

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 wive and the rest of my family.

Milan van der Meer

Contents

Pr	eface		i		
Al	ostra	ct	iii		
Li	st of	Figures and Tables	iv		
Lis	st of	Abbreviations and Symbols	\mathbf{v}		
1	Intr 1.1	oduction Lorem Ipsum 4–5	1 1		
	1.1	Lorem Ipsum 6–7	1		
2	Background 3				
	2.1	Introduction	3		
	2.2	Background Knowledge	3		
	2.3 2.4	Word2Vec	7 8		
	2.4 2.5	Conclusion	8		
3	The	Final Chapter	9		
	3.1	The First Topic of this Chapter	9		
	3.2	The Second Topic	10		
	3.3	Conclusion	11		
4	Con	Conclusion			
\mathbf{A}	The	First Appendix	17		
		More Lorem	17		
		Lorem 51	18		
В		Last Appendix	19		
		Lorem 20-24	19 20		
Bi	Bibliography				

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 Figures and Tables

List of Figures

2.1	A simple presentation of a perceptron	4
2.2	A more complex network made by connecting multiple perceptrons	4
2.3	General vocabulary for a multilayer network	5
2.4	A small change on the weights, only has a small impact on the output	5
2.5	Visual representation of the terminology for a neural network	6

List of Tables

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" according to [1]

c Speed of light

E Energy

m Mass

 π 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

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1.2 Lorem Ipsum 6–7

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1. Introduction

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Chapter 2

Background

2.1 Introduction

In this chapter

2.2 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.

2.2.1 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.

2.2.2 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.

2.2.3 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 2.1). Each input has a corresponding real numbered weight. The output is decided on the following equation:

$$output = \begin{cases} 0 & \text{if } \sum_{j} w_{j} x_{j} \leq \text{ threshold} \\ 1 & \text{if if } \sum_{j} w_{j} x_{j} > \text{ threshold} \end{cases}$$
 (2.1)

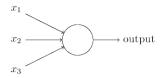


FIGURE 2.1: A simple presentation of a perceptron.

We can build a network by connecting multiple perceptrons (see figure 2.2. By building these networks, more complex decisions can be made.

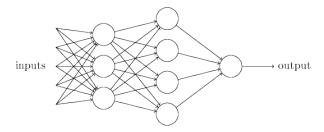


FIGURE 2.2: A more complex network made by connecting multiple perceptrons.

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

In figure 2.3, 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.

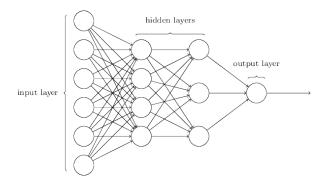


FIGURE 2.3: General vocabulary for a multilayer network.

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 2.4). 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.

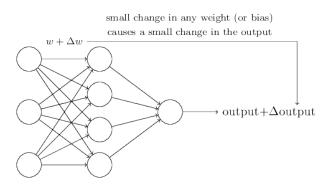


FIGURE 2.4: A small change on the weights, only has a small impact on the output.

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 σ is the sigmoid function. This results in the following formula:

$$\frac{1}{1 + exp(-\sum_{j} w_j x_j - b)} \tag{2.2}$$

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

$$\Delta output \approx \sum_{j} \frac{\partial output}{\partial w_{j}} \Delta w_{j} + \frac{\partial output}{\partial b} \Delta b$$
 (2.3)

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.

2.2.4 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 2.5.

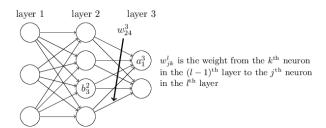


FIGURE 2.5: Visual representation of the terminology for a neural network.

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

$$a^l = \sigma(w^l a^{l-1} + b^l) \tag{2.4}$$

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_i^L :

$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L) \text{ with } z_j^L = \sum_k w_{jk}^L a_k^{L-1} + b_j^L$$
 (2.5)

This can be written as a neat vector equation:

$$\delta^L = (a^L - y) \circ \sigma'(z_i^L) \tag{2.6}$$

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:

$$\delta^l = ((w^{l+1})^T \delta^{l+1}) \circ \sigma'(z_i^L) \tag{2.7}$$

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:

$$\frac{\partial C}{\partial w_{jk}^l} = a_k^{l-1} \delta_j^l. \tag{2.8}$$

$$\frac{\partial C}{\partial b_j^l} = \delta_j^l. \tag{2.9}$$

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

2.3 Word2Vec

2.3.1 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.

2.3.2 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 θ of $p(c|w;\theta)$ to maximize:

$$\underset{\theta}{\arg\max} \tag{2.10}$$

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

2.3.3 Negative-sampling

2.3.4 Neural Networks

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/

2.4 DeepWalk

2.5 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 3

The Final Chapter

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3.1 The First Topic of this Chapter

3.1.1 Item 1

Sub-item 1

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3.3 Conclusion

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Chapter 4

Conclusion

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

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Fusce mauris. Vestibulum luctus nibh at lectus. Sed bibendum, nulla a faucibus semper, leo velit ultricies tellus, ac venenatis arcu wisi vel nisl. Vestibulum diam. Aliquam pellentesque, augue quis sagittis posuere, turpis lacus congue quam, in hendrerit risus eros eget felis. Maecenas eget erat in sapien mattis porttitor. Vestibulum porttitor. Nulla facilisi. Sed a turpis eu lacus commodo facilisis. Morbi fringilla, wisi in dignissim interdum, justo lectus sagittis dui, et vehicula libero dui cursus dui. Mauris tempor ligula sed lacus. Duis cursus enim ut augue. Cras ac magna. Cras nulla. Nulla egestas. Curabitur a leo. Quisque egestas wisi eget nunc. Nam feugiat lacus vel est. Curabitur consectetuer.

Suspendisse vel felis. Ut lorem lorem, interdum eu, tincidunt sit amet, laoreet vitae, arcu. Aenean faucibus pede eu ante. Praesent enim elit, rutrum at, molestie non, nonummy vel, nisl. Ut lectus eros, malesuada sit amet, fermentum eu, sodales cursus, magna. Donec eu purus. Quisque vehicula, urna sed ultricies auctor, pede lorem egestas dui, et convallis elit erat sed nulla. Donec luctus. Curabitur et nunc. Aliquam dolor odio, commodo pretium, ultricies non, pharetra in, velit. Integer arcu est, nonummy in, fermentum faucibus, egestas vel, odio.

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.

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[1].

A.1 More Lorem

Quisque facilisis auctor sapien. Pellentesque gravida hendrerit lectus. Mauris rutrum sodales sapien. Fusce hendrerit sem vel lorem. Integer pellentesque massa vel augue. Integer elit tortor, feugiat quis, sagittis et, ornare non, lacus. Vestibulum posuere pellentesque eros. Quisque venenatis ipsum dictum nulla. Aliquam quis quam non metus eleifend interdum. Nam eget sapien ac mauris malesuada adipiscing. Etiam eleifend neque sed quam. Nulla facilisi. Proin a ligula. Sed id dui eu nibh egestas tincidunt. Suspendisse arcu.

A.1.1 Lorem 15–17

Nulla in ipsum. Praesent eros nulla, congue vitae, euismod ut, commodo a, wisi. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Aenean nonummy magna non leo. Sed felis erat, ullamcorper in, dictum non, ultricies ut, lectus. Proin vel arcu a odio lobortis euismod. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Proin ut est. Aliquam odio. Pellentesque massa turpis, cursus eu, euismod nec, tempor congue, nulla. Duis viverra gravida mauris. Cras tincidunt. Curabitur eros ligula, varius ut, pulvinar in, cursus faucibus, augue.

Nulla mattis luctus nulla. Duis commodo velit at leo. Aliquam vulputate magna et leo. Nam vestibulum ullamcorper leo. Vestibulum condimentum rutrum mauris. Donec id mauris. Morbi molestie justo et pede. Vivamus eget turpis sed nisl cursus tempor. Curabitur mollis sapien condimentum nunc. In wisi nisl, malesuada at, dignissim sit amet, lobortis in, odio. Aenean consequat arcu a ante. Pellentesque porta elit sit amet orci. Etiam at turpis nec elit ultricies imperdiet. Nulla facilisi.

In hac habitasse platea dictumst. Suspendisse viverra aliquam risus. Nullam pede justo, molestie nonummy, scelerisque eu, facilisis vel, arcu.

Curabitur tellus magna, porttitor a, commodo a, commodo in, tortor. Donec interdum. Praesent scelerisque. Maecenas posuere sodales odio. Vivamus metus lacus, varius quis, imperdiet quis, rhoncus a, turpis. Etiam ligula arcu, elementum a, venenatis quis, sollicitudin sed, metus. Donec nunc pede, tincidunt in, venenatis vitae, faucibus vel, nibh. Pellentesque wisi. Nullam malesuada. Morbi ut tellus ut pede tincidunt porta. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Etiam congue neque id dolor.

A.1.2 Lorem 18–19

Donec et nisl at wisi luctus bibendum. Nam interdum tellus ac libero. Sed sem justo, laoreet vitae, fringilla at, adipiscing ut, nibh. Maecenas non sem quis tortor eleifend fermentum. Etiam id tortor ac mauris porta vulputate. Integer porta neque vitae massa. Maecenas tempus libero a libero posuere dictum. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Aenean quis mauris sed elit commodo placerat. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos hymenaeos. Vivamus rhoncus tincidunt libero. Etiam elementum pretium justo. Vivamus est. Morbi a tellus eget pede tristique commodo. Nulla nisl. Vestibulum sed nisl eu sapien cursus rutrum.

Nulla non mauris vitae wisi posuere convallis. Sed eu nulla nec eros scelerisque pharetra. Nullam varius. Etiam dignissim elementum metus. Vestibulum faucibus, metus sit amet mattis rhoncus, sapien dui laoreet odio, nec ultricies nibh augue a enim. Fusce in ligula. Quisque at magna et nulla commodo consequat. Proin accumsan imperdiet sem. Nunc porta. Donec feugiat mi at justo. Phasellus facilisis ipsum quis ante. In ac elit eget ipsum pharetra faucibus. Maecenas viverra nulla in massa.

A.2 Lorem 51

Maecenas dui. Aliquam volutpat auctor lorem. Cras placerat est vitae lectus. Curabitur massa lectus, rutrum euismod, dignissim ut, dapibus a, odio. Ut eros erat, vulputate ut, interdum non, porta eu, erat. Cras fermentum, felis in porta congue, velit leo facilisis odio, vitae consectetuer lorem quam vitae orci. Sed ultrices, pede eu placerat auctor, ante ligula rutrum tellus, vel posuere nibh lacus nec nibh. Maecenas laoreet dolor at enim. Donec molestie dolor nec metus. Vestibulum libero. Sed quis erat. Sed tristique. Duis pede leo, fermentum quis, consectetuer eget, vulputate sit amet, erat.

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

Nulla ac nisl. Nullam urna nulla, ullamcorper in, interdum sit amet, gravida ut, risus. Aenean ac enim. In luctus. Phasellus eu quam vitae turpis viverra pellentesque. Duis feugiat felis ut enim. Phasellus pharetra, sem id porttitor sodales, magna nunc aliquet nibh, nec blandit nisl mauris at pede. Suspendisse risus risus, lobortis eget, semper at, imperdiet sit amet, quam. Quisque scelerisque dapibus nibh. Nam enim. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Nunc ut metus. Ut metus justo, auctor at, ultrices eu, sagittis ut, purus. Aliquam aliquam.

Etiam pede massa, dapibus vitae, rhoncus in, placerat posuere, odio. Vestibulum luctus commodo lacus. Morbi lacus dui, tempor sed, euismod eget, condimentum at, tortor. Phasellus aliquet odio ac lacus tempor faucibus. Praesent sed sem. Praesent iaculis. Cras rhoncus tellus sed justo ullamcorper sagittis. Donec quis orci. Sed ut tortor quis tellus euismod tincidunt. Suspendisse congue nisl eu elit. Aliquam tortor diam, tempus id, tristique eget, sodales vel, nulla. Praesent tellus mi, condimentum sed, viverra at, consectetuer quis, lectus. In auctor vehicula orci. Sed pede sapien, euismod in, suscipit in, pharetra placerat, metus. Vivamus commodo dui non odio. Donec et felis.

Etiam suscipit aliquam arcu. Aliquam sit amet est ac purus bibendum congue. Sed in eros. Morbi non orci. Pellentesque mattis lacinia elit. Fusce molestie velit in ligula. Nullam et orci vitae nibh vulputate auctor. Aliquam eget purus. Nulla auctor wisi sed ipsum. Morbi porttitor tellus ac enim. Fusce ornare. Proin ipsum enim, tincidunt in, ornare venenatis, molestie a, augue. Donec vel pede in lacus sagittis porta. Sed hendrerit ipsum quis nisl. Suspendisse quis massa ac nibh pretium cursus. Sed sodales. Nam eu neque quis pede dignissim ornare. Maecenas eu purus ac urna tincidunt congue.

Donec et nisl id sapien blandit mattis. Aenean dictum odio sit amet risus. Morbi purus. Nulla a est sit amet purus venenatis iaculis. Vivamus viverra purus vel

magna. Donec in justo sed odio malesuada dapibus. Nunc ultrices aliquam nunc. Vivamus facilisis pellentesque velit. Nulla nunc velit, vulputate dapibus, vulputate id, mattis ac, justo. Nam mattis elit dapibus purus. Quisque enim risus, congue non, elementum ut, mattis quis, sem. Quisque elit.

Maecenas non massa. Vestibulum pharetra nulla at lorem. Duis quis quam id lacus dapibus interdum. Nulla lorem. Donec ut ante quis dolor bibendum condimentum. Etiam egestas tortor vitae lacus. Praesent cursus. Mauris bibendum pede at elit. Morbi et felis a lectus interdum facilisis. Sed suscipit gravida turpis. Nulla at lectus. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Praesent nonummy luctus nibh. Proin turpis nunc, congue eu, egestas ut, fringilla at, tellus. In hac habitasse platea dictumst.

B.2 Lorem 25-27

Vivamus eu tellus sed tellus consequat suscipit. Nam orci orci, malesuada id, gravida nec, ultricies vitae, erat. Donec risus turpis, luctus sit amet, interdum quis, porta sed, ipsum. Suspendisse condimentum, tortor at egestas posuere, neque metus tempor orci, et tincidunt urna nunc a purus. Sed facilisis blandit tellus. Nunc risus sem, suscipit nec, eleifend quis, cursus quis, libero. Curabitur et dolor. Sed vitae sem. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Maecenas ante. Duis ullamcorper enim. Donec tristique enim eu leo. Nullam molestie elit eu dolor. Nullam bibendum, turpis vitae tristique gravida, quam sapien tempor lectus, quis pretium tellus purus ac quam. Nulla facilisi.

Duis aliquet dui in est. Donec eget est. Nunc lectus odio, varius at, fermentum in, accumsan non, enim. Aliquam erat volutpat. Proin sit amet nulla ut eros consectetuer cursus. Phasellus dapibus aliquam justo. Nunc laoreet. Donec consequat placerat magna. Duis pretium tincidunt justo. Sed sollicitudin vestibulum quam. Nam quis ligula. Vivamus at metus. Etiam imperdiet imperdiet pede. Aenean turpis. Fusce augue velit, scelerisque sollicitudin, dictum vitae, tempor et, pede. Donec wisi sapien, feugiat in, fermentum ut, sollicitudin adipiscing, metus.

Donec vel nibh ut felis consectetuer laoreet. Donec pede. Sed id quam id wisi laoreet suscipit. Nulla lectus dolor, aliquam ac, fringilla eget, mollis ut, orci. In pellentesque justo in ligula. Maecenas turpis. Donec eleifend leo at felis tincidunt consequat. Aenean turpis metus, malesuada sed, condimentum sit amet, auctor a, wisi. Pellentesque sapien elit, bibendum ac, posuere et, congue eu, felis. Vestibulum mattis libero quis metus scelerisque ultrices. Sed purus.

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. LATEX commands can be used here. Blank lines (or the command \par) are not allowed!

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

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