Neural Networks

Programming for Data Science

TECHNISCHE UNIVERSITÄT DRESDEN
Dresden Database Systems Group

Orga

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Examination dates

- For urgent matters: 07.02.2020
- However, we recommend the 03.04.2020.

Neural Networks

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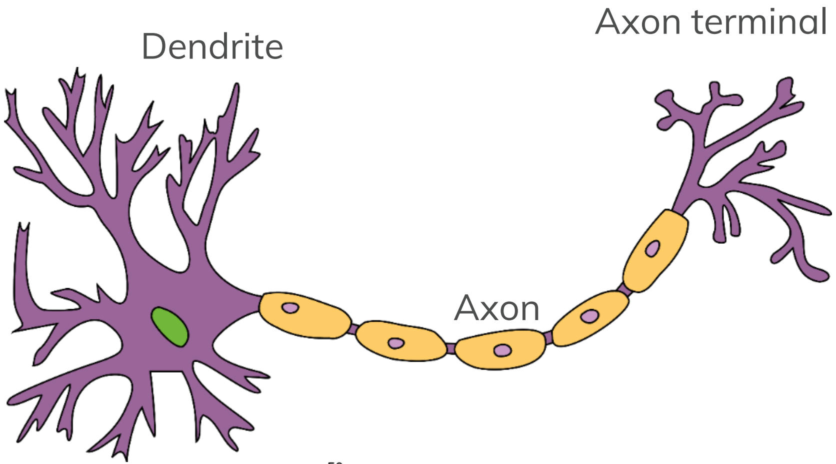
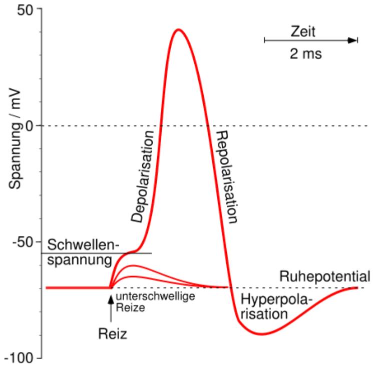
Biological Basics

- Neuron/nerve cell is the structural and functional building block of nervous system
- Cell specializes in receiving, processing and transmitting excitation
- Dendrites receive excitation from other cells
- Axon transmits excitation to other cells
- Transmission: internal electric, external chemical (neurotransmitter, synapses)
- Incoming excitation summed at axon hillock
- If threshold potential is exceeded, action potential is released (all-or-nothing)
- Analog/Digital Converter





Aktionspotential

Neural Networks

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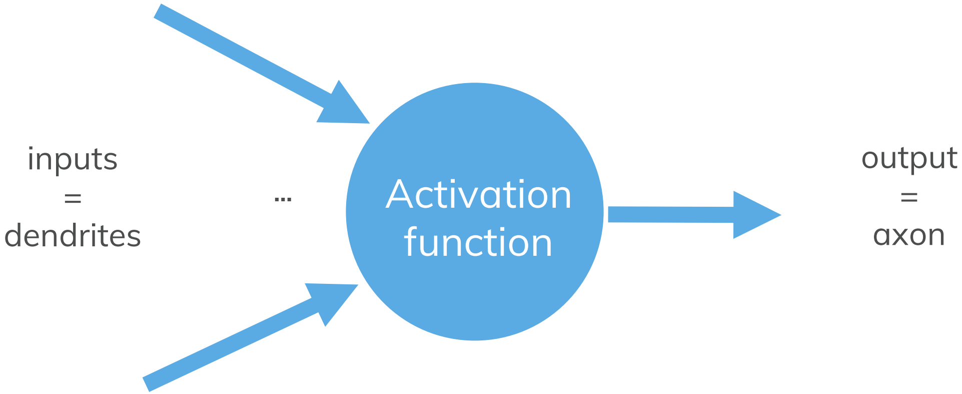
Basics

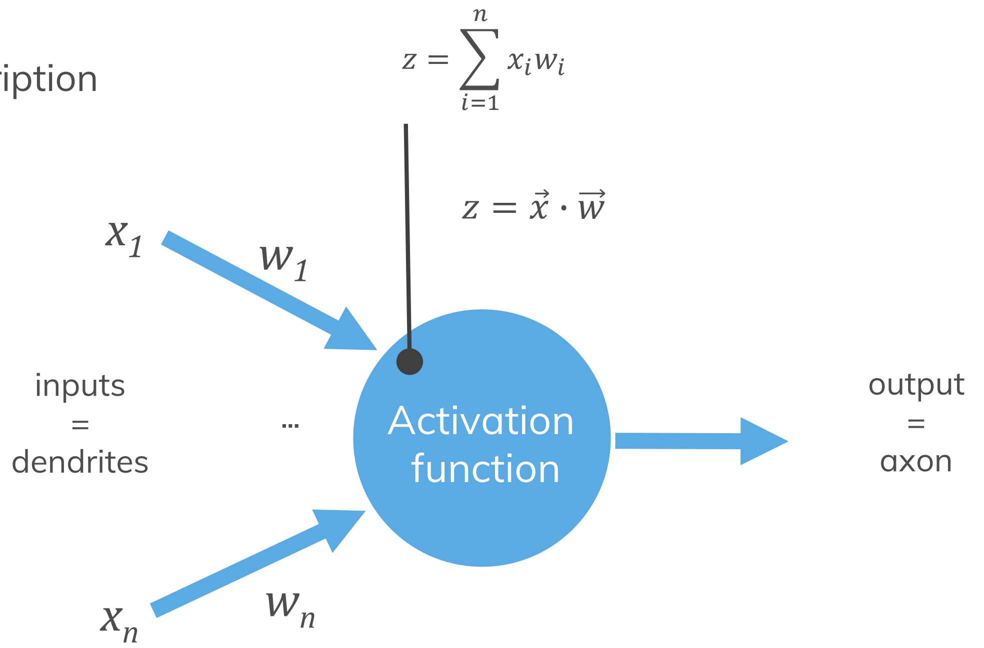
- Core element is the artificial neuron → Perceptron
- Published 1958



Neural Networks

Basics

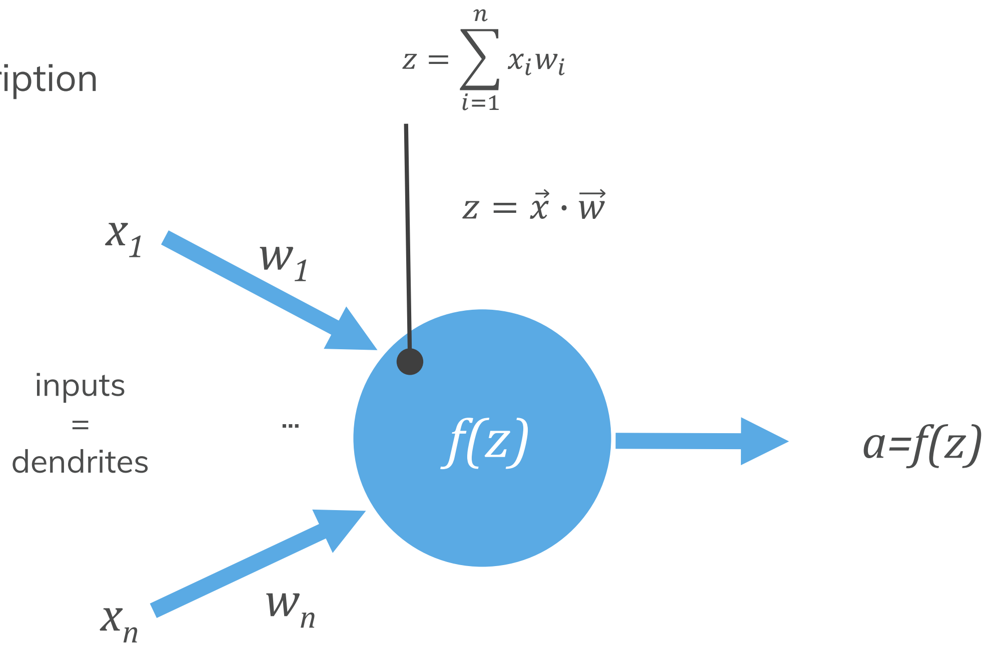
- Mathematical description



Neural Networks

Basics

- Mathematical description



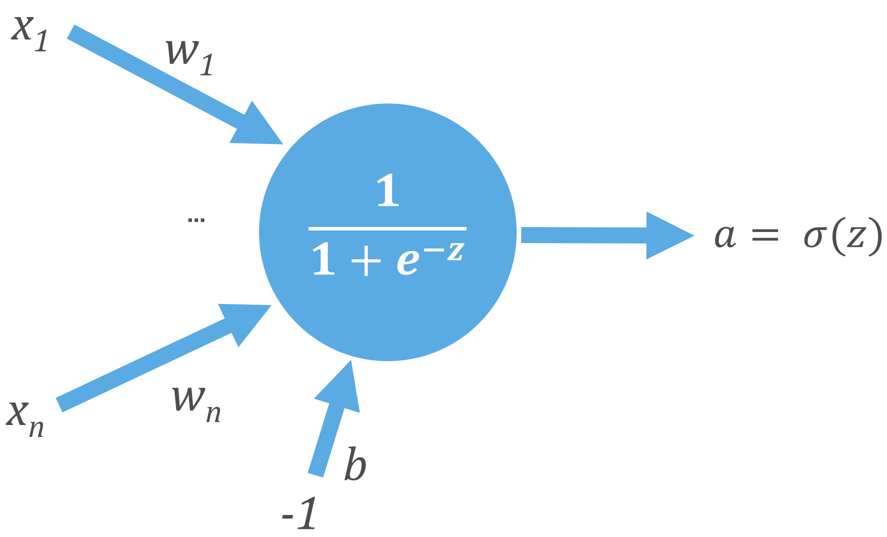
Neural Networks

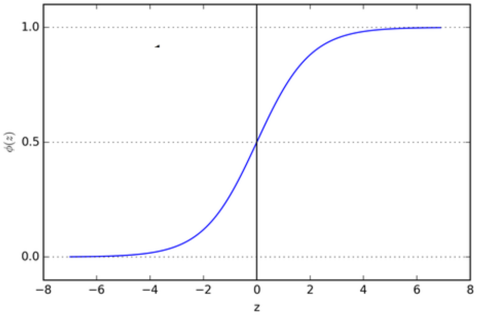
Sigmoid Neuron

- Smoothed Perceptron
- Basic structure is kept
- Inputs and outputs range from 0 to 1
- Activation thresholds are modelled as constant input / bias
- Activation function → Sigmoid function

$$z = b + \sum_{i=1}^{n} x_i w_i$$

$$z = b + \vec{x} \cdot \vec{w}$$





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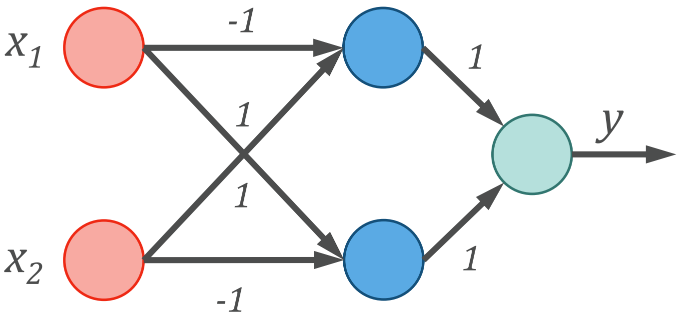
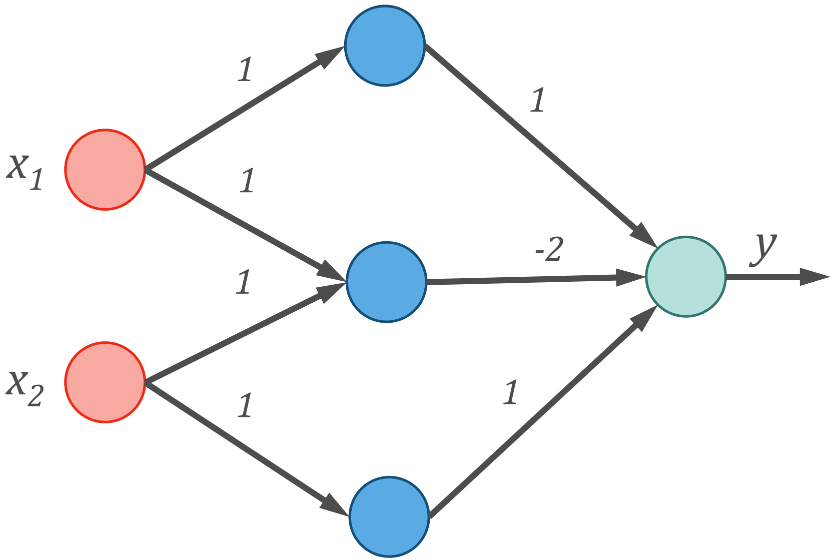
Multilayer Perceptron

- Input layer
- Hidden layer
- Output layer
- Arbitrary Combinations





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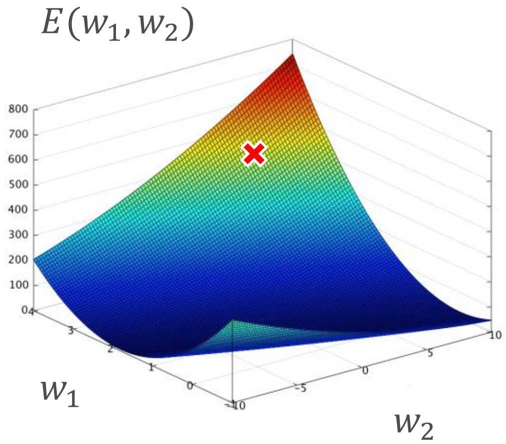
Gradient descent

- → minimize an error function E with multiple parameters
- Example: neuron with two inputs → $E(w_1, w_2)$
- Calculate gradient $\nabla E(w_{1,}w_2)$ → points into direction of biggest increase
- Negative gradient points into direction of biggest reduction
- Gradient is a vector containing the partial derivatives of the error function

$$\nabla E(w_1, \dots, w_n) = < \frac{\partial E}{\partial w_1}, \dots, \frac{\partial E}{\partial w_n} >$$



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Gradient descent

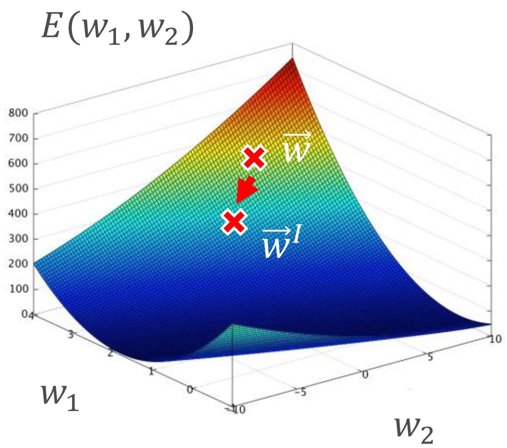
- Gradient is a vector containing the partial derivatives of the error function

$$\nabla E(w_1, \dots, w_n) = < \frac{\partial E}{\partial w_1}, \dots, \frac{\partial E}{\partial w_n} >$$

- Using the gradient, new weights are calculated

$$\vec{w}^I = \vec{w} - \alpha\, \nabla E(\vec{w})$$

- α step size → learning rate
- Step-by-step adjustment until gradient = 0 or smaller than threshold → convergence
- Risk of local minimum → initialization



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Gradient descent

- Gradient is used to calculate new weights

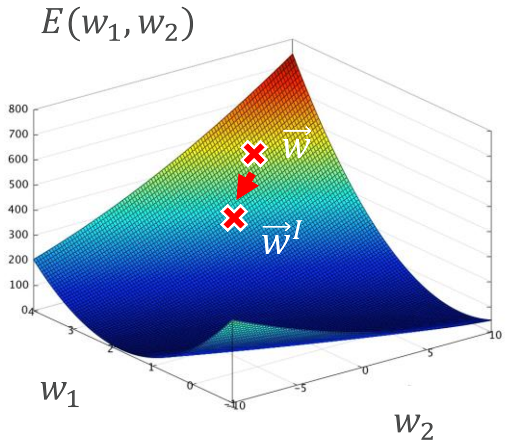
$$\vec{w}^I = \vec{w} - \alpha \nabla E(\vec{w})$$

- Simplified form, actually:

$$\vec{w}^I = \vec{w} - \alpha \nabla \frac{1}{n} \sum_{x=1}^{n} (t_x - a_x)$$

- Consider all *n* training inputs during calculation of average error

- → costly, slow



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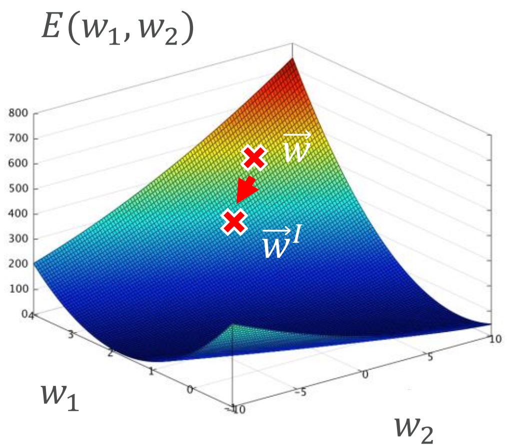
Gradient descent

$$\vec{w}^I = \vec{w} - \alpha \nabla \frac{1}{n} \sum_{x=1}^{n} (t_x - a_x)$$

- Stochastic Gradient Descent → approximation
- Instead of *n* inputs only consider one

$$\vec{w}^I = \vec{w} - \alpha \nabla (t_x - a_x)$$

- Mathematically not optimal, but “good enough“
- Path less direct due to noise/outliers
- More iterations until convergence, BUT greatly reduce cost per iteration



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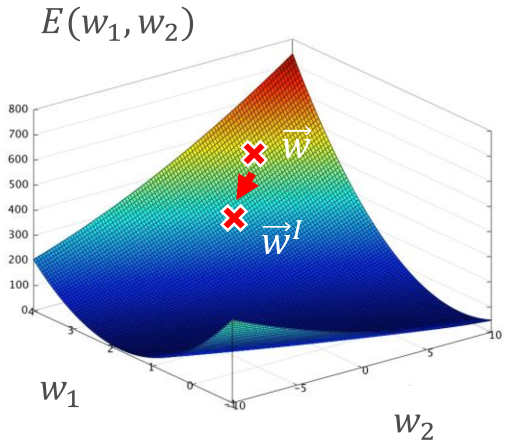
Gradient descent

$$\vec{w}^I = \vec{w} - \alpha \, \nabla \frac{1}{n} \sum_{x=1}^{n} (t_x - a_x)$$

- Mini Batch Gradient Descent → compromise
- Instead of *n* inputs use *m* with *m*<*n*

$$\vec{w}^I = \vec{w} - \alpha \, \nabla \frac{1}{m} \sum_{x=1}^{m} (t_x - a_x)$$

- “Best of both worlds“
- Most common approach for training
- Rule of thumb: $16 \leq m \leq 256$



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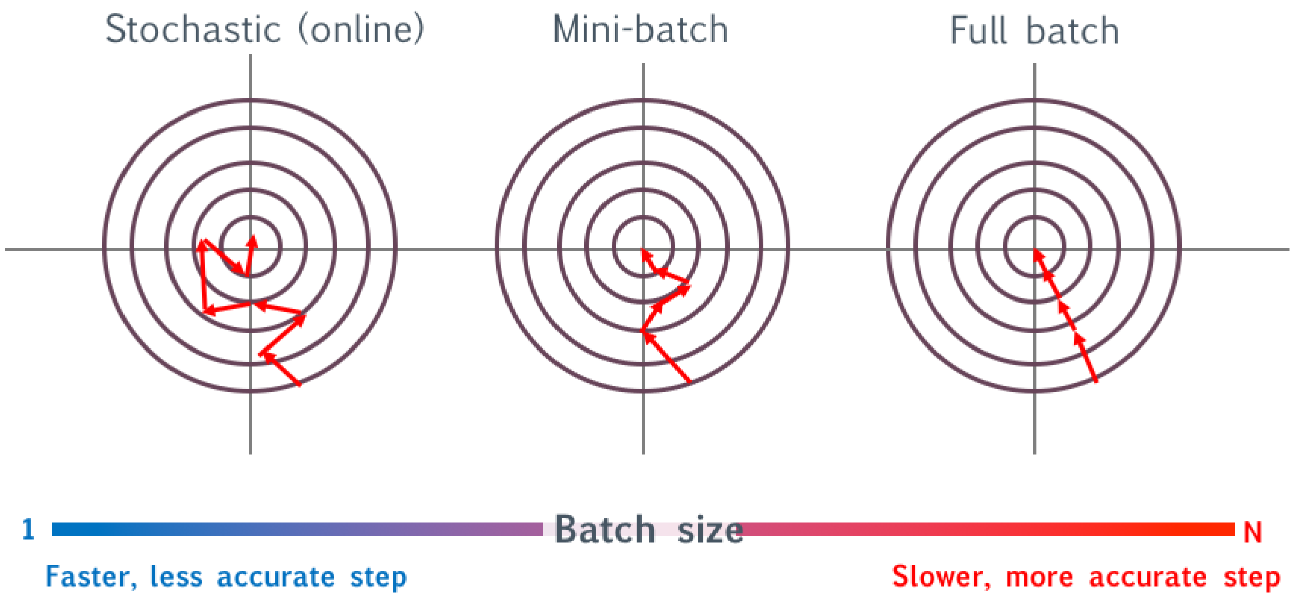
Gradient descent - approaches



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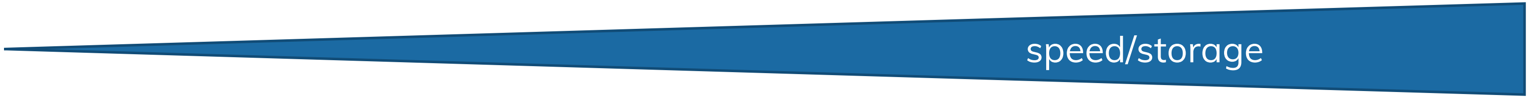
Expansions

- Alternatives to gradient descent
  - Newton‘s method
  - Conjugate gradient method
  - Quasi-Newton method
  - Levenberg-Marquardt Algorithm (only sum-of-squared errors)

- In general these methods converge faster due to usage of Hessian and Jacobian matrices
- Calculation of these matrices requires additional storage space, therefore these methods are not suitable for large networks with thousands of parameters
- Ranking with regards to storage requirements and speed

- Gradient descent < Conjugate gradient < Newton < Quasi Newton < Levenberg-Marquardt



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Backpropagation

- Goal: Calculate $\frac{\partial E}{\partial w_{ij}^l}$ → Chain rule

$$\frac{\partial E}{\partial w_{ij}^l} = \frac{\partial E}{\partial a_j^l} \cdot \frac{\partial a_j^l}{\partial z_j^l} \cdot \frac{\partial z_j^l}{\partial w_{ij}^l}$$

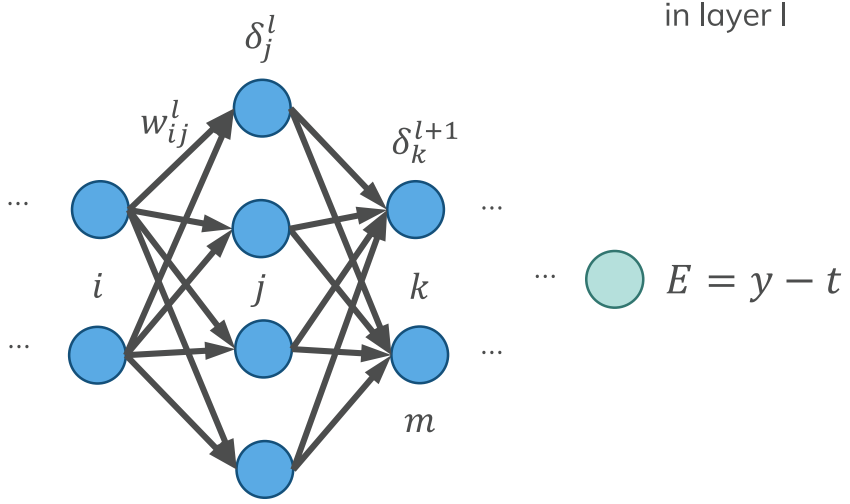
...

$$\frac{\partial E}{\partial w_{ij}^l} = \underbrace{(y - t) \cdot \sigma(z_j^l)(1 - \sigma(z_j^l))}_{\text{Error } \delta_j^l} \cdot a_i^{l-1}$$

$$\delta_j^l = (\sum_{k=1}^{m} w_{jk}^{l+1} \delta_k^{l+1}) \cdot \sigma(z_j^l)(1 - \sigma(z_j^l))$$

- Update weights: $w_{ij}^l = w_{ij}^l - \alpha \delta_j^l a_i^{l-1}$

w_{ij}^l weight from i-th neuron in layer l-1 to j-th neuron in layer l



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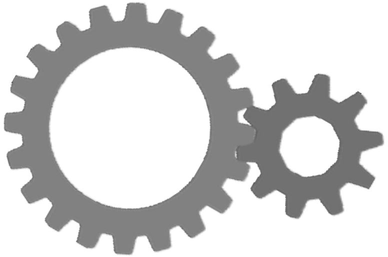
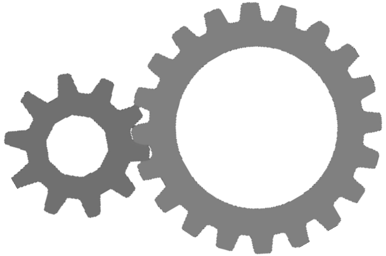
Backpropagation – Problems

Vanishing Gradient



- Backpropagation over multiple layers leads to smaller and smaller changes → greatly decreases learning speed
- $\sigma'(x) \leq 0{,}25$ and $0 < w < 1$
- Repeated multiplication of small values → product gets smaller

Exploding Gradient



- $w_j \sigma'(z_j) > 1$ → too fast and unstable learning in the front layers
- Basic problem: gradients depend on all subsequent layers → more layers mean more instability

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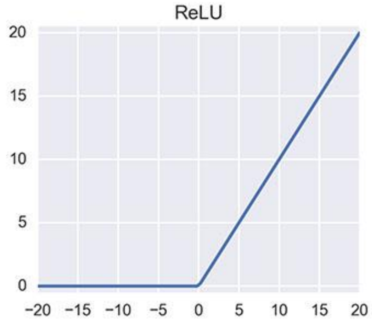
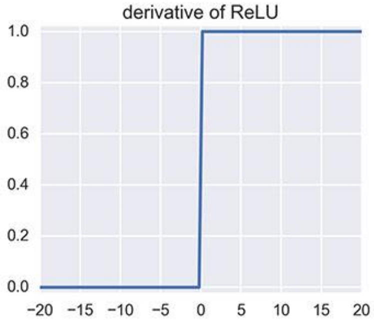
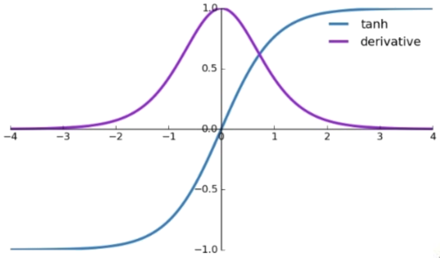
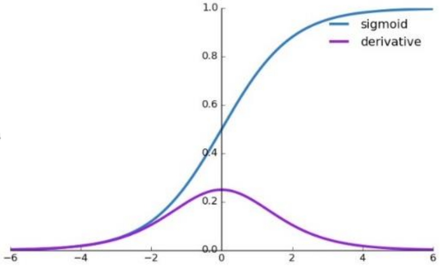
Backpropagation – Activation functions

- Alternatives to sigmoid
- Hyperbolic tangent (tanh): scaled sigmoid $\mathrm{tanh(z)} = 2\sigma(2\mathrm{z}) - 1$, $tanh'(x) \leq 1$
- Rectified Linear Unit (ReLu): $A(z) = \max(0, z)$





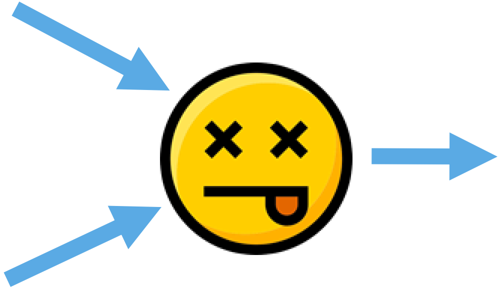




Backpropagation – Activation functions

- Rectified Linear Unit (ReLu): $A(z) = \max(0, z)$

- Pros:
  - no "vanishing gradients"
  - selective neuron activation
  - easy to calculate
  - good performance



- Cons:
  - inflates activation → negative effect on learning
  - Prone to overfitting
  - "dead neuron" problem: if weights of an neuron lead to $z_j \leq 0$, the neuron can never be activated again

- → different variants

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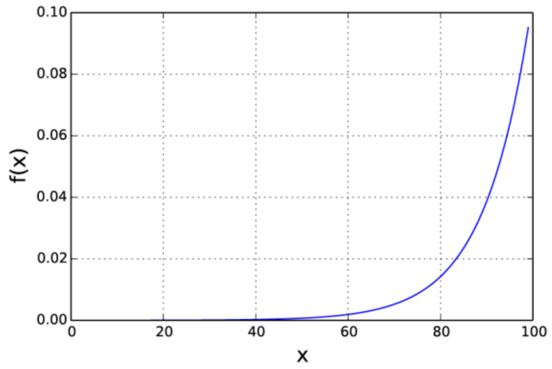
Backpropagation – Activation functions

- Softmax
- Transforms output into probabilities
- → ideal for classification
- Sigmoid allows only two classes
- Generally for output layer

- z is input vector to output layer
- K is number of output neurons



$$softmax(z)_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}}$$

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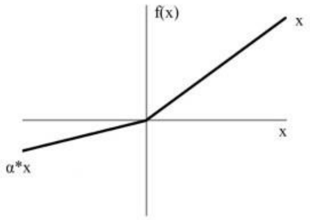
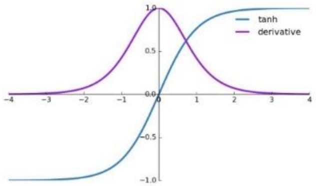
Backpropagation – Activation functions

- What function do I use?
- "Depends on the problem"
- Sigmoid and Tangent suited for classification
- Currently ReLu is considered the best default
- However: Try!
- Why use activation functions at all?
  - Provide non-linearity → make hidden layers useful
  - Linear function of linear functions is linear





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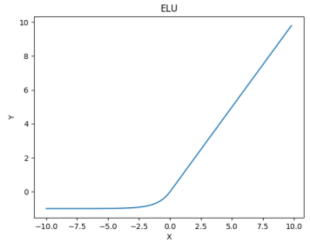

Training – Regularization

- L2 regularization (weight decay)
- Add penalty term to error function

$$E = \frac{1}{2n}(t-y)^2 + \frac{\lambda}{2n}\sum_{w} w^2$$

$\lambda > 0$, n number of training samples

- Favors small weights, big weights have to provide strong improvement
- Trade-off between error minimization and small weights
- Controlled using λ, large λ → small weights, small λ → error minimization

- L1 regularization:

$$E = \frac{1}{2n}(t-y)^2 + \frac{\lambda}{n}\sum_{w} |w|$$

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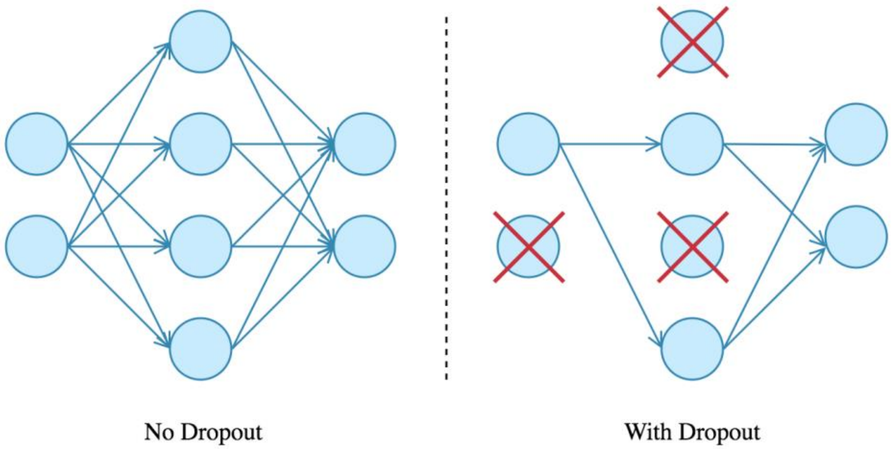
Training – Dropout

- Currently most popular method to prevent overfitting
- In each iteration of trainings, some neurons are “dropped“
- Inputs and output are ignored for these neurons
- Dropout rate typically 20%-50%



Task

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Step 0

- Get the Boston housing price dataset from keras.
- Use the predefined split into training and test data.

Step 1

- Use a funnel MLP* with width (w_1) 512 and depth ($l_{\max}$) 2 to predict the house prices. $\left(w_{l+1} = \frac{w_l}{2}\right)$
- Other parameters: RELU activations, MSE, the Adam optimizer, 100 epochs and a batch size of 32.
- Evaluate the NN on the test data.

Step 2

- Min-max normalize the features. Then, train the same MLP from step 1. Compare the errors.

Step 3

- Use a grid search* to find the best combination of w_1 and $l_{\max}$ for the normalized data.

*use your own implementation

Package suggestions

R

- (data.table)
- keras

python3

- numpy
- pandas
- keras

Exercise Appointment

We compare and discuss the results

- Tuesday, 14.01.2020,
- Consultation: 09.01.2020,
- Please prepare your solutions! Send us your code!

If you have questions, please mail us:

claudio.hartmann@tu-dresden.de Orga + Code + R
lucas.woltmann@tu-dresden.de Tasks + Python