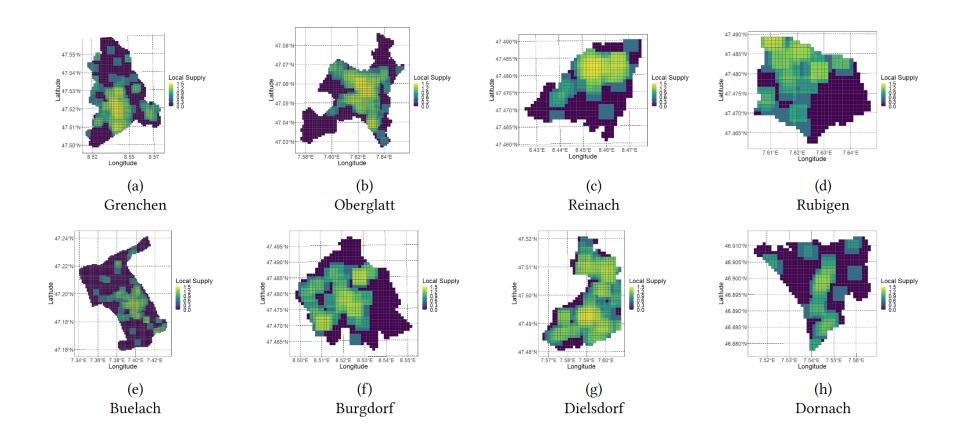
Gears of Neural Networks

Dr. Yves Staudt



Lernziel

Die Studierende sind in der Lage

• die Elemente eines Deep Learning Modells zu bestimmen und zu beschreiben.

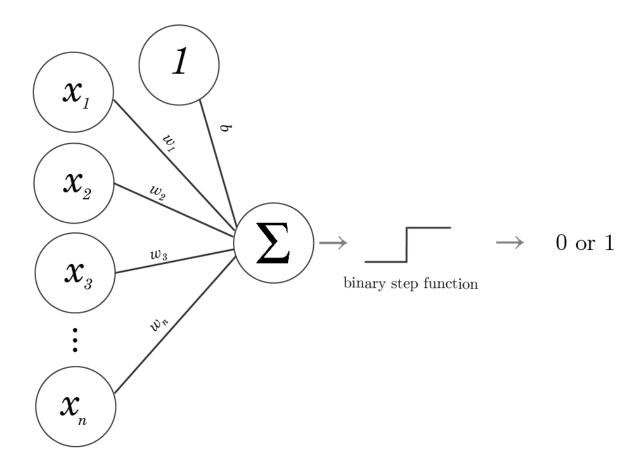


Goal

The goal in deep learning is to optimize the parameters such that the model's predictions on the training data are as close as possible to the true labels



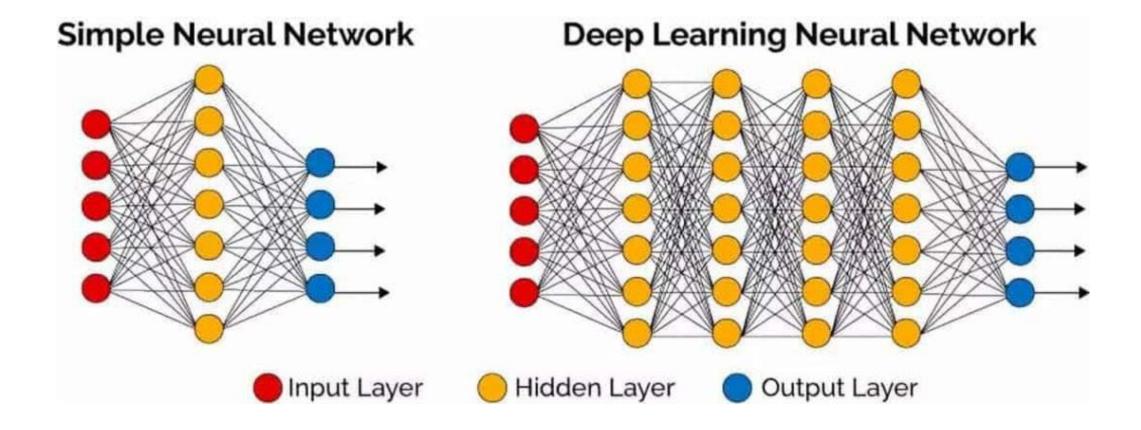
Perceptron Erweiterung



Perceptron mit Aktivierungsfunktion



Deep Learning





Deep Learning

Initialization of the weights

Random initialization:

- Simplest method to randomly initialize the weights using a normal distribution with mean 0 and standard deviation 1
- This is also known as the Glorot initialization or Xavier initialization.

Uniform initialization:

Common method to initialize the weights using a uniform distribution with a specific range, such as [-0.1, 0.1] or [-0.01, 0.01]

Zeroes:

Setting all initial weights to zero

Ones:

Setting all initial weights to one



Choice of Hidden Layers and Nodes

- The choice of the number of hidden nodes and hidden layers in feed forward neural networks depends on the complexity of the problem
- The higher the number of hidden nodes and layers, the higher the complexity
- Some general guidelines:
 - ➤ Start with a simple model 1 hidden layer
 - Common rule of thumb for the number of hidden nodes: number of nodes between the size of the input layer and the output layer

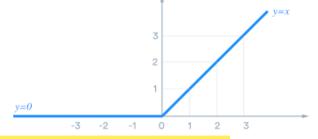
Most common problems can be solved with two hidden layers



Common Activation Functions

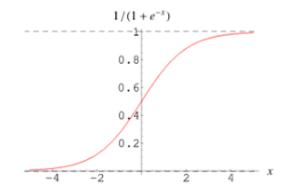


- > ReLU is the most popular activation function for deep learning.
- It is a simple function that returns 0 for negative inputs and the input value for positive inputs.



Sigmoid:

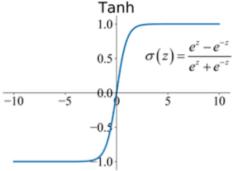
- The sigmoid function is commonly used in feedforward neural networks.
- ➤ It maps any input value to a value between <mark>0 and 1</mark>, which can be interpreted as a probability.



Hyperbolic tangent (tanh):

➤ The hyperbolic tangent function is similar to the sigmoid function, but it maps input values to a range between -1 and 1.





Common Activation Functions for Output

The choice of activation function for the output layer depends on the type of problem you are trying to solve.

Commonly used activation functions for the output layer are:

- Sigmoid:
- > The sigmoid function is commonly used in binary classification problems
- Output is a probability value between 0 and 1.
- Softmax:
- > The softmax function is used in multi-class classification problems
- Output is a probability distribution over multiple classes.
- It normalizes the output values to ensure they sum to 1.

Linear

- The linear activation function is used in regression problems
- Output is a continuous value



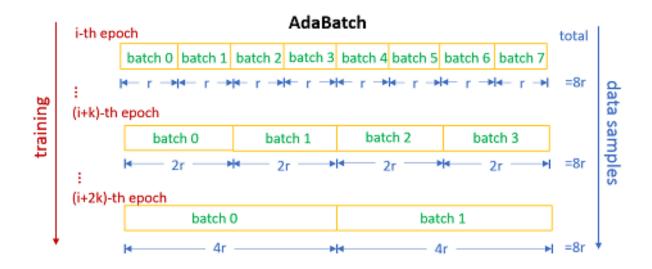
Epochs

- In deep learning, an epoch refers to a single pass over the entire training dataset during the training phase
- One epoch is complete when the model has seen and processed every example in the training set once
- During each epoch, the model updates its parameters (weights and biases) based on the gradients of the loss function with respect to those parameters
- After each epoch, the **model's performance** is typically **evaluated** on a separate validation set
- The number of epochs used to train a deep learning model is a hyperparameter
- If the number of epochs is too low, the model may not be able to converge to an optimal solution, resulting in poor performance.
- If the number of epochs is too high, the model may overfit to the training data
- The number of epochs needed to train a deep learning model depends on the **complexity** of the problem, the size of the dataset, and the architecture of the model



Batches

- In deep learning, a batch refers to a subset of the training data
- Batches are used to update the model's parameters during one iteration of the optimization algorithm
- Batches allow the model to make updates more frequently and efficiently, while also reducing the memory requirements of the optimization process
- By passing each batch through the model, computing the loss function and gradients, and then updating the parameters using an optimizer such as stochastic gradient descent (SGD) or Adam





Choice of the Batches Size

- The choice of batch size is another **important** hyperparameter
- A small batch size can lead to faster convergence and better generalization performance
- A small batch size forces the model to learn more robust features that are relevant across different batches
- A smaller batch size can also slow down training and make the optimization process less stable
- The gradients computed on small batches can be more noisy and less representative of the true gradients on the entire training set
- A larger batch size can lead to faster training and more stable gradients, as the model has more information to work with during each update
- A larger batch size can also result in overfitting



Needed Things for Compilation

For the compilation of a deep learning model we need the following three things:

- Loss function describes how the network will be able to measure its performance on the training data and how it will be able to steer itself in the right direction
- Optimizer is the mechanism through which the network will update itself based on the data
- Metrics monitor the accuracy of the model during training and testing



Loss Functions for Regression

Mean Squared Error (MSE):

- Popular loss function used for regression problems.
- Measures the average squared difference between the predicted and actual values.

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

Mean Absolute Error (MAE):

- Loss function used for regression problems.
- Measures the average absolute difference between the predicted and actual values.

$$MSE = \frac{1}{n} \cdot \sum_{i=1}^{n} |y_i - \hat{y}_i|$$



Loss Functions for Regression

Huber Loss:

- Loss function that is less sensitive to outliers than MSE.
- ➤ Used in regression problems where there are outliers in the data.

Huber Loss =
$$\frac{1}{n} \cdot \sum_{i=1}^{n} L\delta(y_i - \hat{y}_i)$$

where

$$L\delta(x) = \begin{cases} 0.5 \cdot x^2 & \text{if } |x| \le \delta \\ \delta \cdot (|x| - 0.5 \,\delta) & \text{if } |x| > \delta \end{cases}$$



Loss Functions for Classification

Binary Cross-Entropy:

Loss function used for binary classification problems.

Measures the difference between the predicted and actual values using the logarithmic loss.

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

Categorical Cross-Entropy:

Loss function used for multi-class classification problems.

Measures the difference between the predicted and actual values using the logarithmic loss.

$$CE = -\frac{1}{n} \cdot \sum_{i=1}^{n} \sum_{j=1}^{k} y_{ij} \cdot \log(\hat{y}_{ij})$$

Where i is the i-th sample and j the j-th class



Metrics

- The loss function is used to optimize the parameters of the neural network during training
- Evaluation metrics are used to measure the performance of the model on the training and test data
- Evaluation metrics provide insights into its strengths and weaknesses
- In regression problems, the loss function and evaluation metrics are the same
- In classification problems this is not the case



Metric for Classification - Confusion Matrix

		Real classification	
		0	1
Prediction	0	TN	FN
	1	FP	TP



Metric for Classification – Accuracy

Accuracy formula:

$$\frac{TP + TN}{TP + TN + FP + FN}$$



Metric for Classification – Precision/Recall/False Positive Rate/True Negative Rate

Precision also called Predictive Positive Rate:

$$PPV = \frac{TP}{TP + FP}$$

Recall also named Sensitivity or True Positive Rate:

$$TPF = \frac{TP}{TP + FN}$$

False Positive Rate:

$$FPR = \frac{FP}{FP + TN}$$

True negative rate also called Specificity:

$$TNR = \frac{TN}{TN + FP}$$



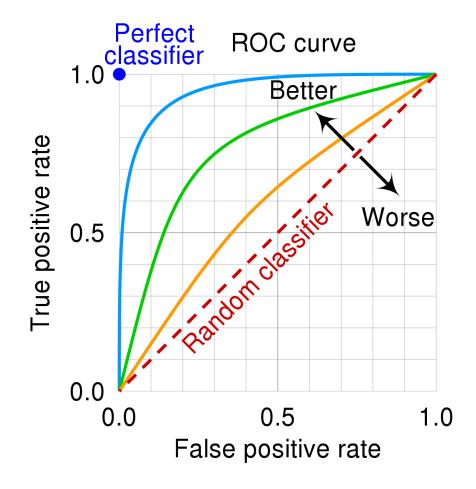
Metric for Classification – F1 Score

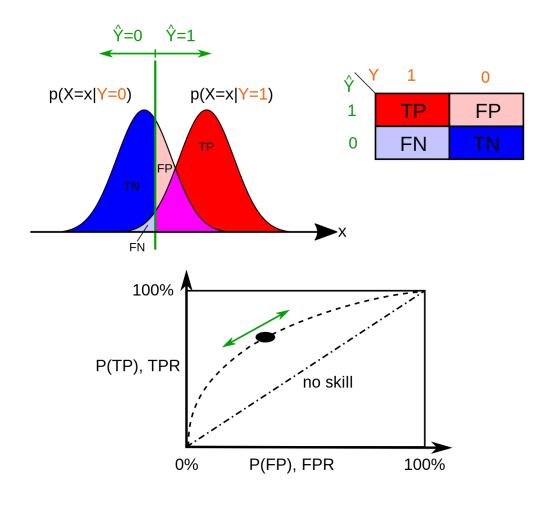
$$F_1 = 2 \frac{precision \cdot recall}{precision + recall} = \frac{2 \cdot TP}{2 \cdot TP + FP + FN}$$

- F1 score reaches its best value at 1
- F1 score worst score at 0



Receiver Operating Characteristic





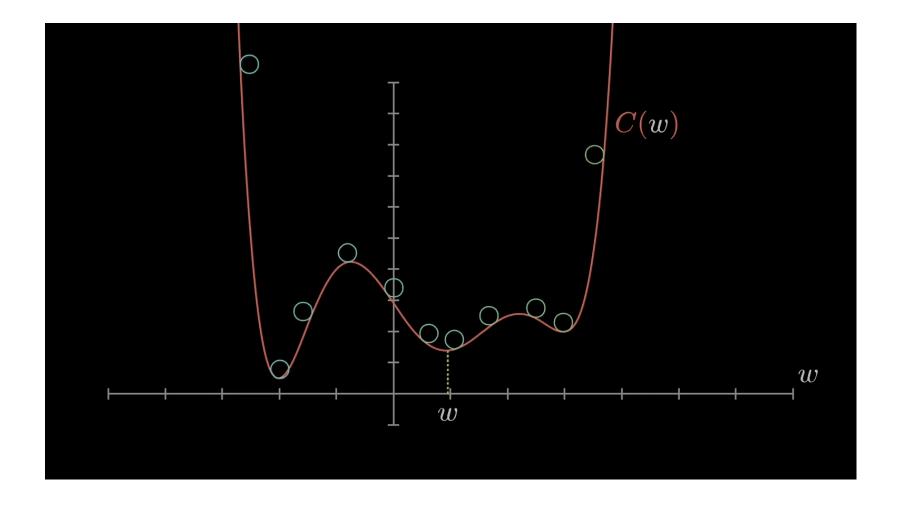


Area under the ROC Curve

- The area under a ROC curve (AUC) is a single scalar value that measures the overall performance of a classifier.
- AUC is within [0.5-1.0]
- AUC = 1: represents a perfect classifier
- AUC is a robust measure



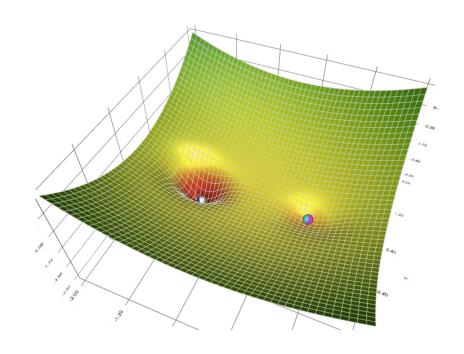
Gradient Descent





Schwierigkeit Gradient Descent

- Das Konvergieren in ein lokales Minimum einer Kostenfunktion
 - Durch wiederholtes Anwenden des gradiellen Abstiegs





Learning Rate

- The learning rate is a critical hyperparameter in deep learning
- The learning rate controls the step size used to update the weights during training
- The learning rate determines how quickly or slowly the model learns from the data
- The learning rate have a significant **impact** on the **performance** of the model
- If the learning rate is too high, the model may fail to converge or even diverge
- If the learning rate is too low, the model may converge very slowly or get stuck in a local minimum of the loss function
- A to low learning rate can prevent the model from finding the global minimum of the loss function.



Application of Learning Rate

To find an **appropriate** learning rate, it's common to start with a relatively high learning rate and **gradually reduce** it during training

To gradually reduce the learning rate is known as learning rate annealing or decay

Some common strategies for learning rate **annealing** include:

- **Step decay**: The learning rate is reduced by a fixed factor after a certain number of epochs
- **Exponential decay**: The learning rate is reduced exponentially over time
- Adaptive learning rate: The learning rate is adjusted dynamically based on the gradients of the loss function



Optimizer

There exists several optimizers

The most common are:

- Stochastic Gradient (SGD)
- Adaptive Moment Estimation (Ada)
- Root Mean Square Propagation (RMSprop)
- Adaptive gradient (Adagrad)



Stochastic Gradient Descent (SGD)

- The most basic optimizer
- Good starting point.
- SGD works by adjusting the weights of the neural network in the direction of the negative gradient of the loss function with respect to the weights
- Variants of SGD: mini-batch SGD, momentum SGD



Adaptive Moment Estimation (Adam)

- Adapative learning rate optimizer
- Very popular in recent years.
- Uses a combination of the first and second moments of the gradients to adapt the learning rate for each parameter.



Root Mean Square Propagation (RMSprop)

- Adaptive learning rate optimizer
- Uses a moving average of the squared gradient to normalize the gradient values



Adaptive Gradient (Adagrad)

- Adaptive learning rate optimizer
- Adapts the learning rate for each parameter based on the history of the gradients for that parameter.



Fragen





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Vielen Dank für Ihre Aufmerksamkeit. Grazia fitg per l'attenziun. Grazie per l'attenzione.

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