Computing the Optimal Path in Stochastic Dynamical Systems

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MONTCLAIR STATE UNIVERSITY

/ COMPUTING THE OPTIMAL PATH IN STOCHASTIC
DYNAMICAL SYSTEMS /

by

Martha Bauver

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ABSTRACT

Title of Thesis: COMPUTING THE OPTIMAL PATH IN STOCHASTIC DYNAMICAL SYSTEMS

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In stochastic systems, one is often interested in finding the optimal path that maximizes the probability of escape from a metastable state or of switching between metastable states. Even for simple systems it may be impossible to find an analytic form of the optimal path, and in high-dimensional systems, this is almost always the case.

The optimal path is of great importance, since it represents the most likely path of a rare switching or escape event. For instance, the optimal path for an infectious disease model represents a switching from an infectious state to the extinction of the disease within the population, which is both rare and a desirable outcome. Knowledge of this trajectory to extinction will add to our understanding of how to control and, potentially, eradicate infectious disease outbreaks around the world.

To find the optimal path, we present a constructive methodology that is used to compute the path numerically. The method utilizes finite-time Lyapunov exponents, statistical selection criteria, and a Newton-based iterative minimizing scheme. The method is fully demonstrated using an epidemiology model and a population model. We first present a two-dimensional system that has an analytical solution for the optimal path. The numerical solution found using our computational method agrees well with the analytical result. We next present the computational method to find the optimal path in a higher-dimensional system for which no analytic solution exists. The final example represents a specific type of optimal path for which no numerical method has been shown to succeed.

While our interest in this methodology lies primarily with its use in epidemiology models, the methodology can be applied to a broad range of systems for which the path between states is unknown.
COMPUTING THE OPTIMAL PATH IN STOCHASTIC
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A THESIS

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# Contents

1 Introduction ................................................................. 7  
   1.1 Epidemiology and the use of Stochastic Models ............... 7  

2 General Theory ............................................................ 9  
   2.1 Master Equation Formalism ........................................... 9  
   2.2 Finite-Time Lyapunov Exponents (FTLE) ......................... 11  
   2.3 Iterative Action Minimizing Method (IAMM) ...................... 12  

3 The 1D and 2D SIS Models .............................................. 14  
   3.1 Introduction .................................................................. 14  
   3.2 Steady States and Stability Analysis .............................. 15  
   3.3 The 1D and 2D SIS stochastic models ............................. 15  

4 1D SIS Results .............................................................. 16  
   4.1 Finite-Time Lyapunov Exponents ................................. 16  
   4.2 High Value FTLE Point Harvesting ............................... 17  
   4.3 IAMM Computations .................................................. 18  
   4.4 1D SIS Optimal Path .................................................. 18  

5 2D SIS Results .............................................................. 19  
   5.1 Finite-Time Lyapunov Exponents ................................. 20  
   5.2 High Value FTLE Point Harvesting ............................... 20  
   5.3 IAMM Computations .................................................. 21  
   5.4 2D SIS Optimal Path .................................................. 23  

6 Allee Population Model .................................................. 25  
   6.1 Introduction .............................................................. 25  
   6.2 The Stochastic Allee Model ........................................... 26  
   6.3 Allee Results ............................................................. 27  

7 Summary .......................................................................... 28  
   7.1 A Global Vision .......................................................... 30  

8 Bibliography ..................................................................... 32  

Appendices ........................................................................ 34  
A The Emergence of Dynamical Structures using FTLE Computations 34  
B Additional Projections of 2D SIS Model Results .......................... 36
List of Figures

1 The simplest deterministic compartmental models have two steady states. There is a bifurcation at $R_0 = 1$ that causes a change in stability. For $R_0 < 1$ the extinct state is attracting while the endemic state is repelling. For $R_0 > 1$ the extinct state is repelling while the endemic state is attracting. ........................................... 10

2 (a) The numerical integration of two initially close points on one side of the manifold. After a finite time the two points remain close to one another, and therefore the corresponding FTLE value will be small. (b) The numerical integration of two initially close points on opposite sides of the zero-energy trajectory. After a finite time the two points move a significant distance apart from one another, and therefore the corresponding FTLE value will be large. .......................... 13

3 The SIS model compartmental flow includes birth $\mu N$, infection $\beta SI/N$, recovery $\gamma I$, death of susceptibles $\mu S$, and death of infected individuals $\mu I$. ........................................... 14

4 Generalized solution curves for the 1D SIS model when $R_0 > 1$. The horizontal axis represents the infectious population $i$, and the vertical axis represents the conjugate momentum $p$. The dashed, horizontal line denotes the deterministic dynamics when $p = 0$. The dotted, vertical line denotes the trivial solution when $i = 0$. The third curve, described by Eq. 21, connects the endemic point to the fluctuational extinct point with zero population and non-zero momentum. ........................................... 17

5 The success of IAMM processing is dependent upon the ordering of the initial condition, as illustrated by these 1D SIS figures. Panel (a) contains the initial condition $\mathbf{q}_0$ with color-coded segments; each segment holds an equal number of points. The dashed gray line underlying the points is the analytic optimal path given by Eq. (21). Panels (b) and (c) contain the results after two Newton iterations of the IAMM. In (b) $\mathbf{q}_0$ was ordered from the fluctuational extinct state to the endemic state, whereas in (c) $\mathbf{q}_0$ was ordered from endemic state to fluctuational extinction. Panel (b) shows the extreme repositioning of array points as the IAMM attempts to achieve the desired point ordering from the endemic to the extinct state. The points move so far from the optimal path that, ultimately, the method does not converge to the optimal path. In contrast, (c) reflects minimal repositioning due to IAMM adjustments. All IAMM computations were done using $T_e = 2$. ........................................... 18

6 Average of forward and backward FTLE field for the 1D SIS model. The analytic solution for the optimal path appears as a black curve. The section between the endemic and fluctuational extinct states is overlaid in blue with the optimal path produced by IAMM computations. The FTLE computations were done using a fourth-order Runge-Kutta scheme with $\delta t = 0.02$, a finite time $T = 7$, and a grid resolution of 0.0005 for both $i$ and $p$. Parameter values are $\beta = 5.0, \mu = 0.02, \gamma = 0.98$. ........................................... 19

7 To derive a $p_s$ range for the 2D SIS FTLE computations, a four-dimensional grid is defined and each point is tested using a tolerance of $\mathcal{H} < 10^{-9}$. This figure displays the $p_s \times p_i$ values of those points meeting that tolerance. For all 2D SIS computations, we use parameters $\mu = 0.2, \beta = 104$ and $\gamma = 100$. .......................... 20
These figures indicate the location of all points having an FTLE value greater than 4.25 after completion of FTLE processing for the 2D SIS model. Since the points are four dimensional, we display them using two companion figures, where Panel (a) describes the \((s, i)\) location and Panel (b) describes the \((p_s, p_i)\) location of each selected point.

Panel (a) contains the \((s, i)\) coordinates and panel (b) contains the \((p_s, p_i)\) coordinates of the 1752 points harvested from the FTLE results for use as the initial condition in the IAMM computations for the 2D SIS model. For best results, \(q_0\) should be ordered from the endemic state to the fluctuational extinct state. The harvested points cannot be ordered properly since \(p_s\) is not monotonic. We substitute the ordered array plotted in panel (c) for the actual \((p_s, p_i)\) coordinates of panel (b), and pair it with a sorted \((s, i)\) array plotted in panel (a) to obtain an ordered initial guess \(q_0\). The green circle denotes the endemic steady state, while the red circle denotes the fluctuational extinction steady state.

The 2D SIS results from the IAMM, obtained using \(T_e = 13\) for 50 iterations of the Newton method process. Panel (a) contains the final location of all \((s, i)\) coordinates from Fig. 9(a). Panel (b) contains the final location of all \((p_s, p_i)\) coordinates from Fig. 9(c). Together, they represent the optimal path. Although the points appear equally spaced, an examination of the array values shows that is not the case. The central section of the path, between two turns in both views, contains only about 200 of the 1752 point array. The other sections of the path, namely, the exit from the endemic state and the approach to the fluctuational extinct state, are each populated by half of the remaining points. This is due to the fact that very slow dynamics are present near either steady state, while the area of fast dynamics begins and ends with a transition that is, in fact, a change in the direction of the optimal path. The green circle denotes the endemic steady state, while the red circle denotes the fluctuational extinction steady state.

Two projections of the IAMM and FTLE results for the 2D SIS model. The optimal path obtained from the IAMM computation is represented as a black curve. It begins at the endemic steady state (green circle) on the rear surface, and ends at the fluctuational extinct steady state (red circle) in the upper right foreground. Both projections show FTLE values averaged over the missing dimension, so that (a) shows the mean FTLE values of all \(p_s\) slices and (b) shows the mean for all \(s\) slices. In projection (a), the vertical \(p_i\) slices contain areas of of high FTLE values in red that closely correlate to the curve of the optimal path. Projection (b), however, exhibits a widening and splitting of high FTLE regions. On vertical slice \(p_i = -0.0272\), one observes a path diverging from the optimal path. In the vicinity is a critical point, shown as a blue circle in the foreground of (b). This critical point is not part of the optimal path structure. A stability analysis reveals that the point is neither stable nor a saddle point, but from this projection and many others, it does create dynamics that may compete with those along the optimal path. All FTLE computations were done both forward and backward in time using a fourth-order Runge-Kutta scheme with \(\delta t = 0.02\) and a finite time \(T = 10\).
Three steady states delineate the deterministic dynamics of the Allee model. The attracting point $c_0$ is the extinct steady state, the repelling point $c_1$ is the threshold value that separates a growing population from a decaying one, and the attracting point $c_3$ is the carrying capacity.

Zero-energy curves of the Hamiltonian for the stochastic Allee model. The optimal path to extinction (shown in blue) consists of the curve, given by Eq. (26), that connects $c_2$ to $c_1$, and the $p = 0$ deterministic line from $c_1$ to the extinct state $c_0$.

Average of forward and backward FTLE field for the Allee model. The optimal path, given by Eq. (26) and denoted by the blue curve overlay, leaves the deterministic line at the carrying capacity $c_2$ and rejoins the deterministic line at the threshold $c_1$. The optimal path then essentially runs deterministically to the extinct state $c_0$. All FTLE computations were done using a fourth-order Runge-Kutta scheme with $\delta t = 0.1$, a finite time $T = 40$, and a grid resolution of 0.002 in $x$ and 0.001 in $p$. Parameter values are $\lambda = 1.6, \mu = 0.2, \sigma = 3.0$.

IAMM results for the Allee model using 1000 points randomized about the analytical optimal path as the initial condition. After three Newton iterations, the point locations, shown as a black line, have markedly converged to the analytic optimal path (in red). The initial array contained nine points within $10^{-5}$ of $\mathcal{H}(x, p) = 0$, but after IAMM processing 60% of the points meet that tolerance. In order to lessen the effect of deterministic dynamics on IAMM convergence, artificial "endpoints", shown as blue dots, were defined at $x = 0.3101$ and $x = 1.2115$. Consequently, two small portions of the optimal path between these points and the analytic steady states (shown as black dots) are not found. A $T_e$ of 10.2 was used to produce these results.

Time series of FTLE contour plots showing the emergence of structures for the branching annihilation model. The label on each contour plot refers to the time step, i.e. the Step 1 pane represents FTLE values after a single integration, and the Step 60 pane is the final result after 60 integration steps. All FTLE values are an average of separate forward and backward fourth-order Runge-Kutta integration schemes. Each time step is 0.1, and the finite time for the process is $T = 6$. The grid resolution is .01 in both the $x$ and $p$ dimensions. Parameter values are $\lambda = 2.0, \mu = 0.5$.

2D SIS projections with common base $p_s$ by $p_i$.

2D SIS projections with common base $s$ by $p_s$. 
List of Tables

1  SIS Transitions and Rates .................................................. 15
2  2D SIS Domain Definition ................................................... 21
3  Allee Transitions and Rates ............................................... 26
4  Branching Annihilation Transitions ................................. 34
1 Introduction

Stochastic dynamical systems are used to model a wide variety of physical and biological phenomena that change over time. In these types of systems, one often sees rare transition events that are induced by noise which may be internal or external to the system. These noise-induced rare events may be associated with a desirable outcome, such as the extinction of an infectious disease outbreak, or an undesirable outcome, such as the sudden clustering of cancerous cells.

Both internal and external noise can lead to a rare switching event between metastable states or a rare escape event from a metastable state. There are many possible escape or switching paths, but there is one path along which switching or escape is most likely to occur. We call this most likely path the optimal path.

Defining the optimal path is important, since knowledge of the path enables the determination of the mean time to escape from a metastable state or to switch from one metastable state to another metastable state. Such knowledge, when applied to a real world problem such as the possible extinction of a species, allows us to know how quickly total extinction will occur without interventions of some kind.

For most systems, it is impossible to analytically determine the optimal path to escape or switch. Therefore, the optimal path must be determined numerically. This thesis describes a novel methodology for computing the optimal path in higher-dimensional systems where analytical results are not available. Additionally, while our focus is epidemiology and population models, this methodology is general and may be used for finding a path between metastable states for a wide variety of problems.

1.1 Epidemiology and the use of Stochastic Models

One of the major concerns of our time is understanding the outbreak, spread, and control of infectious diseases, where extinction of the disease is the ultimate goal. Even as industrialized nations benefit from robust medical developments that have increased longevity, and from vaccines that have virtually erased fatal childhood diseases in first-world countries, we live with the threat of the next great infectious disease outbreak. In 2009, the annual influenza season featured a return of the H1N1 virus that was responsible for 60.8 million cases and over 12,000 deaths in the United States alone [1]. This outbreak prompted recollections of the Spanish influenza pandemic of 1918-1920, estimated to have killed at least 50 million people worldwide [2]. The ease of modern global travel is an obvious conduit for outbreaks of “new” diseases far from their areas of origin (e.g., HIV, SARS, and Ebola) as well as a means for the reintroduction of well-known diseases, including measles, polio, and diphtheria, into communities where they were once eradicated. Hence, understanding pathways to the extinction of an infectious outbreak is of primary importance.

Mathematical models that replicate disease outbreaks and extinction events are important tools to aid our understanding of disease dynamics. Historically, deterministic compartmental models have been used to understand population dynamics in a range of biological applications [3]. The simplest population models for species generally have two equilibrium levels: the first is the zero, or extinct, population state, and the second represents the carrying capacity, which defines the maximum sustainable population. For realistic sets of parameter values the carrying capacity equilibrium state will be stable, while the extinct state will be unstable. Therefore, there is no way for a population that exists at or near the carrying capacity to go extinct in the deterministic formulation. Nevertheless, one often
hears of the extinction of species. To capture these extinction events, one must consider stochastic effects due to the random interactions of individuals within the population [4, 5].

Similarly, the simplest deterministic compartmental models for infectious disease transmission have two equilibrium states: the first is the extinct state, which contains no infectious individuals; the second is the endemic state where the disease is maintained without external forcing. As with the simple population models described above, for realistic parameter values that lead to a reproductive number $R_0 > 1$, the endemic state will be stable, while the extinct state will be unstable. Once again, there is no way for an endemic disease to deterministically go extinct. However, we often experience disease extinction. Every winter, we observe the rise and fall of the number of infectious individuals around us, as influenza travels through workplaces, schools, and other venues. Even when no control (for example, vaccine or quarantine) is applied, we often can recognize when the disease has run its course and, in our community at least, a local extinction has occurred. As before, in order to capture these types of extinction events in compartmental models, one must consider stochastic effects due to the random interactions of individuals within the population [6-8].

Mathematically, the effect of internal noise due to these random interactions of individuals within the system is described using a master equation. Specifically, the master equation describes the evolution of the probability of $X$ individuals at a particular time $t$ [9, 10]. The master equation is a large, or even infinite, set of differential equations, and in general, it cannot be solved analytically. Therefore, one must resort to approximation methods. Since disease or species extinction is a rare event, an eikonal, or WKB, approximation of the master equation will be used [11-15]. The WKB method transforms the problem into one of classical mechanics. The method leads to the development of a Hamilton-Jacobi equation with Hamiltonian $\mathcal{H}(x, p) = 0$ [16]. The dimensions of the Hamiltonian are twice the dimensions of the original system due to the conjugate momenta variables $p$. The WKB solution amounts to finding a zero-energy trajectory of an effective mechanical system, and at least one of the solutions to the zero-energy Hamiltonian is the optimal path to extinction. There may be other paths to extinction, but the optimal path is the path that maximizes the probability of extinction. Even for simple problems, the optimal path may not have an analytical solution. The numerical computation of the optimal path trajectory has been achieved in the past using a shooting method [16]. However, since the procedure is very sensitive to boundary conditions, it is difficult to implement when analyzing paths far away from bifurcation points [17, 18]. In Refs. 17 and 18 these numerical issues were overcome by computing finite-time Lyapunov exponents (FTLE). The method worked very well for low-dimensional problems, but in high dimensional problems the FTLE results define a region on and around the optimal path, but fail to describe the optimal path itself in the necessary detail.

In this thesis, we describe a novel methodology that combines the use of two numerical methods to compute the optimal path trajectory for high-dimensional models. The method begins by computing finite-time Lyapunov exponents. FTLE computations provide a measure of stretching of initially close particles over a specified finite amount of time. Ridges of high FTLE values are of greatest interest, since it has been shown that a maximal FTLE ridge is equivalent to the optimal path [17, 18]. Therefore, the FTLE provides a means to identify points in close proximity to the optimal path. We then use the FTLE results as an initial guess for the second numerical scheme.

This second scheme is an Iterative Action Minimizing Method (IAMM) [19], which applies a Newton's Method process to the initial guess provided by the FTLE result. The IAMM provides a method to converge rapidly to the optimal path. While the method is
rather straightforward, there are difficulties in computing the trajectory of an unstable path in higher dimensions which lead us to explore other factors that may be influencing the computations.

We illustrate the methodology using a Susceptible-Infectious-Susceptible (SIS) epidemiology model and an Allee population model, both with intrinsic noise. For the SIS system, all processes and methods are demonstrated using a low-dimensional single population model, as well as a high-dimensional two population model. For the Allee system, the single population model has an optimal path that both begins and ends on the deterministic mean-field path. To date, finding such a path using other numerical methods has proven unsuccessful. We present an example in which we have purposely randomized points about the analytic optimal path to mimic placement of high FTLE points in an n-dimensional model. We then demonstrate the use of IAMM with a specific strategy so that the randomized points converge to the optimal path rather than to the nearby deterministic path.

2 General Theory

2.1 Master Equation Formalism

As mentioned in the introduction, the simplest deterministic epidemic compartmental models contain two steady states of differing stability: an extinct state where no infectious individuals are present, and an endemic state where the infection is maintained. The stability of these steady states is determined by the value of the basic reproductive number \( R_0 \), as shown in Fig. 1. The reproductive number can be thought of as the average number of new infectious individuals that one infectious individual generates over the course of the infectious period, in an entirely susceptible population. When \( R_0 < 1 \), the extinct state is stable while the endemic state is unstable; when \( R_0 > 1 \), the extinct state is unstable while the endemic state is stable. It is worth noting that since the model is deterministic, a population at the attracting endemic state can never go extinct.

To capture extinction events, we must consider a stochastic model with internal noise that represents the random interactions of individuals in the population. Therefore, a master equation is used to describe the effect of stochasticity. Let \( X \) be a state variable that represents the number of individuals in a single population. The following theory will be developed for a single population, but it is easily extended to multiple populations \( X_1, X_2, \ldots X_n \) by use of a state vector \( \mathbf{X} \).

The probability density \( \rho(X,t) \) describes the probability of finding \( X \) individuals at time \( t \). Each possible population-changing event (birth, death, infection, migration, etc.) is defined by a transition rate \( W_r(X) \), where \( r \) is a positive or negative integer that defines an incremental change from state \( X \) to state \( X + r \). Then the master equation that provides the time evolution of \( \rho(X,t) \) for a single population is \([9,10]\)

\[
\frac{\partial \rho(X,t)}{\partial t} = \sum_r [W_r(X - r)\rho(X - r,t) - W_r(X)\rho(X,t)].
\]  \(1\)

In general, it is not possible to analytically solve the master equation given by Eq. 1. Let \( X \) be scaled by \( N \), the large parameter of the model. Using \( x = X/N \), the transition rate \( W_r(X) = W_r(Nx) \) can be represented as the following expansion in \( N \),

\[
W_r(Nx) = Nw_r(x) + u_r(x) + \mathcal{O}(1/N),
\]  \(2\)
Figure 1: The simplest deterministic compartmental models have two steady states. There is a bifurcation at $R_0 = 1$ that causes a change in stability. For $R_0 < 1$ the extinct state is attracting while the endemic state is repelling. For $R_0 > 1$ the extinct state is repelling while the endemic state is attracting.

where $x$ and the scaled transition rates $w_r$ and $u_r$ are $\mathcal{O}(1)$.

For $N \gg 1$ we approximate the scaled master equation using the Wentzel-Kramers-Brillouin (WKB) approximation. To account for the rare possibility of extinction, we look for the probability distribution in the form of the WKB ansatz

$$\rho = e^{-NS(x,t)}$$

where $S(x,t)$ is a quantity known as the action [11–13,20]. The WKB ansatz given by Eq. 3 is substituted into the scaled master equation, which is stated in terms of $w_r(x - r/N)$ and $S(x - r/N, t)$, where $r/N$ is small. A Taylor series expansion of these functions of $x - r/N$ is performed, and one arrives at a Hamilton-Jacobi equation $\mathcal{H} = -\partial S/\partial t$. At leading order, the Hamilton-Jacobi equation has the form $\mathcal{H}(x,p) = 0$, where $\mathcal{H}$, known as the effective Hamiltonian, is given as

$$\mathcal{H}(x,p) = \sum_r w_r(x)(e^{pr} - 1); \quad p = \frac{dS}{dx},$$

where $p$ is the conjugate momentum. The solutions to $\mathcal{H}(x,p) = 0$ are the zero-energy curves of the system. At least one solution is the optimal path where the action $S$ is minimized which corresponds to the path that maximizes the probability of extinction.

Hamilton’s equations

$$\dot{x} = \partial \mathcal{H}(x,p)/\partial p, \quad \dot{p} = -\partial \mathcal{H}(x,p)/\partial x$$

describe the system’s dynamics and are easily found from the Hamiltonian given by Eq. 4. The $x$ dynamics along the $p = 0$ deterministic line are described by

$$\dot{x} = \left. \frac{\partial \mathcal{H}(x,p)}{\partial p} \right|_{p=0}$$
which is the rescaled mean-field rate equation associated with the original deterministic problem. For the simple models described by Fig. 1 the deterministic steady states are nodes. It is easy to show that the WKB method has transformed these steady state nodes in the original 1D deterministic system into steady state saddle points in the 2D set of Hamilton’s equations. This allows for escape from the endemic state and provides a path to extinction that did not exist in the original deterministic model. In the models we will discuss, the optimal path leaves the endemic state and arrives at a new extinct point where at least one momentum $p$ value is nonzero.

The complexity of exploring multi-population stochastic models becomes apparent when considering the solution to the generalized set of Hamilton’s equations

$$
\dot{x}_j = \frac{\partial H(x_1,...,x_n,p_1,...p_n)}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial H(x_1,...,x_n,p_1,...p_n)}{\partial x_j}, \quad j = 1,...n
$$

where $n$ is the number of distinct population groups included in a model. After employing the WKB formalism the domain of the system is $\mathbb{R}^{2n}$, and a system of $2n$ equations must be solved to find steady states. Furthermore, since the Hamiltonian is now a function of $2n$ variables, the likelihood that analytic solutions to the zero-energy Hamiltonian equation can be found is greatly reduced. Therefore, we must consider alternate methodologies to compute the optimal path.

### 2.2 Finite-Time Lyapunov Exponents (FTLE)

We consider a velocity field $v : \mathbb{R}^{2n} \times I \to \mathbb{R}^{2n}$ given by Eq. 5 that is defined over time interval $I = [t_i, t_f]$, and the system of equations:

$$
\begin{align*}
\dot{y}(t; t_i, y_0) &= v(y(t; t_i, y_0), t), \quad \text{(8a)} \\
y(t_i; t_i, y_0) &= y_0, \quad \text{(8b)}
\end{align*}
$$

where $y, y_0 \in \mathbb{R}^{2n}$ and $t \in I$. This dynamical system has quantities known as Lyapunov exponents that measure the growth rates of the linearized dynamics about the trajectory of the system. To find the finite-time Lyapunov exponents (FTLE), the Lyapunov exponents are computed on a restricted finite time interval.

To compute FTLE values, we choose a domain of interest and define it as an evenly-spaced grid of $2n$ dimensional points $y = (x, p)$, with initial position $y_0$ defined at the grid points. Then, using Hamilton’s equations (Eq. 5), all points are numerically integrated. The flow map $\phi$ determines the advection of the initial points as follows: [21–24]

$$
\phi^{t_i+T}_{t_i} : y_0 \to \phi^{t_i+T}_{t_i}(y_0) = y(t_i + T; t_i, y_0)
$$

Then the FTLE can be defined as

$$
\sigma(y, t_i + T, T) = \frac{1}{|T|} \ln \sqrt{\lambda_{\text{max}}(\Delta)}, \quad \text{(10)}
$$

where $\lambda_{\text{max}}(\Delta)$ is the maximum eigenvalue of the right Cauchy-Green deformation tensor $\Delta$, which is given as follows:

$$
\Delta(y, t_i + T, T) = \left( \frac{d\phi^{t_i+T}_{t_i}(y(t))}{dy(t)} \right)^* \left( \frac{d\phi^{t_i+T}_{t_i}(y(t))}{dy(t)} \right), \quad \text{(11)}
$$
with * denoting the adjoint.

For a given $y \in \mathbb{R}^{2n}$ at an initial time $t_i$, Eq. 10 gives the maximum finite-time Lyapunov exponent for some finite integration time $T$ (forward or backward), and provides a measure of the sensitivity of a trajectory to small perturbations. The FTLE field given by $\sigma(y, t_i, T)$ can be shown to exhibit ridges of local maxima in phase space. The ridges of the field indicate the location of attracting (backward time FTLE field) and repelling (forward time FTLE field) structures. In two-dimensional (2D) space, the ridge is a curve which locally maximizes the FTLE field so that transverse to the ridge one finds the FTLE to be a local maximum. What is remarkable is that the FTLE ridges correspond to the optimal path trajectories [17, 18]. The basic idea is that since the optimal path is inherently unstable and observed only through many realizations of stochastic experiments, the FTLE shows that locally, the path is also the most sensitive to initial data. Figure 2 shows a schematic that demonstrates why the optimal path corresponds to a maximal FTLE ridge. If one chooses an initial point on either side of the optimal path near the endemic state, the two trajectories will separate exponentially in time since both extinct and endemic states are unstable saddle points.

For single population models, the optimal path is a curve in $\mathbb{R}^2$ with $(x, p)$ coordinates. A contour map of $\sigma$ values as a function of $x$ and $p$ is ideal for showing the maximal FTLE ridge that corresponds to the optimal path. Appendix A shows a step-by-step visualization of the high FTLE ridges that emerge as FTLE computations are performed after each numerical integration step.

For models involving multiple populations, the optimal path is a curve which, in a high-dimensional space, is not easily visualized. A methodology that can extract information about the optimal path from the FTLE field without relying on visual inspection is necessary. Therefore, we use statistical tools to define a threshold cut-off value so that points associated with the highest FTLE values can be identified. Additionally, points associated with deterministic structures, such as those occurring where $p = 0$, can be excluded from selection. In this way, points known to be in the vicinity of the optimal path are identified and selected for inclusion in an array of high FTLE points. For low-dimensional models, this array may produce a nearly complete optimal path. For high-dimensional models, however, such a nice result is less likely. Their known proximity to the optimal path, however, makes the point array highly desirable as initial data for the following method.

### 2.3 Iterative Action Minimizing Method (IAMM)

As described in Section 2.1, the WKB formalism results in a Hamiltonian with a zero-energy curve that is the optimal path connecting two steady state saddle points. The Iterative Action Minimizing Method [19] (IAMM) is a numerical scheme based on Newton's method that computes optimal transition pathways in systems of stochastic differential equations. In particular, given an initial guess of high FTLE-valued points produced by the method described in Sect. 2.2, the IAMM is a useful method for determining the optimal path.

Consider a general situation where a path connecting steady state saddle points $C_a$ and $C_b$ starts at $C_a$ at $t = -\infty$ and ends at $C_b$ at $t = +\infty$. Then a time parameter $t$ exists such that $-\infty < t < +\infty$. For this method, we require a numerical approximation of the time needed to leave the region of $C_a$ and arrive in the region of $C_b$. Therefore, we define a time $T_e$ such that $-\infty < -T_e < t < T_e < +\infty$. Additionally, $C(-T_e) \approx C_a$ and $C(T_e) \approx C_b$. In other words, the solution stays very near the equilibrium $C_a$ for $-\infty < t \leq -T_e$, has a transition region from $-T_e < t < T_e$, and then stays near $C_b$ for $T_e < t < +\infty$. 

12
After numerical integration, points initially remain close pair of points. After a finite time the two points remain close to one another, and therefore the corresponding FTLE value will be small. (b) The numerical integration of two initially close points on opposite sides of the zero-energy trajectory. After a finite time the two points move a significant distance apart from one another, and therefore the corresponding FTLE value will be large.

The interval $[-T_e, T_e]$ is discretized into $N$ segments using a uniform step size $h = (2T_e)/N$. Alternatively, one may map the $[-T_e, T_e]$ interval onto the $[0, 1]$ interval via the linear transformation $t = 2T_e \tau - T_e$ and use a step size of $\tilde{h} = 1/N$ to discretize the interval. It is worth noting that for some problems, such as the Allee system described in Sect. 6, it may be necessary to use a non-uniform step size to resolve sharp transition regions [19].

Given a non-uniform time step $h_k$, one has the time series $t_{k+1} = t_k + h_k$. The derivative of the corresponding function value $q_k$ is approximated using central finite differences by the operator $\delta_h$ given as

$$\frac{d}{dt} q_k \approx \delta_h q_k \equiv \frac{h_k^2 q_{k+1} + (h_k^2 - h_{k-1}^2)q_k - h_k^2 q_{k-1}}{h_k - h_{k-1}^2 + h_k h_{k-1}^2}, \quad k = 0, \ldots, N. \quad (12)$$

Clearly, if a uniform step size is chosen then Eq. 12 simplifies to the familiar form given as

$$\frac{d}{dt} q_k \approx \delta_h q_k \equiv \frac{q_{k+1} - q_{k-1}}{2h}, \quad k = 0, \ldots, N. \quad (13)$$
Thus, one can develop the system of nonlinear algebraic equations

\[
\delta_h x_k - \frac{\partial H(x_k, p_k)}{\partial p} = 0, \quad \delta_h p_k + \frac{\partial H(x_k, p_k)}{\partial x} = 0, \quad k = 0, \ldots, N,
\]

(14)

which is solved using a general Newton's method.

We let \(q_j(x, p) = \{x_{1,j}, \ldots, x_{N,j}, p_{1,j}, \ldots, p_{N,j}\}^T\) be an extended vector of \(2nN\) components that contains the \(j^\text{th}\) Newton iterate, where \(n\) is the number of populations. When \(j = 0\), \(q_0(x, p)\) provides the initial "guess" as to the location of the path that connects \(C_a\) and \(C_b\). In our work, \(q_0\) comes from the results of FTLE computations. Given the \(j^\text{th}\) Newton iterate \(q_j\), the new \(q_{j+1}\) iterate is found by solving the linear system

\[
q_{j+1} = q_j - J^{-1}(q_j) F(q_j),
\]

(15)

where \(F\) is the function defined by Eq. 14 acting on \(q_j\), and \(J\) is the Jacobian. Equation 15 is solved using LU decomposition with partial pivoting.

The IAMM, like any scheme involving Newton’s method, is sensitive to the initial condition. A poor initial guess may lead to erroneous results including convergence to a curve that is not the optimal path or a non-convergent result. It is worth noting that the choice of \(T_e\) can affect the results. These difficulties are addressed in the examples presented.

3 The 1D and 2D SIS Models

3.1 Introduction

The Susceptible-Infected-Susceptible (SIS) model describes a disease without immunity from re-infection. The population is composed of two compartments: Susceptibles \(S\) and Infecteds \(I\). An individual is born susceptible. Then, through contact, the individual may become ill and be classified as infectious. After a specified period, the individual has recovered and is returned to the susceptible compartment. Removal by death is possible from both compartments, but we assume no disease-related deaths in this model.

\[
\begin{align*}
S \xrightarrow{\beta SI/N} I \\
\mu N \xrightarrow{\gamma I} I \\
\mu S \xrightarrow{\gamma I} I
\end{align*}
\]

Figure 3: The SIS model compartmental flow includes birth \(\mu N\), infection \(\beta SI/N\), recovery \(\gamma I\), death of susceptibles \(\mu S\), and death of infected individuals \(\mu I\).

In the SIS compartmental model shown in Fig. 3, we assume a constant total population so that \(N = S + I\). Rates are defined as follows: \(\mu\) is a birth/death rate, \(\beta\) is the mass action contact rate, and \(\gamma\) is the recovery rate. The events affecting each compartment are used to formulate two mean-field equations that describe the system’s behavior over time:

\[
\begin{align*}
\frac{dS}{dt} &= \mu N - (\beta SI)/N + \gamma I - \mu S \\
\frac{dI}{dt} &= (\beta SI)/N - \gamma I - \mu I
\end{align*}
\]

(16a) (16b)
3.2 Steady States and Stability Analysis

At a steady state, \( dS/dt = dI/dt = 0 \). Two such solutions are found:

- \( S = N, I = 0 \), the disease free equilibrium where no infection exists.
- \( S = N \frac{\mu + \gamma}{\beta}, I = N(1 - \frac{\mu + \gamma}{\beta}) \), the endemic equilibrium of persistent infection.

We begin by linearizing about the disease free state using the Jacobian of Eqs. 16, which is

\[
J(S, I) = \begin{bmatrix}
-\frac{\beta I}{N} - \mu & -\frac{\beta S}{N} + \gamma \\
\frac{\beta I}{N} & \frac{\beta S}{N} - (\mu + \gamma)
\end{bmatrix}
\]

(17)

It is then evaluated at the disease free equilibrium:

\[
J(N, 0) = \begin{bmatrix}
-\mu & -\beta + \gamma \\
0 & \beta - (\mu + \gamma)
\end{bmatrix}
\]

(18)

Eigenvalues obtained from Eq. 18 are \( \lambda_1 = -\mu \) and \( \lambda_2 = \beta - (\mu + \gamma) \). Since \( \mu \) is a positive rate no greater than 1, \( \lambda_1 \) is always negative. Therefore, the extinct state is stable when \( \lambda_2 < 0 \), which occurs when \( \beta / (\mu + \gamma) < 1 \). A similar, although more algebraically challenging, linearization about the endemic state shows that it is stable when \( \beta / (\mu + \gamma) > 1 \).

The two steady states, then, attract or repel based upon the comparison of \( \beta \) to \( \mu + \gamma \). When \( \beta < \mu + \gamma \), both \( \lambda_1 \) for the extinct state are negative, so it is stable and attracts. Meanwhile, the endemic state is unstable and repels. The dynamics reverse when \( \mu + \gamma < \beta \). The extinct state now has a positive and a negative eigenvalue. Therefore, the extinct state repels while the endemic state attracts. This ratio, \( \beta / (\mu + \gamma) \), crucial to the dynamics of the SIS model, is called the reproductive number \( R_0 \). The variation in dynamics based on \( R_0 \) is shown in Fig. 1.

3.3 The 1D and 2D SIS stochastic models

A population at the endemic state can never go extinct in the deterministic SIS model just described. To understand how extinction can occur, we must include stochastic effects due to the random interaction of individuals in the population. We do this using the master equation and WKB formalism as described in Sec. 2.1. Using state variable \( X = (S, I) \) to represent the two compartmental model, a list of transitions for all possible events is formulated, as shown in Table 1.

<table>
<thead>
<tr>
<th>Event</th>
<th>S Transitions</th>
<th>I Transitions</th>
<th>Scaled Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Birth</td>
<td>( W_{+1} = \mu N )</td>
<td></td>
<td>( \mu )</td>
</tr>
<tr>
<td>Infection</td>
<td>( W_{-1} = \beta SI/N )</td>
<td>( W_{+1} = \beta SI/N )</td>
<td>( \beta si )</td>
</tr>
<tr>
<td>Recovery</td>
<td>( W_{+1} = \gamma I )</td>
<td>( W_{-1} = \gamma I )</td>
<td>( \gamma i )</td>
</tr>
<tr>
<td>Death</td>
<td>( W_{-1} = \mu S )</td>
<td>( W_{-1} = \mu I )</td>
<td>( \mu s, \mu i )</td>
</tr>
</tbody>
</table>
Scaling by the constant population size $N$ produces new variables $s = S/N$ and $i = I/N$, so that $s + i = 1$. Then the Hamiltonian arising from the WKB method for the 2D SIS model is

$$H(s, i, p_s, p_i) = \mu(e^{p_s} - 1) + \beta s i (e^{-p_s} + p_i - 1) + \gamma i (e^{p_s} - p_i - 1) + \mu s (e^{-p_s} - 1) + \mu i (e^{-p_i} - 1).$$ (19)

We can simplify the 2D model using the constant population assumption so that $S = N - I$ or $s = 1 - i$ in the scaled variables. This relation allows one to formulate a simplified 1D mean-field equation for the infectious individuals. The associated 1D stochastic SIS model is obtained by considering only the transitions in Table 1 affecting the infected population. The resulting Hamiltonian for the 1D SIS model is

$$H(i, p) = \beta(1 - i)i(e^p - 1) + (\mu + \gamma)i(e^{-p} - 1),$$ (20)

where we have omitted the $p_i$ subscript since there is only one momentum variable for a single population model.

4 1D SIS Results

We begin by finding the analytical zero energy solutions for the 1D SIS Hamiltonian given by Eq. 20. The solution $i = 0$ represents extinction; a second solution is $p = 0$, which corresponds to the deterministic mean-field equation. The third solution is the optimal path and is given by

$$p = \ln \left( \frac{\mu + \gamma}{\beta(1 - i)} \right).$$ (21)

Next we find the analytical critical points of Hamilton’s equations

$$\dot{i} = \beta(1 - i)e^p - (\mu + \gamma)i e^{-p},$$ (22a)

$$\dot{p} = \beta(2i - 1)(e^p - 1) - (\mu + \gamma)(e^{-p} - 1).$$ (22b)

The trivial solution $(i, p) = (0, 0)$ is associated with the deterministic extinct state $(S, I) = (N, 0)$. A second critical point $(i, p) = (1 - [(\mu + \gamma)/\beta], 0)$ is associated with the endemic state. Note that the deterministic mean-field endemic $(S, I)$ point was an attracting node for $R_0 > 1$, but the endemic $(i, p)$ state found using Hamilton’s equations is a saddle point, allowing for a path to escape from the endemic level. A third critical point $(0, \ln[(\mu + \gamma)/\beta])$, called the fluctuational extinction point, represents a new disease-free state with non-zero noise, distinguishing it from the deterministic extinct point $(0, 0)$. As shown in Fig. 4, all critical points for the SIS model are metastable saddle points.

We will now describe the use of the FTLE and IANM numerical schemes to compute the optimal path. Our numerical results will be compared with the analytical solution given by Eq. 21. Although we know the analytic solution of the optimal path for the 1D SIS model, our objective is to present a useful methodology when no solution is known. In Sec. 5 we will consider the 2D SIS model, where an analytic solution of the optimal path is not available.

4.1 Finite-Time Lyapunov Exponents

We compute the FTLE field using Hamilton’s equations. There are two important components for producing an accurate FTLE field for any model: (1) a domain that is both sufficiently large and sufficiently meshed must be chosen and (2) a finite time $T$ must
be chosen large enough to capture the dynamics of the system. The critical points of Hamilton's equations are our primary source for boundary information. For the 1D SIS model, we use the critical points of Eqns. 22(a)-(b) to define domain boundaries of at least $0 \leq i \leq (1 - (\mu + \gamma)/\beta)$ and $\ln((\mu + \gamma)/\beta) \leq p \leq 0$. We recommend that the FTLE domain extend a small distance beyond these boundaries to fully capture the system dynamics.

The numerical integration step size is given as $\delta t$. One must consider that a point within the domain may be integrated beyond the domain boundaries. We use hard domain boundaries for our FTLE computations. A point integrated outside of the domain is no longer integrated, and the FTLE value last assigned to it remains unchanged. Although some points are advected outside the domain on the initial integration step, using a relatively small $\delta t$ value minimizes this, with the end result being a more accurate FTLE field.

4.2 **High Value FTLE Point Harvesting**

We wish to harvest points along the high value FTLE ridge that forms a pathway from the endemic point to the fluctuational extinction point as shown in Fig. 6. These points will serve as an initial guess of the optimal path for IAMM computations. To harvest these points, we define a threshold that is three standard deviations above the mean of the 1D SIS FTLE data. Additional restrictions limit consideration to only those points occurring between the endemic and fluctuational extinction points. Specifically, for parameters $\beta = 5.0, \mu = 0.02, \text{ and } \gamma = 0.98$, we limit the range of $i$ and $p$ to $0.001 < i < 0.8$ and $-1.6 < p < -0.001$. This also eliminates points in close proximity to the deterministic $p = 0$ line and the extinction $i = 0$ line from selection. The selection process yields an array of about 10,000 points that,
when plotted, closely approximate the optimal path defined by Eq. 21.

Since the Iamm computation involves the inversion of a matrix with dimensions dependent on the number of array points, it is desirable to reduce the number of points. We evaluate the coordinates of each point in the Hamiltonian given by Eq. 20 and those yielding a value within a tolerance of $5.0 \times 10^{-5}$ to $\mathcal{H} = 0$ are chosen. This produces the 994 point array shown in Fig. 5(a).

4.3 Iamm Computations

For the 1D SIS model, it seems unnecessary to iterate the 994 point $q_0$ initial condition using Iamm; the points appear to lie directly on the optimal path [Fig. 5(a)]. However, performing the Iamm computation reveals information that is useful when finding the optimal path for higher dimensional models.

In particular, the order of the initial condition is of primary importance. The SIS optimal path flows from the endemic state to the fluctuational extinct state. Figure 5 illustrates the differing outcomes when $q_0$ is ordered from the fluctuational extinct state to the endemic state [Fig. 5(b)] compared to when $q_0$ mimics the correct flow [Fig. 5(c)]. The extreme adjustments revealed in 5(b) reflect an attempt to reorder the points. Repositioning of points away from the path is fundamentally disruptive, making divergence more likely.

![Figure 5](image)

Figure 5: The success of Iamm processing is dependent upon the ordering of the initial condition, as illustrated by these 1D SIS figures. Panel (a) contains the initial condition $q_0$ with color-coded segments; each segment holds an equal number of points. The dashed gray line underlying the points is the analytic optimal path given by Eq. (21). Panels (b) and (c) contain the results after two Newton iterations of the Iamm. In (b) $q_0$ was ordered from the fluctuational extinct state to the endemic state, whereas in (c) $q_0$ was ordered from endemic state to fluctuational extinction. Panel (b) shows the extreme repositioning of array points as the Iamm attempts to achieve the desired point ordering from the endemic to the extinct state. The points move so far from the optimal path that, ultimately, the method does not converge to the optimal path. In contrast, (c) reflects minimal repositioning due to Iamm adjustments. All Iamm computations were done using $T_e = 2$.

4.4 1D SIS Optimal Path

Figure 6 demonstrates complete agreement of the FTLE results and the Iamm results with the analytical optimal path given by Eq. 21. Specifically, Fig. 6 shows an average of
the forward and backward FTLE field for the 1D SIS model as filled contours. The three analytical zero-energy solution curves of the Hamiltonian agree well with the red, maximal FTLE ridges. Both the analytical optimal path in black and the final IAMM optimal path in blue appear as overlays on the maximal FTLE ridge.

5 2D SIS Results

We begin by determining whether the Hamiltonian for the 2D SIS model, given by Eq. 19, has any zero-energy analytic solutions. One solution is the deterministic plane where both $p_s$ and $p_i$ are zero, and another is the non-infectious plane where $i$ and $p_s$ are both zero. Since neither of these solutions represents the optimal path, we must find it numerically.

We find the analytical critical points of Hamilton’s equations

$$
\begin{align*}
\dot{s} &= \mu e^{p_s} - \beta s i e^{-p_s + p_i} + \gamma i e^{p_s - p_i} - \mu s e^{-p_s}, \\
\dot{i} &= \beta s i e^{-p_s + p_i} - \gamma i e^{p_s - p_i} - \mu i e^{-p_i}, \\
\dot{p}_s &= -[\beta i (e^{-p_s + p_i} - 1) + \mu (e^{-p_s} - 1)] , \\
\dot{p}_i &= -[\beta s (e^{-p_s + p_i} - 1) + \gamma (e^{p_s - p_i} - 1) + \mu (e^{-p_i} - 1)].
\end{align*}
$$

(23a) (23b) (23c) (23d)
Figure 7: To derive a $p_s$ range for the 2D SIS FTLE computations, a four-dimensional grid is defined and each point is tested using a tolerance of $\mathcal{H} < 10^{-9}$. This figure displays the $p_s \times p_i$ values of those points meeting that tolerance. For all 2D SIS computations, we use parameters $\mu = 0.2, \beta = 104$ and $\gamma = 100$.

The point $(s, i, p_s, p_i) = (1, 0, 0, 0)$ represents the deterministic extinct state. The endemic state is defined at $((\gamma + \mu)/\beta, 1 - ((\mu + \gamma)/\beta), 0, 0)$, while the fluctuational extinct state is found at $(1, 0, 0, \ln((\mu + \gamma)/\beta))$. A stability analysis of these three points show that all are metastable saddle points. Two additional critical points also are found. We will discuss their influence later in these results.

5.1 Finite-Time Lyapunov Exponents

The critical points of Eqs. 23(a)-(d) define domain boundaries of at least $(\gamma + \mu)/\beta \leq s \leq 1, 0 \leq i \leq (1 - [(\mu + \gamma)/\beta])$ and $\ln[(\mu + \gamma)/\beta] \leq p_i \leq 0$. However, $p_s$ is zero at both the endemic and fluctuational extinction steady states, revealing no information as to its range. FTLE computations could be used in a guess-and-check manner to deduce the range of $p_s$, but this is a time-consuming choice. A quicker alternative is derived from our knowledge that the optimal path contains points that evaluate $\mathcal{H}$ to be zero. We define a four-dimensional grid based on the three known domains and use a broad guess for the range of $p_s$. Then each grid point is evaluated in the Hamiltonian, and the points that meet a chosen tolerance are selected. A visual inspection of the selected points, shown in Fig. 7, leads us to defines a minimum $p_s$ value of -0.04.

For all 2D SIS computations, we use parameters $\mu = 0.2, \beta = 104$ and $\gamma = 100$. Table 2 contains the dimensions of the domain used for 2D SIS calculations.

5.2 High Value FTLE Point Harvesting

Just as for 1D SIS, we need to select points along the high FTLE ridge to serve as an initial guess in IAMM computations. In order to determine a useful FTLE value threshold we consider that our domain grid describes a data array with over $10^8$ points, so using three standard deviations above the mean as a threshold yields far too many points. Instead, we
Table 2: 2D SIS Domain Definition

<table>
<thead>
<tr>
<th></th>
<th>Lower Limit</th>
<th>Upper Limit</th>
<th>Grid Dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s$</td>
<td>0.954</td>
<td>1.0012</td>
<td>119</td>
</tr>
<tr>
<td>$i$</td>
<td>-0.002</td>
<td>0.038</td>
<td>101</td>
</tr>
<tr>
<td>$p_s$</td>
<td>-0.04</td>
<td>0.002</td>
<td>106</td>
</tr>
<tr>
<td>$p_i$</td>
<td>-0.04</td>
<td>0.0016</td>
<td>105</td>
</tr>
</tbody>
</table>

define a maximum FTLE value and, after a few trials, find that an FTLE threshold value of 4.25 identifies about 13,000 points, as shown in Fig. 8.

Figure 8: These figures indicate the location of all points having an FTLE value greater than 4.25 after completion of FTLE processing for the 2D SIS model. Since the points are four dimensional, we display them using two companion figures, where Panel (a) describes the $(s, i)$ location and Panel (b) describes the $(p_s, p_i)$ location of each selected point.

For this harvesting, we also eliminate all points on the deterministic surface, as well as points beyond the boundaries of the optimal path as described in Table 2. Additionally, we eliminate high FTLE points within 0.001 of $i = 0$ since this interval contains a large number of points that provide no significant information.

Keeping in mind the matrix inversion done as part of IAMM processing, we decide to reduce the number of points in $q_0$ further by evaluating each harvested point in the Hamiltonian given by Eq. 19. Those within a tolerance of $2.5 \times 10^{-6}$ to $H = 0$ are retained. The 1752 points meeting this requirement are shown in Figs. 9(a) and (b).

5.3 IAMM Computations

As mentioned in Sect. 4.3, successful IAMM results are more likely when $q_0$ reflects the flow of the optimal path. For the 2D SIS model, the endemic and fluctuational extinction steady states suggest that $s$ monotonically increases and $i$ and $p_i$ monotonically decrease as the optimal path traverses the domain. Since $p_s = 0$ at both steady states, its value must
decrease, and then increase, perhaps repeatedly. Therefore, the harvested points cannot be sorted into a single monotonic ordering that will fulfill all these conditions simultaneously.

Instead we create a hybrid \( q_0 \) for Iamm processing. For the \((s, i)\) coordinates, the points shown in Fig. 9(a) are ordered with \( s \) increasing, and \( i \) decreasing as a secondary sort. For the \((p_s, p_i)\) coordinates, we examine the point plot of the harvested points, shown in Fig. 9(b), and define an ordered array that approximates areas of dense points as a piecewise linear curve, as shown in Fig. 9(c). The section from \( p_i = -0.3 \) to \( 0 \) contains two-thirds of the points, and the remaining one-third populate the lower section. The points of Figs. 9(a) and (c) are combined to produce \( q_0 \).

![Figure 9](image)

Figure 9: Panel (a) contains the \((s, i)\) coordinates and panel (b) contains the \((p_s, p_i)\) coordinates of the 1752 points harvested from the FTLE results for use as the initial condition in the IAMM computations for the 2D SIS model. For best results, \( q_0 \) should be ordered from the endemic state to the fluctuational extinct state. The harvested points cannot be ordered properly since \( p_s \) is not monotonic. We substitute the ordered array plotted in panel (c) for the actual \((p_s, p_i)\) coordinates of panel (b), and pair it with a sorted \((s, i)\) array plotted in panel (a) to obtain an ordered initial guess \( q_0 \). The green circle denotes the endemic steady state, while the red circle denotes the fluctuational extinction steady state.

After just 12 iterations using this initial condition, 90% of the array points met a tolerance of \( 1.5 \times 10^{-6} \) of \( H = 0 \). When the IAMM process continues for a total of 50 iterations, we obtain the optimal path shown in Fig. 10. All points in this array meet a tolerance of \( 5 \times 10^{-7} \).

This successful result was only achieved after we resolved another sensitivity of the IAMM process: the spacing of points in the initial array. Since the harvested points are not evenly spaced, it is likely that some areas are over-represented while others are under-represented. Our initial trials began with a smaller array of about 900 harvested points, and we used the same technique of pairing the actual \( s, i \) values with the approximated \( p_s, p_i \) values to create the initial array. While the array did converge to the optimal path, the results showed a double line of points in the middle portion of the optimal path. The points in this area were not accurate to a stringent tolerance and additional iterations did not improve the result.

We resolved this issue by lowering the harvest threshold to increase the number of initial points. In this instance, and in other problems we explored, the inclusion of more points...
to create a more densely paced initial guess increased the likelihood of converging to the optimal path.

Figure 10: The 2D SIS results from the IAMM, obtained using $T_e = 13$ for 50 iterations of the Newton method process. Panel (a) contains the final location of all $(s, i)$ coordinates from Fig. 9(a). Panel (b) contains the final location of all $(p_s, p_i)$ coordinates from Fig. 9(c). Together, they represent the optimal path. Although the points appear equally spaced, an examination of the array values shows that is not the case. The central section of the path, between two turns in both views, contains only about 200 of the 1752 point array. The other sections of the path, namely, the exit from the endemic state and the approach to the fluctuational extinct state, are each populated by half of the remaining points. This is due to the fact that very slow dynamics are present near either steady state, while the area of fast dynamics begins and ends with a transition that is, in fact, a change in the direction of the optimal path. The green circle denotes the endemic steady state, while the red circle denotes the fluctuational extinction steady state.

5.4 2D SIS Optimal Path

In order to validate the numerically computed IAMM optimal path, we consider a method for visualizing the results so that a comparison can be made with the FTLE simulations. The obvious choice is to develop a set of three dimensional projections of the four-dimensional data. In the case of the IAMM result, one can simply omit one dimension of the final array and project the remaining three coordinate array. But in the case of the FTLE result, each four dimensional point is associated with a unique FTLE value. The omission of one dimension will produce multiple points with the same three-dimensional location but different FTLE values.

We choose to average the FTLE value associated with the same three coordinate locations. For example, in Fig. 11(a), the contour plot is displayed on a grid defined by $(i, p_i, s)$ points. Each location has an associated FTLE value that is the mean of the FTLE values assigned to the 106 points having coordinates $i, p_i$ and $s$ in common, but different $p_s$ coordinates. In other words, we have averaged through the $p_s$ slices.

One flaw in averaging is that it may obscure the minimum and maximum FTLE values. However, a high FTLE ridge in four dimensions is more like a multi-dimensional rope than
a single thread. Hence, the high FTLE values persist for many slices in one or more dimensions. Additionally, use of a finely meshed grid and a domain in the vicinity of the optimal path will control the loss of true FTLE information.

Figure 11 shows two projections of the FTLE field overlaid with the IAMM computed optimal path. The optimal path is shown as a black curve that begins on the rear face and flows to the front of both figures. Areas with high FTLE values appear on the vertical slices in dark red. One can see dominant curves on these red areas that mimic the curve of the optimal path. One can also observe that the high FTLE areas in the vicinity of the optimal path persist, in varying degrees of intensity, through multiple slices of the domain.

Figure 11: Two projections of the IAMM and FTLE results for the 2D SIS model. The optimal path obtained from the IAMM computation is represented as a black curve. It begins at the endemic steady state (green circle) on the rear surface, and ends at the fluctuational extinct steady state (red circle) in the upper right foreground. Both projections show FTLE values averaged over the missing dimension, so that (a) shows the mean FTLE values of all \( p_s \) slices and (b) shows the mean for all \( s \) slices. In projection (a), the vertical \( p_i \) slices contain areas of high FTLE values in red that closely correlate to the curve of the optimal path. Projection (b), however, exhibits a widening and splitting of high FTLE regions. On vertical slice \( p_i = -0.0272 \), one observes a path diverging from the optimal path. In the vicinity is a critical point, shown as a blue circle in the foreground of (b). This critical point is not part of the optimal path structure. A stability analysis reveals that the point is neither stable nor a saddle point, but from this projection and many others, it does create dynamics that may compete with those along the optimal path. All FTLE computations were done both forward and backward in time using a fourth-order Runge-Kutta scheme with \( \delta t = 0.02 \) and a finite time \( T = 10 \).

The projection in Fig. 11(b) reveals an interesting aspect of the 2D SIS dynamics. The view, with \( p_s \) on the \( z \) axis, shows the optimal path fall and then rise. This change of direction occurs near \( p_i = -0.015 \), and the vertical slice in that location shows a widening of the high FTLE ridge. The next vertical slice at \( p_i = -0.027 \) shows a split in the high FTLE ridge, with an upper part that curves with the optimal path, and a lower part that curves downward away from the optimal path.

As previously mentioned, there are two additional real-valued critical points. In Figure 11(b), we include one of them as a blue circle positioned in the foreground at approximately \( i = -0.008, p_s = -0.03, p_i = -0.02 \). It appears that the FTLE values show a path
approaching this critical point, but stability analysis reveals the point is neither stable nor a saddle point. Its presence, however, has led to the harvesting of many high FTLE points that “overshoot” the turn in the optimal path, such as those shown in Fig. 9(b) forming a diagonal line that extends well beyond $p_s = -0.015$. These same footprints then show up in Fig. 11(b) and other projections contained in Appendix B. Although the FTLE provides an initial guess with seemingly multiple paths, one must remember that one of these “paths” does not connect to an extinct point. Moreover, the IAMM uses the initial guess to converge to the correct optimal path.

6 Allee Population Model

The Allee model we present is a single population model. We choose to include it because it possesses an optimal path that is particularly difficult to find numerically. Just as with the SIS examples, the Allee optimal path diverges from the deterministic path at a steady state that has become a saddle point through the Hamiltonian formulation. The optimal path for the SIS model then ends at a new steady state with non-zero momentum. The optimal path for the Allee model, however, travels through a region of non-zero momentum and then rejoins the deterministic path. From there, the optimal path follows deterministic dynamics to extinction. This results in a dynamical system with two paths that traverse the region between the same two points in opposite directions [25]. Most numerical methods that have been used over the years to compute the optimal path fail in this instance. We show, however, that our numerical method successfully captures the optimal path.

6.1 Introduction

The Allee model was formulated as a result of the research of Warder Allee, who observed species in order to determine what contributed to their well-being [26]. The crux of his model is that population density has a direct effect on the growth of a population. His research showed that there exists an interval of population density in which a species exhibits cooperative behavior, and such behavior results in the growth of the population. He observed that a certain level of crowding was beneficial, and helped with combating external attacks such as increased predation or infection. Additionally, he noted that the resources the species requires, such as a healthy environment and food, must be available in sufficient quantities to support the population and engender cooperative behavior.

In contrast, Allee showed that lower population densities often result in a species with decreasing numbers which he attributed to a lack of cooperative behavior. He also noted that extinction was more likely in species with small populations. When he considered the other extreme, an overly dense population, he observed reduced lifespans and a lack of cooperative behavior, often caused by a competition for a stagnant amount of food, water, and other resources necessary for life. Allee concluded that the benefits of cooperation in a population break down both when population density becomes too high or too low.

The dynamical model that describes Allee’s conclusions divides the population density into three intervals. The middle interval, where population growth occurs, is delineated by a minimum value called the threshold and a maximum value called the carrying capacity. These deterministic dynamics are shown in Fig. 12 as a phase line. The steady state $c_1$ represents the threshold, and the steady state $c_2$ represents the carrying capacity. The steady state $c_0$ is the extinct state where the population is zero.
Figure 12: Three steady states delineate the deterministic dynamics of the Allee model. The attracting point $c_0$ is the extinct steady state, the repelling point $c_1$ is the threshold value that separates a growing population from a decaying one, and the attracting point $c_3$ is the carrying capacity.

According to these dynamics, both $c_0$ and $c_3$ are attracting, while $c_1$ is repelling. Consideration of this scenario leads to the conclusion that population extinction is impossible whenever the population exceeds $c_1$. However, extinction of species does occur in nature. To capture these rare extinction events mathematically, one must consider a stochastic Allee model, where the noise is due to the random interactions of the individuals.

### 6.2 The Stochastic Allee Model

As before, we use the master equation and WKB formalism to find the Hamiltonian associated with the stochastic Allee problem. The stochastic Allee population model is represented by the transition processes and associated rates found in Table 3. The first two transitions are required to capture the Allee effect. The death rate of a low-density population is given by $\mu$, and the growth rate of the population when the density is large enough is given by $\lambda$. The negative growth rate for an overcrowded population is provided by $\sigma$, and $K$ is the carrying capacity of the population. In this particular example, all of the transitions are single-step transitions. Therefore, the increment $r$ only takes on the values of $\pm 1$. The scaled transition rates in Eq. 2 also are shown in the final column of Table 3.

<table>
<thead>
<tr>
<th>Event</th>
<th>Expression</th>
<th>Transition</th>
<th>Scaled Transition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Decay</td>
<td>$X \rightarrow 0$</td>
<td>$W_{-1}(X) = \mu X$</td>
<td>$K \mu x$</td>
</tr>
<tr>
<td>Growth</td>
<td>$2X \rightarrow 3X$</td>
<td>$W_1(X) = (\lambda / 2K)(X - 1)$</td>
<td>$(\lambda / 2)(Kx^2 - x)$</td>
</tr>
<tr>
<td>Reduction</td>
<td>$3X \rightarrow 2X$</td>
<td>$W_{-1}(X) = (\sigma / 6K^2)(X - 1)(X - 2)$</td>
<td>$(\sigma / 6)(Kx^3 - 3x^2 + \frac{2}{K})$</td>
</tr>
</tbody>
</table>

Using the scaled transitions, we formulate the following two equations with leading terms of the form $NW_0(r)$ as given in Eq. (2):

$$W_1(Kx) = K\left(\frac{\lambda}{2}x^2\right) - \frac{\lambda}{2}x$$  
and  
$$W_{-1}(Kx) = K(\mu x + \frac{\sigma}{6}x^3) - \frac{\sigma}{2}x^2 + \frac{\sigma}{3K}.$$

Then, the effective Hamiltonian (Eq. (4)) for the Allee model is

$$\mathcal{H}(x, p) = \frac{\lambda}{2}x^2(e^p - 1) + \left(\mu x + \frac{\sigma}{6}x^3\right)(e^{-p} - 1).$$

and the dynamics of the Allee model have been modified to include a path to extinction, as shown in Fig. 13.
Figure 13: Zero-energy curves of the Hamiltonian for the stochastic Allee model. The optimal path to extinction (shown in blue) consists of the curve, given by Eq. (26), that connects $c_2$ to $c_1$, and the $p = 0$ deterministic line from $c_1$ to the extinct state $c_0$.

6.3 Allee Results

Similar to the 1D SIS, the zero-energy solutions are the extinction line $x = 0$, the deterministic line $p = 0$, and the optimal path given by

$$p = \ln \left(\frac{6\mu + \sigma x^2}{3\lambda x}\right).$$

The set of Hamilton's equations for the stochastic Allee model are

$$\dot{x} = \frac{\lambda x^2}{2} e^p - (\mu x + \frac{\sigma x^3}{6}) e^{-p},$$

$$\dot{p} = -[\lambda x(e^p - 1) + (\mu + \frac{\sigma x^2}{2})(e^{-p} - 1)],$$

and have three steady states located at

$$x_0 = 0, \quad x_{1,2} = \frac{3\lambda \pm \sqrt{9\lambda^2 - 24\mu \sigma}}{2\sigma}.$$  

The FTLE results, shown in Fig. 14, illustrate complete agreement with the analytical solution given by Eq. (26). High FTLE ridges appear along all the zero energy curves, and just as with the 1D SIS, an extraction of the points associated with maximal FTLE values yields almost perfect agreement with the optimal path. Any attempt to improve the already excellent result using IAMM seems pointless.

Instead, we present evidence as to the efficacy of the IAMM using a scenario that is analogous to a higher dimensional system. In such systems, maximal FTLE-valued points in the vicinity of the optimal path often define a multi-dimensional region about the path rather than the true path. For this two-dimensional system, we create such a region by randomizing points about the optimal path to replicate the location of high-FTLE points. These random points serve as the initial condition for IAMM processing. In order to mute
Figure 14: Average of forward and backward FTLE field for the Allee model. The optimal path, given by Eq. (26) and denoted by the blue curve overlay, leaves the deterministic line at the carrying capacity $c_2$ and rejoins the deterministic line at the threshold $c_1$. The optimal path then essentially runs deterministically to the extinct state $c_0$. All FTLE computations were done using a fourth-order Runge-Kutta scheme with $\delta t = 0.1$, a finite time $T = 40$, and a grid resolution of 0.002 in $x$ and 0.001 in $p$. Parameter values are $\lambda = 1.6$, $\mu = 0.2$, $\sigma = 3.0$.

the influence of deterministic dynamics, we do not include points in the initial condition that are in the immediate vicinity of the critical points, given by Eq. (28). This results in a “gap” between the steady state locations and the points chosen as the endpoints of the initial condition array. It is worth noting that the part of the path closest to the critical points (where the gap occurs) tends to be the easiest piece of the optimal path to find. More importantly, our method captures the central part of the path, where other methods are known to fail.

To achieve convergence in this problem, we employed a non-uniform step size as described in Sect. 2.3. In particular we used an exponential stretching transformation given by $\tau = 2/(1 + e^{ct})$, where $t$ lies in the interval $[0,1]$. For the results shown in Fig. 15, we chose $c = 5$.

7 Summary

We have developed stochastic dynamical models with internal noise to represent the randomness of interactions, such as those found in the spread of disease or in the growth/decay of a population. It is worth noting that one must include noise to account for rare events such as extinction. Specifically, the internal noise creates pathways between previously stable states; pathways that did not exist in the deterministic model. One of these pathways, the optimal path, is of particular interest since it is the path most likely to result in a rare event, such as the extinction of a population or of an infectious disease.

However, these improvements in the model come with one disadvantage: each population
Figure 15: IAMM results for the Allee model using 1000 points randomized about the analytical optimal path as the initial condition. After three Newton iterations, the point locations, shown as a black line, have markedly converged to the analytic optimal path (in red). The initial array contained nine points within $10^{-5}$ of $H(x,p) = 0$, but after IAMM processing 60% of the points meet that tolerance. In order to lessen the effect of deterministic dynamics on IAMM convergence, artificial “endpoints”, shown as blue dots, were defined at $r = 0.3101$ and $x = 1.2115$. Consequently, two small portions of the optimal path between these points and the analytic steady states (shown as black dots) are not found. A $T_e$ of 10.2 was used to produce these results.

variable is paired with a momentum variable, doubling the complexity of the model. It is not unusual to be unable to find an analytic solution for the optimal path; even a relatively simple model in two variables is now four dimensional. This was our motivation to explore a combination of numerical methods to find the optimal path.

Our methodology began by computing finite-time Lyapunov exponents (FTLE), which have been shown to produce maximal values in the region of the optimal path. We integrated a finely-meshed domain repeatedly and computed FTLE values after each time step in order to produce an $n$-dimensional array of FTLE values. For a single population model, we produced a contour plot for viewing the ridge of points associated with maximal FTLE values that define the optimal path.

In higher dimensional models, the maximal-valued points are not easily viewed, so we chose to identify and extract them from the domain. We used readily available statistical tools to identify those grid points associated with the largest FTLE values, and narrowed the selection by elimination of deterministic regions known to have very high FTLE ridges.

We demonstrated that this statistical extraction technique was highly effective in two-dimensional models. However, results for a four-dimensional model were not as accurate. Observations of those arrays show that high FTLE points are “bunched” together in regions but do not form a distinct path from one critical point to the other. To remedy this, we used a Newton-based scheme called the Iterative Action Minimizing Method (IAMM) to adjust the high-FTLE array coordinates. The final result is a well-defined, distinct path.
that connects the two metastable states.

We demonstrated this methodology and achieved highly accurate results using the SIS epidemiology model. We presented results for a one-population version of the model, and for the compete two-population version. We discussed the sensitivity of IAMM processing to initial conditions, and illustrated ways to improve the likelihood that the method will produce accurate, convergent results along the optimal path. We described a method for viewing the four-dimensional FTLE data using three-dimensional projections. The IAMM optimal path and FTLE values were shown in multiple projections.

We also included an Allee population model in our work. The stochastic formulation for the Allee produces an optimal path that exits the deterministic curve at one saddle point, and rejoins the deterministic path at a different saddle point. This creates two distinct paths, with opposite dynamics, running between a single pair of points. Convergence methods are known to fail for these types of paths, as the dynamics of the deterministic path dominate and disturb convergence along the optimal path.

We showed that this FTLE-IAMM combination is useful to solve for similarly structured optimal paths in higher dimensional systems by using randomized points about the Allee optimal path to approximate an FTLE-produced initial condition. Here we employed a “gap” strategy where the initial condition does not directly connect to the deterministic path. This produced a highly accurate array result that defined most of the optimal path.

7.1 A Global Vision

The developing and testing of this methodology was planned as a precursor to the exploration of models where little is known about the optimal path. In particular, we plan to extend this work to coupled population models. For instance, coupling just two 1D SIS populations produces a fascinating model where one population repeatedly experiences disease extinction, only to be reinfected by its larger companion population. The optimal path may reveal whether we are truly dealing with two populations, or ultimately, do they behave as one. Another goal is the extension of this method to models with three or more compartments, such as those describing Ebola and Dengue fever.

Addressing epidemic disease outbreaks with counter-measures is of primary importance in the world. Health experts need reliable methods to assess whether an outbreak will worsen or if it is on a path towards lessening the number of new infections, potentially leading to a local extinction event. We hope that a reliable methodology for computing the optimal path to extinction for any infectious disease will aid in analyzing disease outbreaks. In areas of the world with efficient health networks, it is possible to make good estimates as to the number of infected individuals and susceptible individuals in a region. Using the optimal path solution, those estimates, when scaled appropriately, can be examined to determine if the real-world levels are on or near the optimal path. If not, control measures can be implemented to move the population levels closer to the path. Once on the path, controls may be lessened, since extinction is now a more likely event.

Linking the theoretical world to the real world is a challenge. Models must reflect the unique way each infectious disease is spread among populations. Dengue fever models consider both human and mosquito populations, since mosquitoes both contract and spread the disease through random contact with humans. Models for Ebola include “deceased infected” populations, since interactions between the living, susceptible population and deceased victims results in new infections. Stochastic real-world models for such diseases easily require the use of ten or more variables. But even in that complex scenario, an optimal path to
extinction exists. Defining these high-dimensional paths may well be marked as a milestone in mathematics and in the control of infectious diseases.
8 Bibliography

References


Appendices

A The Emergence of Dynamical Structures using FTLE Computations

We use a two event branching annihilation model to present a visualization of the way FTLE computations produce a fully formed replica of system dynamics. This model was chosen because all zero energy solution curves can be described analytically, making the FTLE results easily verified.

The branching annihilation transitions and parameters, described in Table 4, lead to the Hamiltonian equation

\[ H(x, p) = xp[\lambda(p + 1) - \frac{\mu}{2}(p + 2)x]. \]  

(29)

Table 4: Branching Annihilation Transitions

<table>
<thead>
<tr>
<th>Event</th>
<th>Transition Expression</th>
<th>Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Branching</td>
<td>1A → 2A</td>
<td>\lambda</td>
</tr>
<tr>
<td>Annihilation</td>
<td>2A → 0</td>
<td>\mu</td>
</tr>
</tbody>
</table>

Using the FTLE computational scheme detailed in Section 2.2 we produce a series of contour plots, shown in Fig. 16, which represent a snapshot of FTLE values along the way to a fully developed FTLE field.

Beginning with the Step 1 and Step 4 panes, we observe a “pool” of points with low FTLE values (in blue) emerging. Then, by Step 8, the locations of three “corners” and some faint structures linking them (in yellow) appear. Specifically, these are the metastable points representing deterministic extinction at (0, 0), the deterministic endemic point at \((\lambda/\mu, 0)\), and the non-deterministic extinction point at (0, -1). The curves are more definitive by Step 12, and by Step 16 the structure of the model is apparent. We clearly see the three zero-energy curves of the model: the deterministic solution \( p = 0 \), the trivial solution \( x = 0 \), and the optimal path \( x = (2\lambda(p + 1))/(\mu(p + 2)) \).

The emergence of the metastable points first is a direct result of the FTLE’s sensitivity to exponential stretching. As illustrated in Fig. 2, grid points in close proximity but on either side of a zero-energy curve will diverge eventually; those points that are very close to the intersection two curves will show the effect of diverging paths first. It is surprising, then, that the central portion of each zero-energy curve is the next clearly emergent structure, as shown in Step 20. Here, the result is due to velocity in and near the transitional regions far from the metastable points, as described in Section 2.3. Grid points on and near those transitional regions move further apart faster than points near the metastable points.

Finally, the bottom row of contour plots show the advantage of using enough time steps to fully reveal the structures. Some may argue that by Step 32, the model is revealed and the visual differences between it and Step 60 are slight. Keeping the ultimate goal of solving high dimensional models in mind, we see that these additional integration steps intensify
the relative differences of FTLE values by Step 60. Our goal is to harvest the highest FTLE-valued points for IAMM processing; these additional processing time steps may improve the likelihood of capturing the best possible candidates for that process.

Figure 16: Time series of FTLE contour plots showing the emergence of structures for the branching annihilation model. The label on each contour plot refers to the time step, i.e. the Step 1 pane represents FTLE values after a single integration, and the Step 60 pane is the final result after 60 integration steps. All FTLE values are an average of separate forward and backward fourth-order Runge-Kutta integration schemes. Each time step is 0.1, and the finite time for the process is $T = 6$. The grid resolution is .01 in both the $x$ and $p$ dimensions. Parameter values are $\lambda = 2.0$, $\mu = 0.5$. 
B Additional Projections of 2D SIS Model Results

These additional projections of the IAMM and FTLE results for the 2D SIS model complement the information shown in Fig. 11. Each projection adds a unique view of the FTLE data to our body of knowledge about the model. The slices in our views are chosen both for the information they contain and for their orientation as part of a clear three dimensional representation of the model.

In all figures, the optimal path obtained from the IAMM computation is represented by a black curve. The path begins at the endemic steady state, represented by a green circle, and ends at the fluctuational extinct steady state, represented by a red circle.

Some projections include the two additional real critical points. A blue circle represents the steady state with approximate location at \((s, i, p_s, p_i) = (0.95, -0.01, -0.03, -0.02)\) for our parameters. Note that the \(i\) value is negative, so the value has no meaning in the context of the 2D SIS model. From dynamics revealed by the FTLE data, this steady state appears to be an attracting one. However, stability analysis show it is neither stable nor metastable, and there is no evidence that a path leads directly to it. The second steady state, represented with a magenta circle, is located at approximately \((0.97, 0.005, -0.01, -0.02)\). Again, it is neither stable nor metastable. However, its location near where the optimal path turns toward the fluctuational extinction point leads us to believe it has influence on those dynamics.

In Fig. 17, the base, or floor slice, displays a diagonal path of high FTLE values that “overshoot” the turn in the optimal path, revealing a system dynamic in which both momentum values increase in magnitude beyond the momentum magnitudes in the optimal path. Projection (a) represents FTLE values averaged through all \(i\) slices. In (a), the high FTLE values produce a very distinct, and perhaps confusing, set of impressions. The diagonal on the \(p_s = 0\) slice (rear left surface) shows the ascent of the optimal path from the endemic to fluctuational extinction level. If nearby \(p_s\) slices were examined, they would also display a similar diagonal structure. The turn in the optimal path toward extinction is visible on the slice at \(p_i = -0.0256\), but that slice also contains evidence of an “overshooting” path.

Figure 17: 2D SIS projections with common base \(p_s\) by \(p_i\).
that appears to head toward the vicinity of the blue critical point. Projection (b) is averaged through all \( s \) slices. The base slice shown is at \( i = 0.0004 \), which offers more detailed view than the slice at \( i = 0 \), where the entire slice is composed of extremely high FTLE values. The fluctuational extinction point is in the rear corner but not visible. This projection does show the curve of the optimal path in slice \( p_i = -0.0256 \), and that slice also displays a wide-based triangle of high FTLE values. This triangle of high values is replicated through many adjacent \( p_i \) slices.

Figure 18: 2D SIS projections with common base \( s \) by \( p_s \).

The projections in Fig. 18 capture the optimal path as it leaves the endemic point at \( p_s = 0 \) in the upper foreground and then semi-spirals to the fluctuational extinct point, also at \( p_s = 0 \), in the rear of both projections. Projection (a) displays a triangle of higher FTLE values at \( p_s = -0.0256 \) and \(-0.0012\), where the highest values run down the central region of the triangle and replicate the optimal path. In projection (b), the base slice at \( s = 1.0004 \) captures the curve of the optimal path, again reinforcing the fact that high FTLE values near the optimal path continue through many layers of the four dimensional FTLE array. The \( p_s = -0.0156 \) slice shows a large area of high FTLE values in the vicinity of the sharp transition in the optimal path. Again, some paths extend beyond the turn, and the possibly attracting critical point (in blue) is visible in the lower right area of projection(b).