameters; however, it does not touch upon the algorithmic learnability of those parameters."

https://en.wikipedia.org/wiki/Universal\_approximation\_theorem

### Why may learning a function fail?

- 1. optimization algorithm may not find the parameters of the function
- 2. overfitting

### "No free lunch" theorem

"There is no strategy - applied on all possible problems - that is better than pure guessing."

https://de.wikipedia.org/wiki/No-free-Lunch-Theoreme

### Alternative network designs

Depth and height do not need to be the only parameters of the architecture of a neural network.

### Possible modifications:

- Add connections that skip a layer and connect layer i to layer i+2
- Do not connect every input of a layer with every output of the preceding layer.

The choice of modifications is very dependent on the actual application!

### Alternative network designs: examples

- · Convolutional networks (for computer vision)
- · Recurrent neural networks (for sequence processing)
  - · Long short-term memories (Google voice, Siri)
- Autoencoder (dimensionality reduction)
- · Deep belief network

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## Architecture Design

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**Output Units** 

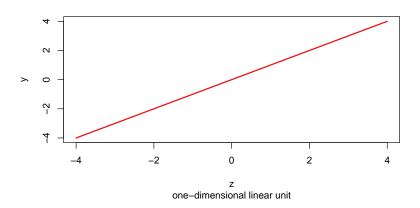
### **Output Units**

The output unit defines what happens to the output  $m{h}$  of the last hidden layer. So it is the last transformation on  $m{x}$ .

The choice of the output unit also determines the cost function.

### Linear units

$$\hat{\boldsymbol{y}} = \boldsymbol{z} = \boldsymbol{W}^T \boldsymbol{h} + \boldsymbol{b}$$



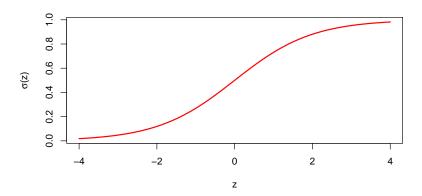
### Linear units

$$\hat{\boldsymbol{y}} = \boldsymbol{z} = \boldsymbol{W}^T \boldsymbol{h} + \boldsymbol{b}$$

- used for predicting the mean of a Gaussion distribution
- easy to handle for optimization algorithms

## Sigmoid units

Sigmoid function: 
$$\sigma(z) = \frac{1}{1+e^{-z}}$$
.



### Sigmoid units

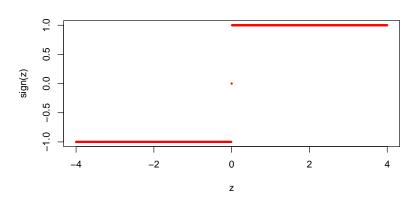
Sigmoid function: 
$$\sigma(z) = \frac{1}{1+e^{-z}}$$
.

$$\hat{y} = \sigma \left( \boldsymbol{w}^T \boldsymbol{h} + b \right)$$

- · applying the sigmoid function on a linear unit
- used for predicting binary outputs
- · problematic: saturation for large absolute values of z

### Perceptron

### Signum function



#### Softmax units

Softmax function: softmax(
$$z$$
) $_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$ .

- · generalization of sigmoid function for multiclass problem
- $\cdot$  used for predicting discrete output with k possible values

# Architecture Design

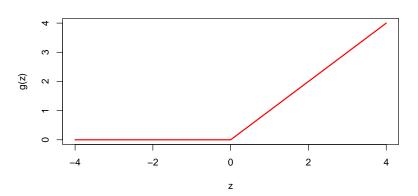
Hidden Units

#### Design of hidden units

- active area of research, not many definitive theoretical guidelines
- · Try out different kinds of units and look which work best.
- · good default choice: Rectified linear units
- · Hidden units do not have to be differentiable.

# Rectified linear units (ReLU)

$$g(z) = \max\{0, z\}$$



#### Rectified linear units (ReLU)

$$g(z) = \max\{0, z\}$$

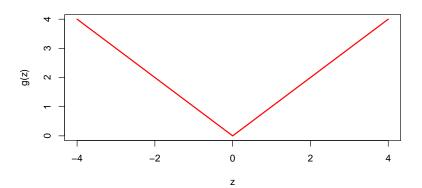
- $\cdot$  typically used with a bias b (set to small, positive value)
- sparse activation
- · not differentiable at zero
- unbounded

There are various generalizations of ReLU:

- · absolute value rectification
- · leaky ReLU
- parametric ReLU (PReLU)

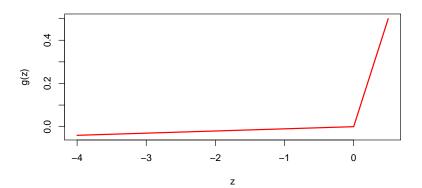
$$h_i = g(\boldsymbol{z}, \boldsymbol{\alpha})_i = \max(0, z_i) + \alpha_i \min(0, z_i)$$

Absolute value rectification:  $\alpha_i = -1 \Rightarrow g(z) = |z|$ .



$$h_i = g(\boldsymbol{z}, \boldsymbol{\alpha})_i = \max(0, z_i) + \alpha_i \min(0, z_i)$$

leaky ReLU:  $\alpha_i = 0.01$ .



$$h_i = g(\boldsymbol{z}, \boldsymbol{\alpha})_i = \max(0, z_i) + \alpha_i \min(0, z_i)$$

parametric ReLU: treat  $\alpha_i$  as learnable parameter.

#### Maxout units

$$g(z)_i = \max z_j$$

- divide z into groups of k values, calculate k linear combinations and take the maximum
- "learning the activation function"
- maxout network with two maxout hidden units can approximate any continuous function (Universal approximation theorem)
- · Goodfellow (2013) Maxout Networks.

# Logistic sigmoid and hyperbolic tangent

Sigmoid function:

$$g(z) = \sigma(z)$$

Hyperbolic tangent function:

$$g(z) = tanh(z)$$

Closely related, because  $tanh(z) = 2\sigma(2z) - 1$ .

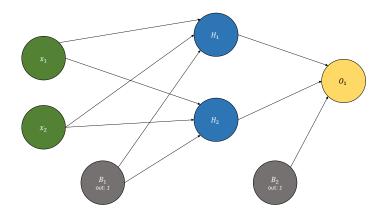
Used e.g. for recurrent networks or autoencoders.

#### Other hidden units

- · radial basis function
- sofplus
- · hard tanh

#### Example: A neural net for the XOR example

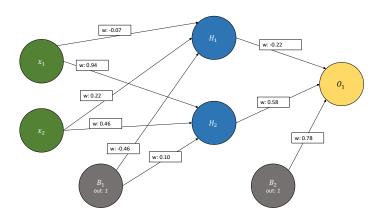
two inputs, one hidden layer with two units



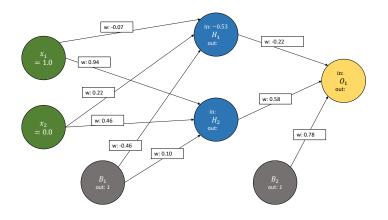
sigmoid activation function for hidden layer and output

# Weight initialisation

initialising random weights for all connections

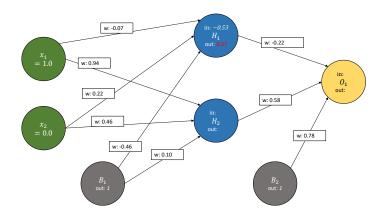


$$x_1 = 1, x_2 = 0$$
:



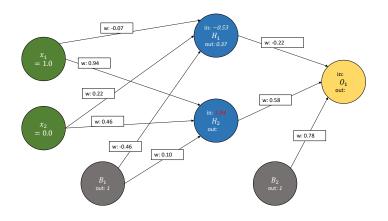
$$H_1$$
: in =  $-0.07 \cdot 1 + 0.22 \cdot 0 + -0.46 \cdot 1 = -0.53$ 

$$x_1 = 1, x_2 = 0$$
:



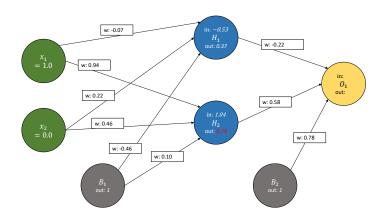
$$H_1$$
: out  $= \frac{1}{1 - e^{-0.53}}$ 

$$x_1 = 1, x_2 = 0$$
:



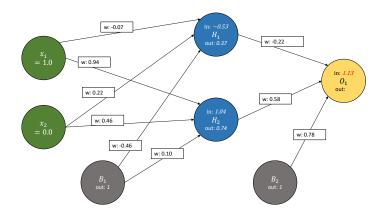
$$H_2$$
: in =  $-0.07 \cdot 1 + 0.22 \cdot 0 + -0.46 \cdot 1 = -0.53$ 

$$x_1 = 1, x_2 = 0$$
:



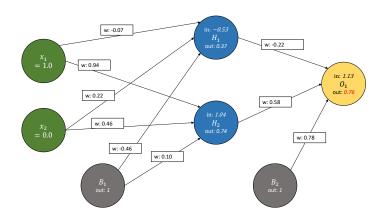
$$H_2$$
: out  $=\frac{1}{1-e^{-0.53}}$ 

$$x_1 = 1, x_2 = 0$$
:



$$O_1$$
: in =  $-0.07 \cdot 1 + 0.22 \cdot 0 + -0.46 \cdot 1 = -0.53$ 

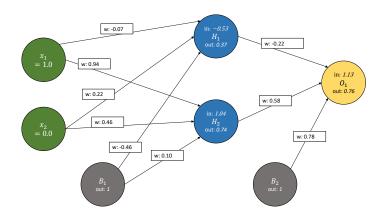
$$x_1 = 1, x_2 = 0$$
:



$$O_1$$
: out  $= \frac{1}{1 - e^{-0.53}}$ 

# Error of the output

Error: 
$$E = f(\boldsymbol{x}) - y = \hat{y} - y$$



$$E = 0.76 - 1 = -0.24$$

#### Total error

Total error can be defined as

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

For our example:

$$E = \frac{1}{2} \left[ (0.73 - 1)^2 + (0.74 - 1)^2 + (0.76 - 1)^2 + (0.76 - 1)^2 \right]$$
  
= 0.12785

**Gradient-Based Learning** 

#### Why gradient-based learning?

- Nonlinearity of neural nets causes loss functions to become non-convex.
- · Convex optimization algorithms do not work anymore.
- · Use iterative, gradient-based optimization.
- Does not guarantee convergence and results may depend heavily on initial parameters.
- For *very large* data sets, it does make sense to train a linear model or SVM by gradient descent, too.

# Gradient-Based Learning

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**Back-Propagation** 

# Forward propagation and back-propagation

#### Forward propagation

The information of the inputs x flows through the hidden units to finally produce  $\hat{y}$  and the cost  $J(\theta)$ .

#### **Back-propagation**

The information of the cost  $J(\theta)$  flows backwards through the hidden units to calculate the gradient.

# Calculating the gradient (output layer)

Total error is defined as:  $E = \frac{1}{2} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2$ 

Gradient of connection from unit i to output  $O_1$ :

$$\frac{\partial E}{\partial w_{O_1,i}} = \frac{\partial E}{\partial out_{O_1}} \cdot \frac{\partial \text{out}_{O_1}}{\partial \text{in}_{O_1}} \cdot \frac{\partial \text{in}_{O_1}}{\partial w_{O_1,i}}$$

If we define  $\delta_{O_1} = (\hat{y}_i - y_i) \cdot \sigma'_{O_1}$ , then we get

$$\frac{\partial E}{\partial w_{O_1,i}} = \delta_{O_1} \text{out}_i,$$

with  $\operatorname{out}_{O_1} = \hat{y}_i$  and  $\frac{\partial \operatorname{out}_{O_1}}{\partial \operatorname{in}_{O_1}} = \sigma'_{O_1}$ .

#### Calculating the gradient (hidden layer)

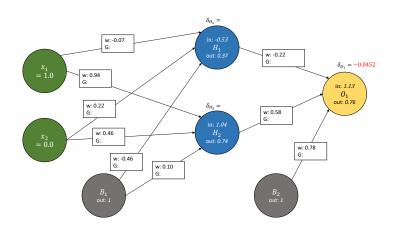
#### Gradient of connection from unit i to unit j:

$$\frac{\partial E}{\partial w_{j,i}} = \frac{\partial E}{\partial out_j} \cdot \frac{\partial \text{out}_j}{\partial \text{in}_j} \cdot \frac{\partial \text{in}_j}{\partial w_{j,i}}$$

Node delta is now defined as  $\delta_j = \sigma'_j \sum_k w_{k,j} \cdot \delta_k$ . We get

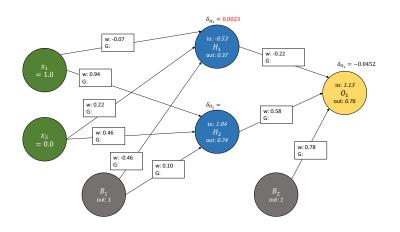
$$\frac{\partial E}{\partial w_{j,i}} = \delta_j \mathsf{out}_i.$$

Delta of output node:



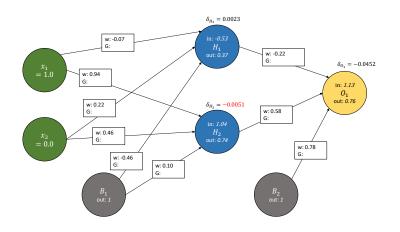
$$\delta_{O_1} = -0.24 \cdot d\sigma(1.13) = -0.24 \cdot \sigma(1.13)(1 - \sigma(1.13)) = -0.0452$$

Delta of hidden node 1:



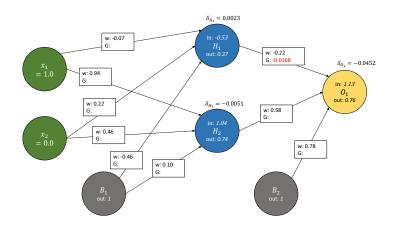
$$\delta_{H_1} = d\sigma(-0.53) \cdot (-0.22 \cdot -0.0452) = 0.0023$$

Delta of hidden node 2:



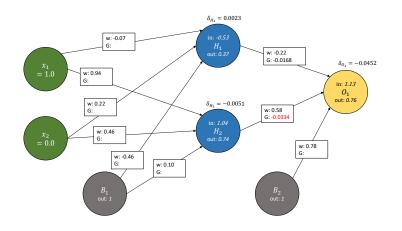
$$\delta_{H_2} = d\sigma(1.04) \cdot (0.58 \cdot -0.0452) = -0.0051$$

#### Gradient from $H_1$ to $O_1$ :



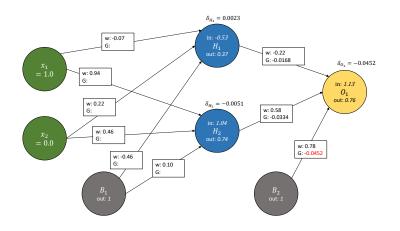
$$G_{O_1,H_1} = 0.37 \cdot -0.0452 = -0.0168$$

#### Gradient from $H_2$ to $O_1$ :



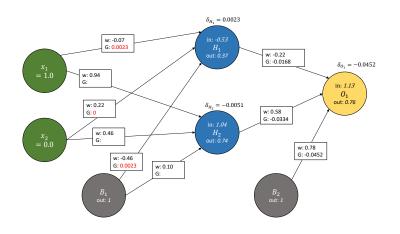
$$G_{O_1,H_2} = 0.74 \cdot -0.0452 = -0.0334$$

#### Gradient from $B_2$ to $O_1$ :



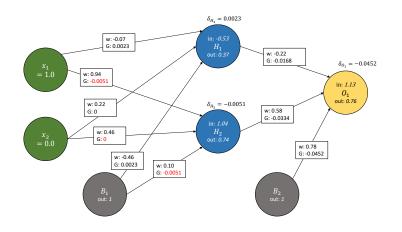
$$G_{O_1,B_2} = 1 \cdot -0.0452 = -0.0452$$

Gradient from  $x_1, x_2, B_1$  to  $H_1$ :



$$G_{H_1,\cdot} = \begin{pmatrix} 0.0023 & 0 & 0.0023 \end{pmatrix}$$

Gradient from  $x_1, x_2, B_1$  to  $H_2$ :



$$G_{H_2,\cdot} = \begin{pmatrix} -0.0051 & 0 & -0.0051 \end{pmatrix}$$

$$\Delta w^{(t)} = -\epsilon \frac{\partial E}{\partial w^{(t)}} + \alpha \Delta w^{(t-1)}$$

- · learning rate  $\epsilon$ 
  - · too high: may fail to converge
  - · too low: very slow learning
- momentum  $\alpha$ 
  - $0 < \alpha < 1$
  - can speed up learning
  - · can help to avoid local minima
- $\epsilon$  and  $\alpha$  have to be determined by trial and error or by experience

### Online vs batch learning

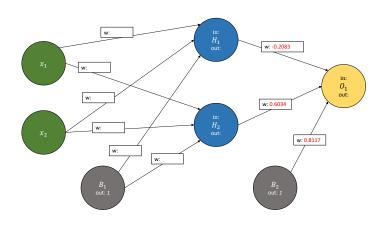
#### · online learning:

- randomly select a training set element, modify weights and repeat
- · can help to avoid local minima, but slow

#### · batch learning:

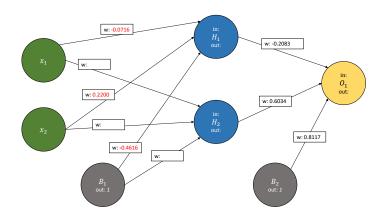
- gradients for each training set element are summed up, then weights are updated
- faster as it incorporates the average error of all elements
- mini-batch: select several training set elements and compute a weight update

New weights  $w_{O_1,:}$ :



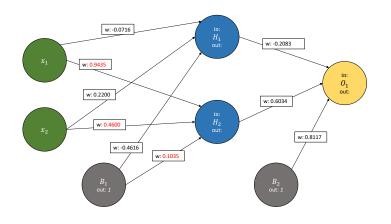
$$w_{O_1,\cdot} = \begin{pmatrix} -0.22 & 0.58 & 0.78 \end{pmatrix} - 0.7 \cdot \begin{pmatrix} -0.0168 & -0.0334 & -0.0452 \end{pmatrix} + 0.3 \cdot 0$$

New weights  $w_{H_1,:}$ :



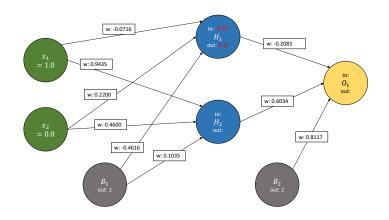
$$w_{H_1,\cdot} = \begin{pmatrix} -0.07 & 0.22 & -0.46 \end{pmatrix} - 0.7 \cdot \begin{pmatrix} 0.0023 & 0 & 0.0023 \end{pmatrix} + 0.3 \cdot 0$$

New weights  $w_{H_2,:}$ :

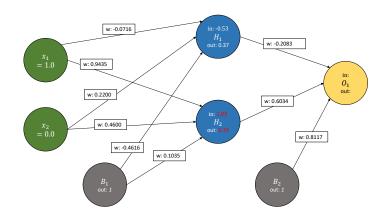


$$w_{H_2,.} = \begin{pmatrix} 0.94 & 0.46 & 0.10 \end{pmatrix} - 0.7 \cdot \begin{pmatrix} -0.0051 & 0 & -0.0051 \end{pmatrix} + 0.3 \cdot 0$$

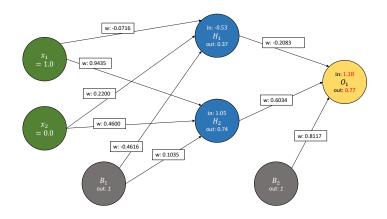
### Test: forward propagation with new weights



### Test: forward propagation with new weights



### Test: forward propagation with new weights



### Total error for new weights

Total error before adjusting weights was 0.12785.

Now:

$$E = \frac{1}{2} [(0.74 - 1)^2 + (0.75 - 1)^2 + (0.77 - 1)^2 + (0.77 - 1)^2]$$
  
= 0.11795

#### Alternative cost function

#### Cross-entropy error function:

$$J = -\frac{1}{n} \sum_{i=1}^{n} \left[ y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i) \right]$$

The node delta for the output layer becomes:  $\delta_O = \hat{y} - y$ .

Cross-entropy error function often performs better than MSE for learning a classification task.

Gradient-Based Learning

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Other Algorithms

### Resilient back-propagation (Rprop)

Rprop weight change:

$$\Delta w_{j,i}^{(t)} = \begin{cases} -\Delta_{j,i}^{(t)}, & \text{if } \frac{\partial E}{\partial w_{j,i}} \\ +\Delta_{j,i}^{(t)}, & \text{if } \frac{\partial E}{\partial w_{j,i}} \\ 0, & \text{otherwise} \end{cases} < 0$$

Modify update values:

$$\Delta_{j,i}^{(t)} = \begin{cases} \eta^{+} \cdot \Delta_{j,i}^{(t-1)}, \text{ if } \frac{\partial E}{\partial w_{j,i}} {}^{(t-1)} \cdot \frac{\partial E}{\partial w_{j,i}} {}^{(t)} > 0\\ \eta^{-} \cdot \Delta_{j,i}^{(t-1)}, \text{ if } \frac{\partial E}{\partial w_{j,i}} {}^{(t-1)} \cdot \frac{\partial E}{\partial w_{j,i}} {}^{(t)} < 0\\ \Delta_{j,i}^{(t-1)}, otherwise \end{cases}$$

There are serveral variants of Rprop: Rprop+, Rprop-, iRprop-, iRprop+.

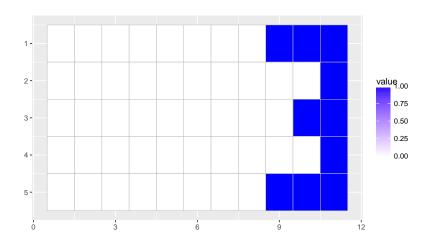
### Levenberg-Marquardt algorithm

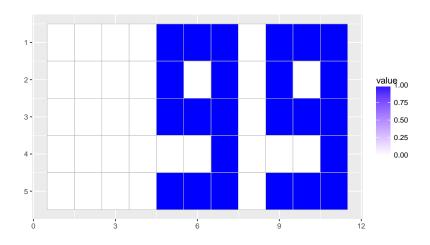
LMA is a very efficient training method for neural networks.

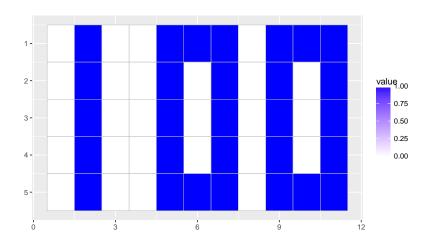
It combines the Gauss-Newton algorithm and the method of gradient descent.

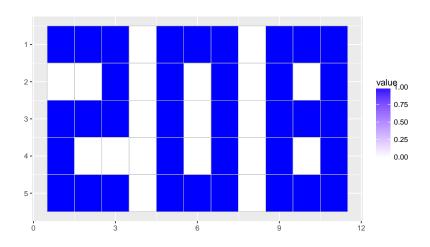
$$W^{(t+1)} = W^{(t)} - (H^{(t)} + \lambda I)^{-1} g^{(t)}$$

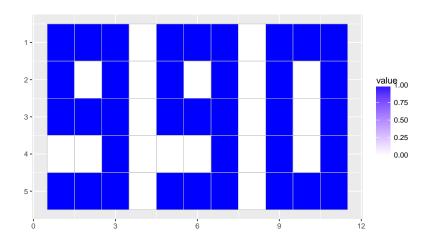
Example Odd/Even











```
print(X[100,1:11])
print(X[100,12:22])
print(X[100,23:33])
print(X[100,34:44])
print(X[100,45:55])
       0 1 0 0 1 1 1 0 1 1 1
##
##
       0 1 0 0 1 0 1 0 1 0 1
##
        0 1 0 0 1 0 1 0 1 0 1
         1 0 0 1 0 1 0 1 0 1
##
         1 0 0 1 1 1 0
##
```

#### Target vector for Odd/Even

```
y \leftarrow rep(c(-1,1), 500)[-1000]
y[5]
y[56]
y[998]
y[999]
## [1] -1
## [1] 1
## [1] 1
## [1] -1
```

#### Perceptron function

- · a single neuron
- uses signum function
- stochastic learning
- weight adjustment:  $w \leftarrow w + \eta \cdot x \cdot y$

### Perceptron function

- · X: feature matrix
- · y: target vector
- · w: weights vector
- · eta: learning rate
- max\_reps: maximum weight update iterations
- max\_error\_rate: stop learning, if missclassification rate ≤ max\_error\_rate

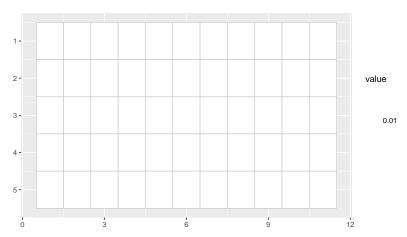
# **Initialising the weights**

```
# number of features and number of obs
m = ncol(X)

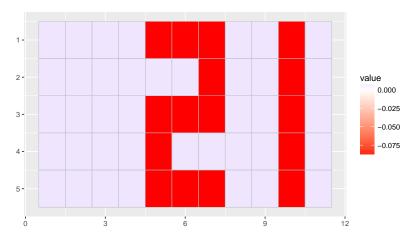
# initial weights:
w = rnorm(m, 1)/10
w = rep(0.01, m)
```

#### **Fitting**

#### Initial weights:

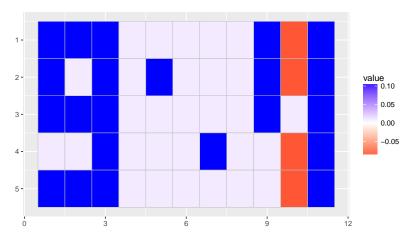


#### 1 iteration:



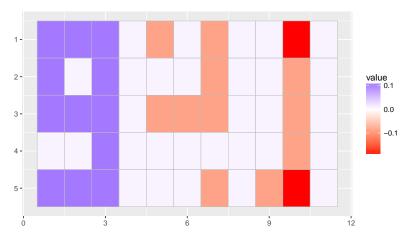
Used number: 21

#### 2 iterations:



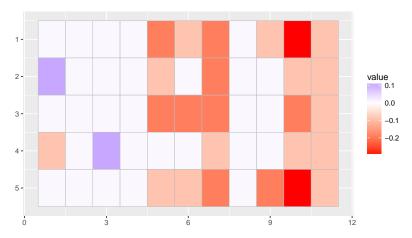
Used numbers: 21, 984

#### 3 iterations:



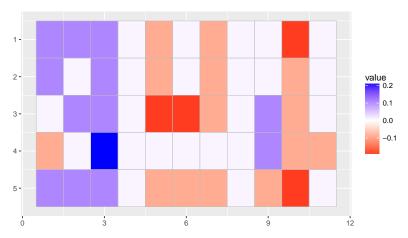
Used numbers: 21, 984, 49

#### 4 iterations:

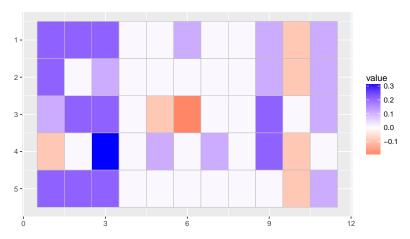


Used numbers: 21, 984, 49, 293

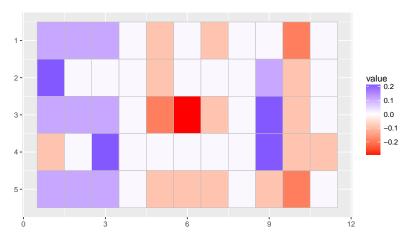
#### 5 iterations:



Used numbers: 21, 984, 49, 293, 372

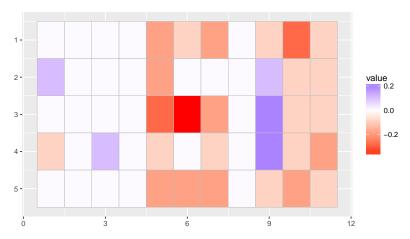


#### 7 iterations:

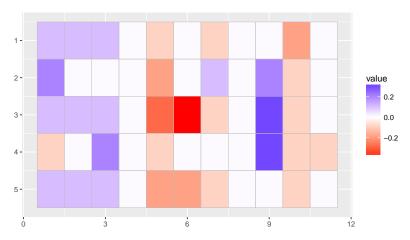


Used numbers: 21, 984, 49, 293, 372, 508, 363

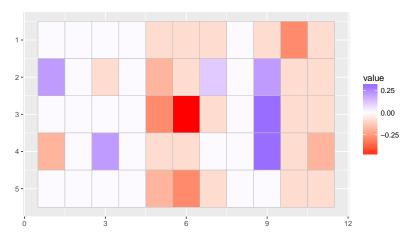
#### 8 iterations:



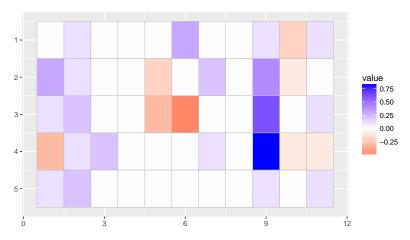
Used numbers: 21, 984, 49, 293, 372, 508, 363, 567

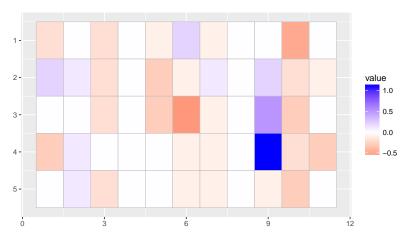


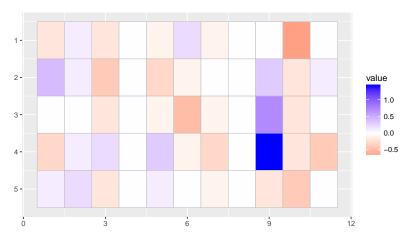
#### 10 iterations:

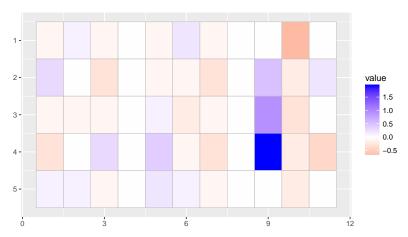


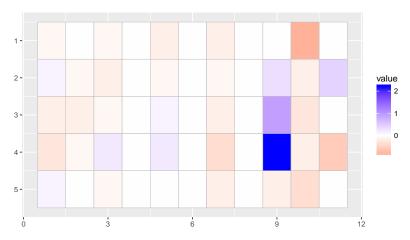
Used numbers: 21, 984, 49, 293, 372, 508, 363, 567, 570, 217



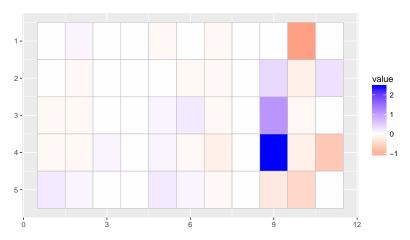








#### Final weights after 70 iterations:



### New targets

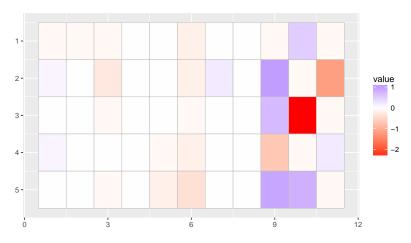
- "multiple of 5"
- "multiple of 4"
- "multiple of 3"

### New target: multiple of 5

```
y = rep(-1, 999)
V[(1:999) \%\% 5 == 0] = 1
set.seed(909)
fit = perceptron(X, y, w, eta = 0.1,
      \max \text{ reps} = 300, \max \text{ error rate} = 0.05)
## [1] "At least 95% of all points correctly classi
## [1] "Number of iterations:"
## [1] 112
```

## Final weights

#### Final weights for "multiple of 5":



#### References

- Bengio, Y., A. Courville and I. Goodfellow (2016) *Deep Learning*. The MIT Press. ISBN: 978-0262035613.
- Heaton, J. (2015) AI for Humans, Volume 3: Deep Learning and Neural Networks.
- Rumelhart, D., G. Hinton and R. Williams (1986a) *Learning representations by back-propagating errors*. Nature, 323, 533–536.
- · Riedmiller, M. (1994) Rprop-description and implementation details.
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- Yu, H., and Bogdan Wilamowski (2011) Levenberg-marquardt training. Industrial Electronics Handbook, 5(12), 1.
- http://people.idsia.ch/~juergen/