OTH
Amberg-Weiden

Deep Learning

Winter Semester 2024/2025

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Multi-Layer Perceptron

Overview

Topics From Last Time: Training Parametric Models – Softmax Regression

- Approaches to multi-class classification
- Properties of the softmax function
- Model approach and error functional for softmax regression
- Softmax regression as a linear neural network

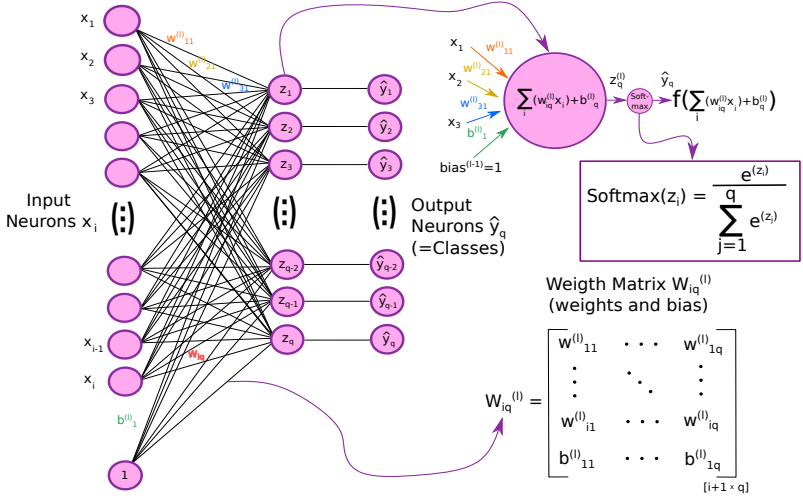
Topics of Today: Multi-Layer Perceptron

- Multilayer architectures
- Activation functions
- Universal approximation theorem
- Backpropagation

Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Multi-Layer Perceptron

Multi-Layer Perceptron

Recap: Softmax Regression as Neural Network



- Affine-linear transformation $z = W^T x + b \rightarrow \hat{y} = softmax(z)$

Multi-Layer Perceptron

Multi-Class vs. Multi-Label Classification

Limits Softmax Regression

- In softmax regression, the relationship between input x and output z is affine-linear
- Many real relationships cannot be mapped with affine-linear functions

Idea

- Add further (hidden) layers to the network
- Without non-linear functions a composition of affine-linear transformations, due to multiple layer, results still in just an affine-linear mapping
- Thereby: Increase the parametric complexity (layer dimensionality)

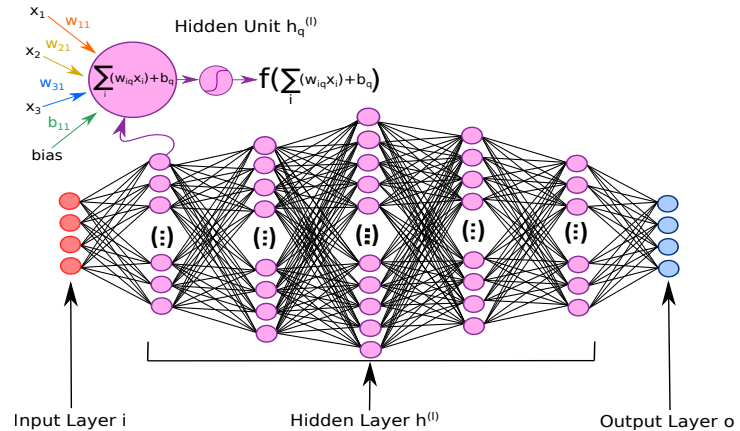
Questions

- What shape does the model function then have?
- Can more complex functions be modelled as a result?

Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Multi-Layer Perceptron

Multi-Layer Perceptron

Multi-Layer Perceptron or (Deep) Feedforward Neural Network



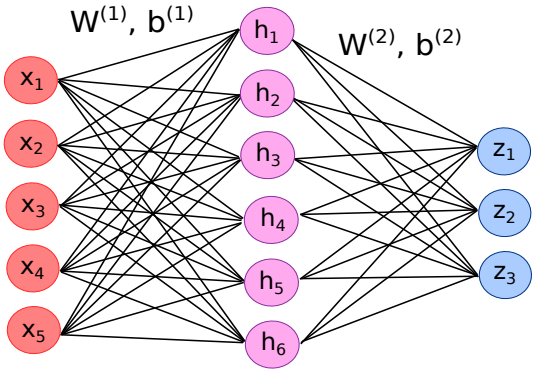
- Forward Pass: $h^{(l)} = W^{T(l)}x + b^{(l)}$, with layer index $l = 1, ..., L$
- Output Layer $z = W^{T(L)}h + b^{(L)}$

Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Multi-Layer Perceptron

Multi-Layer Perceptron

Multi-Layer Perceptron or (Deep) Feedforward Neural Network

- Which dimensionality does $W^{(1)}, b^{(1)}, W^{(2)}$, and $b^{(2)}$ have?
- Provide the forward propagation path of the given model function (network)?
- Interpret the network result in terms of linearity?



Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Multi-Layer Perceptron

Additional Notes

Multi-Layer Perceptron

Non-Linear Activation Function

Observations

- By simply connecting several layers in series, the space of the approximable functions remains linear
- The space is only enlarged by adding non-linear (activation) functions
- This is done by applying non-linear activation functions
- Typically, the same activation function is used for all nodes within a layer
- An application-specific activation function is often used at the output layer

Questions of understanding

- What does the choice of activation function at the output layer depend on?
- What properties would be desirable for activation functions?

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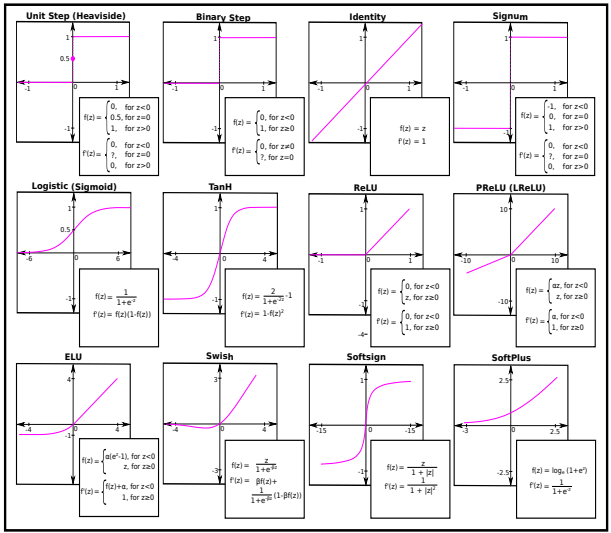
Multi-Layer Perceptron

Frequently Used Non-Linear Activation Function



Multi-Layer Perceptron

Recap: Biological Neuron vs. Mathematical Neuron

- Mathematical model of a biological neuron to represent binary functions
- Perceptron (Rosenblatt 1958): Model with learnable weights

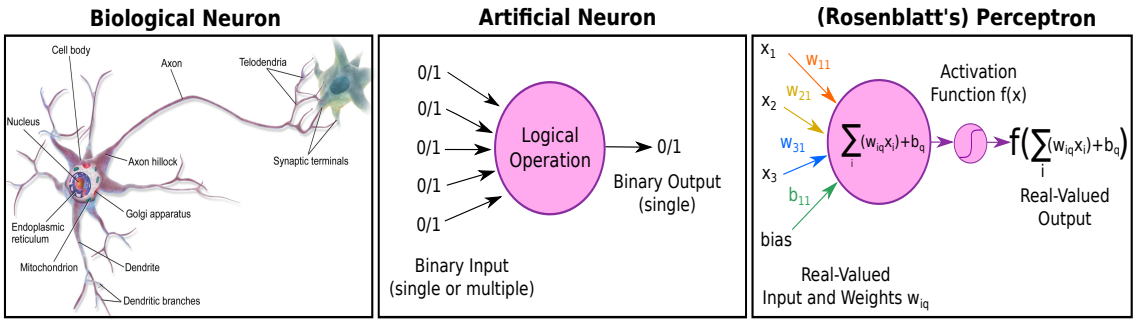


Image by Bruce Blaus (Creative Commons 3.0 - CC BY 3.0), no additional changes, taken from: https://commons.wikimedia.org/wiki/File:Blausen_0657_MultipolarNeuron.png

Source: Christian Bergler, Dissertation "Deep Learning Applied To Animal Linguistics", 2023

Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Einführung

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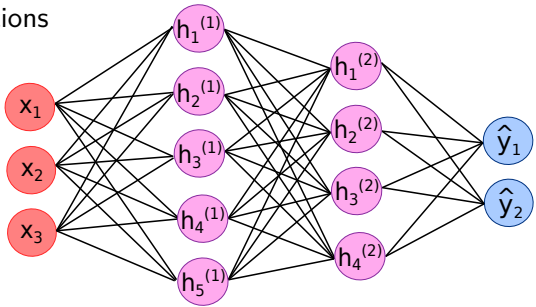
Network Architecture

- The structure of the model function is determined by the topology of the network and the activation functions



- Forward propagation of an input sample $x \in \mathbb{R}^3$ w.r.t. the given architecture:
  - $z^{(1)} = W^{(1)T}x + b^{(1)}$, followed by the network activation: $h^{(1)} = f^{(1)}(z^{(1)})$
  - $z^{(2)} = W^{(2)T}h^{(1)} + b^{(2)}$, followed by the network activation: $h^{(2)} = f^{(2)}(z^{(2)})$
  - $z^{(3)} = W^{(3)T}h^{(2)} + b^{(3)}$, followed by the network activation: $\hat{y} = f^{(3)}(z^{(3)})$

Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Multi-Layer Perceptron

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Model Function & Forward Propagation

Let L be the number of layers of the mesh (without the input layer). Then the model function for an input $\mathbf{x} \in \mathbb{R}^p$ is calculated by

$$\begin{aligned}
\mathbf{z}^{(1)} &:= (\mathbf{W}^{(1)})^T \mathbf{x} + \mathbf{b}^{(1)} , & \mathbf{h}^{(1)} &= f^{(1)}(\mathbf{z}^{(1)}) , \\
&\vdots & &\vdots \\
\mathbf{z}^{(l)} &:= (\mathbf{W}^{(l)})^T \mathbf{h}^{(l-1)} + \mathbf{b}^{(l)} , & \mathbf{h}^{(l)} &= f^{(l)}(\mathbf{z}^{(l)}) , \quad \text{for } l = 2, \ldots, L-1 \\
&\vdots & &\vdots \\
\mathbf{z}^{(L)} &:= (\mathbf{W}^{(L)})^T \mathbf{h}^{(L-1)} + \mathbf{b}^{(L)} , & \hat{\mathbf{y}} &= f^{(L)}(\mathbf{z}^{(L)})
\end{aligned}$$

- Where $f^{(1)}, \ldots, f^{(L)}$ are the activation functions of the individual layers
- Loss/Error/Objective Function: $L(\theta) = L(\hat{y})$

Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Multi-Layer Perceptron

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Number of Layers

Question: How do you choose the number of layers and the number of nodes per layer?

- The number of layers and the number of nodes per layer are hyperparameters
- Additional layers and nodes increase the number of parameters (dimensionality) and can lead to overfitting
- Neural networks should therefore always be regularized (stand-alone lecture about "regularization")
- A middle way must be found between too many and too few parameters θ
- In most cases, only experience or trial and error will help

Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Multi-Layer Perceptron

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Architecture

General: The choice of the architecture and activation functions depends on the task and data situation!

MLP for Classification:

- Output layer with n nodes, where n is the number of classes
- Softmax activation at the output layer
- Frequently: Cross entropy (CE) loss as error function

MLP for Regression

- Output layer with one node
- Linear activation at the output layer
- Frequently: Mean Squared Error (MSE) as loss function

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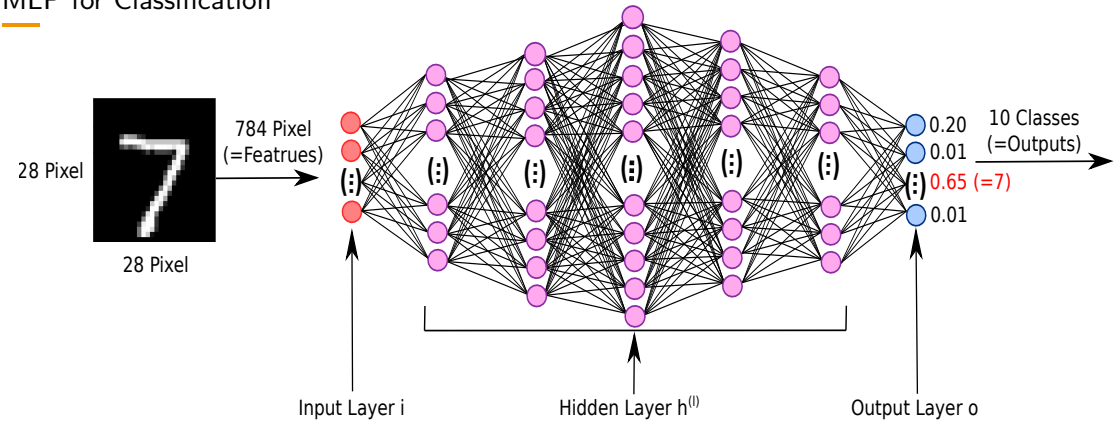
MLP for Classification



- Transforms a given input $x \in \mathbb{R}^{784}$ via forward propagation (forward path) into a final output feature representation $\hat{y} \in \mathbb{R}^{10} \rightarrow$ 10 Classes = 10 Numbers (0-9)

Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Multi-Layer Perceptron

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Loss Function

The choice of loss function depends on the task and data situation. The following loss functions are frequently used in deep learning

Regression

- Mean Squarred Error
- Mean Absolute Error
- Huber

Classification

- (Binary) Cross Entropy
- Hinge
- Kullback-Leibler Divergence

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Definition

Using a neural network with just a single hidden layer (together with a sigmoid activation), any continuous function can be approximated with arbitrary accuracy

Notes:

- The above description is not a rigorous formulation of the theorem in the mathematical sense. To understand it, we lack the basic mathematical knowledge (e.g. convergence in function spaces).
- The theorem is not necessarily of practical relevance, as it does not specify how many nodes the hidden layer must have.
- However, after the first „AI winter“ it has promoted the „confidence“ in deep learning.

Model Training

Training via Gradient Descent

The training of neural networks typically uses the gradient (descent) method (or a variant thereof)

- For this purpose, the partial derivatives of the loss function w.r.t. the weights must be determined
- Therefor, the so-called backpropagation algorithm (backward path) is used, which is based on the chain rule
- The loss function is obtained by summing all samples of the training dataset. Subsequently, the contribution of a sample to the loss function is analyzed

Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Multi-Layer Perceptron

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Backpropagation for MLP's

Forward Propagation

- Forward propagation is the evaluation of the model for a given sample $x \in \mathbb{R}^p$, meaning the calculation of $f(x)$, while f describes the network as function
- The sample is feeded to the network as model input, while the input is successively propagated forward through the model, computing affine linear mappings and the respective activation until the final output layer

Backward Propagation

- Forward propagation takes place from the input layer to the output layer
- For a given sample, the error can be measured at the output layer ($\rightarrow$ Loss, determined by the pre-defined loss function $L(\theta)$)
- This can be propagated back from the output layer to the input layer layer, in order to compute (using the chain rule) the partial derivatives of the loss loss function w.r.t. the weights/parameters $\rightarrow$ This process is called back(ward) propagation

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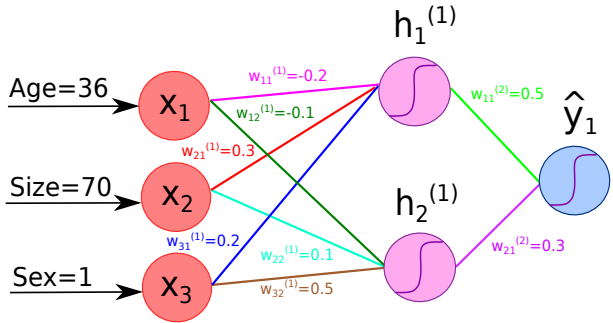
Forward Propagation

- The network uses the sigmoid function in all layers as the respective activation function
- Furthermore, bias terms are omitted for simplification
- Perform the forward propagation for the input $x = [36, 70, 1]^T$



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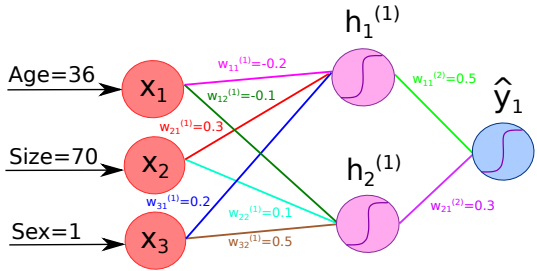
Training Iteration for MLP's

- Forward Propagation:
  - $z^{(1)} = W^{(1)T}x + b^{(1)}$ and $h^{(1)} = \sigma(z^{(1)})$
  - $z^{(2)} = W^{(2)T}h^{(1)} + b^{(2)}$ and $\hat{y} = \sigma(z^{(2)})$
- Computing the Loss:
  - MSE-Loss: $L(\theta) = L(\hat{y}, y) = L_{\theta=(W^{(1)},W^{(2)},b^{(1)},b^{(2)})}(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$



- Backward propagation via "Chain Rule"!

Source: OTH-AW, Electrical Engineering, Media and Computer Science, Fabian Brunner – Vorlesung Deep Learning, Multi-Layer Perceptron

Backward propagation – Partial Derivatives $L(\theta)$ w.r.t to θ $(= W, b)$

$$\frac{\partial L}{\partial W^{(2)}} = \underbrace{\frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{(2)}}}_{\delta^{(2)} := \frac{\partial L}{\partial z^{(2)}}} \frac{\partial z^{(2)}}{\partial W^{(2)}} = (\hat{y} - y)\sigma'(z^{(2)})h^{(1)}$$

$$\frac{\partial L}{\partial b^{(2)}} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial b^{(2)}} = (\hat{y} - y)\sigma'(z^{(2)})$$

$$\frac{\partial L}{\partial W^{(1)}} = \underbrace{\frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial h^{(1)}} \frac{\partial h^{(1)}}{\partial z^{(1)}}}_{\delta^{(1)} := \frac{\partial L}{\partial z^{(1)}}} \frac{\partial z^{(1)}}{\partial W^{(1)}} = (\hat{y} - y)\sigma'(z^{(2)})W^{(2)}\sigma'(z^{(1)})x$$

$$\frac{\partial L}{\partial b^{(1)}} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial h^{(1)}} \frac{\partial h^{(1)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial b^{(1)}} = (\hat{y} - y)\sigma'(z^{(2)})W^{(2)}\sigma'(z^{(1)})$$

Backward propagation – Observations

- For $\delta^{(1)} = \frac{\partial L}{\partial z^{(1)}}$ and $\delta^{(2)} = \frac{\partial L}{\partial z^{(2)}}$ the following relation is given:

$$\delta^{(1)} = \delta^{(2)} \frac{\partial z^{(2)}}{\partial z^{(1)}} = \delta^{(2)} W^{(2)} \sigma'(z^{(1)})$$

- For $\delta^{(1)}$ and $\delta^{(2)}$ the partial derivatives of L according to the weights can be calculated as follows:

$$\frac{\partial L}{\partial W^{(1)}} = \delta^{(1)} \frac{\partial z^{(1)}}{\partial W^{(1)}}, \qquad \frac{\partial L}{\partial b^{(1)}} = \delta^{(1)} \frac{\partial z^{(1)}}{\partial b^{(1)}},$$
$$\frac{\partial L}{\partial W^{(2)}} = \delta^{(2)} \frac{\partial z^{(2)}}{\partial W^{(2)}}, \qquad \frac{\partial L}{\partial b^{(2)}} = \delta^{(2)} \frac{\partial z^{(2)}}{\partial b^{(2)}}$$

- This two-step procedure (first recursive calculation of the quantities $\delta^{(l)}$ from „right to left“, then calculation of the desired derivatives) is transferred to general MLPs with several units per hidden layer

Multi-Layer Perceptron

Training Iteration for MLP's Using Batch-Size B = 1

Recursive Calculation of Variables $\delta^{(l)} = \frac{\partial L}{\partial z^{(l)}}$:

$$\delta^{(L)} = \nabla_{\hat{y}} L \odot f^{(L)'}(z^{(L)}) \ ,$$

$$\delta^{(l)} = \mathbf{W}^{[l+1]} \delta^{[l+1]} \odot f^{(l)'}(z^{(l)}) \ , \quad l = L-1, \ldots, 1$$

Note: where $\odot$ denotes the dot product between matrices.

Calculation of the Partial Derivatives with respect to the Variables $\delta^{(l)}$

$$\frac{\partial L}{\partial b_j^{(l)}} = \delta_j^{(l)} \ , \quad l = 1, \ldots, L$$

$$\frac{\partial L}{\partial w_{kj}^{(l)}} = h_k^{(l-1)} \delta_j^{T(l)} \ , \quad l = 1, \ldots, L$$

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Training Iteration for MLP's Using Batch-Size B > 1

Recursive Calculation of Variables $\delta^{(l)} = \frac{\partial L}{\partial z^{(l)}}$:

$$\delta^{(L)} = \nabla_{\hat{y}} L \odot f^{(L)'}(z^{(L)}) \ ,$$

$$\delta^{(l)} = \delta^{[l+1]} \mathbf{W}^{T[l+1]} \odot f^{(l)'}(z^{(l)}) \ , \quad l = L-1, \ldots, 1$$

Note: where $\odot$ denotes the dot product between matrices.

Calculation of the Partial Derivatives with respect to the Variables $\delta^{(l)}$

$$\frac{\partial L}{\partial b_j^{(l)}} = \delta_j^{(l)} \ , \quad l = 1, \ldots, L$$

$$\frac{\partial L}{\partial w_{kj}^{(l)}} = H_k^{T(l-1)} \delta_j^{(l)} \ , \quad l = 1, \ldots, L$$

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Summary and Outlookk

Summary

- From softmax regression to multi-layer networks
- Activation functions
- Forward propagation
- Backpropagation

Outlook

- Exercise: Implementation from scratch
- Initialisation of the weights
- Regularization
- Deep learning in PyTorch

Further Questions?

https://www.oth-aw.de/hochschule/ueber-uns/personen/bergler-christian/

Source: https://emekaboris.medium.com/the-intuition-behind-100-days-of-data-science-code-c98402cdc92c