A study on Brain Networks

A Thesis

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THESIS CERTIFICATE

This is to certify that the thesis titled A study on Brain networks, submitted by Anand

Uday Gokhale, to the Indian Institute of Technology, Madras, for the award of the

degree of Dual Degree (Bachelor of Technology + Master of Technology), is a bona

fide record of the research work done by him under our supervision. The contents of

this thesis, in full or in parts, have not been submitted to any other Institute or University

for the award of any degree or diploma.

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ABSTRACT

KEYWORDS: Networked Control Systems, Large Scale Systems, Nonlinear Oscillators, Computational Neuroscience, Brain Networks, Target Controllability, Modal Controllability

While dealing with the problem of control of complex networks, in addition to verifying qualitative properties of whether the system is controllable or not, one needs to quantify the effort needed to control the system. This is because the required control effort becomes significantly large, especially when there are constraints on the number of control inputs, rendering the system practically uncontrollable. In the context of Large scale systems, it may not be required to control all the nodes of the network but rather a subset of states called target nodes, in which case the energy requirements reduce substantially with dropping off few nodes for control. Further, with a shift of basis, there may be particular modes within the network that are of interest. In this thesis, we propose some algorithms for minimizing the control effort for target controllability and modal controllability.

This thesis also explores some aspects of computational neuroscience and studies the behaviour of some nonlinear oscillatory models under varying amounts of input load. Connections between models such as the Kuramoto oscillator and Hopf Model are drawn. To conclude, an analysis of the structural and functional states in the brain is analyzed.

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CHAPTER 1

Introduction

In recent years, there is an increased interest in dealing with large systems in a modular form, where the system is modelled as a network of units, and the dynamics of each unit is represented as a combination of the local dynamics and the network dynamics of the system. Such a viewpoint allows the system to be interpreted as a graph of nodes, and allows us to use tools from Graph Theory. These abstractions find applications in the analysis of biological, social and power grid based networks.

A key problem that is central in control theory involves the quantification of the energy required to achieve a target state. Traditionally, the controllability of a system is defined as a the ability of a system to reach any state in its state space through some sequence of inputs. The quantification of whether a system is controllable or not is usually sufficient for the analysis of small scale systems, as the energy requirements for the control of such systems is typically within some practical bounds. However, for large scale systems or networked systems, this does not translate well, and in some cases, the energy required to control a system typically increases exponentially with the size of the system.

For particular use cases, it may be neither feasible nor necessary to control the entire system. Instead, we may be concerned only with the controllability of a subset of the nodes, referred to as target nodes. For example, to contain the rate of infection down in infectious disease, it might be enough to vaccinate 70-80% of the population (the target set) to achieve herd immunity instead of the entire population. The problem then translates to identifying the easiest 70% of the population to vaccinate.

Similar to the study of target nodes, the concept of studying a fixed set of modes of a linear system has gained some popularity in the context of brain networks. Since large scale networks may have ill conditioned modes, the study of modal control allows one to limit their analysis to the well conditioned modes of the system. Further, Modal Controllability metrics provide an estimate of the energy required to reach difficult to reach states in brain networks.

The study of the effects of stimulation of brain networks may prove to be critical in the diagnosis and medication for several brain disorders like Parkinson's disease, Schizophrenia, epilepsy among others. In addition, some evidence suggests it may be even used to optimize performance among healthy individuals by altering cortical plasticity.

However, the effect of stimulus on human brains is not yet fully understood. The recent increase in interest in networked complex systems has led to the development of tools which could be detrimental to the study of stimulus and controllability of brain networks. To attack this problem, we require models for brain dynamics, and then we may study the effects of stimulation on these models. There are some engineering challenges that need to be resolved before brain stimulation is a part of everyday clinical methods. It is still unclear how stimulation influences brain activity in certain regions. An approach to these challenges may be provided by network science.

In this thesis, we start by developing tools for the analysis of networked linear systems, and define some optimization algorithms for target controllability. We also define a new metric for the study of modal controllability. Next, we move on to the problem of brain stimulation. Here, we develop and validate the use of nonlinear models for Brain Networks. We show that in these nonlinear models, the average controllability of each region reduces while performing complex tasks. This is similar to what has been observed empirically in [1]. Next we discuss the differences between functional and structural states in the brain. Functional states are time varying and depend on the task, whereas a structural state is plastic and represents the physical connections in the brain.

This thesis has been organized as follows. Some mathematical preliminaries have been presented in Chapter 2. Chapter 3 describes the optimization algorithms developed for target controllability as well as a metric proposed for modal controllability. Chapter 4 describes some nonlinear models. We also describe our experimental setup for our experiments on brain stimulation.

The sections involving target controllability in this thesis have been adapted from my paper which has been accepted at the Seventh Indian Control Conference (ICC-7). The results involving Modal Controllability have been submitted for peer review at the 25th International Symposium on Mathematical Theory of Networks and Systems 2022.

CHAPTER 2

Preliminaries

2.1 A Network as a Linear system

Consider a network denoted by a directed graph \mathcal{G} , with vertex set \mathcal{V} , $|\mathcal{V}| = n$, and an edge set $\mathcal{E} \subseteq \{\mathcal{V} \times \mathcal{V}, \mathbb{R}\}$. Each element (v_i, v_j, w_{ij}) of the set \mathcal{E} denotes a directed edge from vertex v_i to v_j with an edge weight w_{ij} . Let the adjacency matrix of the graph be $A \in \mathbb{R}^{n \times n}$. Each non-zero entry A_{ij} of A indicates the presence of an edge from vertex v_j to vertex v_i with an edge weight equal to A_{ij} . We define $x_i(k) \in \mathbb{R}$ as the state of vertex v_i , at time instant k, and the network state as $x(k) = [x_1(k) \ x_2(k) \ \dots \ x_n(k)]'$. We consider the network state follows discrete-time linear time-invariant dynamics given by

$$x[k+1] = Ax[k] + B_{\mathcal{K}}u[k],$$
 (2.1)

$$y[k] = C_{\mathcal{T}}x[k], \tag{2.2}$$

where, $x(k) \in \mathbb{R}^n$, $y(k) \in \mathbb{R}^p$, $u(k) \in \mathbb{R}^m$ represents network's state, output and input vectors respectively. Further, the matrix $B_{\mathcal{K}}$ identifies a set of vertices provided with dedicated external control inputs and termed as a driver node set $\mathcal{K} \subseteq \mathcal{V}$, $|\mathcal{K}| = m$. The canonical vectors in \mathbb{R}^n associated with the driver nodes form the columns of the input matrix $B_{\mathcal{K}}$. The output matrix $C_{\mathcal{T}}$ identifies the set of target nodes $\mathcal{T} \subseteq \mathcal{V}$, $|\mathcal{T}| = p$ we wish to control. The matrix $C_{\mathcal{T}} \in \mathbb{R}^{p \times n}$ is constructed using the canonical vectors of the vertices belonging to the set \mathcal{T} , in a similar fashion to $B_{\mathcal{K}}$. Throughout our analysis, we assume the driver node set \mathcal{K} remains the same and hence we denote $B_{\mathcal{K}}$ as B through out the paper.

2.2 Target Controllability

To define the target controllability, we first define the controllability for the entire system as follows:

Definition 2.2.1. A discrete linear dynamical system is said to be controllable over time [0,T], if for any initial state $x_0 \in \mathbb{R}^n$ and final state $x_f \in \mathbb{R}^n$, there exists a discrete control input $u[.]: [0,T-1] \to \mathbb{R}^m$ that drives the system from x_0 at time step k=0 to x_f at time step k=T.

We extend this notion to target controllability by restricting our interest in the final state to the states of target nodes only. Formally,

Definition 2.2.2. A discrete dynamical system is said to be target controllable with respect to the target set $T \subseteq V$, |T| = p over time [0, T], if for any final output $y_f \in \mathbb{R}^p$ and any initial state x_0 , there exists a control input $u[.]: [0, T-1] \to \mathbb{R}^m$ that drives the system from x_0 at time step k = 0 to the final state of the target nodes as y_f at time step k = T.

This definition is very similar to that of output controllability, the key difference being the constraint defined on C.

2.3 Energy metrics for target controllability

Let W be the controllability gramian of a network system \mathcal{G} and $C_{\mathcal{T}}WC'_{\mathcal{T}}$ be invertible. Then for any $y_f \in \mathbb{R}^p$, the sequence of inputs that steers the state from $x_0 = 0$, to the desired target state using the least energy in T steps is given by [2]

$$u^*[k] = B^T(A')^{T-1-k}C'_{\mathcal{T}}(C_{\mathcal{T}}WC'_{\mathcal{T}})^{-1}y_f,$$
$$k = \{1, 2, \dots, T-1\}.$$

Henceforth, we refer to $C_{\mathcal{T}}WC'_{\mathcal{T}}=W_{\mathcal{T}}$. We can verify that the control energy is given by $\sum_{i=0}^{T-1}u'[i]u[i]=y'_fW^{-1}_{\mathcal{T}}y_f$. Now, the unit energy reachable set is given by a hyperellipsoid $\{y_f\in\mathbb{R}^p|y'_fW^{-1}_{\mathcal{T}}y_f\leq 1\}$. Intuitively, a larger reachable set would mean lesser effort is required in controlling the network. Let λ_i,v_i be an eigen-pair for $W_{\mathcal{T}}$. For $y_f=cv_i$,

$$cv_i^T W_{\mathcal{T}}^{-1} cv_i \le 1 \iff c^2 \lambda_i^{-1} \le 1.$$

The axis lengths of the unit energy reachable space correspond to the square roots of the eigenvalues of W_T . Intuitively, a larger reachable set would mean lesser effort is required in controlling the network. Based on the eigenvalues of the gramian, several metrics have been proposed[3]. In our work, we limit ourselves to the following metrics.

1. The trace of the gramian $tr(W_T)$, has been interpreted as average controllability in previous work[4],[3], and is motivated by

$$\frac{p}{\operatorname{tr}(W_{\mathcal{T}})} \le \frac{\operatorname{tr}(W_{\mathcal{T}}^{-1})}{p}.$$

Here, the $\operatorname{tr}(W_{\mathcal{T}}^{-1})$ represents the average energy required to control the system in any direction. This metric is often dominated by the length of the largest axis of the hyperellipsoid. Specifically, when the smallest eigenvalue of the gramian $\lambda_1 \to 0$, the average controllability does not change much, despite the significant change in the ellipsoid. We also note that a high average controllability does not guarantee that $W_{\mathcal{T}}$ is full rank, or that the target is fully controllable.

2. The smallest eigenvalue of the gramian, $\lambda_{\min}(W_{\mathcal{T}})$ represents the shortest axis of the hyperellipsoid, and therefore the least controllable direction in the target space. Physically, the inverse of the smallest gramian represents the inverse of the worst case control energy.

2.4 Set functions, modular and submodular functions

We focus on selection of target node set to optimize the controllability metrics. We formulate the problems as a set function optimization. In this regard, we state the following definitions.

Definition 2.4.1. A set function $f: 2^V \to \mathbb{R}$ is said to be submodular if for all subsets $X \subseteq Y \subseteq V$ and all elements $s \notin Y$,

$$f(X \cup \{s\}) - f(X) \ge f(Y \cup \{s\}) - f(Y).$$
 (2.3)

A function f is said to be supermodular if -f is submodular.

A function is said to be modular, if equality holds in (2.3).

Definition 2.4.2. A set function $f: 2^V \to \mathbb{R}$ is said to be monotone increasing (non-decreasing) if for all subsets $X, Y \subseteq V$, $X \subseteq Y \implies f(X) \leq f(Y)$.

We use the following definition of a modular function[5].

Theorem 2.4.1 (Modularity,[5]). A set function $f: 2^V \to \mathbb{R}$ is modular if and only if for any subset $S \subseteq V$, it can be expressed as

$$f(S) = a(\phi) + \sum_{i \in S} a(i),$$
 (2.4)

for some weight function $a:V\to\mathbb{R}$ and ϕ denoting the null set.

Finally, we also intend to use the following property of submodular functions.

Proposition 1 ([6]). Let a function $f: 2^V \to \mathbb{R}$ be a non-decreasing submodular function of set $S, S \subseteq V$ and for any real number γ , the function

$$f_1(S) = min(f(S), \gamma).$$

Then, $f_1(S)$ is submodular function

2.5 Cauchy's Interlacing Theorem

We use Cauchy's Interlacing theorem [7] that relates the eigenvalues of a symmetric matrix to that of its submatrix.

Theorem 2.5.1. Let M be a $n \times n$ symmetric matrix. Let N = PMP', where $P \in \mathbb{R}^{m \times n}$ is an orthogonal projection matrix. If the eigenvalues of M are $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$, and those of N are $\mu_1 \leq \mu_2 \leq \ldots \leq \mu_m$. Let $j \in \{1, 2, \ldots, m\}$. Then, $\lambda_j \leq \mu_j \leq \lambda_{n-m+j}$. Specifically, when m = n - 1, we have $\lambda_j \leq \mu_j \leq \lambda_{j+1}$.

2.6 An extension to Cauchy Schwarz inequality

Lemma 2.6.1. Consider a symmetric, positive definite matrix $Q \in \mathbb{R}^{n \times n}$. For any $x \in \mathbb{R}^n$, $||x||_2 = 1$, we have

$$\mathbf{x}'Q\mathbf{x}\mathbf{x}'Q^{-1}\mathbf{x} \ge 1.$$

Since Q is positive definite and symmetric, it can be diagonalized by an orthogonal

matrix([7]), i.e,

$$Q=P'DP, \quad \text{and} \quad \label{eq:Q}$$

$$Q=P'D^{-1}P.$$

where P is orthogonal, and . Orthogonal matrices preserve norms, so $\|Px\|_2 = 1$. Let y = Px. The LHS of our inequality is now reduced to

$$y'Dyy'D^{-1}y = \sum_{i=0}^{n} d_i y_i^2 \sum_{i=0}^{n} \frac{y_i^2}{d_i},$$

where d_i is the i^{th} diagonal element of D.

Since Q is positive definite, $d_i > 0$, and since $\|y\|_2 = 1$, $\sum_{i=1}^n y_i^2 = 1$. Applying Cauchy-Schwarz,

$$\sum_{i=0}^{n} d_i y_i^2 \sum_{i=0}^{n} \frac{y_i^2}{d_i} \ge \sum_{i=1}^{n} \frac{\sqrt{i}}{\sqrt{i}} y_i^2 = 1.$$

CHAPTER 3

Modal and target controllability

3.1 Target Controllability

To motivate the problems addressed in this paper, we first show that controlling a target set rather than the entire network reduces the worst case control energy required. In our experiments on a random sparse connected graph with 20 nodes, and 2 driver nodes, the worst case control energy increased as the size of the target set increased, as illustrated in Figure 3.1. In this particular example, for a target involving 95% of the nodes the worst case energy drop by 97.41%. A target set involving 90% of the nodes had a drop of 99.7% in the worst case energy. It is seen that energy needed for control exponentially decay with the number of target nodes. This property can be verified from the Cauchy's interlacing Theorem 2.5.1, and is formally proved in [2].

In our first problem, we would like to select the set of target nodes such that the average controllability of the target set is maximized.

Problem 3.1.1. Given a network G, select a target set T of size p such that the target set T maximizes average controllability over all candidate sets T of size p. Formally, the problem is stated as

$$\underset{\mathcal{T} \subseteq \mathcal{V}}{\operatorname{arg \, max}} \quad tr(W_{\mathcal{T}}) \tag{3.1}$$

$$subject \ to \quad |\mathcal{T}| = p.$$

This problem is solved using Algorithm 3.1.3.1.

Next, we seek to solve the problems involving the worst case energy required to control the network.

Problem 3.1.2. Given a set of driver nodes K, and a worst case energy bound β^{-1} , find the largest possible set of target nodes T, such that the energy required to transfer the

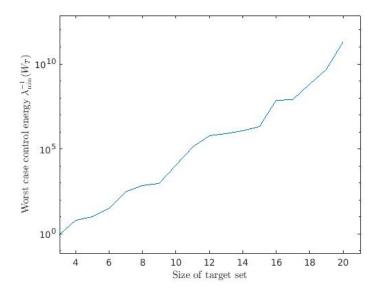


Figure 3.1: The worst case control energy vs Target set size

states of target nodes to one unit in any direction in the state space and does not exceed the worst case energy limit. Formally, the problem is stated as,

$$\max |\mathcal{T}|$$
subject to $\lambda_{\min}(W_{\mathcal{T}}) > \beta$. (3.2)

It is known that $\lambda_{\min}(W_{\mathcal{T}})$ is neither submodular nor supermodular function. We, therefore, state a sufficient condition for the constraint that involves a submodular monotone increasing function. This reduces the size of our constraint set, but allows us to use existing literature on submodular set functions. Our algorithm for this modified version of the problem is given in Algorithm 3.1.3.2. The final problem we are interested in involves bounding the size of the target set, and optimize the worst case control energy

Problem 3.1.3. . Given a network G of size n, and a limit on the number of target nodes $p, p \leq n$, we would like to find the best set of target nodes T of size p that maximizes $\lambda_{\min}(W_T)$. Formally, the problem is stated as

$$\max \quad \lambda_{\min}(W_{\mathcal{T}})$$
subject to $|\mathcal{T}| = p$. (3.3)

This problem is addressed in Section 3.1.3.3

3.1.1 Results

3.1.2 Modularity properties of Energy Based metrics

The following theorem analyzes the property of the average controllability with respect to the target node set.

Theorem 3.1.1. Given a network \mathcal{G} , let \mathcal{V}, \mathcal{T} be the set of nodes in \mathcal{G} , set of target nodes respectively and $C_{\mathcal{T}}$ be the output matrix corresponding to the target set \mathcal{T} . The set function $f: 2^{\mathcal{V}} \to \mathbb{R}$ that maps the subsets of \mathcal{V} to a real value is given by

$$f(\mathcal{T}) = tr\Big(C_{\mathcal{T}}\Big(\sum_{\tau=0}^{T-1} A^{\tau}BB'(A')^{\tau}\Big)C'_{\mathcal{T}}\Big),$$

is a modular function.

Proof.

$$\mathbf{tr}\Big(W_{\mathcal{T}}\Big) = \mathbf{tr}\Big(C_{\mathcal{T}}\Big(\sum_{\tau=0}^{T-1} A^{\tau}BB'(A')^{\tau}\Big)C'_{\mathcal{T}}\Big)$$
$$= \sum_{j\in\mathcal{T}}\Big(\sum_{\tau=0}^{T-1} A^{\tau}BB'(A')^{\tau}\Big)_{jj} = \sum_{j\in\mathcal{T}} \mathbf{tr}\Big(W_{\{j\}}\Big).$$

Since we show that the function is modular over the target set, we are guaranteed to get an optimal solution for any problem involving maximizing average controllability.

In order to solve problems involving worst case control energy, we introduce a function, that provides sufficient conditions for the constraints in our problems. We show that these functions, are submodular, and monotone increasing. Such an approach has been taken in [8]. However, the main focus in [8] is to select a set of driver nodes that maximizes the minimum eigenvalue of a submatrix of a Laplacian matrix, which is obtained after removing rows and columns corresponding to the input node set. Our aim is to find the maximum dimension of the target set such that minimum eigenvalue of the target controllability matrix is above a pre-specified threshold.

Lemma 3.1.1. For a symmetric matrix $H \in \mathbb{R}^{n \times n}$, let V be an indexed set of all columns, and $S \subset V$, and let $\alpha > |V||\max_{1 \leq i,j \leq n}(H_{ij})|$. Let $w \in \mathbb{R}^n \in N(0,I)$ be a vector, where N(0,I) is a gaussian normal variable. If

$$\mathbb{E}(\min w'(\alpha D(S) + H)w, 0) = 0,$$

then, $H(V \setminus S)$ is positive semidefinite.

Proof. Let us consider the function Q_1 defined as,

$$Q_1(S) = \mathbb{E}[\min(w'(H + \alpha D(S))w, 0)]. \tag{3.4}$$

Now, suppose that $H + \alpha D(S)$ is not positive semidefinite, and let there exist some set $U \in \mathbb{R}^n$, such that $u \in U$ if and only if $u'(H + \alpha D(S))u < 0$. Due to our assumption of $H + \alpha D(S)$ not being positive semidefinite, U is non empty. Let $f_w : \mathbb{R}^n \to \mathbb{R}$ represent the probability distribution of w. Now,

$$Q_1(S) = \int_{\mathbb{R}^n} \min(u'(H + \alpha D(S))u, 0) f_w(u) du$$

$$= \int_U \min(u'(H + \alpha D(S))u, 0) f_w(u) du$$

$$+ \int_{\mathbb{R}^n \setminus U} \min(u'(H + \alpha D(S))u, 0) f_w(u) du < 0, \tag{3.5}$$

where the last inequality follows because the first term is negative, and the second term is 0. This is a contradiction. Therefore, $H + \alpha D(S)$ is positive semidefinite. Now, by Cauchy's Interlacing Theorem, 2.5.1,

$$\lambda_{\min}(H + \alpha D(S)) \le \lambda_{\min}(H(V \setminus S)).$$

Therefore, if $Q_1(S) = 0$,

$$\lambda_{\min}(H + \alpha D(S)) \ge 0, \implies \lambda_{\min}(H(V \setminus S)) \ge 0.$$

The lower bound placed on α is motivated by a common upper bound used for the eigenvalues of H. The goal is to choose an α with magnitude greater than any

eigenvalue of H(S) for any $S \subseteq V$.

Lemma 3.1.2. For any positive α , a symmetric matrix $H \in \mathbb{R}^{n \times n}$, and a vector $w \in \mathbb{R}^n$; the function $Q_1(S)$ defined as

$$Q(S) = \mathbb{E}(\min(w'(\alpha D(S) + H)w, 0)) = 0,$$

is submodular, and monotone increasing.

A proof for this lemma is available in [8].

We use Lemma 3.1.1 and 3.1.2 to solve Problem 3.1.2. Since the lemma gives a sufficient condition for the constraint in the problem, we replace the constraint with this sufficient condition. While this shrinks the feasible set, the Q(S) we have chosen is still a reasonably tight bound for the constraint. However, since Lemma 3.1.1 is only applied to positive semidefinite matrices, using this for Problem 3.1.3 requires further manipulation, which is discussed later in Section 3.1.3.3.

3.1.3 Algorithms for selection of Target nodes for optimizing controllability metrics

3.1.3.1 Selection of target set for optimizing average controllablity

Given a network \mathcal{G} , the aim is to maximize average controllability for a set of target nodes. Formally, given a driver node set \mathcal{K} , we find a set of target nodes \mathcal{T} such that

$$\underset{\mathcal{T} \subseteq \mathcal{V}}{\operatorname{arg \, max}} \quad \operatorname{tr}(W_{\mathcal{T}}) \tag{3.6}$$
 subject to $|\mathcal{T}| \leq p$.

In other words, pick a target set containing at most p nodes that maximizes average controllability. We propose an algorithm with a guaranteed optimal solution in Algorithm 3.1.3.1. This algorithm is motivated by Theorem 3.1.1, where we show that average controllability is modular over the set \mathcal{T} .

Algorithm 1: For Choosing Optimal target nodes for maximizing average controllability

```
input: System matrices A, B, and the limit on the number of target nodes p output: A list of target nodes \mathcal{T} W \leftarrow \operatorname{gramian}(A, B) \mathcal{T} \leftarrow \{\} for i \leftarrow 1 to p do | \operatorname{temp} \leftarrow \operatorname{arg} \max\{W_{ii}, i \notin \mathcal{T}\} | \mathcal{T} \leftarrow \mathcal{T} \cup \{\operatorname{temp}\} end return \mathcal{T}
```

3.1.3.2 Maximizing the target set for a given bound on worst case control energy

We consider the following problem,

$$\max \quad |\mathcal{T}| \tag{3.7}$$
 subject to $\lambda_{\min}(W_{\mathcal{T}}) > \beta$,

where we would like to control as many nodes as possible, as long as our worst case control energy is bounded.

Let $\hat{W} = W - \beta I$. Using Lemma 3.1.1, a sufficient condition for the constraint is given by Q(S) = 0, where $S = \mathcal{V} \setminus \mathcal{T}$. Choosing α as per Lemma 3.1.1, our problem is equivalent to the following problem,

$$\min |S|$$
subject to $Q(S) = 0$, (3.8)

where $Q(S) = \mathbb{E}(\min(w'(\alpha D(S) + \hat{W})w, 0))$, and the expectation is taken over $w \in N(0, I)$. Further, from Lemma 3.1.2 we know that Q is submodular and monotone non decreasing. We propose a greedy algorithm proposed in Algorithm 3.1.3.2 to solve the problem. As shown in [9], this algorithm returns a set S such that

$$\frac{|S|}{|S^*|} \le 1 + \log \left(\frac{f(V) - f(\phi)}{f(V) - f(S_{T-1})} \right),$$

where S^* is the optimal solution, and S_{T-1} is the set returned at the second-to-last iteration of the algorithm.

Algorithm 2: For Choosing Optimal target nodes given a worst case energy constraint

```
input: system matrices A, B, \beta

output: A list of target nodes \mathcal{T}

Choose \alpha as per Lemma 3.1.1

W \leftarrow \operatorname{gramian}(A, B)

\hat{W} \leftarrow W - \beta I

S \leftarrow \{\}

while Q_1(S) < 0 do

v^* \leftarrow \operatorname{arg max}\{Q_1(S \cup \{v\}), v \notin S\}

S \leftarrow S \cup \{v^*\}

end

return \mathcal{V} \setminus S
```

3.1.3.3 Minimizing the worst case control energy for a fixed set of target nodes

We consider the following problem,

$$\max \quad \lambda_{\min}(W_{\mathcal{T}}) \tag{3.9}$$
 subject to $|\mathcal{T}| = p$,

where the input nodes, and the number of target nodes p are known. Our algorithm attempts to select the best possible target set to minimize the worst case energy.

 λ_{\min} is neither submodular nor supermodular over the set of target nodes. Therefore, we cannot directly use a greedy algorithm for this problem. Instead, we use Lemma 3.1.1 and 3.1.2 to resolve this problem. Our approach is motivated by extending the previous method, by adapting Algorithm 3.1.3.2, for a changing β . Specifically, every time we add an element to S, we set $\beta = \lambda_2$ where λ_2 is the second smallest eigenvalue of $W + \alpha D(S)$. Practically over large sparse random networks, we also observe that Q(S) rarely crosses 0. This is primarily because gramians for such large networks have eigenvalues spaced reasonably far apart, For example in Figure 3.1, dropping just one node increased the smallest eigenvalue by two orders of magnitude. Improving this algorithm with better optimality bounds is an important direction in future work.

Algorithm 3: For Choosing Optimal target nodes to minimize worst case energy

3.2 Modal Controllability

In this section, we propose modal controllability metrics for both continuous and discrete time systems. The definition of the metric is different in both cases due to the change in the closed form expression of the controllability gramian.

3.2.1 Notation

We represent a continuous linear time invariant system (C-LTI system) by

$$\dot{\mathbf{x}} = A\mathbf{x} + B\mathbf{u},\tag{3.10}$$

and a discrete linear time invariant (D-LTI) system by

$$\mathbf{x}^+ = A\mathbf{x} + B\mathbf{u}.\tag{3.11}$$

In both cases, $\mathbf{x} \in \mathbb{R}^n$ represents the state of a system, $A \in \mathbb{R}^{n \times n}$ is a system matrix, and $B \in \mathbb{R}^{n \times m}$ is termed as an input matrix. $\mathbf{u} \in \mathbb{R}^m$ is the control input.

3.2.2 Continuous time LTI systems

We first present a lower bound on control energy required to control a given mode.

Consider a continuous time LTI system (3.10), and assume that (A, B) is controllable. Let \mathbf{v}_i be a left eigenvector of A, such that $\|\mathbf{v}_i\| = 1$, associated with the eigenvalue λ_i . Let the optimal energy required to traverse one unit in the direction of \mathbf{v}_i be E_i , for a horizon time t, starting from the origin. Then,

$$E_i \ge \left(\mathbf{v}_i'BB'\mathbf{v}_i\frac{e^{2\lambda_i t}-1}{2\lambda_i}\right)^{-1}$$

The optimal control energy for a system to reach v_i starting from the origin is given by

$$E_i = \mathbf{v}_i' W_c^{-1} \mathbf{v}_i$$

where W_c is the controllability gramian. Since (A, B) is controllable, the controllability gramian is symmetric and positive definite. By Lemma 2.6.1, we have

$$E_i \mathbf{v}_i' W_c \mathbf{v}_i \ge 1. \tag{3.12}$$

The controllability gramian, for a time horizon t is given by,

$$W_c(t) = \int_0^t e^{A\tau} BB' e^{A'\tau} d\tau$$

Therefore,

$$\mathbf{v}_i' W_c(t) \mathbf{v}_i = \mathbf{v}_i' \left(\int_0^t e^{A\tau} B B' e^{A'\tau} d\tau \right) \mathbf{v}_i$$

Now, considering $e^{A'\tau}\mathbf{v}_i$, and expanding as per Taylor series, we have

$$e^{A'\tau} \mathbf{v}_i = \left(\sum_{k=0}^{\infty} \frac{(A'\tau)^k}{k!}\right) \mathbf{v}_i$$
$$= \left(\sum_{k=0}^{\infty} \frac{(A')^k \mathbf{v}_i \tau^k}{k!}\right)$$
$$= \left(\sum_{k=0}^{\infty} \frac{\lambda_i^k \tau^k \mathbf{v}_i}{k!}\right)$$
$$= e^{\lambda \tau} \mathbf{v}_i$$

Using this result, we have,

$$\mathbf{v}_{i}'W_{c}(t)\mathbf{v}_{i} = \int_{0}^{t} e^{\lambda_{i}\tau} \mathbf{v}_{i}'BB'\mathbf{v}_{i}e^{\lambda_{i}\tau}d\tau$$
$$= \mathbf{v}_{i}'BB'\mathbf{v}_{i}\frac{e^{2\lambda_{i}t} - 1}{2\lambda_{i}}$$

From Equation (3.12) and the equation above, the theorem follows. Based on this theorem, we define a metric for controllability of C-LTI systems. Let M_i be the metric to control the i^{th} mode using a given input and a time horizon t, defined as,

$$M_i(t) = \left(\mathbf{v}_i' B B' \mathbf{v}_i \frac{e^{2\lambda_i t} - 1}{2\lambda_i}\right)$$

where B is the input matrix, and \mathbf{v}_i is the normalized eigenvector associated with the i^{th} mode, and λ_i is the eigenvalue associated with the i^{th} mode.

Since our metric is a function of the eigenvalue, it quantifies difficulty to control along a particular mode. It can be used to quantify the difficulty of controlling more than one mode as well. For the setup described in Theorem 1, we have

$$\sum_{i \in \mathcal{T}} E_i \ge \left(\sum_{i \in \mathcal{T}} \frac{1}{M_i(t)}\right),\,$$

for a set of modes \mathcal{T} . Motivated by this inequality, we define, to control a set of modes \mathcal{T} ,

$$M(\mathcal{T},t) = \left(\sum_{i \in \mathcal{T}} \frac{1}{M_i(t)}\right)^{-1}.$$

We also note that if the system is stable, all the eigenvalues have a negative real part. In this case we extend our metric to the infinite horizon case, as $t \to \infty$, and if A is stable,

$$\sum_{i \in \mathcal{T}} E_i \ge \sum_{i \in \mathcal{T}} \left(\mathbf{v}_i' B B' \mathbf{v}_i \frac{1}{2|\lambda_i|} \right)^{-1},$$

where the inequality follows as finite horizon energy control is always higher than the infinite horizon case.

3.2.3 Discrete Time LTI Systems

We extend these ideas to discrete time systems, starting with a lower bound for control energy along a mode in the discrete time case. Let us consider a discrete time LTI system (3.11) and assume (A, B) is controllable. Let \mathbf{v}_i be a left eigenvector of A, associated with the eigenvalue λ_i . Let the optimal energy required to traverse one unit in the direction of \mathbf{v}_i be E_i , for a time horizon t, starting from the origin. Then,

$$E_i \ge \left(\mathbf{v}_i' B B' \mathbf{v}_i \frac{1 - \lambda_i^{2(t+1)}}{1 - \lambda_i^2}\right)^{-1}.$$

The optimal control energy for a system to reach v_i starting from the origin is given by

$$E_i = \mathbf{v}_i' W_c^{-1}(t) \mathbf{v}_i,$$

where W_c is the controllability gramian. Since (A, B) is controllable, the controllability gramian is symmetric and positive definite. By Lemma 2.6.1, we have.

$$E_i \mathbf{v}_i' W_c(t) \mathbf{v}_i \ge 1. \tag{3.13}$$

The controllability gramian, for a time horizon t is given by ,

$$W_c(t) = \sum_{k=0}^t A^k B B'(A')^k.$$

Therefore,

$$\mathbf{v}_{i}'W_{c}(t)\mathbf{v}_{i} = \mathbf{v}_{i}'\left(\sum_{k=0}^{t} A^{k}BB'(A')^{k}\right)\mathbf{v}_{i}$$

$$= \sum_{k=0}^{t} \mathbf{v}_{i}'A^{k}BB'(A')^{k}\mathbf{v}_{i}$$

$$= \mathbf{v}_{i}'BB'\mathbf{v}_{i}\sum_{k=0}^{t} \lambda_{i}^{2k}.$$

The theorem follows from Equation (3.13) and the above equation. Based on this theorem, we define another metric for discrete time systems. We consider the following

metric M_i^d to control the i^{th} mode for a given input matrix B, for a time horizon t,

$$M_i^d(t) = \left(\mathbf{v}_i' B B' \mathbf{v}_i \frac{1 - \lambda_i^{2(t+1)}}{1 - \lambda_i^2}\right)^{-1}.$$

Similar to the continuous time case, we extend this notion to multiple modes. For the setup described in Theorem 3, we have

$$\sum_{i \in \mathcal{T}} E_i \ge \sum_{i \in \mathcal{T}} \left(\mathbf{v}_i' B B' \mathbf{v}_i \frac{1 - \lambda^{2(t+1)}}{1 - \lambda_i^2} \right)^{-1}.$$

The proof for this statement follows from the theorem, by summing across modes. Subsequently, we define the following metric across modes. For a given set of modes, \mathcal{T} and a time horizon t, we have,

$$M^d(\mathcal{T}, t) = \left(\sum_{i \in \mathcal{T}} \frac{1}{M_i^d(t)}\right)^{-1}.$$

In the limiting case, as $t \to \infty$, when A is stable, we have,

$$\sum_{i \in \mathcal{T}} E_i \ge \sum_{i \in \mathcal{T}} \left(\mathbf{v}_i' B B' \mathbf{v}_i \frac{1}{1 - \lambda_i^2} \right)^{-1},$$

based on a similar argument to the C-LTI case.

3.2.4 Discussion

In this section, we discuss the factors affecting our defined metrics, and discuss their relationship with existing metrics.

3.2.5 Factors affecting the metric

A lower bound for the energy required to control a mode, in both the discrete and the continuous time case, is inversely related to $\mathbf{v}_i B B' \mathbf{v}_i$. Since the eigenvector \mathbf{v}_i is normalized, this term only depends on the magnitude of the columns in the input matrix, and the angle between the column of the input matrix and the eigenvector. This is in line with the PBH test, as when the two vectors are orthogonal, the system is uncontrollable.

Further, a key feature of our metric is the ability to compare the ease of controlling a system across modes. This allows us to study optimization problems where we consider the optimization of the ease of control across a range of modes. Specifically, in the discrete case, we note that modes with eigenvalues closer to unity are easier to control. This is in part due to the natural response of the system. This result is consistent with the findings in [10] for the case of continuous time systems.

3.2.5.1 Similarity to past metrics

In [11], the cosine of the angle between an input column and the modal vector is declared as a metric. Our metric is strongly correlated with that metric, but our metric has the added benefit of allowing comparison across modes. Specifically, while considering the modal controllability of the i^{th} mode from the j^{th} input column, if we consider the metric in [11], it is given by $\cos(\theta)_{ij}$. Whereas our metric for controlling the i^{th} mode from the j^{th} input is:

$$M_i = \frac{\|\mathbf{b}_j\|^2 \cos^2(\theta)_{ij}}{1 - \lambda_i^2},$$

where \mathbf{b}_j is the j^{th} input, and λ_i is the eigenvalue associated with the i^{th} mode.

3.2.5.2 Similarity to eigenvector centrality

We extend our ideas to linear network systems, by studying the relationship between our metric and the eigenvector centrality measure. In network science, there are several centrality measures ([12]) such as degree, pagerank, and eigenvector centrality among others. Specifically we focus on the eigenvector centrality measure. The eigenvector centrality measure computes the influence of a node in a network. In practice, this centrality measure can be represented by the entries of the dominant eigenvector of the adjacency matrix. Specifically, if the dominant eigenvalue is λ , and the associated eigenvector is \mathbf{v} , the centrality measure of the i^{th} node is given by \mathbf{v}_i . In the case of linear network systems, each column of the B matrix is a canonical vector. Therefore, our metric for infinite horizon, for the control of the dominant mode from the i^{th} input

reduces to

$$M_{dom} = \frac{\mathbf{v}_i^2}{1 - \lambda^2}. (3.14)$$

We show that this is true for a 100 node Erdos-Renyi random network ([13]), by plotting M_{dom} against the eigenvector centrality in Fig. 3.2.

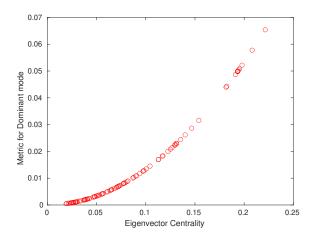


Figure 3.2: The eigenvector centrality vs Our metric

3.2.6 Algorithms for controllability

In this section, we formulate and propose solutions to two main problems involving the metric. We restrict our analysis to network systems with discrete time LTI dynamics in the infinite horizon case, but the same analysis can be extended to continuous time systems and finite horizon cases as well.

3.2.6.1 Identification of driver nodes

We first consider the problem of identification of the best driver nodes, to minimize the lower bound on the control effort required to move along a given mode i. Formally, given a mode \mathbf{v}_i , and a constraint of selecting any k driver nodes, we intend to minimize the inverse of our metric,

$$\min \quad \left(\mathbf{v}_i' B_{\mathcal{K}} B_{\mathcal{K}}' \mathbf{v}_i \frac{1}{1 - \lambda_i^2}\right)^{-1}$$
 subject to $|\mathcal{K}| = k$.

Since $B_{\mathcal{K}}B'_{\mathcal{K}} = \sum_{j \in \mathcal{K}} \mathbf{b}_j \mathbf{b}'_j$ for a network system, our problem reduces to

$$\min \quad \left(\sum_{j \in \mathcal{K}} \mathbf{v}_i' \mathbf{b}_j \mathbf{b}_j' \mathbf{v}_i \frac{1}{1 - \lambda_i^2}\right)^{-1}$$
 subject to $|\mathcal{K}| = k$.

Since $\frac{1}{1-\lambda_i^2}$ is a constant for a given mode, and $\mathbf{v}_i'\mathbf{b}_j\mathbf{b}_j'\mathbf{v}_i = \left\|\mathbf{b}_j'\mathbf{v}_i\right\|_2^2 \geq 0$, the problem can be restated as,

$$\max \left(\sum_{j \in \mathcal{K}} \mathbf{v}_i' \mathbf{b}_j \mathbf{b}_j' \mathbf{v}_i \right)$$
 subject to $|\mathcal{K}| = k$.

The function being maximized here is of the form described in Theorem 2.4.1. Therefore, this problem can be solved by using a sorting algorithm and choosing the nodes associated with the top k values of $\mathbf{v}_i'\mathbf{b}_j\mathbf{b}_j'\mathbf{v}_i$.

3.2.6.2 Identification of easy to control modes

For our second problem, we assume that the driver nodes are fixed, and we seek to identify the top m modes that are easiest to control. Formally, we express our optimization problem as

$$\min \quad \sum_{i \in \mathcal{T}} \left(\mathbf{v}_i' B B' \mathbf{v}_i \frac{1}{1 - \lambda_i^2} \right)^{-1}$$
 subject to $|\mathcal{T}| = m$.

This can also be converted to a maximization problem,

$$\max \sum_{i \in \mathcal{T}} \left(\mathbf{v}_i' B B' \mathbf{v}_i \frac{1}{1 - \lambda_i^2} \right)$$
 subject to $|\mathcal{T}| = m$. (3.16)

This problem also involves the maximization of a modular function, as the function being optimized is of the form described in Theorem 2.4.1. This problem can also be solved by a sorting algorithm, by computing $\mathbf{v}_i'BB'\mathbf{v}_i\frac{1}{1-\lambda_i^2}$. for each mode, and selecting the top m modes.

3.2.7 Numerical Example

We consider a network following the topology of the IEEE-14 bus system given in [14] as an illustrating example. The network consists of 14 buses represented as nodes and 20 transmission lines that constitute the edges of the network. Similar to [15], we choose symmetric edge weights corresponding to resistance values of transmission lines that connect the buses in the power grid, as shown in Figure 3.3. The objective is to

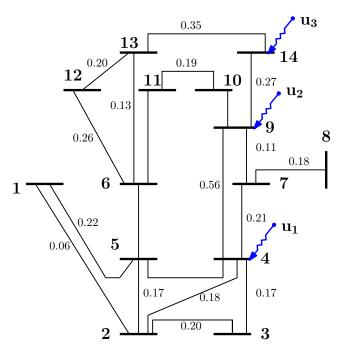


Figure 3.3: Network topology of IEEE-14 bus system. Thick lines represent buses and thin lines are transmission lines.

choose k driver nodes where k=3, which minimizes the lower bound on control effort required to move along the dominant mode of the system. In this example, the dominant mode is corresponding to the eigenvalue 0.764. Since the adjacency matrix is a stable matrix, we compute the functional value of the objective function given in (3.15) for each input node and sort them in descending order of their contribution. The best 3 nodes that minimize the lower bound on energy required to drive the system along the direction of the dominant mode are 4, 9, 14, respectively. In the second experiment, we choose node 4 as a driver node. We are interested in identifying the top m modes(m=3) that are easiest to control from the driver node 4. We compute the objective function in

(3.16) for each mode and sort them in decreasing order. In this case, the best 3 modes that the input at node 4 can drive with little effort are correspond to eigenvalues 0.764, -0.681, -0.383.

CHAPTER 4

Oscillator networks And Brain networks

4.1 Mathematical Analysis of the networked Hopf Model

The system equations are given by

$$\dot{x}_n = (a_n - x_n^2 - y_n^2)x_n - \omega_n y_n + G \sum_{p=1}^N C_{np}(x_p - x_n) + \beta_n \eta_n + u_n$$
 (4.1)

$$\dot{y}_n = (a_n - x_n^2 - y_n^2)y_n + \omega_n x_n + G \sum_{p=1}^N C_{np}(y_p - y_n) + \beta_n \eta_n$$
(4.2)

On converting to polar coordinates (r_n, θ_n) , ignoring the noise term, we have for \dot{r}_n ,

$$r_n \dot{r}_n = x_n \dot{x}_n + y_n \dot{y}_n$$

$$r_n \dot{r}_n = (a_n - r_n^2) r_n^2 + G \sum_{p=1}^N C_{np} (x_p x_n - x_n^2 + y_p y_n - y_n^2) + x_n u_n$$

$$r_n \dot{r}_n = (a_n - r_n^2) r_n^2 + G \sum_{p=1}^N C_{np} (r_n r_p \cos(\theta_p - \theta_n) - r_n^2) + u_n r_n \cos \theta_n$$

$$\dot{r}_n = (a_n - r_n^2) r_n + G \sum_{p=1}^N C_{np} (r_p \cos(\theta_p - \theta_n) - r_n) + u_n \cos \theta_n$$

For $\dot{\theta}_n$,

$$(\sec^2 \theta_n)\dot{\theta}_n = \frac{\dot{y}_n x_n - \dot{x}_n y_n}{x_n^2}$$

$$\frac{\dot{\theta}_n}{\cos^2 \theta_n} = \frac{\omega_n r_n^2 + G \sum_{p=1}^N C_{np} (x_n y_p - x_p y_n) - y_n u_n}{x_n^2}$$

$$\dot{\theta}_n = \omega_n + G \sum_{p=1}^N C_{np} \frac{r_p}{r_n} \sin(\theta_p - \theta_n) - \sin \theta_n \frac{u_n}{r_n}$$

The equations in when written in polar form lead to the Kuramoto oscillator equations. This result has some interesting consequences discussed in Chapter 5.

4.2 Functional and Structural Matrices

Within the human brain, connections are rapidly evolving and only some connections are active at any given point of time, depending on the task being performed by the brain. Further, The nonlinearities appearing in large scale complex networks may often have unknown dynamics. As a result, The adjacency matrix of the system alone is not enough to quantify the system. In order to derive properties of the system due to internal dynamics and external stimulus, a new connectivity matrix must be generated. In the context of brain networks, this connectivity matrix is referred to as the functional matrix and is derived using information theoretic measures.

In literature [16], [17], the main methods of quantifying these connections are cross correlations and transfer entropy.

Since the Hopf model tends to synchronize phases, cross correlations aren't a good measure of connectivity. Instead, Transfer entropy is a better measure of the connectivity in our particular use case. Further, Transfer entropy is also asymmetric, and therefore induces a sense of causality into our connectivity matrix.

CHAPTER 5

Applications to Brain Networks

5.1 Experimental Setup

In our experiments, we consider an underlying structural matrix generated using the Watts Strogatz Model, for N=11 nodes. We run a simulated version of the Hopf dynamical system for t=0 to t=2 seconds. For the first second (0<= t<1), the stimulus is in a low state. For the next second (1<=t<=2), we increase the stimulus to a high state. The stimulus is fixed beforehand, and is scaled based on whether the system is supposed to be in a high state or a low state. Based on the generated time series, we construct two functional state matrices, one representing a low state, and another representing a high state. These matrices represent a functional connectivity matrix whose edge weights are obtained by calculating transfer entropy between the time series for two regions, followed by a sparsification procedure. The average controllability of each node in both matrices is computed. Our approach is summarized in Figure 5.1

5.2 Design Choices

We made several design choices in our experimental setup which are described below

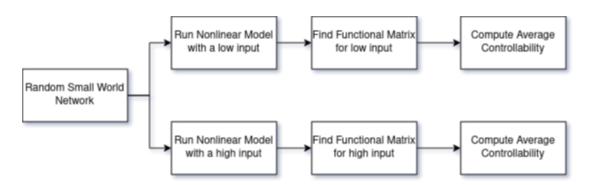


Figure 5.1: The Experimental Setup

5.2.1 The Watts Strogatz model

We use the Watts Strogatz Model to generate small world networks. This is because the structural network in a real brain also shares a similar degree distribution.

5.2.2 Transfer Entropy is a better option than cross correlations

We choose Transfer Entropy as it captures causality and is asymmetric in nature, and hence is a better estimate of connection strengths.

5.2.3 Stimulus Levels

Given two functional states, we define generated by the stimulus with a lower L-2 norm as the Low state, and the other one as a High State. The Dynamics of the Low state are not dominated by the stimulus, and as a result, the system is more easily controllable.

5.3 Results

5.3.1 Validation of the use of Hopf and Kuramoto Models

First, we validate the use of the Hopf Model. Particularly, we aim to replicate the empirical results observed in [1]. In [1], an observation is made linking more complex tasks to a decrease in overall controllability of the brain network. In our case, we model a complex task using a perturbation of larger magnitude, represented by the high state. The low state represents a task with significantly lower magnitude. As shown in the figure, the low state has a higher controllability. This is depicted in Figure fig. 5.2.

5.3.2 Functional and Structural Matrices

We claim that the functional matrix and the structural matrix are independent entities. The functional matrix is computed using information theoretic measures applied on the time series data generated using the underlying model being used. The structural matrix

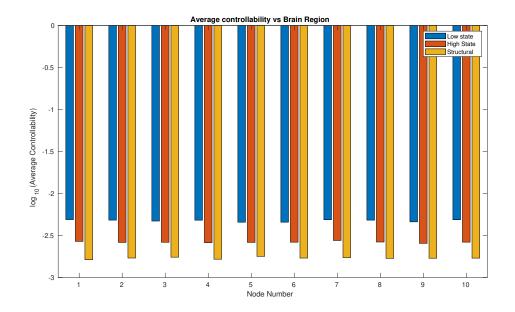


Figure 5.2: Controllability vs task complexity

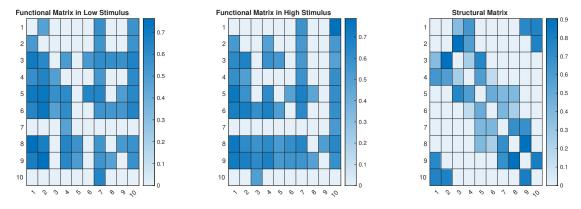


Figure 5.3: Functional and Structural Matrices

represents the underlying physical connections in the brain. For our experiment, we consider a small world structural network as shown in the Figure fig. 5.3. We note the formation of causal hubs in the functional matrix that represents a hierarchical structure among the different nodes. For example, nodes 8 and 9 are hubs in the high state, whereas the structural matrix has no key hubs. This is depicted in Figure fig. 5.3. In a real brain, this would mean that our brain has a different set of connections active depending on the task, and the brain network is continuously rewiring depending on the task it is performing and its complexity.

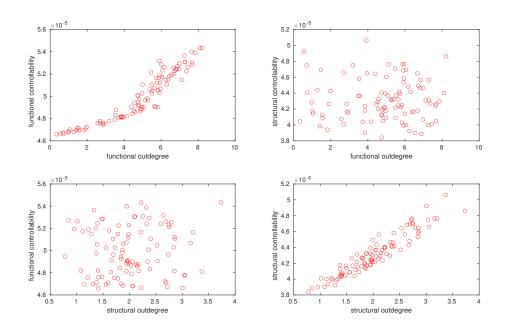


Figure 5.4: Functional and Structural Controllability

5.3.3 Functional and Structural Controllability

To further drive home the difference between functional and structural controllability, we show that functional controllability is correlated with functional outdegree, and not structural outdegree. Similarly, structural controllability is correlated with structural outdegree and not functional outdegree. This is depicted in Figure fig. 5.4.

CHAPTER 6

Conclusion and Future work

In this thesis, we considered the study of networked systems from the perspective of linear networks and nonlinear networked systems, in the context of brain networks. In the analysis of Linear networks, we considered the problem of target controllability and modal controllability.

For target controllability, we have considered the problem of optimal selection of target nodes in complex dynamical networks. We considered two energy related metrics, namely average controllability and worst case control energy. In general, these problems involve combinatorial optimization. However, we have related these metrics to set functions that are either modular, or submodular. This allows us to use a greedy algorithm for an optimal or near optimal solution. Future work will include finding better bounds on the least eigenvalue, that give some guarantees regarding the tightness of the bounds. We will also work on extending these ideas to other gramian based metrics.

We have also considered the problem of modal controllability for large scale systems. We define two energy related metrics, which serve as a lower bound for the control effort required to move along a given mode. We extend our metric to cover multiple modes of the network system. We study the relationship of these metrics with existing metrics and other centrality measures, showing that it is closely related to the eigenvector centrality. We also formulate two problems regarding the optimization of the metrics, in an effort to minimize the control effort required. Our approach to solve these problems are illustrated using a power network example.

In the context of brain networks, we validate the use of two nonlinear oscillatory models using a property relating controllability and task complexity. We define a functional matrix in the context of these states, and compare it with the structural states, in an attempt to show that the functional state captures properties of the system that are not visible in the structural state. Cognitively demanding task conditions reveal large scale functional patterns. Different functional states exhibit varying controllability properties, reflecting different cognitive functions. These task dependent variations

of functional states can serve as a means to identify various neurological disorders. In the future, diseases could be modelled by forcing synchronization/de-synchronization of regions in the nonlinear model, and we could calculate what stimuli returns the brain to a normal state.

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