

To the Graduate Council:

I am submitting herewith a dissertation written by Rachel Natalie Graves entitled “A Method to Accomplish the Optimal Control of Continuous Dynamical Systems with Impulse Controls via Discrete Optimal Control and Utilizing Optimal Control Theory to Explore the Emergence of Synchrony.” I have examined the final electronic copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Mathematics.

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**A Method to Accomplish the Optimal
Control of Continuous Dynamical Systems
with Impulse Controls via Discrete Optimal
Control and Utilizing Optimal Control
Theory to Explore the Emergence of
Synchrony.**

A Dissertation
Presented for the
Doctor of Philosophy
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Rachel Natalie Graves
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Dedication

To Viggo.

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Abstract

This research concerns the development of new optimal control methodologies and applications. In the first chapter we consider systems of ordinary differential equations subject to a restricted number of impulse controls. Examples of such systems include tumor growth, in which case the impulsive control is the administration of medication, and ecological invasion, in which case the impulse control is the release of predator species. Impulse control problems are typically solved via related partial differential equations known as quasi-variational inequalities. We show that these types of impulse control problems can be formulated as a discrete optimal control problems. Furthermore, this formulation is advantageous because it simplifies numerical calculations. In the second chapter we consider how optimal control can be used to investigate the emergence of synchrony in networks of coupled oscillators. In particular, we apply optimal control to a network of Kuramoto oscillators with time-varying coupling in order to relate network synchrony to network connectivity. To the best of our knowledge this is the first such use of optimal control theory.

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Chapter 1

Introduction

Optimal control theory has been used to address problems in the fields of medicine, finance, logistics, ecology, wild life management, public policy, and robotics to name a few [4, 16, 29, 15]. As a result, the theory, which was originally developed to treat systems of ordinary differential equations, has been adapted to treat models described by partial differential equations, stochastic differential equations, difference equations, differential equations with measures, and discrete-continuous or hybrid systems[16, 15, 29, 2, 20]. That said, there are two prominent strategies for solving optimal control problems, Pontryagin's Maximum Principle and dynamic programming. When employing the first strategy, the optimal control is characterized in terms of the optimal state and adjoint variables through the fact that it maximizes a certain function called the Hamiltonian. When employing the second strategy, the principle of optimality is used to derive the partial differential equation that governs the value function. The optimal control is then characterized in terms of the optimal state through the format of the value function. In this thesis we adapt optimal control theory to better treat a specific class of impulse control problems, and then use optimal control theory to investigate the emergence of synchrony in a network of coupled oscillators.

In the second chapter of this dissertation we consider how optimal control theory can be tailored to better address a specific class of impulse control problems. These problems take place on a finite time horizon $[0, T]$. The state is governed by a system of ordinary differential equations and a control which instantaneously alters its value at discrete times. The number of impulses, and the value of the impulses are bounded, while the times at which the impulses occur are chosen freely. An impulse control consists of a sequence of vectors $\{u_i\}$, $i = 0, \dots, N - 1$, which determine the value of the impulses and a sequence of times $\{T_i\}$, $i = 1, \dots, N$, at which the impulses occur. We require that $T_N = T$, and define $T_0 = 0$.

Given an impulse control, the state dynamics are as follows:

For $i = 0, \dots, N - 1$, and $t \in (T_i, T_{i+1})$

$$\dot{x}(t) = g(x, t),$$

$$x(T_{i+1}^+) = G(x(T_{i+1}^-), u_i),$$

$$x(0) = c_0,$$

In the equations above $x(t)$ is the value of the state, the continuous dynamics are described by the function $g(x, t)$, the discrete dynamics are described by the function $G(x, u_i)$, and N is the number of impulses that can occur. In addition, $x(T_{i+1}^+)$ is the value of the state just after control vector u_i is applied, while $x(T_{i+1}^-)$ is the value of the state just before control vector u_i is applied. Examples

of such problems include the control of tumor growth through the administration of medication, and the control of an invasive species through the release of predator species. We will solve two example impulse control problems. In the first problem a population of invasive plants is controlled by the removal of vegetation. In the second problem, mold is controlled by the application of fungicide.

In order to have a concrete reference in the discussion that follows we will describe the fungicide example now. In this example, the state has two components, x^1 and x^2 , which represent the concentration of fungus and fungicide respectively. Given a sequence of control vectors and times $\{u_i\}$, $i = 0, \dots, N-1$ and times $\{T_i\}$, $i = 0, \dots, N$ the state dynamics are as follows:

For $i = 0, \dots, N-1$, and $t \in (T_i, T_{i+1})$

$$\frac{dx^1}{dt} = r(M - x^1(t)) - x^1(t)x^2(t),$$

$$\frac{dx^2}{dt} = -kx^2(t),$$

$$x^2(T_{i+1}^+) = x^2(T_{i+1}^-) + u_i,$$

$$x^1(0) = x_0^1,$$

$$x^2(0) = x_0^2.$$

The objective functional for the problem is

$$J(u) = \sum_{i=0}^{N-1} u_i^2 + x_1(T).$$

Impulse control problems can be solved via dynamic programming [2, 4]. The value function Φ is then characterized by a partial differential equation termed a quasi-variational inequalities (Q.V.I.). Unfortunately, Q.V.I.s are often fully nonlinear, and difficult to solve numerically. For example, the Q.V.I. that characterizes the value function of the fungicide example is:

$$\max \left\{ \frac{\partial \Phi}{\partial t} - \frac{\partial \Phi}{\partial x^1} (r(M - x^1) - x^1 x^2) - \frac{\partial \Phi}{\partial x^2} (-kx^2), \Phi(x, t) - M\Phi(x, t) \right\} = 0$$

$$\Phi(x, T) = x^1(T),$$

where

$$M\Phi(x, t) = \inf_{0 \leq u \leq 1} [Bu^2 + \Phi((x^1, x^2 + u), t)]$$

A second method of solving impulse control problems with a restricted number of impulses is developed in [16]. In this method, termed the method of discontinuous time change, the original optimal impulse control problem is transformed to an auxiliary continuous control problem. An application of Pontryagin's Maximum Principle to the auxiliary problem allows one to characterize the optimal impulse controls for the original problem. This method, however, requires the impulse function to satisfy certain robustness conditions.

In the next chapter we show how impulse control problems with a restricted number of impulses can be formulated as discrete optimal control problems. This formulation is advantageous because it simplifies numerical calculations. As noted in [16], impulse control problems with a restricted

number of impulses can be formulated as nonlinear programming problems. An application of a Kuhn-Tucker type theory to the reformulated problem yields optimality conditions[6]. Although it can be difficult to solve nonlinear programming problems numerically, discrete optimal control problems are highly structured nonlinear programming problems. As a result of their additional structure, the Kuhn-Tucker theory yields considerably more information when it is applied to discrete optimal control problems. This information allows optimal controls to be characterized in terms of adjoint variables and the corresponding states. Optimal controls are then found numerically by using a forward backward sweep algorithm [15].

Previously, Pierce and Schumitzky used nonlinear programming to solve impulse control problems with a restricted number of impulses [18, 19]. Their method of solution, however, applies only to linear systems, as their primary objective was to handle continuous state constraints. The method of solution that we present in chapter two applies to both linear and nonlinear systems.

In the third chapter of this thesis we consider how optimal control can be used to investigate the emergence of synchrony in networks of coupled oscillators. Many biological networks are known to exhibit synchrony. However, it is difficult to identify the mechanisms of biological synchrony because it is often impossible to directly observe the network topology, the functional form of the inter-oscillator coupling, or the roster of network members. For this reason, biological researchers have employed mathematics to glean information about network structures from empirical observations of network dynamics. For example, Ermentrout and Kopell were able to characterize the structure of the swimming central pattern generator of the lamprey eel by analyzing its dynamics [13]. Meanwhile, mathematicians have devised methods to analyze the existence and stability of a network's various synchronous states as a function of the network's parameters. Much attention has been devoted to one network in particular, the Kuramoto network [14, 1, 25, 12]. The Kuramoto network is a famous system of differential equations that is used to model emergent synchrony. Meaning that, whatever the initial distribution of oscillators' phases, if the inter-oscillator coupling is strong enough the oscillators will assume similar phases. Because this model is so tractable we employ a variation of it in our analysis.

The Kuramoto model is a system of nonlinear, coupled, ordinary differential equations:

$$\frac{dx_i}{dt} = \omega_i + \frac{K}{N} \sum_{k=1}^N \sin(x_j(t) - x_i(t)),$$

where N is the number of oscillators in the network, x_i is the phase of the i th oscillator and ω_i is the natural velocity of the i th oscillator. The coefficient, K , is called the coupling strength.

To quantify the network's state it is useful to introduce the complex valued order function,

$$r(t)e^{i\psi(t)} = \frac{1}{N} \sum_{j=1}^N e^{ix_j(t)}.$$

The angle, ψ , corresponds to the centroid of the oscillator phases [25]. The magnitude, r , of the order function provides a convenient measure of network synchrony, with $r(t) = 1$ corresponding to collective synchrony, and $r(t) = 0$ corresponding to incoherence (i.e. the oscillators' phases are evenly distributed around the unit circle). We will refer to $r(t)$ as the order parameter.

Many papers have explored the stability of the network's steady states in the limit as the number of oscillators in the network tends to infinity [1, 25, 27, 28]. More recent works have focused on the dynamics of networks with a finite number of oscillators, and on networks with time varying

coupling [1, 24, 34]. These papers share the primary goal of establishing sufficient conditions for the stability of the synchronization manifold, in terms of the strength with which the oscillators are coupled. In this research we focus instead on network objectives. Our analysis is accomplished via optimal control theory. Optimal control theory is an obvious way to achieve synchronization in man-made physical networks. Our goal, however, is to adapt optimal control theory so that it can be used to identify synchrony promoting structures and mechanisms in biological networks. As a preliminary step in this direction we apply optimal control to a network of Kuramoto oscillators with time-varying coupling in order to relate network synchrony to network connectivity. To the best of our knowledge this is the first such use of optimal control theory.

We consider the following generalization of the Kuramoto model.

For $i = 1, \dots, N$

$$\frac{dx_i}{dt} = \omega_i + \frac{1}{N} \sum_{j=1}^N u_{ij}(t) \sin(x_j(t) - x_i(t)).$$

Note here that the coupling strengths, u_{ij} , are allowed to vary between oscillator pairs and through time. Throughout this dissertation we assume that network synchrony is desirable, and that there is a cost associated with network connectivity. The coupling strengths, u_{ij} , are control variables, and their magnitudes, $|u_{ij}|$, are a measure of network connectivity. We will set $u_{ii} \equiv 0$ so that there are $N(N - 1)$ control variables to be determined.

To construct a framework on which to formulate optimal control problems we quantify the terms network synchrony and network connectivity cost. We define the network synchrony to be the average value of the order parameter squared:

$$\frac{1}{T} \int_0^T r^2(t) dt.$$

We define the connectivity cost to be the average value of the coupling strengths squared:

$$\frac{1}{TN(N - 1)} \int_0^T \sum_{i \neq j} u_{ij}(t)^2 dt.$$

With these definitions in hand, we address the following three questions.

- (1) How can the network obtain a prescribed level of synchrony while maintaining the lowest possible connectivity cost?
- (2) How can the network achieve the greatest level of synchrony for a fixed connectivity cost?
- (3) How can we maximize synchrony less a weighted connectivity cost?

After formulating and analyzing optimal control problems, numerical simulations allow us to quantitatively answer each of these questions for specific networks. In addition, we observe that in each case the optimal network, unlike the standard Kuramoto network, is not a mean-field network (i.e. the oscillators are not coupled to the average phase), inter-oscillator repulsion can promote synchrony, and due in part to the quadratic form of our objective functional, the oscillators in an optimal network should be coupled continuously.

Chapter 2

A Method to Accomplish the Optimal Control of Continuous Dynamical Systems with Impulse Controls via Discrete Optimal Control

2.1 Introduction

Many biological processes are modeled as continuous dynamical systems in which states evolve according to differential equations. Tumor growth and ecological invasions are examples of such processes. Meanwhile, human interventions into these processes are often discrete. For example, the administration of drugs, the application of pesticides, and the release of predators are all essentially discrete tasks. As a result many biological control problems give rise to impulse control problems. In this paper we consider how optimal control theory can be tailored to better address a specific class of impulse control problems. These problems take place on a finite time interval $[0, T]$, on which the state dynamics are governed by a system of ordinary differential equations and an impulse control which instantaneously alters the value of the state at discrete times. In addition, the number of impulses, and the value of the impulses are bounded, while the instants at which the impulses occur are chosen freely. An impulse control consists of a sequence of vectors $\{u_i\}$, $i = 0, \dots, N - 1$, which determine the magnitude of the impulses and a sequence of instants $\{T_i\}$, $i = 1, \dots, N$, at which the impulses are applied. In addition we require that $T_N = T$ and define $T_0 = 0$. Given an impulse control, the state dynamics can be written as follows:

For $i = 0, \dots, N - 1$, and $t \in (T_i, T_{i+1})$

$$\begin{aligned}\dot{x}(t) &= g(x, t), \\ x(T_i^+) &= G(x(T_i^-), u_i), \\ x(0) &= c_0\end{aligned}$$

where $x(t)$ is the value of the state, the continuous dynamics are described by the function $g(x, t)$, the discrete dynamics are described by the function $G(x, u_i)$, and N is the number of impulses that are applied.

Impulse control problems can be solved via dynamic programming [4, 2]. The PDEs that

result are termed quasi-variational inequalities (Q.V.I.s). Unfortunately, Q.V.I.'s are often fully nonlinear, and difficult to solve numerically. One popular numerical method requires the original impulse control problem to be approximated by a discrete optimal control problem. Meanwhile, our method reformulates the original control problem as an equivalent discrete control problem.

A second method of solving impulse control problems with a restricted number of impulses is developed in [16]. In this method, termed the method of discontinuous time change, the original optimal impulse control problem is transformed to an auxiliary continuous control problem. An application of Pontryagin's Maximum Principle to the auxiliary problem allows one to characterize the optimal impulse controls for the original problem. This method, however, may only be applied to problems in which the impulse function satisfies certain robustness conditions.

In this dissertation we show how impulse control problems with a restricted number of impulses can be formulated as discrete optimal control problems. This formulation is advantageous because it significantly simplifies numerical calculations. As noted in [16], impulse control problems with a restricted number of impulses can be formulated as nonlinear programming problems, so that a Kuhn-Tucker type theory yields optimality conditions [6]. Although it may be quite difficult to solve the general nonlinear programming problem numerically, these problems are discrete optimal control problems, which are highly structured nonlinear programming problems. As a result of their additional structure, the Kuhn-Tucker theory yields a considerably more information when it is applied to discrete optimal control problems. This information allows one to characterize the optimal controls in terms of adjoint variables and corresponding states. Optimal controls are then found numerically by using a forward backward sweep algorithm. Previously, Pierce and Schumitzky used nonlinear programming to solve impulse control problems with a restricted number of impulses at fixed and variable application times[18, 19]. Their method of solution, however, applies only to linear systems, as their primary objective was to handle continuous state constraints. The method of solution that we present here applies to both linear and nonlinear systems.

In the next section we will outline the method by which impulse control problems with a restricted number of impulse controls can be formulated as discrete optimal control problems. We will then use this method to solve two example impulse control problems in sections 2.3 and 2.4. The first problem concerns the control of an invasive plant. The second problem concerns the control of mold. Finally, in section 2.5 we present our conclusions.

2.2 Formulating the Problem

First we set some notation. The state of the system at time t will be represented by a vector $x(t) \in \mathbb{R}^M$. Superscripts will denote vector components so that $x^j(t)$ is the value of the j^{th} component of x at time t . Subscripts will denote time steps so that u_i^j will denote the value of the j^{th} component of the vector u at the time of the i^{th} control action.

In the absence of control, the state, $x(t)$, is modeled by a continuous dynamical system:

$$\dot{x}(t) = g(x(t), t), t \in [0, T],$$

where we assume that $g \in C$ in t and $g \in C^1$ in x .

An impulse control for this system takes the form of a sequence of control vectors and times, $\{u_i, \tau_i\}_{i=0}^{N-1}$, where N is the number of actions to be implemented, $u_i \in \mathbb{R}^L$ is the i^{th} control vector, $\tau_0 \geq 0$ is the time at which the first control vector, u_0 , is executed, and for $i = 1, \dots, N-1$, $\tau_i \geq 0$, is the time between the execution of u_{i-1} and u_i . The action of the control on the state is determined by a continuously differentiable function $G : \mathbb{R}^M \times \mathbb{R}^L \rightarrow \mathbb{R}^M$. We will refer to

$(u, \tau) = (u_0, \dots, u_{N-1}, \tau_0, \dots, \tau_{N-1})$ as the control schedule. For $n = 1, \dots, N$ we will let $T_n = \sum_{i=0}^{n-1} \tau_i$ denote the time at which the control vector u_{n-1} is executed.

When the control schedule is implemented, the states satisfy the following system:

System I for $j \in I$

$$x^j(T) = c_T^j,$$

for $i = 0, \dots, N-1$

$$\dot{x}(t) = g(x, t), t \in (T_i, T_{i+1})$$

$$x(T_{i+1}^+) = G(x(T_{i+1}^-), u_i)$$

Whenever $x(t)$ satisfies System I for a control schedule (u, τ) we will call (x, u, τ) a trajectory control schedule pair of System I.

The problem at hand is then to find a trajectory control schedule pair, (x^*, u^*, τ^*) , of System I that minimizes a given cost functional subject to various constraints.

We will consider control constraints of the form

$$u_i - a_i \geq 0,$$

$$b_i - u_i \geq 0,$$

and

$$\tau_i \geq 0,$$

and state constraints of the form

$$x(0) = c_0,$$

for $j \in I \subset \{1, \dots, M\}$

$$x^j(T) = c_T^j.$$

The vectors a_i, b_i belong to $\mathbb{R}^L$ and $u_i - a_i \geq 0$ means that each component of the vector $u_i - a_i$ is greater than or equal to zero. In practice, we will also need to impose constraints of the form $\sum_{i=0}^{N-1} \tau_i = T$ on the control schedule. However, we assume that these constraints can be handled by the introduction of artificial state vector components that have both initial and terminal time constraints and so these control constraints do not appear explicitly in the formulation of the generic problem that follows.

We will consider objective functionals of the form,

$$J(u, \tau) = \sum_{i=0}^{N-1} f_i(x(T_i^+), u_i, \tau_i) + f_N(x(T_N^+)),$$

where $f_i, i = 1, \dots, N$ is continuous in all its arguments.

The form of the objective functional is more general than it appears. In particular, by increasing the dimension of the state space, integral terms can be rewritten as discrete terms. To see this, consider an objective functional of the form,

$$J(u, \tau) = \int_0^T f(x(t))dt + \sum_{i=0}^{N-1} f_i(x(T_i^+), u_i, \tau_i) + f_N(x(T_N^+)).$$

Now, define a state component $x^{M+1}(t)$ by

$$x^{M+1}(t) = \int_0^t \hat{f}(x(s), s) ds,$$

where

$$\hat{f}(x^1, \dots, x^{M+1}, t) = f(x^1, \dots, x^M, t),$$

and define $\hat{g} : \mathbb{R}^{M+1} \times \mathbb{R} \rightarrow \mathbb{R}^{M+1}$ by

$$\hat{g}^j(x^1, \dots, x^{M+1}, t) = g^j(x^1, \dots, x^M, t)$$

, for $j = 1, \dots, M$ and

$$\hat{g}^{M+1}(x^1, \dots, x^{M+1}, t) = \hat{f}(x^1, \dots, x^{M+1}, t).$$

Also, define

$$\hat{G}^j(x^1, \dots, x^{M+1}, u_i) = G^j(x^1, \dots, x^M, u_i)$$

for $j = 1, \dots, M$ and

$$G^{M+1}(x^1, \dots, x^{M+1}, u_i) = x^{M+1}$$

. Finally if we let $\hat{c}_0 = (c_0, 0)$ then the new state evolves according to the following system:

System I'

For $i = 1, \dots, N - 1$

$$\dot{x}(t) = \hat{g}(x, t), t \in (T_i, T_{i+1})$$

$$x(T_{i+1}^+) = \hat{G}(x(T_{i+1}^-), u_i),$$

Furthermore, the objective functional, $J(u, \tau)$, is

$$J(u, \tau) = \sum_{i=0}^{N-1} \hat{f}_i(x(T_i^+), u_i, \tau_i) + \hat{f}_N(x(T_N^+)),$$

where

$$\hat{f}_i(x^1, \dots, x^{M+1}, u_i, \tau_i) = f_i(x^1, \dots, x^M, u_i, \tau_i)$$

and

$$\hat{f}_N(x^1, \dots, x^{M+1}) = f_N(x^1, \dots, x^M) + x^{M+1}.$$

Therefore it suffices to consider discrete cost functionals.

Finally, we impose terminal time constraints on the state:

The impulse control problem is then stated as follows:

Problem I

Find a trajectory control schedule pair (x^*, u^*, τ^*) of System I that minimizes

$$J(u, \tau) = \sum_{i=0}^{N-1} f_i(x(T_{i-1}^+), u_i, \tau_i) + f_N(x(T_{N-1}^+))$$

subject to the constraints

$$u_i - a_i \geq 0,$$

$$b_i - u_i \geq 0,$$

$$\tau_i \geq 0,$$

$$x(0) = c_0,$$

and for all $j \in I \subset \{1, \dots, M\}$

$$x^j(T) = c_T^j.$$

To formulate the problem as a discrete optimal control problem for $i = 0, \dots, N - 1$ we define a discrete state X_{i+1} which is equal to the state x directly after control action i is executed:

$$X_{i+1} = x(T_{i+1}^+) = G(x(T_{i+1}^-), u_i).$$

We also impose constraints at the initial and final times:

$$X_0 = c_0,$$

for $j \in I$

$$X_0^j = c_T^j.$$

In order to express X_{i+1} as a function of X_i we introduce an auxiliary function $y_i(x, t) : \mathbb{R}^M \times \mathbb{R} \rightarrow \mathbb{R}^M$. The characterization of $y_i(x, t)$ depends on whether or not the system is autonomous.

The Autonomous Case

If the system is autonomous then $y(x, t)$ is the solution to the initial value problem:

$$\begin{aligned} \dot{y}(y_0, t) &= g(y(y_0, t)), \\ y(y_0, 0) &= y_0. \end{aligned}$$

Now, for $t \in [0, \tau_i)$,

$$y(X_i, t) = x(t + T_i),$$

and

$$y(X_i, \tau_i) = x(T_{i+1}^-)$$

With this definition in place the discrete states evolve according to the following system of difference equations:

System II

For $i = 0, \dots, N - 1$

$$X_{i+1} = G(x(T_{i+1}^-), u_i) = G(y(X_i, \tau_i), u_i).$$

The objective functional, $J(u, \tau)$, is

$$J(u, \tau) = \sum_{i=0}^{N-1} f_i(X_i, u_i, \tau_i) + f_N(X_N).$$

Problem I may be restated as a discrete control problem.

Problem II

Find a trajectory control schedule pair (X^*, u^*, τ^*) of System II that minimizes

$$J(u, \tau) = \sum_{i=0}^{N-1} f_i(X_i, u_i, \tau_i) + f_N(X_N)$$

subject to the constraints

$$u_i - a_i \geq 0,$$

$$b_i - u_i \geq 0,$$

$$\tau_i \geq 0,$$

$$X_0 = c_0,$$

and for all $j \in I$

$$X_N^j = c_T^j.$$

With this definition in place the discrete states evolve according to the following system of difference equations:

System II

for $i = 0, \dots, N - 1$

$$X_{i+1} = G(x(T_i^-), u_i) = G(y_i(X_i, \tau_i), u_i)$$

and the objective functional, $J(u, \tau)$, is

$$J(u, \tau) = \sum_{i=0}^{N-1} f_i(X_i, u_i, \tau_i) + f_N(X_N).$$

Now Problem I may be restated as a discrete control problem.

Problem II

Find a trajectory control schedule pair (X^*, u^*, τ^*) of System II that minimizes

$$J(u, \tau) = \sum_{i=0}^{N-1} f_i(X_i, u_i, \tau_i) + f_N(X_N)$$

subject to the constraints

$$u_i - a_i \geq 0,$$

$$b_i - u_i \geq 0,$$

$$\tau_i \geq 0,$$

$$X_0 = c_0,$$

and for all $j \in I$

$$X_N^j = c_T^j$$

At this point we have succeeded in formulating the original impulse control problem as a discrete optimal control problem. Discrete optimal control problems are a special class of nonlinear programming problems, and so, at this stage one could proceed to solve the discrete optimal control problem by using any applicable nonlinear programming algorithm. As you can imagine, the nonlinear programming problems that arise from impulse control problems tend to be highly nonlinear and so this may not be an easy task. Discrete optimal control problems, however, have a great deal more structure than the general nonlinear programming problem, and so the necessary conditions

which characterize the solutions to nonlinear programming problems yield more information when applied to discrete optimal control problems. In particular, the necessary conditions determine a system of difference equations that characterize the adjoint variables. This characterization is the content of the following theorem.

Solutions to Problem II are characterized by the following theorem which follows from Theorems 3.4.22 (page 64) of Canon, Cullum and Polak [6] (See also Lenhart and Workman (page 199) [15].) If there exists a solution to problem II, then this theorem guarantees the existence of a set of adjoint vectors, $p_0, \dots, p_N$, which satisfy a certain system of difference equations and a set of nonnegative multiplier vectors $\mu_0^1, \dots, \mu_{N-1}^1, \mu_0^2, \dots, \mu_{N-1}^2$ in $\mathbb{R}^L$, and nonnegative scalars $\mu_0^3, \dots, \mu_{N-1}^3$, which satisfy a zero sum condition that relates to the control constraints. (Note that by introducing vectors μ_i^1, μ_i^2 and scalars μ_i^3 for $i = 1, \dots, N-1$ we have deviated from our convention of using superscripts to denote vector components. Instead the vector μ_i^1 corresponds to the lower bound on the control at the i th time step, the vector μ_i^2 corresponds to the upper bound on the control at the i th time step, and the scalar μ_i^3 corresponds to the lower bound on the size of the i th time step.)

Theorem 2.2.1. *If (X^*, u^*, τ^*) is a solution to Problem I then there exists adjoint vectors $p_0, \dots, p_N$ in $\mathbb{R}^M$, vectors, $\mu_0^1, \dots, \mu_{N-1}^1, \mu_0^2, \dots, \mu_{N-1}^2 \geq 0$ in $\mathbb{R}^L$, scalars $\mu_0^3, \dots, \mu_{N-1}^3 \geq 0$ and a scalar $\lambda \geq 0$ with the following properties:*

$$p_i = p_{i+1} \frac{\partial G}{\partial y}(y_i(X_i, \tau_i), u_i) \frac{\partial y_i}{\partial x}(X_i, \tau_i) + \lambda \frac{\partial f_i}{\partial x}(X_i, u_i, \tau_i).$$

If $j \notin I$,

$$p_N^j = \lambda \frac{\partial f_N}{\partial x^j}(X_N).$$

$$\langle \mu_i^1, a - u_i \rangle + \langle \mu_i^2, u_i - b \rangle - \mu_i^3 \tau_i = 0.$$

In addition, for $i = 0, \dots, N-1$, the Hamiltonian $H_i : \mathbb{R}^M \times \mathbb{R}^L \times \mathbb{R}^M \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$, defined by

$$H_i(X_i, u_i, \tau_i, p_{i+1}, \lambda) = \lambda f_i(X_i, u_i, \tau_i) + \langle p_{i+1}, G(y_i(X_i, \tau_i), u_i) \rangle + \langle \mu_i^1, a - u_i \rangle + \langle \mu_i^2, u_i - b \rangle + \mu_i^3(-\tau_i)$$

satisfies the following conditions:

for $j = 1, \dots, L$

$$\frac{\partial H_i}{\partial u_i^j}(X_i^*, u_i^*, \tau_i^*, p_{i+1}, \lambda) = 0$$

$$\frac{\partial H_i}{\partial u_i^j}(X_i^*, u_i^*, \tau_i^*, p_{i+1}, \lambda) = 0.$$

In the statement of the previous theorem we employed the substitution

$$\frac{\partial G}{\partial X_i}(y_i(X_i, \tau_i), u_i) = \frac{\partial G}{\partial y}(y_i(X_i, \tau_i), u_i) \frac{\partial y_i}{\partial x}(X_i, \tau_i).$$

In order to utilize this theorem we need to solve for $\frac{\partial y_i}{\partial x}(X_i, \tau_i)$. If the system of differential equations governing the state is exactly solvable then $\frac{\partial y_i}{\partial x}(X_i, \tau_i)$ can be calculated explicitly. Otherwise,

we note that $\frac{\partial y_i}{\partial x}(X_i, \tau_i)$ satisfies the following ordinary differential equation:

$$\frac{\partial y_i}{\partial x}(X_i, t) = \frac{\partial f}{\partial y}(y_i(X_i, t), t) \frac{\partial y_i}{\partial x}(X_i, t)$$

$$\frac{\partial y_i}{\partial x}(X_i, 0) = I.$$

Then, in practice, the solution to Problem II can be found numerically by executing a forward backward sweep in which the matrix $\frac{\partial y_i}{\partial x}(X_i, \tau_i)$ is updated by using its ordinary differential equation with each iteration.

2.2.1 The Nonautonomous Case

If the system is nonautonomous then in order to express X_{i+1} as a function of X_i we introduce discrete states, T_i , for $i = 0, \dots, N$, which satisfy the difference equation

$$T_{i+1} = T_i + \tau_i$$

and

$$T_0 = 0,$$

and for $i = 1, \dots, N$ we let

$$y_i(x, t) : \mathbb{R}^M \times [0, \tau_{i-1}] \rightarrow \mathbb{R}^M$$

denote the solution to the initial value problem:

$$\begin{aligned} \dot{y}_i(y_0, t) &= g(y_i(y_0, t), t + T_{i-1}), \\ y_i(y_0, 0) &= y_0, \end{aligned}$$

where $\dot{\cdot}$ denotes the derivative with respect to t . Note that y_i is a function of an initial condition, $y_0 \in \mathbb{R}^M$, and time. And so, for $t \in [0, \tau_{i-1})$,

$$\begin{aligned} y_i(X_i, t) &= X_i + \int_0^t g(y_i(X_i, s), s + T_{i-1}) ds = X_i + \int_{T_{i-1}}^{T_{i-1}+t} g(y_i(X_i, s - T_{i-1}), s) ds \\ &= x(T_{i-1}^+) + \int_{T_{i-1}}^{T_{i-1}+t} g(x(s), s) ds = x(t + T_{i-1}). \end{aligned}$$

and

$$y_i(X_i, \tau_{i-1}) = x(T_i^-).$$

With these definitions in place the discrete states evolve according to the following system of difference equations:

System II

For $i = 0, \dots, N - 1$

$$X_{i+1} = G(x(T_i^-), u_i) = G(y_i(X_i, \tau_i), u_i)$$

$$T_{i+1} = T_i + \tau_i.$$

Now we can state the discrete optimal control problem:

Problem II Find a trajectory control schedule pair, (X^*, T^*, u^*, τ^*) , of System II that minimizes

$$J(u, \tau) = \sum_{i=0}^{N-1} f_i(X_i, u_i, \tau_i) + f_N(X_N)$$

subject to the constraints

$$\begin{aligned} u_i - a_i &\geq 0, \\ b_i - u_i &\geq 0, \\ \tau_i &\geq 0, \\ X_0 &= c_0, \end{aligned}$$

and for all $j \in I$

$$X_N^j = c_T^j$$

Solutions to Problem II are characterized by the following theorem which follows from Theorems 3.4.22 (page 64) of Canon, Cullum and Polak [6] (See also Lenhart and Workman (page 199) [15].)

Theorem 2.2.2. *If (X^*, T^*, u^*, τ^*) is a solution to the discrete control problem then there exists adjoint vectors $p_0, \dots, p_N$ in $\mathbb{R}^M$, adjoint scalars, $r_0, \dots, r_N$, vectors, $\mu_0^1, \dots, \mu_{N-1}^1, \mu_0^2, \dots, \mu_{N-1}^2 \geq 0$ in $\mathbb{R}^L$, scalars $\mu_0^3, \dots, \mu_{N-1}^3 \geq 0$ and a scalar $\lambda \geq 0$ with the following properties:*

$$p_i = p_{i+1} \frac{\partial G}{\partial y}(y_i(X_i, \tau_i), u_i) \frac{\partial y_i}{\partial x}(X_i, \tau_i) + \lambda \frac{\partial f_i}{\partial x}(X_i, u_i, \tau_i).$$

If $j \notin I$,

$$p_N^j = \lambda \frac{\partial f_N}{\partial x^j}(X_N).$$

$$r_i = p_{i+1} \frac{\partial G}{\partial y}(y_i(X_i, \tau_i), u_i) \frac{\partial y_i}{\partial T_i}(X_i, \tau_i) + r_{i+1}.$$

$$\langle \mu_i^1, a - u_i \rangle + \langle \mu_i^2, u_i - b \rangle - \mu_i^3 \tau_i = 0.$$

In addition, for $i = 0, \dots, N-1$, the Hamiltonian

$$\begin{aligned} H_i(X_i, T_i, u_i, \tau_i, p_{i+1}, \lambda) &= \lambda f_i(X_i, u_i, \tau_i) \\ &+ \langle p_{i+1}, G(y_i(X_i, \tau_i), u_i) \rangle \\ &+ r_{i+1} (T_i + \tau_i) \\ &+ \langle \mu_i^1, a - u_i \rangle + \langle \mu_i^2, u_i - b \rangle + \mu_i^3 (-\tau_i) \end{aligned}$$

satisfies the following conditions: for $j = 1, \dots, L$

$$\frac{\partial H_i}{\partial u_i^j}(X_i^*, T_i^*, u_i^*, \tau_i^*, p_{i+1}, \lambda) = 0$$

$$\frac{\partial H_i}{\partial \tau_i}(X_i^*, T_i^*, u_i^*, \tau_i^*, p_{i+1}, \lambda) = 0.$$

In the statement of Theorem 2.2.2 we employed the substitution,

$$\frac{\partial G}{\partial T_i}(y_i(X_i, \tau_i), u_i) = \frac{\partial G}{\partial y}(y_i(X_i, \tau_i), u_i) \frac{\partial y_i}{\partial T_i}(X_i, \tau_i).$$

We need to solve for $\frac{\partial y_i}{\partial T_i}(X_i, \tau_i)$. If the system of differential equations governing the state is exactly solvable then $\frac{\partial y_i}{\partial T_i}(X_i, \tau_i)$ can be calculated explicitly. Otherwise, we note that $\frac{\partial y_i}{\partial T_i}(X_i, \tau_i)$ satisfies the following ordinary differential equation:

$$\frac{\partial y_i}{\partial T_i}(X_i, t) = \frac{\partial g}{\partial y}(y_i(X_i, t), t) \frac{\partial y_i}{\partial T_i}(X_i, t) + \frac{\partial g}{\partial t}(y_i(X_i, t), t)$$

$$\frac{\partial y_i}{\partial T_i}(X_i, 0) = 0.$$

The discrete optimal control problem can be solved numerically by executing a forward backward sweep in which the matrix $\frac{\partial y_i}{\partial T_i}(X_i, \tau_i)$ is updated by using its ordinary differential equation with each iteration.

At this point we have reformulated the original impulse control problem as a discrete optimal control problem and outlined a numerical algorithm which consists of solving systems of ordinary differential equations. As a result, we believe this method to be a considerable simplification of the standard method which relies on partial differential equations.

Next we illustrate the technique by applying it to a particular, exactly solvable, ODE system.

2.3 Example 1: Invasive Plants

In this example we consider a biological system with two components, designed to produce and store energy. The size of the energy storage component will be denoted by x^1 , and the size of the energy production component will be denoted by x^2 . We will consider the system as a population of invasive plants, so that x^1 denotes the mass of the population's roots, and x^2 denotes the mass of the population's vegetation. The objective is to minimize the size of the plant colony plus a weighted control cost over a fixed interval of time $[0, T]$ by periodically removing a portion of the vegetation. The number of control applications, N , is also fixed in advance. We would like to emphasize that this is a toy problem which was designed solely to illustrate our method of solution.

If the system develops according to the following system of differential equations with M and A positive constants,

$$\frac{dx^1}{dt} = Mx^2 - Ax^1 \tag{2.1}$$

$$\frac{dx^2}{dt} = Ax^1 \tag{2.2}$$

we find that in the absence of control the states at time t are given by:

$$x^1(t) = a \frac{\theta_1}{A} e^{\theta_1 t} + b \frac{\theta_2}{A} e^{\theta_2 t} \tag{2.3}$$

$$x^2(t) = a e^{\theta_1 t} + b e^{\theta_2 t}. \tag{2.4}$$

Here $\theta_1 = \frac{-A + \sqrt{A^2 + 4AM}}{2}$, $\theta_2 = \frac{-A - \sqrt{A^2 + 4AM}}{2}$, and the constants a and b are chosen to meet initial conditions $x^1(0) = x_0^1$, $x^2(0) = x_0^2$. Note that $\theta_1 > 0$ and $\theta_2 < 0$. Therefore, in the long run, the ratio of vegetation to roots approaches $\frac{\theta_1}{A}$.

The growth of the population is limited by a control which removes a portion, u_i , of the vegetative mass at N discrete times, T_i , $i = 0, \dots, N-1$. Because the control acts solely on x^2 , and because the systems's growth is informed by the ratio of x^2 to x^1 , it is reasonable to assume that the control application times will alter the outcome of the control strategy. With these considerations in mind we introduce a second control τ_i which determines the length of time between control applications. We require that:

$$\sum_{i=0}^{N-1} \tau_i = T. \quad (2.5)$$

After incorporating the control, we arrive at a system of difference equations:
for $i = 0, \dots, N-1$

$$\begin{aligned} X_{i+1}^1 &= (a_i \frac{\theta_1}{A} e^{\theta_1 \tau_i} + b_i \frac{\theta_2}{A} e^{\theta_2 \tau_i}) \\ X_{i+1}^2 &= ((1 - u_i)(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i})), \end{aligned}$$

with constraints:

$$\begin{aligned} X_0^1 &= x_0^1 \\ X_0^2 &= x_0^2 \\ 0 &\leq u_i \leq 1 \\ 0 &\leq \tau_i. \end{aligned}$$

Here i is the time step, τ_i is the size of the i th time step, X_i^1 is the mass of the roots at the beginning of the i th time step, X_i^2 is the mass of the vegetation at the beginning of the i th time step, and u_i is the proportion of the vegetation that is removed at the end of the i th time step. Note that the mass of vegetation removed at the end of the i th time step is $u_i(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i})$. Note also that X_{i+1}^1 and X_{i+1}^2 depend on the state of the system at the previous time through the coefficients a_i and b_i , where

$$\begin{aligned} a_i &= \frac{AX_i^1 - \theta_2 X_i^2}{\theta_1 - \theta_2} \\ b_i &= \frac{X_i^2 \theta_1 - AX_i^1}{\theta_1 - \theta_2}. \end{aligned}$$

Note that $\theta_1 \neq \theta_2$ since $A^2 + 4AM \neq 0$, and that $a_i > 0$ if $x_0^1 \neq 0$.

Observe that the mass of the roots at the beginning of the i th time step is positive unless the initial mass of the roots is zero and the size of the i th time step is zero. Also, the mass of the vegetation just before the i th control application is equal to $a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i}$, which is positive unless the mass of the vegetation at the beginning of the i th time step is zero and the size of the i th time step is zero. These observations follow from (2.1) and (2.2) or direct substitution of a_i and b_i into (2.3) and (2.4).

Next, given a trajectory control schedule pair (X_i, u_i, τ_i) , we define the objective functional as

follows:

$$J(u_i, \tau_i) = f(X^1, X^2, u, \tau) = \sum_{i=0}^{N-1} f_i(X_i^1, X_i^2, u_i, \tau_i) + f_N(X_N^1, X_N^2),$$

where

$$f_i(X_i^1, X_i^2, u_i, \tau_i) = Bu_i^2(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i}) + X_i^1 + X_i^2$$

for

$$i = 0, \dots, N-1,$$

and

$$f_N(X_N^1, X_N^2) = X_N^1 + X_N^2.$$

We see that the objective is to minimize the biomass of the invasive plant, measured at each time step, and the weighted cost of implementing the control. We have assumed that the cost of each control action is proportional to the product of the mass of vegetation removed, $u_i(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i})$, and the proportion of the vegetation removed, u_i . Therefore, the cost of removing a fixed mass of vegetation decreases as the mass of the vegetative component of the invasion increases. This feature of the cost function reflects a decrease in search costs as the size of the vegetative component increases [8]. The constant B determines the relative importance of each part of the objective functional.

Our goal is to find the optimal control strategy for fixed T and N . We begin by introducing an artificial state variable X^3 to incorporate the constraint (2.5). We have some freedom to choose the difference equation that governs X^3 . In principle any first order difference equation ensuring that $\sum_{i=0}^{N-1} \tau_i = T$ will do. And so, we select the following equation for computational ease.

$$X_{i+1}^3 = X_i^3 e^{\theta_2 \tau_i}$$

$$i = 0, \dots, N$$

$$X_0^3 = 1$$

$$X_N^3 = e^{\theta_2 T}.$$

Because the state now has an additional component we redefine the objective functional f so that it has five arguments,

$$f(X^1, X^2, X^3, u, \tau) = f(X^1, X^2, u, \tau).$$

In order to characterize an optimal control we will form the Hamiltonian, set its derivative with respect to u and τ to be zero, and solve. However, because of the final time constraint, $\sum_{i=0}^{N-1} \tau_i = T$, the difference equation for X^3 is overdetermined. As a result, it is nontrivial to show that the multiplier, λ , which corresponds to the objective functional in the Hamiltonian, is nonzero, and this is crucial to our control characterization. In order to show that λ is nonzero, it is convenient to formulate this problem as a nonlinear programming problem. And so, we introduce the following notation: Let

$$z = (X^1, X^2, X^3, u, \tau) \in \mathbb{R}^{3(N+1)+2N}.$$

For $i = 0, \dots, N - 1$, $j = 1, \dots, 3$ define the functions,

$$G_{i+1}^j : \Re^{3(N+1)+2N} \rightarrow \Re,$$

as follows:

$$\begin{aligned} G_{i+1}^1(z) &= X_{i+1}^1 - (a_i \frac{\theta_1}{A} e^{\theta_1 \tau_i} + b_i \frac{\theta_2}{A} e^{\theta_2 \tau_i}) \\ G_{i+1}^2(z) &= X_{i+1}^2 - ((1 - u_i)(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i})) \\ G_0^1(z) &= X_0^1 - c_0^1 \\ G_0^2(z) &= X_0^2 - c_0^2 \\ G_0^3(z) &= X_0^3 - 1 \\ G_{N+1}^3(z) &= X_N^3 - e^{\theta_2 T} \end{aligned}$$

For $i = 0, \dots, N - 1$, $j = 1, 2, 3$ define the functions $Q_i^j : \Re^{3(N+1)+2N} \rightarrow \Re$ as follows

$$\begin{aligned} Q_i^1(z) &= -u_i \\ Q_i^2(z) &= u_i - 1 \\ Q_i^3(z) &= -\tau_i \end{aligned}$$

Note that the functions $G_{i+1}^1(z)$ and $G_{i+1}^2(z)$ depend on the states X_i^1 and X_i^2 through the coefficients a_i and b_i .

With this notation in place we restate the optimal control problem as an equivalent nonlinear programming problem:

Find $z^* \in \Re^{3(N+1)+2N}$ satisfying

- For $i = 0, \dots, N - 1$, $j = 1, 2, 3$

$$Q_i^j(z^*) \leq 0, \tag{2.6}$$

- For $i = 0, \dots, N$, $j = 1, 2, 3$

$$G_i^j(z^*) = 0, \tag{2.7}$$

- For $i = 0, \dots, N + 1$

$$G_i^3(z^*) = 0 \tag{2.8}$$

and

-

$$f(z^*) \leq f(z) \tag{2.9}$$

for all z satisfying (2.6), (2.7) and (2.8).

The existence of solutions to this problem is immediate since the objective functional is continuous on a nonempty bounded subset of $\Re^{3(N+1)+2N}$.

Solutions to the problem are characterized by using Theorem 3.4.22, page 64, of Canon, Cullum, and Polak [6].

If z^* is a solution to the nonlinear programming problem then there exists a scalar $\lambda \geq 0$, vectors $p_0, \dots, p_{N+1}$ in $\Re^3$ and vectors $\mu_0, \dots, \mu_N \geq 0$ in $\Re^3$ so that

•

$$\lambda \nabla f(z^*) - \sum_{i=0}^{N+1} \sum_{j=0}^3 p_i^j \nabla G_i^j(z^*) + \sum_{i=0}^N \sum_{j=0}^3 \mu_i^j \nabla Q_i^j(z^*) = 0, \quad (2.10)$$

•

$$\sum_{i=0}^N \sum_{j=0}^3 \mu_i^j Q_i^j(z^*) = 0, \quad (2.11)$$

and

•

$$(\lambda, p_0, \dots, p_{N+1}) \neq 0 \quad (2.12)$$

In order to characterize an optimal control, we need to show that the multiplier λ is nonzero. If, however, when evaluated at z^* , the gradients of G_i^j together with the gradients of Q_i^j such that $\mu_i^j \neq 0$ (i.e. the gradients of the active inequality constraints) are linearly independent then $\lambda \neq 0$ will follow from (2.10) and (2.12). In the lemma that follows the ∇G_i^j gradients run over all possible indices, i.e. for $j = 1, 2, i = 0, \dots, N$, and for $j = 3, i = 0, \dots, N + 1$. The ∇Q_i^j gradients are limited to those that correspond to active inequality constraints with $j \in 1, 2, 3$, and $i \in 0, \dots, N - 1$.

Lemma. If z^* is a solution to the nonlinear programming problem then, when evaluated at z^* , the gradients, ∇G_i^j together with the gradients of the active inequality constraints, ∇Q_i^j form a linearly independent set.

Proof. First note that if these gradients are to form a linearly independent set then there can be no more than $\Re^{3(N+1)+2N}$ of them. However, if z^* solves the nonlinear programming problem then $\sum_{i=0}^N \tau_i = T$. Therefore, at least one of the constraints, $Q_0^3, \dots, Q_{N-1}^3$, is inactive. Without loss of generality we will assume that Q_{N-1}^3 is inactive. Also, for $i = 0, \dots, N - 1$, at most one of the constraints, Q_i^1, Q_i^2 , is active. Since the gradient of Q_i^1 is negative the gradient of Q_i^2 , the linear independence of the set of gradients is not affected by which constraint is active. Without loss of generality, we will assume that Q_i^2 is active. Therefore, in the worst case scenario, we need to show that when evaluated at z^* the gradients of G_i^j , together with the gradients of Q_i^2 for $i = 0, \dots, N - 1$, and the gradients of Q_i^3 for $i = 0, \dots, N - 2$ are linearly independent. This set has $\Re^{3(N+1)+2N}$ vectors. We will proceed by showing that the matrix whose rows consist of these gradient vectors has full rank. As we will see in a moment, it is convenient to shift ∇G_N^3 to the final row, and so,

the matrix of interest has the following form:

$$\begin{bmatrix}
 \nabla G_0^1 \\
 \vdots \\
 \nabla G_N^1 \\
 \nabla G_0^2 \\
 \vdots \\
 \nabla G_N^2 \\
 \nabla G_0^3 \\
 \vdots \\
 \nabla G_{N-1}^3 \\
 \nabla G_{N+1}^3 \\
 \nabla Q_0^2 \\
 \vdots \\
 \nabla Q_{N-1}^2 \\
 \nabla Q_0^3 \\
 \vdots \\
 \nabla Q_{N-2}^3 \\
 \nabla G_N^3
 \end{bmatrix} \quad (2.13)$$

Now, note that for $i = 0, \dots, N-1$ we have that

$$\nabla Q_i^2 = (0, \dots, 0, \overbrace{1}^{u_i}, 0, \dots, 0),$$

and for $i = 1, \dots, N-2$ we have that

$$\nabla Q_i^3 = (0, \dots, 0, \overbrace{1}^{\tau_i}, 0, \dots, 0).$$

Also,

$$\nabla G_0^1 = (\overbrace{1}^{x_0^1}, 0, \dots, 0, 0, \dots, 0),$$

$$\nabla G_0^2 = (0, \dots, 0, \overbrace{1}^{x_0^2}, 0, \dots, 0),$$

and

$$\nabla G_0^3 = (0, \dots, 0, \overbrace{1}^{x_0^3}, 0, \dots, 0).$$

In addition, for $i = 1, \dots, N$, the gradients ∇G_i^1 have the form

$$\left(0, \dots, 0, \frac{\partial G_i^1}{\partial X_{i-1}^1}, \overbrace{1}^{X_i^1}, 0, \dots, 0, \frac{\partial G_i^1}{\partial X_{i-1}^2}, 0, \dots, 0, \frac{\partial G_i^1}{\partial X_{i-1}^3}, 0, \dots, 0, \frac{\partial G_i^1}{\partial u_{i-1}}, 0, \dots, 0, \frac{\partial G_i^1}{\partial \tau_{i-1}}, 0, \dots, 0 \right),$$

for $i = 1, \dots, N$, the gradients ∇G_i^2 have the form

$$\left(0, \dots, 0, \frac{\partial G_i^2}{\partial X_{i-1}^1}, 0, 0, \dots, 0, \frac{\partial G_i^2}{\partial X_{i-1}^2}, \overbrace{1}^{X_i^2}, 0, \dots, 0, \frac{\partial G_i^2}{\partial X_{i-1}^3}, 0, \dots, 0, \frac{\partial G_i^2}{\partial u_{i-1}}, 0, \dots, 0, \frac{\partial G_i^2}{\partial \tau_{i-1}}, 0, \dots, 0 \right),$$

and for $i = 1, \dots, N-1$, the gradients ∇G_i^3 have the form

$$\left(0, \dots, 0, \frac{\partial G_i^3}{\partial X_{i-1}^1}, 0, 0, \dots, 0, \frac{\partial G_i^3}{\partial X_{i-1}^2}, 0, \dots, 0, \frac{\partial G_i^3}{\partial X_{i-1}^3}, \overbrace{1}^{X_i^3}, 0, \dots, 0, \frac{\partial G_i^3}{\partial u_{i-1}}, 0, \dots, 0, \frac{\partial G_i^3}{\partial \tau_{i-1}}, 0, \dots, 0 \right).$$

Finally, ∇G_{N+1}^3 is

$$\nabla G_{N+1}^3 = (0, \dots, 0, \overbrace{1}^{X_N^3}, 0, \dots, 0),$$

and ∇G_N^3 is

$$\left(0, \dots, 0, \frac{\partial G_N^3}{\partial X_{i-1}^1}, 0, 0, \dots, 0, \frac{\partial G_N^3}{\partial X_{i-1}^2}, 0, \dots, 0, \frac{\partial G_N^3}{\partial X_{i-1}^3}, \overbrace{1}^{X_i^3}, 0, \dots, 0, \frac{\partial G_N^3}{\partial u_{i-1}}, 0, \dots, 0, \frac{\partial G_N^3}{\partial \tau_{N-1}} \right),$$

and

In particular, the gradient matrix has ones along its diagonal, until the final row, where the final entry is

$$\frac{\partial G_N^3}{\partial \tau_{N-1}} = -X_{N-1}^3 e^{\theta_2 \tau_{N-1}} \neq 0.$$

Since X_{i+1}^3 depends only on X_i^3 and τ_i and since the final $2N$ rows of the matrix, which correspond to the control constraints, are diagonal, the final $2(N) + N + 1$ rows of the matrix easily reduce to diagonal form. Similarly, since X_{i+1}^1 and X_{i+1}^2 depend only on X_i^1, X_i^2, u_i and τ_i , the first $2(N+1)$ rows of the matrix reduce to upper triangular form. Therefore, the entire matrix reduces to upper triangular form, and so, it has full rank. $\square$

It follows from Corollary 3.4.28 on page 65 of Canon, Cullum and Polak that the multiplier λ is nonzero, and so we will set $\lambda = 1$ [6].

From here on we will let u_i and τ_i denote the optimal controls at time step i . We proceed to form the Hamiltonian:

$$\begin{aligned}
H_i &= \lambda \left(Bu_i^2 (a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i}) + X_i^1 + X_i^2 \right) \\
&+ p_{i+1}^1 \left(a_i \frac{\theta_1}{A} e^{\theta_1 \tau_i} + b_i \frac{\theta_2}{A} e^{\theta_2 \tau_i} \right) \\
&+ p_{i+1}^2 \left((1 - u_i) (a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i}) \right) \\
&+ p_{i+1}^3 (X_i^3 e^{\theta_2 \tau_i}) + \mu_i^1 (-u_i) + \mu_i^2 (u_i - 1) + \mu_i^3 (-\tau_i).
\end{aligned}$$

Recall that the coefficients a_i and b_i depend on the values of the states X_i^1 and X_i^2 .

The adjoint variables are defined by the following difference equations:

$$\begin{aligned}
p_i^1 &= \frac{\partial H}{\partial X_i^1} \\
&= 1 + \frac{ABu_i^2}{\theta_1 - \theta_2} (e^{\theta_1 \tau_i} - e^{\theta_2 \tau_i}) + \frac{p_{i+1}^1}{\theta_1 - \theta_2} (\theta_1 e^{\theta_1 \tau_i} - \theta_2 e^{\theta_2 \tau_i}) \\
&+ \frac{p_{i+1}^2 A}{\theta_1 - \theta_2} (e^{\theta_1 \tau_i} - e^{\theta_2 \tau_i}) (1 - u_i) \\
p_i^2 &= \frac{\partial H}{\partial X_i^2} \\
&= 1 + \frac{Bu_i^2}{\theta_1 - \theta_2} (\theta_1 e^{\theta_2 \tau_i} - \theta_2 e^{\theta_1 \tau_i}) + \frac{p_{i+1}^1 \theta_1 \theta_2}{A (\theta_1 - \theta_2)} (e^{\theta_2 \tau_i} - e^{\theta_1 \tau_i}) \\
&+ \frac{p_{i+1}^2}{\theta_1 - \theta_2} (\theta_1 e^{\theta_2 \tau_i} - \theta_2 e^{\theta_1 \tau_i}) (1 - u_i) \\
p_i^3 &= \frac{\partial H}{\partial X_i^3} \\
&= p_{i+1}^3 e^{\theta_2 \tau_i},
\end{aligned}$$

with the final time constraints:

$$\begin{aligned}
p_N^1 &= 1 \\
p_N^2 &= 1 \\
p_N^3 &= c,
\end{aligned}$$

where the constant c is chosen so that $X_N^3 = e^{\theta_2 T}$.

Note that since $\theta_1 > 0$ and $\theta_2 < 0$ we can see from the adjoint equations that $p_i^1 > 0$ and $p_i^2 > 0$.

We can now characterize the optimal controls by setting the derivatives of the Hamiltonian with respect to u_i and τ_i equal to zero. Differentiating the Hamiltonian with respect to u_i we find that:

$$0 = 2Bu_i(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i}) - p_{i+1}^2 (a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i}) - \mu_i^1 + \mu_i^2. \quad (2.14)$$

which implies that

$$u_i = \frac{p_{i+1}^2}{2B} + \frac{\mu_i^1 - \mu_i^2}{(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i})}, \quad (2.15)$$

provided that the denominator,

$$(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i}) = x^2(T_i^-) \neq 0.$$

When the denominator is equal to zero, equations (2.14) and (2.15) do not yield any information about u_i . Note, however, that if

$$(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i}) = x^2(T_i^-) = 0,$$

then u_i affects neither the objective functional nor the trajectory of the state. Therefore, the value of u_i does not matter in this case, and so we can limit our analysis to the case that

$$(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i}) = x^2(T_i^-) > 0.$$

If $0 < u_i < 1$, then $\mu_i^1 = \mu_i^2 = 0$. And so, equation (2.15) implies that

$$0 < u_i = \frac{p_{i+1}^2}{2B} < 1.$$

In particular, we can check that

$$u_i = \max(0, \min(1, \frac{p_{i+1}^2}{2B})).$$

If $u_i = 1$, then $\mu_i^1 = 0$. And so, equation (7) implies that

$$\frac{p_{i+1}^2}{2B} = 1 + \frac{\mu_i^2}{(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i})} \geq 1.$$

Again, we can write

$$u_i = \max(0, \min(1, \frac{p_{i+1}^2}{2B})).$$

Finally, if $u_i = 0$ then $\mu_i^2 = 0$. And so, equation (2.14) implies that

$$\frac{p_{i+1}^2}{2B} = -\frac{\mu_i^1}{(a_i e^{\theta_1 \tau_i} + b_i e^{\theta_2 \tau_i})} \leq 0.$$

Therefore, in every case we have that

$$u_i = \max(0, \min(1, \frac{p_{i+1}^2}{2B})).$$

Taking the derivative of the Hamiltonian with respect to τ_i we find that

$$\mu_i^3 = k_1 e^{\theta_1 \tau_i} + k_2 e^{\theta_2 \tau_i}, \tag{2.16}$$

where

$$k_1 = p_{i+1}^1 a_i \frac{\theta_1^2}{A} + p_{i+1}^2 (1 - u_i) a_i \theta_1 + B u_i^2 a_i \theta_1 > 0$$

and

$$k_2 = p_{i+1}^1 b_i \frac{\theta_2^2}{A} + p_{i+1}^2 (1 - u_i) b_i \theta_2 + p_{i+1}^3 \theta_2 X_i^3 + B u_i^2 b_i \theta_2.$$

Now we will consider two cases, $\tau_i > 0$ and $\tau_i = 0$.

If $\tau_i > 0$ then $\mu_i^3 = 0$. And so, equation (9) implies that $k_2 < 0$, $|k_1| < |k_2|$, and

$$0 < \tau_i = \frac{\log -\frac{k_2}{k_1}}{(\theta_1 - \theta_2)}.$$

In particular,

$$\tau_i = \max \left(0, \frac{\log -\frac{k_2}{k_1}}{(\theta_1 - \theta_2)} \right).$$

If $\tau_i = 0$ then equation (9) implies that $0 \leq \mu_i^3 = k_1 + k_2$. And so, this case has two subcases, either $k_2 \geq 0$ or $k_2 < 0$ and $|k_1| > |k_2|$. If $k_2 < 0$ and $|k_1| > |k_2|$ then

$$\frac{\log -\frac{k_2}{k_1}}{(\theta_1 - \theta_2)} < 0.$$

And so, we can write

$$\tau_i = \max \left(0, \frac{\log -\frac{k_2}{k_1}}{(\theta_1 - \theta_2)} \right).$$

If $k_2 \geq 0$ then

$$\frac{\log -\frac{k_2}{k_1}}{(\theta_1 - \theta_2)}$$

is undefined. However, the first case shows that if $k_2 \geq 0$ then $\tau_i = 0$. And so, we characterize τ_i as follows: If $k_2 < 0$ then

$$\tau_i = \max \left(0, \frac{\log -\frac{k_2}{k_1}}{(\theta_1 - \theta_2)} \right).$$

If $k_2 \geq 0$ then

$$\tau_i = 0.$$

Numerical Simulations

Now that we have characterized the optimal control we can solve for it numerically by using a forward backward sweep algorithm [15]. In the first simulation the parameters are $x_0^1 = 1$, $x_0^2 = \frac{\theta_1}{A}$, $B = 3$, $A = .25$, $M = 1$, $T = 3$, and $N = 7$. Figure 2.1 shows the proportion of the vegetative biomass that is removed at each control application time. Note that the optimal control schedule cuts the vegetative biomass twice at the initial time. This is because the cost of the control is quadratic. Figures 2.2 and 2.3 show the state trajectories that correspond to the optimal control schedule. For comparison, we also show the proportion of vegetative biomass that is removed by an optimal control with fixed, equidistant, application times and the corresponding state trajectories.

The value of the objective functional for the optimal control with fixed application times is 18.22. The value of the objective functional for the optimal control schedule is 10.73. This shows that we can reduce the value of the objective functional by optimizing the time at which the control is applied.

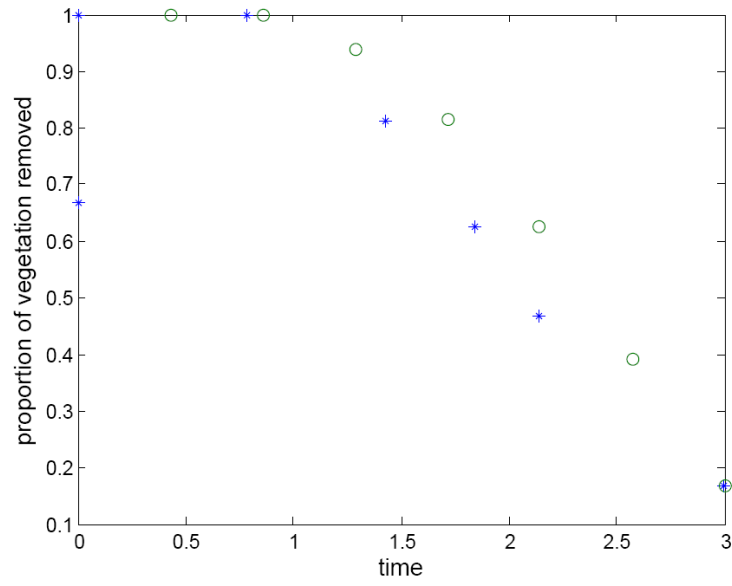


Figure 2.1: The proportion of the vegetative biomass removed by an optimal control schedule (*) and an optimal control with fixed application times (o).

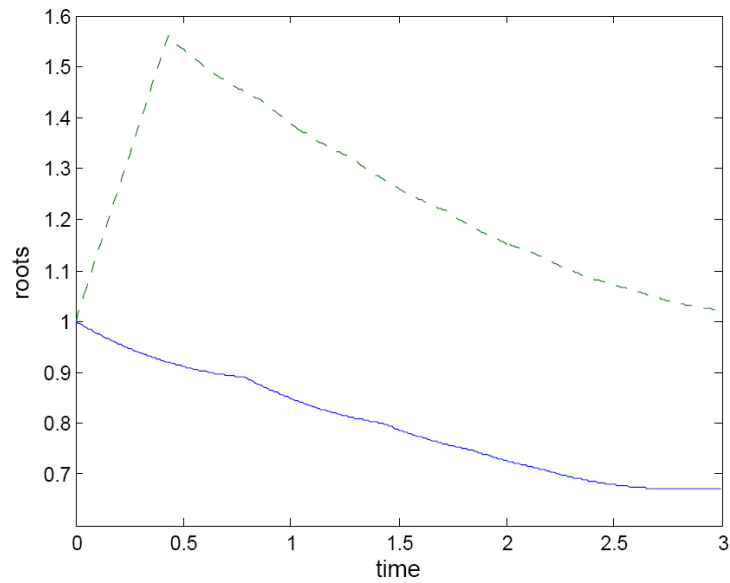


Figure 2.2: The root biomass when it is controlled by an optimal control schedule (-) and when it is controlled by an optimal control with fixed application times (-).

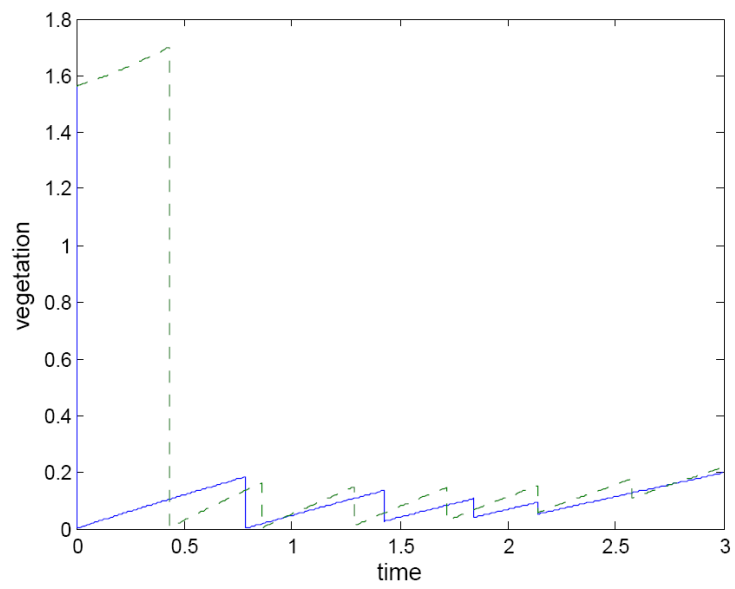


Figure 2.3: The vegetative biomass when it is controlled by an optimal control schedule (-) and when it is controlled by an optimal control with fixed application times (-).

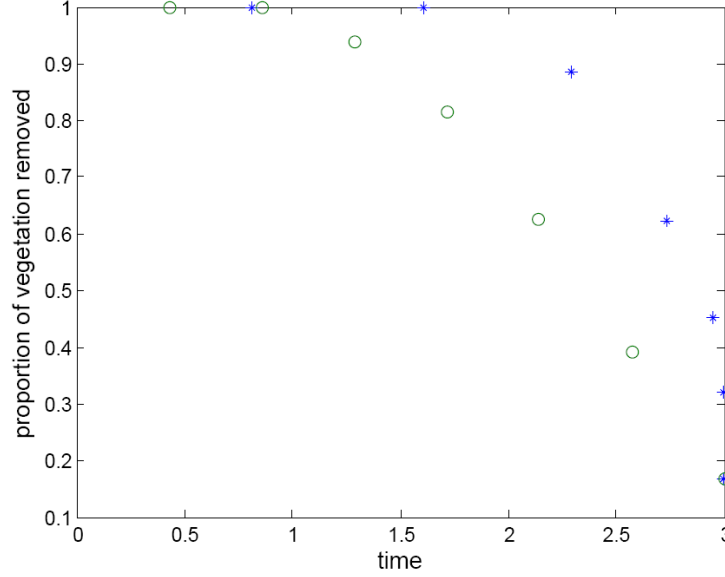


Figure 2.4: The proportion of the vegetative biomass removed by an optimal control schedule (*) and an optimal control with fixed application times (o).

In the next simulation we set $x_0^2 = 0$ and hold the other parameters constant. Figure 2.4 shows the proportion of the vegetative biomass that is removed by both the optimal control schedule and the optimal control with fixed application times. Figures 2.5 and 2.6 show the corresponding state trajectories. The value of the objective functional for the optimal control with fixed application times is 7.54. The value of the objective functional for the optimal control schedule is 6.58. Again, we see that we reduce the value of the objective functional by optimizing the times at which the control is applied.

Figures 2.1 and 2.4 demonstrate that an optimal control schedule may differ significantly from a fixed time control schedule. For example, in the first set of figures, when the ratio of vegetative biomass to root biomass is at its asymptotic value, the optimal control schedule immediately executes a control application. In the second set of figures when the vegetative biomass is zero the optimal control schedule waits longer than the fixed time optimal control before executing a control application.

2.4 Example 2: Fungicide

In this example a fungus infestation is controlled by the periodic application of fungicide. The objective is to minimize the concentration of fungus at the final time and the cost of applying the control. The number of control applications and the final time are fixed in advance. The state has two components, x^1 and x^2 , which represent the concentration of fungus and fungicide respectively. The continuous state dynamics are as follows:

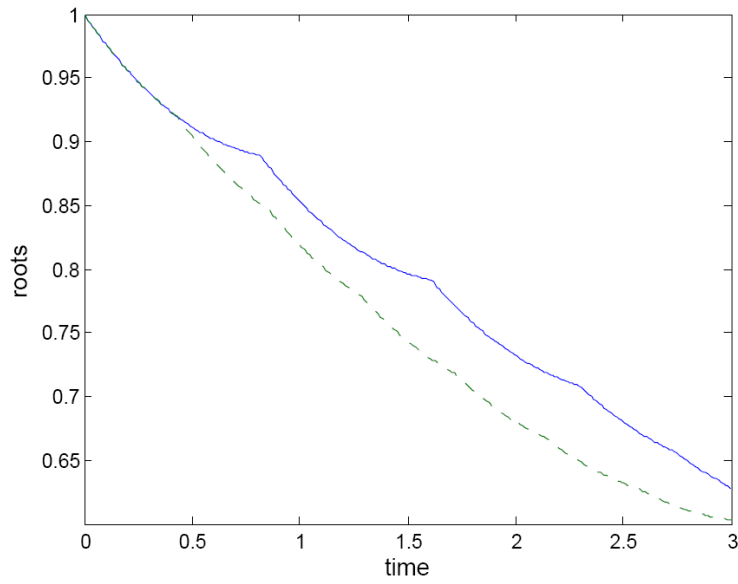


Figure 2.5: The root biomass when it is controlled by an optimal control schedule (-) and when it is controlled by an optimal control with fixed application times (-).

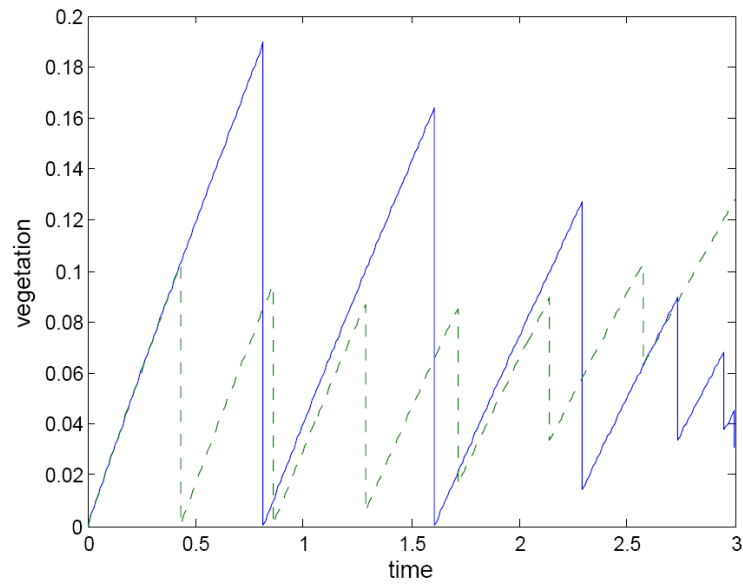


Figure 2.6: The vegetative biomass when it is controlled by an optimal control schedule (-) and when it is controlled by an optimal control with fixed application times (-).

$$\frac{dx^1}{dt} = r(M - x^1(t)) - x^1(t)x^2(t) \quad (2.17)$$

$$\frac{dx^2}{dt} = -kx^2(t) \quad (2.18)$$

$$x^1(0) = x_0^1 \quad (2.19)$$

$$x^2(0) = x_0^2 \quad (2.20)$$

If the system is left undisturbed, the concentrations of fungus and fungicide at time t are given by:

$$\begin{aligned} x^1(t) &= x_0^1 e^{-rt} \exp \left[\frac{x_0^2}{k} (e^{-kt} - 1) \right] \\ &\quad + r M e^{-rt} \exp \left[\frac{x_0^2}{k} (e^{-kt} - 1) \right] \int_0^t e^{rs} \exp \left[\frac{x_0^2}{k} (1 - e^{-ks}) \right] ds \\ x^2(t) &= x_0^2 e^{-kt}. \end{aligned}$$

We limit the growth of the fungus by increasing the concentration of fungicide by u_i units at discrete points, T_i , in time. A second control τ_i determines the time between control applications. If we let T denote the final time, and N denote the number of control applications, we require that,

$$0 \leq u_i \leq C,$$

$$0 \leq \tau_i$$

and

$$\sum_{i=0}^{N-1} \tau_i = T. \quad (2.21)$$

Recall that

$$T_i = \sum_{i=0}^{N-1} \tau_i.$$

If (x^1, x^2, u, τ) is a trajectory control schedule pair, we define the objective functional as follows:

$$J(u, \tau) = x^1(T) + B \sum_{i=0}^{N-1} u_i^2.$$

We see that the objective functional is the sum of the cost of the fungus infestation, which is proportional to the concentration of fungicide at the final time, and the cost of the control, which is quadratic. The balancing parameter B determines the relative importance of each type of cost.

Now we are ready to formulate the problem as a discrete optimal control problem. We define the discrete states X_{i+1}^1 and X_{i+1}^2 to be the concentration of fungus and fungicide, respectively, just after the i th control is applied. After incorporating the control, we arrive at a system of difference equations:

$$\begin{aligned}
X_{i+1}^1 &= X_i^1 e^{-r\tau_i} \exp \left[\frac{X_i^2}{k} (e^{-k\tau_i} - 1) \right] \\
&+ rM e^{-r\tau_i} \exp \left[\frac{X_i^2}{k} (e^{-k\tau_i} - 1) \right] \int_0^{\tau_i} e^{rs} \exp \left[\frac{X_i^2}{k} (1 - e^{-ks}) \right] ds \\
X_{i+1}^2 &= X_i^2 e^{-k\tau_i} + u_i,
\end{aligned}$$

with constraints

$$\begin{aligned}
X_0^1 &= x_0^1 \\
X_0^2 &= x_0^2 \\
0 &\leq u_i \leq C \\
0 &\leq \tau_i \leq T + \epsilon. \\
\sum_{i=0}^{N-1} \tau_i &= T
\end{aligned}$$

Here i denotes the time step, τ_i is the size of the i th time step, and u_i is amount by which the concentration of fungicide is increased at the end of the i th time step.

Next we introduce an artificial discrete state variable X^3 to incorporate constraint $\sum_{i=0}^{N-1} \tau_i = T$. We select the following equation for computational ease:

for $i = 1, \dots, N-1$

$$\begin{aligned}
X_{i+1}^3 &= X_i^3 e^{-k\tau_i} \\
X_0^3 &= 1 \\
X_N^3 &= e^{-kT}.
\end{aligned}$$

Finally, we express the objective functional in terms of the discrete states.

$$J(u, \tau) = X^1(T) + B \sum_{i=0}^{N-1} u_i^2,$$

where (X^1, X^2, X^3, u, τ) is a trajectory control schedule pair.

We will forgo formulating the analogous nonlinear programming problem for this example, note however, that the existence of solutions to the problem is immediate because the objective functional is continuous on a nonempty bounded subset of $\mathfrak{R}^{2(N+1)+2N}$. In addition, the fact that the multiplier, λ , which corresponds to the objective functional in the Hamiltonian, is nonzero, follows exactly as it did in the previous example. Therefore, we will take $\lambda = 1$ in the statement of the necessary conditions.

Now, we are ready to state necessary conditions for optimality in terms of the discrete state variables.

Let u_i^* and τ_i^* denote optimal controls and $(X_i^1)^*, (X_i^2)^*, (X_i^3)^*$ denote the corresponding states.

Utilizing Theorem 3.4.22 and Corollary 3.4.28 page 65 of Canon Cullum and Polak, we find that for $i = 1, \dots, N$ there exist adjoint variables p_i^1, p_i^2, p_i^3 and nonnegative multipliers $\mu_i^1, \mu_i^2, \mu_i^3$ with the following properties:

If we define the Hamiltonian function $H_i(X_i^1, X_i^2, X_i^3, p_{i+1}^1, p_{i+1}^2, p_{i+1}^3, u_i, \tau_i)$ as follows:

$$\begin{aligned}
& H_i(X_i^1, X_i^2, X_i^3, p_{i+1}^1, p_{i+1}^2, p_{i+1}^3, u_i, \tau_i) \\
= & u_i^2 + p_{i+1}^1 \left(X_i^1 e^{-r\tau_i} \exp \left[\frac{X_i^2}{k} (e^{-k\tau_i} - 1) \right] \right) \\
& + p_{i+1}^1 \left(r M e^{-r\tau_i} \exp \left[\frac{X_i^2}{k} (e^{-k\tau_i} - 1) \right] \int_0^{\tau_i} e^{rs} \exp \left[\frac{X_i^2}{k} (1 - e^{-ks}) \right] ds \right) \\
& + p_{i+1}^2 (X_i^2 e^{-k\tau_i} + u_i) + p_{i+1}^3 (X_i^3 e^{-k\tau_i}) \\
& + \mu_i^1(-u_i) + \mu_i^2(u_i - C) + \mu_i^3(-\tau_i) + \mu_i^4(\tau_i - (T + \epsilon))
\end{aligned}$$

then, the adjoint variables are characterized by the following system of difference equations:

$$\begin{aligned}
p_i^1 &= \frac{\partial H}{\partial X_i^1} \\
&= p_{i+1}^1 \left(e^{-r\tau_i^*} \exp \left[\frac{(X_i^2)^*}{k} (e^{-k\tau_i^*} - 1) \right] \right) \\
p_i^2 &= \frac{\partial H}{\partial X_i^2} \\
&= p_{i+1}^1 \left(\frac{(X_i^1)^*}{k} (e^{-k\tau_i^*} - 1) e^{-r\tau_i^*} \exp \left[\frac{(X_i^2)^*}{k} (e^{-k\tau_i^*} - 1) \right] \right) \\
&+ p_{i+1}^1 \left(\frac{rM}{k} (e^{-k\tau_i^*} - 1) e^{-r\tau_i^*} \exp \left[\frac{(X_i^2)^*}{k} (e^{-k\tau_i^*} - 1) \right] \right) \\
&* \int_0^{\tau_i^*} e^{rs} \exp \left[\frac{(X_i^2)^*}{k} (1 - e^{-ks}) \right] ds \\
&+ p_{i+1}^1 \left(r M e^{-r\tau_i^*} \exp \left[\frac{(X_i^2)^*}{k} (e^{-k\tau_i^*} - 1) \right] \right) \\
&* \int_0^{\tau_i^*} \frac{e^{rs}}{k} (1 - e^{-ks}) \exp \left[\frac{(X_i^2)^*}{k} (1 - e^{-ks}) \right] ds \\
&+ p_{i+1}^2 (e^{-k\tau_i^*}) \\
p_i^3 &= \frac{\partial H}{\partial X_i^3} \\
&= p_{i+1}^3 e^{-k\tau_i^*},
\end{aligned}$$

with the boundary conditions

$$p_N^1 = 1$$

$$p_N^2 = 0$$

$$p_N^3 = c.$$

In addition, the multipliers, $\mu_i^1, \mu_i^2, \mu_i^3$, satisfy the following zero sum condition:

$$\mu_i^1(-u_i^*) + \mu_i^2(u_i^* - C) + \mu_i^3(-\tau_i^*) = 0.$$

Finally, the derivatives of the Hamiltonian with respect to u_i and τ_i are zero when evaluated at

$$\left((X_i^1)^*, (X_i^2)^*, (X_i^3)^*, p_{i+1}^1, p_{i+1}^2, p_{i+1}^3, u_i^*, \tau_i^* \right).$$

We note that the adjoint equations together with the fact that $(X_i^1)^* \geq 0$ and $(X_i^2)^* \geq 0$ imply that $p_i^1 > 0$ and $p_i^2 \leq 0$.

We can now characterize an optimal control by differentiating the Hamiltonian along an optimal trajectory. Setting the derivative of the Hamiltonian with respect to u_i equal to zero and utilizing the convexity of the Hamiltonian with respect to u_i , we find that:

$$u_i^* = \max \left(0, \min \left(C, \frac{-p_{i+1}^2}{2B} \right) \right), \quad (2.22)$$

Setting the derivative of the Hamiltonian with respect to τ_i equal to zero we find that

$$\mu_i^3 = p_{i+1}^1 \left(r(M - X_{i+1}^1) - X_{i+1}^1 X_i^2 e^{-k\tau_i} \right) - p_{i+1}^2 k X_i^2 e^{-k\tau_i} - p_{i+1}^3 k X_i^3 e^{-k\tau_i}, \quad (2.23)$$

where we have used the continuous state dynamics to simplify the expression.

Solving for τ_i we find that

$$\tau_i = -\frac{1}{k} \log \frac{\mu_i^3 - p_{i+1}^1 r(M - X_{i+1}^1)}{-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3} \quad (2.24)$$

Now we will consider two cases $\tau_i > 0$, and $\tau_i = 0$.

If $\tau_i > 0$ then $\mu_i^3 = 0$. And so, equation (2.24) implies that

$$0 < \tau_i = -\frac{1}{k} \log \frac{-p_{i+1}^1 r(M - X_{i+1}^1)}{-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3}.$$

In particular,

$$\tau_i = \max \left(0, -\frac{1}{k} \log \frac{-p_{i+1}^1 r(M - X_{i+1}^1)}{-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3} \right)$$

in this case. Note also that the state dynamics and the fact that $p_{i+1}^1 > 0$ ensure that

$$-p_{i+1}^1 r(M - X_{i+1}^1) \leq 0.$$

Therefore, $\tau_i > 0$ implies that

$$-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3 \leq 0$$

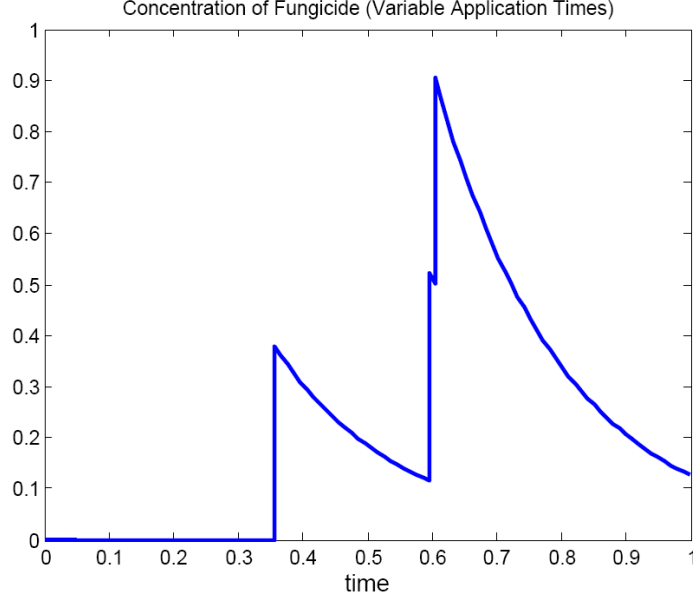


Figure 2.7: The concentration of fungicide that results from an optimal control schedule.

If $\tau_i = 0$ then equation (2.23) implies that

$$-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3 = \mu_i^3 - p_{i+1}^1 r (M - X_{i+1}^1)$$

In particular, we see that if

$$-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3 \leq 0$$

then we must also have that

$$\mu_i^3 - p_{i+1}^1 r (M - X_{i+1}^1) \leq 0$$

, which yields

$$0 = -\frac{1}{k} \log \frac{\mu_i^3 - p_{i+1}^1 r (M - X_{i+1}^1)}{-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3} \geq -\frac{1}{k} \log \frac{-p_{i+1}^1 r (M - X_{i+1}^1)}{-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3}.$$

In particular,

$$\tau_i = \max \left(0, -\frac{1}{k} \log \frac{-p_{i+1}^1 r (M - X_{i+1}^1)}{-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3} \right)$$

in this case.

Now we can characterize an optimal τ_i as follows:

- If

$$-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3 \geq 0$$

then $\tau_i = 0$.

- If

$$-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3 \leq 0$$

then

$$\tau_i^* = \max \left(0, -\frac{1}{k} \log \frac{-p_{i+1}^1 r (M - X_{i+1}^1)}{-p_{i+1}^1 X_{i+1}^1 X_i^2 - p_{i+1}^2 k X_i^2 - p_{i+1}^3 k X_i^3} \right).$$

Numerical Simulations

The control characterization allows us to find controls that satisfy the necessary conditions. Figures 2.7 and 2.8 show the concentration of fungus and fungicide that result from the optimal control schedule. For comparison, figures 2.9 and 2.10 show the concentration of fungus and fungicide that result from an optimal control with fixed application times at equal intervals. The parameters for both systems are $x_0^1 = .5, x_0^2 = 0, B = .1, k = 5, r = .5, M = 1, C = 1, T = 1$, and $N = 4$. The value of the objective functional for the optimal control schedule is .64 the value of the objective functional for the optimal control with fixed application times is .66.

2.5 Conclusions

We have developed a method to reformulate impulse control problems with a restricted number of impulses as discrete optimal control problems. This solution strategy was advantageous because it allowed us to avoid the difficulties that are associated with Q.V.I.s and the method of discontinuous time change. In particular, when using this method the impulse functions are not required to satisfy robustness conditions, as in the method of discontinuous time change, and the discrete systems that are associated with this method are easier to solve numerically than the Q.V.I.s. In addition, we successfully used this method to solve two example impulse control problems in which the systems of ordinary differential equations governing the state dynamics were exactly solvable. In the future we will use this method to solve impulse control problems with more complicated state dynamics.

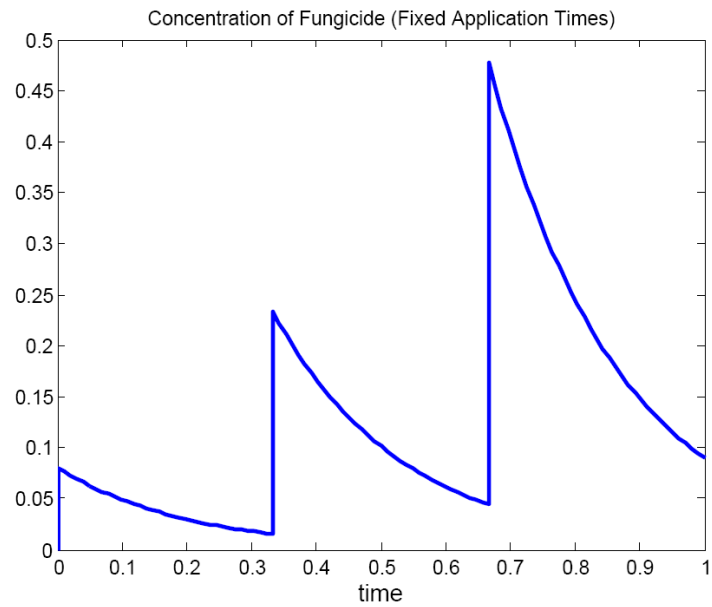


Figure 2.8: The concentration of fungicide that results from an optimal control with fixed application times.

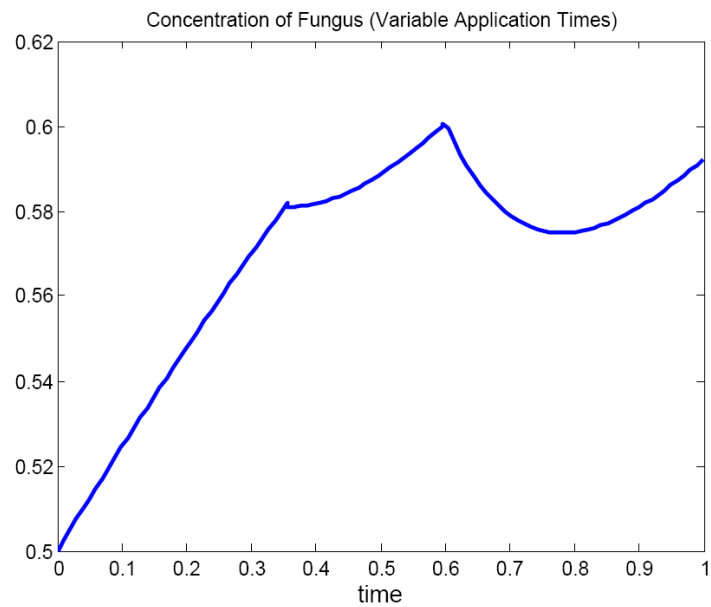


Figure 2.9: The concentration of fungus that results from an optimal control schedule.

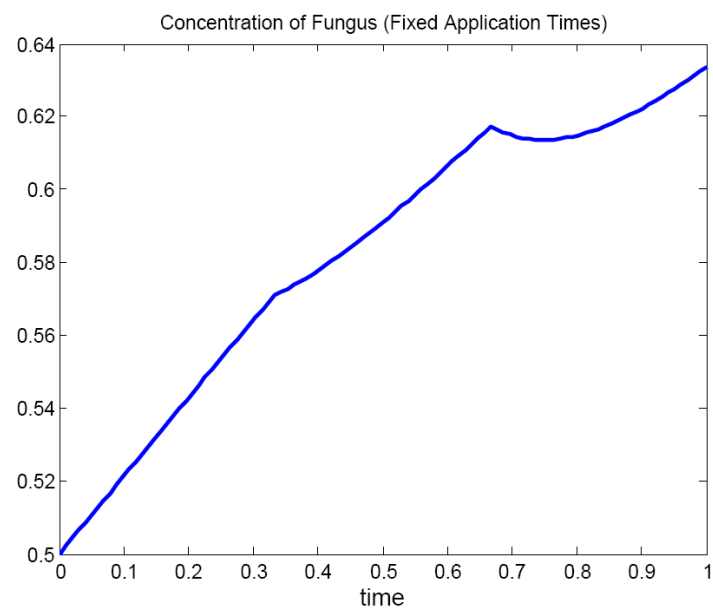


Figure 2.10: The concentration of fungus that results from an optimal control with fixed application times.

Chapter 3

Utilizing Optimal Control Theory to Explore the Emergence of Synchrony in a Network of Kuramoto Oscillators

3.1 Introduction

Many biological networks are known to exhibit synchrony [26, 5, 33, 17, 7]. Because synchrony is both beautiful and important many researchers have devoted their time to understanding how it emerges. Often, very little is known about the biological networks that exhibit synchrony. In particular, it may be difficult or even impossible to know the topology, the functional form of the coupling, or even the exact members of a biological network. For this reason, biological researchers have employed mathematics to glean information about network structures from empirical observations of network dynamics. For example, the following observations have been made about the activity of the neural network which runs through the spinal cord of the lamprey eel and is responsible for the rhythmic undulations that propel the animal through the water, i.e. the swimming central pattern generator (CPG) of the lamprey eel: The CPG produces traveling waves of electrical activity. The wave frequency is proportional to the speed at which the animal swims. The wavelength, however, is constant at about one body length, whatever the frequency. In addition, waves may travel in either direction, allowing the animal to swim backwards and forwards, and any cord segment of sufficient length is capable of producing traveling waves. These observations allowed Koppel and Ermentrout to characterize the structure of the CPG by analyzing the existence of stable phase-locked solutions in a chain of nonlinear coupled oscillators as a function of the coupling type (i.e. synaptic vs. electronic) and configuration (i.e. nearest neighbor vs. long range) [13]. There have also been many interesting and purely mathematical papers along these same lines. That is, mathematicians have devised methods to analyze the existence and stability of a network's various synchronous states as a function of the network's parameters. Much attention has been devoted to one network in particular, the Kuramoto network [1, 25, 12]. The Kuramoto network is a famous mathematical model of emergent synchrony. That is to say, whatever the initial distribution of oscillators' phases, if the coupling is strong enough, their phases will cluster together. Many papers have explored the stability of the network's steady states in the limit as the number of oscillators in the network tends to infinity [1, 25, 27, 28]. More recent works have focused on the dynamics of finite oscillator networks and on networks with time varying coupling [1, 24, 34]. Many of these papers share the goal of establishing sufficient conditions for the stability

of the synchronization manifold, in terms of the strength with which the oscillators are coupled.

In this dissertation we will not investigate network steady states, but instead focus on network objectives. Our analysis is accomplished via optimal control theory. An introduction to this theory can be found in [15]. Optimal control theory is an obvious way to achieve synchronization in man-made physical networks. Our goal, however, is to adapt optimal control theory so that it can be used to identify synchrony promoting structures and mechanisms in biological networks. As a preliminary step in this direction we consider how a network of Kuramoto oscillators can best achieve synchrony through time. The term “best” is quantified below. In fact, we will consider three distinct objective functionals. The oscillator coupling is sinusoidal, but the strengths with which the oscillators are coupled varies freely in time and between oscillator pairs. In particular, at any instant in time oscillator i may push oscillator j away, pull oscillator j toward itself, or not influence oscillator j at all. The control characterizations and numerical simulations allow us to answer two basic questions about an optimal network:

- Should the oscillators be coupled with continuous controls or with bang-bang controls?
- Is the optimal network a mean-field network?

In the next section, we introduce our model and quantify the terms network synchrony and connectivity cost. The following three sections present three different control problems which relate network synchrony to network connectivity cost. In the final section of this article we summarize our observations and suggest future directions of research.

3.2 The Model

Networks of phase oscillators are typically modeled by systems of coupled ordinary differential equations. In 1975, Kuramoto introduced an elegant and tractable network model that is capable of producing collective synchrony. Since then Kuramoto’s model and variations of it have been studied extensively [14, 25, 28, 27]. Because this model is so tractable we employ a variation of it in our analysis.

The Kuramoto model is a system of nonlinear, coupled, ordinary differential equations:

$$\frac{dx_i}{dt} = \omega_i + \frac{K}{N} \sum_{j=1}^N \sin(x_j(t) - x_i(t)),$$

where N is the number of oscillators in the network, x_i is the phase of the i th oscillator and ω_i is the natural velocity of the i th oscillator. The coefficient, K , is called the coupling strength.

To quantify the network’s state it is useful to introduce the complex valued order function,

$$r(t)e^{i\psi(t)} = \frac{1}{N} \sum_{j=1}^N e^{ix_j(t)}.$$

The angle, ψ , corresponds to the centroid of the oscillator phases [25]. The magnitude, r , of the order function provides a convenient measure of network synchrony, with $r(t) = 1$ corresponding to collective synchrony, and $r(t) = 0$ corresponding to incoherence (i.e. the oscillators’ phases are evenly distributed around the unit circle). We will refer to $r(t)$ as the order parameter.

Kuramoto noticed that the state dynamics can be rewritten in terms of the order parameter, as follows:

$$\frac{dx_i}{dt} = \omega_i + r(t)K \sin(\psi(t) - x_i(t)),$$

so that each oscillator is coupled to the mean phase with coupling strength $Kr(t)$. For this reason the Kuramoto model is called a *mean-field* model.

We consider the following generalization of the Kuramoto model.

For $i = 1, \dots, N$

$$\frac{dx_i}{dt} = \omega_i + \frac{1}{N} \sum_{j=1}^N u_{ij}(t) \sin(x_j(t) - x_i(t)).$$

Note here that the coupling strengths, u_{ij} , are allowed to vary between oscillator pairs and through time. The coupling matrix is not assumed to be symmetric, that is, in general $u_{ij} \neq u_{ji}$. We will set $u_{ii} \equiv 0$, and so, there are $N(N-1)$ coupling strengths to be determined.

Throughout this dissertation we assume that network synchrony is desirable, and that there is a cost associated with network connectivity. The coupling strengths, u_{ij} , are the control variables, and their magnitudes, $|u_{ij}|$, are a measure of network connectivity.

To construct a framework on which to formulate optimal control problems we quantify the terms network synchrony and network connectivity cost. We define the network synchrony to be the average value of the order parameter squared:

$$\frac{1}{T} \int_0^T r^2(t) dt.$$

We define the connectivity cost to be the average value of the coupling strengths squared:

$$\frac{1}{TN(N-1)} \int_0^T \sum_{i \neq j} u_{ij}(t)^2 dt.$$

We will address the following three questions.

- (1) How can the network obtain a prescribed level of synchrony while maintaining the lowest possible connectivity cost?
- (2) How can the network achieve the greatest level of synchrony for a fixed connectivity cost?
- (3) How can we maximize synchrony less a weighted connectivity cost?

We begin each section by formulating an optimal control problem that corresponds to one of the above questions. After the problem is formulated we proceed to show the existence of optimal coupling strengths, u_{ij} , and to characterize the optimal coupling strengths with the aid of Pontryagin's Maximum Principle. The characterization of the optimal coupling strengths is nontrivial for the first two problems, due to the multitude of controls and the integral constraints that are imposed on the controls and states. The constraints are handled by the introduction of an artificial state variables which have two boundary conditions. Because the artificial states' dynamics are overdetermined, the control problems may be abnormal. Finally, numerical simulations are presented. Each numerical simulation answers one of the three questions listed above for a specific network.

3.3 Minimizing the Connectivity of a Network with Fixed Synchrony

3.3.1 Formulating the Problem

In this section we find the coupling strengths, $u_{ij}(t)$, that drive a network to a prescribed level of synchrony at the minimal possible connectivity cost. In particular, we are interested in seeing how much we can improve upon the efficiency of a Kuramoto network by allowing the coupling strengths to vary between oscillators and through time. As a result the prescribed level of synchrony will be that produced by the Kuramoto network with $K = c$, i.e. $u_{ij} \equiv c$, with $c > 0$. Given c , we will find the coupling strengths, $u_{ij}(t)$, that minimize

$$\int_0^T \sum_{i \neq j} u_{ij}^2(t) dt,$$

subject to the prescribed synchrony

$$\int_0^T r^2(t) dt = A.$$

In this equation A is the synchrony obtained by an identical set of oscillators, interacting through the Kuramoto network with $u_{ij}(t) \equiv c$.

Next, we define the control set. Let U be the set of all matrix valued functions, $u : [0, T] \rightarrow [-M, M]^{N \times (N-1)}$, such that each component u_{ij} is a Lebesgue measurable function. The requirement that $|u_{ij}(t)| \leq M$ *a.e.* is a matter of theoretical convenience. We shall assume throughout this paper that M is very large so that it does not affect the value of the optimal control.

To incorporate the constraint $\int_0^T r^2(t) dt = A$ into the problem, we introduce an artificial state variable x_{N+1} , which satisfies:

$$\frac{dx_{N+1}}{dt} = \frac{1}{N^2} \left[\left(\sum_{i=1}^N \sin x_i(t) \right)^2 + \left(\sum_{i=1}^N \cos x_i(t) \right)^2 \right] \quad (3.1)$$

$$= \frac{1}{N^2} \sum_{i,j=1}^N \sin x_i(t) \sin x_j(t) + \cos x_i(t) \cos x_j(t) \quad (3.2)$$

$$= \frac{1}{N^2} \sum_{i,j=1}^N \cos(x_i(t) - x_j(t)) = r^2(t) \quad (3.3)$$

In addition we impose the initial and final time constraints:

$$x_{N+1}(0) = 0,$$

$$x_{N+1}(T) = A,$$

Finally, we will assume that the initial oscillator phases are fixed, i.e., for $i = 1, 2, \dots, N$,

$$x_i(0) = x_i^0.$$

We will say that a vector, $x(t) = (x_1(t), \dots, x_N(t), x_{N+1}(t))$, corresponds to the control $u(t)$ if the components of $x(t)$ are absolutely continuous functions such that for $i = 1, \dots, N$,

$$\frac{dx_i}{dt} = \omega_i + \frac{1}{N} \sum_{j=1}^N u_{ij}(t) \sin(x_j(t) - x_i(t)),$$

$$x_i(0) = x_i^0,$$

$$\frac{dx_{N+1}}{dt} = \frac{1}{N^2} \left[\left(\sum_{i=1}^N \sin x_i(t) \right)^2 + \left(\sum_{i=1}^N \cos x_i(t) \right)^2 \right] = \frac{1}{N^2} \sum_{i,j=1}^N \cos(x_i(t) - x_j(t)) = r^2(t),$$

and

$$x_{N+1}(0) = 0.$$

In this case we will call $(x(t), u(t))$ a trajectory-control pair.

Now we can define the set of admissible controls, U_{ad} . Let $(x(t), u(t))$ be a trajectory-control pair, with $u \in U$. We will say that $u \in U_{ad}$ if $x_{N+1}(T) = A$. In addition, we know that $U_{ad} \neq \emptyset$, because the control with $u_{ij}(t) \equiv c$ for all i, j belongs to U_{ad} by design.

Finally we define the objective functional,

$$J(u) = \int_0^T \sum_{i \neq j} u_{ij}^2(t) dt.$$

Within this framework the problem may be stated as follows:

Problem I

Find a trajectory-control pair $(x^*(t), u^*(t))$ so that $u^* \in U_{ad}$, and

$$J(u^*) = \min_{u \in U_{ad}} J(u).$$

3.3.2 Existence of an Optimal Control

Now we will show that Problem I has a solution.

Theorem 3.3.1. *There exists a solution, $(x^*(t), u^*(t))$, to Problem I.*

Proof. Choose a sequence $\{u^m\}$ in U_{ad} so that $J(u^m) \rightarrow \min_{u \in U_{ad}} J(u)$. Now since each control component, u_{ij}^m , is $L^2[0, T]$, bounded there exists an L^2 function, u^* with components, u_{ij}^* , and a weakly converging subsequence, which we will also denote by $\{u^m\}$, so that $u_{jk}^m \rightharpoonup u_{jk}^*$ for all j, k . Then, if x^m is the state associated with u^m , we have that for $j \in \{1, \dots, N\}$

$$\frac{dx_j^m}{dt} = \omega_j + \frac{1}{N} \sum_{k=1}^N u_{jk}^m(t) \sin(x_k^m(t) - x_j^m(t)),$$

and so for $t_2 > t_1$

$$\begin{aligned}
|x_j^m(t_2) - x_j^m(t_1)| &\leq \left| \int_{t_1}^{t_2} \omega_j + \frac{1}{N} \sum_{k=1}^N u_{jk}^m(t) \sin(x_k^m(t) - x_j^m(t)) dt \right| \\
&\leq (t_2 - t_1) \max_i \{\omega_i\} + \frac{1}{N} \int_{t_1}^{t_2} \sum_i |u_{ij}(t)| dt \\
&\leq (t_2 - t_1) \max_i \{\omega_i\} + (t_2 - t_1)(M).
\end{aligned}$$

Therefore if $K = \max_{i \in \{1, \dots, N\}} (\omega_i, M)$ and $(t_2 - t_1) \leq \frac{\epsilon}{K}$ then $|x_j^m(t_2) - x_j^m(t_1)| \leq \epsilon$. And so, for $j \in \{1, \dots, N\}$ the functions, $\{x_j^m\}$, are equicontinuous. Furthermore, we have

$$\begin{aligned}
|x_j^m(s)| &= \left| x_j^0 + \int_0^s \omega_j + \frac{1}{N} \sum_{k=1}^N u_{jk}^m(t) \sin(x_k^m(t) - x_j^m(t)) dt \right| \\
&\leq \max_i \{x_i^0\} + T \max_i \{\omega_i\} + TM,
\end{aligned}$$

so that, for $j \in \{1, \dots, N\}$, the functions, $\{x_j^m\}$, are uniformly bounded. Also the functions, x_{N+1}^m , are trivially equicontinuous and uniformly bounded. Therefore, by Arzela-Ascoli, for $j \in \{1, \dots, N, N+1\}$, there exists a subsequence, $\{x_j^m\}$, converging uniformly to x_j^* in $C[0, T]$. In particular,

$$x_{N+1}^*(T) = \lim_{m \rightarrow \infty} x_{N+1}^m(T) = A.$$

Next we will show that

$$\frac{dx_j^*}{dt} = \omega_j + \frac{1}{N} \sum_{k=1}^N u_{jk}^*(t) \sin(x_k^*(t) - x_j^*(t))$$

in $H^1[0, T]$. First note that

$$\begin{aligned}
&\lim_{m \rightarrow \infty} \int_0^T \sum_k u_{j,k}^*(t) \sin(x_k^*(t) - x_j^*(t)) - u_{jk}^m(t) \sin(x_k^m(t) - x_j^m(t)) dt \\
&= \lim_{m \rightarrow \infty} \int_0^T \sum_k (u_{j,k}^*(t) - u_{jk}^m(t)) \sin(x_k^*(t) - x_j^*(t)) dt \\
&+ \lim_{m \rightarrow \infty} \int_0^T \sum_k [\sin(x_k^*(t) - x_j^*(t)) - \sin(x_k^m(t) - x_j^m(t))] u_{jk}^m(t) dt \\
&= 0.
\end{aligned}$$

The second integral converges to zero by the weak convergence of the controls and the third integral converges to zero by the uniform convergence of the states and the L^∞ bound on the controls. Therefore, for all $v \in C_c^\infty[0, T]$,

$$\begin{aligned}
\int_0^T v'(t)x^*(t)dt &= \lim_{m \rightarrow \infty} \int_0^T v'(t)x_j^m(t)dt \\
&= \lim_{m \rightarrow \infty} - \int_0^T v \left[\omega_j + \frac{1}{N} \sum_{k=1}^N u_{jk}^m(t) \sin(x_k^m(t) - x_j^m(t)) \right] dt \\
&= - \int_0^T v(t) \left[\omega_j + \frac{1}{N} \sum_{k=1}^N u_{jk}^*(t) \sin(x_k^*(t) - x_j^*(t)) \right] dt
\end{aligned}$$

The first equality follows from the uniform convergence of the states, the second via integration by parts, and the final equality follows from the note above. Furthermore by the uniform convergence of the states,

$$\frac{dx_{N+1}^*}{dt} = \frac{1}{N^2} \sum_{i,j} \cos(x_i^*(t) - x_j^*(t)) = r^2(t).$$

Next we will show that $\text{esssup}(u_{ij}^*) \leq M$ for all i, j . Assume toward a contradiction that $\text{esssup}(u_{ij}^*) > M$ for some i, j . Then we can assume without loss of generality that there exists a set E with $\mu(E) > 0$ such that $u_{ij}(t)^* > M$ for $t \in E$. Then the weak convergence of the controls yields:

$$\mu(E)M < \int_E u_{ij}^*(t)dt = \lim_{m \rightarrow \infty} \int_E u_{ij}^m(t)dt \leq \lim_{m \rightarrow \infty} \mu(E)M = \mu(E)M,$$

which is a contradiction.

Finally since the L^2 norm is lower semicontinuous with respect to weak convergence,

$$J(u^*) = \int_0^T \sum_{j,k} u_{jk}^*(t)^2 dt \leq \liminf \int_0^T \sum_{j,k} u_{jk}^m(t)^2 dt = \min_{u \in U} J(u).$$

Therefore u^* is optimal and the desired existence result is proved. $\square$

3.3.3 Characterization of the Optimal Control

The right hand sides of the differential equations for the states can be used to define $N+1$ functions from $[\mathfrak{R}^{N+1}, \mathfrak{R}^{N \times (N-1)}]$ to $\mathfrak{R}$. For notational convenience we will denote these functions by

$$\frac{dx_i}{dt}(x, u).$$

Now we define $g(x, u) : [\mathfrak{R}^{N+1}, \mathfrak{R}^{N \times (N-1)}] \rightarrow \mathfrak{R}^{N+1}$ to be the vector valued function

$$g(x, u) := \left(\frac{dx_1}{dt}(x, u), \dots, \frac{dx_{N+1}}{dt}(x, u) \right)',$$

where $'$ denotes the transpose. We also define the function $f(x, u)$ by,

$$f(x, u) := \sum_{i=1}^N u_{ij}^2,$$

and the Hamiltonian function, $H : \mathfrak{R}^{N+1} \times \mathfrak{R}^{N \times (N-1)} \times \mathfrak{R}^{N+1} \times \mathfrak{R} \rightarrow \mathfrak{R}$ by,

$$\begin{aligned}
H(x, u, y, y_0) &= y'g(x, u) + y_0f(x, u) \\
&= \sum_{i=1}^N y_i \left(\omega_i + \frac{1}{N} \sum_j u_{ij} \sin(x_j - x_i) \right) \\
&+ \frac{y_{N+1}}{N^2} \left[\left(\sum_j \sin x_j \right)^2 + \left(\sum_j \cos x_j \right)^2 \right] \\
&+ y_0 \sum_{i,j} u_{ij}^2
\end{aligned}$$

An application of results from [29] characterizes the solutions of problem *I*.

Theorem 3.3.2. *If (x^*, u^*) is a solution to Problem I then there exists a pair $(y_0, y(t))$ so that the following conditions are met:*

- (i) *The map $y : [0, T] \rightarrow \mathfrak{R}^{N+1}$ is absolutely continuous;*
- (ii) *$y_0 \in \mathfrak{R}$ and $y_0 \leq 0$;*
- (iii) *$(y_0, y(t)) \neq (0, 0)$ for every $t \in [0, T]$;*
- (iv) *the adjoint differential equation holds, that is,*

$$\frac{dy}{dt} = -\frac{\partial H}{\partial x}(x^*(t), u^*(t), y(t), y_0);$$

- (v) *the Hamiltonian maximization condition holds, that is,*

$$H(x^*(t), u^*(t), y(t), y_0) = \max_{u \in [-M, M]^{N \times (N-1)}} \{H(x^*(t), u(t), y(t), y_0)\};$$

- (vi) *and the transversality condition,*

$$y_i(T) = 0$$

for $i = 1, 2, \dots, N$ holds.

The adjoint equations may be written out componentwise: For $i = 1, 2, \dots, N$

$$\begin{aligned}
\frac{dy_i}{dt} &= \frac{1}{N} \sum_{j \neq i, j=1}^N (y_i(t)u_{ij}^*(t) - y_j(t)u_{ji}^*(t)) \cos(x_j^*(t) - x_i^*(t)) \\
&- \frac{2y_{N+1}(t)}{N^2} \sum_{j=1}^N \sin(x_j^*(t) - x_i^*(t))
\end{aligned}$$

and

$$\frac{dy_{N+1}}{dt} = 0.$$

In particular we see that y_{N+1} is constant.

At this point we would like to characterize an optimal coupling strength, u_{ij} , by setting the derivative of the Hamiltonian with respect to u_{ij} equal to zero and solving. However, the resulting characterization will depend on whether or not $y_0 = 0$. If $y_0 = 0$ then the Hamiltonian is linear in u_{ij} and so on every interval an optimal coupling strength is either bang-bang or singular. On the other hand, if $y_0 \neq 0$, then we arrive at the usual characterization of u_{ij} from which it follows that u_{ij} is continuous. Here we would like to emphasize that by characterizing the adjoint variable y_0 , we can answer a fundamental question about optimal oscillator coupling, that is: *Should oscillators be coupled with continuous controls or with bang-bang controls?* When $y_0 \neq 0$ the answer is that any optimal control is continuous.

For an unconstrained optimal control problem $y_0 \neq 0$ is immediate. For constrained problems, it has become somewhat customary to assume that $y_0 \neq 0$ as well, although this need not be the case. Given the importance of y_0 in characterizing an optimal coupling, we will make no such assumption. Instead, over the next few pages we will show that under fairly mild conditions y_0 is indeed nonzero, that is, any optimal coupling is continuous.

The next theorem will be used to show that the Hamiltonian is monotonically increasing along an optimal trajectory-control pair. It is an adaptation to measurable controls of Lemma 15.1 (page 53) of Fleming and Rishel [9], which only applies to piecewise continuous controls. In replacing piecewise continuous controls with measurable ones we lose the full strength of the lemma. In particular the statement

$$\frac{d}{dt}H(x^*(t), u^*(t), y(t), y_0, t) = \frac{\partial H}{\partial t}(x^*(t), u^*(t), y(t), y_0, t)$$

is replaced by

$$\frac{d}{dt}H(x^*(t), u^*(t), y(t), y_0, t) \geq \frac{\partial H}{\partial t}(x^*(t), u^*(t), y(t), y_0, t).$$

As a result, the well known result that the Hamiltonian is constant along an optimal trajectory when the system is autonomous is weakened to, the Hamiltonian is monotonically increasing along an optimal trajectory, when the system is autonomous and the controls are measurable but not necessarily piecewise continuous. This lemma will aid us in showing that y_0 is nonzero.

Theorem 3.3.3. *Let $h(t, u) : \mathbb{R}^1 \times \mathbb{R}^m \rightarrow \mathbb{R}$ be differentiable and Lipschitz continuous with respect to t , and let $u^*(t) : [0, T] \rightarrow \mathbb{R}^m$ be measurable. Let U be a closed subset of $\mathbb{R}^m$.*

If

$$\max_{u \in U} h(t, u) = h(t, u^*(t)) \tag{3.4}$$

then $h(t, u(t))$ is differentiable a.e. on $[0, T]$ and

$$\frac{d}{dt}h(t, u(t)) \geq \frac{\partial h}{\partial t}(t, u(t)).$$

In particular if $\frac{\partial h}{\partial t}(t, u(t)) \equiv 0$, then $h(t, u(t))$ is monotonically increasing on $[0, T]$.

Proof. Since $h(t, u)$ is Lipschitz there exists a positive constant W so that

$$\begin{aligned} \frac{h(s + \tau, u^*(s)) - h(s, u^*(s))}{\tau} &\leq \frac{h(s + \tau, u^*(s + \tau)) - h(s, u^*(s))}{\tau} \\ &\leq \frac{h(s + \tau, u^*(s + \tau)) - h(s, u^*(s + \tau))}{\tau} \leq W. \end{aligned} \quad (3.5)$$

The first and second inequalities follow from equation (3.7), and the final inequality follows from the assumption that $h(t, u)$ is Lipschitz with respect to t . In particular, we have that $h(t, u(t))$ is also Lipschitz continuous. Therefore, by Theorem 7.20 of Rudin [21], $h(t, u(t))$ is absolutely continuous and differentiable a.e. on $[0, T]$. And so, (3.8) implies that

$$\frac{d}{dt}h(t, u(t)) \geq \frac{\partial h}{\partial t}(t, u(t)).$$

In particular, if $\frac{\partial h}{\partial t}(t, u(t)) \equiv 0$ then $h(t, u(t))$ is monotonically increasing on $[0, T]$. □

Lemma 3.3.1. The Hamiltonian is monotonically increasing along an optimal trajectory-control pair, that is, if $s < t$ then

$$H(x^*(t), u^*(t), y(t), y_0) \geq H(x^*(s), u^*(s), y(s), y_0)$$

Proof. Apply Theorem 3.3.3 to the function $h : \mathbb{R}^{N \times N} \times [0, T] \rightarrow \mathbb{R}$ defined by

$$h(t, u) = H(x^*(t), u, y(t), y_0) = y'(t)g(x^*(t), u) + y_0f(x^*(t), u).$$

In this definition $x^*(t)$ and $y(t)$ are the state and adjoint vectors that correspond to the control $u^*(t)$. Note that the chain rule, the adjoint equations, and the fact that g does not depend explicitly on t imply that

$$\begin{aligned} \frac{\partial h}{\partial t} &= -y'(t)g_x(x^*(t), u^*(t))g(x^*(t), u) - y_0f_x(x^*(t), u^*(t))g(x^*(t), u) \\ &+ y'(t)g_x(x^*(t), u)g(x^*(t), u^*(t)) + y_0f_x(x^*(t), u)g(x^*(t), u^*(t)). \end{aligned}$$

In particular,

$$\left. \frac{\partial h}{\partial t} \right|_{u=u^*(t)} \equiv 0.$$

Therefore,

$$\frac{d}{dt}H(x(t), u(t), y(t), y_0) \geq 0.$$

And so, $H(x(t), u(t), y(t), y_0)$ is monotonically increasing as claimed. □

Theorem 3.3.1 and Lemma 3.3.1 will now be used to show that if M is large enough and the oscillators are not identical, then $y_0 \neq 0$. Specifically we have the following theorem.

Theorem 3.3.4. *If the following conditions are met, then $y_0 \neq 0$.*

(i) The oscillators are not identical. That is, there exists at least one pair $\{i, j\}$ such that, $\omega_i \neq \omega_j$.

(ii) For all $i \in \{1, \dots, N\}$,

$$\max_j M |\sin(x_i(0) - x_j(0))| > |\omega_i|.$$

(iii) $M(M-1) > \frac{T}{A} c^2 N(N-1)$.

In summary, if there is some variability in the oscillators' natural velocities, if the oscillators are not in phase initially, and if M is large enough, then $y_0 \neq 0$.

Proof. We begin by showing that not both y_0 and y_{N+1} are equal to zero. Let $(x^*(t), u^*(t))$ be an optimal trajectory control pair. Assume toward a contradiction that $y_0 = y_{N+1} = 0$. Then we see that

$$0 = H(x^*(T), u^*(T), y(T), y_0) \geq H(x^*(0), u^*(0), y(0), y_0) \quad (3.6)$$

$$= \sum_i y_i(0) \left(\omega_i + \sum_j u_{ij}^*(0) \sin(x_j^*(0) - x_i^*(0)) \right). \quad (3.7)$$

The first equality holds because $y_{N+1} = y_0 = 0$ and $y_i(T) = 0$, and the second because the Hamiltonian is monotonically increasing along an optimal trajectory. In particular, since the Hamiltonian is maximized along the optimal trajectory by the optimal control we have that

$$0 \geq \max_{u \in [-M, M]^{N \times N}} \{H(x^*(0), u, y(0), y_0)\}.$$

According to assumption (ii) of this theorem, for each $i \in \{1, \dots, N\}$ there exists an index j_i so that

$$M |\sin(x_i^*(0) - x_{j_i}^*(0))| > |\omega_i|.$$

If we define the matrix u by $u_{ij} = 0$ if $j \neq j_i$, and $u_{ij_i} = M \operatorname{sgn}(y_i(0) \sin(x_{j_i}^*(0) - x_i^*(0)))$, we see that

$$H(x^*(0), u, y(0), y_0) \geq \sum_{i=1}^N |y_i(0)| (-|\omega_i| + M |\sin(x_{j_i}^*(0) - x_i^*(0))|).$$

Since we are now under the assumption that $y_0 = y_{N+1} = 0$, condition (iii) of Theorem 3.2 (the characterization of an optimal control) implies that there exists $k \in \{1, \dots, N\}$ such that $y_k(0) \neq 0$. Therefore, the right hand side of the above inequality is strictly greater than zero. This, however, violates the requirement that an optimal control maximize the Hamiltonian along the optimal trajectory, because, according to (3.10), $H(x^*(0), u^*(0), y(0), y_0) \leq 0$. Therefore, not both y_0 and y_{N+1} are zero.

We will show that $y_0 \neq 0$ by showing that $y_0 = 0$ contradicts the optimality of u^* . Toward this goal define the set S as follows:

$$S := \{t : r^2(t) \neq 0\}.$$

Note that since $0 \leq r^2(t) \leq 1$ and $\int_0^T r^2(t) dt = A$, the measure of S is greater than or equal to A .

Now we will show that if $y_0 = 0$, then $\max_{ij} |u_{ij}^*(t)| = M$ for all $t \in S$, and we will show that this contradicts the optimality of u^* under assumption (iii) of this theorem (i.e. under the assumption that $M > \sqrt{\frac{T}{A}} cN$).

Assume toward a contradiction that $y_0 = 0$. Then we must have that $y_{N+1} \neq 0$, and so the Hamiltonian becomes

$$\begin{aligned} H(x^*(t), u^*(t), y(t), 0) &= \sum_i y_i(t) \left(\omega_i + \frac{1}{N} \sum_j u_{ij}(t) \sin(x_j^*(t) - x_i^*(t)) \right) \\ &+ \frac{y_{N+1}}{N^2} \sum_{ij} \cos(x_j^*(t) - x_i^*(t)). \end{aligned}$$

Therefore, by the Maximum Principle, for all $\{i, j\}$ and, at each point $t \in [0, T]$, either $u_{ij}^*(t) = \pm M$, or $y_i(t) \sin(x_j^*(t) - x_i^*(t)) = 0$ (i.e. the singular case).

As it stands, the condition $y_i(t) \sin(x_j^*(t) - x_i^*(t)) = 0$, tells us nothing about the coupling strength u_{ij} , and so, it cannot help us to contradict its optimality. Often times, constraints of this type are differentiated with respect to time in order to yield control characterizations. However, the multitude of controls prevents us from employing this strategy. Instead we will use the Maximum Principle to show that on every interval in S the singular case can be ruled out for at least one pair $\{i, j\}$. This result contradicts the optimality of the control under the assumptions of this theorem.

Assume there exists an open interval $E \subset S$ such that $\max_{ij} |u_{ij}^*(t)| < M$ for all $t \in E$. Then, for all $\{i, j\}$ and for all $t \in E$,

$$y_i(t) \sin(x_j^*(t) - x_i^*(t)) = 0.$$

Therefore, for all $\{i, j\}$ and for all $t \in E$ either $y_i(t) = 0$ or $\sin(x_j^*(t) - x_i^*(t)) = 0$. In fact for all i we must have $y_i(t) \equiv 0$ in E . To see this note that if there exists i and $t^* \in E$ such that $y_i(t^*) \neq 0$ then $\sin(x_j^*(t^*) - x_i^*(t^*)) = 0$ for all j . Also since y_i is continuous there exists an open interval I about t^* in E on which $y_i(t) \neq 0$ so that for all j we have $\sin(x_j^*(t) - x_i^*(t)) \equiv 0$ in I . Therefore for all j , $x_j^*(t) - x_i^*(t)$ is a multiple of π and

$$0 \equiv \frac{d(\sin(x_j^*(t) - x_i^*(t)))}{dt} = \cos(x_j^*(t) - x_i^*(t))(\omega_j - \omega_i) = \pm(\omega_j - \omega_i)$$

in I , contradicting assumption (i) of this theorem.

Then, for all $i \in \{1, \dots, N\}$ we must have $y_i(t) \equiv 0$ in E , which yields

$$0 \equiv \frac{dy_i}{dt} = -\frac{2y_{N+1}}{N^2} \sum_j \sin(x_j^*(t) - x_i^*(t)).$$

Now, since $y_{N+1} \neq 0$, we have that

$$\begin{aligned} 0 &\equiv \sum_j \sin(x_j^*(t) - x_i^*(t)) \\ &= \cos x_i^*(t) \sum_j \sin x_j^*(t) - \sin x_i^*(t) \sum_j \cos x_j^*(t) \\ &= a \cos x_i^*(t) + b \sin x_i^*(t) \end{aligned}$$

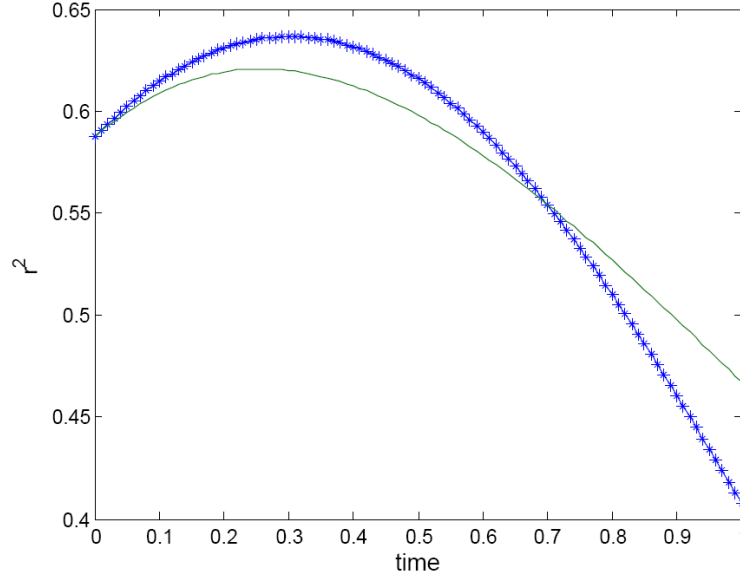


Figure 3.1: The evolution of r^2 for $N = 10$, $T = 1$, and $c = 1$. The starred line corresponds to the controlled network. The solid line corresponds to the Kuramoto network.

in E , where $a = \sum_j \sin x_j^*(t)$, and $b = -\sum_j \cos x_j^*(t)$.

Note also that not both a and b are zero, because if they were then $r^2(t) = 0$, which would contradict the assumption that $t \in E \subset S$. Therefore, the vectors $(\cos x_i^*(t), \sin x_i^*(t))$ all belong to the one dimensional vector space spanned by (a, b) . And so, for all pairs (i, j) , $(\cos x_i^*(t), \sin x_i^*(t)) = \alpha_j(t)(\cos x_j(t), \sin x_j(t))$, for some nonzero $\alpha_j(t)$. But this implies that $x_i(t) \equiv x_j(t) \pmod{\pi}$. Again we have arrived at $\sin(x_j(t) - x_i(t)) = 0$ in E which has already been shown to contradict assumption (1) of this theorem. Therefore at almost every point $t \in S$ there exists at least one pair (i, j) , such that $|u_{ij}^*(t)| = M$. This yields:

$$\int_0^T \sum_{i \neq j} u_{ij}^{*2}(t) dt \geq \int_S \sum_{i \neq j} u_{ij}^{*2}(t) dt \geq AM(M-1) > TN(N-1)c^2 = \int_0^T \sum_{i \neq j} c^2 dt,$$

which contradicts the optimality of u^* because $u_{ij} \equiv c$ forms an admissible control. $\square$

Since we have shown that $y_0 \neq 0$, taking $y_0 = 1$ we can characterize an optimal control by maximizing the Hamiltonian pointwise along the optimal trajectory:

$$u_{ij}^* = \max \left(-M, \min \left(\frac{y_i(t) \sin(x_j^* - x_i^*)}{2N}, M \right) \right).$$

3.3.4 Numerical Simulations

The characterization of an optimal control allows us to find controls that satisfy the necessary

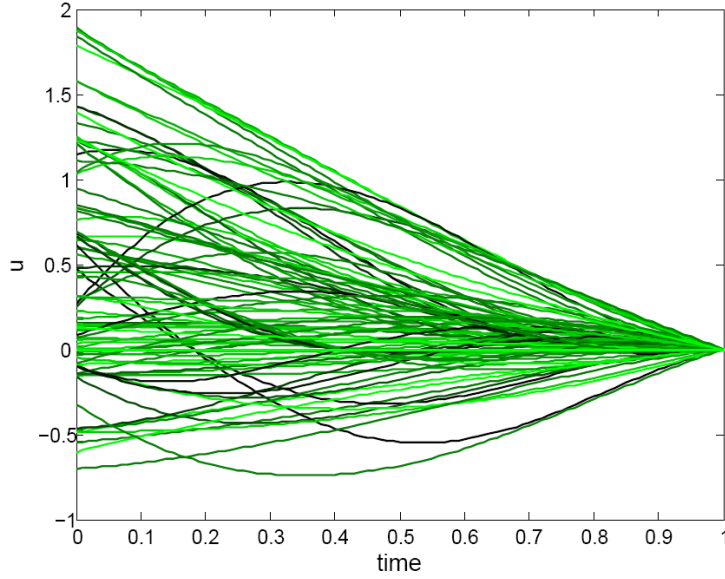


Figure 3.2: The coupling strengths, $u_{ij}(t)$, for $N = 10$, $T = 1$, $c = 1$

conditions by using a forward backward sweep algorithm. In all of these simulations we choose the bound M on the magnitude of the controls to be large, $M = 1000$, so that it is not attained.

First we simulate the evolution of a network of ten oscillators. The final time is 1. The oscillators' natural velocities are drawn from a normal distribution with mean 20 and standard deviation 1. The oscillators' initial phases are drawn from a uniform distribution on the interval $[0, \pi]$. The network synchrony, $\frac{1}{T} \int_0^T r^2 dt$, is equal to the synchrony achieved by an identical set of oscillators connected through a Kuramoto network with $u_{ij}(t) \equiv 1$ ($c = 1$).

Figure 3.1 plots r^2 for both the controlled and Kuramoto networks ($u_{ij} \equiv 1$). Note that with these parameters the order parameter of both networks increases and then declines. The synchrony of both networks is 0.5700. The controlled network's connectivity cost is 0.2333, while that of the Kuramoto network is 1. These results indicate that networks with time varying coupling are able to achieve equal levels of synchrony as Kuramoto networks while being much less connected.

Figure 3.2 shows the evolution of the controls. From this figure we see that the controlled network is not a mean-field network, that is, the oscillators are not coupled to the mean phase. (If the network was a mean-field network, we would have $u_{ij} = u_i$. As a result, Figure 3.2 would appear to have at most $N = 10$ controls.) Also note that some negative coupling does occur. Negative coupling implies that the oscillators are actually repelling one another. This result is interesting because it suggests that repulsion can facilitate the development of synchrony. The shade of the line that corresponds to u_{ij} corresponds to the magnitude of the difference in the natural velocities of i th and j th oscillator (i.e. $|\omega_i - \omega_j|$). The greater the difference in the natural velocities of two oscillators the darker the shade of the coupling strength that connects them.

In our next simulation the final time is lengthened to 2. The other parameters are held constant.

Figure 3.3 plots r^2 for both the controlled and Kuramoto networks ($u_{ij} \equiv 1$). The synchrony of both networks is 0.2677. The controlled network's connectivity cost is 0.0783, while that of the Kuramoto network is 1.

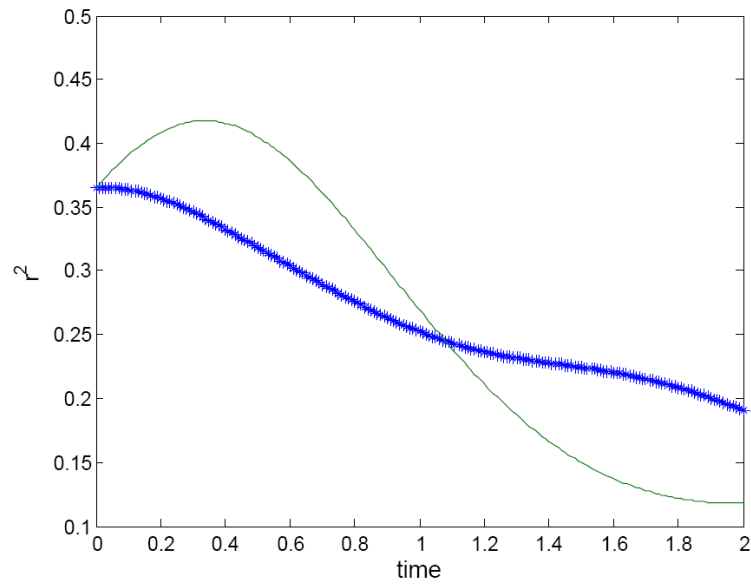


Figure 3.3: The evolution of r^2 for $N = 10$, $T = 2$, and $c = 1$. The starred line corresponds to the controlled network. The solid line corresponds to the Kuramoto network.

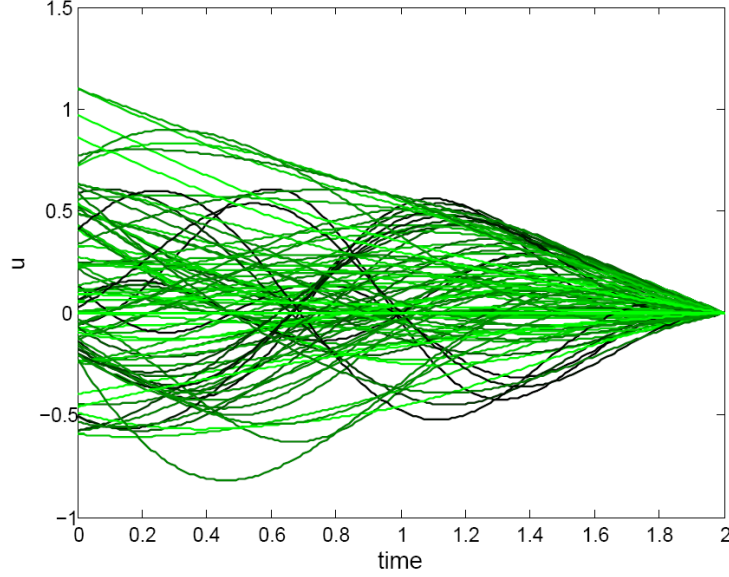


Figure 3.4: The coupling strengths, $u_{ij}(t)$, for $N = 10$, $T = 2$, $c = 1$

Figure 3.4 shows the evolution of the controls. From this figure we see that lengthening the time length to 2 has not qualitatively changed the control strategy.

In the next simulation we increase the value of the parameter c to 3. As a result, the network synchrony is equal to the synchrony achieved by an identical set of oscillators interacting through a Kuramoto network with $u_{ij}(t) \equiv 3$. The other parameters are held constant.

Figure 3.5 plots r^2 for both the controlled and Kuramoto networks ($u_{ij} \equiv 3$). The synchrony of both networks is 0.6769. The controlled network's connectivity cost is 2.194, while that of the Kuramoto network is 9.

Figure 3.6 shows the evolution of the controls. From this figure we see that increasing the synchrony of the network has increased the magnitude of the controls.

Finally, we reduce the standard deviation in the natural velocities of the oscillators to .1. This increases the importance of the coupling relative to the natural velocity in determining an oscillator's dynamics. As a result, the network synchronizes more easily. The effect is similar to what would occur if we increased the network connectivity (i.e. the average coupling strength squared). However, for large connectivity costs the numerical algorithm may not converge, while convergence is not a problem for networks of oscillators that have a small standard deviation in their natural velocities. The final time, the initial phases, the mean of the oscillator's natural velocities, and the upper bound on the network connectivity cost are the same as in the previous simulation. The network synchrony is constrained to be that of an identical set of oscillators interacting through a Kuramoto network with $u_{ij} \equiv 3$.

Figure 3.7 plots r^2 for both the controlled and Kuramoto networks ($u_{ij} \equiv 3$). The synchrony of both networks is 0.8042. The controlled network's connectivity cost is 2.1926, while that of the Kuramoto network is 9.

Figure 3.8 shows the evolution of the controls. From this figure we see that increasing the size of the network does not qualitatively alter the control strategy.

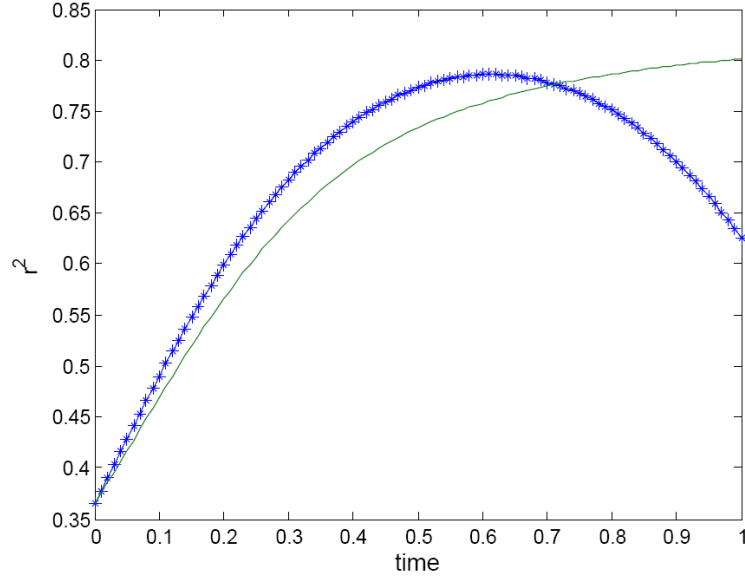


Figure 3.5: The evolution of r^2 for $N = 10$, $T = 1$, and $c = 3$. The starred line corresponds to the controlled network. The solid line corresponds to the Kuramoto network.

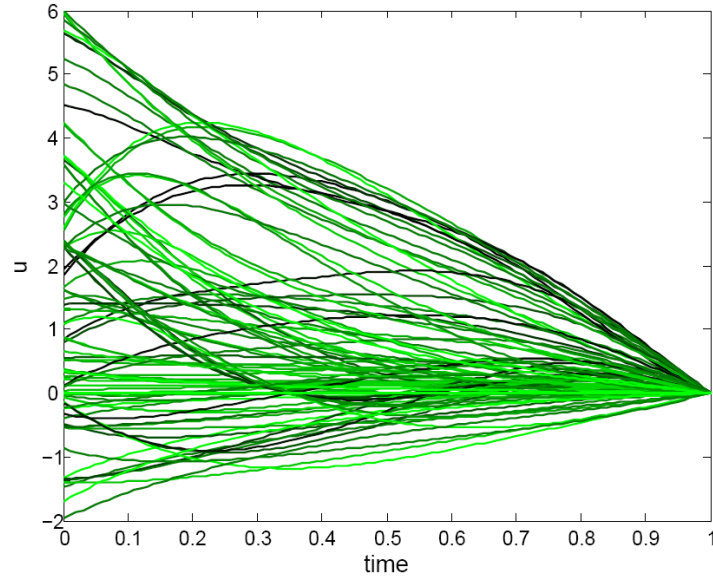


Figure 3.6: The coupling strengths, $u_{ij}(t)$, for $N = 10$, $T = 1$, $c = 3$

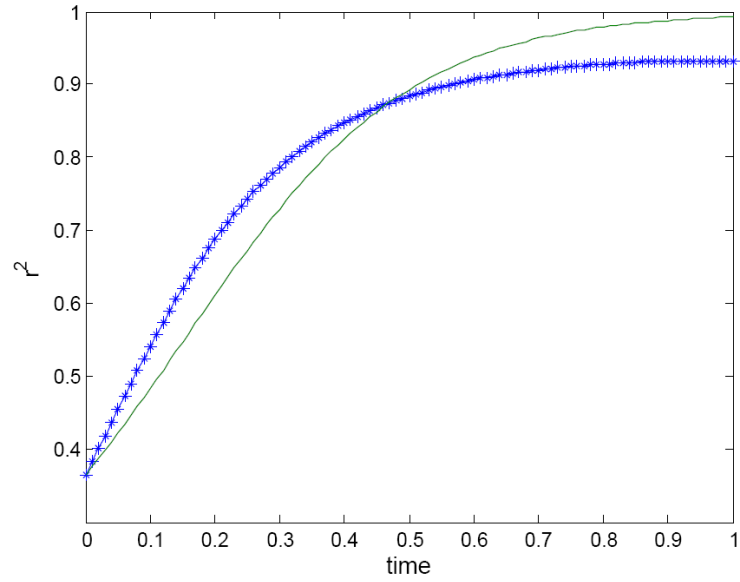


Figure 3.7: The evolution of r^2 for $N = 10$, $T = 1$, and $c = 1$. The starred line corresponds to the controlled network. The solid line corresponds to the Kuramoto network.

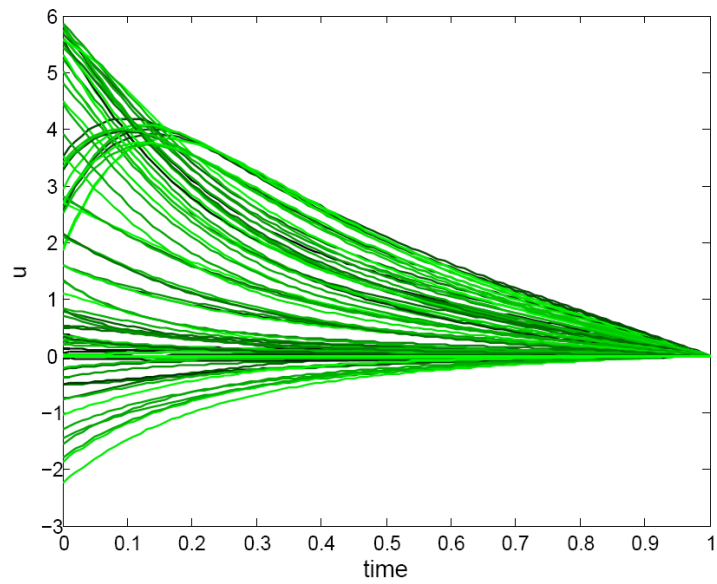


Figure 3.8: The coupling strengths, $u_{ij}(t)$, for $N = 24$, $T = 1$, $c = 1$

3.4 Maximizing the Synchrony of a Network with Bounded Connectivity

3.4.1 Formulating the Problem

In this section we find the coupling strengths, u_{ij} , that maximize the network synchrony while keeping the connectivity cost below a prescribed bound. In particular, we are interested in seeing how much we can improve upon the synchrony of a Kuramoto network by allowing the coupling strengths to vary between oscillators and through time. As a result the prescribed bound on the connectivity cost, C , will be the connectivity cost of the Kuramoto network with $u_{ij} \equiv c$. Now given c we will find the coupling strengths, $u_{ij}(t)$, that maximize

$$\int_0^T r^2(t) dt$$

subject to,

$$\int_0^T \sum_{i \neq j} u_{ij}^2 dt \leq C = N(N-1)c^2T.$$

As in the previous problem we define the control set, U , to be the set of all matrix valued functions, $u : [0, T] \rightarrow [-M, M]^{N \times (N-1)}$, such that each component u_{ij} is a measurable function.

To incorporate the constraint $\int_0^T \sum_{i \neq j} u_{ij}^2 dt \leq C$ into the problem we introduce an artificial state variable x_{N+1} , which satisfies:

$$\begin{aligned} \frac{dx_{N+1}}{dt} &= \sum_{i \neq j} u_{ij}^2(t) \\ x_{N+1}(0) &= 0. \end{aligned}$$

We will also assume that the initial oscillator phases are fixed, that is, for $i = 1, \dots, N$,

$$x_i(0) = x_i^0.$$

We will say that a vector, $x(t) = (x_1(t), \dots, x_N(t), x_{N+1}(t))$, corresponds to the control $u \in U$ if the components of $x(t)$ are absolutely continuous functions that satisfy the following conditions: For $i = 1, \dots, N$,

$$\begin{aligned} \frac{dx_i}{dt} &= \omega_i + \frac{1}{N} \sum_{j=1}^N u_{ij}(t) \sin(x_j(t) - x_i(t)), \\ x_i(0) &= x_i^0, \\ \frac{dx_{N+1}}{dt} &= \sum_{i \neq j} u_{ij}^2(t), \end{aligned}$$

and

$$x_{N+1}(0) = 0.$$

In this case we will call $(x(t), u(t))$ a trajectory-control pair.

Now we can define the set of admissible controls. Let $(x(t), u(t))$ be a trajectory-control pair

with $u \in U$. We will say that $u \in U_{ad}$ if $x_{N+1}(T) \leq C$. It is clear that $U_{ad} \neq \emptyset$ since the control $u_{ij} \equiv c$ for $i \neq j$ belongs to U_{ad} .

Finally we define the objective functional,

$$J(u) = \int_0^T r^2(t) dt.$$

Within this framework the problem may be stated as follows:

Problem II

Find a trajectory-control pair (x^*, u^*) so that $u^* \in U_{ad}$, and

$$J(u^*) = \max_{u \in U_{ad}} J(u).$$

3.4.2 Existence of an Optimal Control

It is straightforward to show that Problem II has a solution. The proof that an optimal control exists for Problem II is similar to that of Problem I.

Theorem 3.4.1. *There exists a solution, (x^*, u^*) , to Problem II.*

Proof. Choose a sequence $\{u^m\}$ in U_{ad} so that $J(u^m) \rightarrow \max_{u \in U_{ad}} J(u)$. Since each control component, u_{ij} , is $L^2[0, T]$ bounded, there exist L^2 functions u_{ij}^* and a subsequence $\{u^m\}$ so that $u_{ij}^m \rightharpoonup u_{ij}^*$ weakly in L^2 . The structure of the state system implies that the state components x_i^m with $i \in \{1, \dots, N\}$ associated with the controls u^m are uniformly bounded and equicontinuous and so by the Arzela-Ascoli Theorem for $i \in \{1, \dots, N\}$ there exists a subsequence $\{x_i^m\}$ converging uniformly to x_i^* in $C[0, T]$. Uniform convergence of the states and weak convergence of the controls yields

$$\frac{dx_i^*}{dt} = \omega_j + \frac{1}{N} \sum_{j=1}^N u_{ij}^*(t) \sin(x_j^* - x_i^*)$$

in $H^1[0, T]$, as desired, meaning x^* is the state corresponding to u^* . Also, since the norm is lower semicontinuous with respect to weak convergence, $u^* \in U_{ad}$, that is,

$$x_{N+1}^*(T) = \int_0^T \sum_{j \neq k} u_{jk}^*(t)^2 dt \leq \liminf_m \int_0^T \sum_{j \neq k} u_{jk}^m(t)^2 dt = \liminf_m x_{N+1}^m(T) \leq C.$$

Finally, because the state components x_i^m with $i \in \{1, \dots, N\}$ converge uniformly, x^* maximizes the objective functional.

$$J(u^*) = \int_0^T r^*(t)^2 dt = \lim_{m \rightarrow \infty} \int_0^T r^m(t)^2 dt = \lim_{m \rightarrow \infty} J(u^m)$$

Therefore u^* is optimal and the desired existence result is proved. $\square$

3.4.3 Characterization of the Optimal Control

The right hand sides of the differential equations for the states can be used to define $N + 1$ functions from $[\mathfrak{R}^{N+1}, \mathfrak{R}^{N \times (N-1)}]$ to $\mathfrak{R}$. For notational convenience we will denote these functions by

$$\frac{dx_i}{dt}(x, u).$$

Now we can define $g(x, u) : [\mathfrak{R}^{N+1}, \mathfrak{R}^{N \times (N-1)}] \rightarrow \mathfrak{R}^{N+1}$ to be the vector valued function

$$g(x, u) := \left(\frac{dx_1}{dt}(x, u), \dots, \frac{dx_{N+1}}{dt}(x, u) \right)',$$

where $'$ denotes the transpose. We also define the function $f(x, u)$ by,

$$f(x, u) := \frac{1}{N^2} \left[\left(\sum_j \sin x_j \right)^2 + \left(\sum_j \cos x_j \right)^2 \right],$$

and the Hamiltonian function, $H : \mathfrak{R}^{N+1} \times \mathfrak{R}^{N \times (N-1)} \times \mathfrak{R}^{N+1} \times \mathfrak{R} \rightarrow \mathfrak{R}$ by,

$$H(x, u, y, y_0) = y'g(x, u) + y_0f(x, u) \quad (3.8)$$

$$= \sum_{i=1}^N y_i \left(\omega_i + \frac{1}{N} \sum_j u_{ij} \sin(x_j - x_i) \right) \quad (3.9)$$

$$+ y_{N+1} \sum_{i \neq j} u_{ij}^2 \quad (3.10)$$

$$+ \frac{y_0}{N^2} \left[\left(\sum_j \sin x_j \right)^2 + \left(\sum_j \cos x_j \right)^2 \right]$$

. An application of the results from [29] characterizes the solutions of problem *II*.

Theorem 3.4.2. *If (x^*, u^*) is a solution to Problem II, then there exists a pair $(y_0, y(t))$ so that the following conditions are met,*

- (i) *The map $y : [0, T] \rightarrow \mathfrak{R}^{N+1}$ is absolutely continuous;*
- (ii) *$y_0 \in \mathfrak{R}$ and $y_0 \geq (0)$;*
- (iii) *$(y_0, y(t)) \neq (0, 0)$ for every $t \in [0, T]$;*
- (iv) *the adjoint differential system holds, that is,*

$$\frac{dy}{dt} = -\frac{\partial H}{\partial x}(x^*(t), u^*(t), y(t), y_0);$$

- (v) *the Hamiltonian maximization condition holds, that is,*

$$H(x^*(t), u^*(t), y(t), y_0) = \max_{u \in U_{ad}} \{H(x^*(t), u(t), y(t), y_0)\};$$

- (vi) *and the transversality condition,*

$$y_i(T) = 0$$

for $i = 1, \dots, N$ holds.

The adjoint equations may be written out componentwise. For $i = (1, \dots, N)$

$$\frac{dy_i}{dt} = \frac{1}{N} \sum_{j \neq i, j=1}^N (y_i(t)u_{ij}^*(t) - y_j(t)u_{ji}^*(t)) \cos(x_j^*(t) - x_i^*(t)) - \frac{2y_0}{N^2} \sum_{j=1}^N \sin(x_j^*(t) - x_i^*(t))$$

and

$$\frac{dy_{N+1}}{dt} = 0.$$

In particular, we see that y_{N+1} is constant.

At this point we would like to characterize an optimal coupling strength, u_{ij} , by setting the derivative of the Hamiltonian with respect to u_{ij} equal to zero and solving. For reasons analogous to those presented in Problem I the resulting characterization will depend on whether or not the adjoint variable $y_{N+1} = 0$.

The next lemma states that the Hamiltonian is monotone increasing along an optimal trajectory-control pair. This lemma will aid us in characterizing the optimal control.

Lemma 3.4.1. The Hamiltonian is monotonically increasing along an optimal trajectory-control pair, that is, if $s < t$ then

$$H(x^*(t), u^*(t), y(t), y_0) \geq H(x^*(s), u^*(s), y(s), y_0)$$

The proof of Lemma 3.4.1 is like that of Lemma 3.3.1, but with y_{N+1} in place of y_0 .

Theorem 3.4.2 and Lemma 3.4.1 will now be used to show that if M is large enough and the oscillators are not identical then $y_{N+1} \neq 0$. This allows us to characterize the optimal control in terms of the adjoint and state variables by setting the derivative of the Hamiltonian with respect to each control component to zero.

Theorem 3.4.3. *Let A be the synchrony obtained by an identical system of oscillators governed by the mean-field control $u_{ij} \equiv c$ for $i \neq j$. Then, if the following conditions are met, $y_{N+1} \neq 0$.*

(i) $A \neq 0$.

(ii) *The oscillators are not identical. That is, for some i and j $\omega_i \neq \omega_j$.*

(iii) *For all $i \in \{1, \dots, N\}$,*

$$\max_j M |\sin(x_i(0) - x_j(0))| > |\omega_i|.$$

(iv) $M > \sqrt{\frac{C}{A}}$

In summary, if an identical set of oscillators coupled via the admissible Kuramoto network, $u_{ij} \equiv c$, has nonzero order, if there is some variability in the oscillators' natural velocities, if the oscillators are not in phase initially, and if M is large enough, then $y_0 \neq 0$. Note that the first condition is always satisfied if the order parameter is initially nonzero.

Proof. We begin by showing that not both y_0 and y_{N+1} are equal to zero. Let $(x^*(t), u^*(t))$ be an optimal trajectory-control pair. Assume toward a contradiction that $y_0 = y_{N+1} = 0$. Then we see

that

$$0 = H(x^*(T), u^*(T), y(T), 0) \geq H(x^*(0), u^*(0), y(T), 0) \quad (3.11)$$

$$\geq \sum_{i=1}^N y_i(0) \left(\omega_i + \sum_j u_{ij}^*(0) \sin(x_j^*(0) - x_i^*(0)) \right). \quad (3.12)$$

The first equality holds because $y_{N+1} = y_0 = 0$ and $y_i(T) = 0$ for $i = 1, 2, \dots, N$, and the second holds because the Hamiltonian is monotone increasing along an optimal trajectory. In particular, since the Hamiltonian is maximized along the optimal trajectory by the optimal control we have that

$$0 \geq \max_{u \in [-M, M]^{N \times N}} \{H(x^*(0), u, y(0), 0)\}.$$

Now, by condition (iii) of Theorem 4.2, there exists $k \in \{1, \dots, N\}$ such that $y_k(0) \neq 0$. In addition by assumption (iii) of this theorem for each $i \in \{1, \dots, N\}$ there exists an index j_i so that

$$M |\sin(x_i^*(0) - x_{j_i}^*(0))| > |\omega_i|.$$

And so, if we define the matrix u by $u_{ij} = 0$ if $j \neq j_i$, and $u_{ij_i} = M \operatorname{sgn}(y_i(0) \sin(x_{j_i}^*(0) - x_i^*(0)))$, we see that

$$H(x^*(0), u, y(0), y_0) \geq \sum_{i=1}^N |y_i(0)| (-|\omega_i| + M |\sin(x_{j_i}^*(0) - x_i^*(0))|) > 0,$$

which contradicts the Maximum Principle. Therefore, not both y_0 and y_{N+1} are zero.

Now we will show that $y_{N+1} \neq 0$ by showing that $y_{N+1} = 0$ implies that u^* is not admissible, that is $y_{N+1} = 0$ implies that $\int_0^T \sum u_{ij}^{*2}(t) dt > C$. Toward this goal define the set S as follows:

$$S := \{t : r^2(t) \neq 0\}.$$

Note that since $0 \leq r^2(t) \leq 1$, and u^* is an optimal control the measure of S is greater than or equal to A . Now we will proceed by showing that if $y_{N+1} = 0$ then

$$\max_{ij} |u_{ij}^*(t)| = M$$

for all $t \in S$, and this will contradict the admissibility of u^* under assumption (4) of this theorem (i.e. under the assumption that $M > \sqrt{\frac{C}{A}}$.)

Assume toward a contradiction that $y_{N+1} = 0$. Then we must have that $y_0 \neq 0$, and so the Hamiltonian becomes

$$\begin{aligned} H(x^*(t), u^*(t), y(t), y_0) &= \sum_i y_i(t) \left(\omega_i + \frac{1}{N} \sum_j u_{ij}^* \sin(x_j^*(t) - x_i^*(t)) \right) \\ &+ \frac{y_0}{2N^2} \sum_{ij} \cos(x_i^*(t) - x_j^*(t)). \end{aligned}$$

Here we used equations (1) – (3) on page 5. Therefore by the Maximum Principle either $u_{ij}^*(t) = \pm M$, or $y_i(t) \sin(x_j^*(t) - x_i^*(t)) = 0$ at every point $t \in [0, T]$.

If there exists an open interval $E \subset S$ such that $\max_{ij} |u_{ij}^*(t)| < M$ for all $t \in E$, then for all (i, j) and for all $t \in E$, $y_i(t) \sin(x_j^*(t) - x_i^*(t)) = 0$. And so, for all (i, j) and for all $t \in E$ either $y_i(t) = 0$ or $\sin(x_j^*(t) - x_i^*(t)) = 0$. In fact for all i we must have $y_i(t) \equiv 0$ in E . To see this note that if there exists i and $t^* \in E$ such that $y_i(t^*) \neq 0$ then $\sin(x_j^*(t^*) - x_i^*(t^*)) = 0$ for all j . Also since y_i is continuous there exists an open interval I about t^* in E on which $y_i(t) \neq 0$ so that for all j we have $\sin(x_j^*(t) - x_i^*(t)) \equiv 0$ in I . Therefore for all (i, j)

$$0 \equiv \frac{d(\sin(x_j^*(t) - x_i^*(t)))}{dt} = \cos(x_j^*(t) - x_i^*(t))(\omega_j - \omega_i) = \pm(\omega_j - \omega_i)$$

in I , contradicting assumption (2) of this theorem. Therefore, for all $i \in \{1, \dots, N\}$, we must have $y_i(t) \equiv 0$ in E , which yields

$$0 \equiv \frac{dy_i}{dt} = \frac{y_0}{2N^2} \sum_j \sin(x_j^*(t) - x_i^*(t)).$$

Now, since $y_0 \neq 0$, we have that

$$\begin{aligned} 0 &\equiv \sum_j \sin(x_j^*(t) - x_i^*(t)) \\ &= \cos x_i^*(t) \sum_j \sin x_j^*(t) - \sin x_i^*(t) \sum_j \cos x_j^*(t) \\ &= a \cos x_i^*(t) + b \sin x_i^*(t) \end{aligned}$$

in E , where $a = \sum_j \sin x_j^*(t)$, and $b = -\sum_j \cos x_j^*(t)$. Note also that not both a and b are zero, because if they were then $r^2(t) = 0$, which would contradict the assumption that $t \in E \subset S$. Therefore for all i , $(\cos x_i^*(t), \sin x_i^*(t))$ is in the one dimensional vector space spanned by (a, b) . And so, for all pairs (i, j) , $(\cos x_i^*(t), \sin x_i^*(t)) = \alpha_j(t)(\cos x_j^*(t), \sin x_j^*(t))$, for some nonzero $\alpha_j(t)$. But this implies that $x_i^*(t) \equiv x_j^*(t) \pmod{\pi}$. Again we have arrived at $\sin(x_j^*(t) - x_i^*(t)) \equiv 0$ in E which has already been shown to contradict assumption (2) of this theorem. Therefore at almost every point $t \in S$ there exists u_{ij}^* such that $|u_{ij}^*(t)| = M$. This yields:

$$\int_0^T \sum_{ij} u_{ij}^{*2}(t) dt \geq \int_S \sum_{ij} u_{ij}^{*2}(t) dt \geq AM^2 > C,$$

which contradicts the admissibility of the control u^* . $\square$

Taking $y_{N+1} = 1$, we characterize an optimal control by the fact that it maximizes the Hamiltonian:

$$u_{ij}^* = \max \left(-M, \min \left(\frac{-y_i(t) \sin(x_j^* - x_i^*)}{2N}, M \right) \right). \quad (3.13)$$

The next theorem states that an optimal network will be as connected as possible, that is, the connectivity cost will be equal to C .

Theorem 3.4.4. *Let (x^*, u^*) be an optimal trajectory control pair. If*

- (i) $y_{N+1} \neq 0$,
- (ii) u^* is not identically equal to zero, and
- (iii) Controls with $|u_{ij}(t)| \equiv M$ for all ij are not admissible, that is,

$$\int_0^T \sum_{ij} u_{ij}^2(t) dt = T(NM)^2 > C,$$

then $x_{N+1}^*(T) = C$.

Note that Theorem 3.4.3 provides us with conditions under which condition (i) of this theorem is guaranteed to hold, assumption (ii) of this theorem is easy to check numerically, and assumption (iii) of this theorem is satisfied if M is large enough.

Proof. Suppose that assumptions (i), (ii), and (iii) of this theorem are met, and that $x_{N+1}^*(T) < C$. Assumption (i) implies that u^* is continuous through its characterization (3.16). The continuity of u^* along with assumptions (ii) and (iii) imply that there exists an open interval I and an index pair (i, j) so that $u_{ij}^*(t) \notin \{-M, 0, M\}$ for all $t \in I$. Since u^* maximizes the Hamiltonian along the optimal trajectory,

$$H_{u_{ij}}(x^*(t), u^*(t), y(t), y_0) = 0$$

in I . In addition, since $x_{N+1}(T) < C$, we can find continuous functions $h(t)$ with support in I so that the control variation u^ϵ defined by

$$u_{ij}^\epsilon = u_{ij}^* + \epsilon h(t),$$

$$u_{kl}^\epsilon = u_{kl}^*, (k, l) \neq (i, j)$$

is admissible for ϵ small enough. Note that we can easily find continuous functions $h(t)$ so that the corresponding state trajectory satisfies either

$$x_{N+1}^\epsilon(T) < x_{N+1}^*(T)$$

or

$$x_{N+1}^*(T) > x_{N+1}^\epsilon(T).$$

Let

$$g(x, u) := \left(\frac{dx_1}{dt}(x, u), \dots, \frac{dx_{N+1}}{dt}(x, u) \right)'.$$

and

$$f(x, u) := \frac{1}{N^2} \left[\left(\sum_j \sin x_j \right)^2 + \left(\sum_j \cos x_j \right)^2 \right],$$

as before. Then, following the development of the necessary conditions presented by Lenhart and Workman [15], we see that

$$y_0 J(u^\epsilon) = \int_0^T y_0 f(x^\epsilon, u^\epsilon, t) + \frac{d}{dt}(y(t)' x^\epsilon(t)) dt + y(0)' x^\epsilon(0) - y(T)' x^\epsilon(T).$$

Taking the limit of the difference quotient, $\frac{J(x^\epsilon, u^\epsilon) - J(x^*, u^*)}{\epsilon}$ as $\epsilon \rightarrow 0$ yields

$$\begin{aligned}
0 &\geq \frac{d}{d\epsilon} y_0 J(u^\epsilon) \Big|_{\epsilon=0} \\
&= \int_0^T (y_0 f_{u_{ij}}(t, x^*(t), u^*(t)) + y(t)' g_{u_{ij}}(t, x^*(t), u^*(t))) h(t) dt \\
&\quad - y_{N+1}(T) \frac{\partial x_{N+1}^\epsilon}{\partial \epsilon}(T) \Big|_{\epsilon=0} \\
&= y_{N+1} \frac{\partial x_{N+1}^\epsilon}{\partial \epsilon}(T) \Big|_{\epsilon=0}. \tag{3.14}
\end{aligned}$$

The first equality follows from the chain rule, the adjoint equations, the fact that $y_i(T) = 0$ for $i = (1, 2, \dots, N)$ and the fact that $u_{kl}^\epsilon = u_{kl}^*$ if $(k, l) \neq (i, j)$. The second equality follows from that fact that $\text{supp} h(t) \subset I$ and that

$$y_0 f_{u_{ij}}(t, x^*(t), u^*(t)) + y(t)' g_{u_{ij}}(t, x^*(t), u^*(t)) = H_{u_{ij}}(t, x^*(t), y(t), u^*(t)) = 0$$

in I . Since we can choose h so that either

$$\frac{\partial x_{N+1}^\epsilon}{\partial \epsilon}(T) \Big|_{\epsilon=0} \geq 0,$$

or

$$\frac{\partial x_{N+1}^\epsilon}{\partial \epsilon}(T) \Big|_{\epsilon=0} \leq 0,$$

3.17 implies that $y_{N+1} = 0$, which contradicts assumption i . □

3.4.4 Numerical Simulations

The characterization of an optimal control allows us to find controls that satisfy the necessary conditions by using a forward backward sweep algorithm. As in the simulations from Problem I we choose the upper bound M on the magnitude of the controls to be large, $M = 1000$, so that it is never attained.

First we simulate the evolution of a network of ten oscillators. The final time is 1. The oscillators' natural velocities were drawn from a normal distribution with mean 20 and standard deviation 1. The oscillators' initial phases were drawn from a uniform distribution on the interval $[0, \pi]$. The network connectivity cost, $\frac{1}{T(N-1)(N)} \int_0^T \sum_{i \neq j} u_{ij}^2(t) dt$, is equal to the connectivity cost of an identical set of oscillators connected through a Kuramoto network with $u_{ij}(t) \equiv 1$ for $i \neq j$, (i.e. $c = 1$).

Figure 3.9 plots the order parameter squared for both the controlled and Kuramoto networks. The controlled network's synchrony is .5293, while that of the Kuramoto network is .3715. These results indicate that networks with time varying coupling are able to achieve greater synchrony than Kuramoto networks with the same connectivity cost.

Figure 3.10 shows the evolution of the controls. We can see from the figure that, as in the previous simulation, this controlled network is not a mean-field network. This network also has some negative coupling.

In the next simulation we decrease the standard deviation in the oscillator's natural velocities to .1. The other parameters are held constant.

Figure 3.11 plots the order parameter squared for both the controlled and Kuramoto ($u_{ij} \equiv 1$) networks. The controlled network's synchrony is .6933, while that of the Kuramoto network is .5534. We see that decreasing the standard deviation in the oscillator's natural velocities increases the network synchrony for both the Kuramoto and controlled networks.

Figure 3.12 shows the evolution of the controls. We can see from the figure that, as in the previous simulations, the controlled network is not a mean-field network. This network also has some negative coupling.

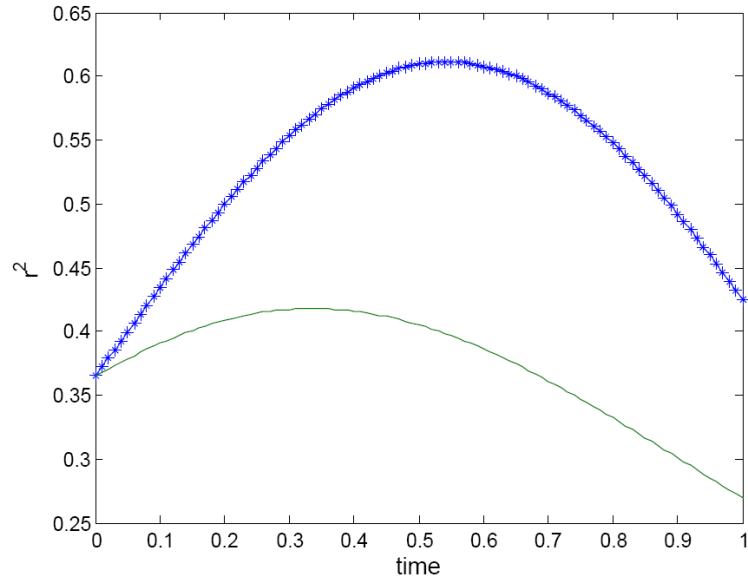


Figure 3.9: The evolution of r^2 for $N = 10$, $T = 1$, and $c = 1$. The starred line corresponds to the controlled network. The solid line corresponds to the Kuramoto network.

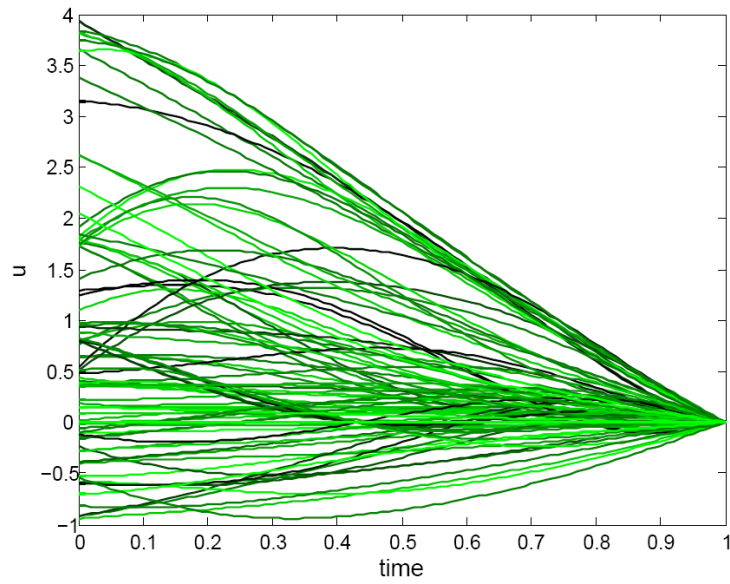


Figure 3.10: The coupling strengths, $u_{ij}(t)$, for $N = 10$, $T = 1$, $c = 1$

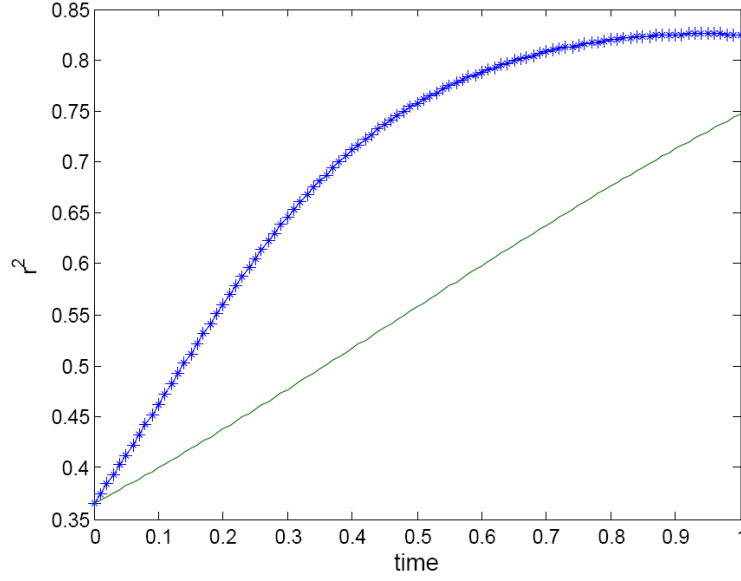


Figure 3.11: The evolution of r^2 for $N = 10$, $T = 1$, and $c = 1$. The starred line corresponds to the controlled network. The solid line corresponds to the Kuramoto network.

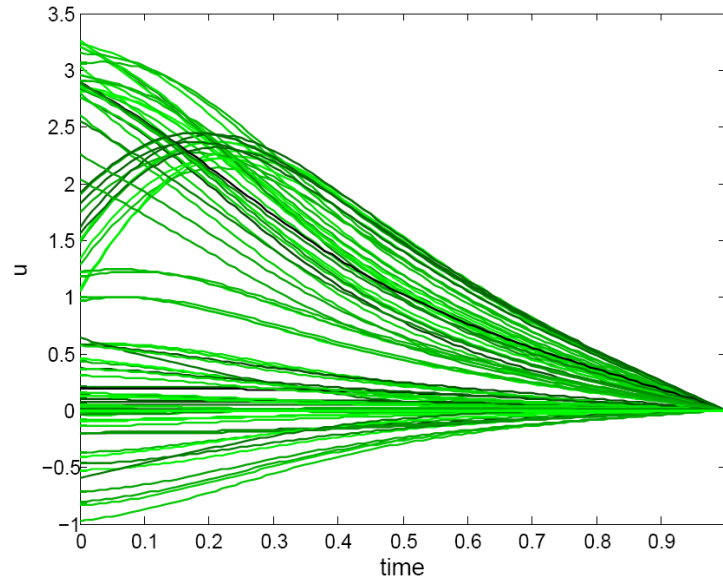


Figure 3.12: The coupling strengths, $u_{ij}(t)$, for $N = 10$, $T = 1$, $c = 1$

3.5 Balancing Network Order and Connectivity

3.5.1 Formulating the Problem

In this section we consider an intermediate problem. Here we will find the coupling strengths, u_{ij} , that maximize network synchrony minus a weighted connectivity cost. In particular, we will find the coupling strengths that maximize,

$$J(u) := \int_0^T r^2(t)dt - B \int_0^T \sum_{i \neq j} u_{ij}^2(t)dt.$$

Note that in this formulation we have dropped the coefficients, $\frac{1}{TN(N-1)}$ and $\frac{1}{T}$ from the connectivity cost and network synchrony respectively.

We define the set of admissible controls, U , to be the set of all matrix valued functions, $u : [0, T] \rightarrow [-M, M]^{N \times (N-1)}$, such that each component u_{ij} is a measurable function.

We will say that a vector, $x(t) = (x_1(t), \dots, x_N(t))$, corresponds to the control $u(t)$ if the components of $x(t)$ are absolutely continuous functions that satisfy the following conditions: For $i = 1, \dots, N$,

$$\frac{dx_i}{dt} = \omega_i + \frac{1}{N} \sum_{j=1}^N u_{ij}(t) \sin(x_j - x_i)$$

and

$$x_i(0) = x_i^0.$$

In this case we will call (x, u) a trajectory-control pair.

Within this framework the problem may be stated as follows:

Problem III

Find a trajectory-control pair (x^*, u^*) so that $u^* \in U$, and

$$J(x^*, u^*) = \min_{u \in U} J(x, u).$$

Note that this problem is simpler than the previous two because it does not have any state or control constraints at the final time.

3.5.2 Existence of an Optimal Control

It is straight forward to show that there exists a solution to Problem III.

Theorem 3.5.1. *There exists a solution, (x^*, u^*) , to Problem III.*

Proof. To show the existence of an optimal control we select a sequence of controls $\{u^m\}$ in U so that $J(u^m) \rightarrow \max_{u \in U} J(u)$. Then since each control u_{ij}^m is bounded in $L^2[0, T]$ there exists a function u^* in U and a weakly converging subsequence $\{u^m\}$ so that $u_{ij}^m \rightharpoonup u_{ij}^*$. Note that this implies that u^* satisfies $\text{esssup}(u_{ij}) \leq M$ as before. Also we see that the states x^m associated with the controls u^m are uniformly bounded and equicontinuous, and so by Arzela-Ascoli there exists a subsequence $\{x_j^m\}$ converging uniformly to x_j^* in $C[0, T]$. Uniform convergence of the states and

weak convergence of the controls yields

$$\frac{dx_j^*}{dt} = \omega_j + \frac{1}{N} \sum_{k=1}^N u_{jk}^*(t) \sin(x_k^* - x_j^*)$$

in $H^1[0, T]$, as desired. Thus, x^* is the state corresponding to u^* . In addition,

$$\begin{aligned} \lim_{m \rightarrow \infty} J(u^m) &= \lim_{m \rightarrow \infty} \frac{1}{N^2} \int_0^T \left[\left(\sum_{i=1}^N \sin x_i^m \right)^2 + \left(\sum_{i=1}^N \cos x_i^m \right)^2 \right] dt - B \int_0^T \sum_{i \neq j} u_{ij}^m(t) dt \\ &= \frac{1}{N^2} \int_0^T \left[\left(\sum_{i=1}^N \sin x_i^* \right)^2 + \left(\sum_{i=1}^N \cos x_i^* \right)^2 \right] dt - \lim_{m \rightarrow \infty} B \int_0^T \sum_{i \neq j} (u_{ij}^m)^2(t) dt \\ &\geq \frac{1}{N^2} \int_0^T \left[\left(\sum_{i=1}^N \sin x_i^* \right)^2 + \left(\sum_{i=1}^N \cos x_i^* \right)^2 \right] dt - B \int_0^T \sum_{ij} (u_{ij}^*)^2(t) dt. \end{aligned}$$

Note that $\lim_{m \rightarrow \infty} J(u^m)$ exists because u^m is a maximizing sequence and $J(u)$ is bounded in U , and that

$$\lim_{m \rightarrow \infty} \frac{1}{N^2} \int_0^T \left[\left(\sum_{i=1}^N \sin x_i^m \right)^2 + \left(\sum_{i=1}^N \cos x_i^m \right)^2 \right] dt$$

exists because the states converge uniformly. Therefore,

$$\lim_{m \rightarrow \infty} B \int_0^T \sum_{i \neq j} (u_{ij}^m)^2(t) dt$$

must also exist, and so, it is valid to break the limit of the sum as the sum of the limits, in the calculation above. In addition the first limit is passed through the integral by the strong convergence of the states and the second by the lower-semicontinuity of the norm with respect to weak convergence. Therefore u^* is an optimal control. $\square$

3.5.3 Characterization of the Optimal Control

The characterization of the optimal control follows from Pontryagin's Maximum Principle.

Theorem 3.5.2. *Given a solution (x^*, u^*) to Problem III, there exists N adjoint variables, y_i , and a nonzero N dimensional vector, λ , such that the Hamiltonian:*

$$\begin{aligned} H(t, x, y, u) &= \frac{1}{N^2} \left[\left(\sum_j \sin x_j \right)^2 + \left(\sum_j \cos x_j \right)^2 \right] - B \sum_{i \neq j} u_{ij}^2 \\ &\quad + \sum_i y_i \left(\omega_i + \frac{1}{N} \sum_j u_{ij} \sin(x_j - x_i) \right) \end{aligned}$$

is constant along the optimal trajectory and is maximized pointwise by the optimal control. In

addition the adjoint variables satisfy for $i = 1..N$,

$$\frac{dy_i}{dt} = \frac{1}{N} \sum_{j=1}^N (y_i u_{ij}^* - y_j u_{ji}^*) \cos(x_j^* - x_i^*) - \frac{2}{N^2} \sum_{j=1}^N \sin(x_j^* - x_i^*),$$

and

$$y_i(T) = 0.$$

This allows us to characterize an optimal control in terms of the corresponding states and adjoints, namely:

$$u_{ij}^* = \max \left(-M, \min \left(\frac{y_i(t) \sin(x_j^* - x_i^*)}{2BN}, M \right) \right).$$

3.5.4 Uniqueness and Sufficient Conditions

Next we will show that given any fixed final time, T , the solution of the optimality system is unique if the number of oscillators, N , is large enough. Since any optimal control is necessarily a solution of the optimality system, it follows that the optimal control is unique and that the necessary conditions are in fact sufficient. The proof relies on the fact that the adjoint functions, $y_i(t)$, are bounded, independent of the bound, M , on the control. This result follows from the next lemma:

Lemma 3.5.1. Suppose that k_N and p_N are positive sequences such that

$$\lim_{N \rightarrow \infty} p_N = \bar{p}$$

and

$$\lim_{N \rightarrow \infty} k_N = 0.$$

Then, given $\epsilon > 0$ there exists $\bar{N}$ so that if $N \geq \bar{N}$ and $g(t) : [0, T] \rightarrow \Re$ satisfies:

$$\begin{aligned} g(t) &\geq 0, \\ g(0) &= 0, \\ g'(t) &\leq p_N + k_N g^2(t), \end{aligned}$$

then,

$$g(t) \leq \bar{p}t + \epsilon.$$

Proof. Fix $\epsilon > 0$ and note that since

$$\lim_{N \rightarrow \infty} \frac{\sqrt{p_N}}{\sqrt{k_N}} \tan\left(\sqrt{k_N p_N t}\right) = \bar{p}t,$$

there exists $\bar{N}$ so that for $N \geq \bar{N}$

$$\frac{\sqrt{p_N}}{\sqrt{k_N}} \tan\left(\sqrt{k_N p_N t}\right) \leq \bar{p}t + \epsilon$$

Now, assume that $N \geq \bar{N}$,

$$\begin{aligned} g(t) &\geq 0, \\ g(0) &= 0, \end{aligned}$$

and

$$g'(t) \leq p_N + k_N g^2(t).$$

It follows from the assumptions on g that

$$\begin{aligned} \frac{g'(t)}{p_N + k_N g^2(t)} &\leq 1 \Rightarrow \\ \int_0^t \frac{g'(s)}{p_N + k_N g^2(s)} ds &\leq \int_0^t ds \Rightarrow \end{aligned}$$

$$\frac{1}{\sqrt{k_N p_N}} \arctan \left(\frac{\sqrt{k_N} g(t)}{\sqrt{p_N}} \right) \leq t \Rightarrow$$

$$g(t) \leq \frac{\sqrt{p_N}}{\sqrt{k_N}} \tan \left(\sqrt{k_N p_N} t \right) \leq \bar{p} t + \epsilon.$$

□

Now let $g_i(t) = y_i(T - t)$, so that:

$$g'_i(t) = -\frac{1}{N} \sum_j^N (g_i(t) u_{ij}(T - t) - g_j(t) u_{ji}(T - t)) \cos(x_j(T - t) - x_i(T - t))$$

$$+ \frac{2}{N^2} \sum_j^N \sin(x_j(T - t) - x_i(T - t)),$$

$$g_i(0) = 0.$$

Theorem 3.5.3. *Given a fixed final time T , there exists N large enough so that the functions $g_i(t)$ and therefore, the adjoint functions, $y_i(t)$ for $i = 1, \dots, N$, are bounded in absolute value, and this bound is independent of the bound M on the magnitude of u_{ij} .*

It is necessary that the bound on the absolute value of the adjoint function, $y_i(t)$, be independent of the bound M on the magnitude of the controls because throughout this paper we assume that M is very large.

Proof.

$$\frac{1}{2} \frac{d}{dt} (g_i^2(t)) = -g_i(t) \frac{1}{N} \sum_j^N (g_i(t) u_{ij}(T - t) - g_j(t) u_{ji}(T - t)) \cos(x_j(T - t) - x_i(T - t))$$

$$+ g_i(t) \frac{2}{N^2} \sum_j^N \sin(x_j(T - t) - x_i(T - t))$$

$$\leq \frac{g_i^2}{2N} + \frac{1}{2N} \left(\sum_j^N (g_i(t) u_{ij}(T - t) + g_j(t) u_{ji}(T - t)) \cos(x_j(T - t) - x_i(T - t)) \right)^2$$

$$+ \frac{g_i^2}{N} + \frac{1}{N^3} \left(\sum_j^N \sin(x_j(T - t) - x_i(T - t)) \right)^2$$

$$\leq \frac{3}{2N} g_i^2 + \frac{1}{2} \sum (g_i u_{ij} - g_j u_{ji})^2 + \frac{1}{N}$$

$$\leq \frac{3}{2N} g_i^2 + \sum (g_i - g_j)^2 u_{ij}^2 + (u_{ij} - u_{ji})^2 g_j^2 + \frac{1}{N}$$

$$\leq \frac{3}{2N} g_i^2 + \frac{2}{B^2 N^2} \sum (g_i^2 + g_j^2) g_i^2 + (g_i^2 + g_j^2) g_j^2 + \frac{1}{N}$$

$$\leq \frac{3}{2N} g_i^2 + \frac{4}{B^2 N} g_i^4 + \frac{4}{B^2 N^2} \sum g_j^4 + \frac{1}{N}.$$

It follows that

$$\frac{d}{dt} \sum g_i^2 \leq \left[\frac{3}{2N} + \frac{8}{NB^2} \right] \left(\sum g_i^2 \right)^2 + 1 + \frac{3}{2N},$$

with $k(N) = \left\lceil \frac{3}{2N} + \frac{8}{NB^2} \right\rceil$ and $p(N) = 1 + \frac{3}{2N}$, the previous lemma shows there exists N large enough so that $|y_i(t)| \leq 2T$. □

Now we are ready to prove the following theorem.

Theorem 3.5.4. *Given a fixed final time T , there exists N large enough so that the solution to the optimality system is unique.*

Proof. Given two solutions, (x, y) and $(\bar{x}, \bar{y})$ to the optimality system make the change of variables $x_i = e^{kt} v_i$, $y_i = e^{-kt} w_i$. Then v satisfies:

Meanwhile w_i satisfies:

$$\begin{aligned}
& \frac{1}{2} (w_i(0) - \bar{w}_i(0))^2 + k \int_0^T (w_i - \bar{w}_i)^2 dt \\
&= \frac{1}{N} \int_0^T e^{kt} \left(\sum_j (y_i u_{ij} - y_j u_{ji}) \cos(x_j - x_i) - (\bar{y}_i \bar{u}_{ij} - \bar{y}_j \bar{u}_{ji}) \cos(\bar{x}_i - \bar{x}_j) \right) (w_i - \bar{w}_i) dt \\
&\quad - \frac{2}{N^2} \int_0^T e^{kt} \left(\sum_j \sin(x_j - x_i) - \sin(\bar{x}_j - \bar{x}_i) \right) (w_i - \bar{w}_i) dt \\
&\leq \frac{3}{2N} \int_0^T (w_i - \bar{w}_i)^2 dt \\
&\quad + \frac{1}{2N} \int_0^T e^{2kt} \left(\sum_j (y_i u_{ij} - y_j u_{ji}) \cos(x_j - x_i) - (\bar{y}_i \bar{u}_{ij} - \bar{y}_j \bar{u}_{ji}) \cos(\bar{x}_i - \bar{x}_j) \right)^2 dt \\
&\quad + \frac{1}{N^3} \int_0^T e^{2kt} \left(\sum_j \sin(x_j - x_i) - \sin(\bar{x}_j - \bar{x}_i) \right)^2 dt \\
&\leq \frac{3}{2N} \int_0^T (w_i - \bar{w}_i)^2 dt \\
&\quad + \int_0^T e^{2kt} \sum_j ((y_i u_{ij} - y_j u_{ji}) - (\bar{y}_i \bar{u}_{ij} - \bar{y}_j \bar{u}_{ji}))^2 \cos^2(x_j - x_i) dt \\
&\quad + \int_0^T e^{2kt} \sum_j (\cos(x_j - x_i) - \cos(\bar{x}_j - \bar{x}_i))^2 (\bar{y}_i \bar{u}_{ij} - \bar{y}_j \bar{u}_{ji})^2 dt \\
&\quad + \frac{2}{N^2} \int_0^T e^{2kt} \sum (x_i - \bar{x}_i)^2 + (x_j - \bar{x}_j)^2 dt
\end{aligned}$$

$$\begin{aligned}
&\leq \frac{3}{2N} \int_0^T (w_i - \bar{w}_i)^2 dt \\
&+ 4 \int_0^T e^{2kt} \sum_j (y_i - \bar{y}_i)^2 u_{ij}^2 + (u_{ij} - \bar{u}_{ij})^2 \bar{y}_i^2 dt \\
&+ 4 \int_0^T e^{2kt} \sum_j (y_j - \bar{y}_j)^2 u_{ji}^2 + (u_{ji} - \bar{u}_{ji})^2 \bar{y}_j^2 dt \\
&+ 2 \int_0^T \sum_j ((x_j - \bar{x}_j)^2 + (x_i - \bar{x}_i)^2) \frac{16T^4}{N^2 B^2} dt \\
&+ \frac{2}{N^2} \int_0^T e^{2kt} \sum (x_i - \bar{x}_i)^2 + (x_j - \bar{x}_j)^2 dt \\
&\leq \frac{3}{2N} \int_0^T (w_i - \bar{w}_i)^2 dt \\
&+ \frac{4T^2}{B^2 N^2} \int_0^T e^{2kt} \sum_j (y_i - \bar{y}_i)^2 + (y_i \sin(x_j - x_i) - \bar{y}_i \sin(\bar{x}_j - \bar{x}_i))^2 dt \\
&+ \frac{4T^2}{B^2 N^2} \int_0^T e^{2kt} \sum_j (y_j - \bar{y}_j)^2 + (y_j \sin(x_i - x_j) - \bar{y}_j \sin(\bar{x}_i - \bar{x}_j))^2 dt \\
&+ \frac{32T^4}{N^2 B^2} \int_0^T e^{2kt} \sum_j (x_j - \bar{x}_j)^2 dt + \frac{32T^4}{N B^2} \int_0^T e^{2kt} (x_i - \bar{x}_i)^2 dt \\
&+ \frac{2}{N^2} \int_0^T e^{2kt} \sum (x_j - \bar{x}_j)^2 dt + \frac{2}{N} \int_0^T e^{2kt} (x_i - \bar{x}_i)^2 dt
\end{aligned}$$

$$\begin{aligned}
&\leq \frac{3}{2N} \int_0^T (w_i - \bar{w}_i)^2 dt \\
&+ \frac{4T^2}{B^2 N} \int_0^T e^{2kt} (y_i - \bar{y}_i)^2 dt \\
&+ \frac{8T^2}{B^2 N^2} \int_0^T e^{2kt} \sum_j (y_i - \bar{y}_i)^2 \sin^2(x_j - x_i) + (\sin(x_j - x_i) - \sin(\bar{x}_j - \bar{x}_i))^2 \bar{y}_i^2 dt \\
&+ \frac{4T^2}{B^2 N} \int_0^T e^{2kt} \sum_j (y_j - \bar{y}_j)^2 dt \\
&+ \frac{8T^2}{B^2 N^2} \int_0^T e^{2kt} \sum_j (y_j - \bar{y}_j)^2 \sin^2(x_i - x_j) + (\sin(x_i - x_j) - \sin(\bar{x}_i - \bar{x}_j))^2 \bar{y}_j^2 dt \\
&+ \frac{32T^4}{N^2 B^2} \int_0^T e^{2kt} \sum_j (x_j - \bar{x}_j)^2 dt + \frac{32T^4}{NB^2} \int_0^T e^{2kt} (x_i - \bar{x}_i)^2 dt \\
&+ \frac{2}{N^2} \int_0^T e^{2kt} \sum_j (x_j - \bar{x}_j)^2 dt + \frac{2}{N} \int_0^T e^{2kt} (x_i - \bar{x}_i)^2 dt \\
&\leq \frac{3}{2N} \int_0^T (w_i - \bar{w}_i)^2 dt \\
&+ \frac{12T^2}{B^2 N} \int_0^T e^{2kt} (y_i - \bar{y}_i)^2 dt + \frac{64T^4}{B^2 N^2} \int_0^T e^{2kt} \sum_j (x_j - \bar{x}_j)^2 + (x_i - \bar{x}_i)^2 dt \\
&+ \frac{12T^2}{B^2 N^2} \int_0^T e^{2kt} \sum_j (y_j - \bar{y}_j)^2 dt + \frac{64T^4}{B^2 N^2} \int_0^T e^{2kt} \sum_j (x_j - \bar{x}_j)^2 + (x_i - \bar{x}_i)^2 dt \\
&+ \frac{32T^4}{N^2 B^2} \int_0^T e^{2kt} \sum_j (x_j - \bar{x}_j)^2 dt + \frac{32T^4}{NB^2} \int_0^T e^{2kt} (x_i - \bar{x}_i)^2 dt \\
&+ \frac{2}{N^2} \int_0^T e^{2kt} \sum_j (x_j - \bar{x}_j)^2 dt + \frac{2}{N} \int_0^T e^{2kt} (x_i - \bar{x}_i)^2 dt \\
&\leq \left[\frac{3}{2N} + \frac{12T^2}{B^2 N} \right] \int_0^T (w_i - \bar{w}_i)^2 dt + \frac{12T^2}{B^2 N^2} \int_0^T \sum_j (w_j - \bar{w}_j)^2 dt \\
&+ \left[\frac{128T^4}{B^2 N} + \frac{32T^4}{NB^2} + \frac{2}{N} \right] \int_0^T e^{4kt} (v_i - \bar{v}_i)^2 dt + \left[\frac{128T^4}{B^2 N^2} + \frac{32T^4}{N^2 B^2} + \frac{2}{N^2} \right] \int_0^T e^{4kt} \sum_j (v_j - \bar{v}_j)^2 dt.
\end{aligned}$$

Summing these equations over all indices we find:

$$\begin{aligned}
k \left(\sum_i \|w_i - \bar{w}_i\|_{L^2}^2 + \|v_i - \bar{v}_i\|_{L^2}^2 \right) &\leq \frac{c_1(T)}{N} \sum \|w_i - \bar{w}_i\|_{L^2}^2 \\
&+ \frac{e^{4kT} c_2(T)}{N} \sum \|v_i - \bar{v}_i\|_{L^2}^2
\end{aligned}$$

Now if we can choose k so that

$$k > c_1(T), \quad (3.15)$$

then for any $N \in \mathbb{N}$

$$k > \frac{c_1(T)}{N}.$$

Therefore, if N is so large that

$$N > \frac{e^{2kT} c_2(T)}{k}, \quad (3.16)$$

the solution is unique.

Of course we can always choose k so that inequality (3.18) is satisfied, therefore the optimality system has a unique solution when N is large. It follows that the necessary conditions for optimality are also sufficient. $\square$

Alternately, the solution to the optimality system is unique for arbitrary N if T is small enough. To see this fix N and let $T_k = \frac{1}{k}$. Since $c_2(T)$ is positive, monotonically increasing, and bounded below

$$\lim_{k \rightarrow \infty} \frac{e^{4kT_k} c_2(T_k)}{k} = 0. \quad (3.17)$$

In particular, for k large enough

$$N \geq 1 > \frac{e^{4kT_k} c_2(T_k)}{k}. \quad (3.18)$$

If k is large enough that (3.20) holds, then, for $T < T_k$

$$N \geq \frac{e^{4kT_k} c_2(T_k)}{k} \geq \frac{e^{4kT} c_2(T)}{k},$$

that is, (3.19) holds. Fix $k > \max\{c_1(1), 1\}$ so that the inequality (3.20) holds. Then, because $c_1(T)$ is monotonically increasing with respect to T we see that for $T \leq T_k$

$$k > c_1(1) > c_1(T) > \frac{c_1(T)}{N},$$

that is (3.18) holds. Therefore, inequalities (3.18) and (3.19) are satisfied and the solution of the optimality system is unique for arbitrary N if $T \leq T_k$.

3.5.5 Numerical Simulations

The characterization of an optimal control allows us to find control strategies that satisfy the necessary conditions by using a forward backward sweep algorithm. As before, we choose the bound on the magnitude of the controls to be large, $M = 1000$.

First we simulate a network of ten oscillators. The final time is 1. The oscillators' natural velocities are drawn from a normal distribution with standard deviation 1 and mean 20. The oscillators' initial phases are drawn from a uniform distribution on the interval $[0, \pi]$. The balancing parameter is $B = .01$, so that the connectivity cost is relatively unimportant. In this simulation the value of the objective functional is found to be .4657.

Figure 3.13 plots the order parameter squared, $r^2(t)$, for the controlled network.

Figure 3.14 shows the evolution of the controls. Again we see that the controlled network is not a mean-field network and that it exhibits some negative coupling.

In the next simulation we decrease the value of the balancing parameter B to .001, so that the connectivity cost is of less importance than in the previous simulation. The other parameters are held constant. In this simulation the value of the objective functional is .6453.

Figure 3.15 plots the order parameter squared for the controlled network. As expected, decreasing the importance of the connectivity cost increases the value of the order parameter.

Figure 3.16 shows the evolution of the controls. Again we see that the controlled network is not a mean-field network and that it exhibits some negative coupling. Also, we see that increasing the importance of the connectivity cost by a factor of 10 decreases the magnitude of the controls by the same factor.

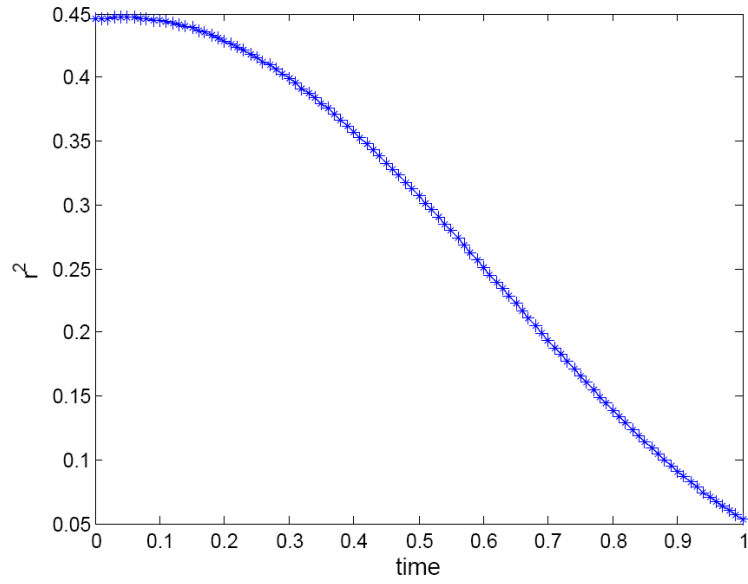


Figure 3.13: The evolution of r^2 for $N = 10$, $T = 1$, and $B = .01$.

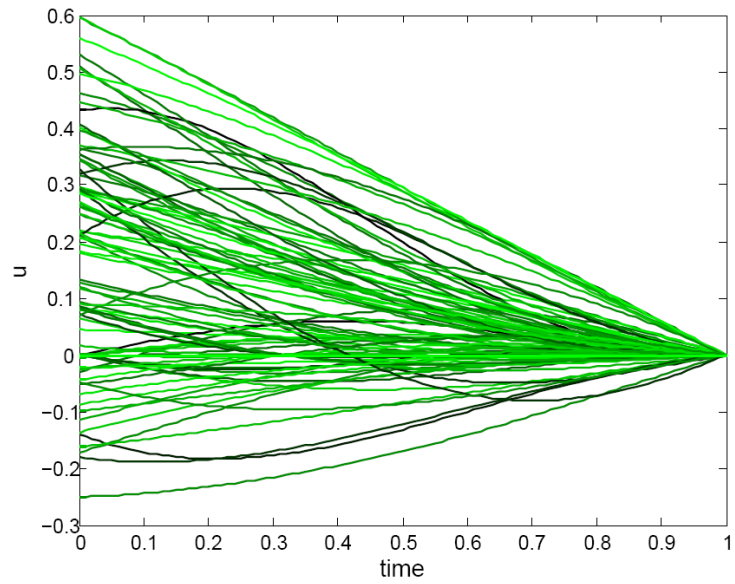


Figure 3.14: The coupling strengths, $u_{ij}(t)$, for $N = 10$, $T = 1$, and $B = .01$

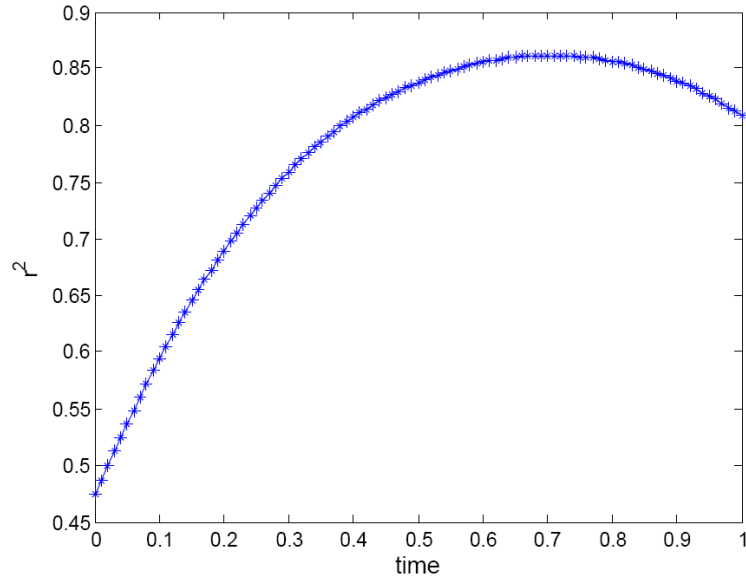


Figure 3.15: The evolution of r^2 for $N = 10$, $T = 1$, and $B = .001$.

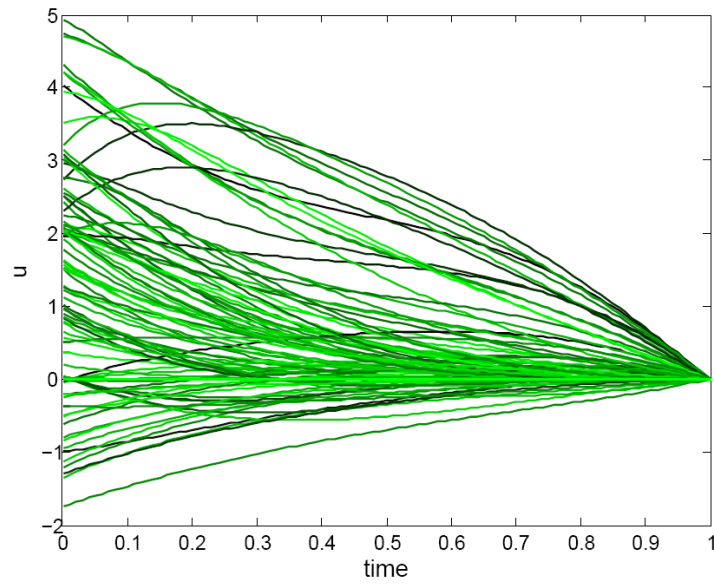


Figure 3.16: The coupling strengths, $u_{ij}(t)$, for $N = 10$, $T = 1$, and $B = .001$

3.6 Conclusions

In this paper we used optimal control to find the most efficient way for a network of nonlinear oscillators to achieve synchronization. We addressed this problem in three ways.

- (1) How can the network obtain a prescribed level of synchrony while maintaining the lowest possible connectivity cost?
- (2) How can the network achieve the greatest level of synchrony for a fixed connectivity cost?
- (3) How can we maximize synchrony less a weighted connectivity cost?

Questions (1) and (2) led to Problems I and II for which the control characterizations were nontrivial. In each case, in order to characterize optimal coupling strengths, we had to determine whether or not a specific adjoint variable that was introduced to handle either a state or control constraint was nonzero. If the adjoint variable of interest was nonzero, then the corresponding optimal coupling strengths would be continuous. If the adjoint variable of interest was zero the oscillators might be coupled through bang-bang controls. For each problem, we showed that under fairly mild conditions, the adjoint variable of interest was nonzero. As a result, we were able to answer a fundamental question about the optimal coupling strengths: The optimal coupling strengths are continuous. The characterization of an optimal control for Problem III also showed that the optimal coupling strengths are continuous.

After characterizing an optimal control we ran a variety of numerical simulations and made several observations. First of all, we noticed that unlike the Kuramoto network, the controlled networks were not mean-field networks. This means that the oscillators were not coupled to the mean phase through time. In addition, we noted that each controlled network exhibited some repulsion between oscillators.

These results suggest many future directions of research. It would be interesting to perform the same analysis on networks with diverse types of coupling. In particular, Ermentrout identifies two distinct types of coupling, synaptic and electronic[13]. In electronic coupling oscillators with the same phase cannot influence one another. While in synaptic coupling oscillators can influence one another, despite having the same phase[13]. Because the coupling in the Kuramoto network is sinusoidal it is also electronic. Would repulsion still occur if the coupling was synaptic? Would the optimal coupling coefficients still be continuous, or would bang-bang coupling coefficients be preferred? One could consider alternate objective functionals to see if this alters the optimal coupling strategy. For example one might try to minimize the time it takes the network to achieve some threshold order, or to maximize the value of the network's order parameter at a fixed final time. Or one could attempt to optimize more complex dynamics, such as traveling waves in a chain of oscillators. Finally, specific oscillator configurations could be considered, for example oscillator chains, oscillators on a lattice with diffusive coupling, or a ring of oscillator groups [12]. In summary, our results suggest that optimal control could be used to investigate synchrony in a variety of biological networks.

Chapter 4

Summary and Future Directions

In this thesis, we devised a method to solve a specific class of impulse control problems and also investigated the emergence of synchrony in a network of coupled oscillators.

First, we showed that impulse control problems with a restricted number of impulses can be reformulated as discrete optimal control problems. The optimal controls are then characterized in terms of the corresponding discrete states and adjoint variables. Our solution strategy is advantageous because it allows one to avoid the difficulties that are associated with QVIs and the method of discontinuous time change. In particular, when using this method the impulse functions are not required to satisfy robustness conditions, as in the method of discontinuous time change, and the discrete systems are easier to solve numerically than the QVIs. We applied this method to two example impulse control problems in which the systems of ordinary differential equations that governed the states were exactly solvable. After characterizing the optimal controls we solved for them numerically using a forward backward sweep algorithm.

Many medical and biological control problems give rise to impulse control problems. As a result, our method of solving impulse control problems could address a variety of urgent and exciting questions. Most models for such applications would not be exactly solvable. We will implement our techniques for systems that are not exactly solvable, which will open doors for many applications.

Currently medical researchers are debating the merits of supervised treatment interruptions (STI) or “drug holidays”, in which a patient ceases to take medication for some period of time [31]. Some evidence suggests that STI may stimulate the body’s immune system and reduce side effects [31]. However, these ideas are highly contentious within the medical community. Our method of solving impulse control problems could be used to design optimal treatment schedules for diseases such as cancer and HIV. In the process, we would gain valuable insight into the efficacy STI.

We would also like to extend this method to systems of partial differential equations. This extension would be of great mathematical interest as there are many open questions in this field. Also, it would be a valuable tool to ecologists. The control of invasive species is of paramount importance because of the threat that invasives pose to biodiversity and the economy [8]. This method could be used to design specific control strategies while helping to answer questions of fundamental interest to ecologists. For example, ‘Should control efforts be focuses on the leading edge of an invasion or at the epicenter’ This work could extend the work by Whittle et al. [32] on invasions with several foci.

As a second project we used optimal control theory to investigate the emergence of synchrony in a Kuramoto type network. Despite differences in their natural velocities, oscillators in a standard

Kuramoto network are able to achieve synchrony through mean-field coupling. In order to better understand how a network of nonlinear, non identical oscillators achieves synchrony we allowed the coupling strengths to vary between oscillator pairs and through time. After quantifying the network synchrony and the network connectivity cost we solved three related optimal control problems. In particular, we formulated and solved an optimal control problem for each of the following three questions.

- (1) How can the network obtain a prescribed level of synchrony while maintaining the lowest possible connectivity cost?
- (2) How can the network achieve the greatest level of synchrony for a fixed connectivity cost?
- (3) How can we maximize synchrony less a weighted connectivity cost?

In each case, the control characterization showed that, due in part to the quadratic form of the objective functional, optimal coupling strengths are continuous in time.

After characterizing the optimal coupling strengths we ran a variety of numerical simulations. These simulations revealed that in each case the optimal network, unlike the standard Kuramoto network, is not a mean-field network (i.e. the oscillators are not coupled to the average phase), and that inter-oscillator repulsion can promote synchrony.

Scientists have long been interested in the ability of non identical oscillators, such as fireflies or the pace-maker cells of the heart to synchronize. Our results suggest that optimal control could be used to investigate synchrony in a variety of biological and social networks.

For example, optimal control could be used to determine how the inherit differences between biological or social oscillators influence network structure. As a first step in this direction we could investigate how the natural velocity distribution affects the optimal coupling strengths in the Kuramoto network. By varying the natural velocity distribution over many numerical simulations one could probe for links between the optimal network structure and the velocity distribution. For example, does the variance in the coupling strength scale with the variance in the velocity distribution? Is the shape of the distribution related to the network clustering coefficient? The conclusions from this work would only apply to the Kuramoto network. However, extensions on other coupled systems could be used to discover paradigms that promote consensus in opinion networks. Researchers have already began to explore the effects of complex topologies on opinion networks [5, 35, 3, 10]. However, the actors (nodes) in these models have identical dynamics [5]. Optimal control could be used to study how population diversity effects the formation of consensus. For example, in an opinion network where actotrs are differentiated by a single parameter one might determine whether or not consensus is facilitated when the strength of the link between two actors scales with the difference in their parameters.

Finally optimal control could be used to explore the structure of cortical networks. For example, cortical networks are characterized by recurrent motifs, or patterns of interconnectedness [5, 22]. However, the function of these motifs remains unclear. Vega et al. hypothesized that motifs may enhance synchronization [30]. Optimal control could be used to test such hypotheses. Evolutionary optimization algorithms have already been used to explain observed patterns of cortical connectivity [23, 11]. However, these studies neglected the plasticity of cortical networks [5], while optimal control theory is well suited to investigate connectivity in networks such as these that evolve through time.

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Vita

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