Recap: Embeddings

Represent text data in neural networks

- Map words to indices
- Embeddings
  - Way to represent input data
  - Word2Vec: Concrete method to calculate/train embeddings
  - Well suited as input for neural networks
  - Pre-trained embeddings
    - Easy to use
    - Trained on very large corpora
    - Allow to incorporate some kind of knowledge into our own models that we don't have to annotate

Hausaufgabe 5

Designen und trainieren Sie ein neuronales Netzwerk, um die vorher benutzten handgeschriebenen Ziffern zu erkennen. Fügen Sie dabei einige selbstgeschriebene Ziffern in den Datensatz ein.

UNIVERSITÄT ZU KÖLN

Machine Learning: Overfitting & Sequence Labeling

VL Sprachliche Informationsverarbeitung

Nils Reiter

nils.reiter@uni-koeln.de

January 11, 2024

Winter term 2023/24

INSTITUT FÜR DIGITAL HUMANITIES

UNIVERSITÄT ZU KÖLN

Section 1

Overfitting

Introduction

- ‘Fitting’: Train a model on data (= “fit” it to the data)
  - Underfitting: The model is not well fitted to the data, i.e., accuracy is low
  - Overfitting: The model is fitted too well to the data, i.e., accuracy is high

Introduction

- 'Fitting': Train a model on data (= "fit" it to the data)
  - Underfitting: The model is not well fitted to the data, i.e., accuracy is low
  - Overfitting: The model is fitted too well to the data, i.e., accuracy is high

Why is overfitting a problem?

Introduction

- ‘Fitting’: Train a model on data (= “fit” it to the data)
  - Underfitting: The model is not well fitted to the data, i.e., accuracy is low
  - Overfitting: The model is fitted too well to the data, i.e., accuracy is high

Why is overfitting a problem?

- We want to the model to behave well “in the wild”
- It needs to generalize from training data
- If it is overfitted, it works very well on training data, and very badly on test data

Intuition

$\simeq$ Learning by heart

Example

- Learning by heart gets you through the test
  - I.e., systems achieve high performance

Intuition

$\simeq$ Learning by heart

Example

- Learning by heart gets you through the test
  - I.e., systems achieve high performance
- You are unable to apply your knowledge to situations not exactly as in the test
  - I.e., system performance is lower in the wild

Intuition

≃ Learning by heart

Example

- Learning by heart gets you through the test
  - I.e., systems achieve high performance
- You are unable to apply your knowledge to situations not exactly as in the test
  - I.e., system performance is lower in the wild

Real-World Examples

- Collection of real-world examples of overfitting: `https://stats.stackexchange.com/questions/128616/whats-a-real-world-example-of-overfitting`

Real-World Examples

- Collection of real-world examples of overfitting: `https://stats.stackexchange.com/questions/128616/whats-a-real-world-example-of-overfitting`
- Machine learning for COVID-19 detection on chest scans Roberts et al. (2021)
  - "none of the models identified are of potential clinical use due to methodological flaws and/or underlying biases" Roberts et al. (2021, 200)
  - "Using a public dataset alone without additional new data can lead to community-wide overfitting on this dataset. Even if each individual study observes sufficient precautions to avoid overfitting, the fact that the community is focused on outperforming benchmarks on a single public dataset encourages overfitting." Roberts et al. (2021, 212)

Overfitting and Neural Networks

⚠ Overfitting is not a purely technical problem – no purely technical solution

Classical machine learning

- Feature selection can avoid relying on irrelevant features
- But this is only one source for overfitting

Overfitting and Neural Networks

⚠ Overfitting is not a purely technical problem – no purely technical solution

Classical machine learning

- Feature selection can avoid relying on irrelevant features
- But this is only one source for overfitting

Neural networks are overfitting machines

- Layered architecture ⇒ Any relation between x and y can be learned
  - including a fixed set of if/else rules

Techniques against overfitting (besides critical thinking and use of brain)

- Regularization
- Dropout

Section 2

Regularization

Intuition

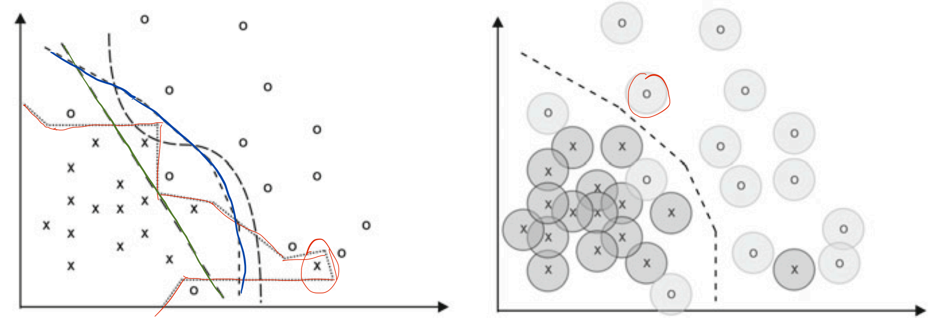


Figure: Visual representation of regularization results (Skansi, 2018, 108)

Formalization

- Formally, regularization is a parameter added to the loss

$$J(\vec{w}) = J_{\text{original}}(\vec{w}) + R$$

L^2-Regularization

L^2-Norm (a. k. a. Euclidean norm) Tikhonov (1963)

- Given a vector $\vec{x} = (x_1, x_2, \ldots, x_n)$,
  its L^2 norm is $L^2(\vec{x}) = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} = ||\vec{x}||_2$

L^2-Regularization

L^2-Norm (a. k. a. Euclidean norm) Tikhonov (1963)

- Given a vector $\vec{x} = (x_1, x_2, \dots, x_n)$,
  its L^2 norm is $L^2(\vec{x}) = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} = ||\vec{x}||_2$
- In practice, we drop the square root and calculate L^2 norm of the weight vector during training:

$$(||\vec{w}||_2)^2 = \sum_{i=0}^{n} w_i^2$$

L^2-Regularization

L^2-Norm (a. k. a. Euclidean norm) Tikhonov (1963)

- Given a vector $\vec{x} = (x_1, x_2, \ldots, x_n)$,
  its L^2 norm is $L^2(\vec{x}) = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} = ||\vec{x}||_2$
- In practice, we drop the square root and calculate L^2 norm of the weight vector during training:

$$(||\vec{w}||_2)^2 = \sum_{i=0}^{n} w_i^2$$

- Regularization rate λ: Factor that expresses how much we want (another hyperparameter)

$$J(\vec{w}) = J_{\text{original}}(\vec{w}) + \frac{\lambda}{n}||w||_2^2 \qquad \text{with } n \text{ for the batch size}$$

L_2-Regularization

- What does it do?

L_2-Regularization

- What does it do?
  - If weights $\vec{w}$ are large: Loss is increased more
  - Large weights are only considered if the increased loss is “worth it”, i.e., if it is counterbalanced by a real error reduction
  - Small weights are preferred

Implementation

- In Keras, most layers support additional arguments for regularization:
  - `kernel_regularizer`, `bias_regularizer`, `activity_regularizer`
    - Applied to weights, constant term, neuron output (= result of activation function)
    - Docs: `https://keras.io/api/layers/regularizers/`

Implementation

- In Keras, most layers support additional arguments for regularization:
  - `kernel_regularizer`, `bias_regularizer`, `activity_regularizer`
    - Applied to weights, constant term, neuron output (= result of activation function)
    - Docs: `https://keras.io/api/layers/regularizers/`
  - Argument value: Regularization function with parameter(s)
    - Layer-specific

Implementation

- In Keras, most layers support additional arguments for regularization:
  - `kernel_regularizer`, `bias_regularizer`, `activity_regularizer`
    - Applied to weights, constant term, neuron output (= result of activation function)
    - Docs: `https://keras.io/api/layers/regularizers/`
  - Argument value: Regularization function with parameter(s)
    - Layer-specific

λ

```
ffnn.add(layers.Dense(5,
  activation="sigmoid",
  activity_regularizer=regularizers.l2(0.2)))
```

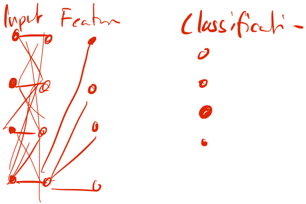
Section 3

Dropout

Dropout

- Regularization: Numerically combatting overfitting
- Dropout: Structurally combatting overfitting Hinton et al. (2012)

Dropout



- Regularization: Numerically combatting overfitting
- Dropout: Structurally combatting overfitting — Hinton et al. (2012)
  - A new hyperparameter $\pi = [0; 1]$
  - In each epoch, every weight is set to zero with a probability of π

[Dropout] prevents complex co-adaptations in which a feature detector is only helpful in the context of several other specific feature detectors. Instead, each neuron learns to detect a feature that is generally helpful for producing the correct answer given the combinatorially large variety of internal contexts in which it must operate.

Hinton et al. (2012, 1)

Dropout

Example

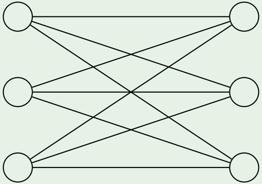


Figure: Dropout $\pi = 0.5$, visualized

Dropout

Example

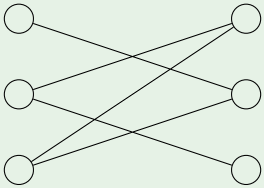


Figure: Dropout $\pi = 0.5$, visualized, Epoch 0

Dropout

Example

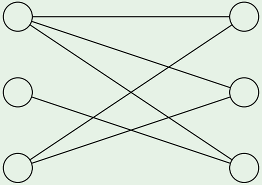


Figure: Dropout $\pi = 0.5$, visualized, Epoch 1

Dropout

Example

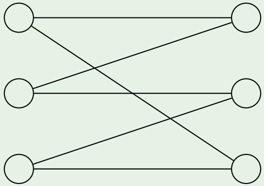


Figure: Dropout $\pi = 0.5$, visualized, Epoch 2

Dropout
Implementation

- Why?
  - Dropout forces the network to learn redundancies
  - Use in the first layers, where features are detected

Dropout

Implementation

- Why?
  - Dropout forces the network to learn redundancies
  - Use in the first layers, where features are detected
- Implementation
  - In Keras, dropout is realized as additional layer
  - Applies to the layer before the dropout layer

```
model.add(layers.Dense(20)) # edges are dropped here
model.add(layers.Dropout(0.5)) # dropout layer (not a real layer though)
model.add(layers.Dense(10)) # no edges dropped
```

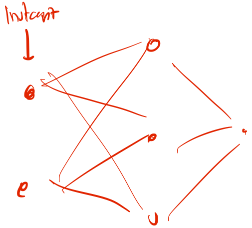
Section 4

Sequence Labeling

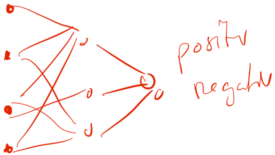
Motivation

- Language works sequentially
    - Word meaning depends on context

Motivation



- Language works sequentially
  - Word meaning depends on context
- Feedforward neural networks
  - One instance at a time
  - E.g., one sentence with four tokens ➔ positive/negative



Motivation

- Language works sequentially
  - Word meaning depends on context
- Feedforward neural networks
  - One instance at a time
  - E.g., one sentence with four tokens ➔ positive/negative
- Conceptually not adequate for natural language
- Length of influencing context varies

Motivation

- Language works sequentially
  - Word meaning depends on context
- Feedforward neural networks
  - One instance at a time
  - E.g., one sentence with four tokens ➔ positive/negative
- Conceptually not adequate for natural language
- Length of influencing context varies
- Recurrent neural networks are one solution to this problem

Sequence Labeling

- So far: Classification
- Sequence labeling
  - Special case of classification
  - Instances are organized sequentially and not independent of each other
    - I.e.: The prediction of a class for one item influences the next

Sequence Labeling

- So far: Classification
- Sequence labeling
  - Special case of classification
  - Instances are organized sequentially and not independent of each other
    - I.e.: The prediction of a class for one item influences the next

Example (Part of speech tagging)

- "the dog barks" $\rightarrow$ "DET NN VBZ"
- Predicting "DET VBZ NN" is extremely unlikely, because verbs usually don't follow determiners

Towards Recurrent Neural Networks

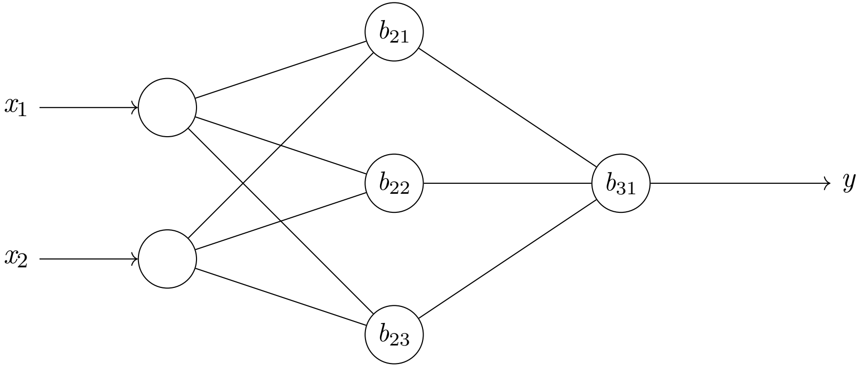


Figure: A feedforward neural network with 1 hidden layer (same picture as before)

Towards Recurrent Neural Networks

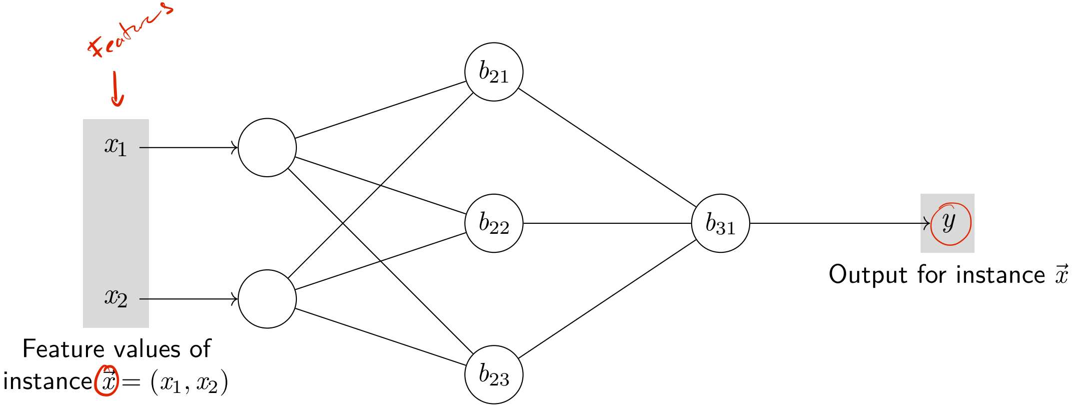


Figure: A feedforward neural network with 1 hidden layer (same picture as before)

Towards Recurrent Neural Networks

To work with sequences, we need to include the sequence into the model

Notation

$X = \boxed{(\vec{X}_1, \vec{X}_2, \ldots)}$ The input data set containing a sequence of instances
(e.g., a sequence of words)

$\vec{X}_i = (x_1, x_2, \ldots)$ One instance with feature values
(e.g., embedding dimensions)

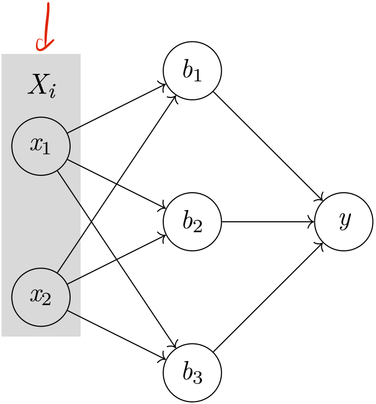
0.5

Y_i Output for instance X_i

X_1	x_1 x_2
X_2	x_1 x_2
X_3	x_1 x_2

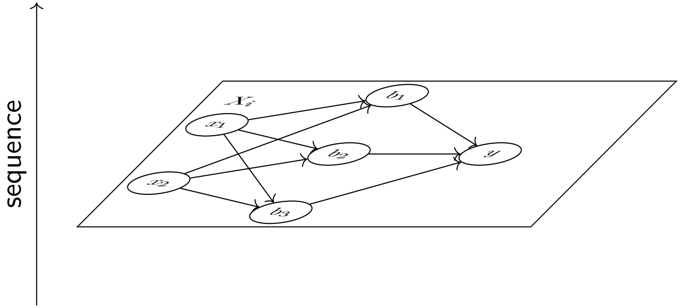
Recurrent Neural Networks

Example



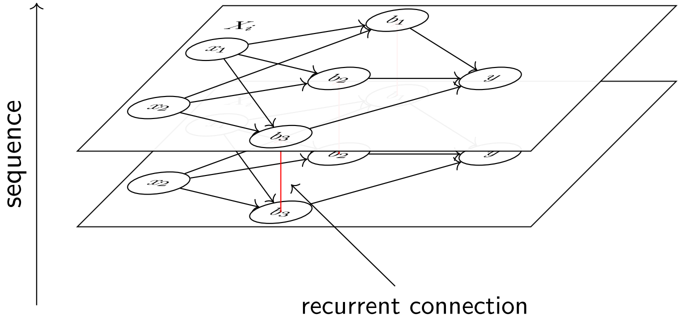
Recurrent Neural Networks

Example



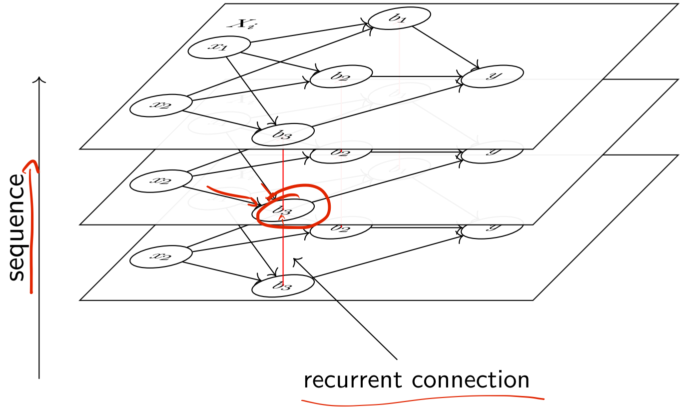
Recurrent Neural Networks

Example



Recurrent Neural Networks

Example



Recurrent Neural Networks

- FFNN, CNN: Weights between neurons
- RNN: Additional weights for recurrent connections

	x_1	x_2	x_3
X_1	0.5		
X_2		0.7	
X_3			-0.8

Recurrent Neural Networks

- FFNN, CNN: Weights between neurons
- RNN: Additional weights for recurrent connections

Input shape

- Before: Network gets at one object at a time, potentially with multiple features
- Now: Network gets sequence of objects at a time, each one potentially with multiple features
- RNN layers need 2D input:
  - Length of input sequences (if needed, padded)
  - Number of features (dimensions)
    - (this is where embeddings would go)
- For training, we need multiple sequences, making the training data 3D

Demo

- Simple task: Learn to count distances
  - Given a sequence of 1s and 0s, predict a 1 two steps after an input-1
  - E.g.: "010010001" becomes "000100100"
  - Model has to learn to count the distance
  - Training data can easily be generated

Demo

- Simple task: Learn to count distances
  - Given a sequence of 1s and 0s, predict a 1 two steps after an input-1
  - E.g.: “010010001” becomes “000100100”
  - Model has to learn to count the distance
  - Training data can easily be generated

demo

Implementation in keras

W → P
W → P
W → P

- `tf.keras.layers.SimpleRNN`
  - Documentation: `https://keras.io/api/layers/recurrent_layers/simple_rnn/`
    Selected parameters:
  - `recurrent_dropout=0.0` Dropout for recurrent links
  - `return_sequences=False` Wether to continue the network with the entire sequence or just the last element

True für SL

```
model.add(layers.SimpleRNN(...))
```

BIO Scheme

- POS-Tagging is easy, because structurally simple: Each token is assigned to one class
- Named entity recognition (and many other tasks) is complicated
  - Not every token is part of a named entity (NE)
  - Many named entities span multiple tokens
  - We distinguish NEs based on the ontological type of the referent
    - PERson, ORGanization, LOCation, ...

BIO Scheme

- POS-Tagging is easy, because structurally simple: Each token is assigned to one class
- Named entity recognition (and many other tasks) is complicated
  - Not every token is part of a named entity (NE)
  - Many named entities span multiple tokens
  - We distinguish NEs based on the ontological type of the referent
    - PERson, ORGanization, LOCation, ...
- BIO scheme
  - How to represent NE annotations token-wise
  - Each token gets a label
    - B: Beginning of a NE
    - I: Inside of a NE
    - O: Outside of a NE (the majority of tokens)

BIO Scheme

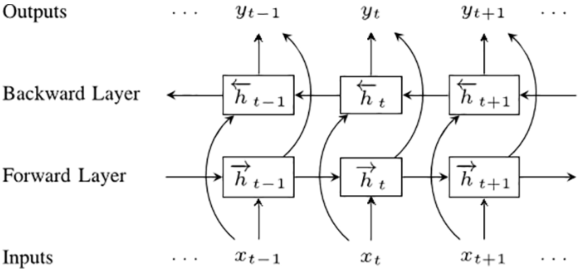
- POS-Tagging is easy, because structurally simple: Each token is assigned to one class
- Named entity recognition (and many other tasks) is complicated
  - Not every token is part of a named entity (NE)
  - Many named entities span multiple tokens
  - We distinguish NEs based on the ontological type of the referent
    - PERson, ORGanization, LOCation, …
- BIO scheme
  - How to represent NE annotations token-wise
  - Each token gets a label
    - B: Beginning of a NE
    - I: Inside of a NE
    - O: Outside of a NE (the majority of tokens)
- Why B: Marking the beginning allows to recognize multiple multi-word NEs in direct sequence
  - "…hat Peter Paulus Maria Müller geküsst" → "O B-PER I-PER B-PER I-PER O"

Directions

- In a regular RNN, the sequence is processed in one direction
- Simple extension: two recurrent layers for both directions

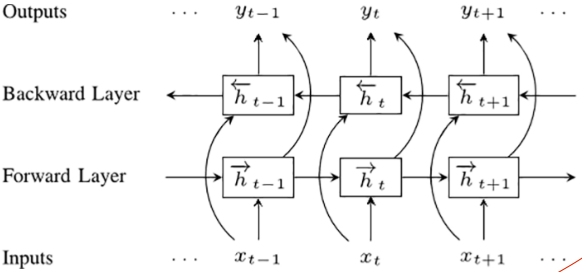
Directions

- In a regular RNN, the sequence is processed in one direction
- Simple extension: two recurrent layers for both directions



Directions

- In a regular RNN, the sequence is processed in one direction
- Simple extension: two recurrent layers for both directions



B

```
model.add(layers.Bidirectional(layers.SimpleRNN(...)))
```

Section 5

Summary

Summary

Sequence Labeling

Overfitting

- Bla