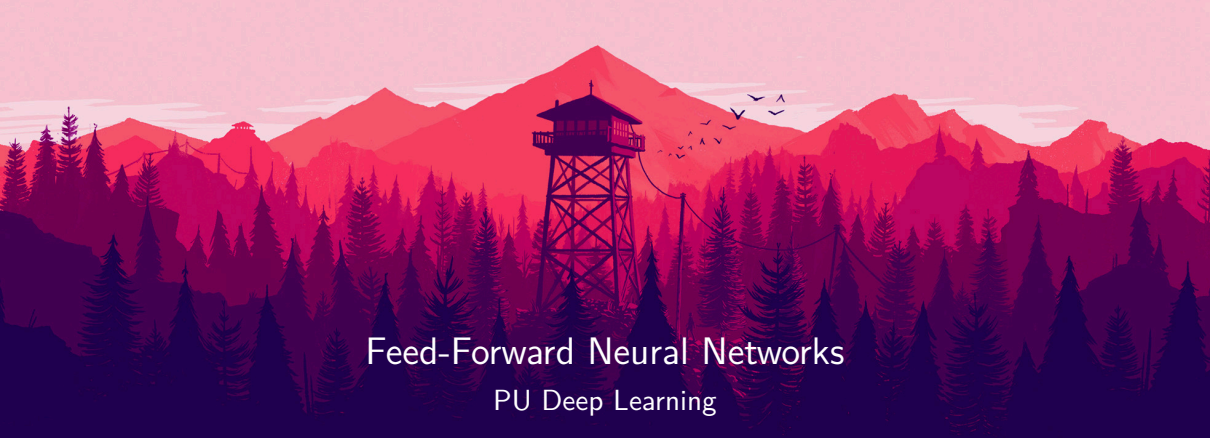


Feed-Forward Neural Networks

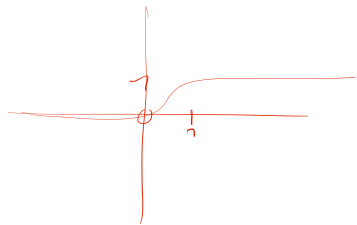
PU Deep Learning

Nils Reiter, nils.reiter@uni-koeln.de

May 18, 2021 (Summer term 2021)

Recap

- Classification
  - Assign previously known labels to instances
  - Different algorithms, wide range of applications
- Logistic Regression
  - Classification method based on $h(x) = \frac{1}{1+e^{-(ax+b)}}$
  - Core ingredient of artificial neural networks
- Gradient Descent
  - Learning algorithm for logistic regression
  - Core ingredient of learning artificial neural networks
- `scikit-learn`
  - Python library for machine learning



Today

Neural Networks

Deep Learning Library `keras`

Exercise

Section 1

Neural Networks

From a Logistic Regression to a Neuron

- Hypothesis function of logistic regression:

$$h(x) = \frac{1}{1 + e^{-(ax+b)}}$$

Maps one value to another (just like many other functions)

From a Logistic Regression to a Neuron

- Hypothesis function of logistic regression:

$$h(x) = \frac{1}{1 + e^{-(ax+b)}}$$

  Maps one value to another (just like many other functions)

- Further parameterization:

$$h(x) = \sigma(ax + b) \qquad \text{with } \sigma(x) = \frac{1}{1 + e^{-x}}$$

From a Logistic Regression to a Neuron

- Hypothesis function of logistic regression:

$$h(x) = \frac{1}{1 + e^{-(ax+b)}}$$

  Maps one value to another (just like many other functions)

- Further parameterization:

$$h(x) = \sigma(ax + b) \qquad \text{with } \sigma(x) = \frac{1}{1 + e^{-x}}$$

$\Rightarrow$ We can insert other functions as well!

What is a neural network?

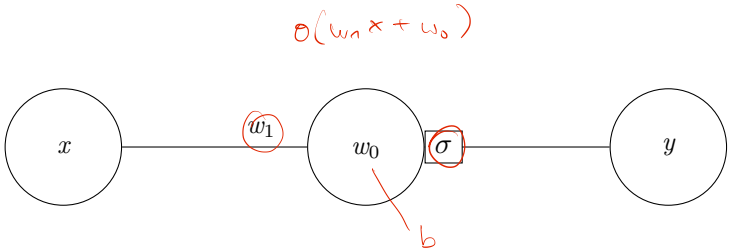


Figure: 1 neuron (with logistic activation) = logistic regression (with 1 feature)

What is a neural network?

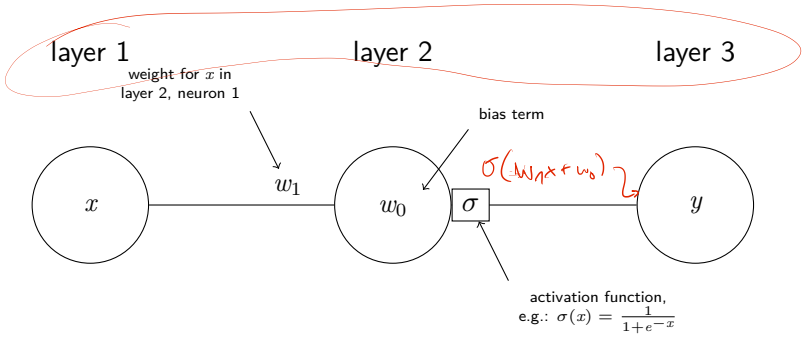


Figure: 1 neuron (with logistic activation) = logistic regression (with 1 feature)

What is a neural network?

Example

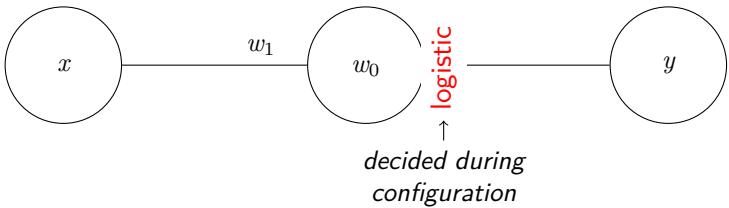


Figure: 1 neuron (with logistic activation) = logistic regression (with 1 feature)

What is a neural network?

Example

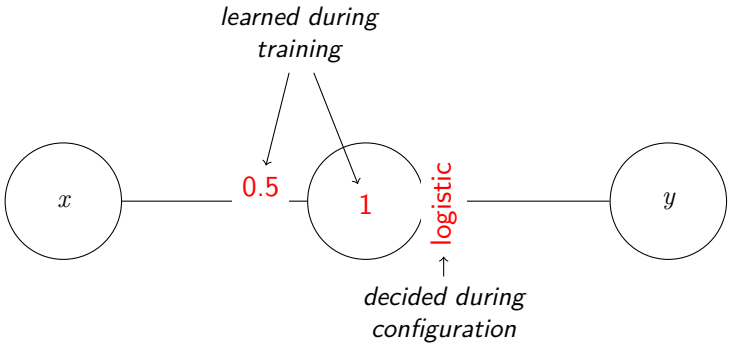


Figure: 1 neuron (with logistic activation) = logistic regression (with 1 feature)

What is a neural network?

Example

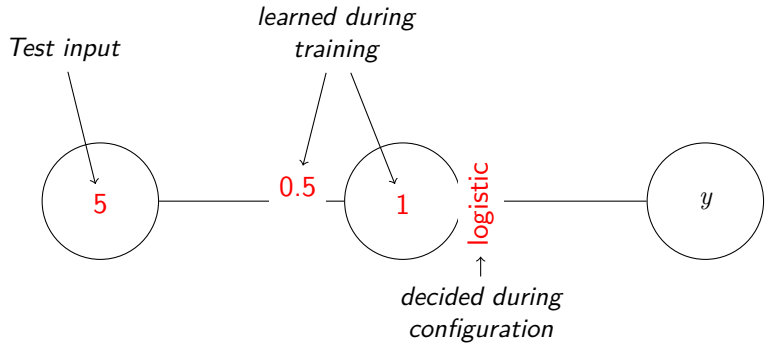


Figure: 1 neuron (with logistic activation) = logistic regression (with 1 feature)

What is a neural network?

Example

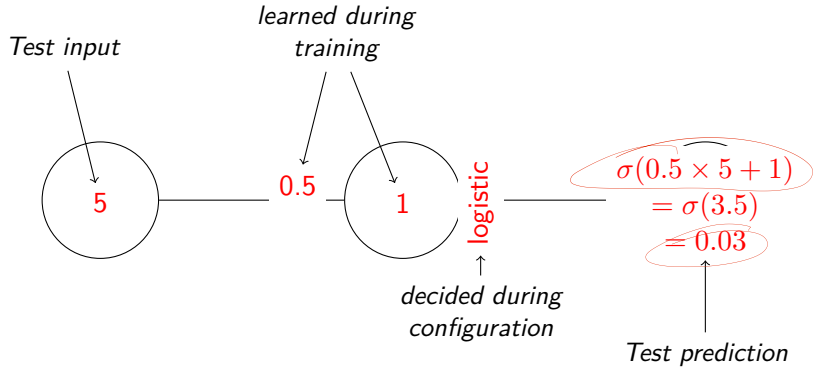
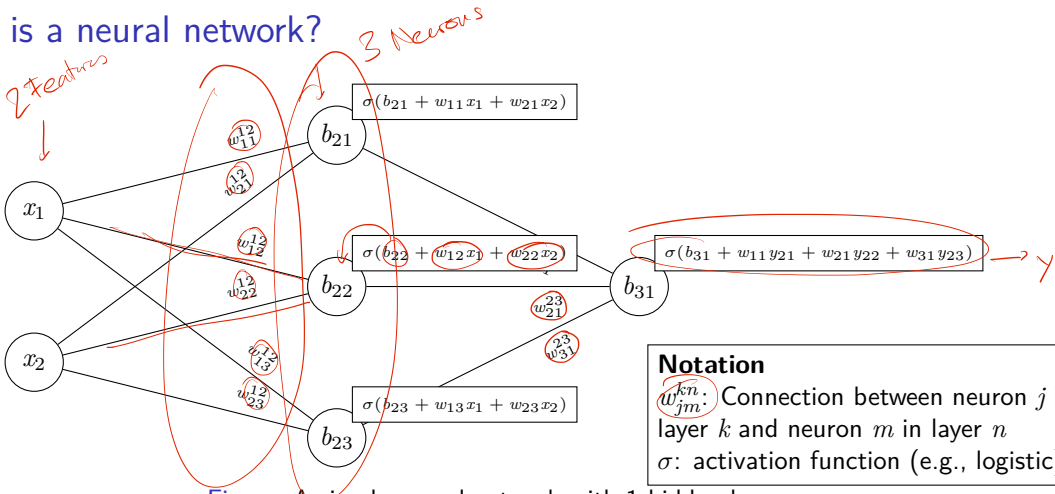


Figure: 1 neuron (with logistic activation) = logistic regression (with 1 feature)

What is a neural network?



Notation

w^{kn}_{jm}: Connection between neuron j in layer k and neuron m in layer n

σ: activation function (e.g., logistic)

Figure: A simple neural network with 1 hidden layer

Prediction Model: Forward Pass

- If we have all the weights, bias terms, numbers of neurons and layers, we can compute the output of the network
  - Conceptually: Applying functions in sequence: $y = f_3(f_2(f_1(x)))$ (one per layer)

Prediction Model: Forward Pass

- If we have all the weights, bias terms, numbers of neurons and layers, we can compute the output of the network
  - Conceptually: Applying functions in sequence: $y = f_3(f_2(f_1(x)))$ (one per layer)
- Practically, a lot of the computation happens in matrices
  - Hidden layer
    - Weights from input to hidden: $W_{1,2} = \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \end{bmatrix}$
    - Biases $B_2 = (b_{21}, b_{22}, b_{23})$

Prediction Model: Forward Pass

- If we have all the weights, bias terms, numbers of neurons and layers, we can compute the output of the network
  - Conceptually: Applying functions in sequence: $y = f_3(f_2(f_1(x)))$ (one per layer)
- Practically, a lot of the computation happens in matrices
  - Hidden layer
    - Weights from input to hidden: $W_{1,2} = \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \end{bmatrix}$
    - Biases $B_2 = (b_{21}, b_{22}, b_{23})$
- Hidden layer computation
  - $f_2(X) = \sigma((W_{1,2}^T X) + B_2)$

Prediction Model: Forward Pass

- If we have all the weights, bias terms, numbers of neurons and layers, we can compute the output of the network
  - Conceptually: Applying functions in sequence: $y = f_3(f_2(f_1(x)))$ (one per layer)
- Practically, a lot of the computation happens in matrices
  - Hidden layer
    - Weights from input to hidden: $W_{1,2} = \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \end{bmatrix}$
    - Biases $B_2 = (b_{21}, b_{22}, b_{23})$
- Hidden layer computation
  - $f_2(X) = \sigma((W_{1,2}^{\intercal} X) + B_2)$
- Deep learning involves a lot of matrix multiplication
  - GPUs are highly optimized for this
  - Hint: Gaming-GPUs that support CUDA are also usable for deep learning

Feed-Forward Neural Networks

- The above is called a »feedforward neural network«
  - Information is fed only in forward direction

Feed-Forward Neural Networks

- The above is called a »feedforward neural network«
  - Information is fed only in forward direction
- Configuration choices
  - Activation function (next slide)
  - Layer size: Number of neurons in each layer
  - Number of layers
  - Loss function
  - Optimizer
- Training choices
  - Epochs/batches
  - Training status displays

Feed-Forward Neural Networks

Activation Functions

All neurons of one layer have the same

Popular choices:

- **logistic** $y = \sigma(x) = \frac{1}{1+e^{-x}}$ – ›squashes‹ everything to a value between 0 and 1
- **relu** $y = \max(0, x)$ – Makes everything negative to 0
- **softmax** Scales a vector such that values sum to 1 (probability distribution)

Training: »Backpropagation«

- Similar to gradient descent
- But
  - A lot more parameters
  - Because of multiple layers: Vanishing gradients
    - Backpropagation involves a lot of multiplication
    - Factors are between zero and one

    $\Rightarrow$ Numbers get very small very quickly

Training: »Backpropagation«

- Similar to gradient descent
- But
  - A lot more parameters
  - Because of multiple layers: Vanishing gradients
    - Backpropagation involves a lot of multiplication
    - Factors are between zero and one
    - $\Rightarrow$ Numbers get very small very quickly
- Training choice: Batches and epochs

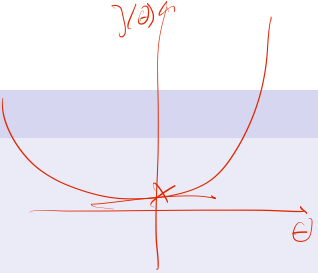
Training a Feedforward Neural Network I

Stochastic Gradient Descent (SGD)

- Gradient Descent
  - Apply θ to all training instances
  - Calculate loss over entire data set
- Stochastic Gradient Descent
  - Data set in random order
  - Calculate loss for every single instance, then update weights

Training a Feedforward Neural Network II

When to stop the training



- Logistic regression (last week): Stop in minimum
- In theory, that's what we want
- In practice
  - We usually are not exactly in the minimum
  - It's not important to be exactly in the minimum

$\Rightarrow$ Fixed number of iterations over the data set (= number of epochs)

Batches vs. Epochs

batch Number of instances used before updating weights

epochs Number of iterations over all instances

Section 2

Deep Learning Library `keras`

keras

- `https://keras.io`
- High-level Python API for deep learning
- Built on top of tensorflow
- Pattern: 1. Layout the network, 2. set hyper parameters, 3. run training

Listing: Installing Keras

```
1 pip install keras
```

Configuration

- Sequential API: Linear topology of layers
  - We will use mainly this
- Functional API: Graph of layers

Configuration

- Sequential API: Linear topology of layers
  - We will use mainly this
- Functional API: Graph of layers

Listing: Sequential API

```
# model layout
model = Sequential()
model.add(...)
model.add(...)

# hyperparameter specification
model.compile(loss=...,
  optimizer=...)

# training
model.fit(..., epochs=...,
  batch_size=...)
```

Listing: Functional API

```
# model layout
in = ...
out = Dense(10)(in)
model = Model(inputs=in,
  outputs=out)

# hyperparameter specification
model.compile(loss=...,
  optimizer=...)

# training
model.fit(..., epochs=...,
  batch_size=...)
```

Configuration

Two most basic layer types

- Dense: »Just your regular densely-connected NN layer.«
  - https://keras.io/api/layers/core_layers/dense/

```
layer = Dense(3, # number of neurons
  activation = activations.sigmoid, # activation function
  name = "dense layer 7" # useful for debugging/visualisation
  ... # more options, see docs
)
```

- Input: Marks layers to accept data
  - https://keras.io/api/layers/core_layers/input/

```
layer = Input(shape=(15,) # number of input dimensions/features
  name = "input layer", # useful for debugging/visualisation
  ... # see docs
)
```

Shape

- Description of the dimensionality of the data
- A vector of numbers, describing the elements for each dimension
- Python tuple
  - List with fixed length: `x = (5,3,1) #a tuple`
  - ⚠ Tuple with one element printed as `(5,)` or `5`

Shape

- Description of the dimensionality of the data
- A vector of numbers, describing the elements for each dimension
- Python tuple
  - List with fixed length: `x = (5,3,1) #a tuple`
  - ⚠ Tuple with one element printed as `(5,)` or `5`

```
1 x = np.zeros(5) # array([0., 0., 0., 0., 0.])
2 x.shape # returns (5,)
3 x = np.zeros((3,5))
4 # array([[0., 0., 0., 0., 0.],
5 #         [0., 0., 0., 0., 0.],
6 #         [0., 0., 0., 0., 0.]])
7 x.shape # returns (3,5)
```

np.zeros((3, 5, 7))

A Full Example

```
1  import numpy as np
2  from tensorflow import keras
3  from tensorflow.keras import layers
4
5  # create a random data set
6  train = np.random.randn(100)
7  train = train.reshape([4,25])
8  y_train = train[0]
9  x_train = np.rot90(train[1:])
10
11 # setup the model architecture
12 model = keras.Sequential()
13 model.add(layers.Input(shape=(3,)))
14 model.add(layers.Dense(5, activation="sigmoid"))
15 model.add(layers.Dense(1, activation="softmax"))
16
17 # compile it
18 model.compile(loss="mean_squared_error",optimizer="sgd",metrics=["accuracy"])
19
20 # train it
21 model.fit(x_train, y_train, epochs=100, batch_size=5)
```

Section 3

Exercise

Exercise 06

https://github.com/idh-cologne-deep-learning/exercise-06