

# Learning a Disease Embedding using Generalized Word2Vec Approaches.

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Thesis submitted for the degree of  
Master of Science in Engineering:  
Computer Science, specialisation  
Artificial Intelligence

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# Preface

I would like to thank everybody who kept me busy the last year, especially my promotor and my assistants. I would also like to thank the jury for reading the text. My sincere gratitude also goes to my wife and the rest of my family.

*Milan van der Meer*

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# Abstract

The **abstract** environment contains a more extensive overview of the work. But it should be limited to one page.

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# List of Abbreviations and Symbols

## Abbreviations

|      |                            |
|------|----------------------------|
| LoG  | Laplacian-of-Gaussian      |
| MSE  | Mean Square error          |
| PSNR | Peak Signal-to-Noise ratio |

## Symbols

|       |   |
|-------|---|
| 42    | “The Answer to the Ultimate Question of Life, the Universe, and Everything”<br>according to <a href="#">[1]</a> |
| $c$   | Speed of light  |
| $E$   | Energy  |
| $m$   | Mass  |
| $\pi$ | The number pi   |



# Chapter 1

## Introduction

The first contains a general introduction to the work. The goals are defined and the modus operandi is explained.

### 1.1 Lorem Ipsum 4–5

Quisque ullamcorper placerat ipsum. Cras nibh. Morbi vel justo vitae lacus tincidunt ultrices. Lorem ipsum dolor sit amet, consectetur adipiscing elit. In hac habitasse platea dictumst. Integer tempus convallis augue. Etiam facilisis. Nunc elementum fermentum wisi. Aenean placerat. Ut imperdiet, enim sed gravida sollicitudin, felis odio placerat quam, ac pulvinar elit purus eget enim. Nunc vitae tortor. Proin tempus nibh sit amet nisl. Vivamus quis tortor vitae risus porta vehicula.

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### 1.2 Lorem Ipsum 6–7

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Sed commodo posuere pede. Mauris ut est. Ut quis purus. Sed ac odio. Sed vehicula hendrerit sem. Duis non odio. Morbi ut dui. Sed accumsan risus eget odio. In hac habitasse platea dictumst. Pellentesque non elit. Fusce sed justo eu urna porta tincidunt. Mauris felis odio, sollicitudin sed, volutpat a, ornare ac, erat. Morbi quis dolor. Donec pellentesque, erat ac sagittis semper, nunc dui lobortis purus, quis congue purus metus ultricies tellus. Proin et quam. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos hymenaeos. Praesent sapien turpis, fermentum vel, eleifend faucibus, vehicula eu, lacus.

# Chapter 2

## Context

### 2.1 Introduction

In this chapter

Context: Depends on chosen problem (Extracting knowledge from EHR )

Problem: info out of EHR State of the art:

Explain Disease codes DiseaseProgression Explain Danish paper, Matrix group America (recommender), Querying

### 2.2 Electronic Health Records

An electronic health records (EHR) is a collection of data about a patient at a certain point in time. It is stored digitally and thus can be part of a large number of patients over a long time period.

#### 2.2.1 Disease Codes

An important part of EHRs is applying methods which are uniform and well documented. This makes it easy to store and extract data from large-scale databases of EHRs. A part of an EHR consists of the diagnosis of the patient. It provides information about the disease trajectory of the patient and allows analysis on the health situation of a patient. With a uniform system for classifying diseases, it is possible to provide a general picture on health situations of populations.

#### ICD-10

The International Statistical Classification of Diseases and Related Health Problems (ICD) is a medical classification list made by the World Health Organization (WHO). The ICD contains more than 14,400 codes about diseases, disorders, injuries, and other related health conditions. It also provides hierarchical categories for those codes to allow a more general overview of diseases.

## MedDRA

The Medical Dictionary for Regulatory Activities (MedDRA) provides medical terminology in the form of disease codes. It doesn't provide hierarchical categories.

## 2.3 EHR Analytics

EHRs provide a massive amount of data which could be used to create useful insights. Those insights can be offered on an individual level, which means a right intervention to the right patient at the right time. EHR analytics can be used to have a personalized care for patients and benefits the healthcare system by cutting costs and improved outcomes.

In the following sections we talk about current EHR analytic methods.

### 2.3.1 Querying

Analytics on EHRs is still done through querying a database. A specialist can have a certain idea about correlations between conditions or patients. He can support this idea by finding cases in EHRs for example.

This method is based on the knowledge and experience of a specialist. The information has to be actively be sought after and thus a lot of other information is never found. Also complex relations aren't easily found and maybe too subtle to be found by a querying language.

### 2.3.2 Recommender Systems

An EHR of a patient can be transformed into a matrix structure, see figure 2.1. On these matrix structures, feature extraction methods can be applied similar to recommender systems. This can, for example, be done by defining patient similarities. So when a patient is similar to a previous patient, his treatment can be based on previous experiences.

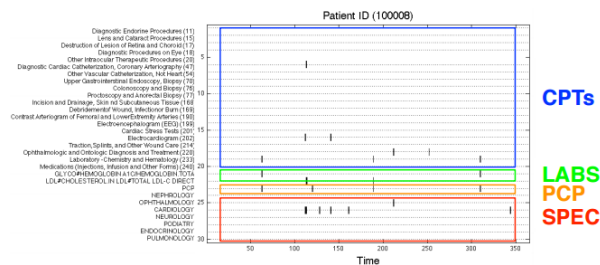


FIGURE 2.1: An example of an EHR transformed into a matrix structure.

### 2.3.3 Statistical Analysis

A combination of statistical methods and graph clustering are applied to obtain disease trajectories. To have any significance using those methods, a large set of EHRs need to be used.

These techniques have been applied to Danish EHRs. The study identifies temporal correlations between pairs of diagnoses. The pairs are further clustered into larger disease trajectories based on the diagnoses they shared. Based on the clusters, patients can be categorized into certain trajectories and retrieve a more personal care. An example of a cluster graph can be found in figure 2.2.

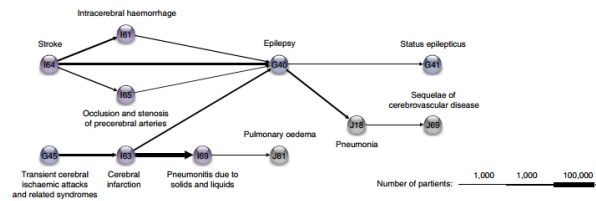


FIGURE 2.2: A cerebrovascular disease trajectory cluster for the Danish population.

<http://www.who.int/classifications/icd/en/>

<http://arxiv.org/pdf/1112.1668v1.pdf>

[https://en.wikipedia.org/wiki/Electronic\\_health\\_record#Technical\\_features](https://en.wikipedia.org/wiki/Electronic_health_record#Technical_features)

[file:///media/milan/Data/Chrome%20Downloads/EHRAnalytics\\_Stateoftheheart%20\(1\).pdf](file:///media/milan/Data/Chrome%20Downloads/EHRAnalytics_Stateoftheheart%20(1).pdf)

<http://www.meddra.org/>

<https://www.siam.org/meetings/sdm13/sun.pdf>

Jimeng Sun, Fei Wang, Jianying Hu, Shahram Edabollahi: Supervised patient similarity measure of heterogeneous patient records. SIGKDD Explorations 14(1): 16-24 (2012)

[https://books.google.co.uk/books?id=eZmjIVtVtucC&pg=PA96&lpg=PA96&dq=querying+ehr&source=AM3VVXy\\_n-&sig=epPrp87M\\_ZixVmikVJKto8IvyIM&hl=nl&sa=X&ved=0ahUKEwjQ3MzouPrLAhXFhQD5I4ChDoAQgbMAA#v=onepage&q=querying%20ehr&f=false](https://books.google.co.uk/books?id=eZmjIVtVtucC&pg=PA96&lpg=PA96&dq=querying+ehr&source=AM3VVXy_n-&sig=epPrp87M_ZixVmikVJKto8IvyIM&hl=nl&sa=X&ved=0ahUKEwjQ3MzouPrLAhXFhQD5I4ChDoAQgbMAA#v=onepage&q=querying%20ehr&f=false)

Towards Heterogeneous Temporal Clinical Event Pattern Discovery: A Convolutional Approach

<http://www.nature.com/ncomms/2014/140617/ncomms5022/pdf/ncomms5022.pdf>

## 2.4 Conclusion

The final section of the chapter gives an overview of the important results of this chapter. This implies that the introductory chapter and the concluding chapter don't need a conclusion.



# Chapter 3

## Background

### 3.1 Introduction

In this chapter

### 3.2 Background Knowledge

We assume a basic knowledge of general computer science concepts as algorithms, statistics, time complexity, linear algebra, basic graph theory, optimization, and heuristics.

#### 3.2.1 Machine Learning

Machine learning is a data driven approach with as goal to build a model which can be used to make predictions or decisions. This task is done by algorithms which are able to learn models based on examples given by the designer. In machine learning there are 3 types of problems, namely supervised learning, unsupervised learning, and reinforcement learning.

Supervised learning is concerned with the learning task where there are examples given with their corresponding label. Unsupervised learning is similar to supervised learning only no labels are given. We won't go into reinforcement learning.

We can also classify to problems according to the desired output of our model. Those main tasks consist of classification, regression, clustering, and dimension reduction.

#### 3.2.2 Time Series Analysis

A time series consists of data points over a certain time period. We refer to this as a sequence of states. Where a state represents a data point and can differ from a single value to more complex representations like pictures.

The domain of time series analysis handles around extracting information or relations from a time series. It can have different goals like forecasting, classification, or exploratory.

### 3.2.3 Neural Networks

A neural network is a machine learning approach based on biological neural networks.

#### Perceptron

The basic component of a neural network is a perceptron. A perceptron take multiple binary inputs and has a single binary output (see figure 3.1). Each input has a corresponding real numbered weight. The output is decided on the following equation:

$$output = \begin{cases} 0 & \text{if } \sum_j w_j x_j \leq \text{threshold} \\ 1 & \text{if } \sum_j w_j x_j > \text{threshold} \end{cases} \quad (3.1)$$

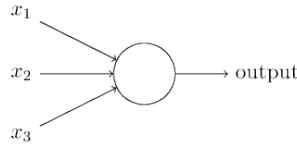


FIGURE 3.1: A simple presentation of a perceptron.

We can build a network by connecting multiple perceptrons (see figure 3.2. By building these networks, more complex decisions can be made.

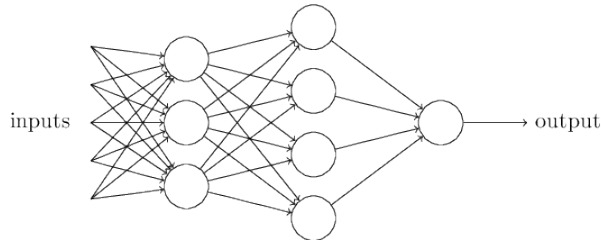


FIGURE 3.2: A more complex network made by connecting multiple perceptrons.

Now we have seen how a general network is constructed, we look at some vocabulary.

In figure 3.3, we see a four-layer network. As mentioned on the figure, we call the first layer the input layer, the last layer the output layer, and the layers in between are called hidden layers. Sometime multiple layer networks are referred to as multilayer perceptrons or MLPs.



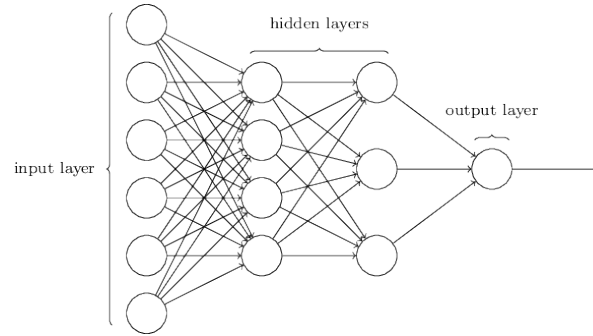


FIGURE 3.3: General vocabulary for a multilayer network.

### Training a network

To train a neural network, we input an example with a known label. The network will have a certain output based on the current weights. When this output is incorrect, it should be possible to adjust the weights with as effect that the network now has as output the correct label. Of course, this change in weights, should only effect the output by a small bit (see figure 3.4). The reason for this is that otherwise all the previous images could now be labeled incorrectly. So, the concept of training a neural network means, adjusting the weights in a way that the behavior of the network doesn't change completely on the previous seen pictures but that the current picture is labeled correctly.

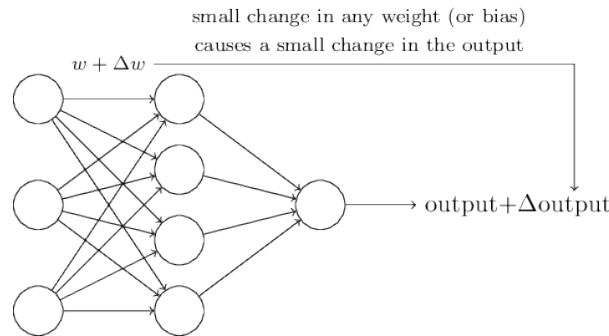


FIGURE 3.4: A small change on the weights, only has a small impact on the output.

To achieve this effect, we change our known perceptrons to sigmoid neurons. A sigmoid neuron has the same basics as a perceptron. It still has inputs but now it also has a bias  $b$ . The inputs still have weights but the weights can now range between 0 and 1. The output is now calculate with  $\sigma(w * x + b)$  where  $\sigma$  is the sigmoid function. This results in the following formula:

$$\frac{1}{1 + \exp(-\sum_j w_j x_j - b)} \quad (3.2)$$

### 3. BACKGROUND

---

The sigmoid function makes it possible to calculate the gradient and makes the output a linear combination of  $\Delta w_j$  and  $\Delta b$  as  $\Delta output$  is approximated by

$$\Delta output \approx \sum_j \frac{\partial output}{\partial w_j} \Delta w_j + \frac{\partial output}{\partial b} \Delta b \quad (3.3)$$

Because of the linearity, it is now possible to choose changes for the weights and biases to achieve a correct output. By adjusting the weights, we will train our network to achieve a higher accuracy.

#### 3.2.4 Backpropagation

Backpropagation is an algorithm which is used to train neural networks. It calculates the gradient of a chosen loss function with respect to the individual weights. With the gradient, the weights are updated and the loss function is minimized.

##### Terminology

We use  $w_{jk}^l$  to denote the weight corresponding to the connection between the  $k^{th}$  node in the  $(l-1)^{th}$  layer to the  $j^{th}$  node in the  $l^{th}$  layer. We use  $b_j^l$  for the bias of the  $j^{th}$  node in the  $l^{th}$  layer and  $a_j^l$  for the activation of the  $j^{th}$  node in the  $l^{th}$  layer. See figure 3.5.

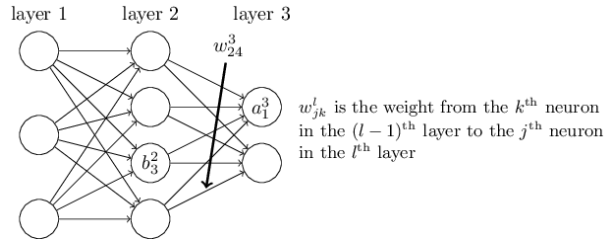


FIGURE 3.5: Visual representation of the terminology for a neural network.

We can now convert these notation to a vector representation. We remove the indexes for the node numbers which results in the following:

$$a^l = \sigma(w^l a^{l-1} + b^l) \quad (3.4)$$

##### Cost function

AS mentioned before, backpropagation has as goal to calculate the partial derivatives of the cost function  $C$  with respect to each weight and bias.

The cost function has to fulfill certain criteria. The first one is that it needs to be possible to write it as a summation over cost functions for individual training examples. Secondly, it needs to be derivable. And lastly, the cost function is a function of the activations of the last layer.

### Fundamental equations

Backpropagation has 4 equations. They allow us to calculate the error for each node and adjust the weights based on the gradient descent.

First we calculate the error of each node which is based on how much the cost function is influenced by each activation and on how much the activation function is influenced by  $z_j^L$ :

$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L) \text{ with } z_j^L = \sum_k w_{jk}^L a_k^{L-1} + b_j^L \quad (3.5)$$

This can be written as a neat vector equation:

$$\delta^L = (a^L - y) \circ \sigma'(z_j^L) \quad (3.6)$$

The next equation explains why the algorithm is called backpropagation. The equation calculates each layers error vector based on the layer after it, it propagates the error back over the layers:

$$\delta^l = ((w^{l+1})^T \delta^{l+1}) \circ \sigma'(z_j^L) \quad (3.7)$$

With those 2 equations we calculate the error in each layer of the neural network. Those errors can be used to calculate the derivatives of the cost function with respect to the weights and the biases:

$$\frac{\partial C}{\partial w_{jk}^l} = a_k^{l-1} \delta_j^l. \quad (3.8)$$

$$\frac{\partial C}{\partial b_j^l} = \delta_j^l. \quad (3.9)$$

When the derivatives are calculated, we can apply the gradient descent and update the weights and biases accordingly. This process represents the learning of a neural network.

<http://neuralnetworksanddeeplearning.com/chap1.html>

## 3.3 Word2Vec

### 3.3.1 Motivation

In natural language processing tasks, a good representation of words helps learning algorithms perform better. A representation is learned which maps words to vectors in a low-dimensional space compared to the vocabulary size. In this representation, we try to map context-similar words close to each other in the new vector space. We could say in an informal way: a linguistic background is made which the learning algorithm can use.

### 3.3.2 Skip-gram

One way of learning a word2vec representation of a corpus  $Text$ , is by using the skip-gram model.

Based on given words  $w$  and their contexts  $c$ , we set the parameter  $\theta$  of  $p(c|w; \theta)$  to maximize:

$$\arg \max_{\theta} \prod_{(w,c) \in D} p(c|w; \theta) \quad (3.10)$$

with  $D$  the set of all word and context pairs we extract from the corpus.

#### Finding word-context pairs

Given a sequence of words, we define their context based on n-gram. In figure 3.6, n-gram is explained on the sentence "This is a sentence".

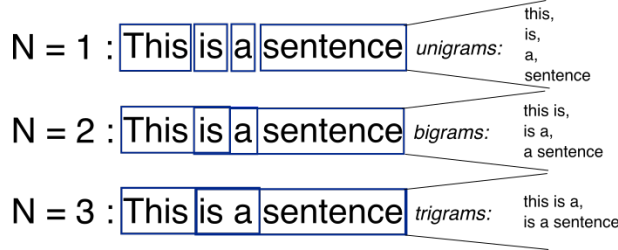


FIGURE 3.6: Explanation of n-gram.

For the Skip-gram model, we define the context of a word  $w_t$  as  $w_{t+j}$  with  $j$  between  $-c$  and  $c$ . A larger  $c$  results in more training examples and thus can lead to a higher accuracy but will have a longer training time.

#### Parameterization

We start with rewriting the conditional probability using soft-max:

$$p(c|w; \theta) = \frac{e^{v_c * v_w}}{\sum_{c' \in C} e^{v_{c'} * v_w}} \quad (3.11)$$

where  $v_c$  and  $v_w$  are vector representations for  $c$  and  $w$ , and  $C$  is the set of all available contexts. This means that the parameters  $\theta$  are  $v_{c_i}$  and  $v_{w_i}$ . Computing the optimal parameters is very expensive because you need to calculate this over all contexts  $c'$ . We also switch from product to sum by taking the logs:

$$\arg \max_{\theta} \sum_{(w,c) \in D} \log p(c|w; \theta) = \sum_{(w,c) \in D} (\log e^{v_c * v_w} - \log \sum_{c'} e^{v_{c'} * v_w}) \quad (3.12)$$

### 3.3.3 Negative Sampling

To compute the vectors using the Skip-gram model more efficiently, we introduce negative sampling.

Instead of calculating  $\sum_{c' \in C} e^{v_{c'} * v_w}$  over all contexts, we make a set  $D'$  which consists of randomly sampled word-context pairs. With this new set, we remove the costly term  $\sum_{c' \in C} e^{v_{c'} * v_w}$  and replace it with  $\sum_{(w,c) \in D'} e^{v_{c'} * v_w}$ .

In a less formal way: we are not making sure that if words appear in the same context, their vectors are more similar than all the other word vectors, but only of several vectors chosen randomly. This makes the Skip-gram model usable in terms of speed.

### 3.3.4 Neural Networks

When the word2vec algorithm is trained using the Skip-gram model, one will have a lookup table. This table contains the mapping of words to their vector representation. This lookup table can be found by training a 2-layer neural network with as goal function the function described in the previous section. The training can be done with Gradient Descent for example.

The trained 2-layer neural network can be placed in front of another neural network. It will convert the words to their vector representation and feed into the next neural network. It is empirically shown that this can improve the results of the neural network by putting the lookup table in front of it. As mentioned before, in a way, you offer background knowledge to the neural network.

<http://papers.nips.cc/paper/5021-distributed-representations-of-words-and-phrases-and-their-compositionality.pdf>

<http://arxiv.org/pdf/1402.3722v1.pdf>

<http://colah.github.io/posts/2014-07-NLP-RNNs-Representations/>

[http://homepages.inf.ed.ac.uk/ballison/pdf/lrec\\_skipgrams.pdf](http://homepages.inf.ed.ac.uk/ballison/pdf/lrec_skipgrams.pdf)

<http://recognize-speech.com/images/Antonio/Unigram.png>

<http://stackoverflow.com/questions/27860652/word2vec-negative-sampling-in-layman-term>

## 3.4 DeepWalk

DeepWalk is an approach where graph structured data is transformed into sequences of vertices. Word2vec is then applied on those sequences to learn a good vector representation for the vertices.

In figure 3.7, we see an overview of the DeepWalk algorithm. It exist of two parts.

---

**Algorithm 1** DEEPWALK( $G, w, d, \gamma, t$ )

---

**Input:** graph  $G(V, E)$   
 window size  $w$   
 embedding size  $d$   
 walks per vertex  $\gamma$   
 walk length  $t$

**Output:** matrix of vertex representations  $\Phi \in \mathbb{R}^{|V| \times d}$

- 1: Initialization: Sample  $\Phi$  from  $\mathcal{U}^{|V| \times d}$
- 2: Build a binary Tree  $T$  from  $V$
- 3: **for**  $i = 0$  to  $\gamma$  **do**
- 4:    $\mathcal{O} = \text{Shuffle}(V)$
- 5:   **for each**  $v_i \in \mathcal{O}$  **do**
- 6:      $\mathcal{W}_{v_i} = \text{RandomWalk}(G, v_i, t)$
- 7:     SkipGram( $\Phi, \mathcal{W}_{v_i}, w$ )
- 8:   **end for**
- 9: **end for**

---

FIGURE 3.7: Overview of the DeepWalk algorithm.

First a random walk generator. For each vertex  $v_i$  of the graph  $G$ , it will generate a random walk of length  $t$ . It will do this  $\gamma$  times but the order to which the vertices are traversed, is randomly ordered each pass. With those walks, a sequence of vertices is generated.

Secondly, those vertices are used for word2vec. This process is explained in section 3.3.

<http://arxiv.org/pdf/1403.6652v2.pdf>

### 3.5 Conclusion

The final section of the chapter gives an overview of the important results of this chapter. This implies that the introductory chapter and the concluding chapter don't need a conclusion.

## Chapter 4

# Future Work

### 4.1 Introduction

In this chapter

Normalisation Mapping Disease Codes Distributed RNN

### 4.2 Generalization

### 4.3 Distributed Word2Vec

MapReduce

### 4.4 Classification Patients

As mentioned in section 3.3, a trained 2-layer neural network can be placed before another neural network and function as a lookup table. In this section, we discuss a possible neural network which allows us to further investigate the effectiveness of our word2vec approach to classify patients.

#### 4.4.1 Problem Definition

The medical history of a patient is seen as a time series with as datapoints an EHR. Based on the time series, we want to classify it into different disease trajectories. A patient who is classified into a specific disease trajectory, can be treated more specifically.

The medical data of multiple patients is a 3 dimensional tensor, see figure 4.1. This data structure is the input structure for a neural network.

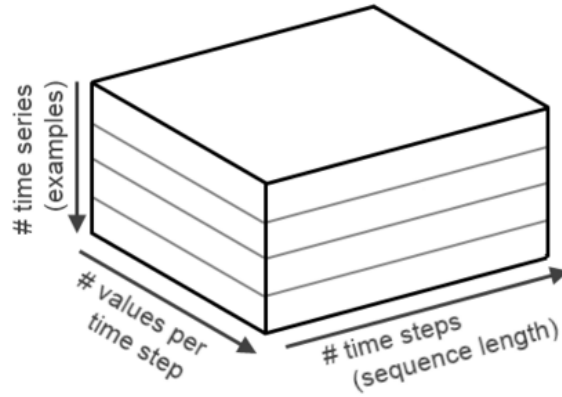


FIGURE 4.1: Overview of the data structure for medical data with a time aspect.

Medical data has some problems which we will discuss. It often consists of long time periods. This means there could be a long range of dependencies between events. In the context of training neural networks, this can cause a problem known as the vanishing gradient problem. Patients don't have regular intervals in their medical data. The irregular intervals need to be transformed to regular intervals otherwise the time aspect won't be consistent throughout the data. The standardization of the attributes needs to be taken into account. Preferably some sort of normalization should be applied as well. Medical data has a high dimensionality. A lot of parameters need to be taken into account to retrieve accurate results. This causes the well known problem: Curse of Dimensionality. It causes the data to be sparse and therefore, more data is needed. Especially in medical data where outliers are important.

### 4.4.2 Approach

Vanishing gradient padding Word2Vec standardization Recurrent -> high dimension

### 4.4.3 Neural Network

We mentioned the reasons on why we choose a Long Short Term Memory (LSTM) approach as a recurrent neural network solution. In this section we explain in more detail why LSTM handles the vanishing problem and long-term dependencies.

First we shortly repeat the structure of a neural network in figure 4.2. We see the input, different layers with their perceptrons, and  $\sigma$  as the activation function.



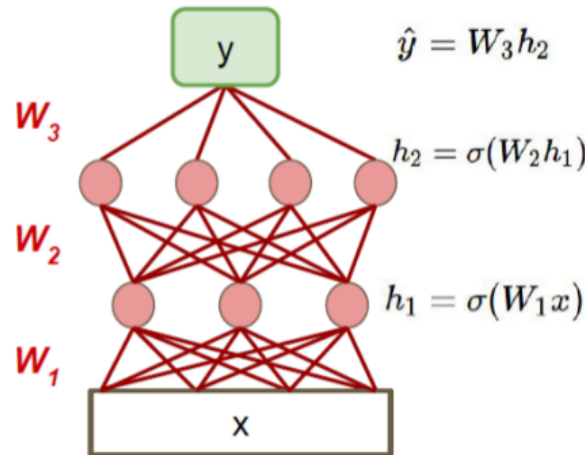


FIGURE 4.2: A general structure of a neural network.

## Recurrent Neural Network

### LSTM

<http://deeplearning4j.org/usingrnns>

Supervised Sequence Labelling with Recurrent Neural Networks

Phenotyping of Clinical Time Series with LSTM Recurrent Neural Networks

IMEC Technical talk by Jaak Simm

Missing covariate data in medical research: To impute is better than to ignore

Recurrent Neural Networks for Missing or Asynchronous Data

Development of a Database of Health Insurance Claims: Standardization of Disease Classifications and Anonymous Record Linkage

Machine Learning Based Missing Value Imputation Method for Clinical Dataset

Modeling Temporal Dependencies in High- Dimensional Sequences: Application to Polyphonic Music Generation and Transcription

Long short-term memory neural network for traffic speed prediction using remote microwave sensor data

Noisy Time Series Prediction using a Recurrent Neural Network and Grammatical Inference

Neural Networks for Time Series Processing Constructing a Non-Linear Model with Neural Networks for Workload Characterization

<http://colah.github.io/posts/2015-08-Understanding-LSTMs>

A Critical Review of Recurrent Neural Networks for Sequence Learning

Bidirectional Recurrent Neural Networks Optimization of Hidden Markov Models and Neural Networks

LONG SHORT-TERM MEMORY

LSTM: A Search Space Odyssey

### 4.5 Conclusion

The final section of the chapter gives an overview of the important results of this chapter. This implies that the introductory chapter and the concluding chapter don't need a conclusion.

## Chapter 5

# Conclusion

The final chapter contains the overall conclusion. It also contains suggestions for future work and industrial applications.

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# Appendices



# Appendix A

## The First Appendix

Appendices hold useful data which is not essential to understand the work done in the master thesis. An example is a (program) source. An appendix can also have sections as well as figures and references<sup>[1]</sup>.

### A.1 More Lorem

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#### A.1.1 Lorem 15–17

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## Appendix B

# The Last Appendix

Appendices are numbered with letters, but the sections and subsections use arabic numerals, as can be seen below.

### B.1 Lorem 20-24

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### B.2 Lorem 25-27

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# Bibliography

- [1] D. Adams. *The Hitchhiker's Guide to the Galaxy*. Del Rey (reprint), 1995.  
ISBN-13: 978-0345391803.

## Master thesis filing card

*Student:* Milan van der Meer

*Title:* Learning a Disease Embedding using Generalized Word2Vec Approaches.

*UDC:* 621.3

*Abstract:*

Here comes a very short abstract, containing no more than 500 words.  $\text{\LaTeX}$  commands can be used here. Blank lines (or the command  $\text{\backslash par}$ ) are not allowed!

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Thesis submitted for the degree of Master of Science in Engineering: Computer Science, specialisation Artificial Intelligence

*Thesis supervisor:* Prof. dr. Roel Wuyts

*Assessors:* Ir. Kn. Owsmuch  
K. Nowsrest

*Mentors:* Ir. An Assistent  
S. Dhooghe