Otto von Guericke Universität Magdeburg

Master's Thesis

Simulation of Brain Functional and Structural Connectivity on Empirical and Randomized Complex Networks

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A thesis submitted in fulfilment of the requirements for the degree of Master of Science

in the

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Integrative Neuroscience

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Declaration of Authorship

I, Şeyma Bayrak, declare that this thesis titled, 'Simulation of Brain Functional and Structural Connectivity on Empirical and Randomized Complex Networks' and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a research degree at this University.
- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.
- Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

Signed:

Date:

"Thanks to my solid academic training, today I can write hundreds of words on virtually any topic without possessing a shred of information, which is how I got a good job in journalism."

Dave Barry

UNIVERSITY NAME (IN BLOCK CAPITALS)

Abstract

Faculty Name
Integrative Neuroscience

Master of Science

Simulation of Brain Functional and Structural Connectivity on Empirical and Randomized Complex Networks

by Şeyma Bayrak

The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

Acknowledgements

The acknowledgements and the people to thank go here, don't forget to include your project advisor…

Contents

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Abbreviations

LAH **L**ist **A**bbreviations **H**ere

Physical Constants

Speed of Light $c = 2.997\ 924\ 58 \times 10^{8}\ \mathrm{ms}^{-\mathrm{S}}$ (exact)

Symbols

a	distance	m
P	power	W (Js^{-1})
ω	angular frequency	$rads^{-1}$

For/Dedicated to/To my…

Chapter 1

Introduction

The purpose of this master's project is to quantify large-scale functional and structural brain networks and the comparison to resting-state functional Magnetic Resonance Imaging (fMRI). The functional brain networks are derived from simulated Blood-Oxygen-Level-Dependendt (BOLD) signals, whereas the structural brain networks are obtained from Diffusion-Weighted Magnetic Resonance Imaging (DWI-MR). The project uses experimental results combined with modelling approaches and implements methods drawn from nonlinear and network science.

The functional connectivities in a typical fMRI experiment are obtained from pre-defined brain regions, whose corresponding time-series of BOLD activity display significant correlations at low-frequencies (< 0.1 Hz). The measured correlated activity patterns are complex, but highly structured and robust. They have been captured not only during brain's activity paradigm, but also during its resting state, i.e. under no stimulations and in the absence of any stimulus driven task. The fMRI-BOLD empirical data used in this project is downloaded from the *1000 Functional Connectome Project* website http://www.nitric.org/). This data set is also referred as functional connectivity matrix (FCM) revealing the correlated activities among the 90 cortical and sub-cortical regions with the automated anatomical labelling (AAL) template as given in Table 1 in Appendix.

The DW-MRI tecnique illustrates the anatomical connection probabilities among the brain regions by investigating the diffusion direction of water molecules, which indirectly. The direction of the fiber tracks in white matter depends indirectly on the diffusion of water molecules. A DW-MRI experiment approximates the existence of a fiber track between regions of interest. The anatomical connection probability (ACP) matrix for the 90 anatomically labelled brain regions considered in this project is obtained from the study of Iturria-Medina et. al. (2008) [1]. Both anatomical and functional connectivities are defined on the same cortical and sub-cortical regions.

[1] Iturria-Medina et. al. (2008)

Statistical characterisation of the functional brain networks, using methods from graph theory / network science, have revealed some of their key topological properties such as small worldness, modularity or resilience to the attacks [**?**]. This project studies these properties both on the functional and structural brain networks arising from modelled intrinsic brain dynamics. In particular, such conditions that distinguish obtained network topologies from that of random networks will be explored. Several randomization procedures will be considered. They include, but not limited to random networks of Erdos-Renyi-type with the same number of nodes and links as in the empirically derived case. This approach will provide a deeper insight into the underlying processes involved in the observed functional connectivity and their relations to the coupling topology, i.e. brain structural connectivity.

Despite important progress over the past few years, the question how functional connectivity arises from the complex anatomical connectivity still remains poorly understood [VUK14]. The existing models of resting-brain dynamics hypotheize that functional interactions result from a compley interplay between intrinsic brain dynamics and underlying structural connections [RUB09]. In particular they explore the range of conditions at which functional networks emerge from anatomical connections, the role of multiple time-scales in the formation of functional-commectivity networks [HON07], time delays in the signal propagation between the network nodes as well as the system noise [GHO08, GHO08a]. local network oscillations [DEC09, CAB11] and structural disconnection [CAB12].

In this project, the model of resting-state brain activity will be based on the models previously proposed in [VUK13, VUK14]. The key ingredients are coupling topologies of the time-delayed functional interactions which are scaled by the global coupling strength c and subject to uncorrelated Gaussian white noise. The time-delay in the model is considered to happen as a natural effect of finite speed of the signal propagation along the axons. Therefore, velocity v, representing biophysically realistic axonal signal propagation [GH008, GHO08a, DEC09] is another important ingredient of the model.

The rest of the master's thesis is organized in the following order : The Sec. 2 will introduce the empirical data sets of FCM and ACM used in this project. This section will further explain the randomization methods used to construct random graphs. Characterization of those brain networks by using methods od graph theory / network science [RUB09, STA10, NEW10, RUB11] will be done by quantifying global and local network properties such as network density, clustering coefficient, small-worldness etc.. Sec.2 will finally provide an insight to the FitzHugh-Nagumo (FHN) modeled neuronal interactions [14,15 VUK13ten bak!] and Balloon-Windkessel hemodynamic model [16 -VUK13ten bak]. The Sec. 3 will illustrate the effect of coupling strength c and signal propagation velocity v on the empirically derived brain networks and randomly obtained networks. Additionaly, such parameter regions will be identified, at which the network properties of the emprirical data differ from that of random graphs. Sec.4 will conclude the master's thesis.

Chapter 2

Methods and Models

Graph theory is a mathematical field applicable to a considerable diversity of complex systems such as markets, ecosystems, computer circuits, and gene-gene interactions [Barabasi, 2009]. A graph is defined as an ensemble of vertices (nodes) that are linked with edges. If the edges connect the nodes in a specified direction, the graph is referred to as *directed*, otherwise *undirected*. Moreover, the edges can be assigned a weight yielding a *weighted* graph. A graph with edges of uniform weight is called an *unweighted* graph.

Network science incorporates graph theory applied on a distinct complex domain. Unlike classical graph theory, network science primarily deals with real life networks that are large and complex - neither uniformly random nor ordered [RUB10]. The neuro-anatomical and neuro-physiological data sets derived from DW-MRI and fMRI-BOLD techniques can be constructed as such large-scale complex brain graphs that are undirected and unweighted. Nodes in large-scale brain networks usually represent brain regions, while edges represent anatomical, functional or effective connections (Friston, 1994).

A brain network can be statistically described in terms of its topology, i.e. solely in terms of its connectivity and independently of spatial positions of nodes and edges. Topological measures described in previous studies capture local and global properties of a network, e.g. local and global efficiency, clustering coefficient, transitivity and small-worldness [LAT01, WAT98, NEW03, HUM08].

Methods of graph theory applied to structural and functional systems have shown that both share typical features of many complex networks [BUL09, RUB09, HEU11, VUK14]. However, the essential features of brain's connectivity still remain ambiguous both for functional and structural maps. This project aims to investigate whether the brain does not behave as a completely random circuitry. This idea will be tested by comparing brain graphs to the randomized networks as it was previously noticed by Bullmore and Bassett [BUL11a]. The majority of random graphs here are inspired by Erdős-Rényi type random networks and the configuration model.

In this section, the construction of brain graphs based on empirical functional connectivity matrix (FCM) and anatomical connectivity matrix (ACM) will be first introduced. Then, the topological characteristics of all graphs will be statistically measured and those topological measures will be interpreted neuro-biologically. In particular, it is aimed to explore under which conditions that brain network topologies distinguish from random networks. This approach is expected to provide a deeper insight into the underlying process involved in the observed functional and structural brain connectivity.

2.1 Empirical functional and anatomical connectivity matrices

2.2 The Brain Graph

The brain graphs considered here are derived from two sets of empirical brain connectivity maps: FCM and ACM obtained from fMRI-BOLD and DW-MRI techniques, respectively. Those data sets represent measurements from $N = 90$ cortical and subcortical regions labeled with AAL, represented by nodes in the graph. The nodes can be connected to each other by means of "edges". If the graph is constructed on the FCM, edges are interpreted as correlation strengths between the functional BOLD activity of two nodes. If the graph is built on the ACM, an existing edge is considered as the probability of two nodes to be structurally connected by fiber tracks in white matter.

The brain graphs in this project are generated through binarizing the functional connectivity matrix (FCM) and anatomical connectivity matrix (ACM). Binarization here means converting all the values in a given matrix into 1's and 0's via thresholding. Because of the nature of their definition, both empirical data sets have values between 0 and 1, reflecting a correlation strength in case of FCM or a probability value in case of ACM. We arbitrarily define a threshold value r for the strength of correlations in FCM. Then, the values greater and equal to r are assigned the value 1, while others are set to 0. This thresholding is applied by means of the strength of probability value, p, for the ACM. The binarized matrix is the basis of brain graph construction, and it is commonly known as *adjacency matrix*. The NETWORKX software package in PYTHON is used to built graphs given adjacency matrices. Neither the direction of functional or anatomical connectivity between nodes, nor any other values apart from 0 and 1 are encoded in the adjacency matrices, so that the resulting graphs are considered as "undirected" and "unweighted". In other words, all existing edges are thought to be of uniform weight and nodes interact both ways along an edge connecting them.

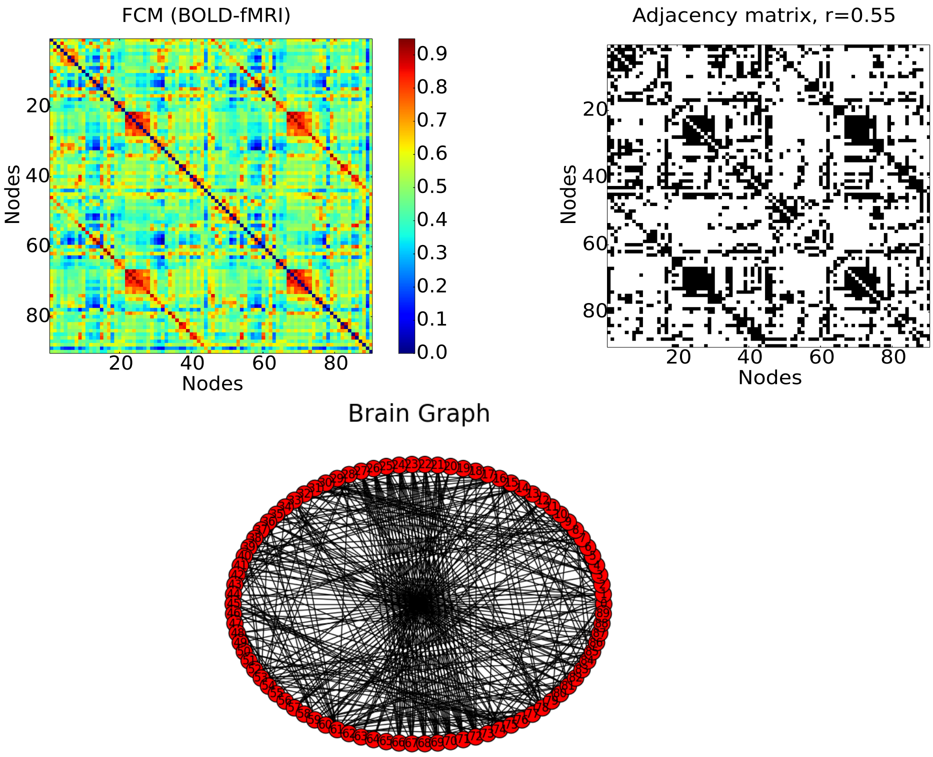

FIGURE 2.1: How to build a brain graph : The empirical data matrix derived from fMRI-BOLD technique (on the upper left) is binarized via a threshold value $r = 0.55$ and its corresponding adjacency matrix is obtained (on the upper right). The black spots represent 1's indicating edges between nodes, whereas the white squares represent 0's implying no connectivity. The brain graph derived from the adjacency matrix (on the bottom) has $N = 90$ nodes, edges represent functionally connected node pairs.

Figure 2.1 illustrates the exemplary construction of a brain graph exemplary from the FCM. All the correlation values among the cortical and sub-cortical regions in the empirical fMRI-BOLD data lie between 0 and 1. The adjacency matrix (AM) is filled out only with 1's and 0's indicating functionally connected and unconnected nodes, whose correlated BOLD activity is equal to or greater than $r = 0.55$. The algorithm NETWORKX builds the corresponding graph of an adjacency matrix. It should be noted that both FCM and AM are symmetric. The AM obtained from an ACM would look similar, but would represent the probability of two nodes to be anatomically connected above a predefined threshold p.

The following sections will cover randomization methods reshuffling the brain graphs and introduce some of the topological concepts characterizing brain graphs as well as random networks.

2.3 Randomization Methods

2.3.1 Erdős-Rényi Type Randomization

Given total number of nodes N and a probability P, Paul Erdős and Alfréd Rényi produced an undirected graph $G(N, P)$, in which the presence of any edge between two nodes is assigned with probability P. One can generalize the total number of edges L in an Erdős-Rényi type random graph as the following: $\binom{N}{2}P$, pointing out a binomial distribution for the edges per node.

It is possible to improve new randomization tools with adaptations in Erdős-Rényi method, i.e. given N and L, an intended graph $G(N, L)$ can be picked uniformly random out of set of all potential graphs having N nodes and L edges. The probability for a graph to be picked among all the others is $\frac{L}{\binom{N}{2}}$. One can study the relevance of $G(N, P)$ and $G(N, L)$ even more detailed, but for the sake of simplicity, Erdős-Rényi model will not discussed further here.

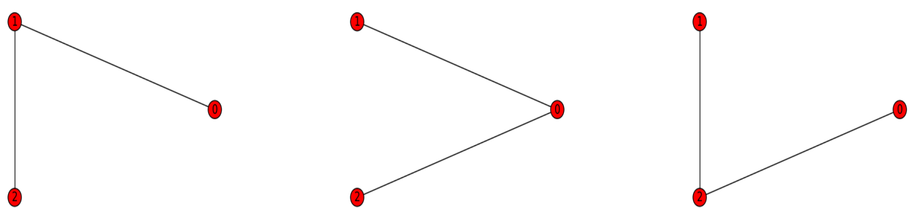

FIGURE 2.2: An illustration to the set of all $G(N, L)$ type random graphs with $N = 3$ and $L = 2$.

Figure 2.2 illustrates all possible graphs having 3 nodes ans 2 edges in total. One of those 3 simple graph is chosen uniformly random for the $G(N, L)$ randomization type means that each graph is chosen with probability $P = \dfrac{1}{3}$.

The $G(N, L)$ type randomization is the first method used to derive random graphs from the adjacency matrices of FCM and ACM in this project. Both matrices have $N = 90$ nodes, however L changes at each brain graph according to the applied threshold and probability level, therefore it is always recalculated.

2.3.2 Double-Edge-Swap Type Randomization

The *degree* of a node is defined as the number of edges connected to that node, from now on it will be denoted with k_i for the node i. The double-edge-swap method manipulates a given graph by swapping two existing edges among four nodes, while keeping the node degrees fixed.

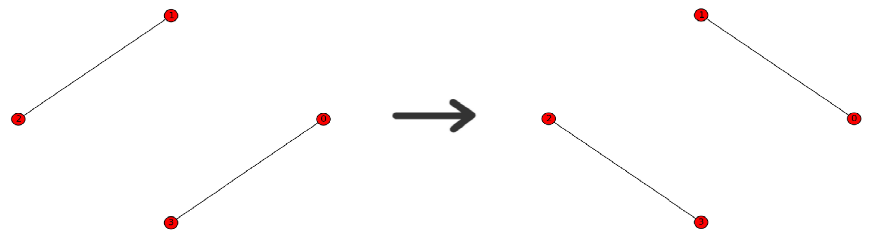

FIGURE 2.3: Swapping edges between 4 nodes

Figure 2.3 illustrates randomly chosen double edges in a sample graph to be swapped. After the existing edges are removed, the new couple of nodes are rewired. The k_i of each node is the same before and after swapping. The *degree distribution* of a graph is a topological property, which reveals a probability distribution of node degrees over whole graph. Although the randomly constructed graphs with the double-edge-swap method based on the brain graphs of FCM and ACM are expected to have the same degree distribution, it is not a unique property identifying a graph.

2.3.3 Configuration Model Randomization

The *degree sequence* of a graph is either ascending or descending sequence of node degrees in a graph. The configuration model intends to return a random graph with given degree sequence. The ideal concept of this model is to assign edges to the nodes randomly until the desired degree sequence is matched. However, the algorithms practicing the configuration model are not so trivial due to self-loops (node is connected to itself) and parallel edges (duplicating edges), which are both undesirable graph properties in this project.

Figure 2.4 points out the relevance of degree sequence to the node degrees. It should be reminded that the degree distribution and the degree sequence are not the same metrics.

The configuration model variant used here is the expected-degree-graph method, which has an option to exclude self-loops and parallel edges. This algorithm receives the list of expected degree sequence as input, $(k_u, k_v, k_m, k_l, ...)$, and assigns edges between

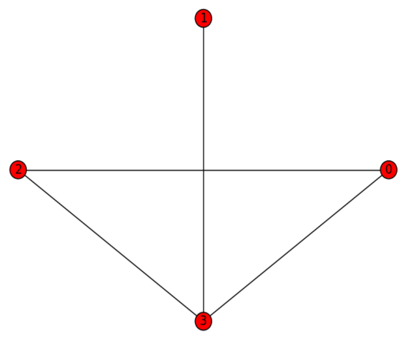

FIGURE 2.4: The degrees of the nodes: $k_0 = 2$, $k_1 = 1$, $k_2 = 2$, $k_3 = 3$ and the degree sequence in non-increasing order in the sample graph : $\{3, 2, 2, 1\}$

nodes with a predefined probability $P_{uv} = \dfrac{k_u k_w}{\sum_i k_i}$. This tool does not guarantee to construct graphs with exactly the same given degree sequence but with the closest possible sequence.

2.3.4 Preserved-Degree-Distribution Type Randomization

The *degree distribution* of a network reflects the probability of a node to have a given number of degree k. The preserved-degree-distribution method randomizes a given undirected network by rewiring its edges randomly while preserving its degree distribution. The method first chooses four target nodes randomly, then flips the edges between those nodes with the probability of $P = 0.5$. The total number of rewirings to be performed is given as an iteration parameter to the method.

2.3.5 Partial Randomization

The partial randomization method reconstructs a graph (say A) with partial rewirings with respect to a second graph (say B) while keeping the degree distribution the same as in A. The analogy of this algorithm is to perform rewirings in the adjacency matrix of A, while avoiding any edge generation which already exist in the B. In other words, the choice of edges to be performed rewirings in A is limited with respect to the B.

In this project, the functional connectivity (FC) adjacency matrix is partially rewired with anatomical connectivity (AC) adjacency matrix. This means doing such rewirings among the nodes in FCM, only if these nodes are not structurally connected in the brain at above a probability value. The same procedure is done to randomize AC adjacency matrix partially with respect to FC adjacency matrix. This time such nodes in ACM are rewired, that do not functionally correlated above a given threshold.

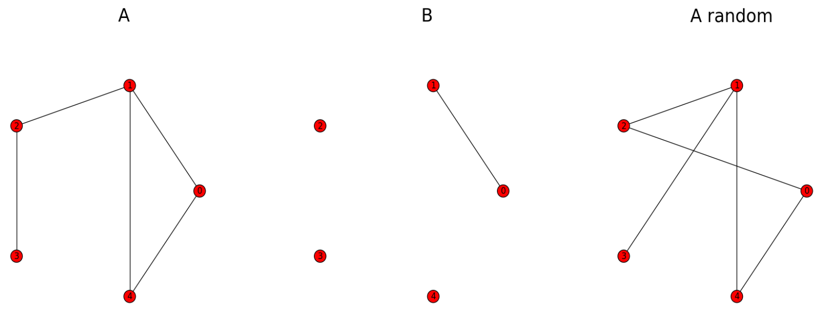

FIGURE 2.5: Graph A is performed a partial randomization with respect to graph B. While the partial randomization tool rewires edges in A, it avoids creating such edges that exist in B.

The brain graph and randomly generated graphs will be identified in terms of their topological properties in the following sections. For simplicity the abbreviations are introduced in the table below.

TABLE 2.1: Abbreviations for the brain graph and the randomly constructed graphs.

Abbreviation	Description	method
R0	the brain graph	NETWORKX
Ra	Erdős-Rényi, G(N,L)	NETWORKX
Rd	double-edge-swap	NETWORKX
Rg	configuration model	NETWORKX
Rh	preserved-degree-distribution	BCT
Rk	partial randomization	BCT

2.4 Network Characterizations

2.4.1 Network Density

The *average degree* $\langle k \rangle$ of a network indicates the ratio of total number of edges L to total number of nodes N in a graph.

$$\langle k \rangle = \frac{2L}{N} \tag{2.1}$$

It should be noted that in order to not count each link twice, the total number of edges is divided by $N/2$ instead of N. The *density* D of a network is a scaled version of average degree measurement. It is formulated as the ratio between L and maximum number of possible edges $\binom{N}{2}$.

$$D = \frac{2L}{N(N-1)} \tag{2.2}$$

The measure of network density can be referred as the total *wiring cost* of the network [RUB10]. The degree, average degree and network density are the key ingredients to characterize the topology of a network further. It has even related clinical evidence that reductions in nodal degree have been associated with greater severity of local amyloid deposition in patients with Alzheimer's disease [Buckner et al. 2009].

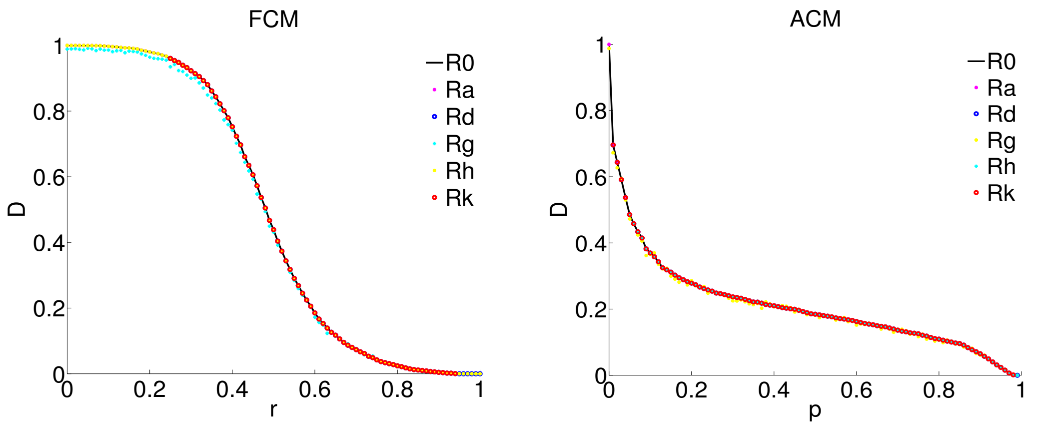

Figure 2.6: Network density of the brain graphs and random graphs of FCM (on the left) and ACM (on the right). The abbreviations are chosen as described in Table 1.

The network density D is presented as probability values lying between 0 and 1 for all the graphs in corresponding threshold r and p ranges. The random networks are built in such ways that they have the same number of N and almost the same D as in the brain graphs. However, the D is not a unique metric identifying a network.

All networks for FCM and ACM seem to be densely connected at lower r and p. The brain graph and randomized graphs of FCM follows an inverse sigmoidal D pattern with decreasing threshold r. The D decreases slower for the ACM graphs graph with the ascending probability p. It should be noted that all the graphs have almost the same D values.

Functional networks are likely to be denser than anatomical networks, as they will typically contain numerous connections between anatomically unconnected regions [DAM09].

2.4.2 Average Clustering Coefficient

The *average clustering coefficient* C of a network is calculated through individual clustering coefficients C_i of single nodes,

$$C = \frac{1}{n}\sum_{i\epsilon N} C_i = \frac{1}{n}\sum_{i\epsilon N}\frac{2t_i}{k_i(k_i-1)} \tag{2.3}$$

where t_i is the number of triangles around node i, k_i is the degree of node i [WAT98]. The clustering coefficient is a measure of segregation, that is the ability for specialized processing to occur within densely interconnected groups of brain regions [RUB10]. It reveals how the individual nodes in a graph cluster together; how many neighbors of a node are neighbors of each other.

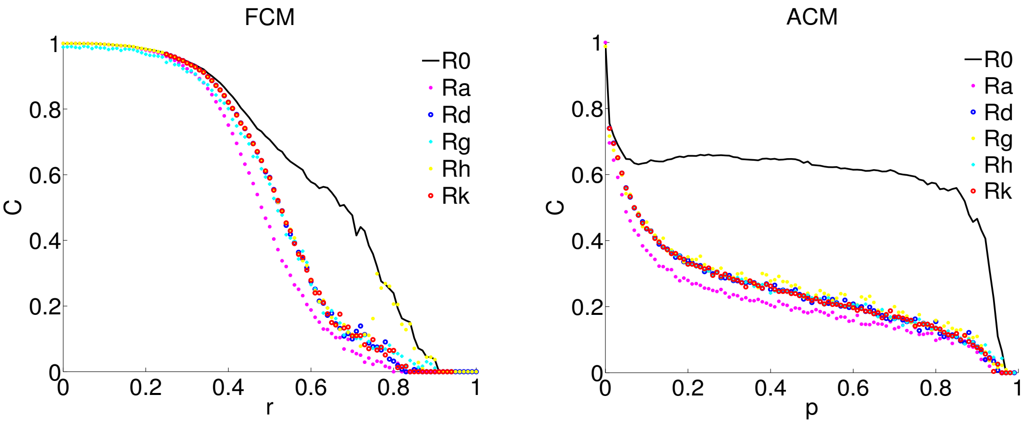

FIGURE 2.7: Average clustering coefficient of the brain graphs and random graphs of FCM (on the left) and ACM (on the left).

Clustering coefficient of a node C_i is a measure of local connectivity and is highly correlated with the local efficiency of the information transfer [LAT01]. The C_i is formulated as the ratio of t_i over all possible edges of the node i; $\binom{k_i}{2}$. The average clustering coefficient C is a normalized version of C_i for the whole network, yielding now a global property. All C values are between 0 and 1. Figure 2.7 shows that at lower threshold, the nodes tend to cluster more due to higher number of existing edges. The empirically obtained brain networks of FCM and ACM have the highest C compared to random graphs. The local information transfer seems to be more efficient in the brain graphs. The randomized graphs of ACM Ra, Rd, Rh and Rk share more nodes with lower degrees compared to $R0$.

2.4.3 Transitivity

Transitivity is a similar measure to the clustering coefficient, it is also a measure for the segregation in the network. The corresponding equation represents the transitivity of a network (Newman, 2003):

$$T = \frac{\sum\limits_{i\epsilon N} 2t_i}{\sum\limits_{i\epsilon N} k_i(k_i - 1)} \tag{2.4}$$

If a node has links to two other nodes, transitivity inquires whether those two other nodes are also connected to each other. Transitivity resembles clustering coefficient, however, it is defined only for the whole network rather than single nodes.

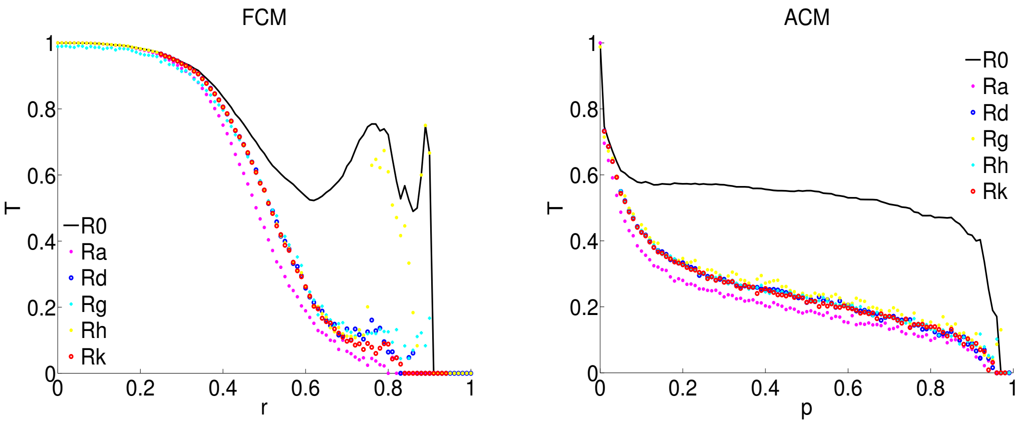

FIGURE 2.8: Transitivity of the brain graphs and random graphs of FCM (on the left) and ACM (on the left).

Transitivity is one of severe shortcomings that real world networks and random networks strongly differ [NEW10]. Transitivity difference between brain graphs and random graphs observed to be more distinguishable than C difference between brain graphs and random graphs when Figure 2.8 is compared to Figure 2.7.

2.5 FitzHugh-Nagumo Model for Neuronal Activity Simulation

2.6 Balloon-Windkessel Model for BOLD Activity Simulation

Chapter 3

Results

Chapter 4

Conclusion

4.0.1 Common LaTeX Math Symbols

There are a multitude of mathematical symbols available for LaTeX and it would take a great effort to learn the commands for them all. The most common ones you are likely to use are shown on this page:
http://www.sunilpatel.co.uk/latexsymbols.html

You can use this page as a reference or crib sheet, the symbols are rendered as large, high quality images so you can quickly find the LaTeX command for the symbol you need.

4.1 Getting Started with this Template

If you are familiar with LaTeX, then you can familiarise yourself with the contents of the Zip file and the directory structure and then place your own information into the '`Thesis.cls`' file. Section 4.3 on page 19 tells you how to do this. Make sure you read section 4.5 about thesis conventions to get the most out of this template and then get started with the '`Thesis.tex`' file straightaway.

If you are new to LaTeX it is recommended that you carry on reading through the rest of the information in this document.

4.1.1 About this Template

This LaTeX Thesis Template is originally based and created around a LaTeX style file created by Steve R. Gunn from the University of Southampton (UK), department of Electronics and Computer Science. You can find his original thesis style file at his site, here:
http://www.ecs.soton.ac.uk/~srg/softwaretools/document/templates/

My thesis originally used the '`ecsthesis.cls`' from his list of styles. However, I knew LaTeX could still format better. To get the look I wanted, I modified his style and also created a skeleton framework and folder structure to place the thesis files in.

This Thesis Template consists of that modified style, the framework and the folder structure. All the work that has gone into the preparation and groundwork means that all you have to bother about is the writing.

Before you begin using this template you should ensure that its style complies with the thesis style guidelines imposed by your institution. In most cases this template style and layout will be suitable. If it is not, it may only require a small change to bring the template in line with your institution's recommendations.

4.2 What this Template Includes

4.2.1 Folders

This template comes as a single Zip file that expands out to many files and folders. The folder names are mostly self-explanatory:

Appendices – this is the folder where you put the appendices. Each appendix should go into its own separate '`.tex`' file. A template is included in the directory.

Chapters – this is the folder where you put the thesis chapters. A thesis usually has about seven chapters, though there is no hard rule on this. Each chapter should go in its own separate '`.tex`' file and they usually are split as:

- Chapter 1: Introduction to the thesis topic
- Chapter 2: Background information and theory
- Chapter 3: (Laboratory) experimental setup
- Chapter 4: Details of experiment 1

- Chapter 5: Details of experiment 2
- Chapter 6: Discussion of the experimental results
- Chapter 7: Conclusion and future directions

This chapter layout is specialised for the experimental sciences.

Figures – this folder contains all figures for the thesis. These are the final images that will go into the thesis document.

Primitives – this is the folder that contains scraps, particularly because one final image in the 'Figures' folder may be made from many separate images and photos, these source images go here. This keeps the intermediate files separate from the final thesis figures.

4.2.2 Files

Included are also several files, most of them are plain text and you can see their contents in a text editor. Luckily, many of them are auxiliary files created by LaTeX or BibTeX and which you don't need to bother about:

Bibliography.bib – this is an important file that contains all the bibliographic information and references that you will be citing in the thesis for use with BibTeX. You can write it manually, but there are reference manager programs available that will create and manage it for you. Bibliographies in LaTeX are a large subject and you may need to read about BibTeX before starting with this.

Thesis.cls – this is an important file. It is the style file that tells LaTeX how to format the thesis. You will also need to open this file in a text editor and fill in your own information (such as name, department, institution). Luckily, this is not too difficult and is explained in section 4.3 on page 19.

Thesis.pdf – this is your beautifully typeset thesis (in the PDF file format) created by LaTeX.

Thesis.tex – this is an important file. This is the file that you tell LaTeX to compile to produce your thesis as a PDF file. It contains the framework and constructs that tell LaTeX how to layout the thesis. It is heavily commented so you can read exactly what each line of code does and why it is there. After you put your own information into the '`Thesis.cls`' file, go to this file and begin filling it in – you have now started your thesis!

vector.sty – this is a LaTeX package, it tells LaTeX how to typeset mathematical vectors. Using this package is very easy and you can read the documentation on the site (you just need to look at the '`vector.pdf`' file):
http://www.ctan.org/tex-archive/macros/latex/contrib/vector/

lstpatch.sty – this is a LaTeX package required by this LaTeX template and is included as not all TeX distributions have it installed by default. You do not need to modify this file.

Files that are *not* included, but are created by LaTeX as auxiliary files include:

Thesis.aux – this is an auxiliary file generated by LaTeX, if it is deleted LaTeX simply regenerates it when you run the main '`.tex`' file.

Thesis.bbl – this is an auxiliary file generated by BibTeX, if it is deleted, BibTeX simply regenerates it when you run the main tex file. Whereas the '`.bib`' file contains all the references you have, this '`.bbl`' file contains the references you have actually cited in the thesis and is used to build the bibliography section of the thesis.

Thesis.blg – this is an auxiliary file generated by BibTeX, if it is deleted BibTeX simply regenerates it when you run the main '`.tex`' file.

Thesis.lof – this is an auxiliary file generated by LaTeX, if it is deleted LaTeX simply regenerates it when you run the main '`.tex`' file. It tells LaTeX how to build the 'List of Figures' section.

Thesis.log – this is an auxiliary file generated by LaTeX, if it is deleted LaTeX simply regenerates it when you run the main '`.tex`' file. It contains messages from LaTeX, if you receive errors and warnings from LaTeX, they will be in this '`.log`' file.

Thesis.lot – this is an auxiliary file generated by LaTeX, if it is deleted LaTeX simply regenerates it when you run the main '`.tex`' file. It tells LaTeX how to build the 'List of Tables' section.

Thesis.out – this is an auxiliary file generated by LaTeX, if it is deleted LaTeX simply regenerates it when you run the main '`.tex`' file.

So from this long list, only the files with the '`.sty`', '`.bib`', '`.cls`' and '`.tex`' extensions are the most important ones. The other auxiliary files can be ignored or deleted as LaTeX and BibTeX will regenerate them.

4.3 Filling in the '`Thesis.cls`' File

You will need to personalise the thesis template and make it your own by filling in your own information. This is done by editing the '`Thesis.cls`' file in a text editor.

Open the file and scroll down, past all the '`\newcommand`...' items until you see the entries for '`University Name`', '`Department Name`', etc....

Fill out the information about your group and institution and ensure you keep to block capitals where it asks you to. You can also insert web links, if you do, make sure you use the full URL, including the '`http://`' for this.

The last item you should need to fill in is the Faculty Name (in block capitals). When you have done this, save the file and recompile '`Thesis.tex`'. All the information you filled in should now be in the PDF, complete with web links. You can now begin your thesis proper!

4.4 The '`Thesis.tex`' File Explained

The `Thesis.tex` file contains the structure of the thesis. There are plenty of written comments that explain what pages, sections and formatting the LaTeX code is creating. Initially there seems to be a lot of LaTeX code, but this is all formatting, and it has all been taken care of so you don't have to do it.

Begin by checking that your information on the title page is correct. For the thesis declaration, your institution may insist on something different than the text given. If this is the case, just replace what you see with what is required.

Then comes a page which contains a funny quote. You can put your own, or quote your favourite scientist, author, person, etc... Make sure to put the name of the person who you took the quote from.

Next comes the acknowledgements. On this page, write about all the people who you wish to thank (not forgetting parents, partners and your advisor/supervisor).

The contents pages, list of figures and tables are all taken care of for you and do not need to be manually created or edited. The next set of pages are optional and can be deleted since they are for a more technical thesis: insert a list of abbreviations you have used in the thesis, then a list of the physical constants and numbers you refer to and finally, a list of mathematical symbols used in any formulae. Making the effort to fill these tables means the reader has a one-stop place to refer to instead of searching the internet and references to try and find out what you meant by certain abbreviations or symbols.

The list of symbols is split into the Roman and Greek alphabets. Whereas the abbreviations and symbols ought to be listed in alphabetical order (and this is *not* done automatically for you) the list of physical constants should be grouped into similar themes.

The next page contains a one line dedication. Who will you dedicate your thesis to?

Finally, there is the section where the chapters are included. Uncomment the lines (delete the '`%`' character) as you write the chapters. Each chapter should be written in its own file and put into the 'Chapters' folder and named '`Chapter1`', '`Chapter2`, etc...Similarly for the appendices, uncomment the lines as you need them. Each appendix should go into its own file and placed in the 'Appendices' folder.

After the preamble, chapters and appendices finally comes the bibliography. The bibliography style (called '`unsrtnat`') is used for the bibliography and is a fully featured style that will even include links to where the referenced paper can be found online. Do not under estimate how grateful you reader will be to find that a reference to a paper is just a click away. Of course, this relies on you putting the URL information into the BibTeX file in the first place.

4.5 Thesis Features and Conventions

To get the best out of this template, there are a few conventions that you may want to follow.

One of the most important (and most difficult) things to keep track of in such a long document as a thesis is consistency. Using certain conventions and ways of doing things (such as using a Todo list) makes the job easier. Of course, all of these are optional and you can adopt your own method.

4.5.1 Printing Format

This thesis template is designed for single sided printing as most theses are printed and bound this way. This means that the left margin is always wider than the right (for binding). Four out of five people will now judge the margins by eye and think, "I never noticed that before.".

The headers for the pages contain the page number on the right side (so it is easy to flick through to the page you want) and the chapter name on the left side.

The text is set to 11 point and a line spacing of 1.3. Generally, it is much more readable to have a smaller text size and wider gap between the lines than it is to have a larger text size and smaller gap. Again, you can tune the text size and spacing should you want or need to. The text size can be set in the options for the '`\documentclass`' command at the top of the '`Thesis.tex`' file and the spacing can be changed by setting a different value in the '`\setstretch`' commands (scattered throughout the '`Thesis.tex`' file).

4.5.2 Using US Letter Paper

The paper size used in the template is A4, which is a common – if not standard – size in Europe. If you are using this thesis template elsewhere and particularly in the United States, then you may have to change the A4 paper size to the US Letter size. Unfortunately, this is not as simple as replacing instances of '`a4paper`' with '`letterpaper`'.

This is because the final PDF file is created directly from the LaTeX source using a program called '`pdfTeX`' and in certain conditions, paper size commands are ignored and all documents are created with the paper size set to the size stated in the configuration file for pdfTeX (called '`pdftex.cfg`').

What needs to be done is to change the paper size in the configuration file for `pdfTeX` to reflect the letter size. There is an excellent tutorial on how to do this here:
http://www.physics.wm.edu/~norman/latexhints/pdf_papersize.html

It may be sufficient just to replace the dimensions of the A4 paper size with the US Letter size in the `pdftex.cfg` file. Due to the differences in the paper size, the resulting margins may be different to what you like or require (as it is common for Institutions to dictate certain margin sizes). If this is the case, then the margin sizes can be tweaked by opening up the `Thesis.cls` file and searching for the line beginning with, '`\setmarginsrb`' (not very far down from the top), there you will see the margins specified. Simply change those values to what you need (or what looks good) and save. Now your document should be set up for US Letter paper size with suitable margins.

4.5.3 References

The '`natbib`' package is used to format the bibliography and inserts references such as this one [**?**]. The options used in the '`Thesis.tex`' file mean that the references are listed in numerical order as they appear in the text. Multiple references are rearranged in numerical order (e.g. [**? ?**]) and multiple, sequential references become reformatted to a reference range (e.g. [**? ? ?**]). This is done automatically for you. To see how you use references, have a look at the '`Chapter1.tex`' source file. Many reference managers allow you to simply drag the reference into the document as you type.

Scientific references should come *before* the punctuation mark if there is one (such as a comma or period). The same goes for footnotes[1]. You can change this but the most important thing is to keep the convention consistent throughout the thesis. Footnotes themselves should be full, descriptive sentences (beginning with a capital letter and ending with a full stop).

To see how LaTeX typesets the bibliography, have a look at the very end of this document (or just click on the reference number links).

4.5.4 Figures

There will hopefully be many figures in your thesis (that should be placed in the 'Figures' folder). The way to insert figures into your thesis is to use a code template like this:

```
\begin{figure}[htbp]
  \centering
    \includegraphics{Figures/Electron.pdf}
    \rule{35em}{0.5pt}
  \caption[An Electron]{An electron (artist's impression).}
  \label{fig:Electron}
\end{figure}
```

Also look in the source file. Putting this code into the source file produces the picture of the electron that you can see in the figure below.

Sometimes figures don't always appear where you write them in the source. The placement depends on how much space there is on the page for the figure. Sometimes there is not enough room to fit a figure directly where it should go (in relation to the text) and so LaTeX puts it at the top of the next page. Positioning figures is the job of LaTeX and so you should only worry about making them look good!

Figures usually should have labels just in case you need to refer to them (such as in Figure 4.1). The '`\caption`' command contains two parts, the first part, inside the square brackets is the title that will appear in the 'List of Figures', and so should

[1]Such as this footnote, here down at the bottom of the page.

Figure 4.1: An electron (artist's impression).

be short. The second part in the curly brackets should contain the longer and more descriptive caption text.

The '`\rule`' command is optional and simply puts an aesthetic horizontal line below the image. If you do this for one image, do it for all of them.

The LaTeX Thesis Template is able to use figures that are either in the PDF or JPEG file format.

4.5.5 Typesetting mathematics

If your thesis is going to contain heavy mathematical content, be sure that LaTeX will make it look beautiful, even though it won't be able to solve the equations for you.

The "Not So Short Introduction to LaTeX" (available here) should tell you everything you need to know for most cases of typesetting mathematics. If you need more information, a much more thorough mathematical guide is available from the AMS called, "A Short Math Guide to LaTeX" and can be downloaded from:
`ftp://ftp.ams.org/pub/tex/doc/amsmath/short-math-guide.pdf`

There are many different LaTeX symbols to remember, luckily you can find the most common symbols here. You can use the web page as a quick reference or crib sheet and because the symbols are grouped and rendered as high quality images (each with a downloadable PDF), finding the symbol you need is quick and easy.

You can write an equation, which is automatically given an equation number by LaTeX like this:

```
\begin{equation}
E = mc^{2}
  \label{eqn:Einstein}
\end{equation}
```

This will produce Einstein's famous energy-matter equivalence equation:

$$E = mc^2 \tag{4.1}$$

All equations you write (which are not in the middle of paragraph text) are automatically given equation numbers by LaTeX. If you don't want a particular equation numbered, just put the command, '`\nonumber`' immediately after the equation.

4.6 Sectioning and Subsectioning

You should break your thesis up into nice, bite-sized sections and subsections. LaTeX automatically builds a table of Contents by looking at all the '`\chapter{}`', '`\section{}`' and '`\subsection{}`' commands you write in the source.

The table of Contents should only list the sections to three (3) levels. A '`\chapter{}`' is level one (1). A '`\section{}`' is level two (2) and so a '`\subsection{}`' is level three (3). In your thesis it is likely that you will even use a '`\subsubsection{}`', which is level four (4). Adding all these will create an unnecessarily cluttered table of Contents and so you should use the '`\subsubsection*{}`' command instead (note the asterisk). The asterisk (*) tells LaTeX to omit listing the subsubsection in the Contents, keeping it clean and tidy.

4.7 In Closing

You have reached the end of this mini-guide. You can now rename or overwrite this pdf file and begin writing your own '`Chapter1.tex`' and the rest of your thesis. The easy work of setting up the structure and framework has been taken care of for you. It's now your job to fill it out!

Good luck and have lots of fun!

Guide written by —
Sunil Patel: www.sunilpatel.co.uk

Appendix A

Appendix Title Here

Write your Appendix content here.