Welcome to INFO216:
Knowledge Graphs
Spring 2022

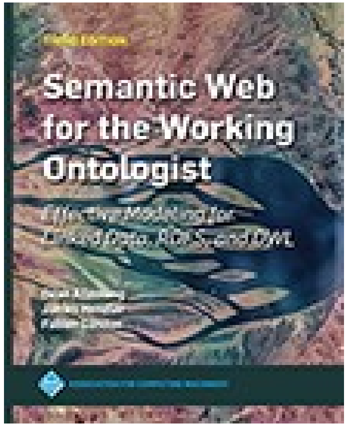
Andreas L Opdahl
<Andreas.Opdahl@uib.no>

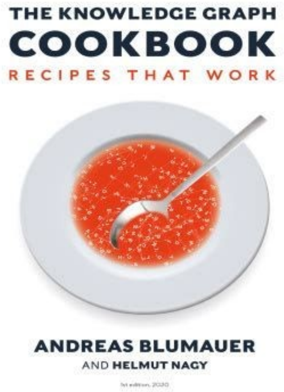
Session 12: Graph embeddings

- Themes:
  - *KGs and machine learning (ML)*
  - *what are embeddings?*
    - word embeddings
    - how to find and use them
    - other types of embeddings
  - *what are graph embeddings?*
    - how to find them...
    - ...and what to use them for

Readings

- Material at http://wiki.uib.no/info216:
  - Introduction to Machine Learning
  - Introduction to Word Embeddings
  - Introduction to Knowledge Graph Embeddings
- Supplementary (links in the wiki):
  - Mikolov et al's original word2vec paper
  - Bordes et al's original TransE paper
  - TorchKGE documentation (for the labs):
    - https://torchkge.readthedocs.io/en/latest/index.html





KGs and
Machine Learning (ML)

What are the connections?

- *Knowledge graphs are well matched with machine learning!*
- Preparing inputs to ML (varying origins, formats, modalities…)
  - also managing outputs from ML
- Infusing world knowledge into ML
  - common sense knowledge, world knowledge (domain and general), …
- As a native ML technique

A micro-introduction to machine learning (ML)

- Sole purpose: to be able to understand and use KG embeddings
- *How to make computers do useful things based on examples (training data)*
  Supervised learning:
  - training materials comprise input-output value pairs as examples
- *Unsupervised learning:*
  - training materials comprise only input examples
- Several other variants: *semi-supervised, reinforcement learning*, …
- Learning KG (and other) embeddings is *unsupervised*

Train, evaluate, and test

- Training examples can be split in three:
  - *training data* are used to train the model
  - *validation data* are used to optimise hyper-parameters and monitor progress
  - *test data* are used only for final evaluation
  - 60%-20%-20% or 80%-10%-10% split is common
    - also minimum requirements for test examples
- *k-fold cross-validation:*
  - training and validation data are split in *k* folds
  - *k-1* folds are used for training, *1* for validation
  - repeated *k* times for each validation fold
  - finally, the measures are averaged

Epochs and batches

- We can go through the training data many times
  - each time is an *epoch*
- We can go through the training examples in groups
  - each group is called a *batch*
- Each example creates a *loss*
- So:
  - training consists of many epochs
  - each epoch consists of many batches
  - each batch consists of many training examples
  - each training example creates a loss
  - after each batch, steps are taken to minimise future loss

Evaluation measures

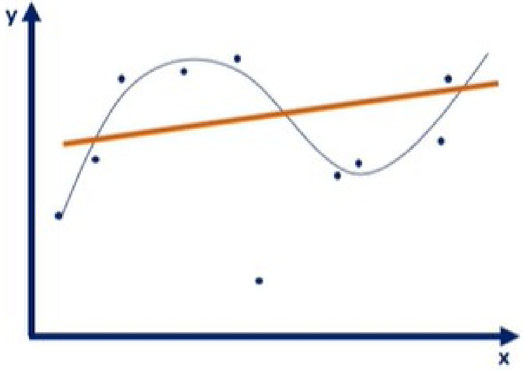
- Results without ranking:
  - *accuracy (A):* ratio of correct results
  - there are lots of others:
    - precision (P), recall (R), F1 = 2PR/(P+R), ...
- Ranked results:
  - *Hit@n:* number of correct results in the "top n", e.g., Hit@10
  - *Mean Rank*: average rank of the correct results
  - *Mean Reciprocal Rank (MRR):* average inverse rank of the correct results, example:
    - the correct results have rank 1, 3, 28
    - MRR = (1/1 + 1/3 + 1/28) / 3
- Other measures for other data types, e.g., time series data

Under- and overfitting

- Underfitting:
  - we have not trained for long enough, too few epocs
  - there is more to learn from the training data
  - high loss, weak validation measures
- Overfitting:
  - we have trained for too long, too many epocs
  - the model has specialised on the training data
  - low loss, weak validation measures

Underfitting and overfitting

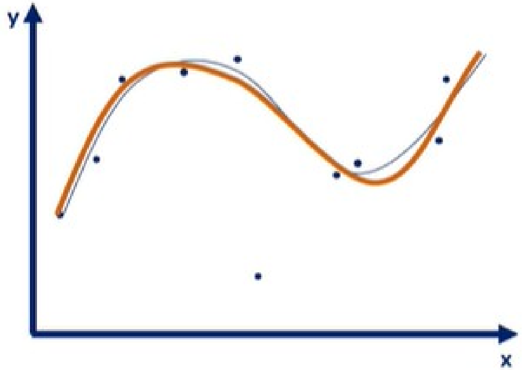
An **underfitted** model



Doesn't capture any logic

- High loss
- Low accuracy

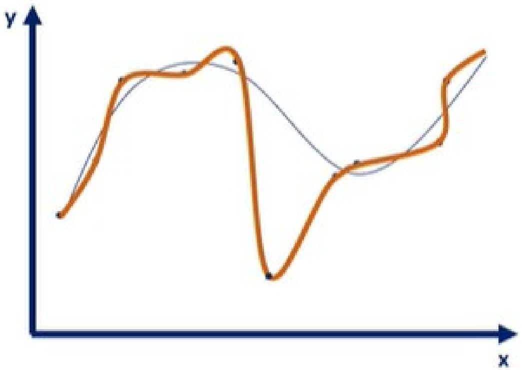
A **good** model



Captures the underlying logic of the dataset

- Low loss
- High accuracy

An **overfitted** model



Captures all the noise, thus "missed the point"

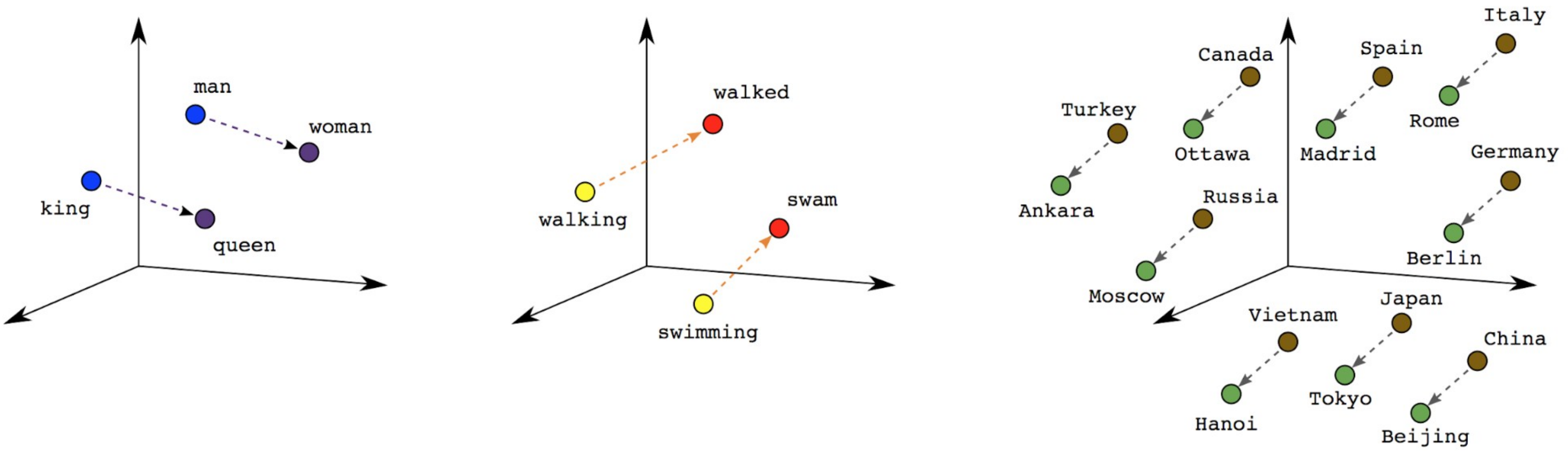
- Low loss
- Low accuracy

https://365datascience.com/tutorials/machine-learning-tutorials/overfitting-underfitting/

What are embeddings?

How can we represent the meaning of words?

- By designation (e.g., textual descriptions in a dictionary)
- As nodes in a network (e.g., in WordNet or a knowledge graph)
- Formally (e.g., adding axioms to)
- As *vectors* in a *latent semantic space*!



Male-Female Verb Tense Country-Capital

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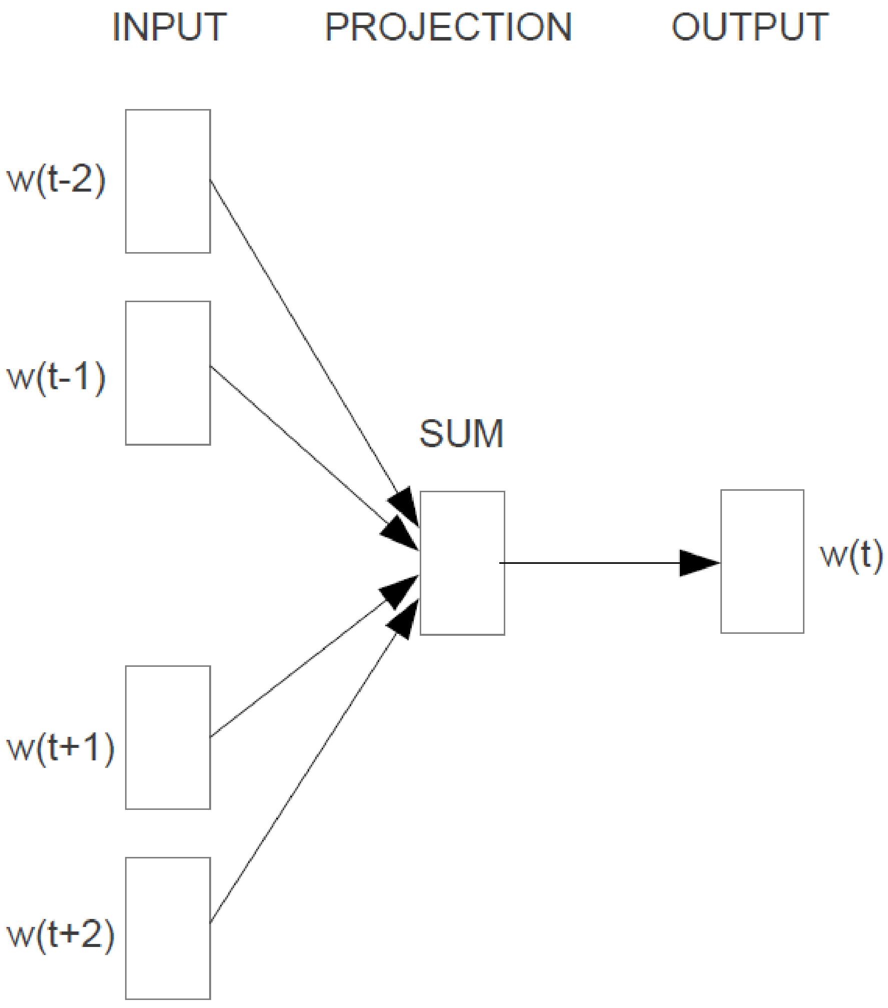
- As *vectors* in a *latent semantic space*!
  - [0.01 0.62 0.03 … 0.41]
  - similar words are close to one another
  - relative positions between words can be systematic
    - [Paris] – [France] + [Italy] ≈ [Rome]
  - distances between words can represent relations
    - [J. K. Rowling] + [influenced by] ≈ [J. R. R. Tolkien]
- Important use: as inputs to deep neural networks that process NL text

How to learn the vectors?

- CBOW (Continuous Bag of Words):
  - part of *word2vec*
  - neural network with one hidden layer
  - trained on large corpus of NL text (1.6 billion words)
  - input examples: sentences with one word missing
  - expected output: the missing word
  - the weights in the neural network are used as word vectors
- Also: Skip-gram, GloVe, FastText, …
- Ubiquitous as *inputs to deep neural networks that process NL text*



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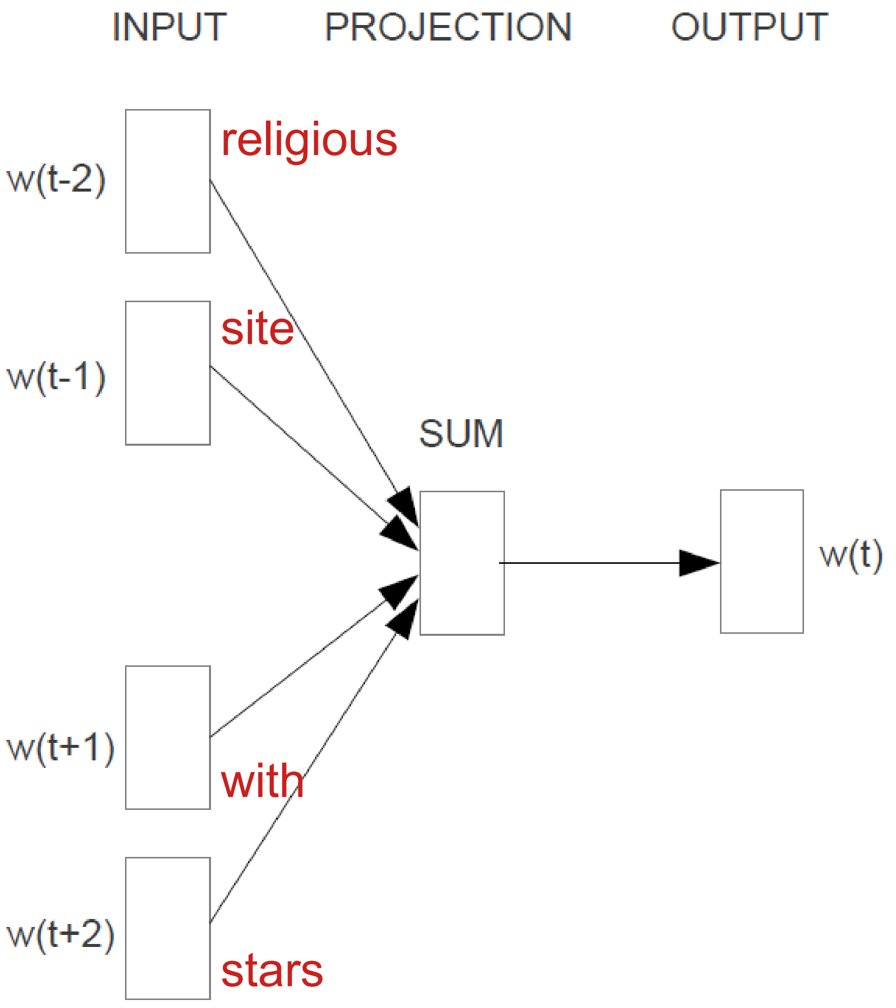

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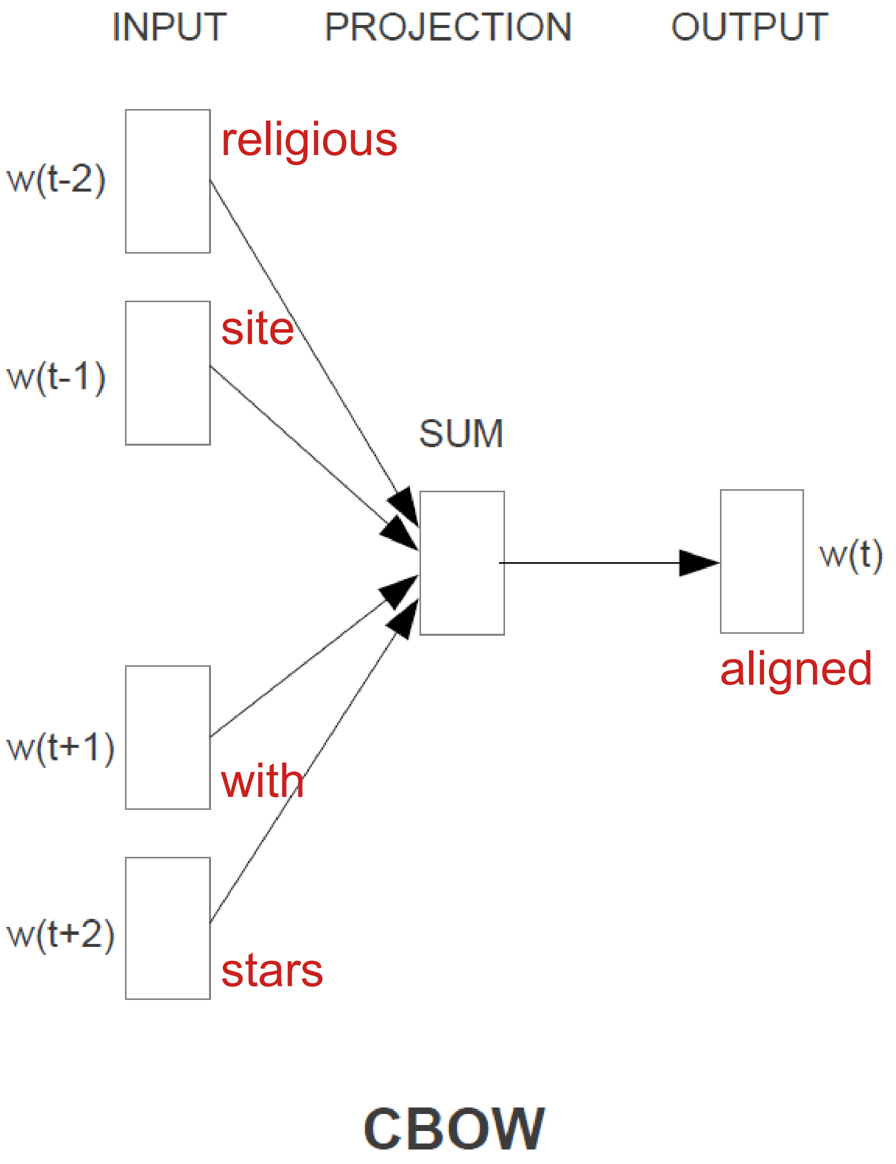
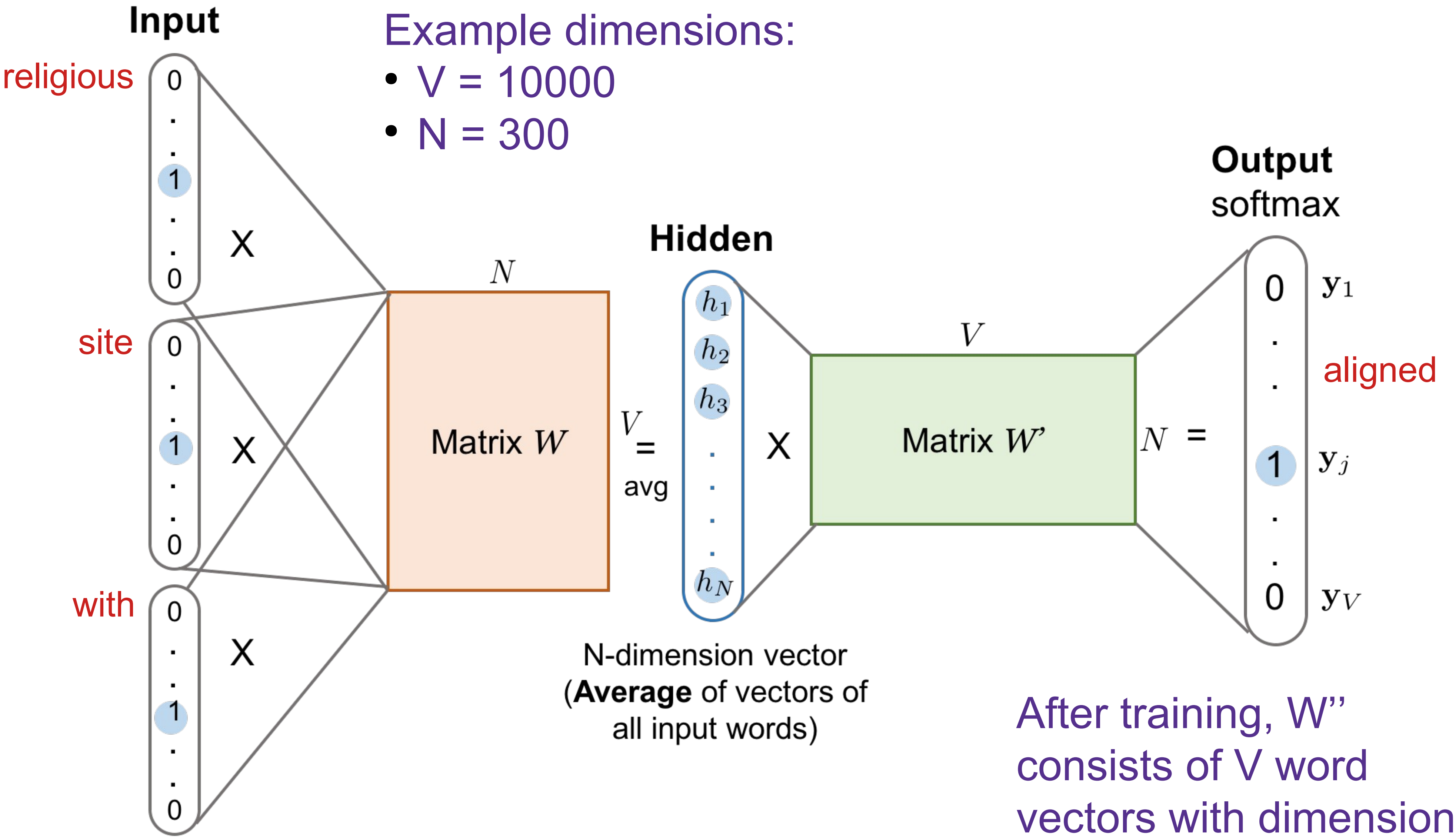


Example dimensions:

- V = 10000
- N = 300



After training, W''
consists of V word
vectors with dimension N

Word similarity

- Extremely powerful and much used, *but be careful*
- The distributional hypothesis:
  - "words that occur in the same contexts tend to have similar meanings" (Harris 1954)
  - hence, word similarity can be measured in terms of vector similarity
  - *this is not true in general*
    - synonyms will often appear close to the same words
    - *but so will many antonyms* ("love", "hate")
  - syntagmatic similarity:
    the words are able to combine in sentences with the same other words
  - paradigmatic similarity:
    the words can be substituted with one another

Other types of embeddings

- The idea has caught on:
  - phrase embeddings (“baseball bat”, “linear algebra”, …)
  - word piece embeddings ([lin-] + [-ear], [al-] + [-ge-]+ [-bra])
- Contextual embeddings (ELMo):
  - how to deal with words that are
    - homonymous (different words that look/sound the same)
    - polysemous (same word form has several meanings)
    - words have different embeddings in different neighbourhoods
- Sentence and paragraph embeddings:
  - transformer models with attention
  - BERT and descendants, e.g., S-BERT
- *Graph embeddings!*

What are graph embeddings?

How can we represent the meaning of graphs?

- By designation (e.g., textual descriptions) of nodes and edges
- By URIs defined in open KGs and standard vocabularies
- Formally (e.g., using description logic)
- As *vectors* in a *latent semantic space*!
  - node vectors
  - edge vectors
  - graph vectors

What can we do with graph embeddings?

- Graph completion and validation:
  - node classification: given a node which type should it have?
  - link prediction: given a node and a edge, what should be at the end?
  - relation prediction: given two nodes, which edge type should link them?
  - triple classification: given two nodes and an edge, is the triple correct?
- Graph (or sub-graph) classification:
  - what type of entity/situation/event does the graph represent?
  - which class does the graph represent?
- Input to deep networks:
  - perhaps in combination with text, images, ...
  - deep multi-stream networks
  - early or late fusion of streams

How to learn the vectors?

- Early and simple example:
  - *Deepwalk* (2014)
- Algorithm:
  1) drop a marker randomly onto a graph node
  2) let the marker traverse the graph randomly along edges for *n* steps
     - additional parameters can guide traversal
  3) treat each resulting walk of *n* nodes as a sentence of *n* words
  4) feed a corpus of *n*-node walks into CBOW or similar
- *Instead of a vector for each word, this produces a vector for each node*
- Limitations:
  - all relations are equal
  - sampling may not fully exploit graph structure

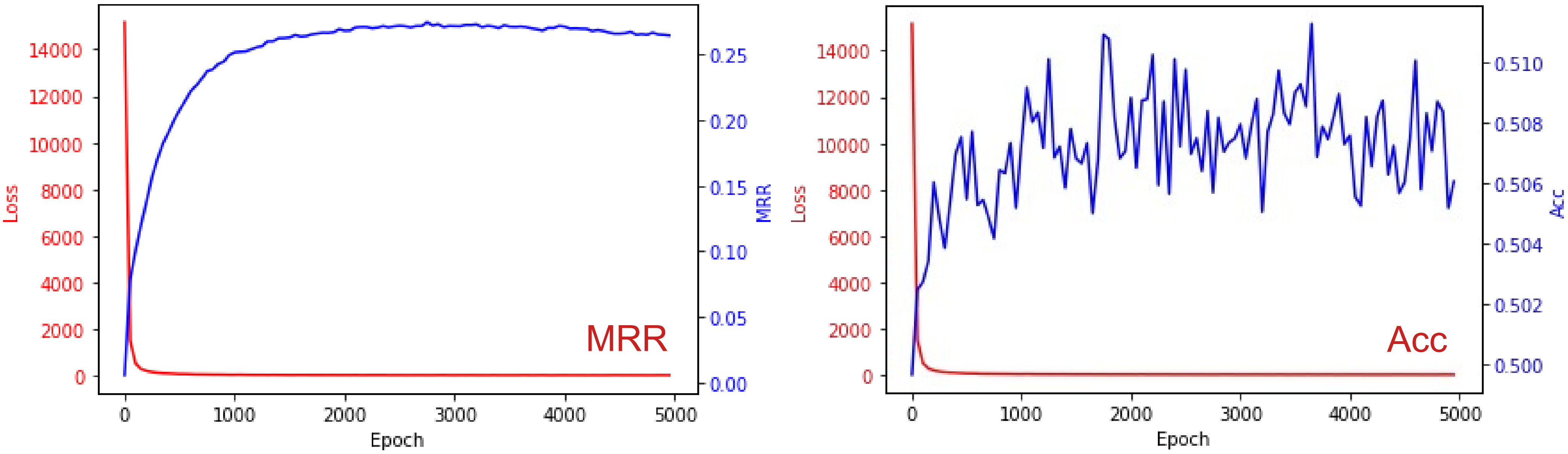
Translational embeddings (TransE)

- The *translational property:*
  - *if* $(h, r, t) \in KG$, *then* $[h] + [r] \approx [t]$
- Approach:
  - start out with random vectors for nodes and edges
  - repeat:
    - for each $(h, r, t) \in KG$, generate corrupted (h', r, t') that is *not* in KG (because either h' or t' is changed)
    - adjust vectors to
      - *minimise* $dist([h] + [r], [t])$
      - *maximise* $dist([h'] + [r], [t'])$
      - loss is $L = \gamma + dist([h] + [r], [t]) - dist([h'] + [r], [t'])$

Evaluation

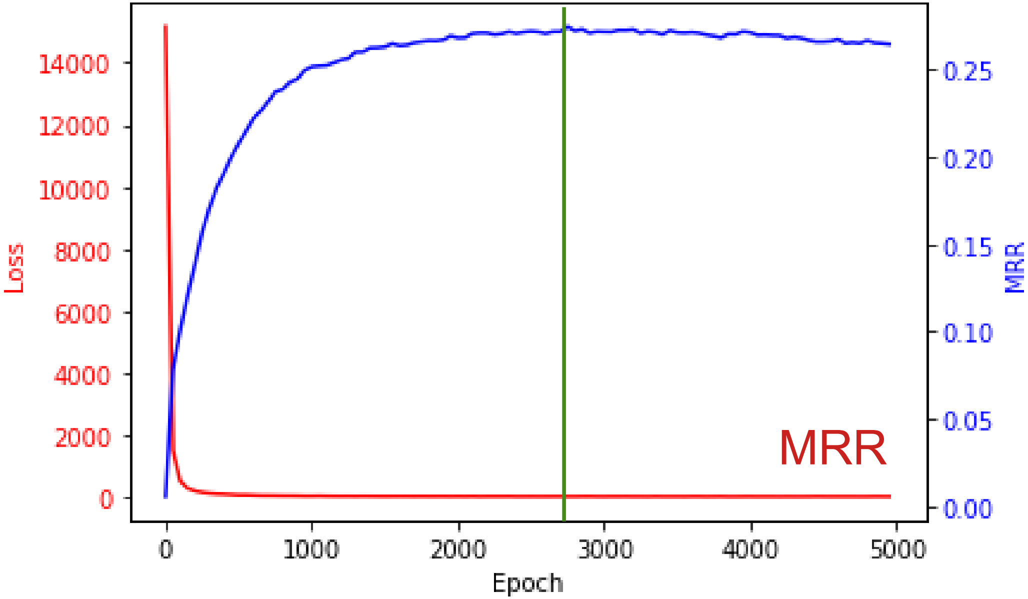
- *Link prediction:*
  - h + r ≈ which t?
  - MRR, Mean Rank, Hit@n (@10).
  - filtered and raw variants
- *Relation prediction:*
  - h – t ≈ which r?
  - MRR, Mean Rank, Hit@n (@10).
  - filtered and raw variants
- *Relation classification:*
  - are (h, t, r) and (h’, t, r’) in KG?
  - accuracy (A)

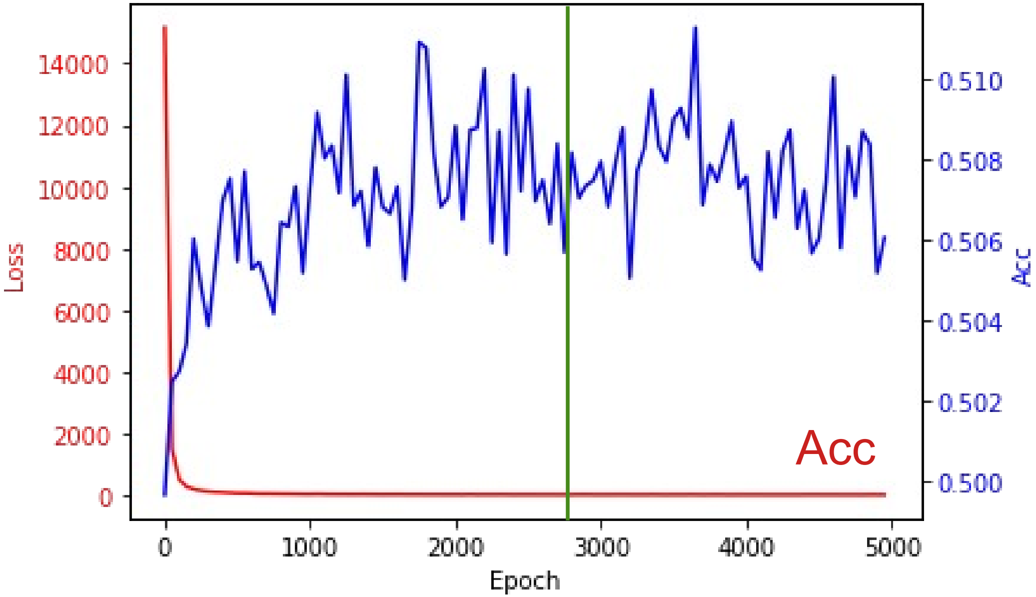
Learning curves



TransE on FB15k237 with 5000 epochs

Learning curves





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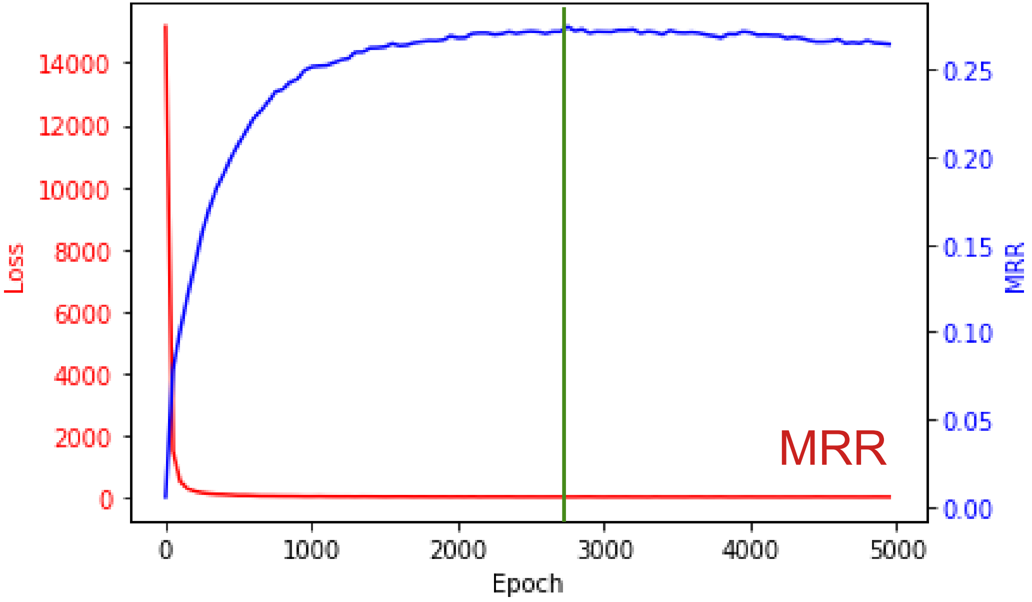
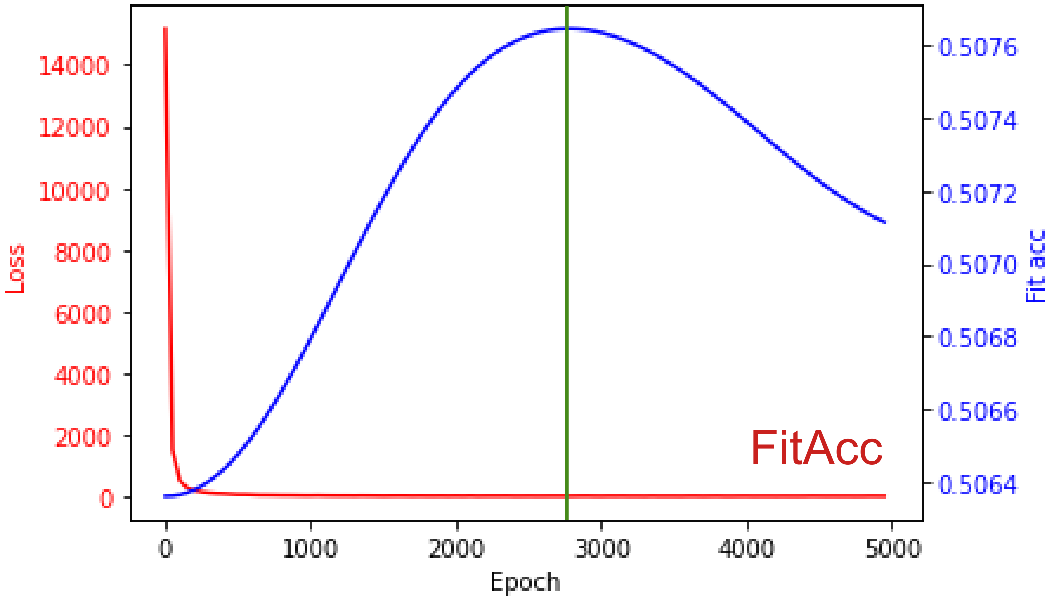
Learning curves





TransE on FB15k237 with 5000 epochs

Datasets and pre-trained models

- Datasets:
  - Freebase extract (FB15k)
  - WordNet synsets (WN)
  - both have problems with training/validation/test overlap:
    - use FB15k237 and WN18RR instead
- Pre-trained models:
  - for example TransE already trained on FB15k237

DATA SET	WN	FB15K	FB1M
ENTITIES	40,943	14,951	1×10^6
RELATIONSHIPS	18	1,345	23,382
TRAIN. EX.	141,442	483,142	17.5×10^6
VALID EX.	5,000	50,000	50,000
TEST EX.	5,000	59,071	177,404

Limitations

- *TransE* is powerful and simple, but has limitations:
  - works best for 1-1 relations
  - trained on corrupted (h’, r, t) and (h, r, t’) variants, but never (h, r’, t)
  - therefore bad on relation prediction
  - several derivations:
    - *TransH, TransR, TransD, TorusE,* …
  - more recent developments:
    - *Graph Neural Netwoks (GNNs)*
    - e.g., *Graph Convolutional Networks (CGNs)*
    - combines ideas from:
      - Convolutional Neural Networks (CNNs)
      - big graph databases

Next week:
Wrapping Up