CENTER FOR SCALABLE DATA ANALYTICS AND
ARTIFICIAL INTELLIGENCE

IOM AI School

TOPIC: Deep Learning – Theory and Practice

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GEFÖRDERT VOM
Bundesministerium für Forschung, Technologie und Raumfahrt

SACHSEN
Diese Maßnahme wird gefördert durch die Bundesregierung aufgrund eines Beschlusses des Deutschen Bundestages. Diese Maßnahme wird mitfinanziert durch Steuermittel auf der Grundlage des von den Abgeordneten des Sächsischen Landtags beschlossenen Haushaltes.

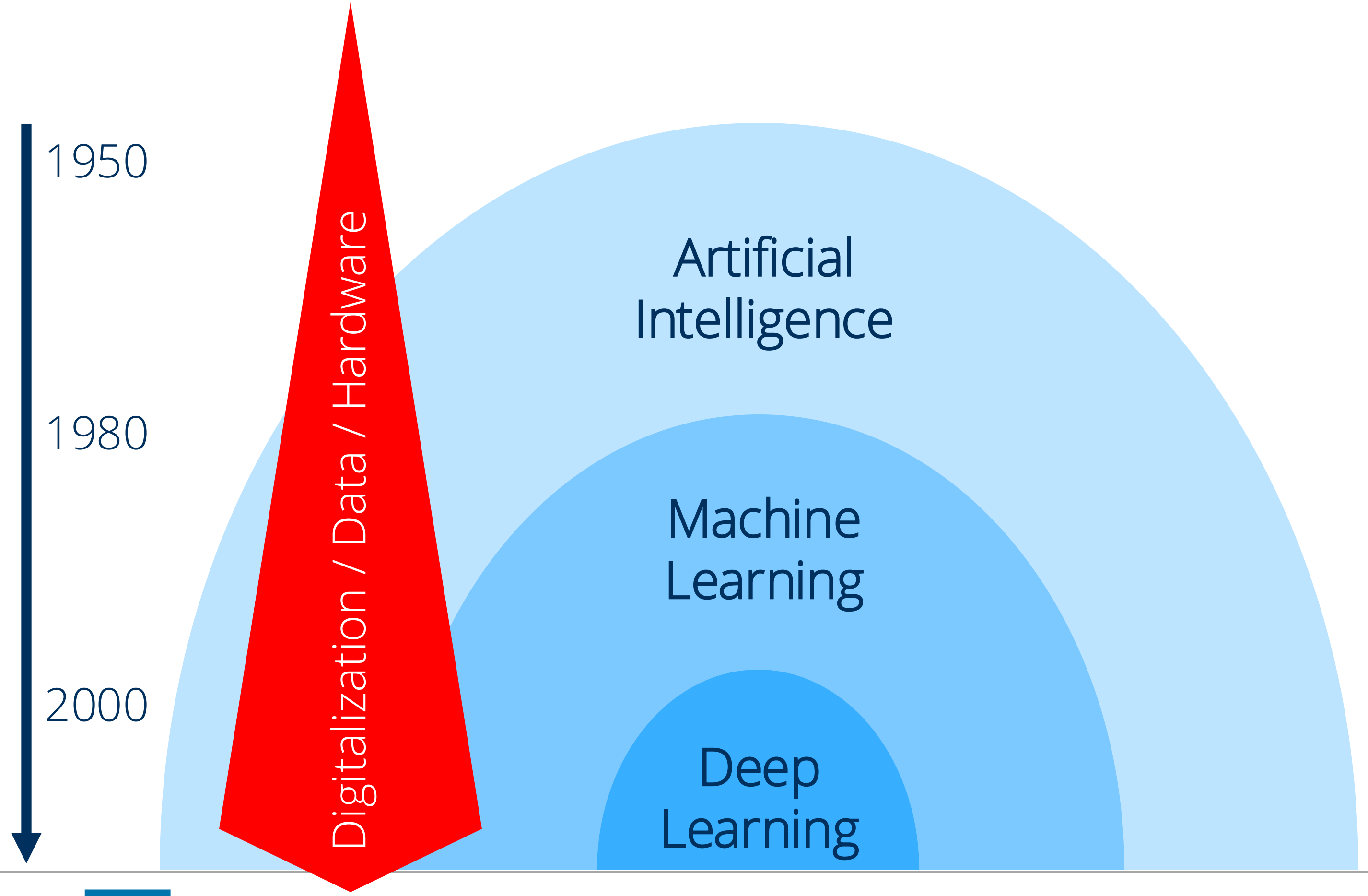
Using materials from Laura Zigutyte, Michaela Unger (EKFZ, TU Dresden), Robert Haase (ScaDS.AI, Leipzig University)

AGENDA

- Areas of Artificial Intelligence (AI)
- Neural Networks and Deep Learning
- Neural Network Architectures
- Practice: Neural Network for Regression

Areas of Artificial Intelligence

Historical phases of AI



Programs mimic intelligent human behavior

Programs independently identify connections and patterns in (structured) data.

Use of neural networks with many layers

Areas of Artificial Intelligence

Model Family

Areas, paradigms, model families (not exhaustive)

Artificial Intelligence

Machine Learning

- Linear Models
- Decision Trees
- Kernel-based
- Clustering
- Ensembles
- ...

Neural Networks

- Feed-Forward
- ...

Deep Learning

- Autoencoder
- CNN
- RNN
- Transformer
- ...

Paradigms

- Supervised
- Unsupervised
- Reinforcement
- Semi-Supervised
- Self-Supervised

Problems

- Regression
- Classification
- Clustering
- Dimension reduction
- Anomaly detection
- Sequence-to-sequence
- Recommendations
- Generative modeling
- Time series prediction
- ...

Areas of Artificial Intelligence
Paradigms - Supervised Learning

Procedure

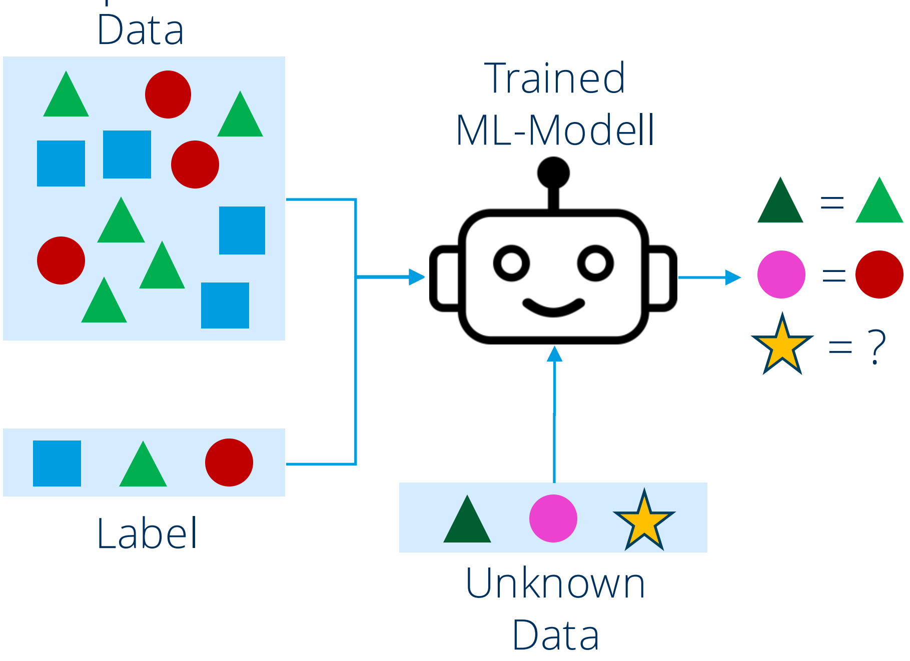
- ML models are trained using pre-labeled data
- Input data and the desired target values (ground truth) are provided for training
- Prediction of target values on new, previously unknown input data of the same format

Application examples

- Classification, Regression
- Anomaly Detection
- Generative modeling

Algorithm / model type examples

- Linear Regression
- Decision Trees & Random Forest (DT & RF)
- Support-Vector-Machines (SVM)
- Neural Networks (NN)



Areas of Artificial Intelligence
Paradigms - Unsupervised Learning

Procedure

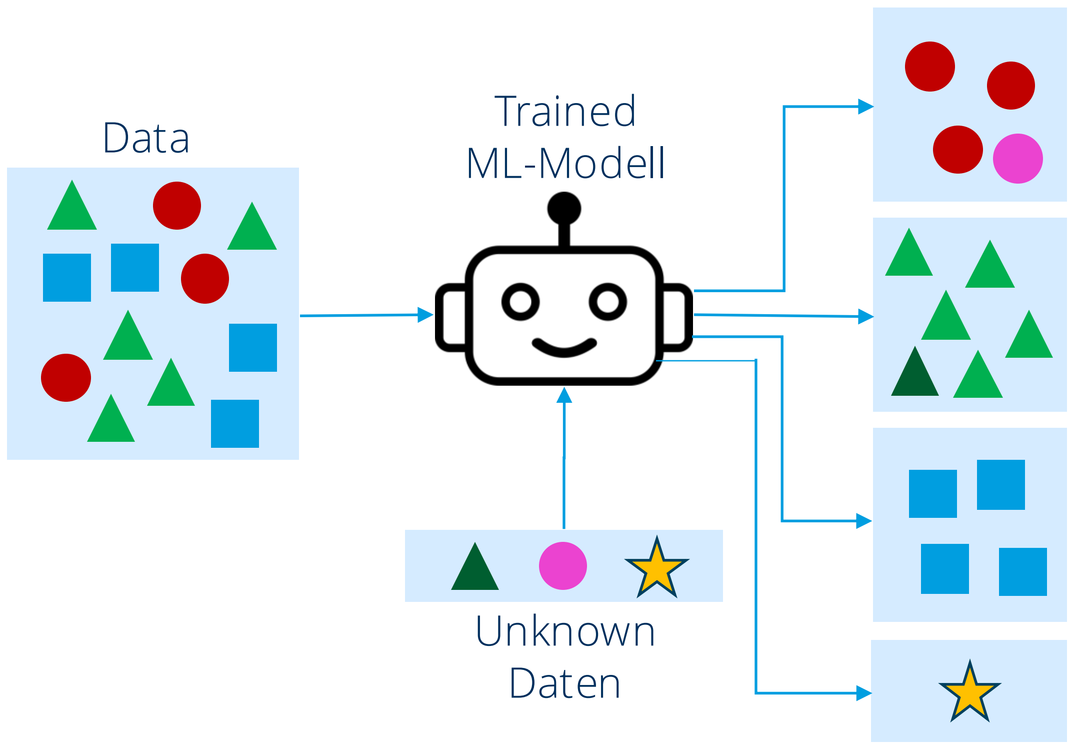
- ML models are trained with unlabeled data
- Models independently recognize patterns, structures, and correlations

Application examples

- Clustering
- Dimensionality Reduction
- Anomaly Detection

Algorithm / model type examples

- K-Means Clustering
- Principal Component Analysis (PCA)
- Autoencoder



Areas of Artificial Intelligence
Paradigms - Reinforcement Learning

Procedure

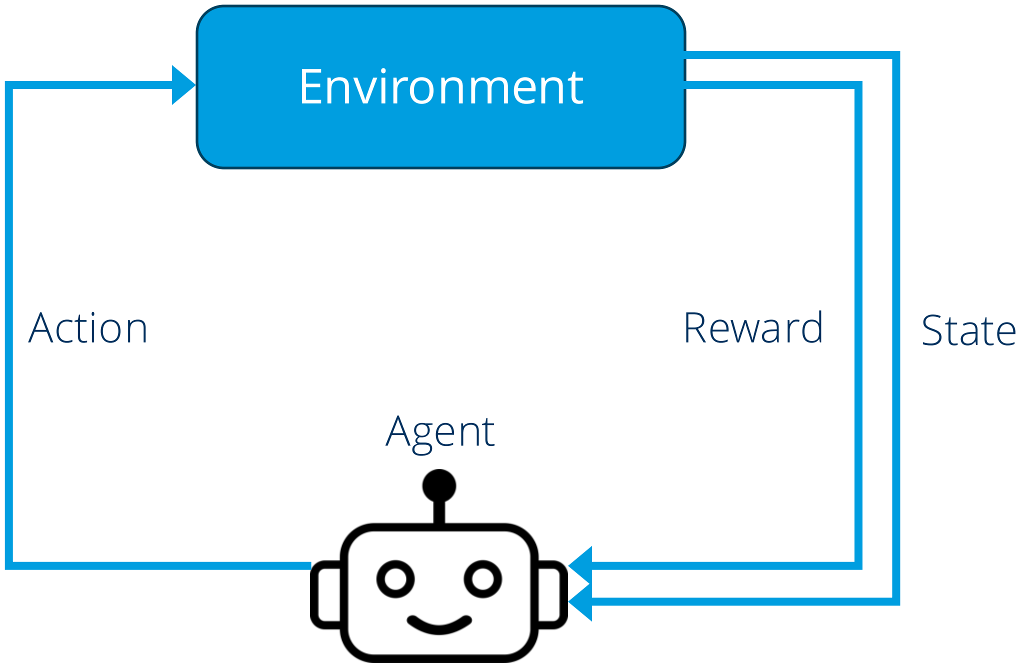
- An agent is trained to maximize a specific reward in an environment through trial and error
- Rules define the possible actions the agent can take
- Rewards (or punishments) influence the agent's behavior

Application examples

- Game agents, e.g., in chess or Go
- Automation systems, robotics
- Simulations

Algorithm / model type examples

- Q-Learning
- Markov Decision Processes (MDP)
- Monte Carlo Methods



Areas of Artificial Intelligence
Paradigms - Mixed Forms

Semi-Supervised

- A small dataset with labeled samples
- A larger dataset with unlabeled samples from the same distribution
- Training on labeled data → model assigns “pseudo-labels” to unlabeled data
- Include data with the most reliable “pseudo-labels” in further training (human-in-the-loop)

Self-Supervised

- Data is not labeled; required labels are generated by the model itself
- The model generates its own “practice questions” and answers from the raw data
- In doing so, it learns useful patterns from the data
- Example: Cover words in a sentence and then guess them – no label necessary

Areas of Artificial Intelligence
Linear models vs. non-linear models

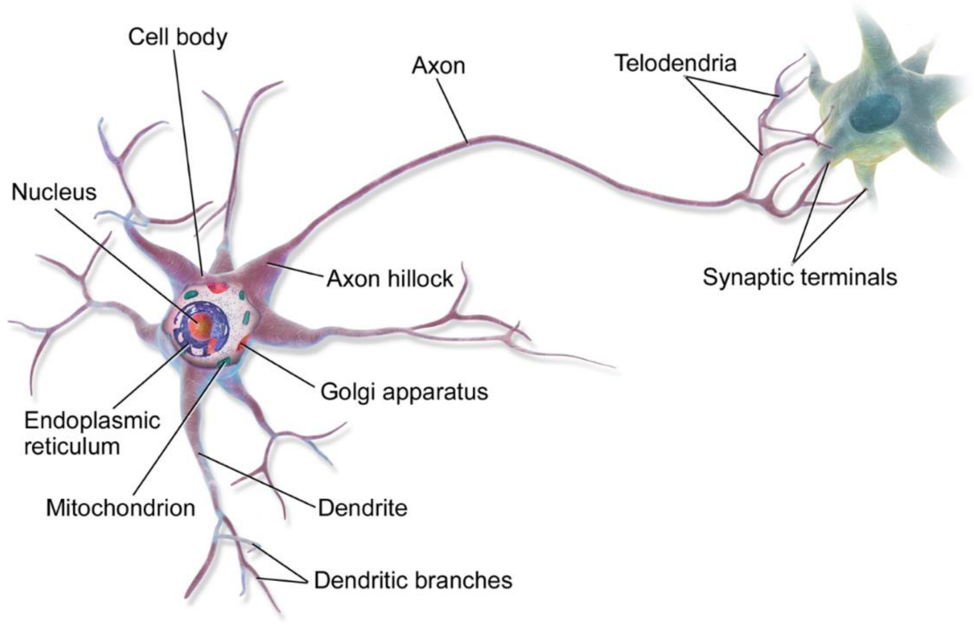
- Linear model ≠ plotting a straight line / curve
- Linearity refers to model parameters

A model is linear if its prediction is a linear combination of the features.
(e.g., weighted sum of input data)

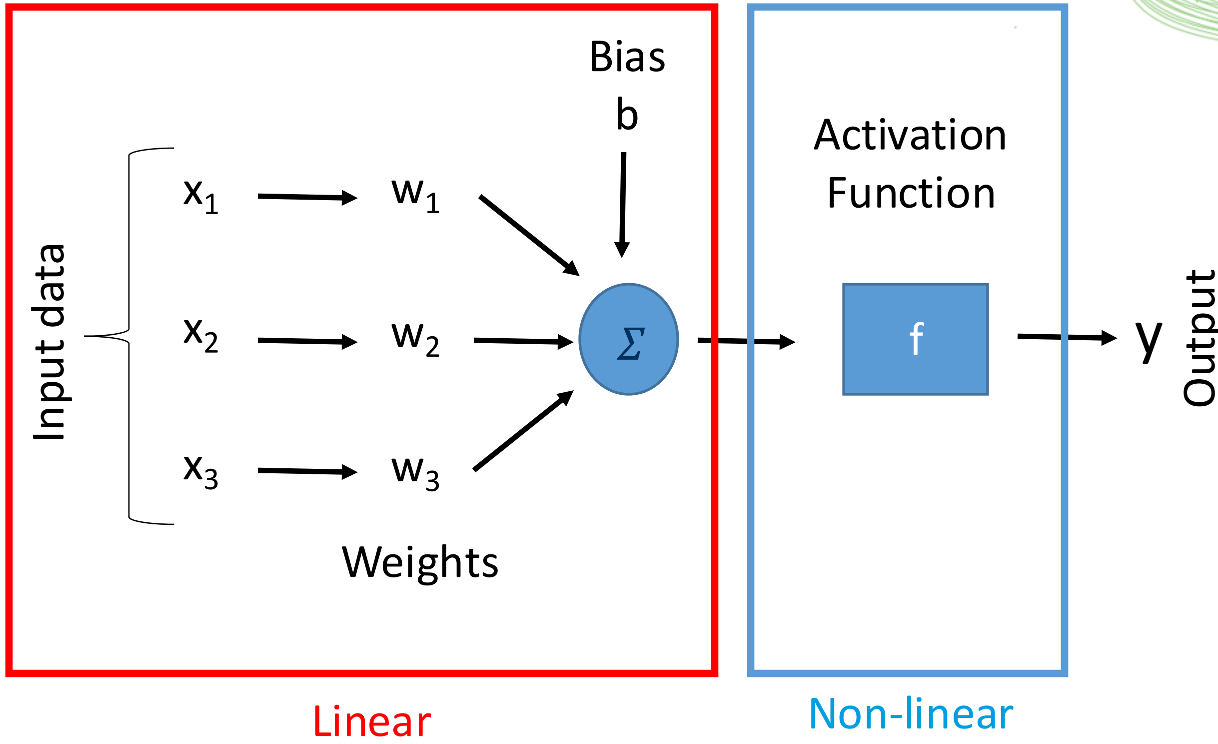
- Linear models
  - Easy to interpret, based on well-understood principles, fast and efficient training
  - Can only model simple, linear relationships in the data
  - Examples: Linear or logistic regression, ARIMA, linear SVM, etc.
- Non-linear models
  - Allows to model complex, non-linear relationships in the data
  - More difficult to interpret, complex training with more parameters, often more data required
  - Examples: Decision tree, kernel SVM, k-NN, neural networks, etc.

Neural Networks and Deep Learning
Basic Architecture

Neurons from a biological perspective



Neuron in Data Science

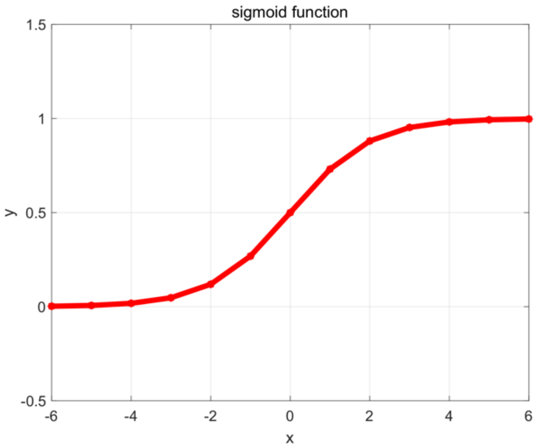


$$y = f(w_1x_1 + w_2x_2 + w_3x_3 + \mathrm{b})$$

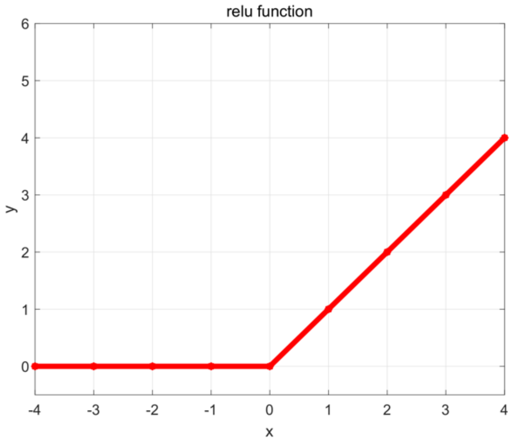
Neural Networks and Deep Learning
Basic Architecture

Activation-Function

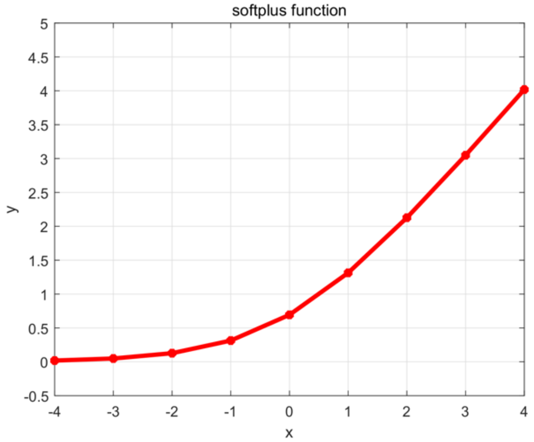
- Non-linear transformation of the linear combination of input features



(**a**) The curve of sigmoid function



(**c**) The curve of ReLu function



(**d**) The curve of softplus function

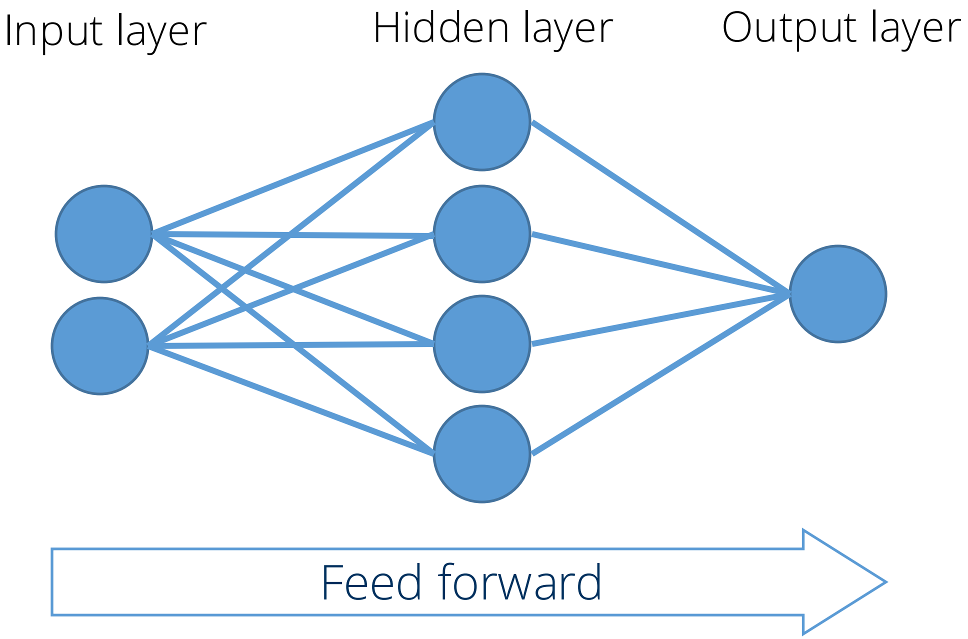
Source: Wang, Y., Li, Y., Song, Y., & Rong, X. (2020). The Influence of the Activation Function in a Convolution Neural Network Model of Facial Expression Recognition. Applied Sciences, 10(5), 1897. https://doi.org/10.3390/app10051897, OpenAccess

- More examples and explanations: https://en.wikipedia.org/wiki/Activation_function

Neural Networks and Deep Learning
Basic Architecture

Multi-Layer Perceptron

- Several layers of neurons: Input → Hidden → Output
- Neurons in one layer are fully connected to those in the next layer (Fully-Connected, Dense)
- Information flows through the network from input to output only (Feed Forward)



„**Deep Learning**"
Neural networks with **many** hidden layers

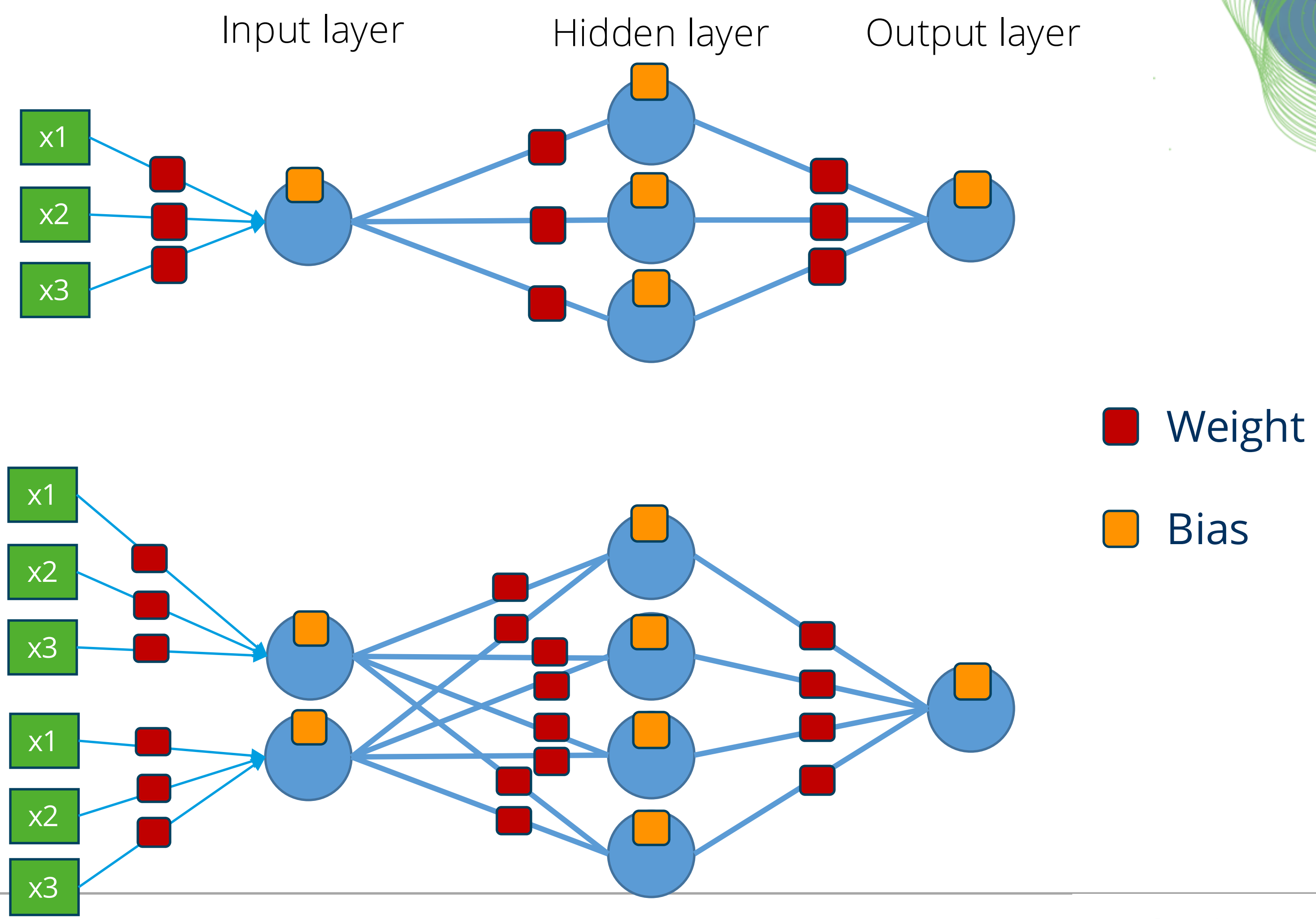
Neural Networks and Deep Learning
Basic Architecture

Data input and information flow

(Fully-Connected Feed-Forward)

Year	m^2	Zip-Code	Price
1991	234	12345	xxxxx
1896	400	54638	xxxxx
2005	185	95463	xxxxx

x1	x2	x3	T

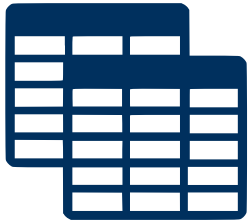


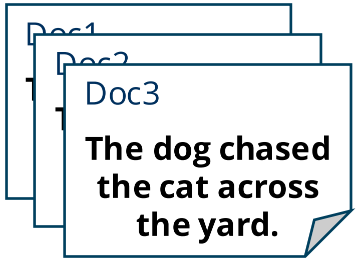
$$y = f(w_1 x_1 + w_2 x_2 + w_3 x_3 + b)$$

Neural Networks and Deep Learning
Data Processing

Processing and conversion of input data

- Create features that can be used and learned by ML models / neural networks
- Goal: Turn input data into numerical representation so a neural network can process them





Is the data representative?

Handling of missing data

Handling of outliers

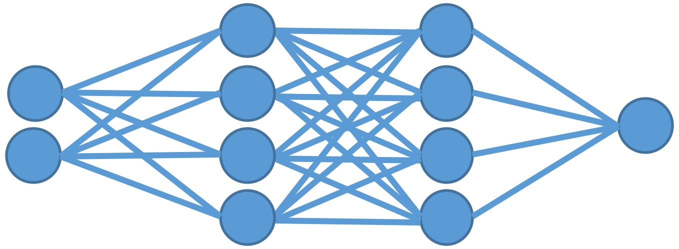
Feature selection

Data scaling / normalization

Embeddings

Train-test-split

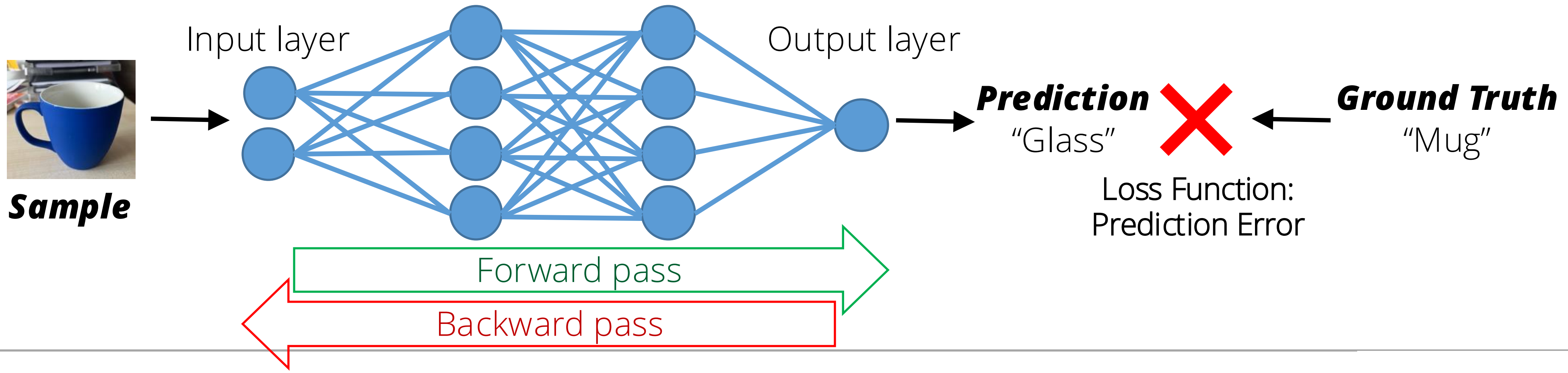
…



Neural Networks and Deep Learning
Training Process

Learning through “Back Propagation”

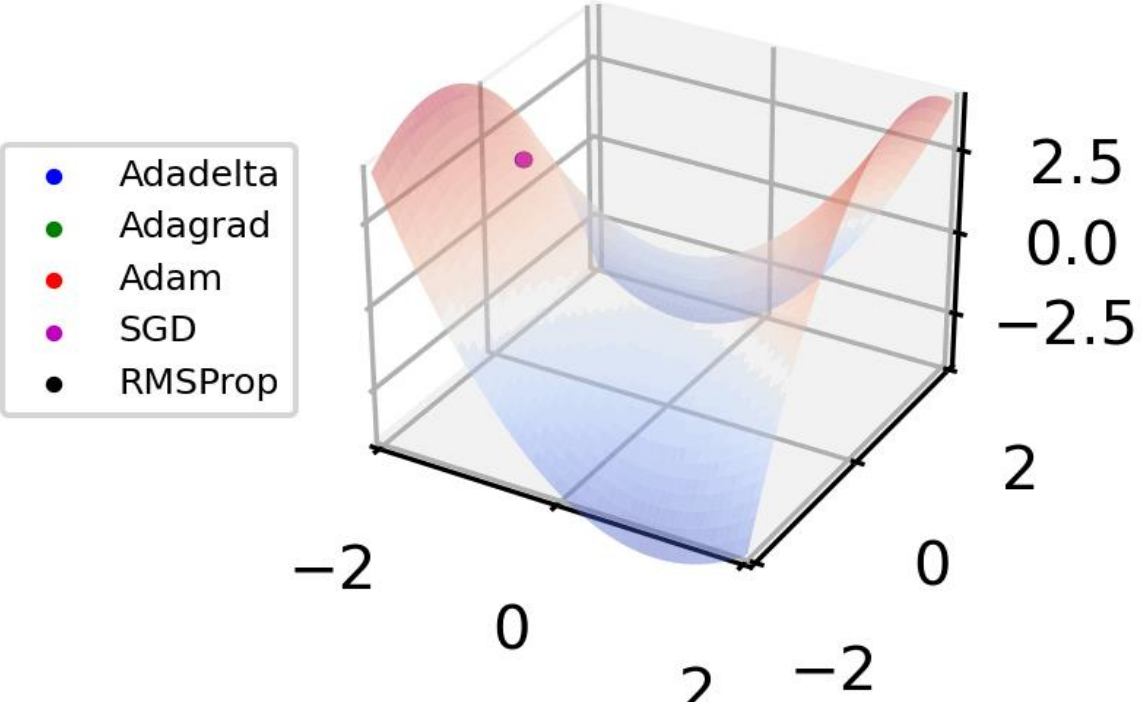
- Step 1: Initialize weights of all neurons with small random values
- Step 2: Send data point (**sample**) through the network for prediction (**forward pass**)
- Step 3: Compare prediction with known label for the sample (supervised learning with **ground truth**), calculate error between prediction and ground truth (via **loss function**)
- Step 4: Starting with the output layer (**backward pass**), adjust the weights in the neurons with the goal to minimize the calculated error (e.g., via **gradient descent**)
- Repeat steps 2-4 for each sample in training data (one **epoch**), running through this for several epochs



Neural Networks and Deep Learning
Training Process

Weight Adjustment – Optimization via Gradient Descent

- Gradient descent updates weights to minimize an objective function → loss function → error
- Optimizer follows the steepest descent (slope) on the loss function
- Learning rate controls the step size
  → too large = overshoot
  → too small = slow training
- Training may get stuck in local minima instead of reaching best global solution
- Different optimizer algorithms improve training

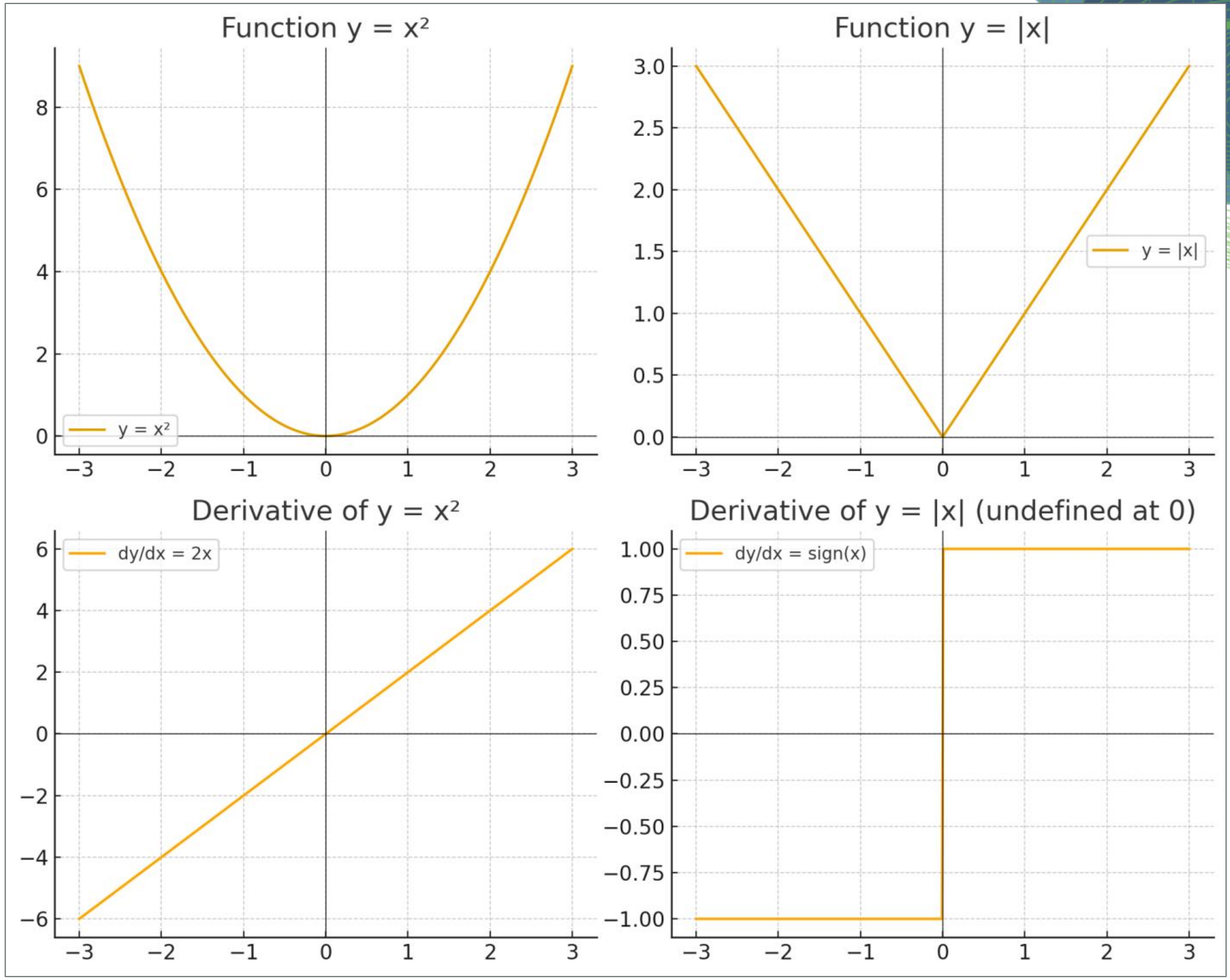


Source: VirtualVistas - Own work, https://commons.wikimedia.org/w/index.php?curid=139889895, CC BY-SA 4.0

Neural Networks and Deep Learning
Training Process

Loss Function

- Needs to be a differentiable function to compute a slope
- Derivate must be defined for all points
- Example:
  - Mean Squared Error: $(y\_true – y\_predicted)^2$



Neural Networks and Deep Learning
Training Process

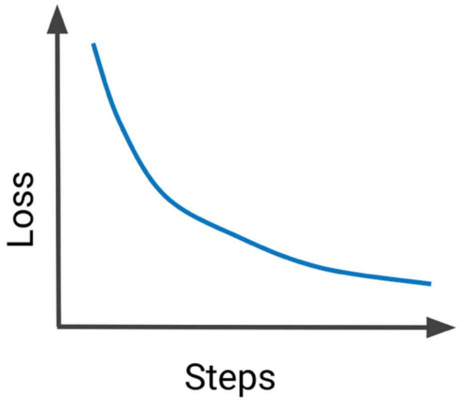
Architecture and Training Parameters (Hyperparameters)

- Model parameters = learned by the neural network during training (weights, biases)
- Model architecture choices
  - Layer types and arrangement
  - Number of neurons per layer
  - Type of activation function
  - …
- Training parameter
  - Number of samples / batches per epoch
  - Number of epochs
  - Optimization method and learning rate
  - …
- Hyperparameter optimization → find the best configuration for the architecture and the training

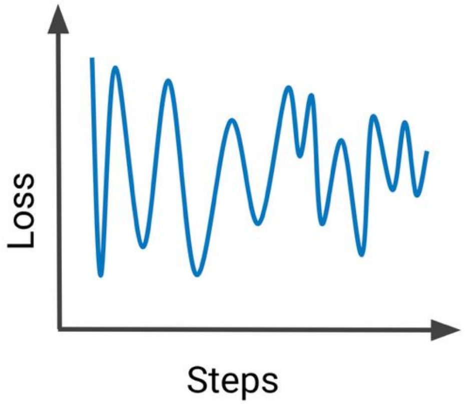
Neural Networks and Deep Learning
Training Process

But how can we check how well the training process is going?

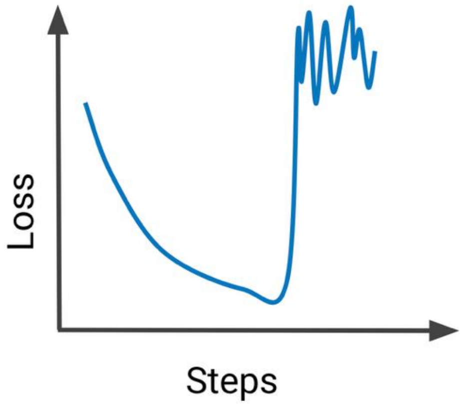
- Plot the loss curve to see how the loss (error) develops over time (steps / epochs)



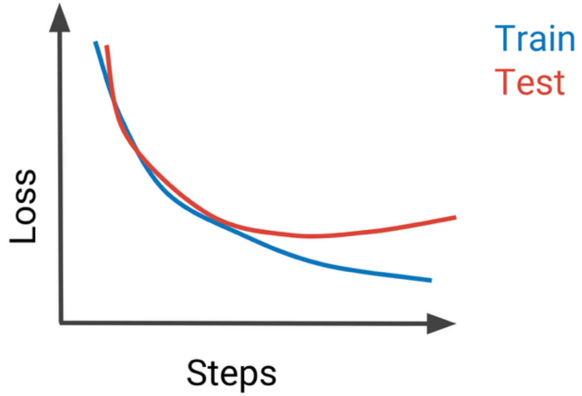
Ideal loss curve



Oscillating training
- Bad training data
- Learning rate too high



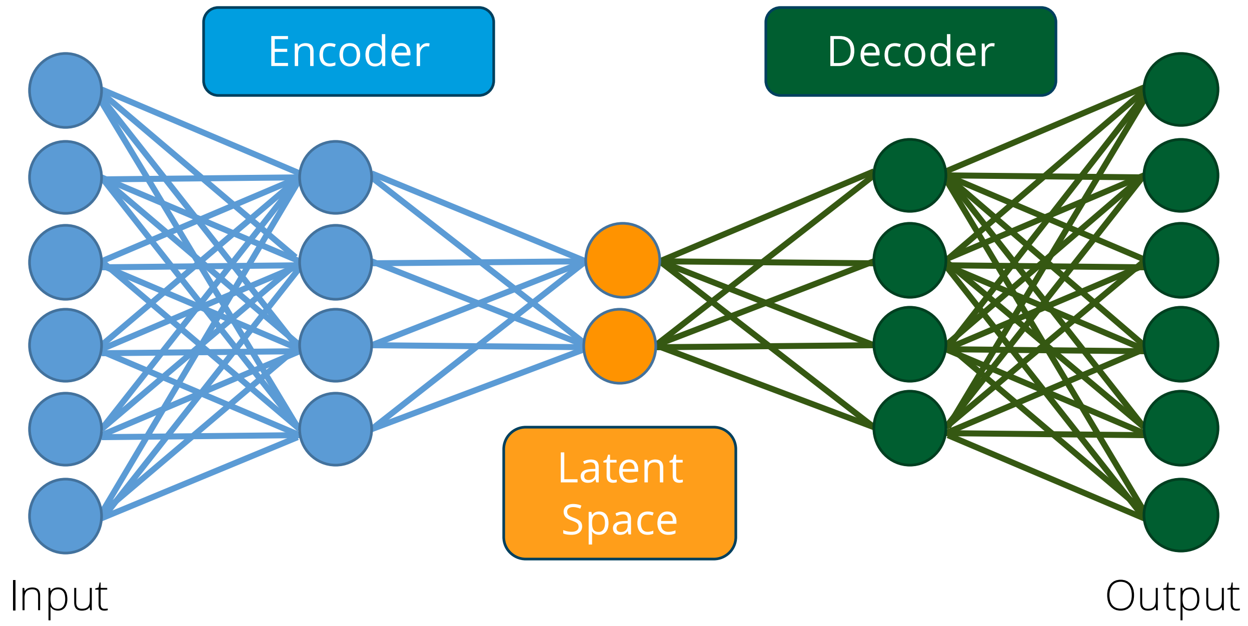
Disturbed training
- Outliers in data
- Missing values (NaN)



Overfitting on training data
Bad generalizing for new data

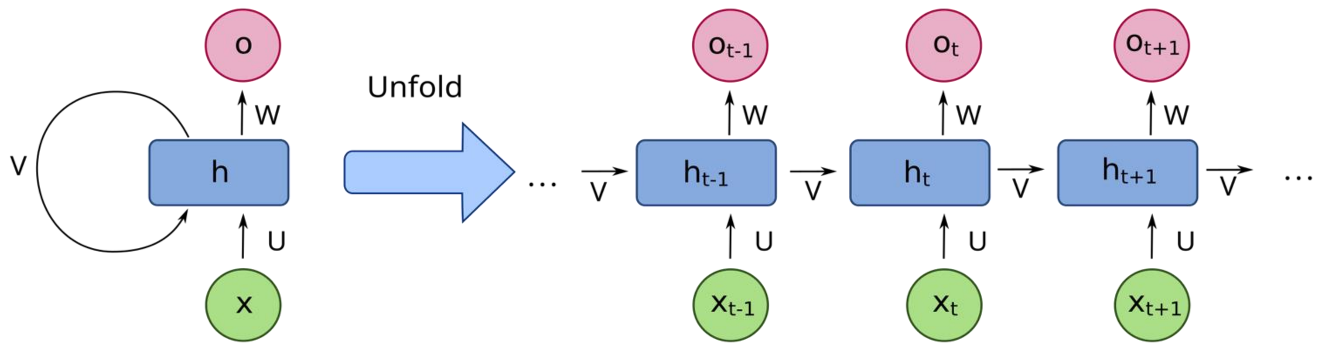
Neural Network Architectures
Autoencoder

- Neural network for data compression (encoder) and reconstruction (decoder)
- Most important information (properties of features) get embedded in low-dimensional latent space
- Training aims to minimize the error during reconstruction
- Applications, e.g., dimensionality reduction or anomaly detection (large error = anomaly)



Neural Network Architectures
Recurrent Neural Network (RNN / LSTM / GRU)

- Neural network for modeling sequences
- Implements “memory” with the help of “feedback loops”
- Information no longer flows only from input to output (feed forward), but is also fed back into the neurons of previous hidden layers
- Variants of this enable, among other things, “long short-term memory” (LSTM)



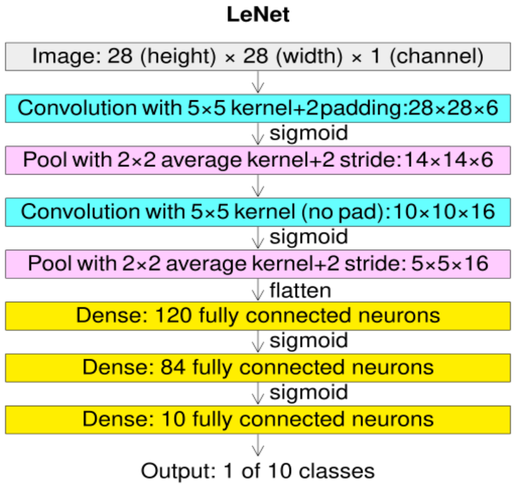
Source: fdeloche, https://commons.wikimedia.org/w/index.php?curid=60109157, CC BY-SA 4.0

x – Input
h – Hidden (Memory)
o – Output
U, V, W – according Weights

Unfold…”roll up” over time:
At time t, the previous state t-1 is incorporated via V
At time t+1, the previous state t is incorporated via V
…

Neural Network Architectures
Convolutional Neural Network (CNN)

- Neural network with different layer types for extracting local to global features from input data
  - Convolutional Layer (Convolution)
  - Pooling Layer (Aggregation)
  - Dropout Layer (Regularization)
  - Fully Connected Layer (Classification)
- Application mostly in image processing (object recognition, classification)



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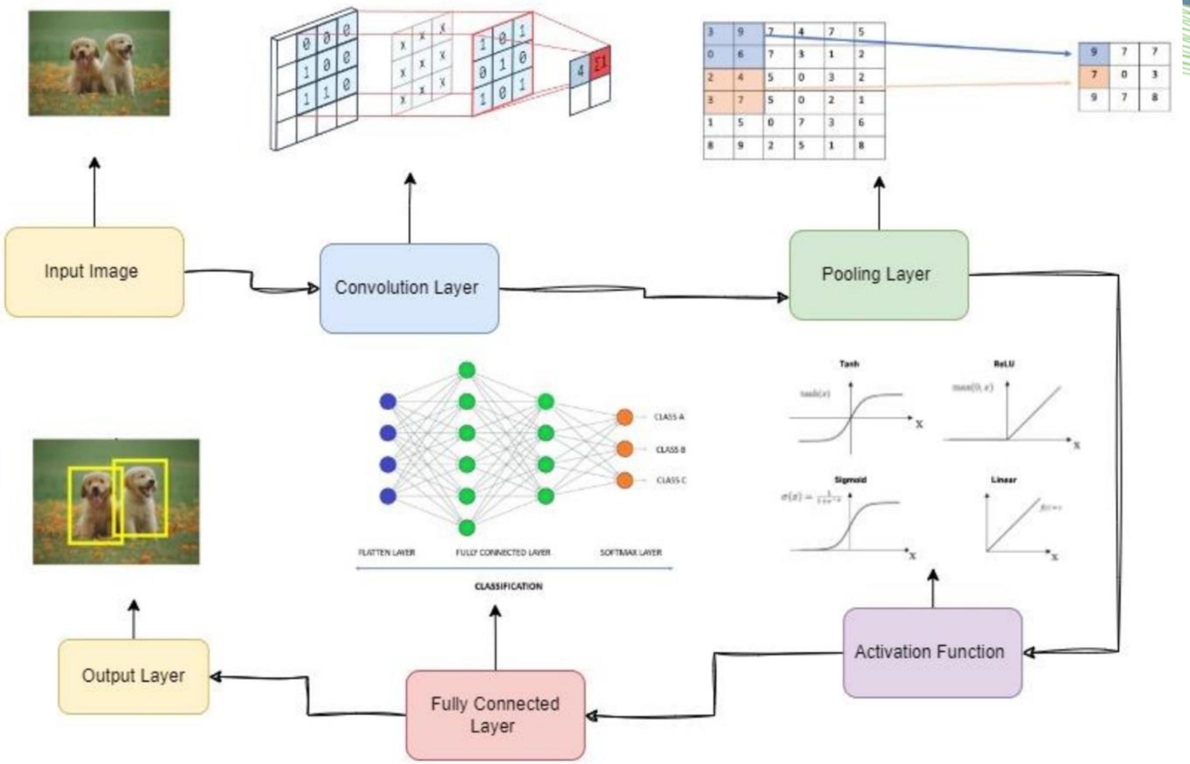


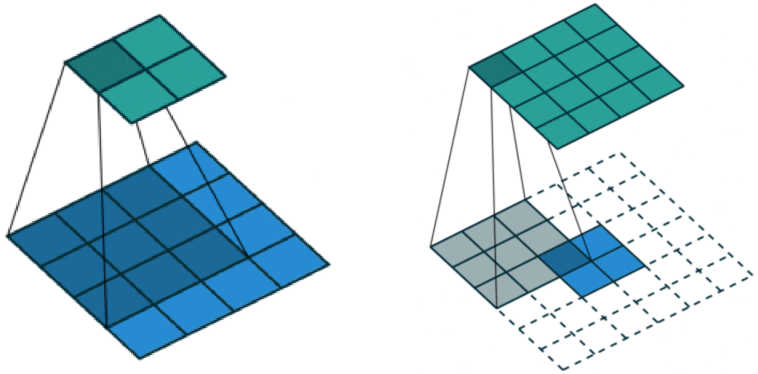
Source: Taye, M. M. (2023). Theoretical Understanding of Convolutional Neural Network: Concepts, Architectures, Applications, Future Directions. *Computation*, *11*(3), 52. https://doi.org/10.3390/computation11030052, OpenAccess

Neural Network Architectures
Convolutional Neural Network (CNN)

- Convolutional Layer – <u>not</u> fully connected
- Kernel moves over input and extracts features by applying element-wise multiplications and sums
  → kernels are small weight matrices that are learned during training

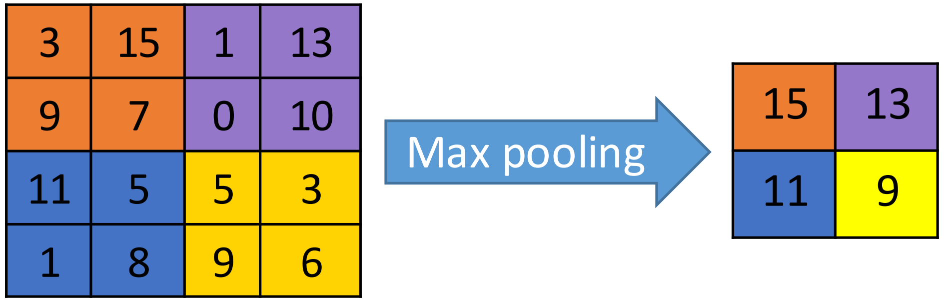
0	2	0
2	1	2
0	2	0

3x3 Kernel



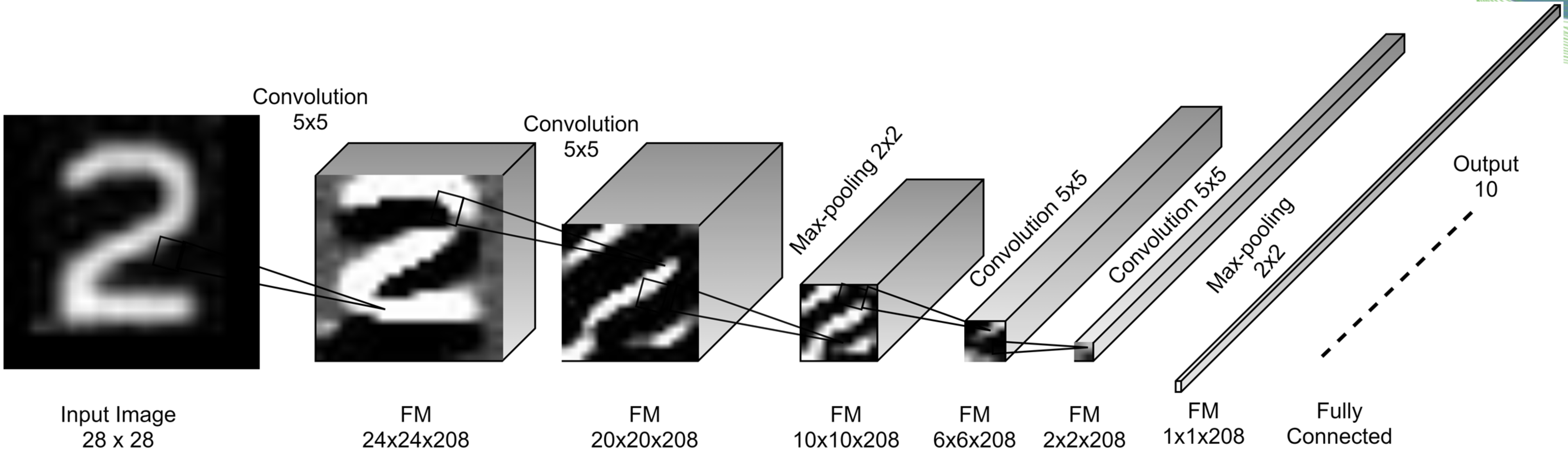
Quellen:
Vincent Dumoulin and Francesco Visin (2018). A guide to convolution arithmetic for deep learning. *arXiv*. https://doi.org/10.48550/arXiv.1603.07285
Vincent Dumoulin, Francesco Visin, https://github.com/vdumoulin/conv_arithmetic, MIT

- Pooling Layer aggregates input (e.g., max, avg, …), introduces robustness to variations in the data
- Dropout randomly removes connections during training to prevent overfitting



Neural Network Architectures
Convolutional Neural Network (CNN)

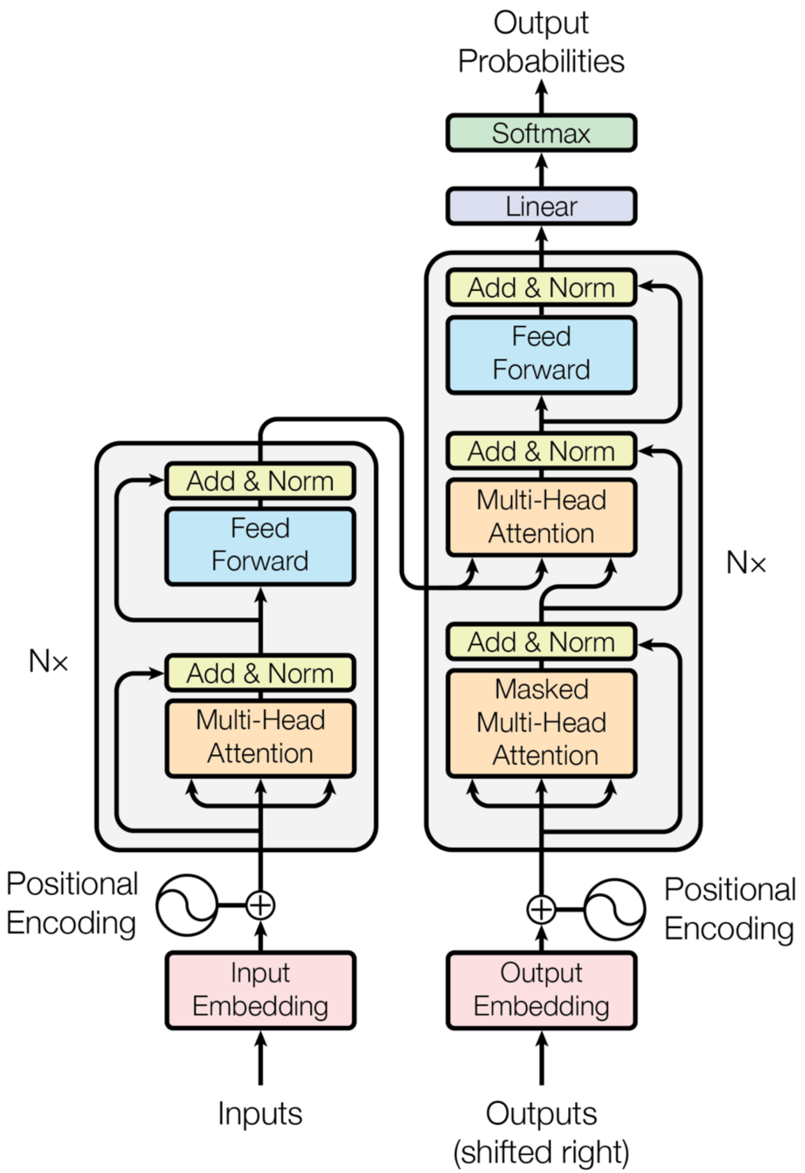
- Convolutional Neural Network – the full image



Source: Salemdeeb M, Ertürk S. 2021. Full depth CNN classifier for handwritten and license plate characters recognition. PeerJ Computer Science 7:e576 https://doi.org/10.7717/peerj-cs.576, CC-BY4.0

Neural Network Architectures
Transformer

- Complex, multi-component, multi-layer deep learning-based model for generative AI, sequence modelling…
- Consists of various components, grouped into encoders and decoders



Quelle: Vaswani et al (2017), https://arxiv.org/abs/1706.03762

Neural Network Architectures
Transformer

Transformer architecture explained

Encoder Block
Process input data, extract meaning

Add & Norm
Stabilize training process

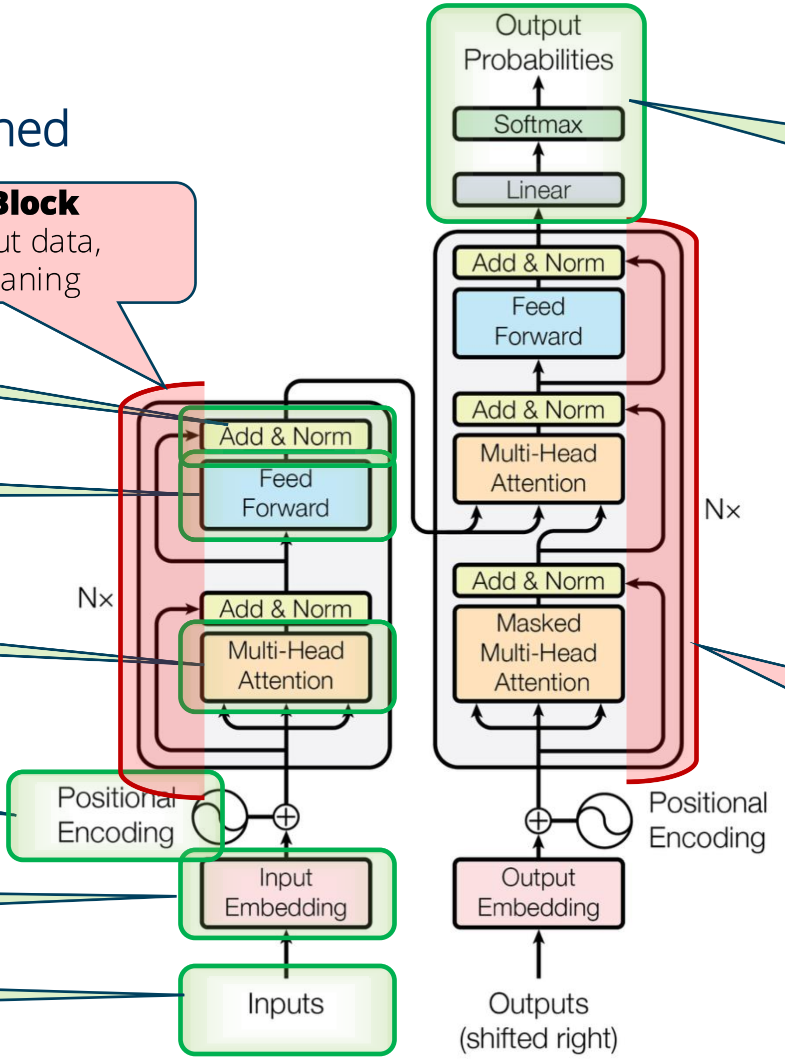
Feed Forward
Neural network, non-linear transformation

Multi-Head Attention
Compute relationships between embeddings

Positional Encoding
Enrich embeddings with positional information

Embeddings
Compute embeddings from tokens

Tokenizer
Compute tokens from input text data



Output
Probability for next token

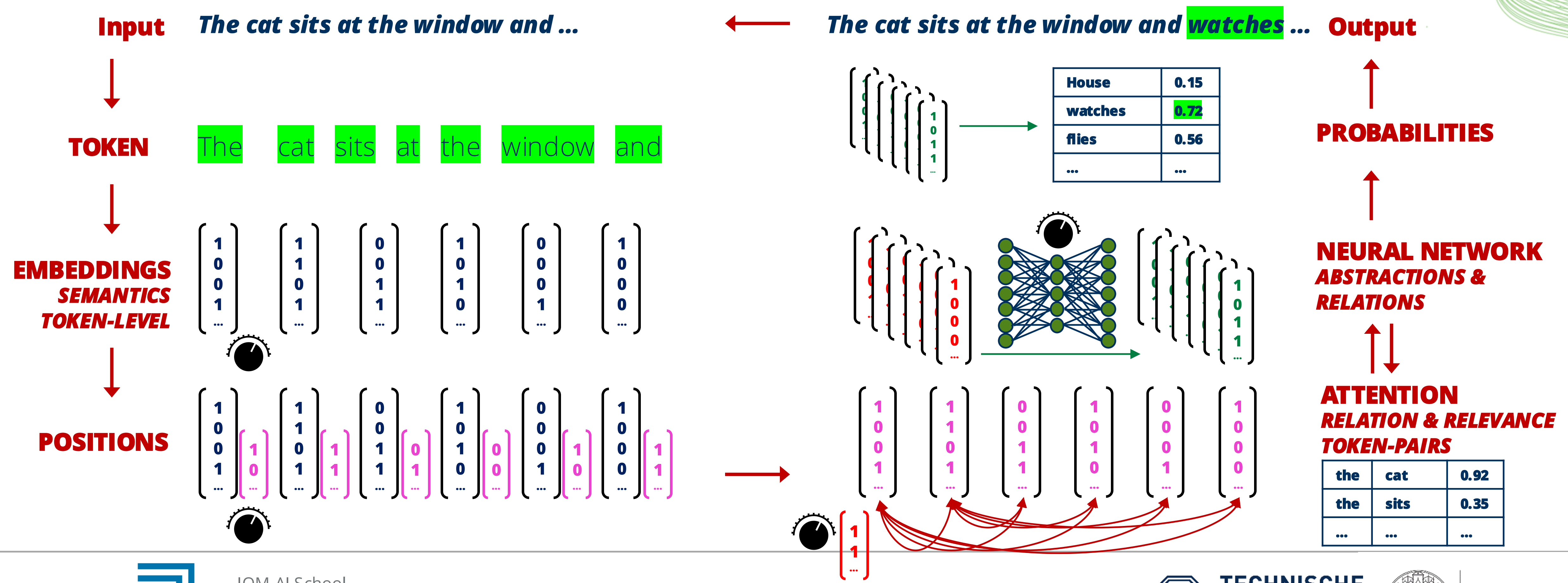
Decoder Block
Merge previous token / prediction and current encoder output to predict next token

Source: Vaswani et al (2017), https://arxiv.org/abs/1706.03762

Neural Network Architectures
Transformer

Weights for almost all operations
“Adjustment screws”

Transformer – High level view on the process



House	0.15
watches	0.72
flies	0.56
…	…

the	cat	0.92
the	sits	0.35
…	…	…

Practical exercise

- Build and train a neural network for a regression problem
- Covering model training, hyperparameter optimization, monitoring the training process, model evaluation
- Leveraging the Python libraries
  - pytorch – open-source deep learning framework
  - optuna – open-source framework for hyperparameter optimization