LINEAR RESPONSE IN DYNAMICAL SYSTEMS: OPTIMISATION AND FINITE-TIME COHERENT SETS

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The linear response of a dynamical system refers to changes to properties of the system under small external perturbations. We consider two applications of linear response theory to dynamical systems. In the first application (covering two settings) we consider the optimal perturbation that (i) maximises the linear response of the equilibrium distribution of the system, (ii) maximises the linear response of the expectation of a specified observable and (iii) maximises the linear response of the rate of convergence of the system to the equilibrium distribution. We also consider problems (i) and (ii) in the time-dependent situation where the governing dynamics is not stationary. We initially solve these problems for finite-state Markov chains. We numerically apply the theory developed in the finite-state setting to stochastically perturbed dynamical systems, where the Markov chain is replaced by a matrix representation of an approximate annealed transfer operator for the random dynamical system. In the second setting, we consider problems (ii) and (iii) for Hilbert-Schmidt integral operators with stochastic kernels. By representing a deterministic dynamical system with additive noise as an integral operator, we develop theory to compute optimal map perturbations that address problems (ii) and (iii); we also provide numerical examples in this setting.

The second application of linear response is to finite-time coherent sets. Finite-time coherent sets represent minimally mixing objects in general nonlinear dynamics and are spatially mobile features that are the most predictable in the medium term. Under a small parameter change to the dynamical system, one can ask about the rate of change of the location and shape of the coherent sets, and one can also ask about the mixing properties (how much more or less mixing) with respect to the parameter change. We answer these questions by developing linear response theory for the eigenfunctions of the dynamic Laplace operator, from which one readily obtains the linear response of the corresponding coherent sets. We construct efficient numerical methods based on a recent finite-element approach and provide numerical examples.

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Abstract

The linear response of a dynamical system refers to changes to properties of the system under small external perturbations. We consider two applications of linear response theory to dynamical systems. In the first application (covering two settings) we consider the optimal perturbation that (i) maximises the linear response of the equilibrium distribution of the system, (ii) maximises the linear response of the expectation of a specified observable and (iii) maximises the linear response of the rate of convergence of the system to the equilibrium distribution. We also consider problems (i) and (ii) in the time-dependent situation where the governing dynamics is not stationary. We initially solve these problems for finite-state Markov chains. We numerically apply the theory developed in the finite-state setting to stochastically perturbed dynamical systems, where the Markov chain is replaced by a matrix representation of an approximate annealed transfer operator for the random dynamical system. In the second setting, we consider problems (ii) and (iii) for Hilbert-Schmidt integral operators with stochastic kernels. By representing a deterministic dynamical system with additive noise as an integral operator, we develop theory to compute optimal map perturbations that address problems (ii) and (iii); we also provide numerical examples in this setting.

The second application of linear response is to finite-time coherent sets. Finite-time coherent sets represent minimally mixing objects in general nonlinear dynamics and are spatially mobile features that are the most predictable in the medium term. Under a small parameter change to the dynamical system, one can ask about the rate of change of the location and shape of the coherent sets, and one can also ask about the mixing properties (how much more or less mixing) with respect to the parameter change. We answer these questions by developing linear response

theory for the eigenfunctions of the dynamic Laplace operator, from which one readily obtains the linear response of the corresponding coherent sets. We construct efficient numerical methods based on a recent finite-element approach and provide numerical examples.

Contents

Chapter 1

Introduction

Response theory aims to describe how various properties of a dynamical system (e.g. the dynamics of the ocean or the climate) change when the dynamics governing the system is perturbed. Linear response considers the first-order change in quantities of interest (e.g. average temperature) with respect to a parameter change to the dynamics of the system. To illustrate the basic idea of linear response, we consider the following theoretically simple setting of finite-state Markov chains [65]. Suppose we have a finite state space $\{1, \ldots, n\}$ and an $n \times n$ probability transition matrix $M \in \mathbb{R}^{n \times n}$ (i.e. the matrix containing the probabilities of transitioning between individual states) describing the dynamics over the state space. Suppose there exists a unique invariant probability vector $\mathbf{f}_M \in \mathbb{R}^n$ such that $M\mathbf{f}_M = \mathbf{f}_M$. Furthermore, suppose that for a small parameter $\varepsilon \in \mathbb{R}$ and a matrix $m \in \mathbb{R}^{n \times n}$, the matrix $M + \varepsilon m$ (i.e. the "small perturbation" of M by m) also possesses a unique probability vector $\mathbf{f}_{M+\varepsilon m} \in \mathbb{R}^n$ such that $(M + \varepsilon m)\mathbf{f}_{M+\varepsilon m} = \mathbf{f}_{M+\varepsilon m}$. If for all sufficently small ε it is possible to write $\mathbf{f}_{M+\varepsilon m} = \mathbf{f}_M + \varepsilon \mathbf{u}_1 + \varepsilon^2 \mathbf{u}_2 + \ldots$, then the vector $\mathbf{u}_1$ is the linear response of the invariant vector to the perturbation m. A central part of linear response theory in dynamical systems is to prove the existence of linear response for various dynamical systems and to obtain a formula for it using only information from the unperturbed system (M and $\mathbf{f}_M$ in this example) and the perturbing force (the matrix m).

Early work in response theory, in the setting of statistical mechanics, was [59]; in this work, the perturbation of statistical quantities (e.g. the average temperature) of a system resulting from the change of the governing dynamics was studied. The rigorous mathematical study of linear response began from the work [76],

who, for uniformly hyperbolic dynamics, derived response formulae for the Sinai-Bowen-Ruelle measure (a distinguished measure preserved under the dynamics of the system). Since the work of [76], there has been much interest in the existence (or lack of) of linear response for various dynamical systems. The work of [17,45,46] extended the results in [76] by introducing modern functional analytic methods to address the existence of linear response. Linear response results for one-dimensional dynamical systems [8,9,12,13,58] and (partially) hyperbolic systems [11,22,77,83] have been obtained; there are also results for the existence of linear response for random dynamical systems [7,16,40,49]. In terms of applications, there has been a development of rigorous results for the numerical computation of linear response [6,73]. Applications of linear response theory to Earth's climate [1,18,66,74] have seen success and have motivated new questions, like the numerical validation for applications of linear response [44,82]; see the survey [43] for a recent review of the applicability of response theory to climate science.

In this thesis we consider two problems grounded in the ideas of linear response; the first is in line with trends exploring different questions relating to linear response and the second is to use the idea of linear response to investigate mixing properties of smooth dynamical systems. In the first problem we consider finding optimal perturbations that maximise response. Aside from theoretical curiosity, knowledge of these optimal perturbations can provide valuable information: in the context of applicability to climate models, the optimal perturbations could signify perturbation "directions" that should be avoided.

The systems we consider for the first problem, in Chapters 2 and 3, are stochastically perturbed dynamical systems. An example of such a system is one whose trajectories are given by

$$x_{n+1} = T(x_n) + \omega_n,$$

where $T : X \to X$, $X \subseteq \mathbb{R}^n$, is a deterministic system and ω_n is an i.i.d. process on X distributed according to some probability density ρ. To study the behaviour of the stochastic dynamics, one can form the annealed transfer operator

$$Lg(x) = \int_X \rho(x - T(y))g(y)\ d\ell(y) = \int_X k(x,y)g(y)\ d\ell(y), \tag{1.0.1}$$

where $k(x,y) = \rho(x - T(y))$ (see e.g. [62]). Under certain conditions, the operator L acting on $L^2(X)$ has a unique invariant density f. With this representation, we consider the following optimization problems:

OP1 We consider the problem of finding the infinitesimal perturbation δk to the kernel k so as to maximise the L^2 norm of the linear response δf to this perturbation. A motivation for this is to obtain an upper bound on the expectations of all L^2 normalised observables. This follows by noting that $|\mathbb{E}_{\delta f}(c)| := \left| \int_X c(x)\delta f(x)dx \right| \leq \|c\|_{L^2}\|\delta f\|_{L^2}$ and therefore $\sup_{\|c\|_{L^2}=1} |\mathbb{E}_{\delta f}(c)| \leq \|\delta f\|_{L^2}$.

OP2 We consider the problem of finding the perturbation δk so as to maximise the expectation $\mathbb{E}_{\delta f}(c)$ for a specific observable $c \in L^2(X)$. That is, for a specific observation function, we want to know the perturbation direction that increases the expectation the most.

OP3 We consider the problem of finding the perturbation δk that maximises the rate of convergence to the invariant measure of the dynamical system.

In Chapter 2 we address **OP1**–**OP3** in the setting of finite-state Markov chains. **OP1** requires the maximisation of an ℓ^2-norm and is therefore a non-convex problem. We reformulate the problem to a setting where the solution is an eigenvector to an eigenvalue problem; when reformulating to the eigenvalue problem, we provide explicit construction of the finite-dimensional feasible space, allowing us to easily obtain the optimal solution from the eigenvector. We also provide sufficient conditions for the uniqueness of the optimal solution. For **OP2** we use the method of Lagrange multipliers to solve the optimisation problem and obtain a closed form solution. We answer **OP3** by first computing the derivative of the second largest eigenvalue of the transition probability matrix with respect to the perturbing parameter; we note that from here we begin to use the term linear response for the first-order change of the spectral data and not just for the first-order change of the invariant vector. Similarly to **OP2**, we use Lagrange multipliers to obtain an explicit solution to the optimal perturbation for **OP3**. We then consider **OP1**–**OP2** in the non-homogeneous case where the stochastic dynamics is now an application of a finite sequence of stochastic transition matrices. We apply the methods used to solve **OP1**–**OP2** in the homogeneous case (i.e. one application of a stochastic

transition matrix) to this setting and obtain similar results as in the corresponding homogeneous sections. We conclude the chapter with applications to stochastically perturbed one-dimensional maps. Using the Ulam discretisation method, we obtain matrix representations for the annealed transfer operator (1.0.1) allowing us to apply the above methods to compute the optimal kernel perturbations.

Questions involving optimisation of linear response have been considered in [42] and [56]. In [42] the authors, in the setting of deterministic perturbations of expanding maps, consider the problem of finding the perturbations achieving a prescribed linear response. In their setting they show that there are many allowable perturbations achieving the prescribed response and then address the question of finding the minimal norm solution to this problem. In contrast to the optimisation problem in [42], we consider *stochastic* perturbations that *maximises* the ℓ^2-norm of the linear response. In [56], the problem posed in [42] is considered in the setting of smooth dynamics; [56] considers perturbations coming from smooth conjugacy that achieves a prescribed linear response and discusses how the problem of finding the perturbation that achieves a minimum norm of the linear response can be solved. In this article, the optimisation problem is not attempted, only an approach to the solution is presented. In contrast to [56], we pose and solve our norm optimisation problem **OP1**. The idea of identifying the unique perturbations that address the optimisation problems **OP1** and **OP2** is to our knowledge the original contribution of Chapter 2 and has no precedents. There are several studies addressing the mixing question **OP3** and we will discuss these shortly.

In Chapter 3 we extend the finite-dimensional work in Chapter 2 to address **OP2** and **OP3** in the setting of Hilbert-Schmidt integral operators. To show the linear response for the invariant density we use the differentiability of the transfer operator with respect to the perturbing parameter. For the linear response of the eigenvalues, we use standard results and formulae for perturbation of isolated eigenvalues (see e.g. [54] and [50]). By considering specific perturbations to the kernel k, we obtain explicit formulae for the linear response of the invariant vector and the second eigenvalue with respect to kernel perturbations. As in Chapter 2, we apply the method of Lagrange multipliers to a obtain an explicit formula for the

optimal kernel perturbation for **OP2**. A study in the literature that incorporates linear response of the expectation within an optimisation problem is [81]. In the setting of Langevin dynamics, the authors use the linear response of the expectation of a specific observable in the context of a gradient descent procedure to solve an optimal control problem. In contrast to this work, we consider the maximisation of the linear response of the expectation for a specified observable.

We continue in Chapter 3 by solving **OP3** in the setting of Hilbert-Schmidt integral operators. As in Chapter 2, we also use the method of Lagrange multipliers and obtain an explicit solution for the optimal perturbation that enhances mixing by analysing the perturbation of the second largest eigenvalue of the Hilbert-Schmidt integral operator. In the literature, there are a few related perturbative approaches addressing **OP3**. In [29] the authors consider driving a noninvariant density to a target density in one time step. More precisely, they find a perturbation (which is the kernel of a Hilbert-Schmidt integral operator) so that after an application of the perturbation and the dynamics, an initial density is as close as possible to the target density in the L^2-norm. The approach taken in this thesis to enhance mixing is similar to theirs in that we also consider kernel perturbations. The main difference to their approach is that we use the linear response of the eigenvalue of a Hilbert-Schmidt integral operator (i.e. a spectral method) to pose the optimisation problem **OP3**, while they enhance mixing by determining the optimal perturbations at each step of the dynamics that push the noninvariant density to the invariant density (i.e. a non-spectral method).

Some ideas and methods from [29] were used in [47], where the authors consider the problem of perturbing the flow to transport an initial measure to a final measure in finite time. To solve this problem, they minimise an objective function involving the norms of differences between measures and the (fixed) number of steps required to push the initial measure to the final one. To address the problem of optimal enhancement of mixing, they chose the final measure to be "uniform over a compact phase space". In contrast to [47], we enhance mixing via spectral-based methods and we do not require the specification of an initial and final measure.

For the remainder of Chapter 3, we apply the theory developed for Hilbert-Schmidt integral operators to deterministic systems with additive noise. For these systems, we consider the problem of perturbing the deterministic part to maximise the linear response of the expectation of an observable and to enhance mixing. We again obtain explicit formulae for the optimal perturbations. Prior to our work in Chapter 2, the idea of enhancing mixing by spectral methods was considered in [38]. In this work, the authors perturb the drift/velocity part of periodically driven flows to enhance mixing. The spectral approach in this thesis is similar to theirs in that they set up the optimisation problem to enhance mixing by considering the perturbation of an eigenvalue of an operator (in their setting this was an infinitesimal generator on the time-expanded phase space). In contrast to their work, we solve our optimisation problem using the method of Lagrange multipliers which allows us to obtain an explicit formula for the optimal perturbation.

The method/approach we use to enhance mixing (originally considered in Chapter 2 but motivated by [38]) is also considered in [34]. In this work, the authors consider perturbations to the velocity field of the Fokker-Planck equation to enhance mixing (via Lagrange multipliers). Similar to the spectral approach in [38], they form an optimisation problem from a differentiablity result (see [57]) of the eigendata of the Fokker-Planck equation with respect to drift/velocity perturbations. The primary difference of the results in Chapter 3 to the work of [34] is that we obtain optimal map perturbations to enhance mixing for deterministic systems with additive noise while they consider drift/velocity perturbations of the Fokker-Planck equation. We conclude Chapter 3 with numerical experiments which consider optimal kernel and map perturbations to the Pomeau-Manneville map and a weakly mixing interval exchange map.

In Chapter 4 we turn our attention away from optimisation problems and apply linear response ideas to finite-time coherent sets. Finite-time coherent sets are subsets of the phase space that do not mix rapidly in a finite period of time and therefore are important in the analysis of fluid transport. The concept of finite-time coherent sets was initially developed in [39] and used to isolate the Antarctic polar vortex as the slowest mixing object in the stratosphere over the south pole. This

concept was further developed theoretically in [27]. Aside from applications to the polar vortex, coherent sets have been used to track mesoscale eddies in the South Atlantic [30,31,33] and in the North Atlantic [37].

We consider in Chapter 4 a family of smooth volume-perserving maps $T_\varepsilon : \Omega \to T_\varepsilon(\Omega)$, where Ω is a submanifold of X and ε is the perturbing parameter. Following the setting of [28], we identify finite-time coherent sets as those sets that continue to have a small boundary size relative to volume as they are evolved by the dynamics. Coherent sets are obtained from the dynamic Laplacian operator Δ_ε^D. The dynamic Laplacian is an elliptic operator and one can solve the weak form of the dynamic Laplacian eigenproblem:

$$\int_\Omega \Delta_\varepsilon^D u_\varepsilon \cdot \varphi \, d\ell = \int_\Omega \lambda_\varepsilon u_\varepsilon \cdot \varphi \, d\ell,$$

for all φ in an appropriate function space. From the eigenfunctions u_ε the coherent sets are computed [28].

When the map $\varepsilon \mapsto T_\varepsilon$ is sufficiently differentiable, we prove in Chapter 4 that the maps $\varepsilon \mapsto u_\varepsilon$ and $\varepsilon \mapsto \lambda_\varepsilon$ are also differentiable. We then derive a formula for the linear response. The derivative of eigenfunctions of the dynamic Laplacian immediately yields derivatives of the corresponding finite-time coherent sets with respect to ε. We also obtain a formula for the derivative of the eigenvalues with respect to the parameter, which quantify the instantaneous rate of change of mixing as the parameter is varied. Building on the FEM-based approaches in [33] we develop numerical schemes for numerically computing the linear response and illustrate these with experiments on the standard map and the rotating double gyre. In these experiments we observe that even for large extrapolation values, the first-order approximations of the perturbed eigenvectors, computed using linear response, produce coherent sets that are very close to the true coherent sets (obtained from finite difference of the perturbed dynamics).

In the literature, linear response of eigenvalues of transfer operators and generators of periodically and aperiodically driven flows, relating to finite-time coherent sets, have been studied in [34, 38]. These works also provide methods to optimise

the system to extremise the linear response and optimally enhance or destroy coherent sets. In these articles, they consider the Fokker-Planck equation and analyse finite-time coherent sets using the ideas in [27]. In [27], coherent sets are obtained from the eigendata of a linear operator which is constructed from the composition of the transfer operator with a "diffusion operator" that encodes small scale diffusive dynamics. In [28], the dynamic Laplacian is shown to be a zero-diffusion limit operator capturing the small diffusion effects of the operator theoretic method in [27]. In contrast to the coherent set analysis in [34, 38], we analyse and develop the perturbation theory of finite-time coherent sets that are identified by the dynamic Laplacian.

I note that the content of the thesis has been or will be published in three journal articles. Chapter 2 has been published in [2]; my contributions to this paper include the setup and derivation of the optimal solution to the norm optimisation problem (Section 2.2 of the thesis), the proof of necessary and sufficient conditions in the Lagrange multiplier methods (Sections 2.3 and 2.4), the derivation of the optimal linear response for the non-homogeneous setting (Section 2.5) and the algorithms for the optimal solutions (Appendix A.1). Chapter 3 is a collaboration with Gary Froyland and Stefano Galatolo; my contributions to it include the derivation of the explicit formulae for the optimal *kernel* perturbations and the corresponding approximation results (Section 3.3, modulo the existence and uniqueness results for the general optimisation problem). Also, the derivation of the explicit formulae for the optimal *map* perturbations and the corresponding approximation results (Section 3.5). Finally, my contributions to Chapter 4, which is a collaboration with the preliminary preprint [3], include the linear response existence proof (Section 4.3), the derivation of the explicit linear response formulae and the extension of the results to the Neumann boundary conditions (Section 4.4). Also, the derivation of the matrix in Proposition 4.5.1.

Chapter 2

Optimal Linear Responses for Markov Chains and Stochastically Perturbed Dynamical Systems

In this chapter we pose and solve problems relating to optimal linear responses for finite-state Markov chains. In Section 2.1 we set up the fundamentals of linear response in finite dimensions. Section 2.2 tackles the problem of finding the perturbation that maximises the linear response of the equilibrium measure in an ℓ^2 sense. We first treat the easier case where the transition matrix for the Markov chain is positive, before moving to the situation of a general irreducible aperiodic Markov chain. In both cases we provide sufficient conditions for a unique optimum, and present explicit algorithms, including `MATLAB` code to carry out the necessary computations. We illustrate these algorithms with a simple analytic example. In Section 2.3 we solve the problem of maximising the linear response of the expectation with respect to a particular observable, while in Section 2.4 we demonstrate how to find the perturbation that maximises the linear response of the rate of convergence to equilibrium. In both of these sections, we provide sufficient conditions for a unique optimum, present explicit algorithms, code, and treat an analytic example. Section 2.5 considers the linear response problems for a finite sequence of (in general different) stochastic transition matrices. Section 2.6 applies the theory of Sections 2.2–2.4 to stochastically perturbed one-dimensional chaotic maps. We develop a numerical scheme to produce finite-rank approximations of the transfer (Perron-Frobenius) operators corresponding to the stochastically perturbed maps. These finite-rank approximations have a stochastic matrix representation, allowing the preceding theory to be applied.

2.1 Notation and Setting

We follow the notation and initial setup of [65]. Consider a column stochastic transition matrix $M = (M_{ij}) \in \mathbb{R}^{n\times n}$ of a mixing Markov chain on a finite state space $\{1, \dots, n\}$. More precisely, we assume that M satisfies:

1. $0 \leq M_{ij} \leq 1$ for every $i, j \in \{1, \dots, n\}$;
2. $\sum_{i=1}^{n} M_{ij} = 1$ for every $j \in \{1, \dots, n\}$;
3. there exists $N \in \mathbb{N}$ such that $M_{ij}^N > 0$ for every $i, j \in \{1, \dots, n\}$.

Let $\mathbf{f}_M = (f_1, \dots, f_n)^\top \in \mathbb{R}^n$ denote the invariant probability vector of M, i.e. the probability vector such that $M\mathbf{f}_M = \mathbf{f}_M$. We note that the existence and the uniqueness of $\mathbf{f}_M$ follow from the above assumptions on M. Moreover, let us consider perturbations of M of the form $M + \varepsilon m$, where $\varepsilon \in \mathbb{R}$ and $m \in \mathbb{R}^{n\times n}$. In order to ensure that $M + \varepsilon m$ is also a column stochastic matrix, we need to impose some conditions on m and ε. For a fixed $m = (m_{ij}) \in \mathbb{R}^{n\times n}$, we require that

$$\sum_{i=1}^{n} m_{ij} = 0 \quad \text{for every } j \in \{1, \dots, n\}. \tag{2.1.1}$$

Furthermore, we assume that $\varepsilon \in [\varepsilon_-, \varepsilon_+]$ and $\varepsilon_- < \varepsilon_+$, where

$$\varepsilon_+ := \max_{\varepsilon}\{\varepsilon \in \mathbb{R} : M_{ij} + \varepsilon m_{ij} \geq 0 \text{ for every } i, j \in \{1, \dots, n\}\}$$

and

$$\varepsilon_- := \min_{\varepsilon}\{\varepsilon \in \mathbb{R} : M_{ij} + \varepsilon m_{ij} \geq 0 \text{ for every } i, j \in \{1, \dots, n\}\}.$$

Let us denote the invariant probability vector of the perturbed transition matrix $M + \varepsilon m$ by $\mathbf{f}_{M+\varepsilon m}$. We remark that by decreasing $[\varepsilon_-, \varepsilon_+]$ we can ensure that the invariant probability vector $\mathbf{f}_{M+\varepsilon m}$ remains unique. If we write

$$\mathbf{f}_{M+\varepsilon m} = \mathbf{f}_M + \sum_{j=1}^{\infty} \varepsilon^j \mathbf{u}_j, \tag{2.1.2}$$

where $\varepsilon \in \mathbb{R}$ is close to 0, then $\mathbf{u}_1$ is defined as the *linear response* of the invariant probability vector $\mathbf{f}_M$ to the perturbation εm.

By summing the entries of both sides of (2.1.2) and comparing ε orders, we must have that the column sum of the vector $\mathbf{u}_1$ is zero. On the other hand, since $\mathbf{f}_{M+\varepsilon m}$ is an invariant probability vector of $M+\varepsilon m$, we have that

$$(M+\varepsilon m)\left(\mathbf{f}_M+\sum_{j=1}^{\infty}\varepsilon^j\mathbf{u}_j\right)=\mathbf{f}_M+\sum_{j=1}^{\infty}\varepsilon^j\mathbf{u}_j. \tag{2.1.3}$$

By expanding the left-hand side of (2.1.3), we obtain

$$(M+\varepsilon m)\left(\mathbf{f}_M+\sum_{j=1}^{\infty}\varepsilon^j\mathbf{u}_j\right)=\mathbf{f}_M+\varepsilon(M\mathbf{u}_1+m\mathbf{f}_M)+O(\varepsilon^2).$$

Hence, it follows from (2.1.2) and (2.1.3) that the linear response $\mathbf{u}_1$ satisfies

$$(\mathrm{Id}-M)\mathbf{u}_1=m\mathbf{f}_M \tag{2.1.4}$$

and

$$\mathbf{1}^\top\mathbf{u}_1=0, \tag{2.1.5}$$

where $\mathbf{1}^\top=(1,\dots,1)\in\mathbb{R}^n$. By Theorem 2 [55], the linear system (2.1.4)–(2.1.5) has a unique solution given by

$$\mathbf{u}_1=Qm\mathbf{f}_M, \tag{2.1.6}$$

where

$$Q=\left(\mathrm{Id}-M+\mathbf{f}_M\mathbf{1}^\top\right)^{-1} \tag{2.1.7}$$

is the *fundamental matrix* of M.

We note that (2.1.6) is a standard linear response formula, holding in more general settings, such as where M is replaced by a transfer operator with a spectral gap (see [10] and [45]). In the rest of the chapter, we will denote $\mathbf{f}_M$ simply by $\mathbf{f}$.

2.2 Maximising the Euclidean Norm of the Linear Response of the Invariant Measure

Our aim in this section is to find the perturbation m that will maximise the Euclidean norm of the linear response. We will start by considering the case when M has all positive entries and later we will deal with the general case when $M \in \mathbb{R}^{n\times n}$ is the transition matrix of an arbitrary mixing Markov chain.

2.2.1 The Kronecker Product

In this subsection, we will briefly introduce the Kronecker product and some of its basic properties. These results will be used to convert some of our optimisation problems into simpler, smaller, and more numerically stable forms.

Definition 2.2.1. *Let $A = (\mathbf{a}_1|\dots|\mathbf{a}_n) = (a_{ij})$ be an $m \times n$ matrix and B a $p \times q$ matrix. The $mp \times nq$ matrix given by*

$$\begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{pmatrix}$$

is called the Kronecker product of A and B and is denoted by $A \otimes B$. Furthermore, the vectorization of A is given by the vector

$$\widehat{A} := \begin{pmatrix} \mathbf{a}_1 \\ \vdots \\ \mathbf{a}_n \end{pmatrix} \in \mathbb{R}^{mn}.$$

The following result collects some basic properties of the Kronecker product.

Proposition 2.2.2 ([63])**.** *Let A, B, C, D be $m \times n$, $p \times q$, $n \times n$ and $q \times q$ matrices respectively, and let $\alpha \in \mathbb{R}$. Then, the following identities hold:*

(i) $(A \otimes B)(C \otimes D) = AC \otimes BD$;

(ii) $\alpha A = \alpha \otimes A = A \otimes \alpha$;

(iii) $(A \otimes B)^\top = A^\top \otimes B^\top$, *where $A^\top$ denotes the transpose of A;*

(iv) $\mathrm{Rank}(A \otimes B) = (\mathrm{Rank}(A)) \cdot (\mathrm{Rank}(B))$;

(v) *let* $\lambda_1, \ldots, \lambda_n$ *be the eigenvalues of* C *and* $\mu_1, \ldots, \mu_q$ *be the eigenvalues of* D*. Then, the* nq *eigenvalues of* $C \otimes D$ *are given by* $\lambda_i \mu_j$*, for* $i = 1, \ldots, n$ *and* $j = 1, \ldots, q$*. Moreover, if* $\boldsymbol{x}_1 \ldots, \boldsymbol{x}_n$ *are linearly independent right eigenvectors of* C *corresponding to* $\lambda_1, \ldots, \lambda_n$ *and* $\boldsymbol{y}_1 \ldots, \boldsymbol{y}_q$ *are linearly independent right eigenvectors of* D *corresponding to* $\mu_1, \ldots, \mu_q$*, then* $\boldsymbol{x}_i \otimes \boldsymbol{y}_j$ *are linearly independent right eigenvectors of* $C \otimes D$ *corresponding to* $\lambda_i \mu_j$*;*

(vi) *for any* $n \times p$ *matrix* E*, we have* $\widehat{AEB} = (B^\top \otimes A)\widehat{E}$*.*

2.2.2 An Alternative Formula for the Linear Response of the Invariant Measure

As a first application of the Kronecker product, we give an alternative formula for the linear response (2.1.6). Using Proposition 2.2.2(vi) and noting that $Qm\mathbf{f}$ is an $n \times 1$ vector, we can write

$$Qm\mathbf{f} = \widehat{Qm\mathbf{f}} = \left(\mathbf{f}^\top \otimes Q\right) \widehat{m} = W\widehat{m}, \tag{2.2.1}$$

where $W = \mathbf{f}^\top \otimes Q$. The dimension of W is $n \times n^2$. We now have two equivalent formulas for the linear response: (2.1.6) in terms of the matrix m and (2.2.1) in terms of the vectorization $\widehat{m}$. In Sections 2.2.3 and 2.2.4, the formula (2.2.1) will be predominately used.

2.2.3 Positive Transition Matrix M

We first assume that the transition matrix is positive, i.e. $M_{ij} > 0$ for every $i, j \in \{1, \ldots, n\}$. In some situations, positivity is a strong assumption; in Section 2.2.4 we handle general (aperiodic and irreducible) stochastic M. We will find the perturbation m that maximises the Euclidean norm of the linear response. More precisely, we consider the following optimisation problem:

$$\max_{m \in \mathbb{R}^{n \times n}} \quad \|Qm\mathbf{f}\|_2^2 \tag{2.2.2}$$

$$\text{subject to} \quad m^\top \mathbf{1} = \mathbf{0} \tag{2.2.3}$$

$$\|m\|_F^2 - 1 = 0, \tag{2.2.4}$$

where $\|\cdot\|_2$ is the Euclidean norm and $\|\cdot\|_F$ is the Frobenius norm defined by $\|A\|_F^2 = \sum_i \sum_j |a_{ij}|^2$, for $A = (a_{ij})$. We note that the constraint (2.2.3) corresponds to the condition (2.1.1), while (2.2.4) is imposed to ensure the existence (finiteness) of the solution. Furthermore, we observe that a solution to the above optimisation problem exists since we are maximising a continuous function on a compact subset of $\mathbb{R}^{n\times n}$.

Reformulating Problem (2.2.2)–(2.2.4) in Vectorized Form

We begin by reformulating (2.2.2)–(2.2.4) in order to obtain an equivalent optimisation problem over a space of vectors as opposed to a space of matrices. Using (2.2.1), we can write the objective function in (2.2.2) as $\|W\widehat{m}\|_2^2$. Similarly, we can rewrite the constraint (2.2.3) in terms of $\widehat{m}$. More precisely, we have the following auxiliary result. Let Id_n denote an identity matrix of dimension n.

Lemma 2.2.3. *The constraint (2.2.3) can be written in the form $A\widehat{m} = \mathbf{0}$, where A is an $n \times n^2$ matrix given by*

$$A = Id_n \otimes \mathbf{1}^\top. \tag{2.2.5}$$

Proof. Since $\mathbf{1}^\top m$ is a $1 \times n$ vector, we have that $\widehat{\mathbf{1}^\top m} = m^\top \mathbf{1}$. Furthermore, using Proposition 2.2.2(vi), we have that $m^\top \mathbf{1} = \widehat{\mathbf{1}^\top m} = \widehat{\mathbf{1}^\top m \mathrm{Id}_n} = \left(\mathrm{Id}_n \otimes \mathbf{1}^\top\right)\widehat{m} = A\widehat{m}$. □

We also observe that $\|m\|_F^2 = \sum_i \sum_j |m_{ij}|^2 = \|\widehat{m}\|_2^2$. Consequently, we can rewrite constraint (2.2.4) in terms of the Euclidean norm of the vector $\widehat{m}$. Let A be as in (2.2.5). Our optimisation problem (2.2.2)–(2.2.4) is therefore equivalent to the following:

$$\max_{\widehat{m}\in\mathbb{R}^{n^2}} \quad \|W\widehat{m}\|_2^2 \tag{2.2.6}$$

$$\text{subject to} \quad A\widehat{m} = \mathbf{0} \tag{2.2.7}$$

$$\|\widehat{m}\|_2^2 - 1 = 0. \tag{2.2.8}$$

Reformulating Problem (2.2.6)–(2.2.8) to Remove Constraint (2.2.7)

Finally, we reformulate (2.2.6)–(2.2.8) to solve it as an eigenvalue problem. Consider the subspace V of $\mathbb{R}^{n^2}$ given by

$$V = \left\{ \mathbf{x} \in \mathbb{R}^{n^2} : A\mathbf{x} = \mathbf{0} \right\}. \tag{2.2.9}$$

We can write V as $V = \text{span}\{\mathbf{v}_1, \ldots, \mathbf{v}_\ell\}$, where $\mathbf{v}_k \in \mathbb{R}^{n^2}$, $k \in \{1, \ldots, \ell\}$ form a basis of V. Note that $\ell = n^2 - n$. Indeed, it follows from Proposition 2.2.2(iv) and (2.2.5) that $\text{Rank}(A) = \text{Rank}(\text{Id}_n)\,\text{Rank}(\mathbf{1}^\top) = n$; thus, by and thus by the rank-nullity theorem, we have that $\ell = n^2 - n$.

Taking $\widehat{m} \in V$ and writing

$$E = (\mathbf{v}_1 | \ldots | \mathbf{v}_\ell), \tag{2.2.10}$$

we conclude that there exists a unique $\boldsymbol{\alpha} \in \mathbb{R}^\ell$ such that $\widehat{m} = E\boldsymbol{\alpha}$. Hence, $\boldsymbol{\alpha} = E^+\widehat{m}$, where E^+ denotes the left inverse of E given by $E^+ := (E^\top E)^{-1}E^\top$. Note that since E has full rank, we have that $E^\top E$ is non-singular (see p.43, [14]) and therefore E^+ is well-defined. Using the above identities, we obtain

$$W\widehat{m} = WE\boldsymbol{\alpha} = WEE^+\widehat{m}. \tag{2.2.11}$$

Let

$$U = WEE^+. \tag{2.2.12}$$

Since the only assumption on $\widehat{m}$ was that $\widehat{m} \in V$, the problem (2.2.6)–(2.2.8) is equivalent to the following:

$$\max_{\widehat{m} \in \mathbb{R}^{n^2}} \quad \|U\widehat{m}\|_2^2 \tag{2.2.13}$$

$$\text{subject to} \quad \|\widehat{m}\|_2^2 - 1 = 0. \tag{2.2.14}$$

The solution $\widehat{m}^*$ to the problem (2.2.13)–(2.2.14) is the ℓ^2-normalised eigenvector corresponding to the largest eigenvalue of the $\ell \times \ell$ matrix $U^\top U$ (see p.281, [69]).

In the particular case when $\{\mathbf{v}_1, \ldots, \mathbf{v}_\ell\}$ is an orthonormal basis of V, we have that $E^\top E = \mathrm{Id}_\ell$ and therefore $\|\widehat{m}\|_2^2 = \boldsymbol{\alpha}^\top E^\top E \boldsymbol{\alpha} = \boldsymbol{\alpha}^\top \boldsymbol{\alpha} = \|\boldsymbol{\alpha}\|_2^2$. Using (2.2.11), we conclude that the optimisation problem (2.2.13)–(2.2.14) further simplifies to

$$\max_{\boldsymbol{\alpha} \in \mathbb{R}^\ell} \quad \|\widetilde{U}\boldsymbol{\alpha}\|_2^2 \tag{2.2.15}$$

$$\text{subject to} \quad \|\boldsymbol{\alpha}\|_2^2 - 1 = 0, \tag{2.2.16}$$

where

$$\widetilde{U} = WE. \tag{2.2.17}$$

The solution $\boldsymbol{\alpha}^*$ to (2.2.15)–(2.2.16) is the eigenvector corresponding to the largest eigenvalue of $\widetilde{U}^\top \widetilde{U}$. Finally, we note that the relationship between the solutions of (2.2.13)–(2.2.14) and (2.2.15)–(2.2.16) is given by

$$\widehat{m}^* = E\boldsymbol{\alpha}^*. \tag{2.2.18}$$

An Optimal Solution and Optimal Objective Value

For positive M, we can now derive an explicit expression for E and thus obtain an explicit form for the solution of the optimisation problem (2.2.2)–(2.2.4). We will do this by considering the reformulation (2.2.15)–(2.2.16) of our original problem (2.2.2)–(2.2.4). Let V_0 denote the null space of $\mathbf{1}^\top$. An orthonormal basis for V_0 is the set $\{\mathbf{x}_1, \ldots, \mathbf{x}_{n-1}\}$, where

$$\mathbf{x}_i = \frac{\widetilde{\mathbf{x}}_i}{\|\widetilde{\mathbf{x}}_i\|_2}, \quad \text{for } i \in \{1, \ldots, n-1\} \tag{2.2.19}$$

and

$$\widetilde{\mathbf{x}}_1 = \begin{pmatrix} 1 \\ -1 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix}, \ \widetilde{\mathbf{x}}_2 = \begin{pmatrix} 1 \\ 1 \\ -2 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \ldots, \widetilde{\mathbf{x}}_{n-1} = \begin{pmatrix} 1 \\ \vdots \\ \vdots \\ \vdots \\ 1 \\ -(n-1) \end{pmatrix}. \tag{2.2.20}$$

Let B be an $n \times (n-1)$ matrix given by

$$B = (\mathbf{x}_1 | \dots | \mathbf{x}_{n-1}). \tag{2.2.21}$$

Therefore, we can take

$$E = \mathrm{Id}_n \otimes B \tag{2.2.22}$$

in (2.2.10). Using Proposition 2.2.2(i), (2.2.1) and (2.2.17), we have $\widetilde{U} = WE = \mathbf{f}^\top \otimes QB$. Hence, it follows from Proposition 2.2.2(i) and (iii) that $\widetilde{U}^\top \widetilde{U} = \mathbf{f}\mathbf{f}^\top \otimes B^\top Q^\top QB$. By Proposition 2.2.2(v), the eigenvector corresponding to the largest eigenvalue λ of $\widetilde{U}^\top \widetilde{U}$ is given by $\boldsymbol{\alpha}^* = \mathbf{f} \otimes \mathbf{y}$, where $\mathbf{y}$ is the eigenvector corresponding to the largest eigenvalue (which we denote by κ) of an $(n-1) \times (n-1)$ matrix $B^\top Q^\top QB$. From Proposition 2.2.2(v), $\lambda = \kappa \|\mathbf{f}\|_2^2$ is the eigenvalue corresponding to $\boldsymbol{\alpha}^*$. Hence, it follows from (2.2.18) and (2.2.22) that *an optimal perturbation is*

$$\widehat{m}^* = E\boldsymbol{\alpha}^* = (\mathrm{Id}_n \otimes B)(\mathbf{f} \otimes \mathbf{y}) = \mathbf{f} \otimes B\mathbf{y}. \tag{2.2.23}$$

Note that this expression for $\widehat{m}^*$ is an improvement over computing an eigenvector of the $(n^2 - n) \times (n^2 - n)$ matrix $\widetilde{U}^\top \widetilde{U}$ because we only need to find $\mathbf{y}$, which is an eigenvector of an $(n-1) \times (n-1)$ matrix.

Taking into account (2.2.14), we must have $\|\widehat{m}^*\|_2^2 = 1$ and thus

$$1 = \widehat{m}^{*\top} \widehat{m}^* = (\mathbf{f}^\top \mathbf{f})(\mathbf{y}^\top B^\top B\mathbf{y}) = \|\mathbf{f}\|_2^2 \cdot \|\mathbf{y}\|_2^2,$$

as $B^\top B = \mathrm{Id}_{n-1}$ (columns of B form an orthonormal basis of V_0). Hence, $\mathbf{y}$ must satisfy

$$\|\mathbf{y}\|_2^2 = \frac{1}{\|\mathbf{f}\|_2^2}. \tag{2.2.24}$$

Finally, using Proposition 2.2.2(ii), (2.2.1) and (2.2.23), we obtain

$$W\widehat{m}^* = (\mathbf{f}^\top \otimes Q)(\mathbf{f} \otimes B\mathbf{y}) = \mathbf{f}^\top \mathbf{f} QB\mathbf{y} = \|\mathbf{f}\|_2^2 QB\mathbf{y},$$

and therefore *the optimal objective value is*

$$\|W\widehat{m}^*\|_2^2 = \|\mathbf{f}\|_2^4 \mathbf{y}^\top B^\top Q^\top Q B\mathbf{y} = \|\mathbf{f}\|_2^4 \mathbf{y}^\top (\kappa \mathbf{y}) = \kappa \|\mathbf{f}\|_2^4 \cdot \|\mathbf{y}\|_2^2 = \kappa \|\mathbf{f}\|_2^2 = \lambda. \quad (2.2.25)$$

We impose the normalisation condition (2.2.24) for $\mathbf{y}$ throughout the chapter when dealing with positive M. Note that replacing $\widehat{m}^*$ with $-\widehat{m}^*$ in (2.2.25) yields the same Euclidean norm of the response.

The issue of dependency of optimal solutions $\widehat{m}^*$ and optimal objective values λ on the selected set of orthonormal columns for B will be treated in full generality in Proposition 2.2.7. There we show the optimal objective value is independent of the orthonormal basis vectors forming the columns of B (or alternatively the columns of E), and provide a sufficient condition for an optimal m^* to be independent of this choice (up to sign).

2.2.4 General Transition Matrix M for Mixing Markov Chains

In the general setting, when M is a transition matrix of an arbitrary mixing Markov chain, we consider the following optimisation problem:

$$\begin{aligned} \max_{m \in \mathbb{R}^{n\times n}} \quad & \|Qm\mathbf{f}\|_2^2 && (2.2.26)\\ \text{subject to} \quad & m^\top \mathbf{1} = \mathbf{0} && (2.2.27)\\ & \|m\|_F^2 - 1 = 0 && (2.2.28)\\ & m_{ij} = 0 \text{ if } M_{ij} = 0 \text{ or } 1. && (2.2.29) \end{aligned}$$

The (complicating) constraint (2.2.29) models the natural situation of probabilistic fluctuations occurring only where nonzero probabilities already exist. We note that the solution to the optimisation problem (2.2.26)–(2.2.29) exists since we are again maximising a continuous function on a compact subset of $\mathbb{R}^{n\times n}$.

Reformulating Problem (2.2.26)–(2.2.29) in Vectorized Form

As in the positive M case, we want to find a matrix A so that the constraints (2.2.27) and (2.2.29) can be written in terms of $\widehat{m}$ in the linear form (2.2.7). Let $\mathcal{M} := \{i : \widehat{M}_i \in \{0,1\}\} = \{\gamma_1, \ldots, \gamma_j\} \subset \{1, 2, \ldots, n^2\}$, where $\widehat{M}$ denotes the vectorization of M. Proceeding as in the proof of Lemma 2.2.3, it is easy to verify

that constraints (2.2.27) and (2.2.29) can be written in the form (2.2.7), where A is a $k \times n^2$ matrix ($k \geq n$) given by

$$A = \begin{pmatrix} \mathrm{Id}_n \otimes \mathbf{1}^\top \\ \mathbf{e}_{\gamma_1}^\top \\ \vdots \\ \mathbf{e}_{\gamma_j}^\top \end{pmatrix}, \tag{2.2.30}$$

where the $\mathbf{e}_i$s in (2.2.30) are the i-th standard basis vectors in $\mathbb{R}^{n^2}$. As in the positive M case, the term $\mathrm{Id}_n \otimes \mathbf{1}^\top$ in (2.2.30) corresponds to the constraint (2.2.27), while all other entries of A are related to constraints (2.2.29). We conclude that we can reformulate the optimisation problem (2.2.26)–(2.2.29) in the form (2.2.6)–(2.2.8) with A given by (2.2.30).

Explicit Construction of an Orthonormal Basis of the Null Space of the Matrix A in (2.2.30)

Proceeding as in the positive M case, we want to simplify the optimisation problem (2.2.6)–(2.2.8) by constructing a matrix E as in (2.2.10), whose columns form an orthonormal basis for the null space of A. We first note that E is an $n^2 \times \ell$ matrix, where ℓ is the nullity of A. Let us begin by computing ℓ explicitly.

Lemma 2.2.4. *The nullity of the matrix A in (2.2.30) is $n^2 - (n + n_1)$, where n is the dimension of the square matrix M and n_1 is the number of zero entries in M.*

Proof. Let $Y = \{\mathbf{v} = (v_1, \ldots, v_n) \in \mathbb{R}^n : v_i = 1 \text{ for some } 1 \leq i \leq n\}$. Assume first that M doesn't contain any columns that belong to Y and consider $\mathbf{M}_j$, the j-th column of M. Note that the j-th row of A is given by

$$(\underbrace{0, \ldots, 0}_{n(j-1)}, \underbrace{1, \ldots, 1}_{n}, \underbrace{0, \ldots, 0}_{n(n-j)}). \tag{2.2.31}$$

On the other hand, for every zero in $\mathbf{M}_j$, we have the following row in A

$$(\underbrace{0, \ldots, 0}_{n(j-1)}, \underbrace{0, \ldots, 0, 1, 0, \ldots, 0}_{n}, \underbrace{0, \ldots, 0}_{n(n-j)}), \tag{2.2.32}$$

where 1 is in a position corresponding to the position of the zero entry in $\mathbf{M}_j$. Since $\mathbf{M}_j \notin Y$, we have that the number of rows of the form (2.2.32) in A is at most $n-2$. Therefore, we obviously have that the set spanned by row (2.2.31) and rows (2.2.32) is linearly independent. Moreover, since all other rows of A have only zeros on places where vectors in (2.2.31) and (2.2.32) have nonzero entries, and since j was arbitrary, we conclude that rows of A are linearly independent and that $\mathrm{Rank}(A) = n + n_1$. This immediately implies that the nullity of A is $n^2 - (n + n_1)$.

The general case when M can have columns that belong to Y can be treated similarly. Indeed, it is sufficient to note that each $\mathbf{M}_j \in Y$ will generate $n+1$ rows in A (given again by (2.2.31) and (2.2.32)) but only form a subspace of dimension $n = 1 + (n-1)$ and $n-1$ is precisely the number of zero entries in $\mathbf{M}_j$. □

For A given by (2.2.30) written in the form

$$A = (A_1 | \dots | A_n), \quad \text{where } A_i \in \mathbb{R}^{k \times n}, \tag{2.2.33}$$

let V be defined as in (2.2.9). We aim to construct a matrix E as in (2.2.10) whose columns form an orthonormal basis for V. We first need to introduce some additional notation. For a matrix $J \in \mathbb{R}^{p_1 \times p_2}$ and a set $\mathfrak{s} = \{l_1, \dots, l_s\} \subset \{1, \dots, p_1\}$, we define $J[\mathfrak{s}]$ to be the matrix consisting of the rows $l_1, \dots, l_s$ of J. We note that $J[\mathfrak{s}]$ is an $s \times p_2$ matrix.

Note that A_i in (2.2.33) can be written as

$$A_i = \begin{pmatrix} 0_{i_1 \times n} \\ \mathbf{1}_n^\top \\ 0_{i_2 \times n} \\ \mathrm{Id}_n[R_i] \\ 0_{i_3 \times n} \end{pmatrix}, \tag{2.2.34}$$

where $R_i := \{j : M_{ji} \in \{0, 1\}\}$ and for some $i_c \in \{0, 1, \dots, n^2\}$, $c \in \{1, 2, 3\}$, such that $\sum_{c=1}^{3} i_c = k - |R_i| - 1$; recall A has k rows (see (2.2.30)). It follows from (2.2.34) that the null space of A_i is the same as the null space of the matrix

$\widetilde{A}_i := \begin{pmatrix} \mathbf{1}_n^\top \\ \mathrm{Id}_n[R_i] \end{pmatrix}$. Let $r_i \in \{0, \ldots, n-1\}$ denote the number of zeros in the i-th column of M. It follows from the arguments in the proof of Lemma 2.2.4 that

$$\mathrm{Rank}(\widetilde{A}_i) = r_i + 1. \tag{2.2.35}$$

In particular, when $r_i = n - 1$, the nullity of $\widetilde{A}_i$ is zero.

The first step in constructing an explicit E is provided by the following result, where $\mathrm{diag}(B_1, \ldots, B_n)$ denotes the block matrix with diagonal blocks $B_1, \ldots, B_n$.

Proposition 2.2.5. *Define the matrix $E = diag(B_1, \ldots, B_n)$, where B_i is the matrix whose columns form an orthonormal basis of the null space of A_i (if this null space is trivial, we omit the block B_i). The columns of E form an orthonormal basis for the null space of A.*

Proof. We begin by showing that $V = \mathrm{null}(A) \subset \mathrm{col}(E)$ (the column space of E). For $\mathbf{w} \in V$, we write $\mathbf{w} = (\mathbf{w}_1^\top, \ldots, \mathbf{w}_n^\top)^\top$, where $\mathbf{w}_i \in \mathbb{R}^n$ for $1 \leq i \leq n$. From (2.2.33) we have that $A\mathbf{w} = \sum_{i=1}^n A_i \mathbf{w}_i$. Using (2.2.34), we have

$$A_i \mathbf{w}_i = \begin{pmatrix} 0_{i_1 \times n} \\ \mathbf{1}_n^\top \mathbf{w}_i \\ 0_{i_2 \times n} \\ \mathbf{w}_i[R_i] \\ 0_{i_3 \times n} \end{pmatrix}, \text{ and thus } A\mathbf{w} = \begin{pmatrix} \mathbf{1}_n^\top \mathbf{w}_1 \\ \vdots \\ \mathbf{1}_n^\top \mathbf{w}_n \\ \mathbf{w}_1[R_1] \\ \vdots \\ \mathbf{w}_n[R_n] \end{pmatrix}.$$

Since $A\mathbf{w} = \mathbf{0}$, we conclude that $A_i \mathbf{w}_i = \mathbf{0}$ for each $i \in \{1, \ldots, n\}$. Thus, each $\mathbf{w}_i$ can be written as a linear combination of columns of B_i and therefore, $\mathbf{w}$ can be written as a linear combination of columns of E; thus, $V \subset \mathrm{col}(E)$. The orthonormality of the columns of E follows from the orthonormality of the columns of B_i. Since B_i has full column rank, the number of columns of E equals the sum of the rank of the B_i's. The number of columns of E can be computed as $\sum_{i=1}^n \mathrm{Rank}(B_i)$ $= \sum_{i=1}^n \mathrm{Nullity}(A_i) = \sum_{i=1}^n n - \mathrm{Rank}(A_i) = n^2 - (n + n_1) = \mathrm{Nullity}(A)$, where the second last equality follows from (2.2.35) and the fact that $n_1 = \sum_{i=1}^n r_i$, and the

last equality follows from Lemma 2.2.4. Thus, the columns of E form a basis for the null space of A. □

The final step is to construct the matrices B_i, $1 \leq i \leq n$, explicitly.

Proposition 2.2.6. *Assume that $r_i < n-1$ and let $\widetilde{B}_i = (\mathbf{x}_1|\dots|\mathbf{x}_{(n-1)-r_i}) \in \mathbb{R}^{(n-r_i)\times((n-1)-r_i)}$, where $\mathbf{x}_i$ form the orthonormal basis of the null space of $\mathbf{1}_{n-r_i}^\top$ having the form (2.2.19). Furthermore, let $B_i \in \mathbb{R}^{n\times((n-1)-r_i)}$ be a matrix defined by the conditions:*

$$B_i[R_i] = 0_{r_i\times((n-1)-r_i)} \quad \text{and} \quad B_i[\{1,\dots,n\}\setminus R_i] = \widetilde{B}_i. \tag{2.2.36}$$

Then, the columns of B_i form an orthonormal basis for the null space of A_i.

Proof. Since the null spaces of the matrices A_i and $\widetilde{A}_i$ coincide, it is sufficient to show that the columns of B_i form an orthonormal basis for the null space of $\widetilde{A}_i$. We first note that the orthonormality of $\mathbf{x}_1,\dots,\mathbf{x}_{n-1-r_i}$ in $\mathbb{R}^{n-r_i}$ directly implies that the columns of B_i form an orthonormal set in $\mathbb{R}^n$, since the j-th column of B_i is built from $\mathbf{x}_j$ by adding zeroes in appropriate places that are independent of j. Furthermore, since $\mathbf{x}_1,\dots,\mathbf{x}_{n-1-r_i}$ are in the null space of $\mathbf{1}_{n-r_i}^\top$, we have that the columns of B_i belong to the null space of $\mathbf{1}_n^\top$. Moreover, it follows from the first equality in (2.2.36) that columns of B_i are also orthogonal to all other rows of $\widetilde{A}_i$. Consequently, we conclude that all columns of B_i lie in the null space of $\widetilde{A}_i$. Finally, by (2.2.35) we have that the nullity of $\widetilde{A}_i$ is $n-r_i-1$, which is the same as the number of columns of B_i, and therefore columns of B_i span the null space of $\widetilde{A}_i$. □

Using Propositions 2.2.5 and 2.2.6, and exploiting block structure, we can arrive at a computationally convenient form of $\widetilde{U} = WE$: Noting that $\mathbf{f}^\top \otimes Q = (1 \otimes Q)(\mathbf{f}^\top \otimes \mathrm{Id}_n) = Q(\mathbf{f}^\top \otimes \mathrm{Id}_n)$ (which follows from Proposition 2.2.2(i) and (ii), respectively), we have

$$\widetilde{U} = WE = (\mathbf{f}^\top \otimes Q)E = Q(\mathbf{f}^\top \otimes \mathrm{Id}_n)\mathrm{diag}(B_1,\dots,B_n) = Q(f_1B_1|\dots|f_nB_n), \tag{2.2.37}$$

where the second equality follows from (2.2.1) and the third from Proposition 2.2.5.

Solution to Problem (2.2.26)–(2.2.29)

Now that we have constructed an appropriate E (Proposition 2.2.5 gives the form of E and Proposition 2.2.6 provides the specific components of E), we can reformulate our problem (2.2.6)–(2.2.8) (with the matrix A in (2.2.30)), to obtain the optimisation problem (2.2.15)–(2.2.16) with $\widetilde{U}$ as in (2.2.37). A vectorized solution to (2.2.26)–(2.2.29) is given by $\widehat{m}^*$ as in (2.2.18), where $\boldsymbol{\alpha}^*$ again denotes the eigenvector corresponding to the largest eigenvalue, λ, of the matrix $\widetilde{U}^\top\widetilde{U}$. As in the positive M case, both m^* and $-m^*$ yield the same Euclidean norm of the response (2.2.26). Finally, the optimal value may be calculated as $\|Qm^*\mathbf{f}\|_2^2 = \|W\widehat{m}^*\|_2^2 = \|WE\boldsymbol{\alpha}^*\|_2^2 = \|\widetilde{U}\boldsymbol{\alpha}^*\|_2^2 = \lambda\boldsymbol{\alpha}^{*\top}\boldsymbol{\alpha}^* = \lambda$, where the first three equalities follow by (2.2.1), (2.2.18) and (2.2.17), respectively.

A Sufficient Condition for a Unique Optimal Solution and Independence of the Choice of Basis of the Null Space of A

The following result provides an easily checkable sufficient condition (simplicity of the leading eigenvalue of $\widetilde{U}^\top\widetilde{U}$) for the uniqueness of the solution m^* (up to sign) to the problems (2.2.2)–(2.2.4) and (2.2.26)–(2.2.29). Under this condition, the specific choice of basis for the null space of the constraint matrix A is unimportant, and the m^* computed in Algorithms 1 and 2 in Appendix A.1 is independent of this basis choice. Recall that $W = \mathbf{f}^\top \otimes Q$ and A is the matrix of equality constraints (i.e. $A\widehat{m}^* = \mathbf{0}$).

Proposition 2.2.7. *Consider two distinct orthonormal bases for the null space of A and construct matrices $E_1 \neq E_2$ from these bases as in (2.2.10). Then,*

1. *The matrices $\widetilde{U}_i^\top\widetilde{U}_i$ (for $\widetilde{U}_i = WE_i$), $i = 1, 2$ are similar.*
2. *If the largest eigenvalue λ_1 of $\widetilde{U}_1^\top\widetilde{U}_1$ is simple, let $\boldsymbol{\alpha}_i^*$ denote the eigenvector of $\widetilde{U}_i^\top\widetilde{U}_i$ corresponding to λ_1, normalised so that $\|\boldsymbol{\alpha}_i^*\|_2 = 1$, $i = 1, 2$. One then has $\widehat{m}_1^*$ equals $\widehat{m}_2^*$, up to sign, when computed with (2.2.18).*

Proof. Since the columns of E_1 and E_2 span the same space, there exists some matrix $R \in \mathbb{R}^{\ell\times\ell}$ such that $E_2 = E_1R$. Noting that $E_i^\top E_i = \mathrm{Id}_\ell$, $i = 1, 2$, we have that $\mathrm{Id}_\ell = E_2^\top E_2 = R^\top E_1^\top E_1 R = R^\top R$; using the fact that R is square, we also have that $R^\top = R^{-1}$ and hence R is orthogonal. Since $\widetilde{U}_1^\top\widetilde{U}_1 = E_1^\top W^\top W E_1$ and

$\widetilde{U}_2^\top \widetilde{U}_2 = R^{-1} E_1^\top W^\top W E_1 R$, we have that the matrices $\widetilde{U}_1^\top \widetilde{U}_1$ and $\widetilde{U}_2^\top \widetilde{U}_2$ are similar. Using $\boldsymbol{\alpha}_1^* = \pm R\boldsymbol{\alpha}_2^*$, we obtain $\widehat{m}_1^* = E_1\boldsymbol{\alpha}_1^* = \pm E_1 R\boldsymbol{\alpha}_2^* = \pm E_2\boldsymbol{\alpha}_2^* = \pm\widehat{m}_2^*$. □

2.2.5 Algorithms for Solving Problems (2.2.2)–(2.2.4) and (2.2.26)–(2.2.29)

In Appendix A.1 we provide separate algorithms for positive M (problem (2.2.2)–(2.2.4)) and general stochastic (mixing) M (problem (2.2.26)–(2.2.29)): Algorithms 1 and 2 respectively.

2.2.6 Analytic Example

We now explicitly construct the solution for the problem (2.2.26)–(2.2.29) when $M \in \mathbb{R}^{2\times 2}$. Since M is column stochastic and the columns of m sum to zero, we can write

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = \begin{pmatrix} 1 - M_{21} & M_{12} \\ M_{21} & 1 - M_{12} \end{pmatrix}$$

and

$$m = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} = \begin{pmatrix} m_{11} & -m_{22} \\ -m_{11} & m_{22} \end{pmatrix}.$$

We first note that without any loss of generality, we can assume that M is positive. Indeed, if $M_{11} = 0$ then by (2.2.28) and (2.2.29), we have that $m_{11} = 0$ and $m_{22} = \pm\frac{1}{\sqrt{2}}$. Similarly, if $M_{22} = 0$ then $m_{22} = 0$ and $m_{11} = \pm\frac{1}{\sqrt{2}}$. Furthermore, we note that $M_{11} \neq 1$ and $M_{22} \neq 1$ since otherwise M would not be a transition matrix of an ergodic Markov chain. One may calculate that

$$m^* = \begin{cases} \frac{1}{\sqrt{2(M_{12}^2+M_{21}^2)}} \begin{pmatrix} M_{12} & M_{21} \\ -M_{12} & -M_{21} \end{pmatrix}, & \text{if } M_{12} \geq M_{21}; \\ \frac{1}{\sqrt{2(M_{12}^2+M_{21}^2)}} \begin{pmatrix} -M_{12} & -M_{21} \\ M_{12} & M_{21} \end{pmatrix}, & \text{if } M_{21} > M_{12}, \end{cases} \tag{2.2.38}$$

$$\mathbf{u}_1 = \begin{cases} \frac{\sqrt{M_{12}^2+M_{21}^2}}{(M_{12}+M_{21})^2} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}, & \text{if } M_{12} \geq M_{21}; \\ \frac{\sqrt{M_{12}^2+M_{21}^2}}{(M_{12}+M_{21})^2} \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, & \text{if } M_{21} > M_{12}, \end{cases} \tag{2.2.39}$$

and

$$\|\mathbf{u}_1\|_2^2 = \frac{M_{12}^2 + M_{21}^2}{(M_{12} + M_{21})^4}.$$

We see from (2.2.39) that the greatest ℓ^2 response of the invariant probability vector $\mathbf{f} = (M_{12}, M_{21})/(M_{12} + M_{21})$ is achieved by increasing whichever of M_{12} or M_{21} is greatest. Furthermore, as expected $\mathbf{f}$ is most sensitive when M is near diagonal. The minimum value of $\|\mathbf{u}_1\|_2^2$ occurs when $M_{12} = M_{21} = 1$ (value of 1/8) and increases with decreasing values of M_{12} and M_{21}. There is a singularity at $M_{12} = M_{21} = 0$ when the second eigenvalue merges with the eigenvalue 1; see Figure 2.1.

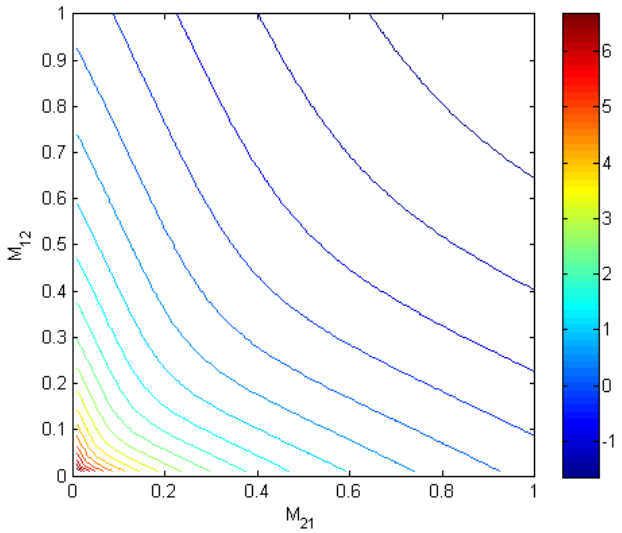


Figure 2.1: Contour plot of $\log_e((M_{12}^2 + M_{21}^2)/(M_{12} + M_{21})^4)$.

2.3 Maximising the Linear Response of the Expectation of an Observable

In this section we consider maximising the linear response of the expected value of a cost vector $\mathbf{c}$ with respect to the invariant probability vector $\mathbf{f}$. The computations developed in this section will be used in Section 2.6 to solve a discrete version of the problem of maximising the linear response of an observable with respect to the invariant measure of a stochastically perturbed dynamical system.

We recall that the linear response to the invariant probability vector $\mathbf{f}$ of an irreducible, aperiodic transition matrix M, under a perturbation matrix m, is denoted

by $\mathbf{u}_1$. We wish to select a perturbation matrix m so that we maximise $\mathbf{c}^\top \mathbf{u}_1$. For $\mathbf{c} \in \mathbb{R}^n$, using (2.1.6), we consider the following problem:

$$\begin{aligned} \max_{m \in \mathbb{R}^{n \times n}} \quad & \mathbf{c}^\top Q m \mathbf{f} && (2.3.1) \\ \text{subject to} \quad & m^\top \mathbf{1} = \mathbf{0} && (2.3.2) \\ & \|m\|_F^2 - 1 = 0 && (2.3.3) \\ & m_{ij} = 0 \text{ if } (i,j) \in N, && (2.3.4) \end{aligned}$$

where $N = \{(i,j) \in \{1,\dots,n\}^2 : M_{ij} = 0 \text{ or } 1\}$. Note that since m_{ij} takes the value 0 for all $(i,j) \in N$, we just need to determine m_{ij} for $(i,j) \notin N$.

We employ Lagrange multipliers (see e.g. §12.3–12.5 [71]). Consider the Lagrangian function

$$\mathcal{L}(m, \boldsymbol{\varrho}, \nu) = \mathbf{w}^\top m \mathbf{f} - \boldsymbol{\varrho}^\top m^\top \mathbf{1} - \nu(\|m\|_F^2 - 1), \tag{2.3.5}$$

where $\mathbf{w}^\top = \mathbf{c}^\top Q \in \mathbb{R}^n$ and $\boldsymbol{\varrho} \in \mathbb{R}^n, \nu \in \mathbb{R}$ are the Lagrange multipliers. Differentiating (2.3.5) with respect to m_{ij}, we obtain

$$\frac{\partial \mathcal{L}}{\partial m_{ij}}(m, \boldsymbol{\varrho}, \nu) = w_i f_j - \varrho_j - 2\nu m_{ij}.$$

Using the first-order optimality (KKT) conditions from the method of Lagrange multipliers (e.g. Theorem 12.1 [71]), we require

$$w_i f_j - \varrho_j - 2\nu m_{ij} = 0 \text{ for } (i,j) \notin N, \tag{2.3.6}$$

$$\sum_{i:(i,j)\notin N} m_{ij} = 0 \text{ for } j \in \{1,\dots,n\}, \tag{2.3.7}$$

$\|m\|_F = 1$, and a regularity condition (LICQ)[1]. Equation (2.3.6) yields $\varrho_j = -2\nu m_{ij} + w_i f_j$ for $(i,j) \notin N$. Using (2.3.7), we calculate

$$\sum_{i:(i,j)\notin N} \varrho_j = |N_j^c| \varrho_j = f_j \sum_{i:(i,j)\notin N} w_i,$$

[1]The regularity condition is that the gradients of all (equality) constraints are linearly independent at the local optimum. A proof of this fact is in Appendix A.2.

where $N_j^c = \{i : (i,j) \notin N\}$. Thus, substituting $\varrho_j = (f_j/|N_j^c|)\sum_{l:(l,j)\notin N} w_l$ we obtain

$$m_{ij}^* = \frac{-\varrho_j + w_i f_j}{2\nu} = \frac{f_j}{2\nu}\left(w_i - \frac{1}{|N_j^c|}\sum_{l:(l,j)\notin N} w_l\right). \tag{2.3.8}$$

We now scale ν to ensure $\|m^*\|_F = 1$. The matrix m^* satisfies the first-order equality constraints (2.3.2)–(2.3.4) and $\frac{\partial \mathcal{L}}{\partial m_{ij}}(m^*, \boldsymbol{\varrho}, \nu) = 0$ for $(i,j) \notin N$. Finally, we determine the sign of ν by checking the standard second order sufficient conditions for m_{ij}^* to be a maximiser (namely (2.3.10) below); see e.g. Theorem 12.6 [71]. We compute

$$\frac{\partial^2 \mathcal{L}}{\partial m_{ij}\partial m_{kl}}(m^*, \boldsymbol{\varrho}, \nu) = -2\nu\delta_{(i,j),(k,l)}; \tag{2.3.9}$$

thus, the Hessian matrix of the Lagrangian function is $H(m^*, \boldsymbol{\varrho}, \nu) = -2\nu\,\mathrm{Id}_{n^2-|N|}$. If $\nu > 0$ one has

$$\mathbf{s}^\top H(m^*, \boldsymbol{\varrho}, \nu)\mathbf{s} < 0, \tag{2.3.10}$$

for any $\mathbf{s} \in \mathbb{R}^{n^2-|N|} \setminus \{\mathbf{0}\}$ (indeed for any $\mathbf{s} \in \mathbb{R}^{n^2} \setminus \{\mathbf{0}\}$).

2.3.1 Algorithm for Solving Problem (2.3.1)–(2.3.4)

See Appendix A.1.

2.3.2 Analytic Example

Suppose that $M \in \mathbb{R}^{2\times 2}$ and we would like to solve (2.3.1)–(2.3.4) for $\mathbf{c} \in \mathbb{R}^2$, $\mathbf{c} \neq a\mathbf{1}$, where $a \in \mathbb{R}$. As in the example in Section 2.2.6, we only need to consider the case when M is positive. Let $\mathbf{w} = Q^\top \mathbf{c}$; one may calculate that

$$m^* = \begin{cases} \frac{1}{\sqrt{2(M_{12}^2+M_{21}^2)}}\begin{pmatrix} M_{12} & M_{21} \\ -M_{12} & -M_{21}\end{pmatrix}, & \text{if } w_1 > w_2; \\ \frac{1}{\sqrt{2(M_{12}^2+M_{21}^2)}}\begin{pmatrix} -M_{12} & -M_{21} \\ M_{12} & M_{21}\end{pmatrix}, & \text{if } w_2 > w_1, \end{cases} \tag{2.3.11}$$

and

$$\mathbf{c}^\top \mathbf{u}_1 = \begin{cases} \frac{\sqrt{M_{12}^2+M_{21}^2}}{\sqrt{2}(M_{12}+M_{21})^2}(c_1 - c_2), & \text{if } w_1 > w_2; \\ \frac{\sqrt{M_{12}^2+M_{21}^2}}{\sqrt{2}(M_{12}+M_{21})^2}(c_2 - c_1), & \text{if } w_2 > w_1. \end{cases} \tag{2.3.12}$$

2.4 Maximising the Linear Response of the Rate of Convergence to Equilibrium

In this section we consider maximising the linear response of the rate of convergence of the Markov chain to its equilibrium measure. We achieve this by maximising the linearised change in the magnitude of the (assumed simple) second eigenvalue λ_2 of the stochastic matrix M. The computations in this section will be applied in Section 2.6 to solve a discrete version of the problem of maximising the linear response of the rate of convergence to equilibrium for some stochastically perturbed dynamical system.

Because M is irreducible and aperiodic, $\lambda_1 = 1$ is the only eigenvalue on the unit circle. Let $\lambda_2 \in \mathbb{C}$ be the eigenvalue of M strictly inside the unit circle with largest magnitude, and assume that λ_2 is simple. Denote by $\mathbf{l}_2 \in \mathbb{C}^n$ and $\mathbf{r}_2 \in \mathbb{C}^n$ the left and right eigenvectors of M corresponding to λ_2. We assume that we have the normalisations $\mathbf{r}_2^*\mathbf{r}_2 = 1$ and $\mathbf{l}_2^*\mathbf{r}_2 = 1$. Considering the small perturbation of M to $M + \varepsilon m$, by standard arguments (e.g. Theorem 6.3.12 [53]), one has

$$\left.\frac{d\lambda_2(\varepsilon)}{d\varepsilon}\right|_{\varepsilon=0} = \mathbf{l}_2^* m \mathbf{r}_2, \tag{2.4.1}$$

where $\lambda_2(\varepsilon)$ is the second largest eigenvalue of $M + \varepsilon m$. We wish to achieve a maximal decrease in the magnitude of λ_2, or equivalently a maximal decrease in the real part of the logarithm of λ_2. Denote by $\Re(\cdot)$ and $\Im(\cdot)$ the real and imaginary parts, respectively. Now $d(\Re(\log\lambda_2(\varepsilon)))/d\varepsilon = \Re(d\log(\lambda_2(\varepsilon))/d\varepsilon) = \Re((d\lambda_2(\varepsilon)/d\varepsilon)/\lambda_2(\varepsilon))$, which, using (2.4.1) becomes

$$\begin{aligned}\Re((d\lambda_2(\varepsilon)/d\varepsilon)/\lambda_2)|_{\varepsilon=0} = \frac{1}{|\lambda_2|^2}\Big(&\left(\Re(\mathbf{l}_2)^\top m\Re(\mathbf{r}_2) + \Im(\mathbf{l}_2)^\top m\Im(\mathbf{r}_2)\right)\Re(\lambda_2) \\ &+ \left(\Re(\mathbf{l}_2)^\top m\Im(\mathbf{r}_2) - \Im(\mathbf{l}_2)^\top m\Re(\mathbf{r}_2)\right)\Im(\lambda_2)\Big).\end{aligned} \tag{2.4.2}$$

Similarly to Section 2.3 we now have the optimisation problem:

$$\begin{aligned}\min_{m\in\mathbb{R}^{n\times n}} \quad &\left(\Re(\mathbf{l}_2)^\top m\Re(\mathbf{r}_2) + \Im(\mathbf{l}_2)^\top m\Im(\mathbf{r}_2)\right)\Re(\lambda_2) \\ &+ \left(\Re(\mathbf{l}_2)^\top m\Im(\mathbf{r}_2) - \Im(\mathbf{l}_2)^\top m\Re(\mathbf{r}_2)\right)\Im(\lambda_2)\end{aligned} \tag{2.4.3}$$

$$\text{subject to} \quad m^\top \mathbf{1} = \mathbf{0} \tag{2.4.4}$$

$$\|m\|_F^2 - 1 = 0 \tag{2.4.5}$$

$$m_{ij} = 0 \text{ if } (i,j) \in N, \tag{2.4.6}$$

where $N = \{(i,j) \in \{1,\dots,n\}^2 : M_{ij} = 0 \text{ or } 1\}$. Note that since m_{ij} takes the value 0 for all $(i,j) \in N$, we just need to solve (2.4.3)–(2.4.5) for $(i,j) \notin N$.

Applying Lagrange multipliers, we proceed as in Section 2.3, with the only change being to replace the expression (2.3.6) with

$$S_{ij} - \varrho_j - 2\nu m_{ij} = 0 \text{ for } (i,j) \notin N, \tag{2.4.7}$$

where

$$S_{ij} := (\Re(\mathbf{l}_2)_i \Re(\mathbf{r}_2)_j + \Im(\mathbf{l}_2)_i \Im(\mathbf{r}_2)_j)\, \Re(\lambda_2) + (\Re(\mathbf{l}_2)_i \Im(\mathbf{r}_2)_j - \Im(\mathbf{l}_2)_i \Re(\mathbf{r}_2)_j)\, \Im(\lambda_2). \tag{2.4.8}$$

Following the steps in Section 2.3 we obtain

$$m^*_{ij} = \frac{-\varrho_j + S_{ij}}{2\nu} = \frac{\left(S_{ij} - \frac{1}{|N_j^c|} \sum_{l:(l,j)\notin N} S_{lj}\right)}{2\nu}, \tag{2.4.9}$$

where $(i,j) \notin N$ and $N_j^c = \{i : (i,j) \notin N\}$. Note that because we are minimising (as opposed to maximising in Section 2.3) we select $\nu < 0$, scaled so that $\|m^*\|_F = 1$.

2.4.1 Algorithm for Solving Problem (2.4.3)–(2.4.6)

See Appendix A.1.

2.4.2 Analytic Example

Suppose that $M \in \mathbb{R}^{2\times 2}$ and we would like to solve (2.4.3)–(2.4.6). As in Section 2.2.6 for $M \in \mathbb{R}^{2\times 2}$, we only need to consider the case when M is positive. One

may calculate that

$$m^* = \begin{cases} \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, & \text{if } M_{11} + M_{22} < 1; \\ \frac{1}{2}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}, & \text{if } M_{11} + M_{22} > 1, \end{cases} \tag{2.4.10}$$

and

$$\left.\frac{d(\Re(\log \lambda_2(\varepsilon)))}{d\varepsilon}\right|_{\varepsilon=0} = \frac{1}{\lambda_2}\mathbf{l}_2^* m^* \mathbf{r}_2 = \begin{cases} \frac{1}{M_{11}+M_{22}-1} = \frac{1}{\lambda_2}, & \text{if } M_{11} + M_{22} < 1; \\ \frac{-1}{M_{11}+M_{22}-1} = \frac{-1}{\lambda_2}, & \text{if } M_{11} + M_{22} > 1. \end{cases} \tag{2.4.11}$$

The optimal choice of m^* depends only on whether M is diagonally dominant or not: if M is diagonally dominant, perturb away from diagonal dominance, and if M is not diagonally dominant, perturb toward diagonal dominance. The linear response of λ_2 has a fixed magnitude of 1.

2.5 Optimising Linear Response for a General Sequence of Matrices

In this section we extend the ideas of Sections 2.2 and 2.3 to derive the linear response of the Euclidean norm of a probability vector $\mathbf{f}$ and the expectation of an observable $\mathbf{c}$, when acted on by a *finite sequence of matrices*. We will then introduce and solve an optimisation problem that finds the sequence of perturbation matrices that achieve these maximal values.

2.5.1 Linear Response for the Probability Vector $\mathbf{f}$

Let $M^{(0)}, M^{(1)}, \ldots, M^{(\tau-1)}$ be a fixed finite sequence of column stochastic matrices. Furthermore, let $m^{(t)}$, $t \in \{0, \ldots, \tau-1\}$, be a sequence of perturbation matrices. Take an arbitrary probability vector $\mathbf{f}^{(0)}$ and set

$$\mathbf{f}^{(t+1)} = M^{(t)}\mathbf{f}^{(t)}, \quad \text{for } t \in \{0, \ldots, \tau-1\}.$$

We now want to derive the formula for the linear response of $\mathbf{f}^{(\tau)}$. We require that

$$(M^{(t)} + \varepsilon m^{(t)})\left(\mathbf{f}^{(t)} + \sum_{i=1}^{\infty} \varepsilon^i \mathbf{u}_i^{(t)}\right) = \mathbf{f}^{(t+1)} + \sum_{i=1}^{\infty} \varepsilon^i \mathbf{u}_i^{(t+1)}, \tag{2.5.1}$$

where $\varepsilon \in \mathbb{R}$. We refer to $\mathbf{u}_1^{(t)}$ as the linear response at time t. By expanding the left-hand side of (2.5.1), we have

$$\left(M^{(t)} + \varepsilon m^{(t)}\right)\left(\mathbf{f}^{(t)} + \sum_{i=1}^{\infty} \varepsilon^i \mathbf{u}_i^{(t)}\right) = \mathbf{f}^{(t+1)} + \varepsilon\left(M^{(t)}\mathbf{u}_1^{(t)} + m^{(t)}\mathbf{f}^{(t)}\right) + O(\varepsilon^2). \quad (2.5.2)$$

Denoting for simplicity $\mathbf{u}_1^{(t)}$ by $\mathbf{u}^{(t)}$, it follows from (2.5.1) and (2.5.2) that

$$\mathbf{u}^{(t+1)} = M^{(t)}\mathbf{u}^{(t)} + m^{(t)}\mathbf{f}^{(t)}. \quad (2.5.3)$$

Set $\mathbf{u}^{(0)} = 0$. Iterating (2.5.3), we obtain that

$$\mathbf{u}^{(\tau)} = \sum_{t=1}^{\tau-1} M^{(\tau-1)} \dots M^{(t)} m^{(t-1)} \mathbf{f}^{(t-1)} + m^{(\tau-1)}\mathbf{f}^{(\tau-1)}. \quad (2.5.4)$$

The Norm Optimisation Problem

It follows from Proposition 2.2.2(vi) that

$$\begin{aligned}
\mathbf{u}^{(\tau)} = \widehat{\mathbf{u}}^{(\tau)} &= \sum_{t=1}^{\tau-1} \left(\mathbf{f}^{(t-1)\top} \otimes \left(M^{(\tau-1)} \cdots M^{(t)}\right)\right) \widehat{m}^{(t-1)} + (\mathbf{f}^{(\tau-1)\top} \otimes \mathrm{Id}_n)\widehat{m}^{(\tau-1)} \\
&= \sum_{t=1}^{\tau-1} W^{(t-1)}\widehat{m}^{(t-1)} + W^{(\tau-1)}\widehat{m}^{(\tau-1)} \\
&= W \begin{pmatrix} \widehat{m}^{(0)} \\ \vdots \\ \widehat{m}^{(\tau-1)} \end{pmatrix} = W\widehat{m},
\end{aligned}$$

where

$$W^{(t)} = \mathbf{f}^{(t)\top} \otimes \left(M^{(\tau-1)} \cdots M^{(t+1)}\right) \quad \text{for } 0 \le t \le \tau - 2, \quad W^{(\tau-1)} = \mathbf{f}^{(\tau-1)\top} \otimes \mathrm{Id}_n$$

and $W = \left(W^{(0)}|W^{(1)}|\dots|W^{(\tau-1)}\right)$. Note that the $W^{(t)}$s are $n \times n^2$ matrices, W is an $n \times \tau n^2$ matrix and $\widehat{m}$ is a τn^2-vector.

We consider the following optimisation problem, which maximises the response of the Euclidean norm of the response $\mathbf{u}^{(\tau)}$:

$$\max_{\widehat{m}\in\mathbb{R}^{\tau n^2}} \quad \|W\widehat{m}\|_2^2 \tag{2.5.5}$$

$$\text{subject to} \quad A^{(t)}\widehat{m}^{(t)} = \mathbf{0} \text{ for } t = 0, \ldots, \tau - 1 \tag{2.5.6}$$

$$\sum_{t=0}^{\tau-1} \|\widehat{m}^{(t)}\|_2^2 - 1 = 0, \tag{2.5.7}$$

where $A^{(t)}$ is the constraint matrix (2.2.30) associated to the matrix $M^{(t)}$ and conditions (2.2.27) and (2.2.29).

Solution to the Norm Optimisation Problem

We want to reformulate the optimisation problem with the constraints (2.5.6) removed. We first note that (2.5.6) can be replaced by $A\widehat{m} = \mathbf{0}$, where

$$A = \operatorname{diag}(A^{(0)}, \ldots, A^{(\tau-1)}). \tag{2.5.8}$$

Let $E^{(t)}$ be an $n^2 \times \ell^{(t)}$ matrix whose columns form an orthonormal basis of the null space of $A^{(t)}$ for $t = 0, \ldots, \tau - 1$, where $\ell^{(t)}$ denotes the nullity of $A^{(t)}$. Then, $E = \operatorname{diag}(E^{(0)}, \ldots, E^{(\tau-1)})$ is a matrix whose columns form an orthonormal basis of the null space of the matrix A in (2.5.8). Thus, if $\widehat{m}$ is an element of the null space of A then, $\widehat{m} = E\boldsymbol{\alpha}$ for a unique $\boldsymbol{\alpha} \in \mathbb{R}^{\sum_{t=0}^{\tau-1}\ell^{(t)}}$. Finally, since $\sum_{t=0}^{\tau-1}\|\widehat{m}^{(t)}\|_2^2 = \|\widehat{m}\|_2^2 = \|E\boldsymbol{\alpha}\|_2^2 = \|\boldsymbol{\alpha}\|_2^2$, we can reformulate the optimisation problem (2.5.5)–(2.5.7) as:

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^{\sum_{t=0}^{\tau-1}\ell^{(t)}}} \quad \|U\boldsymbol{\alpha}\|_2^2 \tag{2.5.9}$$

$$\|\boldsymbol{\alpha}\|_2^2 - 1 = 0, \tag{2.5.10}$$

where

$$U = WE = (W^{(0)}E^{(0)}|\ldots|W^{(\tau-1)}E^{(\tau-1)}). \tag{2.5.11}$$

Arguing as in Section 2.2.4, we conclude that $\widehat{m}^* = E\boldsymbol{\alpha}^*$ maximises the Euclidean norm of the linear response $\mathbf{u}^{(\tau)}$, where $\boldsymbol{\alpha}^* \in \mathbb{R}^{\sum_{t=0}^{\tau-1}\ell^{(t)}}$ is the eigenvector corresponding to the largest eigenvalue of $U^\top U$ (with U as in (2.5.11)). Finally, if

we denote $\mathbf{f}^{(t+1)}(\varepsilon) = \left(M^{(t)} + \varepsilon m^{(t),*}\right)\mathbf{f}^{(t)}$, we choose the sign of $m^{(t),*}$ so that $\|\mathbf{f}^{(t)}\|_2 < \|\mathbf{f}^{(t)}(\varepsilon)\|_2$ for small $\varepsilon > 0$ and for each $t \in \{1, \ldots, \tau\}$; this is possible since $\mathbf{f}^{(t)}$ is independent of $m^{(t)}$.

2.5.2 Linear Response for the Expectation of an Observable

In this section, we consider maximising the linear response of the expected value of an observable $\mathbf{c}$ with respect to the probability vector $\mathbf{f}^{(\tau)}$, when acted on by a *finite sequence of matrices*. More precisely, we consider the following problem: For $\mathbf{c} \in \mathbb{R}^n$

$$\begin{aligned}
\max_{m^{(0)}, m^{(1)}, \ldots, m^{(\tau-1)} \in \mathbb{R}^{n\times n}} \quad & \mathbf{c}^\top \mathbf{u}^{(\tau)} && (2.5.12)\\
\text{subject to} \quad & m^{(t)\top}\mathbf{1} = \mathbf{0} \text{ for } t \in \{0, \ldots, \tau-1\} && (2.5.13)\\
& \sum_{t=0}^{\tau-1} \|m^{(t)}\|_F^2 - 1 = 0 && (2.5.14)\\
& m_{ij}^{(t)} = 0 \text{ if } (i,j) \in N^{(t)} \text{ for } t \in \{0, .., \tau-1\}, && (2.5.15)
\end{aligned}$$

where $N^{(t)} = \{(i,j) \in \{1, \ldots, n\}^2 : M_{ij}^{(t)} = 0 \text{ or } 1\}$. Multiplying (2.5.4) on the left by $\mathbf{c}^\top$ we obtain $\mathbf{c}^\top \mathbf{u}^{(\tau)} = \sum_{t=0}^{\tau-1} \mathbf{w}^{(t)\top} m^{(t)} \mathbf{f}^{(t)}$, where $\mathbf{w}^{(t)\top} = \mathbf{c}^\top M^{(\tau-1)} \ldots M^{(t+1)}$ for $t \in \{0, \ldots, \tau-2\}$ and $\mathbf{w}^{(\tau-1)\top} = \mathbf{c}^\top$. Since $m_{ij}^{(t)} = 0$ for $(i,j) \in N^{(t)}$, we just need to solve (2.5.12)–(2.5.14) for $(i,j) \notin N^{(t)}$.

As in Section 2.3, we solve this problem using the method of Lagrange multipliers. We begin by considering the following Lagrangian function:

$$\begin{aligned}
&\mathcal{L}(m^{(0)}, \ldots, m^{(\tau-1)}, \boldsymbol{\varrho}^{(0)}, \ldots, \boldsymbol{\varrho}^{(\tau-1)}, \nu)\\
&\quad = \sum_{t=0}^{\tau-1} \mathbf{w}^{(t)\top} m^{(t)} \mathbf{f}^{(t)} - \sum_{t=0}^{\tau-1} \boldsymbol{\varrho}^{(t)\top} m^{(t)\top} \mathbf{1} - \nu \left(\sum_{t=0}^{\tau-1} \|m^{(t)}\|_F^2 - 1 \right),
\end{aligned} \tag{2.5.16}$$

where $\boldsymbol{\varrho}^{(t)} \in \mathbb{R}^n$ and $\nu \in \mathbb{R}$ are the Lagrange multipliers. Differentiating (2.5.16) with respect to $m_{ij}^{(t)}$, we obtain

$$\frac{\partial \mathcal{L}}{\partial m_{ij}^{(t)}}(m^{(0)}, \ldots, m^{(\tau-1)}, \boldsymbol{\varrho}^{(0)}, \ldots, \boldsymbol{\varrho}^{(\tau-1)}, \nu) = w_i^{(t)} f_j^{(t)} - \varrho_j^{(t)} - 2\nu m_{ij}^{(t)},$$

where $w_i^{(t)}, f_j^{(t)}, \varrho_j^{(t)} \in \mathbb{R}$ are the elements of the n-vectors $\mathbf{w}^{(t)}, \mathbf{f}^{(t)}$ and $\boldsymbol{\varrho}^{(t)}$ respectively.

Using the first order optimality (KKT) conditions, we require

$$w_i^{(t)} f_j^{(t)} - \varrho_j^{(t)} - 2\nu m_{ij}^{(t)} = 0 \text{ for } (i,j) \notin N^{(t)},$$

$$\sum_{i:(i,j)\notin N^{(t)}} m_{ij}^{(t)} = 0 \text{ for } j \in \{1,\dots,n\}, t \in \{0,\dots,\tau-1\}, \tag{2.5.17}$$

(2.5.14), and a regularity condition, analogous to that treated in Appendix A.2, which follows similarly. We note that $\varrho_j^{(t)} = w_i^{(t)} f_j^{(t)} - 2\nu m_{ij}^{(t)}$. Using (2.5.17), we calculate

$$\sum_{i:(i,j)\notin N^{(t)}} \varrho_j^{(t)} := \left|N_j^{(t),c}\right| \varrho_j^{(t)} = f_j^{(t)} \sum_{i:(i,j)\notin N^{(t)}} w_i^{(t)},$$

where $N_j^{(t),c} = \{i : (i,j) \notin N^{(t)}\}$. Thus, we obtain

$$m_{ij}^{(t),*} = \frac{f_j^{(t)}}{2\nu}\left(w_i^{(t)} - \frac{1}{\left|N_j^{(t),c}\right|} \sum_{i:(i,j)\notin N^{(t)}} w_i^{(t)}\right),$$

where $(i,j) \notin N^{(t)}$. We scale ν to ensure $\sum_{t=0}^{\tau-1} \|m^{(t),*}\|_F^2 = 1$; all first-order optimality conditions are now satisfied. As in Section 2.3, we determine the sign of ν by checking the standard second order sufficient conditions for $m^{(t),*}$, $t \in \{0,\dots,\tau-1\}$, to be a maximiser. We note that the matrices $m^{(t),*}$ satisfy (2.5.13)–(2.5.15) and

$$\frac{\partial \mathcal{L}}{\partial m_{ij}^{(t)}}(m^{(0),*},\dots,m^{(\tau-1),*},\boldsymbol{\varrho}^{(0)},\dots,\boldsymbol{\varrho}^{(\tau-1)},\nu) = 0 \text{ for } (i,j) \notin N^{(t)}.$$

We compute

$$\frac{\partial^2 \mathcal{L}}{\partial m_{ij}^{(t)} \partial m_{kl}^{(t')}}(m^{(0),*},\dots,m^{(\tau-1),*},\boldsymbol{\varrho}^{(0)},\dots,\boldsymbol{\varrho}^{(\tau-1)},\nu) = -2\nu\delta_{(i,j,t),(k,l,t')}.$$

If $\nu > 0$ then $H(m^{(0),*},\dots,m^{(\tau-1),*},\boldsymbol{\varrho}^{(0)},\dots,\boldsymbol{\varrho}^{(\tau-1)},\nu)$, the Hessian of the Lagrangian function, satisfies $\mathbf{s}^\top H(m^{(0),*},\dots,m^{(\tau-1),*},\boldsymbol{\varrho}^{(0)},\dots,\boldsymbol{\varrho}^{(\tau-1)},\nu)\mathbf{s} < 0$ for any $\mathbf{s} \in \mathbb{R}^{\tau n^2} \setminus \{\mathbf{0}\}$. Thus, the second order sufficient conditions for a maximiser are satisfied.

2.6 Numerical Examples of Optimal Linear Response for Stochastically Perturbed Dynamical Systems

We apply the techniques we have developed in Sections 2.2–2.4 to randomly perturbed dynamical systems of the type introduced in Section 1. The annealed Perron-Frobenius (or transfer) operator defined by (1.0.1) is the linear (Markov) operator that pushes forward densities under the annealed (averaged) action of our random dynamical system. We will consider a connected, compact phase space $X \subset \mathbb{R}^d$ and a stochastic[2] kernel $k(x, y)$ in (1.0.1) to handle perturbations near the boundary of X. The kernel k defines the integral operator $Lg(x) = \int_X k(x, y)g(y)\, dy$. We will assume that $k \in L^2(X \times X)$, which guarantees that L is a compact operator on $L^2(X)$; see e.g. Proposition II.1.6 [19]. A sufficient condition for L possessing a unique fixed point in $L^1(X)$ is that there exists a j such that $\int_X \inf_y k^j(x, y)\, dx > 0$, where k^j is the kernel associated with L^j; see Corollary 5.7.1 [62]. This is a stochastic "covering" condition, which is satisfied by our examples, which are generated by transitive deterministic T with bounded additive uniform noise. In summary, we have a unique annealed invariant measure for our stochastically perturbed system and by compactness our transfer operator L has a spectral gap on $L^2(X)$ (i.e. the only element of $\sigma(L)$ on the unit circle is $\{1\}$, which is a simple eigenvalue).

2.6.1 Ulam Projection

To carry out numerical computations, we project the operator L onto a finite-dimensional space spanned by indicator functions on a fine mesh of X. Let $B_n = \{I_1, \ldots, I_n\}$ be a partition of X into connected sets, and set $\mathcal{B}_n = \text{span}\{\mathbf{1}_{I_1}, \ldots, \mathbf{1}_{I_n}\}$. Define a projection $\pi_n : L^1 \to \mathcal{B}_n$ by $\pi_n(g) = \sum_{i=1}^n \left(\frac{1}{\ell(I_i)} \int_{I_i} g\, d\ell\right) \mathbf{1}_{I_i}$, where ℓ is Lebesgue measure; π_n simply replaces $g|_{I_i}$ with its expected value. We now consider the finite-rank operator $\pi_n L : L^1 \to \mathcal{B}_n$; this general approach is known as Ulam's method [80]. When Ulam's method is applied to compact L as above, one achieves convergence of $\pi_n L$ to L in operator norm (and therefore L^2 convergence of the leading eigenvector of $\pi_n L$ to that of L via standard operator perturbation theory); see [21].

[2] $k(x, y) \geq 0$, $\int_X k(x, y)\, dx = 1\ \forall y \in X$.

We calculate

$$\begin{aligned}\pi_n Lg &= \sum_{i=1}^{n}\left(\frac{1}{\ell(I_i)}\int_{I_i} Lg(x)\,dx\right)\mathbf{1}_{I_i}\\ &= \sum_{i=1}^{n}\left(\frac{1}{\ell(I_i)}\int_X \underbrace{\int_{I_i} k(x,y)\,dx}_{:=\psi_i(y)}\, g(y)\,dy\right)\mathbf{1}_{I_i}. \end{aligned} \tag{2.6.1}$$

Putting $g=\sum_{j=1}^{n} g_j\mathbf{1}_{I_j}\in\mathcal{B}_n$, where $g_j\in\mathbb{R}, j=1,\dots,n$, we have

$$\pi_n Lg = \sum_{i=1}^{n}\sum_{j=1}^{n} f_j \underbrace{\frac{\int_{I_j}\psi_i(y)\,dy}{\ell(I_i)}}_{:=M_{ij}}\mathbf{1}_{I_i}, \tag{2.6.2}$$

where M is the matrix representation of $\pi_n L:\mathcal{B}_n\to\mathcal{B}_n$.

In our examples below, $X=[0,1]$ or $X=S^1$, and $k(x,y):=\mathbf{1}_{B_\epsilon(Ty)}(x)/\ell(X\cap B_\epsilon(Ty))$, where $B_\epsilon(Ty)$ denotes an ϵ-ball centred at the point Ty. This definition of k ensures that we do not stochastically perturb points outside our domain X. Our random dynamical systems therefore comprise deterministic dynamics followed by the addition of uniformly distributed noise in an ϵ-ball (with adjustments made near the boundary of X). This choice of k leads to

$$\psi_i(y)=\frac{\int_{I_i}\mathbf{1}_{B_\epsilon(Ty)}(x)\,dx}{\ell(X\cap B_\epsilon(Ty))}=\frac{\ell(I_i\cap B_\epsilon(Ty))}{\ell(X\cap B_\epsilon(Ty))}. \tag{2.6.3}$$

Combining (2.6.2) and (2.6.3) we obtain

$$M_{ij}=\frac{\int_{I_j}\ell(I_i\cap B_\epsilon(Ty))/\ell(X\cap B_\epsilon(Ty))\,dy}{\ell(I_i)}.$$

From now on we assume that $I_i=[(i-1)/n,i/n), i=1,\dots,n$, so that $\mathcal{B}_n$ is a partition of X into equal length subintervals. We now have that $\sum_{i=1}^{n}M_{ij}=1$ for each $j=1,\dots,n$, and so M is a column stochastic matrix. We use the matrix M to numerically approximate the operator L in the experiments below.

Consistent Scaling of the Perturbation m

In Sections 2.6.2–2.6.4 we will think of the entries of the perturbation matrix m as resulting from the matrix representation of the Ulam projection of a perturbation δL of L. To make this precise, we first write $g \in \mathcal{B}_n$ as $g = \sum_{j=1}^n \bar{g}_j \mathbf{1}_{I_j}$, and introduce a projected version of δk: $\pi_n(\delta k) = \sum_{i,j} \bar{\delta k}_{ij} \mathbf{1}_{I_i \times I_j}$, where the matrix $\bar{\delta k}_{ij} = (1/(\ell(I_i)\ell(I_j))) \int_{I_i \times I_j} \delta k(x,y)\, dydx$. We now explicitly compute the Ulam projection of δL:

$$\begin{aligned}
\pi_n \delta L(g)(z) &= (1/\ell(I_i)) \sum_{i=1}^n \left[\int_{I_i} \delta L(g)(x)\, dx \right] \mathbf{1}_{I_i}(z) \\
&= (1/\ell(I_i)) \sum_{i=1}^n \left[\int_{I_i} \int_X \delta k(x,y) g(y)\, dydx \right] \mathbf{1}_{I_i}(z) \\
&= (1/\ell(I_i)) \sum_{i,j=1}^n \bar{g}_j \left[\int_{I_i \times I_j} \delta k(x,y)\, dydx \right] \mathbf{1}_{I_i}(z) \\
&= \sum_{i,j=1}^n \underbrace{\ell(I_j) \bar{\delta k}_{ij}}_{:= m_{ij}} \bar{g}_j \mathbf{1}_{I_i}(z).
\end{aligned}$$

Thus, we have the relationship $m_{ij} = \ell(I_j)\bar{\delta k}_{ij}$ between the matrix representation of the projected version of the operator δL (namely m) and the elements of the projected version of the kernel (namely $\bar{\delta k}$).

We wish to fix the Hilbert-Schmidt norm of $\pi_n \delta L$ to 1.

$$1 = \|\pi_n \delta L\|_{HS}^2 = \|\pi_n \delta k\|_{L^2(X\times X)}^2 = \left\| \sum_{i,j=1}^n \bar{\delta k}_{ij} \mathbf{1}_{I_i \times I_j} \right\|_{L^2(X\times X)}^2 = \sum_{i,j=1}^n \ell(I_i)\ell(I_j) \bar{\delta k}^2. \tag{2.6.4}$$

Since $\|m\|_F^2 = \sum_{i,j=1}^n \ell(I_j)^2 \bar{\delta k}_{ij}^2$, if we assume that $\ell(I_i) = 1/n$, $1 \le i \le n$, we obtain $\|m\|_F = (1/n)^2 \|\bar{\delta k}\|_F^2$ and by (2.6.4) we know $\|\bar{\delta k}\|_F^2 = n^2$. We thus conclude that enforcing $\|m\|_F = 1$ will ensure $\|\pi_n \delta L\|_{HS} = 1$, as required.

Consistent Scaling for f and c

In Sections 2.6.2–2.6.4 we will use vector representations of the invariant density f and an L^2 function c. We write $f = \sum_{i=1}^n \mathbf{f}_i \mathbf{1}_{I_i}$, where $\mathbf{f} \in \mathbb{R}^n$. We normalise so that $\int_X f(x)\, dx = 1$, which means that $\sum_{i=1}^n \mathbf{f}_i = n$. Similarly, we write $c = \sum_{i=1}^n \mathbf{c}_i \mathbf{1}_{I_i}$,

where $\mathbf{c} \in \mathbb{R}^n$. We normalise so that $\int_X c(x)^2\, dx = 1$, which means that $\sum_{i=1}^n \mathbf{c}_i^2 = n$ or $\|\mathbf{c}\|_2 = \sqrt{n}$.

2.6.2 A Stochastically Perturbed Lanford Map

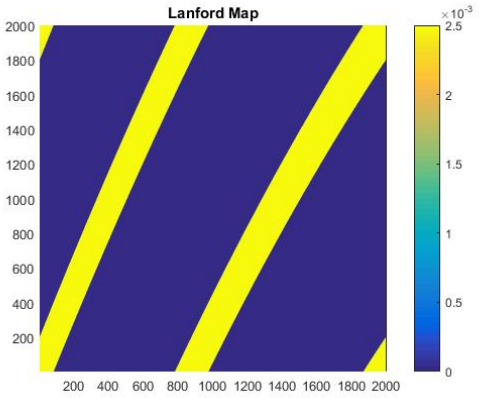
The first example we consider is the stochastically perturbed Lanford map [60]. We will use the numerical solution of the problems (2.2.26)–(2.2.29) and (2.3.1)–(2.3.4) for this map to solve the problem of maximising the L^2 norm of the linear response of the invariant measure and maximising the linear response of the expectation of an observable.

Maximising the Linear Response of the L^2 Norm of the Invariant Measure

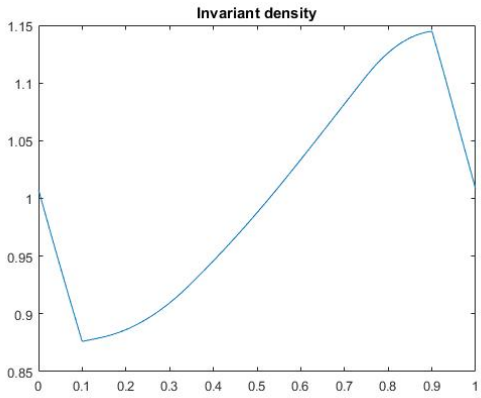
Let $T : S^1 \to S^1$ be the stochastically perturbed Lanford map defined by

$$T(x) = 2x + \frac{1}{2}x(1-x) + \xi \bmod 1, \tag{2.6.5}$$

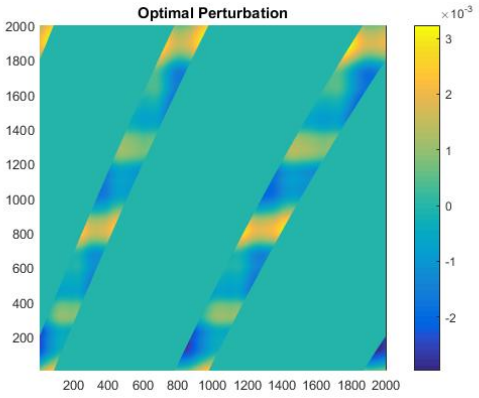
where $\xi \sim \mathcal{U}(0, \frac{1}{10})$ (uniformly distributed on an interval about 0 of radius 1/10). Let $M \in \mathbb{R}^{n\times n}$ be Ulam's discretisation of the transfer operator of the map T with n subintervals. The matrix M will be mixing (aperiodic and irreducible) by arguments similar to those in Proposition 2.3 [26]. Using Algorithm 2 (see Appendix A.1), we solve the problem (2.2.26)–(2.2.29) for the matrix M for $n = 2000$ to obtain the optimal perturbation m^*. The top two singular values of the matrix $\widetilde{U}$, computed using MATLAB, are 35.08 and 33.32 (each with multiplicity one), which we consider to be strong numerical evidence that the leading singular value of $\widetilde{U}$ has multiplicity one. By Proposition 2.2.7 we conclude that our computed m^* is the unique optimal perturbation for the discretised system (up to sign). The sign of the matrix m^* is chosen so that $\|\mathbf{f}_M\|_2 < \|\mathbf{f}_{M+\varepsilon m^*}\|_2$ for $\varepsilon > 0$. Figure 2.2(a) shows the Lanford map and Figure 2.2(b) presents the approximation of the invariant density f of the Lanford map. Figure 2.2(c) presents the optimal perturbation matrix m^* which generates the maximal response. Figure 2.2(d) presents the approximation of the associated linear response $u_1^* = \sum_{i=1}^n \mathbf{u}_1^* \mathbf{1}_{I_i}$, for the perturbation m^*; for this example, we compute $\|u_1^*\|_{L^2}^2 \approx 0.6154$. Figure 2.2(c) shows that the selected perturbation preferentially places mass in a neighbourhood of $x = 0.4$ and $x = 0.95$, consistent with local peaks in the response in Figure 2.2(d).



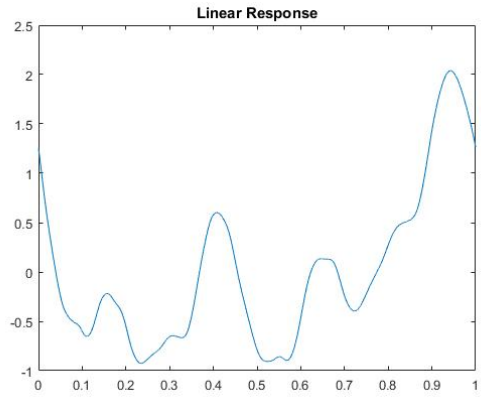
(a) Colourmap of the stochastically perturbed Lanford map. The colourbar indicates the values of the elements of the matrix.



(b) The invariant density f.



(c) The optimal perturbation m^*. The colourbar indicates the values of the elements of the matrix. Note that the aqua colour outside the support of the two branches corresponds to a zero perturbation.



(d) The optimal linear response u_1^*.

Figure 2.2: Solution to the problem of maximising the L^2 norm of the linear response of the stochastically perturbed Lanford map.

Having computed the optimal linear response for a specific n, we verify in Table 2.1 that for various partition cardinalities, the L^2 norm of the approximation of the linear response u_1^* converges. We also verify that $\|f_{M+\varepsilon m^*} - (f_M + \varepsilon u_1^*)\|_{L^2}^2$ is small for small $\varepsilon > 0$. The 10000-fold improvement in the accuracy is consistent with the error terms of the linearisation being of order ε^4 when considering the square of the L^2 norm (because $f_{M+\varepsilon m} = f_M + \varepsilon u_1 + O(\varepsilon^2)$, when we decrease ε from $1/100$ to $1/1000$, the square of the error term of the linearisation is changed by $((1/10)^2)^2 = 1/10000$). The table also illustrates the change in the norm of the

invariant density when perturbed; we see that the norm of the invariant density increases when we perturb M by εm^* and decreases when we perturb by $-\varepsilon m^*$, consistent with the choice of sign of m^* noted above.

n	$\|u_1^*\|_{L^2}^2$	ε	$\|f_{M+\varepsilon m^*} - (f_M + \varepsilon u_1^*)\|_{L^2}^2$	$\|f_{M-\varepsilon m^*}\|_{L^2}^2$	$\|f_M\|_{L^2}^2$	$\|f_{M+\varepsilon m^*}\|_{L^2}^2$
1500	0.6180	1/100	1.35×10^{-9}	1.00713	1.00783	1.00865
		1/1000	1.35×10^{-13}	1.00775	1.00783	1.00790
1750	0.6165	1/100	1.35×10^{-9}	1.00713	1.00783	1.00864
		1/1000	1.34×10^{-13}	1.00775	1.00783	1.00790
2000	0.6154	1/100	1.35×10^{-9}	1.00713	1.00783	1.00864
		1/1000	1.34×10^{-13}	1.00775	1.00783	1.00790

Table 2.1: Numerical results for maximising the linear response of the L^2 norm of the invariant probability measure of the stochastic Lanford Map. Column 1: number of partition elements; Column 2: optimal objective value; Column 3: values of ε; Column 4: linearisation error; Columns 5-7: demonstration that the L^2 norm of the invariant density increases and decreases appropriately under the small perturbation εm^*.

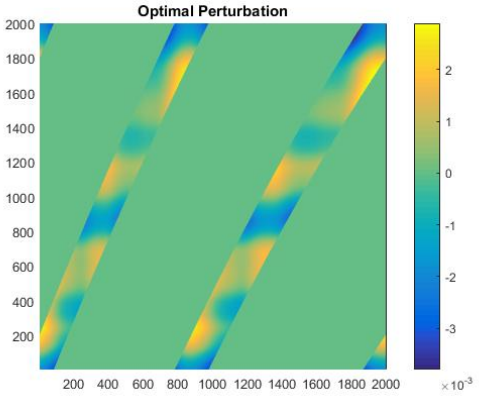
Maximising the Linear Response of the Expectation of an Observable

In this section we find the perturbation that generates the greatest linear response of the expectation

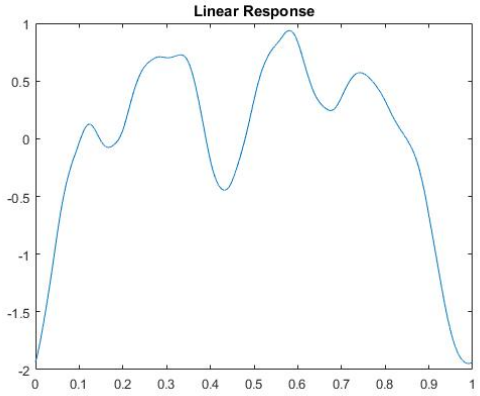
$$\langle c, h\rangle = \int_{[0,1]} c(x)h(x)dx,$$

where $c(x) = \sqrt{2}\sin(\pi x)$ and the underlying dynamics are given by the map (2.6.5). We consider problem (2.3.1)–(2.3.4) with the vector $\mathbf{c} = (c_1, \ldots, c_n) \in \mathbb{R}^n$, where $c_i = \sqrt{2n}\sin(\pi x_i)$ and $x_i = \frac{i-1}{n} + \frac{1}{2n}$, $i = 1, \ldots, n$. Let $M \in \mathbb{R}^{n\times n}$ be the discretisation matrix derived from Ulam's method. We use Algorithm 3 (see Appendix A.1) to solve problem (2.3.1)–(2.3.4). Figure 2.3 presents the optimal perturbation m^* and the associated linear response u_1^* for this problem. Note that the response in Figure 2.3(b) has positive values where $c(x)$ is large and negative values where $c(x)$ is small, consistent with our objective to increase the expectation of c. In this example ($n = 2000$), we obtain $\langle c, u_1^*\rangle \approx 0.2514$.

Table 2.2 provides numerical results for various partition cardinalities n. We see that (i) the value of $\langle c, u_1^*\rangle$ appears to converge when we increase n, (ii) the 100 fold improvement in accuracy is consistent with the error terms of the linearisation being



(a) The optimal perturbation m^*. The colourbar indicates the values of the elements of the matrix.



(b) The optimal linear response u_1^*.

Figure 2.3: Solution to the problem of maximising the expectation of the response of the observable $c(x)$ for the stochastically perturbed Lanford map.

of order ε^2 since $f_{M+\varepsilon m} = f_M + \varepsilon u_1 + O(\varepsilon^2)$, and (iii) the expectation increases if we perturb in the direction εm^* and decreases if we perturb in the direction $-\varepsilon m^*$.

n	$\langle c, u_1^* \rangle$	ε	$\langle c, f_{M+\varepsilon m^*} \rangle - \langle c, f_M + \varepsilon u_1^* \rangle$	$\langle c, f_{M-\varepsilon m^*} \rangle$	$\langle c, f_M \rangle$	$\langle c, f_{M+\varepsilon m^*} \rangle$
1500	0.2520	1/100	-9.70×10^{-6}	0.89434	0.89687	0.89938
		1/1000	-9.73×10^{-8}	0.89662	0.89687	0.89712
1750	0.2517	1/100	-9.68×10^{-6}	0.89434	0.89687	0.89937
		1/1000	-9.71×10^{-8}	0.89662	0.89687	0.89712
2000	0.2514	1/100	-9.67×10^{-6}	0.89434	0.89687	0.89937
		1/1000	-9.69×10^{-8}	0.89662	0.89687	0.89712
5000	0.2503	1/100	-9.61×10^{-6}	0.89435	0.89687	0.89936
		1/1000	-9.63×10^{-8}	0.89662	0.89687	0.89712
7000	0.2501	1/100	-9.60×10^{-6}	0.89436	0.89687	0.89936
		1/1000	-9.62×10^{-8}	0.89662	0.89687	0.89712

Table 2.2: Numerical results for maximising the linear response of the expectation of $c(x) = \sqrt{2}\sin(\pi x)$ for the stochastic Lanford map. Column 1: number of partition elements; Column 2: optimal objective value; Column 3: values of ε; Column 4: linearisation error; Columns 5-7: demonstration that the expected value of the function c increases and decreases appropriately under the small perturbation εm^*.

2.6.3 A Stochastically Perturbed Logistic Map

In this section, we consider the problems of maximising the L^2 norm of the linear response of the invariant measure and maximising the linear response of the expectation of an observable. The underlying deterministic dynamics is given by

the logistic map, and this map is again stochastically perturbed, yielding a linear response (see e.g. the survey [10] for a discussion of the failure of linear response for the deterministic logistic map).

Maximising the Linear Response of the L^2 Norm of the Invariant Measure

Let $T_\xi : [0,1] \to [0,1]$ be the logistic map with noise defined by

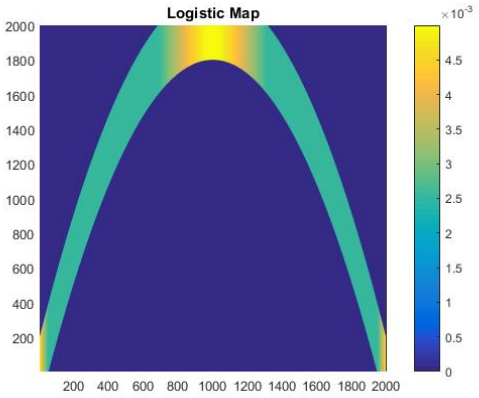
$$T_\xi(x) = 4x(1-x) + \xi_x, \tag{2.6.6}$$

where $\xi_x \sim \mathcal{U}(B_{\frac{1}{10}}(0) \cap [-x, 1-x])$ and $\mathcal{U}(I)$ denotes the uniform distribution on the interval I. Let $M \in \mathbb{R}^{n\times n}$ be Ulam's discretisation of the transfer operator of the map T_ξ with n partitions. We use Algorithm 2 (see Appendix A.1) to solve the optimisation problem (2.2.26)–(2.2.29) with the matrix M, for $n = 2000$, to obtain the optimal perturbation m^*. The top two singular values of $\widetilde{U}$, for this example, were computed in MATLAB to be 36.92 and 29.36 (each with unit multiplicity); thus, by Proposition 2.2.7, m^* is the unique optimal perturbation (up to sign). The sign of the matrix m^* is chosen so that $\|\mathbf{f}_M\|_2 < \|\mathbf{f}_{M+\varepsilon m^*}\|_2$ for $\varepsilon > 0$. Figure 2.4 shows the results for the stochastically perturbed logistic map; for this example we compute $\|u_1^*\|_{L^2}^2 \approx 0.6815$. In the right branch of Figure 2.4(c), we see sharp increases in mass mapped to neighbourhoods of $x = 0.15$ and $x = 0.4$, as well as a sharp decrease in mass mapped to a neighbourhood of $x = 0.25$; these observations coincide with the local peaks and troughs of the response vector shown in Figure 2.4(d). Table 2.3 displays the corresponding numerical results.

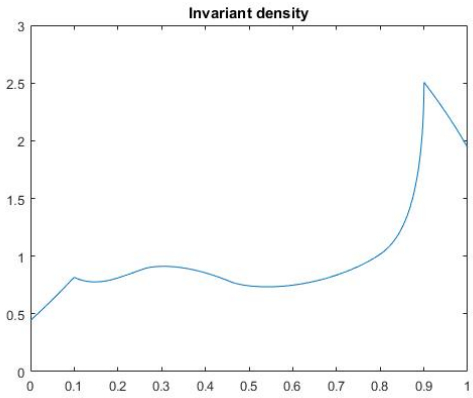
Maximising the Linear Response of the Expectation of an Observable

Using (2.3.1)–(2.3.4), we calculate the perturbation achieving a maximal linear response of $\langle c, f\rangle$, for $c(x) = \sqrt{2}\sin(\pi x)$, for the stochastic dynamics (2.6.6). We again compute with the vector $\mathbf{c} = (c_1, \ldots, c_n) \in \mathbb{R}^n$, where $c_i = \sqrt{2n}\sin(\pi x_i)$ and $x_i = \frac{i-1}{n} + \frac{1}{2n}$, $i = 1, \ldots, n$. We compute the discretisation matrix $M \in \mathbb{R}^{n\times n}$ derived from Ulam's method and make use of Algorithm 3 (see Appendix A.1).

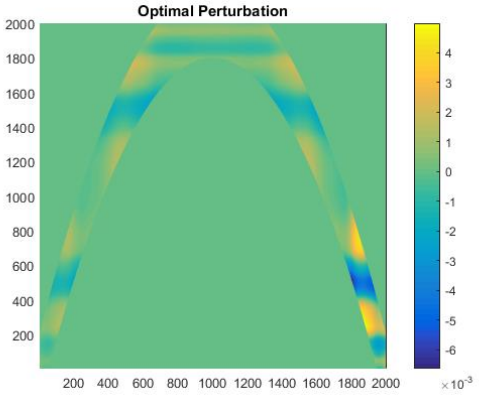
The m^* provoking the greatest linear response in the expectation $\langle c, f\rangle$ is shown in Figure 2.5(a). The linear response corresponding to m^* is shown in Figure 2.5(b); for this example, $\langle c, u_1^*\rangle \approx 0.1187$. The response takes its minimal values at



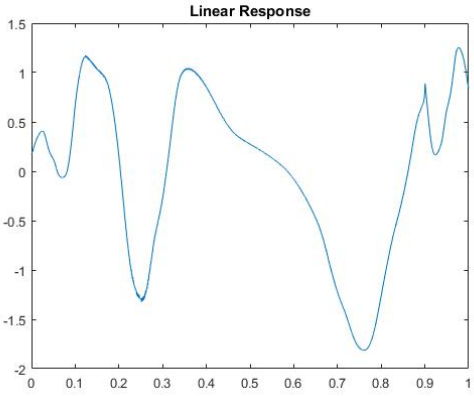
(a) Colourmap of the stochastically perturbed logistic map. The colourbar indicates the values of the elements of the matrix.



(b) The invariant density f.



(c) The optimal perturbation m^*. The colourbar indicates the values of the elements of the matrix.



(d) The optimal linear response u_1^*.

Figure 2.4: Solution to the problem of maximising the L^2 norm of the linear response of the stochastically perturbed logistic map.

$x = 0, x = 1$, where the values of the observable c is also least, and the response is broadly positive near the centre of the interval $[0, 1]$, where the observable takes on large values; both of these observations are consistent with maximising the linear response of the observable c.

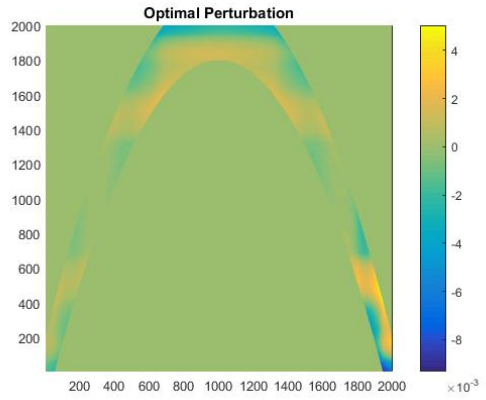
Numerical results for this example are provided in Table 2.4.

2.6.4 A Stochastically Perturbed Double Lanford Map

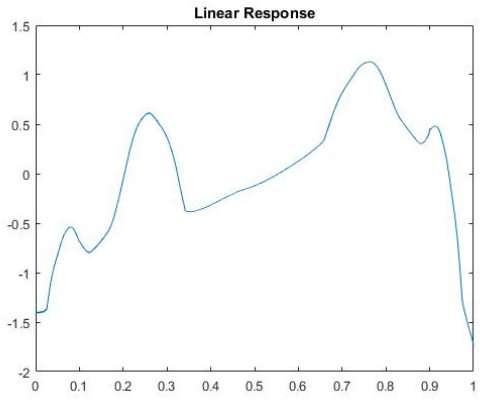
In this last section, we consider the problem of maximising the linear response of the rate of convergence to the equilibrium. The underlying deterministic dynamics

n	$\|u_1^*\|_{L^2}^2$	ε	$\|f_{M+\varepsilon m^*} - (f_M + \varepsilon u_1^*)\|_{L^2}^2$	$\|f_{M-\varepsilon m^*}\|_{L^2}^2$	$\|f_M\|_{L^2}^2$	$\|f_{M+\varepsilon m^*}\|_{L^2}^2$
1500	0.6849	1/100	7.85×10^{-10}	1.21563	1.21711	1.21872
		1/1000	7.87×10^{-14}	1.21696	1.21711	1.21727
1750	0.6829	1/100	7.83×10^{-10}	1.21564	1.21711	1.21872
		1/1000	7.85×10^{-14}	1.21696	1.21711	1.21727
2000	0.6815	1/100	7.81×10^{-10}	1.21564	1.21711	1.21872
		1/1000	7.83×10^{-14}	1.21696	1.21711	1.21727

Table 2.3: Numerical results for maximising the linear response of the L^2 norm of the invariant probability measure of the stochastic logistic map. Column 1: number of partition elements; Column 2: optimal objective value; Column 3: values of ε; Column 4: linearisation error; Columns 5-7: demonstration that the L^2 norm of the invariant density increases and decreases appropriately under the small perturbation εm^*.



(a) The optimal perturbation m^*. The colourbar indicates the values of the elements of the matrix.



(b) The optimal linear response u_1^*.

Figure 2.5: Solution to the problem of maximising the expectation of the response of the observable $c(x)$ for the stochastically perturbed logistic map.

is given by a stochastically perturbed double Lanford map. More explicitly, we consider the map $T : S^1 \to S^1$ defined by

$$T(x) = \begin{cases} \left(T_{Lan}(2x) \mod \frac{1}{2}\right) + \xi \mod 1 & \text{if } 0 \le x \le \frac{1}{2} \\ \left(T_{Lan}\left(2\left(x - \frac{1}{2}\right)\right) \mod \frac{1}{2}\right) + \frac{1}{2} + \xi \mod 1 & \text{if } \frac{1}{2} < x \le 1, \end{cases} \tag{2.6.7}$$

where $T_{Lan}(x) = 2x + \frac{1}{2}x(1-x)$ and $\xi \sim \mathcal{U}(0, \frac{1}{10})$ (uniformly distributed on an interval about 0 of radius 1/10). We have chosen this doubled version of the Lanford

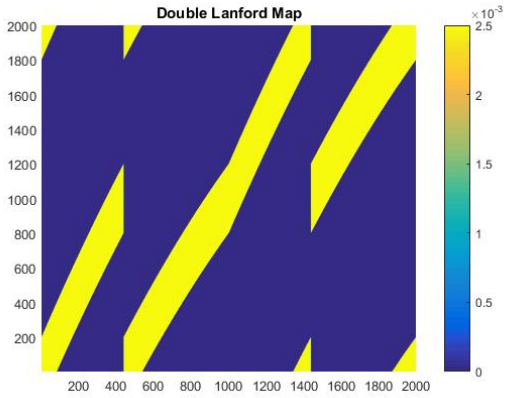
n	$\langle c, u_1^* \rangle$	ε	$\langle c, f_{M+\varepsilon m^*} \rangle - \langle c, f_M + \varepsilon u_1^* \rangle$	$\langle c, f_{M-\varepsilon m^*} \rangle$	$\langle c, f_M \rangle$	$\langle c, f_{M+\varepsilon m^*} \rangle$
1500	0.1190	1/100	-1.89×10^{-6}	0.80009	0.80128	0.80247
		1/1000	-1.89×10^{-8}	0.80116	0.80128	0.80140
1750	0.1189	1/100	-1.89×10^{-6}	0.80009	0.80128	0.80247
		1/1000	-1.88×10^{-8}	0.80116	0.80128	0.80140
2000	0.1187	1/100	-1.88×10^{-6}	0.80009	0.80128	0.80247
		1/1000	-1.88×10^{-8}	0.80116	0.80128	0.80140
5000	0.1182	1/100	-1.87×10^{-6}	0.80010	0.80128	0.80246
		1/1000	-1.87×10^{-8}	0.80116	0.80128	0.80140
7000	0.1181	1/100	-1.87×10^{-6}	0.80010	0.80128	0.80246
		1/1000	-1.87×10^{-8}	0.80116	0.80128	0.80140

Table 2.4: Numerical results for maximising the linear response of the expectation of $c(x) = \sqrt{2}\sin(\pi x)$ for the stochastic logistic map. Column 1: number of partition elements; Column 2: optimal objective value; Column 3: values of ε; Column 4: linearisation error; Columns 5-7: demonstration that the expected value of the function c increases and decreases appropriately under the small perturbation εm^*.

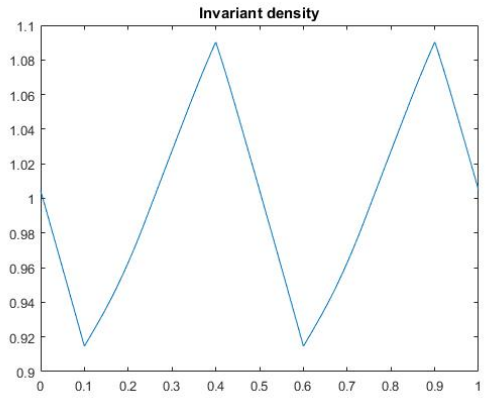
map in order to study a relatively slowly (but still exponentially) mixing[3] system. The subintervals $[0, 1/2]$ and $[1/2, 1]$ are "almost-invariant" because there is only a relatively small probability that points in each of these subintervals are mapped into the complementary subinterval; see Figure 2.6(a).

Let $M \in \mathbb{R}^{n\times n}$ be Ulam's discretisation of the transfer operator of the map T with n partitions. Using Algorithm 4 (see Appendix A.1), we solve problem (2.4.3)–(2.4.6) for the matrix M for $n = 2000$. Figure 2.6 shows the double Lanford map and the approximation of the invariant density f of this map. Figure 2.6(c) shows the optimal perturbation matrix m^* that maximises the linear response of the rate of convergence to the equilibrium and Figure 2.6(d) shows the corresponding linear response u_1^* of the invariant density f. We note that the sign of the matrix m^* is chosen such that the ν in (2.4.9) is negative. The optimal objective is given by $\varrho = \frac{d(\Re(\log \lambda_2(\varepsilon)))}{d\varepsilon}|_{\varepsilon=0} \approx -0.2843$. Figure 2.6(c) shows that most of the large positive values in the perturbation occur in the upper left and lower right blocks of the graph of the double Lanford map, precisely to overcome the almost-invariance of the subintervals $[0, 1/2]$ and $[1/2, 1]$. In order to compensate for these increases,

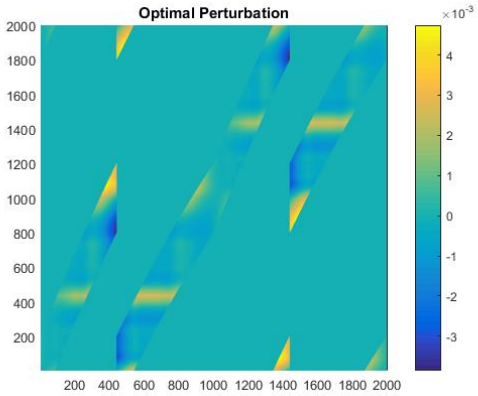
[3]Exponential mixing is guaranteed by expansivity and transitivity of T_{Lan}, which together with the additive noise, yield the stochastic covering condition of Section 2.6.



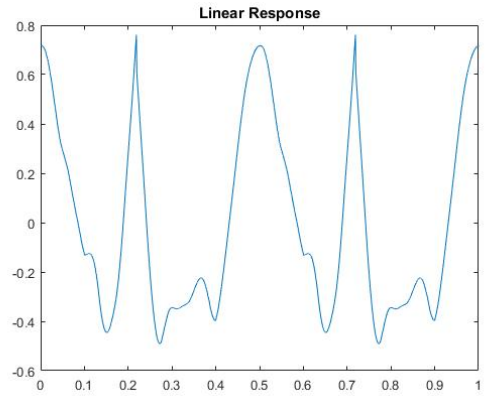
(a) Colourmap of the stochastically perturbed double Lanford map. The colourbar indicates the values of the elements of the matrix.



(b) The invariant density f.



(c) The optimal perturbation m^*. The colourbar indicates the values of the elements of the matrix.



(d) The optimal linear response u_1^*.

Figure 2.6: Solution to the problem of maximising the linear response of the rate of convergence to the equilibrium of the stochastically perturbed double Lanford map.

there are commensurate negative values in the lower left and upper right. The net effect is that more mass leaves each of the almost-invariant sets at each iteration of the stochastic dynamics, leading to an increase in mixing rate.

Table 2.5 illustrates the numerical results. The value of ϱ, namely the estimated derivative of the real part of $\log(\lambda_2)$, minimised over all valid perturbations, is shown in the second column. As n increases, ϱ appears to converge to a fixed value. Let r and l denote the discretised left and right eigenfunctions of $\pi_n L$ corresponding to the second largest eigenvalue, $\pi_n \delta L$ denote the discretised perturbation operator represented by m^*, and $\eta_2 = \langle l, \pi_n \delta L(r) \rangle$, the analogue of (2.4.1). In the

fourth column, we see that the absolute value of the linearisation of the perturbed eigenvalue, $|\lambda_2+\varepsilon\eta_2|$, is close to the absolute value of the optimally perturbed eigenvalue, $|\lambda_2(\varepsilon)^*|$. Finally, to verify the parity of m^* is correct, in Table 5 we observe that the absolute value of the second eigenvalue increases when we perturb in the direction $-\varepsilon m^*$ and decreases as we perturb in the direction εm^*, as required for the perturbation to enhance mixing.

n	ϱ	ε	$\lvert\lambda_2(\varepsilon)^*\rvert - \lvert\lambda_2 + \varepsilon\eta_2\rvert$	$\lvert\lambda_2(-\varepsilon)^*\rvert$	$\lvert\lambda_2\rvert$	$\lvert\lambda_2(\varepsilon)^*\rvert$
1500	-0.2852	1/100	-4.21×10^{-5}	0.84956	0.84715	0.84473
		1/1000	-4.49×10^{-7}	0.84740	0.84715	0.84691
1750	-0.2846	1/100	-4.17×10^{-5}	0.84955	0.84716	0.84473
		1/1000	-4.67×10^{-7}	0.84740	0.84716	0.84691
2000	-0.2843	1/100	-4.26×10^{-5}	0.84955	0.84716	0.84473
		1/1000	-5.57×10^{-7}	0.84740	0.84716	0.84691
5000	-0.2823	1/100	-3.96×10^{-5}	0.84954	0.84716	0.84475
		1/1000	-4.15×10^{-7}	0.84740	0.84716	0.84692
7000	-0.2820	1/100	-3.92×10^{-5}	0.84953	0.84716	0.84475
		1/1000	-4.07×10^{-7}	0.84740	0.84716	0.84692

Table 2.5: Numerical results for the double Lanford Map. Column 1: number of partition elements; Column 2: optimal objective value; Column 3: values of ε; Column 4: linearisation error; Columns 5-7: demonstration that the absolute value of the second eigenvalue increases and decreases appropriately under the small perturbation εm^*.

Chapter 3

Optimal Linear Response for Hilbert-Schmidt Integral Operators and Stochastic Dynamical Systems

In this chapter we will generalise the two optimisation problems considered in Sections 2.3 and 2.4 to Hilbert-Schmidt integral operators; the two optimisation problems are then considered in the setting of deterministic systems with additive noise, which are systems that can be represented as integral operators. In Section 3.1 we obtain linear response formulae for the invariant measure and the dominant eigenvalues of integral-preserving compact operators. In Section 3.2 we introduce the setting and derive the formulae for the linear response of the invariant measure and the dominant eigenvalues of Hilbert-Schmidt integral operators. In Section 3.3 we consider the problems of finding the optimal kernel perturbation to maximise the expectation of a specified observable and to enhance mixing; for both problems we obtain explicit formulae for the optimal perturbations. In Section 3.4 we introduce deterministic systems with additive noise and derive the linear response formulae in this setting. In Section 3.5 we consider the problems of finding the optimal map perturbation to maximise the expectation of a specified observable and to enhance mixing; for both problems we obtain explicit formulae for the optimal perturbation. We conclude in Section 3.6 with numerical applications to stochastically perturbed Pomeau-Manneville map and a weakly mixing interval exchange map.

3.1 Linear Response for Integral-Preserving Compact Operators

In this section we obtain response results for compact operators under suitable perturbations. We consider both the response of the invariant measure and the response of the dominant eigenvalues to the perturbations. In the literature there are several

results describing the way eigenvalues and eigenvectors of suitable classes of operators change when those operators are perturbed in some way (see e.g. [54], [50]). We will consider integral-preserving compact operators, which are not necessarily positive, acting on L^2 that are slightly perturbed in a "differentiable" way.

3.1.1 Existence of Linear Response for the Invariant Measure

Let X be a manifold and let $L^2(X)$ be the space of square integrable functions over the manifold (considered with the Lebesgue measure ℓ). For brevity, we will denote it as simply L^2. To understand the general behaviour of operators preserving the integral, it is important to understand their action on the space of functions having null integral. To this end, let us consider the space of zero average functions

$$V := \left\{ f \in L^2 \ s.t. \ \int f \, d\ell = 0 \right\}.$$

Definition 3.1.1. *We say that an operator $L : L^2 \to L^2$ has exponential contraction of the zero average space V if there are $C \geq 0$ and $\lambda < 0$ such that for all $g \in V$*

$$\|L^n g\|_2 \leq C e^{\lambda n} \|g\|_2 \tag{3.1.1}$$

for all $n \geq 0$.

For $\varepsilon \in [0, \varepsilon_0)$, we consider a family of integral-preserving compact operators $L_\varepsilon : L^2 \to L^2$; we think of L_ε as perturbations of L_0. We say that $f_\varepsilon \in L^2$ is an *invariant function* of L_ε if $L_\varepsilon f_\varepsilon = f_\varepsilon$. We will show that under suitable assumptions the operators L_ε, $\varepsilon \in [0, \varepsilon_0)$, have a family of normalised invariant functions $f_\varepsilon \in L^2$. We also show that for suitable perturbations the invariant functions vary smoothly in L^2 and we obtain an explicit formula for the resulting derivative $\frac{df_\varepsilon}{d\varepsilon}$. We remark that since the operators we consider are not necessarily positive, the invariant functions will not necessarily be positive.

Theorem 3.1.2 (Linear response for integral-preserving compact operators)**.** *Let $L_\varepsilon : L^2 \to L^2$, $\varepsilon \in [0, \varepsilon_0)$, be a family of integral-preserving compact operators: for each $g \in L^2$*

$$\int L_\varepsilon g \, d\ell = \int g \, d\ell. \tag{3.1.2}$$

Then, the operators have invariant functions in L^2: for each ε there is $g_\varepsilon \neq 0$ such that $L_\varepsilon g_\varepsilon = g_\varepsilon$.

Suppose L_0 satisfies the assumption:

(A1) (Mixing of the unperturbed operator) For every $g \in V$,

$$\lim_{n\to\infty} \|L_0^n g\|_2 = 0.$$

Then, the unperturbed operator L_0 has a unique invariant function f_0 such that $\int f_0 \, d\ell = 1$. Furthermore, L_0 has exponential contraction of the zero average space.

If we furthermore suppose that the family of operators L_ε also satisfy the following:

(A2) (L_ε are small perturbations and existence of derivative operator) There exists $K \geq 0$ such that $||L_\varepsilon - L_0||_{L^2\to L^2} \leq K\varepsilon$ for small ε and there is a function $\dot{L}f_0 \in V$ such that

$$\lim_{\varepsilon\to 0} \left\| \frac{(L_\varepsilon - L_0)}{\varepsilon} f_0 - \dot{L}f_0 \right\|_2 = 0.$$

Then, we have the following:

1. *There exists $\varepsilon_2 > 0$ such that for each $0 \leq \varepsilon < \varepsilon_2$, the operator L_ε has a unique invariant functions f_ε such that $\int f_\varepsilon d\ell = 1$.*
2. *The resolvent operator $(Id - L_0)^{-1} : V \to V$ is continuous.*
3. *The linear response formula*

$$\lim_{\varepsilon\to 0} \left\| \frac{f_\varepsilon - f_0}{\varepsilon} - (Id - L_0)^{-1}\dot{L}f_0 \right\|_2 = 0.$$

Proof of Theorem 3.1.2. We start by proving the existence of the invariant functions g_ε for the operators L_ε from the fact that L_ε are compact and integral-preserving. Consider the adjoint operators $L_\varepsilon^* : L^2 \to L^2$ defined by the duality relation $(L_\varepsilon f, g) = (f, L_\varepsilon^* g)$ for all $f, g \in L^2$. Then, by the integral-preserving assumption, we have $(f, L_\varepsilon^* \mathbf{1}) = (L_\varepsilon f, \mathbf{1}) = \int L_\varepsilon f \; d\ell = \int f \; d\ell = (f, \mathbf{1})$. [1] This implies that 1 is in the spectrum of L_ε^* and thus, in the spectrum of L_ε. Since L_ε

[1] We use the notation $\mathbf{1}$ for the constant function and $\mathbf{1}_A$ for the indicator function of the set A.

is compact, its spectrum equals the eigenvalues and we have invariant functions for the operators L_ε.

Now we prove the uniqueness of the normalised invariant function of L_0. Above we proved that L_0 has some invariant function $g_0 \neq 0$. The mixing assumption $(A1)$ implies that $\int g_0 \, d\ell \neq 0$; to see this, we note that if $\int g_0 \, d\ell = 0$, then $g_0 \in V$, and, by $(A1)$, g_0 cannot be a nontrivial fixed point of L_0. We claim that $f_0 = \frac{g_0}{\int g_0 \, d\ell}$ is the unique normalised invariant function for L_0. To see this, suppose there was a second normalised invariant function f_0'; then, $f_0' - f_0$ should be an invariant function in V, which is a contradiction.

To show that L_0 has exponential contraction on V, we first note that for $f \in L^2$, we can write $f = f_0 \int f \, d\ell + [f - f_0 \int f \, d\ell]$. Since $[f - f_0 \int f \, d\ell] \in V$, it follows from $(A1)$ that $L_0^n f \to_{L^2} f_0 \int f \, d\ell$. Thus, the spectrum of L_0 is contained in the unit disk by the spectral radius theorem. Now suppose λ is in the spectrum of L_0 and $|\lambda| = 1$. By the compactness assumption, there is at least an eigenvector f_λ for λ and then we have $||L_0^n(f_\lambda)||_2 = ||f_\lambda||_2$. However, $L_0^n(f_\lambda) \to_{L^2} f_0 \int f_\lambda \, d\ell$, which is not possible unless $\lambda = 1$. Hence, the spectrum of $L_0|_V$ is strictly contained in the unit disk. Thus, by the spectral radius theorem, there is an $n > 0$ such that $||L_0^n|_V||_{L^2 \to L^2} \leq \frac{1}{2}$ and we have exponential contraction of L_0 on V.

From the assumption $||L_\varepsilon - L_0||_{L^2 \to L^2} \leq K\varepsilon$, we have for small enough ε that $||L_\varepsilon^n|_V||_{L^2 \to L^2} \leq \frac{2}{3}$ and therefore, L_ε is also mixing. We can apply the argument above to the operators L_ε and obtain, for each small enough ε, a unique normalised invariant function f_ε. Furthermore, we have

$$\begin{aligned}
\|f_\varepsilon - f_0\|_2 &= \|L_\varepsilon^n f_\varepsilon - L_0^n f_0\|_2 \\
&\leq \|L_\varepsilon^n f_0 - L_0^n f_0\|_2 + \|L_\varepsilon^n f_\varepsilon - L_\varepsilon^n f_0\|_2 \\
&\leq \|L_\varepsilon^n - L_0^n\|_2 \|f_0\|_2 + \|L_\varepsilon^n|_V\|_{L^2 \to L^2} \|f_\varepsilon - f_0\|_2 \\
&\leq \|L_\varepsilon^n - L_0^n\|_2 \|f_0\|_2 + \frac{2}{3}\|f_\varepsilon - f_0\|_2,
\end{aligned}$$

from which we get $\|f_\varepsilon - f_0\|_2 \leq 3\|L_\varepsilon^n - L_0^n\|_{L^2 \to L^2} \|f_0\|_2$. Since $\|L_\varepsilon - L_0\|_{L^2 \to L^2} \leq K\varepsilon$, we have $\|f_\varepsilon - f_0\|_2 \to 0$ as $\varepsilon \to 0$.

Let us consider the resolvent $(\mathrm{Id} - L_0)^{-1}$. Using the exponential contraction of L_0 on V, we now show that $(\mathrm{Id} - L_0)^{-1} : V \to V$ is continuous. We compute

$$\begin{aligned}
\|(\mathrm{Id} - L_0)^{-1}\|_{V\to V} &\leq \|\mathrm{Id}\|_{V\to V} + \left\| \sum_{n=1}^{\infty} L_0^n \right\|_{V\to V} \\
&= 1 + \sup_{\substack{f\in V \\ \|f\|_2=1}} \left\| \sum_{n=1}^{\infty} L_0^n f \right\|_2 \\
&\leq 1 + \sup_{\substack{f\in V \\ \|f\|_2=1}} \sum_{n=1}^{\infty} Ce^{\lambda n}\|f\|_2 \\
&= 1 + \sum_{n=1}^{\infty} Ce^{\lambda n} < \infty,
\end{aligned} \tag{3.1.3}$$

where the last inequality follows from $\lambda < 0$; thus, $(\mathrm{Id} - L_0)^{-1} : V \to V$ is continuous. We remark that since $\dot{L} f_0 \in V$, the resolvent can be computed at $\dot{L} f_0$.

Now we are ready to prove the linear response formula. Since f_0 and f_ε are the invariant functions of L_0 and L_ε, we have

$$(\mathrm{Id} - L_0)\frac{f_\varepsilon - f_0}{\varepsilon} = \frac{1}{\varepsilon}(L_\varepsilon - L_0)f_\varepsilon.$$

By applying the resolvent to both sides we obtain

$$\begin{aligned}
\frac{f_\varepsilon - f_0}{\varepsilon} &= (\mathrm{Id} - L_0)^{-1}\frac{L_\varepsilon - L_0}{\varepsilon} f_\varepsilon \\
&= (\mathrm{Id} - L_0)^{-1}\frac{L_\varepsilon - L_0}{\varepsilon} f_0 + (\mathrm{Id} - L_0)^{-1}\frac{L_\varepsilon - L_0}{\varepsilon}(f_\varepsilon - f_0).
\end{aligned}$$

Moreover, from assumption $(A2)$, we have for sufficiently small ε that

$$\left\| (\mathrm{Id} - L_0)^{-1}\frac{L_\varepsilon - L_0}{\varepsilon}(f_\varepsilon - f_0) \right\|_2 \leq \|(\mathrm{Id} - L_0)^{-1}\|_{V\to V} K \|f_\varepsilon - f_0\|_2.$$

Since we already proved that $\lim_{\varepsilon\to 0} \|f_\varepsilon - f_0\|_2 = 0$, we are left with

$$\lim_{\varepsilon\to 0} \frac{f_\varepsilon - f_0}{\varepsilon} = (\mathrm{Id} - L_0)^{-1}\dot{L} f_0$$

converging in the L^2 norm. □

Remark 3.1.3. *The mixing assumption* $(A1)$ *is required only for the unperturbed operator* L_0*. This requirement is somehow expected by transfer operators associated to random systems having some sort of indecomposability. The assumption is satisfied, for example, if there is an iterate of the transfer operator having a strictly positive kernel, see Corollary 5.7.1 of [62]. In nontrivial cases the assumption can also be verified by a computer aided proof (see [40], Section 5, [41],[68]). The other assumptions of Theorem 3.1.2 can be easily verified in interesting classes of systems and perturbations. In the following sections we apply the theorem to integral operators and suitable perturbations, showing how to perform the necessary estimates.*

Remark 3.1.4. *(spectral picture of* L_0*) As shown in Theorem 3.1.2, if* L_0 *satisfies* $(A1)$ *then the invariant function is unique, up to normalisation; this shows that* 1 *is a simple eigenvalue. Furthermore,* $L^2 = span\{f_0\} \bigoplus V$ *and* L_0 *preserves this direct sum, having only the eigenvalue* 1 *when restricted to the first summand and spectrum strictly inside the unit disk when restricted to* V*. Hence, the spectrum is contained in the unit disk and there is a spectral gap.*

3.1.2 Existence of Linear Response for the Dominant Eigenvalues

In this section we consider the existence of linear response for the "dominant" eigenvalues and provide a formula for the linear response. Let $\mathcal{B}(X_1)$ denote the space of linear operators from the Banach space X_1 to itself and $r(L)$ denote the spectral radius of an operator L; we begin with the following definition.

Definition 3.1.5 ([50], Definition III.7)**.** *Let* $s \in \mathbb{N}_{\geq 0}$*. We say that* $L \in \mathcal{B}(L^2(X))$ *has* s *dominating simple eigenvalues if there exists closed subspaces* H_1 *and* H_2 *such that*

1. $L^2(X) = H_1 \oplus H_2$,
2. $L(H_1) \subset H_1$, $L(H_2) \subset H_2$,
3. $dim(H_1) = s$ *and* $L|_{H_1}$ *has* s *geometrically simple eigenvalues* λ_i, $i = 1, \ldots, s$,
4. $r(L|_{H_2}) < \min\{|\lambda_i| : i = 1, \ldots, s\}$.

We can now state the linear response result for these eigenvalues.

Proposition 3.1.6. *Let* $L_\varepsilon : L^2(X, \mathbb{C}) \to L^2(X, \mathbb{C})$*, where* $\varepsilon \in (-\varepsilon_0, \varepsilon_0) =: I_0$*, be integral-preserving (see (3.1.2)) compact operators. Assume the map* $\varepsilon \mapsto L_\varepsilon$ *is in*

$C^1(I_0, L^2(X,\mathbb{C}))$ and L_0 is mixing (see (A1) in Theorem 3.1.2). Then, $1 \in \sigma(L_0)$ and $r(L_0) = 1$. Let $\mathcal{I} \subset \sigma(L_0) \setminus \{1\}$ be the eigenvalue(s) of maximal modulus; assume they are geometrically simple and let $s := |\mathcal{I}| + 1$. Then there exists an open interval $I_1 \subset I_0$ such that for $\varepsilon \in I_1$, L_ε has s dominating simple eigenvalues. Thus, there exists functions $e_{i,(\cdot)}$, $\hat{e}_{i,(\cdot)} \in C^1(I_1, L^2(X,\mathbb{C}))$ and $\lambda_{i,(\cdot)} \in C^1(I_1,\mathbb{C})$ such that for $\varepsilon \in I_1$ and $i, j = 1, \ldots, s$

(i) $L_\varepsilon e_{i,\varepsilon} = \lambda_{i,\varepsilon} e_{i,\varepsilon}$, $L_\varepsilon^* \hat{e}_{i,\varepsilon} = \lambda_{i,\varepsilon} \hat{e}_{i,\varepsilon}$,

(ii) $\langle e_{i,\varepsilon}, \hat{e}_{j,\varepsilon} \rangle_{L^2(X,\mathbb{C})} = \delta_{i,j}$, *where $\delta_{i,j}$ is the Kronecker delta.*

Furthermore, if we denote by $\dot{\lambda} \in \mathbb{C}$ the value

$$\lim_{\varepsilon \to 0} \left| \frac{\lambda_{i,\varepsilon} - \lambda_{i,0}}{\varepsilon} - \dot{\lambda}_i \right| = 0,$$

then

$$\dot{\lambda}_i = \langle \hat{e}_{i,0}, \dot{L} e_{i,0} \rangle_{L^2(X,\mathbb{C})}, \tag{3.1.4}$$

where $\dot{L} e_{i,0} = \lim_{\varepsilon \to 0} \frac{L_\varepsilon e_{i,0} - L_0 e_{i,0}}{\varepsilon}$.

Proof. From Theorem 3.1.2, and Remark 3.1.4, $1 \in \sigma(L_0)$ and $r(L_0) = 1$.

We now use Theorem III.8 in [50] to obtain the existence of linear response and Corollary III.11 to obtain the formula. We begin by verifying the two hypotheses of Theorem III.8. By assumption, we have that the map $\varepsilon \mapsto L_\varepsilon$ is C^1 and so hypothesis $(H1)$ of Theorem III.8 is satisfied. Since $r(L_0) = 1$, we just need to show that L_0 has s dominating eigenvalues. Let $\lambda_{0,0}$ denote the eigenvalue 1 and let $\mathcal{E} := \{1, \ldots, s\}$ denote the indices of the eigenvalues in $\mathcal{I}$. Since L_0 is a compact operator, the eigenvalues $\lambda_{i,0} \in \mathcal{I}$ are isolated. Let Π_i be the eigenprojection onto the eigenspace of $\lambda_{i,0}$ and $E_i := \Pi_i(L^2(X,\mathbb{C}))$. Define the eigenspaces $E := \bigoplus_{i \in \{0\} \cup \mathcal{E}} E_i$ and $\widetilde{E} := (\mathrm{Id} - \sum_{i \in \{0\} \cup \mathcal{E}} \Pi_i)(L^2(X,\mathbb{C}))$. We thus have:

(1) $L^2(X,\mathbb{C}) = E \oplus \widetilde{E}$.

(2) $L_0(E) \subset (E)$ and $L_0(\widetilde{E}) \subset (\widetilde{E})$.

(3) $\dim(E) = s$ and $L_0|_E$ has s simple eigenvalues $\lambda_{0,0} \cup \mathcal{I}$. This point follows from the assumption that the eigenvalues in $\mathcal{I}$ are geometrically simple and the fact that $\lambda_{0,0}$ is simple (see Theorem 3.1.2).

(4) $r(L_0|_{\widetilde{E}}) < |\lambda_{0,i}|$ where $\lambda_{0,i} \in \mathcal{I}$.

Thus, L_0 satisfies hypothesis $(H2)$ of Theorem III.8 since it has s dominating simple eigenvalues and $r(L_0) = 1$. Hence, from Theorem III.8, the map $\varepsilon \mapsto \lambda_{i,\varepsilon}$ is differentiable at $\varepsilon = 0$.

We can now apply the argument in Corollary III.11 for $\lambda_{i,0}$ to obtain (3.2.9) (the result and proof of Corollary III.11 is for the top eigenvalue; however, the argument still holds for any eigenvalue $\lambda_{i,0}$, $\in \mathcal{I}$ by changing the index value in the proof of the corollary). □

3.2 Application to Hilbert-Schmidt Integral Operators

In this section we apply the results of the previous section to Hilbert-Schmidt integral operators and suitable perturbations. For simplicity we consider $X = [0, 1]$ throughout the chapter and develop the theory in this case. The operators we consider are compact operators on $L^2([0, 1], \mathbb{R})$ (or $L^2([0, 1], \mathbb{C})$) and sometimes for simplicity we will denote $L^2 := L^2([0, 1], \mathbb{R})$.[2] To avoid confusion we point out that in the following we will also consider the space $L^2([0, 1]^2)$ of square integrable real functions on the unit square; this space contains the kernel of the operators we consider.

Let $k \in L^2([0, 1]^2)$ and consider the operator $L : L^2 \to L^2$ defined in the following way: for $f \in L^2$

$$Lf(x) = \int k(x, y)f(y)dy; \tag{3.2.1}$$

such an operator is called a Hilbert-Schmidt integral operator. Such operators may represent the annealed transfer operators of systems having additive noise (see Section 3.4). We now list some well known and basic facts about Hilbert-Schmidt integral operators with kernels in $L^2([0, 1]^2)$:

- The operator $L : L^2 \to L^2$ is bounded and

$$||Lf||_2 \leq ||k||_{L^2([0,1]^2)}||f||_2 \tag{3.2.2}$$

(see [19], Proposition 4.7, II.§4).

[2] We will also denote $L^p := L^p([0, 1], \mathbb{R})$. We will sometimes also write $L^p([0, 1]^n)$ instead of $L^p([0, 1]^n, \mathbb{R})$; this notation will not be used for $L^2([0, 1]^n, \mathbb{C})$.

- If $k \in L^\infty([0,1]^2)$, then

$$||Lf||_\infty \leq ||k||_{L^\infty([0,1]^2)}||f||_1 \tag{3.2.3}$$

  and the operator $L : L^1 \to L^\infty$ is bounded. Furthermore, $\|L\|_{L^p \to L^\infty} \leq \|k\|_{L^\infty([0,1]^2)}$, for $1 \leq p \leq \infty$.
- If for a.e. $y \in [0,1]$ we have

$$\int k(x,y)dx = 1,$$

  then the Hilbert-Schmidt integral operator associated to the kernel k is integral-preserving (satisfies (3.1.2)).
- The operator $L : L^2 \to L^2$ is compact (see [75], §VI.6).

Combining the last two points, we have from Theorem 3.1.2 that such an operator has an invariant function in L^2.

3.2.1 Characterising Valid Perturbations and the Derivative of the Transfer Operator

In this subsection we consider suitable perturbations of integral-preserving Hilbert-Schmidt integral operators such that assumption $(A2)$ of Theorem 3.1.2 can be verified and the derivative operator $\dot{L}$ computed. We begin, however, by first characterising the set of perturbations for which the "integral preserving property" of the operators is preserved.

Consider the set V_{ker} of kernels having zero average in the x direction, defined as

$$V_{\text{ker}} := \left\{ k \in L^2([0,1]^2) : \int k(x,y)dx = 0 \ for \ a.e. \ y \right\}.$$

The following lemma is a characterisation of the perturbations in V_{ker}; such perturbations will send L^2 functions to V as required to apply the resolvent operator. Then we prove that V_{ker} is closed.

Lemma 3.2.1. *Let $A : L^2 \to L^2$ be defined as $Af(x) = \int k(x,y)f(y)dy$. Then, the following are equivalent*

- $A(L^2) \subseteq V$

- $\int k(x,y)dx = 0$ *for a.e.* y.

Proof. Clearly, the second condition implies the first. Conversely, if $\int k(x,y)dx \neq 0$ on a set I of positive measure, then for a sufficently small $\delta > 0$, there is a set S of positive measure such that $\int k(x,y)dx \geq \delta$ or $\int k(x,y)dx \leq -\delta$ for each $y \in S$. Consider $f := \mathbf{1}_S$ and $g := Af$. Then, we have $|\int g(x)dx| \geq \delta$ and $g \notin V$; thus, condition one implies condition two. □

Lemma 3.2.2. *The set* V_{ker} *is a closed vector subspace of* $L^2([0,1]^2)$.

Proof. The fact that V_{ker} is a vector space is clear. For fixed $f \in L^2([0,1])$, the set of $k \in L^2([0,1]^2)$ such that $\int k(x,y)f(y)dx \in V$ is closed. To see this, define the function $K_f : L^2([0,1]^2) \to L^2([0,1])$ as

$$K_f(k) = \int k(x,y)f(y)dy. \tag{3.2.4}$$

By (3.2.2), K_f is continuous. Since V is closed in $L^2([0,1])$, this implies that $K_f^{-1}(V)$ is closed in $L^2([0,1]^2)$. Finally, V_{ker} is closed in $L^2([0,1]^2)$ because $V_{\text{ker}} = \cap_{f \in L^2([0,1])} K_f^{-1}(V)$. □

We now introduce the type of operators and perturbations which we will investigate throughout the chapter. Let $L_\varepsilon : L^2 \to L^2$ be a family of integral operators, with kernels $k_\varepsilon \in L^2([0,1]^2)$, given by

$$L_\varepsilon f(x) = \int k_\varepsilon(x,y)f(y)dy.$$

Lemma 3.2.3. *Let* $k_\varepsilon \in L^2([0,1]^2)$ *for each* $\varepsilon \in [0, \varepsilon_0)$. *Suppose that*

$$k_\varepsilon = k_0 + \varepsilon \cdot \dot{k} + r_\varepsilon, \tag{3.2.5}$$

where $\dot{k},\ r_\varepsilon \in L^2([0,1]^2)$ *and* $||r_\varepsilon||_{L^2([0,1]^2)} = o(\varepsilon)$. *Then, there is a* $K \geq 0$ *such that*

$$||L_\varepsilon - L_0||_{L^2 \to L^2} \leq K\varepsilon. \tag{3.2.6}$$

Furthermore, for every $f \in L^2$,

$$\lim_{\varepsilon \to 0} \left\| \frac{L_\varepsilon f - L_0 f}{\varepsilon} - \int \dot{k}(x,y) f(y) dy \right\|_2 = 0$$

and the derivative operator for this perturbation is given by

$$\dot{L} f(x) = \int \dot{k}(x,y) f(y) dy.$$

Proof. Equation (3.2.6) is a direct application of (3.2.2). We also have

$$\begin{aligned} \frac{L_\varepsilon f - L_0 f}{\varepsilon} &= \int \frac{k_\varepsilon(x,y) - k_0(x,y)}{\varepsilon} f(y) dy \\ &= \int \frac{\varepsilon \dot{k}(x,y) + r_\varepsilon(x,y)}{\varepsilon} f(y) dy \\ &= \int \dot{k}(x,y) f(y) + \int \frac{r_\varepsilon(x,y)}{\varepsilon} f(y) dy. \end{aligned}$$

By (3.2.2), we have

$$\lim_{\varepsilon \to 0} \left\| \int \frac{r_\varepsilon(x,y)}{\varepsilon} f(y) dy \right\|_2 = 0$$

and therefore

$$\lim_{\varepsilon \to 0} \left\| \frac{L_\varepsilon f - L_0 f}{\varepsilon} - \int \dot{k}(x,y) f(y) dy \right\|_2 = 0.$$

□

3.2.2 A Formula for the Linear Response of the Invariant Measure and Continuity with respect to the Kernel

Now we apply Theorem 3.1.2 to Hilbert-Schmidt integral operators and get a linear response formula for L^2 perturbation.

Corollary 3.2.4 (Linear response formula for integral operators)**.** *Suppose $L_\varepsilon : L^2 \to L^2$ are integral-preserving (satisfying (3.1.2)) Hilbert-Schmidt integral operators, with kernels $k_\varepsilon \in L^2([0,1]^2)$ as in (3.2.5). Suppose L_0 satisfies assumption (A1) of Theorem 3.1.2. Then $\dot{k} \in V_{\ker}$, the system has linear response for this perturbation and an explicit formula for it is given by*

$$\lim_{\varepsilon \to 0} \frac{f_\varepsilon - f_0}{\varepsilon} = (Id - L_0)^{-1} \int \dot{k}(x,y) f_0(y) dy \tag{3.2.7}$$

with convergence in L^2.

Proof. Since L_ε, $\varepsilon \in [0, \varepsilon_0)$, is integral perserving, we have $(L_\varepsilon - L_0)(L^2) \subset V$ and therefore, $k_\varepsilon - k_0 \in V_{\ker}$ by Lemma 3.2.1, i.e. $\varepsilon\dot{k} + r_\varepsilon \in V_{\ker}$. Then, for a.e. $y \in [0,1]$ and $\varepsilon \neq 0$, we have

$$\left| \int \dot{k}(x,y)dx \right| \leq \frac{1}{\varepsilon} \int |r_\varepsilon(x,y)|dx \leq \frac{1}{\varepsilon} \|r_\varepsilon\|_{L^2([0,1]^2)}.$$

As $\varepsilon \to 0$, the right hand side approaches 0 and, since $\int \dot{k}(x,y)dx$ is independent of ε, we have $\int \dot{k}(x,y)dx = 0$ for a.e. $y \in [0,1]$, i.e. $\dot{k} \in V_{\ker}$.

Noting that the operators L_ε are compact, integral-preserving and satisfy assumptions $(A1)$ and $(A2)$ (this follows from Lemma 3.2.3), we can apply Theorem 3.1.2 to obtain

$$\lim_{\varepsilon \to 0} \left\| \frac{f_\varepsilon - f_0}{\varepsilon} - (\mathrm{Id} - L_0)^{-1} \int \dot{k}(x,y) f_0(y) dy \right\|_2 = 0.$$

□

Now we show that the linear response associated to a certain infinitesimal perturbation is continuous with respect to the kernel perturbation. This will be used in Section 3.3 for the proof of the existence of solutions of our main optimisation problems.

Consider the transfer operator L_0, having a kernel $k_0 \in L^2([0,1]^2)$, and a set of infinitesimal perturbations $P \subset V_{\ker}$ of k_0. Suppose L_ε is a perturbation of L_0 satisfying the assumptions of Lemma 3.2.3. By Corollary 3.2.4, the linear response will depend on the first order term of the perturbation, $\dot{k} \in P$, allowing us to define the function $R : P \to V$ by

$$R(\dot{k}) := (\mathrm{Id} - L_0)^{-1} \int \dot{k}(x,y) f_0(y) dy. \tag{3.2.8}$$

Here R is well defined thanks to Corollary 3.2.4. Furthermore, we have the following result.

Lemma 3.2.5. *The function $R : P \to V$ defined in (3.2.8) is continuous.*

Proof. The proof is straightforward using (3.2.2). Considering two perturbations $\dot{k}_1$ and $\dot{k}_2$with $||\dot{k}_1 - \dot{k}_2||_{L^2([0,1]^2)} \leq l$ we get

$$\begin{aligned} \|R(\dot{k}_1) - R(\dot{k}_2)\|_2 &= \left\| (\mathrm{Id} - L_0)^{-1} \int [\dot{k}_1(x,y) - \dot{k}_2(x,y)] f_0(y) dy \right\|_2 \\ &\leq l||(\mathrm{Id} - L_0)^{-1}||_{V\to V}||f_0||_2. \end{aligned}$$

□

3.2.3 A Formula for the Linear Response of the Dominant Eigenvalues and Continuity with respect to the Kernel

We begin by applying Proposition 3.1.6 to Hilbert-Schmidt integral operators and obtain a linear response formula for L^2 perturbations. Then we show continuity of the response with respect to the kernel.

Corollary 3.2.6. *Suppose $L_\varepsilon : L^2([0,1],\mathbb{C}) \to L^2([0,1],\mathbb{C})$ are integral-preserving (satisfying (3.1.2)) Hilbert-Schmidt integral operators, with kernels $k_\varepsilon \in L^2([0,1]^2)$ as in (3.2.5). Suppose L_0 satisfies (A1) of Theorem 3.1.2. Let $\lambda_0 \in \mathbb{C}$ be an eigenvalue of L_0 with the largest magnitude strictly inside the unit circle and assume that λ_0 is geometrically simple. Then, there exists $\dot{\lambda} \in \mathbb{C}$ such that*

$$\lim_{\varepsilon\to 0} \left| \frac{\lambda_\varepsilon - \lambda_0}{\varepsilon} - \dot{\lambda} \right| = 0.$$

Furthermore,

$$\begin{aligned} \dot{\lambda} = &\int_0^1 \int_0^1 \dot{k}(x,y) \left(\Re(\hat{e})(x)\Re(e)(y) + \Im(\hat{e})(x)\Im(e)(y)\right) dydx \\ &+ i \int_0^1 \int_0^1 \dot{k}(x,y) \left(\Im(\hat{e})(x)\Re(e)(y) - \Re(\hat{e})(x)\Im(e)(y)\right) dydx, \end{aligned} \tag{3.2.9}$$

where $e \in L^2([0,1],\mathbb{C})$ is the eigenvector of L_0 associated to the eigenvalue λ_0, $\hat{e} \in L^2([0,1],\mathbb{C})$ is the eigenvector of L_0^* associated to the eigenvalue λ_0 and $\dot{L}$ is the operator in Lemma 3.2.3.

Proof. Since $k_\varepsilon \in L^2([0,1]^2)$, the operator $L_\varepsilon : L^2([0,1],\mathbb{C}) \to L^2([0,1],\mathbb{C})$ is compact; by assumption, it also satisfies (3.1.2). From Lemma 3.2.3, the map $\varepsilon \mapsto L_\varepsilon$ is

C^1. Hence, by Proposition 3.1.6, we have $\dot{\lambda} = \langle \hat{e}, \dot{L}e \rangle_{L^2([0,1],\mathbb{C})}$. Finally, we compute

$$\begin{aligned}
\dot{\lambda} = \langle \hat{e}, \dot{L}e \rangle_{L^2([0,1],\mathbb{C})} &= \int_0^1 \hat{e}(x)\overline{\dot{L}e}(x)dx \\
&= \int_0^1 \hat{e}(x)\overline{\int_0^1 \dot{k}(x,y)e(y)dydx} \\
&= \int_0^1 \int_0^1 \dot{k}(x,y)\hat{e}(x)\bar{e}(y)dydx \\
&= \int_0^1 \int_0^1 \dot{k}(x,y)\left(\Re(\hat{e})(x)\Re(e)(y) + \Im(\hat{e})(x)\Im(e)(y)\right)dydx \\
&\quad + i\int_0^1 \int_0^1 \dot{k}(x,y)\left(\Im(\hat{e})(x)\Re(e)(y) - \Re(\hat{e})(x)\Im(e)(y)\right)dydx.
\end{aligned}$$

□

We also have the following.

Lemma 3.2.7. *Let $P \subset L^2([0,1]^2)$ be a family of allowable perturbations. Let $\widetilde{R} : P \to \mathbb{C}$, defined as*

$$\widetilde{R}(\dot{k}) := \lim_{\varepsilon \to 0} \frac{\lambda_\varepsilon - \lambda_0}{\varepsilon},$$

where λ_ε is as in Corollary 3.2.6, denote the linear response of the system to the perturbation $\dot{k}$. Then, the function $\widetilde{R} : P \to \mathbb{C}$ is continuous.

Proof. Consider two perturbations $\dot{k}_1$ and $\dot{k}_2$ with $||\dot{k}_1 - \dot{k}_2||_{L^2([0,1]^2)} \leq l$. Let $H(x,y) := \hat{e}(x)\bar{e}(y)$. We then have

$$\begin{aligned}
|\widetilde{R}(\dot{k}_1) - \widetilde{R}(\dot{k}_2)| &= \left| \int_0^1 \int_0^1 (\dot{k}_1(x,y) - \dot{k}_2(x,y))\hat{e}(x)\bar{e}(y)dydx \right| \\
&= |\langle \dot{k}_1 - \dot{k}_2, \bar{H} \rangle_{L^2([0,1]^2,\mathbb{C})}| \\
&\leq \|\dot{k}_1 - \dot{k}_2\|_{L^2([0,1]^2)} \|H\|_{L^2([0,1]^2,\mathbb{C})} \leq l\|H\|_{L^2([0,1]^2,\mathbb{C})}.
\end{aligned}$$

□

3.3 Optimal Linear Response for Kernel Perturbations

Having studied the linear response properties of Hilbert-Schmidt integral operators in the previous section, we now begin with the central part of the chapter and consider two important optimisation problems. The first problem is to find the

optimal infinitesimal perturbation that maximises the change in the expectation of a given observable and the second problem is to find an optimal infinitesimal perturbation in order to enhance mixing. These problems were considered in the case of finite-state Markov chains in Chapter 2.

In this section, we will show that, in the cases where linear response holds, the problems reduce to the optimisation of a linear continuous functional on a convex set. We show that this problem has a solution and the solution is unique if the set of allowed infinitesimal perturbations is strictly convex. In Subsection 3.3.1 we introduce the abstract setting in which both optimisation problems are situated; we also provide an explicit form of the set of allowable perturbations that we later use to obtain unique solutions to the optimisation problems. In Subsection 3.3.2 we formulate the problem of optimising the expectation of a given observable and obtain an explicit formula for the optimal perturbation. In Subsection 3.3.3 we construct a sequence that approximates the optimal solution obtained in Subsection 3.3.2. In Subsection 3.3.4 we formulate the problem of enhancing mixing and provide an explicit formula for the optimal solution; we conclude in Subsection 3.3.5 by constructing a sequence that approximates the optimal solution.

3.3.1 General Optimisation Setting

We consider the problem of maximising a continuous linear function on the set P. The existence and uniqueness of an optimal perturbation depends on the properties of P. It is natural to think of the set of allowed perturbations P as a convex set because if two kinds of perturbations on the system are possible, then their convex combination (applying the two perturbation with different intensity) should also be possible. We now recall some general results (adapted for our purposes) on optimising a linear continuous functional on convex sets.

The problem is to find $\dot{k}$ such that

$$S(\dot{k}) = \max_{k \in P} S(k), \tag{3.3.1}$$

where $S : \mathcal{H} \to \mathbb{R}$ is a continuous linear function, $\mathcal{H}$ is a separable Hilbert space and $P \subset \mathcal{H}$.

Proposition 3.3.1 (Existence of the optimal solution)**.** *Let P be convex, bounded and closed in $\mathcal{H}$. Then, problem (3.3.1) has at least one solution.*

Proof. Since P is bounded and S is continuous, we have that $\sup_{k\in P} S(k) < \infty$. Consider a maximising sequence k_n such that $\lim_{n\to\infty} S(k_n) = \sup_{k\in P} S(k)$. Then, k_n has a subsequence k_{n_j} converging in the weak topology. Since P is strongly closed and convex in $\mathcal{H}$, we have that it is weakly closed. This implies that $\overline{k} := \lim_{j\to\infty} k_{n_j} \in P$. Also, since $S(k)$ is continuous and linear, it is continuous in the weak topology. Then we have that $S(\overline{k}) = \lim_{j\to\infty} S(k_{n_j}) = \sup_{k\in P} S(k)$ and we get a maximum. □

Uniqueness of the optimal solution will be provided by strict convexity of the feasible set.

Definition 3.3.2. *We say that a convex closed set $A \subseteq \mathcal{H}$ is strictly convex if for every translate A_f of A such that $0 \in A_f$, we have that for each $x, y \in A_f$, $x \neq y$, there is a $\delta > 0$ such that $(1+\delta)\frac{x+y}{2} \in A_f$.*

Proposition 3.3.3 (Uniqueness of the optimal solution)**.** *Suppose P is strictly convex and S is not constant on P.*[3] *Then, the optimal solution to (3.3.1) is unique.*

Proof. First we remark that for the maximisation problem a translation of P is not relevant. Hence, we can assume that $0 \in P$. Since $S(0) = 0$ (because of the linearity of S) and S is not constant, we either have $\max_{k\in P} S(k) > 0$ or $\max_{k\in P} S(k) = 0$ and there is some $k \in P$ such that $S(k) < 0$. Consider the first case and suppose there are two perturbations $k_1, k_2 \in P$, $k_1 \neq k_2$, such that

$$S(k_1) = S(k_2) = \max_{k\in P} S(k) > 0;$$

then

$$\max_{k\in P} S(k) = S\left(\frac{k_1+k_2}{2}\right) > 0.$$

[3] We remark that P could, for example, be entirely contained in the kernel of S. This is possible for certain, not very meaningful, choices of P and S. This assumption is meant to avoid this case.

Since P is strictly convex, there is a $\delta > 0$ such that $(1+\delta)\frac{k_1+k_2}{2} \in P$ and

$$\begin{aligned} S\left((1+\delta)\frac{k_1+k_2}{2}\right) &= (1+\delta)S(k_1) \\ &> S(k_1). \end{aligned}$$

But this contradicts the optimality of k_1; thus, the solution is unique in the case when $\max_{k\in P} S(k) > 0$.

Now consider the second case in which $\max_{k\in P} S(k) = 0$ and there is some $k \in P$ such that $S(k) < 0$. Let $P_1 = P - k$, a translation of the set P; we have that $0, -k \in P_1$ and $S(-k) > 0$. Hence, $\max_{k\in P_1} S(k) > 0$ and we can apply the argument above to deduce the uniqueness of the solution. □

The example below is of a strictly convex set that we will use regularly.

Example 3.3.4. *For $\mathcal{H} = L^2([0,1]^2)$, the intersection of a strong ball of $L^2([0,1]^2)$ with some closed vector subspace is strictly convex according to Definition 3.3.2. The set $P = B_1 \cap V_{\text{ker}}$, where B_1 denotes the unit ball in $L^2([0,1]^2)$, is one natural example of a strictly convex set of allowable perturbations.*

Thus far, we have not required that the perturbed kernel k_ε in (3.2.5) to be a stochastic kernel (i.e. $k_\varepsilon(x,y) \geq 0$ and $\int k_\varepsilon(x,y)dx = 1$). However, such an assumption is natural and, in the last part of this subsection, we will specify a set of allowable perturbations $P_l \subset V_{\text{ker}}$ such that the perturbed kernel $k_\varepsilon := k_0 + \varepsilon\dot{k}$ is non-negative (and thus a stochastic kernel since the condition $\int k_\varepsilon(x,y)dx = 1$ follows from the fact that $\dot{k} \in V_{\text{ker}}$).

Let $k_0 \in L^\infty([0,1]^2)$ be a stochastic kernel. Before we specify the set of allowable perturbations, we note the following result for mixing Hilbert-Schmidt integral operators with essentially bounded stochastic kernels.

Lemma 3.3.5. *Let $L : L^2 \to L^2$ be a Hilbert Schmidt integral operator with a mixing the stochastic kernel $k \in L^\infty([0,1]^2)$ (satisfies (A1) of Theorem 3.1.2). Then, there exists a unique probability density $f \in L^\infty$ such that $Lf = f$.*

Proof. Since k is a stochastic kernel, L_0 satisfies (3.1.2). Thus, we can apply Theorem 3.1.2 to conclude that there exists a unique $f \in L^2$, $\int f\, d\ell = 1$, such that

$Lf = f$. Noting that $k \in L^\infty([0,1]^2)$, we have from inequality (3.2.3) that $f \in L^\infty$. Let k^j be the kernel of the operator L^j. Since k is a stochastic kernel, we have

$$\begin{aligned} |k^2(x,y)| &= \left| \int k(x,z)k(z,y)dz \right| \leq \int |k(x,z)k(z,y)|dz \\ &\leq \|k\|_{L^\infty([0,1]^2)} \int k(z,y)dz = \|k\|_{L^\infty([0,1]^2)}; \end{aligned}$$

from this, it easily follows that $\|k^j\|_{L^\infty([0,1]^2)} \leq \|k\|_{L^\infty([0,1]^2)}$. Thus, for any probability density $g \in L^1$, we have $\|L^j g\|_\infty \leq \|k\|_{L^\infty([0,1]^2)}$; thus, by Corollary 5.2.2 in [62], there exists a probability density $\hat{f}$ such that $L\hat{f} = \hat{f}$. Since f is the unique invariant function with integral 1, we have $\hat{f} = f$; thus, f is a probability density. □

Now, in order that perturbations preserve the non-negativity property of stochastic kernels, we will consider perturbations to k_0 inside the interior of its support. To this end, let $0 < l < 1, F := \{(x,y) \in [0,1]^2 : k_0(x,y) \geq l\}$ and

$$S_{k_0,l} := \{k \in L^2([0,1]^2) : \text{supp}(k) \subseteq F\}.$$

Lemma 3.3.6. *The set $S_{k_0,l}$ is a closed subspace of $L^2([0,1]^2)$.*

Proof. The fact that $S_{k_0,l}$ is a subspace is clear. Let $\{k_n\} \subset S_{k_0,l}$ and suppose $k_n \to_{L^2} k \in L^2([0,1]^2)$; also, suppose $\{(x,y) \in [0,1]^2 : k_0(x,y) < l\}$ is not a null set. Then, we have

$$\int \int_{\{k_0 \geq l\}} (k_n(x,y) - k(x,y))^2 dydx + \int \int_{\{k_0 < l\}} k(x,y)^2 dxdy \to 0.$$

Since $\int \int_{\{k_0 \geq l\}} (k_n(x,y) - k(x,y))^2 dydx \geq 0$, if $\int \int_{\{k_0 < l\}} k(x,y)^2 dxdy > 0$ then we obtain a contradiction; thus, $\int \int_{\{k_0 < l\}} k(x,y)^2 dxdy = 0$ and therefore $k = 0$ a.e. on $\{(x,y) \in [0,1]^2 : k_0(x,y) < l\}$. Hence, $S_{k_0,l}$ is closed. □

Main application: The set of allowable perturbations that we will consider for this section is $P_l := V_{\text{ker}} \cap S_{k_0,l} \cap B_1$, where B_1 is the unit ball in $L^2([0,1]^2)$. Since $S_{k_0,l}$ and V_{ker} are closed subspaces, $V_{\text{ker}} \cap S_{k_0,l}$ is itself a Hilbert space; hence, P_l is strictly convex.

3.3.2 *Explicit Formula for the Optimal Perturbation for Maximising the Expectation of an Observable*

Let $c \in L^\infty$ be a given observable. We consider the problem of finding an infinitesimal perturbation that maximises the expectation of c. The perturbations we consider are to the kernels of Hilbert-Schmidt integral operators and they are of the form (3.2.5).

If we denote by

$$E_{c,\varepsilon} := \int c\ f_\varepsilon\ d\ell$$

the average of c with respect to the perturbed invariant density f_ε, we have

$$\left.\frac{dE_{c,\varepsilon}}{d\varepsilon}\right|_{\varepsilon=0} = \lim_{\varepsilon\to 0}\frac{E_{c,\varepsilon}-E_{c,0}}{\varepsilon} = \lim_{\varepsilon\to 0}\int c\ \frac{f_\varepsilon - f_0}{\varepsilon}\ d\ell = \int c\ R(\dot{k})\ d\ell,$$

where the last equality follows from the weak convergence to $R(\dot{k})$ in L^2 (this follows from the strong L^2 convergence in (3.2.7)). To formalise the problem of finding the optimal perturbation for c, we try to find a perturbation $\dot{k}$ belonging to P_l for which the linear response of the system maximises the value of $\frac{dE_{c,\varepsilon}}{d\varepsilon}$. This is formalised in the following problem: find $\dot{k} \in P_l$ such that

$$\left\langle c, R(\dot{k})\right\rangle_{L^2([0,1],\mathbb{R})} = \max_{k\in P_l}\left\langle c, R(k)\right\rangle_{L^2([0,1],\mathbb{R})}. \tag{3.3.2}$$

Corollary 3.3.7. *The optimisation problem (3.3.2) has a unique solution.*

Proof. We apply the general existence and uniqueness results of Propositions 3.3.1 and 3.3.3 to problem (3.3.2). Let $\mathcal{H} = P_l$ (being a closed subspace of a Hilbert space, P_l is a Hilbert space itself) and $S(k) = \langle c, R(k)\rangle_{L^2([0,1],\mathbb{R})}$. By Lemma 3.2.5, R is continuous; thus, $\langle c, R(k)\rangle_{L^2([0,1],\mathbb{R})}$ is continuous. Since P_l is strictly convex, we can apply Proposition 3.3.3 to obtain the uniqueness of the solution. □

Since the objective function in (3.3.2) is linear in $\dot{k}$, the maximum will occur on $\partial B_1 \cap V_{\ker} \cap S_{k_0,l}$ (i.e. we only need to consider the optimisation over the unit

sphere and not the unit ball). Furthermore, for $f \in L^2$, we have

$$\begin{aligned}\langle f, R(\dot{k})\rangle_{L^2([0,1],\mathbb{R})} &= \langle f - \langle f, f_0\rangle_{L^2([0,1],\mathbb{R})}\mathbf{1} + \langle f, f_0\rangle_{L^2([0,1],\mathbb{R})}\mathbf{1}, R(\dot{k})\rangle_{L^2([0,1],\mathbb{R})} \\ &= \langle f - \langle f, f_0\rangle_{L^2([0,1],\mathbb{R})}\mathbf{1}, R(\dot{k})\rangle_{L^2([0,1],\mathbb{R})},\end{aligned}$$

since $R(\dot{k}) \in V$. From $\int f_0(x)dx = 1$, we have that $f \mapsto \langle f, f_0\rangle_{L^2([0,1],\mathbb{R})}\mathbf{1}$ is a projection onto $\text{span}\{\mathbf{1}\}$ and so $f \mapsto f - \langle f, f_0\rangle_{L^2([0,1],\mathbb{R})}\mathbf{1}$ is a projection onto $\text{span}\{f_0\}^\perp$. Thus, the objective function has the same value for f and the projection of f onto $\text{span}\{f_0\}^\perp$; hence, without loss of generality, we assume that $c \in W := \text{span}\{f_0\}^\perp \cap L^\infty$. Thus, we consider the following reformulation of problem (3.3.2): for $c \in W$

$$\min_{\dot{k} \in V_{\text{ker}} \cap S_{k_0,l}} \quad -\left\langle c, R(\dot{k})\right\rangle_{L^2([0,1],\mathbb{R})} \tag{3.3.3}$$

$$\text{subject to} \quad \|\dot{k}\|^2_{L^2([0,1]^2)} - 1 = 0. \tag{3.3.4}$$

Theorem 3.3.8. *Let $L_0 : L^2 \to L^2$ be a Hilbert-Schmidt integral operator with the stochastic kernel $k_0 \in L^\infty([0,1]^2)$. Suppose that L_0 satisfies $(A1)$ of Theorem 3.1.2 and let $F_y := \{x \in [0,1] : (x,y) \in F\}$. Then, the unique solution to the optimisation problem (3.3.3)–(3.3.4) is*

$$\dot{k}(x,y) = \begin{cases} \frac{f_0(y)}{\alpha}\left(((Id - L_0^*)^{-1}c)(x) - \frac{\int_{F_y}((Id-L_0^*)^{-1}c)(z)dz}{\ell(F_y)}\right) & (x,y) \in F, \\ 0 & \text{otherwise}, \end{cases} \tag{3.3.5}$$

where $\alpha > 0$ is selected so that $\|\dot{k}\|_{L^2([0,1]^2)} = 1$. Furthermore, if k_0 is such that $L_0 : L^1 \to L^1$ is compact, then $\dot{k} \in L^\infty([0,1]^2)$.

Remark 3.3.9. *Using the fact that k_0 is an essentially bounded stochastic kernel, and that $\dot{k} \in L^\infty([0,1]^2) \cap V_{\text{ker}}$, we can first conclude that $k_\varepsilon := k_0 + \varepsilon\dot{k}$ satisfies $\int k_\varepsilon(x,y)dx = 1$ for a.e. y. Secondly, as we are only perturbing at values where $k_0 \geq l > 0$, and since $\dot{k}$ is essentially bounded, there exists a sufficiently small $\varepsilon_0 > 0$ such that $k_\varepsilon \geq 0$ a.e. for all $\varepsilon \in (0, \varepsilon_0)$; thus, for $\varepsilon \in (0, \varepsilon_0)$, k_ε is a stochastic kernel.*

Remark 3.3.10. *A criteria for L_0 to be compact on L^1 (see [25]) is the following: Given $\delta > 0$ there exists $\beta > 0$ such that for a.e. $x \in [0,1]$ and $\gamma \in \mathbb{R}$ with $|\gamma| < \beta$,*

$$\int_{\mathbb{R}} \left|\tilde{k}(x, y+\gamma) - \tilde{k}(x,y)\right| dy < \delta,$$

where

$$\tilde{k}(x,y) = \begin{cases} k_0(x,y) & y \in [0,1], \\ 0 & \text{otherwise.} \end{cases}$$

An example of kernels that satisfy this are:

- *Essentially bounded kernels $k_0 : [0,1] \times [0,1] \to \mathbb{R}$ that are uniformly continuous in the second coordinate.*

See [25] for compactness of L_0 on L^1 in a more general setting.

The following lemma will be needed in our proof of Theorem 3.3.8. Note that this is a different statement to continuity of $(\mathrm{Id} - L_0)^{-1}$, which was treated in the proof of Theorem 3.1.2.

Lemma 3.3.11. *Consider the closed subspace $span\{f_0\}^\perp \subset L^2$ equipped with the L^2 norm. Then, the operator $(Id - L_0^*)^{-1} : span\{f_0\}^\perp \to span\{f_0\}^\perp$ is bounded.*

Proof. We begin by finding the kernel and range of the operator $\mathrm{Id} - L_0^*$. Recall that $L_0(V) \subset V$ and that L_0 has a one-dimensional eigenspace ($\mathrm{span}\{f_0\}$ with eigenvalue 1). Thus, we have $\ker(\mathrm{Id} - L_0) = \mathrm{span}\{f_0\}$ and $\mathrm{ran}(\mathrm{Id} - L_0) \subset V$. Recalling that $L_0 : V \to V$ is compact and $f_0 \notin V$, we have by the Fredholm alternative (see [23], VII.11) that for any $g \in V$, there exists a unique $h \in V$ such that $g = (\mathrm{Id} - L_0)h$. Hence, $\mathrm{ran}(\mathrm{Id} - L_0) = V$. Since V is closed, the range of $\mathrm{Id} - L_0$ is closed and so, by the Closed Range Theorem (Theorem 5.13, IV-§5.2,[54]), we have $\mathrm{ran}((\mathrm{Id} - L_0)^*) = \ker(\mathrm{Id} - L_0)^\perp = \mathrm{span}\{f_0\}^\perp$, which is a co-dimension 1 space, and $\ker((\mathrm{Id} - L_0)^*) = \mathrm{ran}(\mathrm{Id} - L_0)^\perp = V^\perp = \mathrm{span}\{\mathbf{1}\}^{\perp\perp} = \mathrm{span}\{\mathbf{1}\}$, where the last equality follows from Corollary 1.41 in III-§1.8 [54] and the fact that $\mathrm{span}\{\mathbf{1}\}$ is a finite-dimensional closed subspace of L^2.

To prove that $(\mathrm{Id} - L_0^*)^{-1} : \mathrm{span}\{f_0\}^\perp \to \mathrm{span}\{f_0\}^\perp$ is bounded, we will use the Inverse Mapping Theorem (Theorem III.11, [75]). Since the integral operator L_0^* has

an L^2 kernel, by (3.2.2) and the triangle inequality it follows that $\mathrm{Id} - L_0^*$ is bounded. Also, from the Fredholm alternative argument above, $\mathrm{Id} - L_0^*$ is surjective. Thus, to apply the Inverse Mapping Theorem, we just need to show that $\mathrm{Id} - L_0^*$ is injective on $\mathrm{span}\{f_0\}^\perp$. Let $f_1, f_2 \in \mathrm{span}\{f_0\}^\perp$ be such that $(\mathrm{Id} - L_0^*)f_1 = (\mathrm{Id} - L_0^*)f_2$. Thus, $f_1 - f_2 \in \ker(\mathrm{Id} - L_0^*) = \mathrm{span}\{\mathbf{1}\}$ and so $f_1 - f_2 = \gamma\mathbf{1}$ for some $\gamma \in \mathbb{R}$. Since $f_1 - f_2 \in \mathrm{span}\{f_0\}^\perp$, we have that $0 = \int (f_1(x) - f_2(x))f_0(x)dx = \gamma \int f_0(x)dx$ and so $\gamma = 0$ (since $\int f_0(x)dx = 1$), i.e. $f_1 = f_2$; thus, $(\mathrm{Id} - L_0^*)$ is injective and the result follows. □

Proof of Theorem 3.3.8. We will use the method of Lagrange multipliers to derive the expression (3.3.5) from the first-order necessary conditions and then show that such a $\dot{k}$ satisfies the second-order sufficient conditions. To this end, we consider the following Lagrangian function

$$\mathcal{L}(\dot{k}, \lambda) := f(\dot{k}) + \lambda g(\dot{k}),$$

where $f(\dot{k}) := -\langle c, R(\dot{k})\rangle_{L^2([0,1],\mathbb{R})}$, $g(\dot{k}) := \|\dot{k}\|^2_{L^2([0,1]^2)} - 1$ and $\dot{k} \in V_{\mathrm{ker}} \cap S_{k_0,l}$.

Necessary conditions: We want to find $\dot{k}$ and λ that satisfy the first-order necessary conditions:

$$\begin{aligned} g(\dot{k}) &= 0 \\ D_{\dot{k}}\mathcal{L}(\dot{k}, \lambda)\tilde{k} &= 0 \text{ for all } \tilde{k} \in V_{\mathrm{ker}} \cap S_{k_0,l}, \end{aligned}$$

where $D_{\dot{k}}\mathcal{L}(\dot{k}, \lambda) \in \mathcal{B}(L^2([0,1]^2), \mathbb{R})$ is the Frechet derivative with respect to the variable $\dot{k}$ (Theorem 2, §7.7, [67]). Note that since f is linear, we have $(D_{\dot{k}}f)\tilde{k} = f(\tilde{k})$. Also, we have that $(D_{\dot{k}}g)\tilde{k} = 2\langle \dot{k}, \tilde{k}\rangle_{L^2([0,1]^2)}$ since

$$\begin{aligned} &\frac{|g(\dot{k} + \tilde{k}) - g(\dot{k}) - 2\langle \dot{k}, \tilde{k}\rangle_{L^2([0,1]^2)}|}{\|\tilde{k}\|_{L^2([0,1]^2)}} \\ &= \frac{|\|\dot{k} + \tilde{k}\|^2_{L^2([0,1]^2)} - \|\dot{k}\|^2_{L^2([0,1]^2)} - 2\langle \dot{k}, \tilde{k}\rangle_{L^2([0,1]^2)}|}{\|\tilde{k}\|_{L^2([0,1]^2)}} \\ &= \frac{|\langle \dot{k} + \tilde{k}, \dot{k} + \tilde{k}\rangle_{L^2([0,1]^2)} - \langle \dot{k}, \dot{k}\rangle_{L^2([0,1]^2)} - 2\langle \dot{k}, \tilde{k}\rangle_{L^2([0,1]^2)}|}{\|\tilde{k}\|_{L^2([0,1]^2)}} \end{aligned}$$

$$= \frac{|\langle \tilde{k}, \tilde{k} \rangle_{L^2([0,1]^2)}|}{\|\tilde{k}\|_{L^2([0,1]^2)}} = \|\tilde{k}\|_{L^2([0,1]^2)}.$$

Thus, for the necessary conditions of the Lagrange multiplier method to be satisfied, we need that

$$D_{\dot{k}} \mathcal{L}(\dot{k}, \lambda)\tilde{k} = (D_{\dot{k}} f)\tilde{k} + \lambda (D_{\dot{k}} g)\tilde{k} = f(\tilde{k}) + 2\lambda \langle \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2)} = 0 \tag{3.3.6}$$

for all $\tilde{k} \in V_{\ker} \cap S_{k_0,l}$ and

$$g(\dot{k}) = 0. \tag{3.3.7}$$

Noting Lemma 3.3.11 and the fact that $c \in W$, we have

$$\begin{aligned}
&f(\tilde{k}) + 2\lambda \langle \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2)} \\
&\quad = -\langle c, R(\tilde{k}) \rangle_{L^2([0,1],\mathbb{R})} + 2\lambda \langle \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2)} \\
&\quad = -\left\langle c, (\mathrm{Id} - L_0)^{-1} \int \tilde{k}(x,y) f_0(y) dy \right\rangle_{L^2([0,1],\mathbb{R})} + 2\lambda \langle \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2)} \\
&\quad = \left\langle -(\mathrm{Id} - L_0^*)^{-1} c, \int \tilde{k}(x,y) f_0(y) dy \right\rangle_{L^2([0,1],\mathbb{R})} + \langle 2\lambda \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2)} \\
&\quad = \int \int -((\mathrm{Id} - L_0^*)^{-1} c)(x) \tilde{k}(x,y) f_0(y) dy dx + \int \int 2\lambda \dot{k}(x,y) \tilde{k}(x,y) dy dx \\
&\quad = \int \int \left[-((\mathrm{Id} - L_0^*)^{-1} c)(x) f_0(y) + 2\lambda \dot{k}(x,y) \right] \tilde{k}(x,y) dy dx.
\end{aligned} \tag{3.3.8}$$

We claim that

$$\dot{k}(x,y) = \frac{1}{2\lambda} \mathbf{1}_F(x,y) f_0(y) \left(((\mathrm{Id} - L_0^*)^{-1} c)(x) - \frac{1}{\ell(F_y)} \int_{F_y} ((\mathrm{Id} - L_0^*)^{-1} c)(z) dz \right)$$

satisfies the necessary condition (3.3.6). To verify this, we compute

$$\begin{aligned}
f(\tilde{k}) + 2\lambda \langle \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2)} &= \int \int \left[-((\mathrm{Id} - L_0^*)^{-1} c)(x) f_0(y) + 2\lambda \dot{k}(x,y) \right] \tilde{k}(x,y) dy dx \\
&= -\int \int_F f_0(y) \frac{1}{\ell(F_y)} \int_{F_y} ((\mathrm{Id} - L_0^*)^{-1} c)(z) dz \tilde{k}(x,y) dy dx \\
&= 0
\end{aligned}$$

for every $\tilde{k} \in V_{\ker} \cap S_{k_0,l}$ because of Lemma 3.2.1 and the fact that $f_0(y)\frac{1}{\ell(F_y)}\int_{F_y}((\mathrm{Id}-L_0^*)^{-1}c)(z)dz$ is a function of one variable. To check that $\dot{k} \in V_{\ker} \cap S_{k_0,l}$, we first note that $\int_{F_y} \mathbf{1}_F(x,y)dx = \ell(F_y)$ and then we have

$$\begin{aligned}\int \dot{k}(x,y)dx = \frac{f_0(y)}{2\lambda}\Bigg(&\int_{F_y}((\mathrm{Id}-L_0^*)^{-1}c)(x)dx \\ &- \int_{F_y}((\mathrm{Id}-L_0^*)^{-1}c)(z)dz\frac{\int_{F_y}\mathbf{1}_F(x,y)dx}{\ell(F_y)}\Bigg) \\ &= 0.\end{aligned}$$

If we let

$$H(x,y) := \mathbf{1}_F(x,y)f_0(y)\left(((\mathrm{Id}-L_0^*)^{-1}c)(x) - \frac{1}{\ell(F_y)}\int_{F_y}((\mathrm{Id}-L_0^*)^{-1}c)(z)dz\right),$$

then the necessary condition (3.3.7) yields $\lambda = \pm\frac{1}{2}\|H\|_{L^2([0,1]^2)}$; the sign of λ is determined by checking the sufficient conditions.

Sufficient conditions: We want to show that $\dot{k}$ in (3.3.5) is the solution to the optimisation problem (3.3.3)–(3.3.4) by checking that it satisfies the second-order sufficient conditions. We first want to show that the set of Lagrange multipliers $\Lambda(\dot{k})$ (in Definition 3.8, §3.1 [15]) is not empty in our setting; this will enable us to use the second-order sufficient conditions of Lemma 3.65 [15]. Note that in terms of the notation used in [15], we have that $Q = X = V_{\ker} \cap S_{k_0,l}$, $x_0 = \dot{k}$, $Y^* = \mathbb{R}$, $G(x_0) = g(\dot{k})$, $K = \{0\}$, $N_K(G(x_0)) = \mathbb{R}$, $T_K(G(x_0)) = \{0\}$ and $N_Q(x_0) = \{0\}$ (since $Q = X$, see discussion in §3.1 following Definition 3.8). Thus, to show that $\Lambda(\dot{k})$ is not empty, we need to show that $\dot{k}$ and λ satisfy

$$D_{\dot{k}}\mathcal{L}(\dot{k},\lambda)\dot{k} = 0,\ g(\dot{k}) = 0,\ \lambda \in \{0\}^-,\ \lambda g(\dot{k}) = 0, \tag{3.3.9}$$

where $\{0\}^- := \{a \in \mathbb{R} : ax \leq 0\ \forall x \in \{0\}\} = \mathbb{R}$ (this simplification of conditions (3.16) in [15] follows from the discussion following Definition 3.8 in §3.1 and the fact that $\{0\}$ is a convex cone). Since the second condition in (3.3.9) implies the fourth, and since $\lambda \in \mathbb{R}$, we only need to check the first two equalities in (3.3.9). However, these two conditions are implied from the first-order necessary conditions.

Hence, $\Lambda(\dot{k})$ is not empty and thus, to show that $\dot{k}$ is a solution to (3.3.3)–(3.3.4), we need to show that it satisfies the following second-order conditions (see Lemma 3.65): there exists constants $\mu > 0$, $\eta > 0$ and $\beta > 0$ such that

$$\sup_{|\lambda| \leq \mu,\ \lambda \in \Lambda(\dot{k})} D^2_{\dot{k}\dot{k}} \mathcal{L}(\dot{k}, \lambda)(\tilde{k}, \tilde{k}) \geq \beta \|\tilde{k}\|^2_{L^2([0,1]^2)},\ \forall \tilde{k} \in C_\eta(\dot{k}), \tag{3.3.10}$$

where

$$C_\eta(\dot{k}) := \left\{ v \in V_{\ker} \cap S_{k_0,l} : |2\langle \dot{k}, v \rangle_{V_{\ker} \cap S_{k_0,l}}| \leq \eta \|v\|_{V_{\ker} \cap S_{k_0,l}} \ \& \ f(v) \leq \eta \|v\|_{V_{\ker} \cap S_{k_0,l}} \right\}$$

is the approximate critical cone (see equation (3.131), §3.3 [15]). Since $D_{\dot{k}} \mathcal{L}(\dot{k}, \lambda)\tilde{k} = f(\tilde{k}) + 2\lambda \langle \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2)}$ and $\langle \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2)}$ is linear in $\dot{k}$, we have $D^2_{\dot{k}\dot{k}} \mathcal{L}(\dot{k}, \lambda)(\tilde{k}, \tilde{k}) = 2\lambda \langle \tilde{k}, \tilde{k} \rangle_{L^2([0,1]^2)}$. Thus, we conclude that (3.3.10) holds with $\lambda > 0$, $\mu = |\lambda| = \frac{1}{2}\|H\|_{V_{\ker} \cap S_{k_0,l}}$, $\beta = 2\lambda$ and $\eta = \max\left\{2\|\dot{k}\|_{V_{\ker} \cap S_{k_0,l}}, \|c\|_2 \|f_0\|_2 \|(\mathrm{Id} - L_0)^{-1}\|_{V \to V}\right\}$. Since $\dot{k}$ satisfies the necessary conditions (3.3.6) and (3.3.7) with $\lambda > 0$, we conclude that $\dot{k}$ is a solution to the optimisation problem (3.3.3)–(3.3.4). By Corollary 3.3.7, this solution is unique.

Boundedness of the solution: From $L_0 f_0 = f_0$ and $k_0 \in L^\infty([0,1]^2)$, we have by (3.2.3) that $f_0 \in L^\infty$. Let $V_1 := \{f \in L^1 : \int f \, d\ell = 0\}$. We would like to show that $(\mathrm{Id} - L_0)^{-1} : V_1 \to V_1$ is bounded. To obtain this, we first need the exponential contraction of L_0 on V_1. Since L_0 is integral-preserving and compact on L^1, from the argument in the proof of Theorem 3.1.2 we only need to verify the L^1 version of assumption $(A1)$ on V_1. To verify this, we note that for $h \in V_1$, we have $\|L_0 h\|_2 \leq \|L_0 h\|_\infty \leq \|k_0\|_{L^\infty([0,1]^2)} \|h\|_1$ and therefore, $L_0 h \in V$ since L_0 preserves the integral. Thus, for any $h \in V_1$, $\lim_{n\to\infty} \|L_0^n h\|_1 \leq \lim_{n\to\infty} \|L_0^{n-1}(L_0 h)\|_2 = 0$ since L_0 satisfies $(A1)$ on V. Hence, the L^1 version of $(A1)$ holds and L_0 has exponential contraction on V_1. Thus, from the computation (3.1.3) (where V and the L^2 norm is replaced with V_1 and the L^1 norm), it follows that $(\mathrm{Id} - L_0)^{-1} : V_1 \to V_1$ is bounded.

Next, we would like to find the subspace where the operator $(\mathrm{Id} - L_0^*)^{-1}$ is bounded. We will replicate the result of Lemma 3.3.11, however, $(\mathrm{Id} - L_0)^{-1}$ is now acting on L^1, so we make the following remarks:

- Since $f_0 \in L^2 \subset L^1$, we have that $\text{span}\{f_0\} \subset L^2 \subset L^1$; hence, $\text{span}\{f_0\}$ is the subspace we have considered in earlier subsections.
- For a subspace $\mathcal{S}$ of L^1, we have that

$$\mathcal{S}^\perp := \left\{ h \in L^\infty : \int h(x)w(x)dx = 0 \ \forall w \in \mathcal{S} \right\}, \tag{3.3.11}$$

  where we are using the fact that $(L^1)^* = L^\infty$. Also, $\mathcal{S}^\perp$ is a closed subspace of L^∞ (see III-§1.4, [54]).
- For $w \in L^1$ and $h \in L^\infty$, we have, as before, that $L_0 w(x) = \int k_0(x,y)w(y)dy$ and $L_0^* h(y) = \int k_0(x,y)h(x)dx$.

Now, as in Lemma 3.3.11, we have $\ker(\text{Id} - L_0) = \text{span}\{f_0\}$ and $\text{ran}(\text{Id} - L_0) = V_1$. We also have $\text{ran}((\text{Id} - L_0)^*) = \text{span}\{f_0\}^\perp = \{h \in L^\infty : \int h(x)w(x)dx = 0 \ \forall \ w \in \text{span}\{f_0\}\} =: W$ and $\ker((\text{Id} - L_0)^*) = V_1^\perp = \{h \in L^\infty : \int h(x)w(x)dx = 0 \ \forall \ w \in V_1\}$. Next, for $h \in W$, we have

$$\int (L_0^* h)(x) f_0(x)dx = \int h(x)(L_0 f_0)(x)dx = \int h(x) f_0(x)dx = 0;$$

thus, $(\text{Id} - L_0^*)(W) \subset W$. We again, as in Sublemma 3.3.11, apply the Inverse Mapping Theorem to prove that $(\text{Id} - L_0^*)^{-1} : W \to W$ is bounded. From (3.2.3), and the triangle inequality, the operator $\text{Id} - L_0^* : W \to W$ is bounded. Noting that V_1 is a closed co-dimension 1 subspace of L^1, we have $\text{codim}(V_1) = \dim(V_1^\perp)$ (see Lemma 1.40 III-§1.8 [54]); hence, $\dim(\ker(\text{Id} - L_0^*)) = \dim(V_1^\perp) = \text{codim}(V_1) = 1$ and therefore, 1 is a geometrically simple eigenvalue of L_0^*. Thus, $\ker(\text{Id} - L_0^*) = \text{span}\{\mathbf{1}\}$ because $L_0^* \mathbf{1} = \mathbf{1}$. Since $\int f_0 \ d\ell = 1$, $\mathbf{1} \notin \text{span}\{f_0\}^\perp$ and so, by the Fredholm alternative, $\text{Id} - L_0^*$ is a bijection on W. Hence, by the Inverse Mapping Theorem, $(\text{Id} - L_0^*)^{-1}$ is bounded on W. Since $c \in W$, we have $\|(\text{Id} - L_0^*)^{-1} c\|_\infty < \infty$.

To conclude the proof, we now show that $\hat{g}(y) := \frac{1}{\ell(F_y)} \int_{F_y} ((\text{Id} - L_0^*)^{-1} c)(z)dz$ is in L^∞. We compute

$$|\hat{g}(y)| = \left| \frac{1}{\ell(F_y)} \int_{F_y} ((\text{Id} - L_0^*)^{-1} c)(z)dz \right| \leq \|(I - L_0^*)^{-1} c\|_\infty.$$

Since $(\text{Id} - L_0^*)^{-1} c \in L^\infty$, we conclude that $\hat{g} \in L^\infty$; thus, $\dot{k} \in L^\infty([0,1]^2)$. $\square$

Remark 3.3.12. *If we do not require the positivity of k_ε, we can consider the the optimisation problem (3.3.3)–(3.3.4) with $c \in span\{f_0\}^\perp$ (i.e. the observable does not need to be essentially bounded) and $\dot{k} \in V_{\ker}$ (i.e. the allowable perturbations need not be restricted to the space $S_{k_0,l}$). In this case, the optimal solution $\dot{k}$ will be*

$$\dot{k}(x,y) = \left(\frac{((Id - L_0^*)^{-1}c)(x) - \kappa'}{\|(Id - L_0^*)^{-1}c - \kappa'\|_2} \right) \frac{f_0(y)}{\|f_0\|_2},$$

where $\kappa' = \int ((Id - L_0^*)^{-1}c)(z)dz$, and the corresponding linear response is

$$\frac{\|f_0\|_2}{\|(Id - L_0^*)^{-1}c - \kappa'\|_2} (Id - L_0)^{-1} \left((Id - L_0^*)^{-1}c - \kappa' \right).$$

3.3.3 Approximation of the Optimal Response.

In this section we present a result for the approximation of the optimal perturbation (3.3.5) of the optimisation problem (3.3.3)–(3.3.4). We will approximate the solution $\dot{k}$ by approximating the kernel k_0 of the operator L_0 and the observable c.

Proposition 3.3.13. *Let $L_0 : L^1 \to L^1$ be a compact Hilbert-Schmidt integral operator, with the stochastic kernel $k_0 \in L^\infty([0,1]^2)$, satisfying (A1) of Theorem 3.1.2. Let $\{L_n\} \subset \mathcal{B}(L^1)$ be a sequence of compact Hilbert-Schmidt integral operators with stochastic kernels $\{k_n\} \subset L^\infty([0,1]^2)$ such that $\lim_{n\to\infty} \|k_n - k_0\|_{L^\infty([0,1]^2)} = 0$. Then, there exists $n_0 > 0$ such that for each $n \geq n_0$, L_n satisfies assumption (A1) of Theorem 3.1.2 and there exists a unique probability density $f_n \in L^\infty$ such that $L_n f_n = f_n$. Let $\{c_n\} \subset L^\infty$ be such that $c_n \in span\{f_n\}^\perp$ and $\lim_{n\to\infty} \|c_n - c\|_\infty = 0$. Suppose there exists a $\kappa > 0$ such that $\|k_n\|_{L^\infty([0,1]^2)} \leq \kappa$ for all $n \geq n_0$. Then, the sequence of perturbations*

$$\dot{k}_n(x,y) := \begin{cases} \frac{f_n(y)}{\alpha_n} \left(((Id - L_n^*)^{-1}c_n)(x) - \frac{\int_{F_y} ((Id - L_n^*)^{-1}c_n)(z)dz}{\ell(F_y)} \right) & (x,y) \in F, \\ 0 & \text{otherwise}, \end{cases} \tag{3.3.12}$$

where α_n is selected so that $\|\dot{k}_n\|_{L^2([0,1]^2)} = 1$, converges to the optimal perturbation $\dot{k}$ in L^∞ as $n \to \infty$.

Proof. We first show that there exists $n_0 > 0$ such that for each $n \geq n_0$, L_n is mixing and has a unique invariant density $f_n \in L^\infty$ such that $\lim_{n\to\infty} \|f_n - f_0\|_\infty = 0$. From $\|k_n - k_0\|_{L^\infty([0,1]^2)} \to 0$ we have that $\|k_n - k_0\|_{L^2([0,1]^2)} \to 0$; from inequality (3.2.2) this implies that $\|L_n - L_0\|_{L^2 \to L^2} \to 0$. Since L_0 is mixing and L_n converges to L_0 in the operator norm, we have from the argument in the proof of Theorem 3.1.2 that there exists $n_0 > 0$ such that for all $n \geq n_0$, L_n is mixing (satisfies $(A1)$). From Lemma 3.3.5, there exists a unique probability density $f_n \in L^\infty$ such that $L_n f_n = f_n$, where $n \geq n_0$ (similarly, $f_0 \in L^\infty$ is the unique probability density such that $L_0 f_0 = f_0$). We also have that $\|f_n - f_0\|_2 \to 0$ (see the proof of Theorem 3.1.2). Recalling inequality (3.2.3), we have

$$\begin{aligned}\|f_n - f_0\|_\infty &= \|L_n f_n - L_0 f_0\|_\infty \\ &\leq \|k_n - k_0\|_{L^\infty([0,1]^2)} \|f_n\|_1 + \|k_0\|_{L^\infty([0,1]^2)} \|f_n - f_0\|_1;\end{aligned}$$

since $\|f_n - f_0\|_1 \leq \|f_n - f_0\|_2 \to 0$, and from the assumption that $\|k_n - k_0\|_{L^\infty([0,1]^2)} \to 0$, we have $\|f_n - f_0\|_\infty \to 0$.

Before we prove $\|\dot{k}_n - \dot{k}\|_{L^\infty([0,1]^2)} \to 0$ as $n \to \infty$, we note the following. Let $h(x) := ((\mathrm{Id} - L_0^*)^{-1} c)(x)$, $h_n(x) := ((\mathrm{Id} - L_n^*)^{-1} c_n)(x)$, $\hat{g}(y) := \frac{1}{\ell(F_y)} \int_{F_y} h(z)dz$ and $\hat{g}_n(y) := \frac{1}{\ell(F_y)} \int_{F_y} h_n(z)dz$. Also, let $\hat{k}_n(x,y) := f_n(y)\,(h_n(x) - \hat{g}_n(y))$ and $\hat{k}(x,y) := f_0(y)\,(h(x) - \hat{g}(y))$ (i.e. $\dot{k}_n$ and $\dot{k}$ without the normalising constant). We then have

$$\begin{aligned}&|\hat{k}_n(x,y) - \hat{k}(x,y)| \\ &\quad\leq |h_n(x)||f_n(y) - f_0(y)| + |f_0(y)||h_n(x) - h(x)| \\ &\qquad + |\hat{g}_n(y)||f_n(y) - f_0(y)| + |f_0(y)||\hat{g}_n(y) - \hat{g}(y)| \\ &\quad\leq (|h_n(x) - h(x)| + |h(x)|)\,|f_n(y) - f_0(y)| + |f_0(y)||h_n(x) - h(x)| \\ &\qquad + (|\hat{g}_n(x) - \hat{g}(x)| + |\hat{g}(x)|)\,|f_n(y) - f_0(y)| + |f_0(y)||\hat{g}_n(y) - \hat{g}(y)|.\end{aligned}$$

Also, we have that

$$|\hat{g}_n(y) - \hat{g}(y)| \leq \frac{1}{\ell(F_y)} \int_{F_y} |h_n(z) - h(z)|dz \leq \|h_n - h\|_\infty.$$

Since $\dot{k}_n = \hat{k}_n/\|\hat{k}_n\|_{L^2([0,1]^2)}$ (similarly $\dot{k} = \hat{k}/\|\hat{k}\|_{L^2([0,1]^2)}$), if $\|\hat{k}_n - \hat{k}\|_{L^\infty([0,1]^2)} \to 0$ then $\|\hat{k}_n - \hat{k}\|_{L^2([0,1]^2)} \to 0$, which implies $\|\hat{k}_n\|_{L^2([0,1]^2)} \to \|\hat{k}\|_{L^2([0,1]^2)}$ (by the reverse triangle inequality) and therefore $\|\dot{k}_n - \dot{k}\|_{L^\infty([0,1]^2)} \to 0$. Thus, to show $\|\dot{k}_n - \dot{k}\|_{L^\infty([0,1]^2)} \to 0$ as $n \to \infty$, we just need to show that $\|h_n - h\|_\infty \to 0$ as $n \to \infty$.

Let $W_n := \operatorname{span}\{f_n\}^\perp$ and $W := \operatorname{span}\{f_0\}^\perp$, where $^\perp$ is as in (3.3.11). Let $\widehat{\Pi}_0 : L^\infty \to L^\infty$ be defined as $\widehat{\Pi}_0 g = \int g f_0 \, d\ell \mathbf{1}$. Since $\int f_0 \, d\ell = 1$, we have

$$\widehat{\Pi}_0^2 g = \int \int g f_0 \, d\ell \mathbf{1} f_0 \, d\ell \mathbf{1} = \int g f_0 \, d\ell \int f_0 \, d\ell \mathbf{1} = \int g f_0 \, d\ell \mathbf{1} = \widehat{\Pi}_0 g;$$

therefore, $\widehat{\Pi}_0$ is a projection onto $\operatorname{span}\{\mathbf{1}\}$ along $\operatorname{span}\{f_0\}^\perp$(i.e. $\ker(\widehat{\Pi}_0) = \operatorname{span}\{f_0\}^\perp$). Hence, the operator $\Pi_0 := \mathrm{Id} - \widehat{\Pi}_0 : L^\infty \to L^\infty$ is a projection onto $\operatorname{span}\{f_0\}^\perp$ along $\operatorname{span}\{\mathbf{1}\}$. We similarly define $\Pi_n : L^\infty \to L^\infty$ as $\Pi_n g = g - \int g f_n \, d\ell \mathbf{1}$, which is a projection onto $\operatorname{span}\{f_n\}^\perp$ along $\operatorname{span}\{\mathbf{1}\}$. Let $Q_n := (\mathrm{Id} - L_n^*)^{-1}$ and $Q_0 := (\mathrm{Id} - L_0^*)^{-1}$; recalling that $\Pi_0 c = c$ and $\Pi_n c_n = c_n$ (since $c \in W$ and $c_n \in W_n$), we have

$$\begin{aligned}
\|h_n - h\|_\infty &= \|Q_n c_n - Q_0 c\|_\infty \\
&= \|Q_n \Pi_n c_n - Q_n \Pi_n c + Q_n \Pi_n c - Q_0 \Pi_0 c\|_\infty \\
&\le \|Q_n \Pi_n\|_{L^\infty \to L^\infty} \|c_n - c\|_\infty + \|Q_n \Pi_n - Q_0 \Pi_0\|_{L^\infty \to L^\infty} \|c\|_\infty;
\end{aligned}$$

thus, to show $\|h_n - h\|_\infty \to 0$, we need to show that $\|Q_n \Pi_n - Q_0 \Pi_0\|_{L^\infty \to L^\infty} \to 0$ as $n \to \infty$ (which implies $\|Q_n \Pi_n\|_{L^\infty \to L^\infty} \to \|Q_0 \Pi_0\|_{L^\infty \to L^\infty}$ as $n \to \infty$ by the reverse triangle inequality). Noting that $L_n^*(W_n) \subset W_n$, we have $L_n^* \Pi_n = \Pi_n L_n^* \Pi_n$; thus,

$$Q_n \Pi_n = \sum_{i=0}^{\infty} L_n^{*i} \Pi_n = \sum_{i=0}^{\infty} (L_n^* \Pi_n)^i = (\mathrm{Id} - L_n^* \Pi_n)^{-1}.$$

Similarly, we have $Q_0 \Pi_0 = (\mathrm{Id} - L_0^* \Pi_0)^{-1}$. Hence, we have

$$\begin{aligned}
&\|Q_n \Pi_n - Q_0 \Pi_0\|_{L^\infty \to L^\infty} \\
&= \|(\mathrm{Id} - L_n^* \Pi_n)^{-1} - (\mathrm{Id} - L_0^* \Pi_0)^{-1}\|_{L^\infty \to L^\infty} \\
&= \|(\mathrm{Id} - L_n^* \Pi_n)^{-1} (L_0^* \Pi - L_n^* \Pi_n)(\mathrm{Id} - L_0^* \Pi_0)^{-1}\|_{L^\infty \to L^\infty} \\
&\le \|(\mathrm{Id} - L_n^* \Pi_n)^{-1}\|_{L^\infty \to L^\infty} \|L_0^* \Pi_0 - L_n^* \Pi_n\|_{L^\infty \to L^\infty} \|(\mathrm{Id} - L_0^* \Pi_0)^{-1}\|_{L^\infty \to L^\infty},
\end{aligned}$$

where in the second line we used the resolvent identity (Theorem 5.16.1, [52]). We next have

$$\begin{aligned}
&\|L_0^*\Pi_0 - L_n^*\Pi_n\|_{L^\infty\to L^\infty} \\
&\quad = \|L_0^*\Pi_0 - L_0^*\Pi_n + L_0^*\Pi_n - L_n^*\Pi_n\|_{L^\infty\to L^\infty} \\
&\quad \le \|L_0^*\|_{L^\infty\to L^\infty}\|\Pi_0 - \Pi_n\|_{L^\infty\to L^\infty} + \|L_0^* - L_n^*\|_{L^\infty\to L^\infty}\|\Pi_n\|_{L^\infty\to L^\infty}.
\end{aligned}$$

Noting that $(\Pi_0 - \Pi_n)g = \int g(x)(f_n(x) - f_0(x))dx$, we apply Holder's inequality to obtain

$$\begin{aligned}
\|\Pi_0 - \Pi_n\|_{L^\infty\to L^\infty} &= \sup_{\|g\|_\infty=1} \left\| \int g(x)(f_n(x) - f_0(x))dx \right\|_\infty \\
&\le \|f_n - f_0\|_1;
\end{aligned}$$

as $\|f_n - f_0\|_1 \to 0$, we have that $\|\Pi_0 - \Pi_n\|_\infty \to 0$. Also, since $\|L_0^* - L_n^*\|_{L^\infty\to L^\infty} \le \|k_0 - k_n\|_{L^\infty([0,1]^2)} \to 0$, we have that $\|L_0^*\Pi_0 - L_n^*\Pi_n\|_{L^\infty\to L^\infty} \to 0$. Finally, to show that $\|Q_n\Pi_n - Q_0\Pi_0\|_{L^\infty\to L^\infty} \to 0$, and thus conclude the proof, we have the following result.

Sublemma 3.3.14. *There exists an $N > 0$ and $0 < C < \infty$ such that for all $n \ge N$, $\|(Id - L_n^*\Pi_n)^{-1}\|_{L^\infty\to L^\infty} \le C$.*

Proof. We first show that L_0^* is mixing on W. From the proof of Theorem 3.3.8 (see "Boundedness of the solution"), we have that $(\mathrm{Id} - L_0^*)^{-1} : W \to W$ is bounded. Thus, $\sum_{j=0}^\infty L_0^{*j}$ is bounded on $W \subset L^\infty$ and so $\lim_{j\to\infty}\|L_0^{*j}\|_{W\to W} = 0$, i.e. L_0^* is mixing on W.

We now show that $\sum_{j=0}^\infty \|(L_n^*\Pi_n)^j\|_{L^\infty\to L^\infty}$ is bounded using the fact that L_0^* is mixing on W and that $\|L_n - L_0\|_{L^\infty\to L^\infty} \to 0$ as $n \to \infty$. From the mixing of L_0^* on W, we can fix an integer $\mathcal{b} > 1$ such that $\|L_0^{*\mathcal{b}}\|_{W\to W} \le 2\lambda < 1$. Since $\|L_0^*\Pi_0 - L_n^*\Pi_n\|_{L^\infty\to L^\infty} \to 0$ as $n \to \infty$ (see argument prior to this sublemma), there exists an integer N such that for all $n \ge N$, $\|L_0^*\Pi_0 - L_n^*\Pi_n\|_{L^\infty\to L^\infty} < \frac{1-2\lambda}{2}\frac{1}{4}\|k_0\|^{-1}_{L^\infty([0,1]^2)}\kappa^{-1}\mathcal{b}^{-1}$, where κ is from the assumption in the proposition. Let

$\tilde{k}_n^j$ be the kernel of the operator L_n^{*j}; from the proof of Lemma 3.3.5, $\|\tilde{k}_n^j\|_{L^\infty([0,1]^2)} \leq \|\tilde{k}_n\|_{L^\infty([0,1]^2)} = \|k_n\|_{L^\infty([0,1]^2)}$. We also note that

$$\begin{aligned}\|\Pi_0\|_{L^\infty \to L^\infty} &= \sup_{\|g\|_\infty=1} \|\Pi_0 g\|_\infty = \sup_{\|g\|_\infty=1} \left\| g - \int g(y) f_0(y) dy \mathbf{1} \right\|_\infty \\ &\leq \sup_{\|g\|_\infty=1} (\|g\|_\infty + \|g\|_\infty \|f_0\|_1) = 2,\end{aligned}$$

where the last equality follows since f_0 is a probability density (see Lemma 3.3.5); we similarly have $\|\Pi_n\|_{L^\infty \to L^\infty} \leq 2$. Recalling that $\|k_n\|_{L^\infty([0,1]^2)} \leq \kappa$ (from the assumptions in the proposition) and that $(L_n^*\Pi_n)^\mathfrak{b} = L_n^{*\mathfrak{b}}\Pi_n$ (similarly $(L_0^*\Pi_0)^\mathfrak{b} = L_0^{*\mathfrak{b}}\Pi_0$), since $L_n^*(W_n) \subset W_n$ (and $L_0^*(W) \subset W$), we have the following for $n \geq N$

$$\begin{aligned}&\|(L_n^*\Pi_n)^\mathfrak{b}\|_{L^\infty \to L^\infty} \\ &\leq \|L_0^{*\mathfrak{b}}\Pi_0\|_{L^\infty \to L^\infty} + \|(L_0^*\Pi_0)^\mathfrak{b} - (L_n^*\Pi_n)^\mathfrak{b}\|_{L^\infty \to L^\infty} \\ &\leq 2\|L_0^{*\mathfrak{b}}\|_{W \to W} + \left\| \sum_{j=0}^{\mathfrak{b}-1} (L_0^*\Pi_0)^j (L_0^*\Pi_0 - L_n^*\Pi_n)(L_n^*\Pi_n)^{\mathfrak{b}-1-j} \right\|_{L^\infty \to L^\infty} \\ &\leq 2\lambda + \sum_{j=0}^{\mathfrak{b}-1} \|(L_0^*\Pi_0)^j\|_{L^\infty \to L^\infty} \|L_0^*\Pi_0 - L_n^*\Pi_n\|_{L^\infty \to L^\infty} \|(L_n^*\Pi_n)^{\mathfrak{b}-1-j}\|_{L^\infty \to L^\infty} \\ &\leq 2\lambda + 4\sum_{j=0}^{\mathfrak{b}-1} \|L_0^{*j}\|_{L^\infty \to L^\infty} \|L_0^*\Pi_0 - L_n^*\Pi_n\|_{L^\infty \to L^\infty} \|L_n^{*\,\mathfrak{b}-1-j}\|_{L^\infty \to L^\infty} \\ &\leq 2\lambda + 4\sum_{j=0}^{\mathfrak{b}-1} \|\tilde{k}_0^j\|_{L^\infty([0,1]^2)} \|L_0^*\Pi_0 - L_n^*\Pi_n\|_{L^\infty \to L^\infty} \|\tilde{k}_n^{\mathfrak{b}-1-j}\|_{L^\infty([0,1]^2)} \\ &\leq 2\lambda + 4\sum_{j=0}^{\mathfrak{b}-1} \|\tilde{k}_0\|_{L^\infty([0,1]^2)} \|L_0^*\Pi_0 - L_n^*\Pi_n\|_{L^\infty \to L^\infty} \|\tilde{k}_n\|_{L^\infty([0,1]^2)} \\ &= 2\lambda + 4\sum_{j=0}^{\mathfrak{b}-1} \|k_0\|_{L^\infty([0,1]^2)} \|L_0^*\Pi_0 - L_n^*\Pi_n\|_{L^\infty \to L^\infty} \|k_n\|_{L^\infty([0,1]^2)} \\ &\leq 2\lambda + 4\mathfrak{b}\kappa \|k_0\|_{L^\infty([0,1]^2)} \|L_0^*\Pi_0 - L_n^*\Pi_n\|_{L^\infty \to L^\infty} \\ &< 2\lambda + 4\mathfrak{b}\kappa \|k_0\|_{L^\infty([0,1]^2)} \left(\frac{1-2\lambda}{2}\right) \frac{1}{4} \|k_0\|_{L^\infty([0,1]^2)}^{-1} \kappa^{-1} \mathfrak{b}^{-1} \\ &= 2\lambda + \left(\frac{1-2\lambda}{2}\right) = \eta < 1,\end{aligned}$$

where $\eta = 2\lambda + \left(\frac{1-2\lambda}{2}\right)$. Thus, for $m \geq 1$, we have that

$$\|(L_n^*\Pi_n)^{\mathcal{b}m}\|_{L^\infty \to L^\infty} \leq \|(L_n^*\Pi_n)^{\mathcal{b}}\|_{L^\infty \to L^\infty}^m \leq \widehat{C}^{\mathcal{b}m},$$

where $\widehat{C} = \eta^{\frac{1}{\mathcal{b}}} < 1$. For $j > 0$, let $j = \mathcal{b}m + a$, where $m > 0$ and $a \in \{0, \ldots, \mathcal{b} - 1\}$. Since $\kappa \geq \|k_n\|_{L^\infty([0,1]^2)} \geq \|k_n\|_{L^1([0,1]^2)} = 1$ (since k_n is a stochastic kernel), we have

$$\begin{aligned}
\|(L_n^*\Pi_n)^j\|_{L^\infty \to L^\infty} &\leq \|(L_n^*\Pi_n)^{\mathcal{b}m}\|_{L^\infty \to L^\infty} \|(L_n^*\Pi_n)^a\|_{L^\infty \to L^\infty} \\
&\leq \widehat{C}^{\mathcal{b}m} \|L_n^{*a}\Pi_n\|_{L^\infty \to L^\infty} \\
&\leq 2\widehat{C}^{\mathcal{b}m} \|L_n^*\|_{L^\infty \to L^\infty}^a \\
&\leq 2\widehat{C}^{\mathcal{b}m} \|k_n\|_{L^\infty([0,1]^2)}^a \\
&\leq 2\widehat{C}^{\mathcal{b}m} \kappa^a \\
&\leq 2\widehat{C}^{\mathcal{b}m} \kappa^{\mathcal{b}-1} \\
&\leq \widehat{C}' \widehat{C}^{\mathcal{b}m+a} = \widehat{C}' \widehat{C}^j,
\end{aligned}$$

where $\widehat{C}' = 2\kappa^{\mathcal{b}-1}\widehat{C}^{-(\mathcal{b}-1)}$. Finally, since $\widehat{C} < 1$, we have

$$\begin{aligned}
\sum_{j=0}^{\infty} \|(L_n^*\Pi_n)^j\|_{L^\infty \to L^\infty} &= 1 + \sum_{j=1}^{\infty} \|(L_n^*\Pi_n)^j\|_{L^\infty \to L^\infty} \\
&\leq 1 + \sum_{j=1}^{\infty} \widehat{C}' \widehat{C}^j < \infty;
\end{aligned}$$

thus, for $C := 1 + \frac{\widehat{C}'}{1-\widehat{C}}$ and $n \geq N$, the result of the sublemma follows. □

□

Remark 3.3.15. *We note the following link to Chapter 2. Let $\varphi_n : L^\infty \to L^\infty$ be defined as $\varphi_n(g) = \int g f_n \, d\ell\mathbf{1}$. From the proof above, we have that*

$$\begin{aligned}
(Id - L_n^*)^{-1}\Pi_n &= (Id - L_n^*\Pi_n)^{-1} \\
&= (Id - L_n^*(Id - \varphi_n))^{-1} \\
&= (Id - L_n^* + L_n^*\varphi_n)^{-1} \\
&= (Id - L_n^* + \varphi_n)^{-1},
\end{aligned} \tag{3.3.13}$$

where last equality follows from the fact that $\mathbf{1}$ *is an eigenvector of* L_n^* *for the eigenvalue* 1. *Thus, for a function* $c_n \in span\{f_n\}^\perp = W_n$, *we compute* $(Id - L_n^*)^{-1}c_n = (Id - L_n^* + \varphi_n)^{-1}c_n$. *Equation (3.3.13) is used in Section 2.3 (under the notation* $Q^\top$*) to compute the optimal response in the finite dimensional setting .*

3.3.4 Explicit Formula for the Optimal Perturbation to Increase the Mixing Rate

In this section we will investigate the linear response problem for enhancing the rate of mixing. We will begin with a formulation of the optimisation problem and the sufficient condition on the feasible set of allowable perturbations under which the optimisation problem has a unique solution. We conclude by deriving an explicit formula for the optimal solution.

We first state the required assumptions for this, and the following, subsections:

- Let $L_\varepsilon : L^2([0,1],\mathbb{C}) \to L^2([0,1],\mathbb{C})$ be a family of integral operators with kernels $k_\varepsilon \in L^2([0,1]^2,\mathbb{R})$ of the form (3.2.5).
- We assume L_ε satisfies the integral-preserving assumption (3.1.2) and that L_0 satisfies the mixing assumption $(A1)$.
- Let $\lambda_0 \in \mathbb{C}$ denote an eigenvalue of L_0 strictly inside the unit circle with largest magnitude. We assume that λ_0 is geometrically simple. We denote by e and $\hat{e}$ the eigenvectors of L_0 and L_0^*, respectively, corresponding to the eigenvalue λ_0.

To find the kernel perturbations that enhance mixing, we follow the approach taken in Section 2.4 and consider perturbing our original dynamics L_0 in such a way that the modulus of the second eigenvalue of the perturbed dynamics is closer to zero. Equivalently, we want to find perturbations such that the real part of the logarithm of the perturbed second eigenvalue is minimised. The following result provides an explicit formula for the instantaneous change of the real part of the logarithm of the second largest eigenvalue.

Lemma 3.3.16. *Let*

$$\begin{aligned} E(x,y) := &\left(\Re(\hat{e})(x)\Re(e)(y) + \Im(\hat{e})(x)\Im(e)(y)\right)\Re(\lambda_0) \\ &+ \left(\Im(\hat{e})(x)\Re(e)(y) - \Re(\hat{e})(x)\Im(e)(y)\right)\Im(\lambda_0). \end{aligned} \tag{3.3.14}$$

Then

$$\frac{d}{d\varepsilon}\Re\left(\log\lambda_\varepsilon\right)\Big|_{\varepsilon=0} = \frac{\left\langle \dot{k}, E\right\rangle_{L^2([0,1]^2,\mathbb{R})}}{|\lambda_0|^2}.$$

Proof. From (3.2.9), we have that

$$\Re(\dot{\lambda}_0) = \int_0^1\int_0^1 \dot{k}(x,y)\left(\Re(\hat{e})(x)\Re(e)(y) + \Im(\hat{e})(x)\Im(e)(y)\right)dydx \tag{3.3.15}$$

and

$$\Im(\dot{\lambda}_0) = \int_0^1\int_0^1 \dot{k}(x,y)\left(\Im(\hat{e})(x)\Re(e)(y) - \Re(\hat{e})(x)\Im(e)(y)\right)dydx. \tag{3.3.16}$$

Next, we note that

$$\frac{d}{d\varepsilon}\Re(\log\lambda_\varepsilon) = \Re\left(\frac{d}{d\varepsilon}\log\lambda_\varepsilon\right) = \Re\left(\frac{d\lambda_\varepsilon}{d\varepsilon}\frac{1}{\lambda_\varepsilon}\right). \tag{3.3.17}$$

From (3.3.15)–(3.3.17), we obtain

$$\begin{aligned}
\frac{d}{d\varepsilon}\Re\left(\log\lambda_\varepsilon\right)\Big|_{\varepsilon=0} &= \Re\left(\frac{\dot{\lambda}_0}{\lambda_0}\right)\\
&= \Re\left(\frac{\dot{\lambda}_0}{\lambda_0}\frac{\overline{\lambda_0}}{\overline{\lambda_0}}\right)\\
&= \frac{\Re(\dot{\lambda}_0)\Re(\lambda_0) + \Im(\dot{\lambda}_0)\Im(\lambda_0)}{|\lambda_0|^2}\\
&= \frac{\left\langle \dot{k}, E\right\rangle_{L^2([0,1]^2,\mathbb{R})}}{|\lambda_0|^2}.
\end{aligned}$$

□

The formula in the above result provides the objective function for the optimisation problem we will consider for enhancing mixing. Below we state the optimisation problem and the conditions that the set of allowable perturbations must satisfy for a solution to exist and be unique.

Corollary 3.3.17. *Consider the problem of finding $\dot{k} \in P$ such that*

$$\left\langle \dot{k}, E\right\rangle_{L^2([0,1]^2,\mathbb{R})} = \min_{k\in P}\left\langle k, E\right\rangle_{L^2([0,1]^2,\mathbb{R})}, \tag{3.3.18}$$

where $P \subset V_{\ker}$ is the set of allowable perturbations. If P is closed, bounded and convex then there exists at least one solution to the problem. Furthermore, if P is also strictly convex, then there exists a unique solution.

Proof. Since (3.3.18) is a minimisation problem, we apply Propositions 3.3.1 and 3.3.3 with $S(k) = -\langle k, E\rangle_{L^2([0,1]^2,\mathbb{R})}$, which is linear in k, to obtain the result. □

We now would like to obtain a result similar to Theorem 3.3.8 for problem (3.3.18). Since we are interested in kernel perturbations that will ensure that the perturbed kernel k_ε is stochastic, we assume that $k_0 \in L^\infty([0,1]^2, \mathbb{R})$ and we consider the constraint set P_l, as in Section 3.3.1, where $0 < l < 1$. Snce P_l is closed, bounded and strictly convex, from Corollary 3.3.17 we have that problem (3.3.18), with this constraint set, has a unique solution. Furthermore, the objective function of (3.3.18) is linear and therefore, we only need to consider the optimisation problem on $V_{\ker} \cap S_{k_0,l} \cap \partial B_1$. Thus, to obtain the perturbation $\dot{k}$ that will enhance the mixing rate, we solve the following optimisation problem:

$$\min_{\dot{k} \in V_{\ker} \cap S_{k_0,l}} \quad \langle \dot{k}, E\rangle_{L^2([0,1]^2,\mathbb{R})} \tag{3.3.19}$$

$$\text{such that} \quad \|\dot{k}\|^2_{L^2([0,1]^2,\mathbb{R})} - 1 = 0, \tag{3.3.20}$$

where E is defined in (3.3.14).

Theorem 3.3.18. *Let $L_0 : L^2([0,1],\mathbb{C}) \to L^2([0,1],\mathbb{C})$ be a Hilbert-Schmidt integral operator with the stochastic kernel $k_0 \in L^\infty([0,1]^2,\mathbb{R})$. Suppose that L_0 satisfies (A1) of Theorem 3.1.2 and let $F := \{(x,y) \in [0,1]^2 : k_0(x,y) \geq l\}$ and $F_y := \{x \in [0,1] : (x,y) \in F\}$. Then, the unique solution to the optimisation problem (3.3.19)–(3.3.20) is*

$$\dot{k}(x,y) = \begin{cases} \frac{1}{\alpha}\left(\frac{1}{\ell(F_y)}\int_{F_y} E(x,y)dx - E(x,y)\right) & (x,y) \in F \\ 0 & \text{otherwise,} \end{cases} \tag{3.3.21}$$

where E is given in (3.3.14) and $\alpha > 0$ is selected so that $\|\dot{k}\|_{L^2([0,1]^2,\mathbb{R})} = 1$. Furthermore, $\dot{k} \in L^\infty([0,1]^2,\mathbb{R})$.

Proof. The optimisation problem under consideration is very similar to that considered in Theorem 3.3.8; thus, we will refer to the proof of that theorem with the following modifications.

Consider the Lagrangian function

$$\mathcal{L}(\dot{k}, \mu) := f(\dot{k}) + \mu g(\dot{k}),$$

where, in this setting, we have $f(\dot{k}) = \langle \dot{k}, E \rangle_{L^2([0,1]^2,\mathbb{R})}$ and $g(\dot{k}) = \|\dot{k}\|^2_{L^2([0,1]^2,\mathbb{R})} - 1$. Thus, for the necessary conditions of the Lagrange multiplier method to be satisfied, we need that

$$f(\tilde{k}) + 2\mu\langle \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2)} = \langle \tilde{k}, E \rangle_{L^2([0,1]^2,\mathbb{R})} + 2\mu\langle \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2,\mathbb{R})} = 0 \tag{3.3.22}$$

for all $\tilde{k} \in V_{\text{ker}} \cap S_{k_0,l}$ and

$$g(\dot{k}) = 0. \tag{3.3.23}$$

We first note that

$$\langle \tilde{k}, E \rangle_{L^2([0,1]^2,\mathbb{R})} + 2\mu\langle \dot{k}, \tilde{k} \rangle_{L^2([0,1]^2,\mathbb{R})} = \langle \tilde{k}, E + 2\mu\dot{k} \rangle_{L^2([0,1]^2,\mathbb{R})}.$$

Second, we claim that

$$\dot{k}(x,y) = -\mathbf{1}_F(x,y)\frac{1}{2\mu}\left(E(x,y) - \frac{1}{\ell(F_y)}\int_{F_y} E(x,y)dx\right) \tag{3.3.24}$$

satisfies the necessary condition (3.3.22). To see this, let $h(y) := \frac{1}{\ell(F_y)}\int_{F_y} E(x,y)dx$ and so $\dot{k}(x,y) = -\mathbf{1}_F(x,y)\frac{(E(x,y)-h(y))}{2\mu}$. Then, we have

$$\begin{aligned}\langle \tilde{k}, E + 2\mu\dot{k} \rangle_{L^2([0,1]^2,\mathbb{R})} &= \langle \tilde{k}, h \rangle_{L^2([0,1]^2,\mathbb{R})} \\ &= \int\int_F \tilde{k}(x,y)h(y)dydx = 0,\end{aligned}$$

where the last equality follows by Lemma 3.2.1 and the fact that $\tilde{k} \in V_{\ker} \cap S_{k_0,l}$. Finally, we have

$$\begin{aligned}\int \dot{k}(x,y)dx &= -\frac{1}{2\mu}\left(\int_{F_y} E(x,y)dx - \frac{1}{\ell(F_y)}\int_{F_y} E(z,y)dz \int \mathbf{1}_F(x,y)dx\right)\\ &= -\frac{1}{2\mu}\left(\int_{F_y} E(x,y)dx - \frac{1}{\ell(F_y)}\int_{F_y} E(z,y)dz\ \ell(F_y)\right)\\ &= 0\end{aligned}$$

and therefore, (3.3.24) is in $V_{\ker}$. If we let $2\mu = \pm\|\mathbf{1}_F(E-h)\|_{L^2([0,1]^2,\mathbb{R})}$, then $\dot{k}$ in (3.3.24) satisfies both necessary conditions (3.3.22) and (3.3.23).

For the sufficient conditions, we note that in this setting $D^2_{\dot{k}\dot{k}}\mathcal{L}(\dot{k},\lambda)(\tilde{k},\tilde{k})$ is the same as in the proof of Theorem 3.3.8 (since the objectives considered in both this and the other optimisation problem are linear). Hence, the second order sufficient conditions are satisfied with $\mu > 0$. Thus, with $2\mu = \|\mathbf{1}_F(E-h)\|_{L^2([0,1]^2,\mathbb{R})}$, (3.3.21) satisfies the necessary and sufficient conditions; hence (3.3.21) is the unique solution to the optimisation problem (3.3.19)–(3.3.20).

We finally show that $E \in L^\infty([0,1]^2,\mathbb{R})$. Recall that $E(x,y) = \big(\Re(\hat{e})(x)\Re(e)(y) + \Im(\hat{e})(x)\Im(e)(y)\big)\Re(\lambda_0) + \big(\Im(\hat{e})(x)\Re(e)(y) - \Re(\hat{e})(x)\Im(e)(y)\big)\Im(\lambda_0)$. Since $L_0 e = \lambda_0 e$ and $L_0^*\hat{e} = \lambda_0\hat{e}$, from inequality (3.2.3) we have $e, \hat{e} \in L^\infty([0,1],\mathbb{C})$ since $k_0 \in L^\infty([0,1]^2,\mathbb{R})$. Hence, we have that $\Re(e), \Re(\hat{e}), \Im(e), \Im(\hat{e}) \in L^\infty([0,1],\mathbb{R})$ and thus $E \in L^\infty([0,1]^2,\mathbb{R})$. □

Corollary 3.3.19. *If $e, \hat{e}$ and λ_0 are real and $k_0 \geq l$, then the solution to (3.3.19)–(3.3.20) is*

$$\dot{k}(x,y) = sgn(\lambda_0)\frac{e(y)}{\|e\|_2}\left(\frac{\langle \hat{e}, \mathbf{1}\rangle_{L^2([0,1],\mathbb{R})} - \hat{e}(x)}{\|\langle \hat{e}, \mathbf{1}\rangle_{L^2([0,1],\mathbb{R})} - \hat{e}\|_2}\right). \tag{3.3.25}$$

Furthermore, $\ker(\dot{L}) = span\{e\}^\perp$, $ran(\dot{L}) = span\{\hat{e} - \langle \hat{e}, \mathbf{1}\rangle_{L^2([0,1],\mathbb{R})}\mathbf{1}\}$ *and the linear response is*

$$\lim_{\varepsilon\to 0}\frac{f_\varepsilon - f_0}{\varepsilon} = sgn(\lambda_0)\frac{\langle e, f_0\rangle_{L^2([0,1],\mathbb{R})}}{\|e\|_2}(Id - L_0)^{-1}\frac{\langle \hat{e}, \mathbf{1}\rangle_{L^2([0,1],\mathbb{R})} - \hat{e}}{\|\langle \hat{e}, \mathbf{1}\rangle_{L^2([0,1],\mathbb{R})} - \hat{e}\|_2}.$$

Proof. We have $E(x,y) = \lambda_0 \hat{e}(x)e(y)$; thus, the solution to the optimisation problem (3.3.19)–(3.3.20) is

$$\dot{k}(x,y) = \lambda_0 \beta \left(\int_0^1 \hat{e}(x)dx - \hat{e}(x) \right) e(y),$$

where $\beta > 0$ is the normalisation constant such that $\|\dot{k}\|^2_{L^2([0,1]^2,\mathbb{R})} = 1$. More explicitly, from the proof of Theorem 3.3.18, we have that $\beta^{-2} = \|E - h\|^2_{L^2([0,1]^2,\mathbb{R})}$ where $h(y) = \int_0^1 E(x,y)dx$. We can write

$$\begin{aligned}\beta^{-2} &= \int_0^1 \int_0^1 \left(E(x,y) - \int_0^1 E(z,y)dz \right) dydx \\ &= \lambda_0^2 \|e\|_2^2 \|\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}\|_2^2;\end{aligned}$$

hence, $\beta^{-1} = |\lambda_0| \|e\|_2 \|\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}\|_2$. So, we have that

$$\dot{k}(x,y) = sgn(\lambda_0) \frac{e(y)}{\|e\|_2} \frac{\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}(x)}{\|\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}\|_2}.$$

From this we compute

$$\begin{aligned}\dot{L}g(x) &= \int_0^1 \dot{k}(x,y)g(y)dy \\ &= sgn(\lambda_0) \int_0^1 \frac{e(y)}{\|e\|_2} \frac{\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}(x)}{\|\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}\|_2} g(y)dy \\ &= sgn(\lambda_0) \left\langle \frac{e}{\|e\|_2}, g \right\rangle_{L^2([0,1],\mathbb{R})} \frac{\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}(x)}{\|\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}\|_2}.\end{aligned}$$

From the equation above, we see that for any $g \in L^2$, $\dot{L}g \in \text{span}\{\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}\}$; also, for $\alpha(\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}) \in \text{span}\{\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}\}$, where $\alpha \in \mathbb{R}$, the function $g = \alpha \|\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}\|_2 \frac{e}{\|e\|_2}$ is such that $\dot{L}g = \alpha(\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e})$ and thus, $\text{ran}(\dot{L}) = \text{span}\{\langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1} - \hat{e}\}$. If $g \in \text{span}\{e\}^\perp$ then $\dot{L}g = 0$, and if $\left\langle \frac{e}{\|e\|_2}, g \right\rangle_{L^2([0,1],\mathbb{R})} = 0$ then $g \in \text{span}\{e\}^\perp$; thus, $\ker(\dot{L}) = \text{span}\{e\}^\perp$. Since the linear response formula is $\lim_{\varepsilon \to 0} \frac{f_\varepsilon - f_0}{\varepsilon} = (\text{Id} - L_0)^{-1} \dot{L} f_0$, we are done. □

Remark 3.3.20. *Let L_ε be an integral operator with the kernel $k_\varepsilon = k_0 + \varepsilon \dot{k}$, where $\dot{k}$ is as in the result above; thus, we can write $L_\varepsilon = L_0 + \varepsilon \dot{L}$. For $g \in L^2$, we write $g = g_1 + g_2$, where $g_1 \in span\{e\}$ and $g_2 \in span\{e\}^\perp$. From the result*

above, we see that $L_\varepsilon g = L_0 g + \varepsilon \dot{L} g_1$*; that is, to enhance mixing, only* g_1*, the part parallel to* e*, contributes to the perturbation. Furthermore,* $\varepsilon \dot{L} g_1$ *is in the span of* $\hat{e} - \langle \hat{e}, \mathbf{1} \rangle_{L^2([0,1],\mathbb{R})} \mathbf{1}$*, which is the projection of the eigenvector* $\hat{e}$*, corresponding to the second largest eigenvalue of* L_0^**, onto span*$\{\mathbf{1}\}^\perp$ *(the orthogonal complement of the eigenspace corresponding to the largest eigenvalue of* L_0^**).*

3.3.5 Approximation of the Optimal Response

We conclude this section by obtaining a convergence result, similar to Proposition 3.3.13, for the solution (3.3.21).

Proposition 3.3.21. *Let* $L_0 : L^2([0,1],\mathbb{C}) \to L^2([0,1],\mathbb{C})$ *be a Hilbert-Schmidt integral operator, with the stochastic kernel* $k_0 \in L^\infty([0,1]^2)$*, satisfying* $(A1)$ *of Theorem 3.1.2. Let* $\{L_n\} \subset \mathcal{B}(L^2([0,1],\mathbb{C}))$ *be a sequence of Hilbert-Schmidt integral operators with stochastic kernels* $\{k_n\} \subset L^\infty([0,1]^2)$ *such that* $\lim_{n\to\infty} \|k_n - k_0\|_{L^\infty([0,1]^2)} = 0$*. Then, there exists* $n_0 > 0$ *such that for each* $n \geq n_0$*,* L_n *satisfies* $(A1)$ *of Theorem 3.1.2 and there exists* $\lambda_n \in \mathbb{C}$ *and functions* $e_n, \hat{e}_n \in L^\infty([0,1],\mathbb{C})$*, with* $\|e_n\|_2 = 1 = \|\hat{e}\|_2$*, such that* $L_n e_n = \lambda_n e_n$*,* $L_n^* \hat{e}_n = \lambda_n \hat{e}_n, \lim_{n\to\infty} |\lambda_n - \lambda_0| = 0, \lim_{n\to\infty} \|e_n - e\|_\infty = 0$ *and* $\lim_{n\to\infty} \|\hat{e}_n - \hat{e}\|_\infty$*. Let*

$$\begin{aligned} E_n(x,y) := &\left(\Re(\hat{e}_n)(x)\Re(e_n)(y) + \Im(\hat{e}_n)(x)\Im(e_n)(y)\right)\Re(\lambda_n) \\ &+ \left(\Im(\hat{e}_n)(x)\Re(e_n)(y) - \Re(\hat{e}_n)(x)\Im(e_n)(y)\right)\Im(\lambda_n). \end{aligned}$$

Then, the sequence of perturbations

$$\dot{k}_n(x,y) := \begin{cases} \frac{1}{\alpha_n}\left(\frac{1}{\ell(F_y)}\int_{F_y} E_n(x,y)dx - E_n(x,y)\right) & (x,y) \in F, \\ 0 & \text{otherwise}, \end{cases} \tag{3.3.26}$$

where F *and* F_y *are as in Theorem 3.3.18 and* α_n *is selected so that* $\|\dot{k}_n\|_{L^2([0,1]^2,\mathbb{R})} = 1$*, converges to the optimal* $\dot{k}$ *in* L^∞ *as* $n \to \infty$*.*

Proof. From $\lim_{n\to\infty} \|k_n - k_0\|_{L^\infty([0,1]^2,\mathbb{R})} = 0$, and (3.2.2), we have $\lim_{n\to\infty} \|L_n - L_0\|_{L^2\to L^2} = 0$. From this and the assumption that L_0 satisfies $(A1)$, we have from the argument in the proof of Theorem 3.1.2 that there exists $\bar{n}_0 > 0$ such that for all $n \geq \bar{n}_0$, L_n satisfies $(A1)$. Next we show the existence of the approximating

eigenvalues and eigenvectors. Recalling that λ_0 is a geometrically simple isolated eigenvalue, we can use Theorem 3.16 in IV-§3.4 [54] (because of Theorem 2.23 (a) IV-§2.6 and the fact that $L_n \in \mathcal{B}(L^2([0,1]^2,\mathbb{C}))$ and $\lim_{n\to\infty}\|L_n - L_0\|_{L^2\to L^2} = 0$). From Theorem 3.16, and the discussion in IV-§3.5, we conclude that there exists an $n_0 > \bar{n}_0$ and $\{\lambda_n\} \subset \mathbb{C}$ such that for all $n \geq n_0$, λ_n is an eigenvalue of L_n and $\lim_{n\to\infty}|\lambda_n - \lambda_0| = 0$. Let Π_0 be the eigenprojection associated to the eigenvalue λ_0 of L_0; similarly, let Π_n denote the eigenprojection associated to the eigenvalue λ_n of L_n. From Theorem 3.16, we also have that for $n \geq n_0$, λ_n is a geometrically simple eigenvalue of L_n (since $\dim(\Pi_n(L^2([0,1],\mathbb{C}))) = \dim(\Pi_0(L^2([0,1],\mathbb{C}))) = 1$ for $n \geq n_0$) and that $\lim_{n\to\infty}\|\Pi_n - \Pi_0\|_{L^2\to L^2} = 0$. Let $e_n = \frac{\Pi_n e}{\|\Pi_n e\|_2}$; then $L_n e_n = \lambda_n e_n$ and $\|e_n - e\|_2 = \|(\Pi_n - \Pi_0)e\|_2 \leq \|\Pi_n - \Pi_0\|_{L^2\to L^2}\|e\|_2 \to 0$ as $n \to \infty$. From inequality (3.2.2), we also have $\|L_n^* - L_0^*\|_{L^2\to L^2} \leq \|k_n - k_0\|_{L^2([0,1]^2,\mathbb{R})} \to 0$ as $n \to \infty$; thus, we can apply the argument above to conclude that there exists functions $\hat{e}_n \in L^2([0,1],\mathbb{C})$ such that $L_n^*\hat{e}_n = \lambda_n\hat{e}_n$ and $\lim_{n\to\infty}\|\hat{e}_n - \hat{e}\|_2 = 0$.

From inequality (3.2.3) we have $e_n, \hat{e}_n \in L^\infty([0,1],\mathbb{C})$ since $k_n \in L^\infty([0,1]^2,\mathbb{R})$. We now show that $\|e_n - e\|_\infty \to 0$ and $\|\hat{e}_n - \hat{e}\|_\infty \to 0$ as $n \to \infty$. We compute

$$
\begin{aligned}
&\|e_n - e\|_\infty \\
&\quad = \left\| \frac{1}{\lambda_n} L_n e_n - \frac{1}{\lambda_0} L_0 e \right\|_\infty \\
&\quad \leq \left| \frac{1}{\lambda_n} - \frac{1}{\lambda_0} \right| \|L_n e_n\|_\infty + \frac{1}{|\lambda_0|}\|L_n e_n - L_0 e\|_\infty \\
&\quad \leq \left| \frac{1}{\lambda_n} - \frac{1}{\lambda_0} \right| \|k_n\|_{L^\infty([0,1]^2,\mathbb{R})}\|e_n\|_1 + \frac{1}{|\lambda|}(\|(L_n - L_0)e_n\|_\infty + \|L_0(e_n - e)\|_\infty) \\
&\quad \leq \left| \frac{1}{\lambda_n} - \frac{1}{\lambda_0} \right| \|k_n\|_{L^\infty([0,1]^2,\mathbb{R})}\|e_n\|_2 \\
&\qquad + \frac{1}{|\lambda|}(\|k_n - k_0\|_{L^\infty([0,1]^2,\mathbb{R})}\|e_n\|_1 + \|k_0\|_{L^\infty([0,1]^2,\mathbb{R})}\|e_n - e\|_1) \\
&\quad \leq \left| \frac{1}{\lambda_n} - \frac{1}{\lambda_0} \right| \left(\|k_n - k_0\|_{L^\infty([0,1]^2,\mathbb{R})} + \|k_0\|_{L^\infty([0,1]^2,\mathbb{R})}\right)\left(\|e_n - e\|_2 + \|e\|_2\right) \\
&\qquad + \frac{1}{|\lambda|}(\|k_n - k_0\|_{L^\infty([0,1]^2,\mathbb{R})}\left(\|e_n - e\|_2 + \|e\|_2\right) + \|k_0\|_{L^\infty([0,1]^2,\mathbb{R})}\|e_n - e\|_2).
\end{aligned}
\tag{3.3.27}
$$

Hence, as $\|k_n - k_0\|_{L^\infty([0,1]^2,\mathbb{R})} \to 0$, we have that $\|e_n - e\|_\infty \to 0$. The same argument can be used to show $\|\hat{e}_n - \hat{e}\|_\infty \to 0$.

To show that $\lim_{n\to\infty} \|\dot{k}_n - \dot{k}\|_{L^\infty([0,1]^2,\mathbb{R})} = 0$, we need that $\lim_{n\to\infty} \|E_n - E\|_{L^\infty([0,1]^2,\mathbb{R})} = 0$. From the convergence of λ_n, e_n and $\hat{e}_n$ to λ, e and $\hat{e}$, respectively, we have the convergence of $\Re(\lambda_n), \Im(\lambda_n), \Re(e_n), \Im(e_n), \Re(\hat{e}_n), \Im(\hat{e}_n)$ to $\Re(\lambda), \Im(\lambda), \Re(e), \Im(e), \Re(\hat{e}), \Im(\hat{e})$, respectively, where function convergence is in L^∞. Using this, we conclude the convergence of E_n to E in $L^\infty([0,1]^2, \mathbb{R})$. Noting that

$$\begin{aligned}\left|\frac{1}{\ell(F_y)}\int_{F_y} E_n(x,y)dx - \frac{1}{\ell(F_y)}\int_{F_y} E(x,y)dx\right| &\leq \frac{1}{\ell(F_y)}\int_{F_y} |E_n(x,y) - E(x,y)|dx \\ &\leq \|E_n - E\|_{L^\infty([0,1]^2,\mathbb{R})},\end{aligned}$$

the convergence of E_n to E in L^∞ proves the convergence of the integral. Finally, the convergence of the scaling factor α_n follows from the L^∞ convergence of $\frac{1}{m(F_y)}\int_{F_y} E_n(x,y)dx - E_n(x,y)$ and the reverse triangle inequality. Hence, $\|\dot{k}_n - \dot{k}\|_{L^\infty([0,1]^2,\mathbb{R})} \to 0$ as $n \to \infty$.

□

3.4 Linear Response for Map Perturbations

In this section we consider systems (T_ε, ρ) with additive noise in which the dynamics is governed by a stochastic process which is given by the composition of a deterministic map T_ε and the adding of some noise at each iteration. We will assume that the noise is distributed according to a certain Lipschitz kernel ρ and impose a "reflecting boundary" condition that ensures that the dynamics, after the noise, are still in the interval $[0,1]$. More precisely, we consider a random dynamical system with additive noise on $[0,1]$ whose trajectories are given by

$$x_{n+1} = T_\varepsilon(x_n) \hat{+} \omega_n \tag{3.4.1}$$

where

(T1) $T_\varepsilon : [0,1] \to [0,1]$ is a Borel measurable map

(T2) ω_n is an i.i.d. process distributed according to a probability density $\rho \in Lip([-1+\varepsilon_0, 1-\varepsilon_0])$ with Lipschitz constant K.

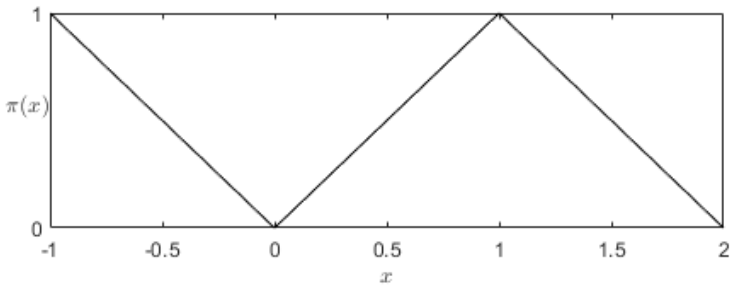


Figure 3.1: The function π.

- $\hat{+}$ is the "boundary reflecting" sum, which we defined as follows: let $\pi : [-1, 2] \to [0, 1]$ be the piecewise linear map

$$\pi(x) = \min_{i \in \mathbb{Z}} |x - 2i|, \tag{3.4.2}$$

see Figure 3.1. Then, for $a, b \in \mathbb{R}$, the sum $\hat{+}$ is defined as

$$a \hat{+} b := \pi(a + b)$$

where $+$ is the usual sum operator on $\mathbb{R}$; by this $a \hat{+} b \in [0, 1]$.

3.4.1 Expressing the Map Perturbation as a Kernel Perturbation

Associated with the process (3.4.1) is an integral-type transfer operator, which we will derive (following the method of §10.5 in [62]). Since $|\pi'(z)| = 1$ for all $z \in [-1, 2]$, the Perron-Frobenius operator $\mathscr{P}_\pi : L^1([-1, 2]) \to L^1([0, 1])$ associated to the map π is simply

$$\mathscr{P}_\pi f(x) = \sum_{z \in \pi^{-1}(x)} f(z) = f(x) + f(-x) + f(2 - x). \tag{3.4.3}$$

For $b \in \mathbb{R}$ consider the shift map τ_b defined by $(\tau_b f)(y) := f(y + b)$ for $f \in Lip([-1, 2])$. For the process (3.4.1), suppose that x_n has the distribution f_n (i.e. $f_n \in L^1$, $f_n \geq 0$ and $\int f_n \, d\ell = 1$). Following [62], §10.5, we note that $T_\varepsilon(x_n)$ and ω_n are independent (since we only need $\omega_0, \ldots, \omega_{n-1}$ to compute $x_1, \ldots, x_n$) and so, the joint density of (x_n, ω_n) is $f_n(y)\rho(z)$. Let $h : \mathbb{R} \to \mathbb{R}$ be a bounded, measurable

function and let $\mathbb{E}$ denote expectation with respect to ℓ; we then compute

$$\begin{aligned}
\mathbb{E}(h(x_{n+1})) &= \mathbb{E}(h(\pi_y(T_\varepsilon(x_n) + \omega_n)) \\
&= \int\int h(\pi(T_\varepsilon(y) + z)) f_n(y)\rho(z)dydz \\
&= \int\int h(\pi(z'))f_n(y)\rho(z' - T_\varepsilon(y))dz'dy \\
&= \int f_n(y) \int h(\pi(z'))(\tau_{-T_\varepsilon(y)}\rho)(z')dz'dy \\
&= \int f_n(y) \int h(z')(\mathscr{P}_\pi \tau_{-T_\varepsilon(y)}\rho)(z')dz'dy,
\end{aligned}$$

where the last equality follows from the duality of the Perron-Frobenius and the Koopman operators. Since $\mathbb{E}(h(x_{n+1})) = \int h(x)f_{n+1}(x)dx$, and h is arbitrary, the map $f_n \mapsto f_{n+1}$ is given by

$$f_{n+1}(z') = \int (\mathscr{P}_\pi \tau_{-T_\varepsilon(y)}\rho)(z')f_n(y)dy$$

for all $z' \in [0,1]$. Thus, the integral operator $L_\varepsilon : L^2([0,1]) \to L^2([0,1])$ associated to the process (3.4.1) is given by

$$L_\varepsilon f(x) = \int k_\varepsilon(x,y)f(y)dy, \tag{3.4.4}$$

where

$$k_\varepsilon(x,y) = (\mathscr{P}_\pi \tau_{-T_\varepsilon(y)}\rho)(x) \tag{3.4.5}$$

and $x, y \in [0,1]$.

Lemma 3.4.1. *The kernel (3.4.5) is a stochastic kernel in $L^\infty([0,1]^2)$.*

Proof. Stochasticity and nonnegativity of k_ε follow from stochasticity and nonnegativity of ρ and the fact that Perron-Frobenius operators preserve these properties. Essential boundedness of k_ε follows from the facts that ρ is Lipschitz (thus essentially bounded), τ is a shift and $\mathscr{P}_\pi$ is constructed from a finite sum.

□

Proposition 3.4.2. *Assume that (T_ε, ρ) satisfies (T1) and (T2) and that k_ε is given by (3.4.5). Suppose that the family of interval maps $\{T_\varepsilon\}_{\varepsilon\in[0,\varepsilon_0)}$ satisfies*

$$T_\varepsilon = T_0 + \varepsilon \cdot \dot{T} + t_\varepsilon,$$

where $\dot{T}, t_\varepsilon \in L^2$ and $\|t_\varepsilon\|_2 = o(\varepsilon)$. Then

$$k_\varepsilon = k_0 + \varepsilon \cdot \dot{k} + r_\varepsilon$$

where $\dot{k} \in L^2([0,1]^2)$ is given by

$$\dot{k}(x,y) = -\left(\mathscr{P}_\pi\left(\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x)\cdot\dot{T}(y) \tag{3.4.6}$$

and $r_\varepsilon \in L^2([0,1]^2)$ satisfies the properties listed in Lemma 3.2.3.

Proof. For almost all x, y we have

$$\begin{aligned} k_\varepsilon(x,y) - k_0(x,y) &= (\mathscr{P}_\pi\tau_{-T_\varepsilon(y)}\rho)(x) - (\mathscr{P}_\pi\tau_{-T_0(y)}\rho)(x) \\ &= (\mathscr{P}_\pi\tau_{-T_\varepsilon(y)}\rho)(x) - (\mathscr{P}_\pi\tau_{-(T_0(y)+\varepsilon\dot{T}(y))}\rho)(x) \qquad (3.4.7) \\ &\quad +(\mathscr{P}_\pi\tau_{-(T_0(y)+\varepsilon\dot{T}(y))}\rho)(x) - (\mathscr{P}_\pi\tau_{-T_0(y)}\rho)(x). \qquad (3.4.8) \end{aligned}$$

We then have that $\|k_\varepsilon - k_0 - \varepsilon\dot{k}\|_{L^2([0,1]^2)}$ is bounded above by sum of the L^2 norm of (3.4.7) and the L^2 norm of (3.4.8) minus $\varepsilon\dot{k}$. We will first show that the L^2 norm of (3.4.7) is $o(\varepsilon)$ and then show that the L^2 norm of (3.4.8) minus $\varepsilon\dot{k}$ is also $o(\varepsilon)$.

Since ρ is uniformly Lipschitz with constant K, we have for a.e. x, y that

$$\begin{aligned} \left|(\tau_{-(T_\varepsilon(y))}\rho)(x) - (\tau_{-(T_0(y)+\varepsilon\dot{T}(y))}\rho)(x)\right| &= \left|\rho(x - T_\varepsilon(y)) - \rho(x - T_0(y) - \varepsilon\dot{T}(y))\right| \\ &= \big|\rho(x - T_0(y) - \varepsilon\dot{T}(y) - t_\varepsilon(y)) \\ &\qquad - \rho(x - T_0(y) - \varepsilon\dot{T}(y))\big| \\ &\le K|t_\varepsilon(y)|; \end{aligned}$$

hence, $|\tau_{-T_\varepsilon}\rho - \tau_{-(T_0+\varepsilon\dot{T})}\rho| \leq K|t_\varepsilon|$. Since $T_0(y) \in [0,1]$ for a.e. $y \in [0,1]$, we have that $\text{supp}(\tau_{-T_0(y)}\rho) \subset [-1,2]$ and hence, we can apply $\mathscr{P}_\pi$ to $\tau_{-T_0(y)}\rho$. To find the interval containing the support of $\tau_{-(T_0(y)+\varepsilon\dot{T}(y))}\rho$ we first note that $|t_\varepsilon| \leq \varepsilon_0$ a.e. since otherwise we would not have $\|t_\varepsilon\|_2 = o(\varepsilon)$. Since $T_\varepsilon = T_0 + \varepsilon\dot{T} + t_\varepsilon$ and $T_\varepsilon(y) \in [0,1]$ for a.e. $y \in [0,1]$, we have that $-\varepsilon_0 \leq T_0 + \varepsilon\dot{T} \leq 1 + \varepsilon_0$. Hence, $\text{supp}(\tau_{-(T_0(y)+\varepsilon\dot{T}(y))}\rho) \subseteq [-1+\varepsilon_0+T_0(y)+\varepsilon\dot{T}(y), 1-\varepsilon_0+T_0(y)+\varepsilon\dot{T}(y)] \subseteq [-1,2]$ and so, we can apply $\mathscr{P}_\pi$ to $\tau_{-(T_0(y)+\varepsilon\dot{T}(y))}\rho$. Then we have

$$\begin{aligned}\left|\mathscr{P}_\pi\tau_{-T_\varepsilon}\rho - \mathscr{P}_\pi\tau_{-(T_0+\varepsilon\dot{T})}\rho\right| &\leq \mathscr{P}_\pi\left(\left|\tau_{-T_\varepsilon}\rho - \tau_{-(T_0+\varepsilon\dot{T})}\rho\right|\right)\\ &\leq K\mathscr{P}_\pi(|t_\varepsilon|) = K|t_\varepsilon|,\end{aligned}$$

where the first inequality follows from the fact that $\mathscr{P}_\pi$ is a Markov operator and the last equality follows from the fact that $\text{supp}(t_\varepsilon) \subseteq [0,1]$. Thus, we have

$$\begin{aligned}&\left(\int_0^1\int_0^1 \left|(\mathscr{P}_\pi\tau_{-(T_\varepsilon(y))}\rho)(x) - (\mathscr{P}_\pi\tau_{-(T_0(y)+\varepsilon\dot{T}(y))}\rho)(x)\right|^2 dxdy\right)^{1/2}\\ &\quad\leq K\left(\int_0^1\int_0^1 |t_\varepsilon(x)|^2 dxdy\right)^{1/2}\\ &\quad= K\|t_\varepsilon\|_2 = o(\varepsilon)\end{aligned}$$

and therefore the L^2 norm of (3.4.7) is $o(\varepsilon)$

Next we show that the L^2 norm of (3.4.8) minus $\varepsilon\dot{k}$ is $o(\varepsilon)$. Noting that

$$\text{supp}\left(\dot{T}(y)\cdot\tau_{-T_0(y)}\frac{d\rho}{dx}\right) \subseteq [-1,2],$$

we have

$$\begin{aligned}&\int_0^1\int_0^1\left(\frac{(\mathscr{P}_\pi\tau_{-(T_0(y)+\varepsilon\dot{T}(y))}\rho)(x) - (\mathscr{P}_\pi\tau_{-T_0(y)}\rho)(x)}{\varepsilon}\right.\\ &\qquad\left.-\left(-\mathscr{P}_\pi\left(\dot{T}(y)\cdot\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x)\right)^2 dxdy\\ &=\int_0^1\int_0^1\left(\mathscr{P}_\pi\left(\frac{\tau_{-(T_0(y)+\varepsilon\dot{T}(y))}\rho - \tau_{-T_0(y)}\rho}{\varepsilon} + \left(\dot{T}(y)\cdot\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)\right)(x)^2 dxdy\end{aligned}$$

$$\leq 7 \int_0^1 \int_{-1}^2 \left(\frac{\left(\tau_{-(T_0(y)+\varepsilon\dot{T}(y))}\rho\right)(x) - \left(\tau_{-T_0(y)}\rho\right)(x)}{\varepsilon} \right.$$
$$\left. - \left(-\dot{T}(y) \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right)(x) \right) \right)^2 dxdy,$$

where in the last line we used Lemma B.1.1 from the Appendix. We next note that

$$\lim_{\varepsilon\to 0} \frac{\rho(x - T_0(y) - \varepsilon\dot{T}(y)) - \rho(x - T_0(y))}{\varepsilon} = -\frac{d\rho}{dx}(x - T_0(y))\dot{T}(y) \tag{3.4.9}$$

for a.e. x, y. Since $\left|\frac{\rho(x-T_0(y)-\varepsilon\dot{T}(y))-\rho(x-T_0(y))}{\varepsilon}\right| \leq K\dot{T}(y)$, by the dominated convergence theorem the limit also converges in L^2. Hence, the L^2 norm of (3.4.8) minus $\varepsilon\dot{k}$ is $o(\varepsilon)$; combining this with the fact that the L^2 norm of (3.4.7) is $o(\varepsilon)$, we have $\lim_{\varepsilon\to 0} \frac{1}{\varepsilon}\|k_\varepsilon - k_0 - \varepsilon\dot{k}\|_{L^2([0,1]^2)} = 0$. We finally conclude from the latter that $\|r_\varepsilon\|_{L^2([0,1]^2)} = o(\varepsilon)$.

□

3.4.2 A Formula for the Linear Response of the Invariant Measure and Continuity with respect to the Map

By considering the kernel form of map perturbations, we can apply Corollary 3.2.4 to obtain the following.

Proposition 3.4.3. *Let $L_\varepsilon : L^2 \to L^2$, $\varepsilon \in [0, \varepsilon_0)$, be integral operators with the kernels k_ε as in (3.4.5). Suppose that L_0 satisfies (A1) of Theorem 3.1.2 and let $f_\varepsilon \in L^2$ be the probability density such that $L_\varepsilon f_\varepsilon = f_\varepsilon$. Then the kernel $\dot{k}$ in (3.4.6) is in V_{ker} and*

$$\lim_{\varepsilon\to 0} \frac{f_\varepsilon - f_0}{\varepsilon} = -(Id - L_0)^{-1} \int_0^1 \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right)(x)\dot{T}(y)f_0(y)dy,$$

with convergence in L^2.

Proof. The result is a direct application of Corollary 3.2.4; we verify its assumptions. From Lemma 3.4.1, k_ε is a stochastic kernel and so L_ε is an integral preserving compact operator. From Proposition 3.4.2, k_ε has the form (3.2.5). Thus, we can apply Corollary 3.2.4 to obtain the result. □

Since we are interested in map perturbations, we will consider the the linear response as a function of the map perturbation; more precisely, let $\widehat{R} : L^2 \to L^2$ be defined as

$$\widehat{R}(\dot{T}) := -(\mathrm{Id} - L_0)^{-1} \int_0^1 \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right) (x) \dot{T}(y) f_0(y) dy. \tag{3.4.10}$$

Lemma 3.4.4. *The function $\widehat{R} : L^2 \to L^2$ is continuous.*

Proof. Let $\dot{T}_1, \dot{T}_2 \in L^2$ be such that $\|\dot{T}_1 - \dot{T}_2\|_2 \leq l$. Then we have

$$\widehat{R}(\dot{T}_1) - \widehat{R}(\dot{T}_2) = -(\mathrm{Id} - L_0)^{-1} \int_0^1 \tilde{k}(x, y) \left(\dot{T}_1(y) - \dot{T}_2(y) \right) dy,$$

where $\tilde{k}(x, y) := \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right) (x) f_0(y)$. Also, $\left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right) (x) \in L^\infty([0,1]^2)$ since $\frac{d\rho}{dx} \in L^\infty$. From inequality (3.2.3), we then have $f_0 \in L^\infty$ and so $\tilde{k} \in L^\infty([0,1]^2)$. Using inequality (3.2.2) we finally have

$$\|\widehat{R}(\dot{T}_1) - \widehat{R}(\dot{T}_2)\|_2 \leq l \|(\mathrm{Id} - L_0)^{-1}\|_{V \to V} \|\tilde{k}\|_{L^2([0,1]^2)}.$$

□

3.4.3 A Formula for the Linear Response of the Dominant Eigenvalues and Continuity with respect to the Map

By expressing map perturbations as kernel perturbations, we are also able to express the linear response of the dominant eigenvalues as a function of the perturbing map $\dot{T}$.

Proposition 3.4.5. *Let $L_\varepsilon : L^2([0,1], \mathbb{C}) \to L^2([0,1], \mathbb{C})$, $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, be integral operators with the kernels k_ε as in(3.4.5). Let $\lambda_{i,\varepsilon}$ be the eigenvalue(s) of L_ε with second largest magnitude strictly inside the unit disk. Suppose that L_0 satisfies (A1) of Theorem 3.1.2 and $\{\lambda_{i,0}\} = \mathcal{I}$ (the unperturbed eigenvalue(s) with second largest magnitude) are geometrically simple. Then*

$$\left. \frac{d\lambda_{i,\varepsilon}}{d\varepsilon} \right|_{\varepsilon=0} = \langle H, \dot{T} \rangle_{L^2([0,1],\mathbb{C})}, \tag{3.4.11}$$

where e is the eigenvector of L_0 associated to the eigenvalue $\lambda_{i,0}$, $\hat{e}$ is the eigenvector of L_0^* associated to the eigenvalue $\lambda_{i,0}$ and

$$H(y) = \bar{e}(y) \int_0^1 \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right) (x) \hat{e}(x) dx.$$

Proof. Since $k_\varepsilon \in L^2([0,1]^2, \mathbb{R})$, $L_\varepsilon : L^2([0,1], \mathbb{C}) \to L^2([0,1], \mathbb{C})$ is compact. From Lemma 3.4.1 we have that k_ε is a stochastic kernel and so L_ε preserves the integral (i.e. it satisfies (3.1.2)). The kernel k_ε is in the form (3.2.5) and so $\varepsilon \mapsto L_\varepsilon$ is C^1 (see Lemma 3.2.3), where the derivative operator $\dot{L}$ is the integral operator with the kernel $\dot{k}$. Using the assumption that L_0 is mixing and $\lambda_{i,0}$ are geometrically simple, we apply Proposition 3.1.6 to obtain $\frac{d\lambda_{i,\varepsilon}}{d\varepsilon}\big|_{\varepsilon=0} = \langle \hat{e}, \dot{L}e \rangle_{L^2([0,1],\mathbb{C})}$. Finally, we compute

$$\begin{aligned}
\langle \hat{e}, \dot{L}e \rangle_{L^2([0,1],\mathbb{C})} &= \int_0^1 \hat{e}(x) \overline{\int_0^1 \dot{k}(x,y) e(y) dy} dx \\
&= \int_0^1 \int_0^1 \hat{e}(x) \dot{k}(x,y) \bar{e}(y) dx dy \\
&= \int_0^1 \bar{e}(y) \int_0^1 \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right) (x) \hat{e}(x) dx \dot{T}(y) dy \\
&= \langle H, \dot{T} \rangle_{L^2([0,1],\mathbb{C})}.
\end{aligned}$$

□

From (3.4.11), the linear response of the dominant eigenvalues is continuous with respect to map perturbations. This follows from Cauchy-Schwarz and the fact that $H \in L^\infty([0,1], \mathbb{C})$; the latter claim follows from the fact that $\left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right) (x) \in L^\infty([0,1]^2, \mathbb{R})$ (see proof of Lemma 3.4.4) and since $e, \hat{e} \in L^\infty([0,1], \mathbb{C})$ (which follows from (3.2.3) and the fact that $k_0 \in L^\infty([0,1]^2, \mathbb{R})$, see Lemma 3.4.1).

3.5 Optimal Linear Response for Map Perturbations

In this section we will obtain the results of Sections 3.3.2–3.3.5 for deterministic systems with additive noise. We begin with a description of the set of allowable map perturbations. Then we obtain an explicit formula for the optimal map perturbation that maximises the expectation of an observable; we then show a convergence result

for the optimal solution. We also obtain an explicit formula for the optimal map perturbation that enhances mixing and conclude with a convergence result for this optimal solution.

3.5.1 The Feasible Set of Perturbations

Before we formulate the optimisation problem, we note that in this setting, we require some restriction on the space of allowable perturbations to T_0 if we are to interpret $\dot{T}$ as a map perturbation. With this in mind, let $\mathcal{b} > 0$ and $\widetilde{F}_{\mathcal{b}} := \{x \in [0,1] : \mathcal{b} \leq T_0(x) \leq 1-\mathcal{b}\}$. Recalling that in Proposition 3.4.2 we are considering L^2 perturbations of the map T_0, that is $\dot{T} \in L^2$, we introduce the following definition and result.

Lemma 3.5.1. *Let*

$$S_{T_0,\mathcal{b}} := \{T \in L^2 : supp(T) \subseteq \widetilde{F}_{\mathcal{b}}\}. \tag{3.5.1}$$

Then $S_{T_0,\mathcal{b}}$ is a closed subspace of L^2.

Proof. It is clear that $S_{T_0,\mathcal{b}}$ is a subspace. To show it is closed, let $\{f_n\} \subset S_{T_0,\mathcal{b}}$ and suppose that $f_n \to_{L^2} f \in L^2$; also suppose that $\widehat{S} := \{x \in [0,1] : T_0(x) < \mathcal{b} \text{ or } T_0(x) > 1-\mathcal{b}\}$ is not a null set. Then, we have

$$\int_{S_{T_0,\mathcal{b}}} (f_n(x) - f(x))^2 dx + \int_{\widehat{S}} f(x)^2 dx \to 0.$$

If $\int_{\widehat{S}} f(x)^2 dx > 0$, we obtain a contradiction since $\int_{S_{T_0,\mathcal{b}}} (f_n(x) - f(x))^2 dx \geq 0$; thus, $\int_{\widehat{S}} f(x)^2 dx = 0$ and so $f = 0$ a.e. on $\widehat{S}$. Hence, $S_{T_0,\mathcal{b}}$ is closed. □

For the remainder of this section, the set of allowable perturbations that we will consider is

$$P_{\mathcal{b}} := S_{T_0,\mathcal{b}} \cap B_1, \tag{3.5.2}$$

where B_1 is the unit ball in L^2. Since $S_{T_0,\mathcal{b}}$ is a closed subspace of L^2, it is itself a Hilbert space and so $P_{\mathcal{b}}$ is strictly convex.

3.5.2 *Explicit Formula for the Optimal Perturbation for Maximising the Expectation of an Observable*

In this section we will consider the problem of finding the optimal map perturbation that maximises the expectation of some observable $c \in L^2$. We begin with a result that ensures a unique solution exists and then derive an explicit expression for the optimal perturbation.

Proposition 3.5.2. *Let P_δ be the set in (3.5.2). Then, the problem of finding $\dot{T} \in P_\delta$ such that*

$$\left\langle c, \widehat{R}(\dot{T}) \right\rangle_{L^2([0,1],\mathbb{R})} = \max_{\dot{h} \in P_\delta} \left\langle c, \widehat{R}(\dot{h}) \right\rangle_{L^2([0,1],\mathbb{R})}, \tag{3.5.3}$$

where $\widehat{R}$ is as in (3.4.10), has a unique solution.

Proof. From Lemma 3.4.4, it follows that $\langle c, \widehat{R}(\dot{h}) \rangle_{L^2([0,1],\mathbb{R})}$ is continuous as a function of $\dot{h}$. Since it is also linear in $\dot{h}$, we can apply Proposition 3.3.1 to conclude that a solution exists. Recalling that P_δ is strictly convex, the uniqueness of the solution follows from Proposition 3.3.3. □

Before we present the explicit formula for the optimal solution, we will reformulate the optimisation problem (3.5.3) to simplify the analysis. We first note that since the objective function in (3.5.3) is linear in $\dot{T}$, the maximum will occur on $S_{T_0,\delta} \cap \partial B_1$. Also, we have that $\widehat{R}(\dot{T}) \in V$; this follows from the fact that $\left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx}\right)\right)(x) f_0(y) \in V_{\text{ker}}$ (since $\dot{k} \in V_{\text{ker}}$, see Proposition 3.4.3) and therefore $\int_0^1 \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx}\right)\right)(x) f_0(y) g(y) dy \in V$ for $g \in L^2$ (see Lemma 3.2.1). Hence, we only need to consider $c \in \text{span}\{f_0\}^\perp$ (see discussion in Section 3.3.2 prior to Theorem 3.3.8). With these remarks, we consider the following reformulation of (3.5.3): for $c \in \text{span}\{f_0\}^\perp$

$$\min_{\dot{T} \in S_{T_0,\delta}} \quad -\left\langle c, \widehat{R}(\dot{T}) \right\rangle_{L^2([0,1],\mathbb{R})} \tag{3.5.4}$$

$$\text{subject to} \quad \|\dot{T}\|_2^2 - 1 = 0. \tag{3.5.5}$$

Theorem 3.5.3. *Let (T_0, ρ) be a deterministic system with additive noise satisfying $(T1)$ and $(T2)$. Suppose the associated transfer operator L_0, with the kernel k_0 as in (3.4.5), satisfies $(A1)$ of Theorem 3.1.2. Let $\mathcal{G} : L^2 \to L^2$ be defined as*

$$\mathcal{G}f(y) := \int_0^1 \left(\mathcal{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right) (x) f(x) dx. \tag{3.5.6}$$

Then, the unique solution to the optimisation problem (3.5.4)–(3.5.5) is

$$\dot{T}(y) = \begin{cases} -\|f_0 \mathcal{G}((Id - L_0^*)^{-1} c) \mathbf{1}_{\widetilde{F}_\delta}\|_2^{-1} f_0(y) \mathcal{G}((Id - L_0^*)^{-1} c)(y) & y \in \widetilde{F}_\delta, \\ 0 & \text{otherwise.} \end{cases} \tag{3.5.7}$$

Furthermore, $\dot{T} \in L^\infty$.

Proof. The proof will follow similarly to that of Theorem 3.3.8. To this end, we consider the following Lagrangian function

$$\mathcal{L}(\dot{T}, \lambda) := f(\dot{T}) + \lambda g(\dot{T}),$$

where $f(\dot{T}) := -\langle c, \widehat{R}(\dot{T}) \rangle_{L^2([0,1],\mathbb{R})}$, $g(\dot{T}) := \|\dot{T}\|_2^2 - 1$ and $\dot{T} \in S_{T_0,\delta}$.

Necessary conditions: We want to find $\dot{T}$ and λ that satisfy the first-order necessary conditions:

$$g(\dot{T}) = 0$$
$$D_{\dot{T}} \mathcal{L}(\dot{T}, \lambda) \tilde{T} = 0 \text{ for all } \tilde{T} \in S_{T_0,\delta},$$

where $D_{\dot{T}} \mathcal{L}(\dot{T}, \lambda) \in \mathcal{B}(L^2, \mathbb{R})$ is the Frechet derivative with respect to the variable $\dot{T}$. Since f is linear, we have $(D_{\dot{T}} f)\tilde{T} = f(\tilde{T})$. Also, we have that $(D_{\dot{T}} g)\tilde{T} = 2\langle \dot{T}, \tilde{T} \rangle_{L^2([0,1],\mathbb{R})}$ (following the computation in Theorem 3.3.8). Thus, for the necessary conditions of the Lagrange multiplier method to be satisfied, we need that

$$D_{\dot{T}} \mathcal{L}(\dot{T}, \lambda) \tilde{T} = (D_{\dot{T}} f)\tilde{T} + \lambda (D_{\dot{T}} g)\tilde{T} = f(\tilde{T}) + 2\lambda \langle \dot{T}, \tilde{T} \rangle_{L^2([0,1],\mathbb{R})} = 0 \tag{3.5.8}$$

for all $\tilde{T} \in S_{T_0,\delta}$ and

$$g(\dot{T}) = 0. \tag{3.5.9}$$

Following the proof of Theorem 3.3.8, we will solve for $\dot{T}$ by rewriting $f(\tilde{T}) + 2\lambda\langle \dot{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})}$ as one inner product on L^2. To this end, we first have that

$$\begin{aligned}
&f(\tilde{T}) + 2\lambda\langle \dot{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})} \\
&= \left\langle c, (\mathrm{Id} - L_0)^{-1} \int_0^1 \left(\mathscr{P}_\pi\left(\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x)\tilde{T}(y)f_0(y)dy \right\rangle_{L^2([0,1],\mathbb{R})} \\
&\quad + 2\lambda\langle \dot{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})} \\
&= \left\langle (\mathrm{Id} - L_0^*)^{-1}c, \int_0^1 \left(\mathscr{P}_\pi\left(\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x)\tilde{T}(y)f_0(y)dy \right\rangle_{L^2([0,1],\mathbb{R})} \\
&\quad + \langle 2\lambda\dot{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})} \\
&= \int_0^1 \int_0^1 ((\mathrm{Id} - L_0^*)^{-1}c)(x) \left(\mathscr{P}_\pi\left(\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x)\tilde{T}(y)f_0(y)dydx \\
&\quad + \langle 2\lambda\dot{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})} \\
&= \int_0^1 \left[\int_0^1 ((\mathrm{Id} - L_0^*)^{-1}c)(x) \left(\mathscr{P}_\pi\left(\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x)dx f_0(y) + 2\lambda\dot{T}(y)\right]\tilde{T}(y)dy \\
&= \int_0^1 \left[f_0(y)\mathcal{G}((\mathrm{Id} - L_0^*)^{-1}c)(y) + 2\lambda\dot{T}(y)\right]\tilde{T}(y)dy.
\end{aligned} \tag{3.5.10}$$

We note that since $c \in \mathrm{span}\{f_0\}^\perp$, we have from Lemma 3.3.11 that $(\mathrm{Id} - L_0^*)^{-1}c \in L^2$ and the above expression is well defined. Now, from (3.5.10), we have that $f(\tilde{T}) + 2\lambda\langle \dot{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})} = \langle f_0\ \mathcal{G}((\mathrm{Id} - L_0^*)^{-1}c) + 2\lambda\dot{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})}$. From this we can conclude that finding $\dot{T}$ and λ that satisfy (3.5.8) and (3.5.9) reduces to finding $\dot{T} \in S_{T_0,\delta}$ and $\lambda \in \mathbb{R}$ that satisfy $\langle f_0\ \mathcal{G}((\mathrm{Id} - L_0^*)^{-1}c) + 2\lambda\dot{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})} = 0$ for all $\tilde{T} \in S_{T_0,\delta}$ and (3.5.9). Using the non-degeneracy of the inner product, we find that

$$\dot{T} = -\frac{H}{2\lambda},$$

where $H = \mathbf{1}_{\widetilde{F}_\delta} f_0\ \mathcal{G}((\mathrm{Id} - L_0^*)^{-1}c)$. The necessary condition (3.5.9) yields $\lambda = \pm\frac{1}{2}\|H\|_2$ and hence we obtain the form (3.5.7); the sign of λ is determined by checking the sufficient conditions.

Sufficient conditions: As in Theorem 3.3.8, we will show that $\dot{T}$ in (3.5.7) is the solution to the optimisation problem (3.5.4)–(3.5.5) by checking that it satisfies the second-order sufficient conditions. We first note that in this setting we have $Q = X = S_{T_0,\delta}$, $x_0 = \dot{T}$, $Y^* = \mathbb{R}$, $G(x_0) = g(\dot{T})$, $K = \{0\}$, $N_K(G(x_0)) = \mathbb{R}$, $T_K(G(x_0)) = \{0\}$ and $N_Q(x_0) = \{0\}$. Thus, to show that $\Lambda(\dot{T})$ is not empty, we need to show that $\dot{T}$ and λ satisfy

$$D_{\dot{T}}\mathcal{L}(\dot{T},\lambda)\dot{T} = 0,\ g(\dot{T}) = 0,\ \lambda \in \{0\}^-,\ \lambda g(\dot{T}) = 0, \tag{3.5.11}$$

where $\{0\}^- := \{\alpha \in \mathbb{R} : \alpha x \leq 0\ \forall x \in \{0\}\} = \mathbb{R}$. Following the argument in Theorem 3.3.8, it is easily verifiable that $\Lambda(\dot{T})$ is not empty. Thus, to show that $\dot{T}$ is a solution to (3.5.4)–(3.5.5), we need to show that it satisfies the following second-order conditions: there exists constants $\mu > 0$, $\eta > 0$ and $\beta > 0$ such that

$$\sup_{|\lambda|\leq\mu,\ \lambda\in\Lambda(\dot{T})} D^2_{\dot{T}\dot{T}}\mathcal{L}(\dot{T},\lambda)(\tilde{T},\tilde{T}) \geq \beta\|\tilde{T}\|_2^2,\ \forall\ \tilde{T} \in C_\eta(\dot{T}), \tag{3.5.12}$$

where $C_\eta(\dot{T}) := \left\{v \in S_{T_0,\delta} : |2\langle \dot{T}, v\rangle_{S_{T_0,\delta}}| \leq \eta\|v\|_{S_{T_0,\delta}} \text{ and } f(v) \leq \eta\|v\|_{S_{T_0,\delta}}\right\}$ is the approximate critical cone. Since $D_{\dot{T}}\mathcal{L}(\dot{T},\lambda)\tilde{T} = f(\tilde{T}) + 2\lambda\langle \dot{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})}$ and $\langle \dot{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})}$ is linear in $\dot{T}$, we have that $D^2_{\dot{T}\dot{T}}\mathcal{L}(\dot{T},\lambda)(\tilde{T},\tilde{T}) = 2\lambda\langle \tilde{T}, \tilde{T}\rangle_{L^2([0,1],\mathbb{R})}$. Thus, we conclude that the second-order condition (3.5.12) holds with $\lambda > 0$, $\mu = |\lambda| = \frac{1}{2}\|H\|_{S_{T_0,\delta}}$, $\beta = 2\lambda$ and $\eta = \max\left\{2\|\dot{T}\|_{S_{T_0,\delta}}, \|H\|_{S_{T_0,\delta}}\right\}$. Since $\dot{T}$ satisfies the necessary conditions (3.5.8) and (3.5.9), with $\lambda > 0$, $\dot{T}$ is a solution to the optimisation problem (3.5.4)–(3.5.5). Using Proposition 3.5.2, we conclude that this solution is unique since the unit ball of the Hilbert space $S_{T_0,\delta}$ is strictly convex.

Boundedness of the solution: We have that $\left(\mathscr{P}_\pi\left(\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x) \in L^\infty([0,1]^2)$ (see proof of Lemma 3.4.4). From (3.2.3), with the kernel $\left(\mathscr{P}_\pi\left(\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x)$, we have that $\mathcal{G}h \in L^\infty$ for any $h \in L^2$. Since $f_0 \in L^\infty$, we have that $f_0\ \mathcal{G}((\mathrm{Id} - L_0^*)^{-1}c) \in L^\infty$. Thus, $H = \mathbf{1}_{\tilde{F}_\delta} f_0\ \mathcal{G}((\mathrm{Id} - L_0^*)^{-1}c) \in L^\infty$ and therefore $\dot{T} \in L^\infty$. □

Corollary 3.5.4. *Suppose there exists an $\mathcal{b} > 0$ such that $\mathcal{b} \leq T_0(x) \leq 1-\mathcal{b}$ for a.e. $x \in [0,1]$. Then, the unique solution to the optimisation problem (3.5.4)–(3.5.5) is*

$$\dot{T} = -\frac{f_0 \; \mathcal{G}\left[(Id - L_0^*)^{-1}c\right]}{\| f_0 \; \mathcal{G}\left[(Id - L_0^*)^{-1}c\right] \|_2}$$

and the linear response with this perturbation is

$$\lim_{\varepsilon \to 0} \frac{f_\varepsilon - f_0}{\varepsilon} = (Id - L_0)^{-1} \mathcal{G}^* \left[\frac{\mathcal{G}\left[(Id - L_0^*)^{-1}c\right] f_0}{\| \mathcal{G}\left[(Id - L_0^*)^{-1}c\right] f_0 \|_2} f_0 \right],$$

where the convergence is in L^2 and $\mathcal{G}^* : L^2 \to L^2$ is the operator

$$\mathcal{G}^* f(y) := \int_0^1 \left(\mathscr{P}_\pi \left(\tau_{-T_0(x)} \frac{d\rho}{dx} \right) \right)(y) f(x) dx.$$

Proof. Since $\mathcal{b} \leq T_0 \leq 1 - \mathcal{b}$, we have that $\widetilde{F}_\mathcal{b} = [0,1]$ and therefore,

$$\dot{T}(y) = -\| f_0 \mathcal{G}((\mathrm{Id} - L_0^*)^{-1}c) \|_2^{-1} f_0(y) \mathcal{G}((\mathrm{Id} - L_0^*)^{-1}c)(y).$$

From Proposition 3.4.2, we have that $\dot{k}(x,y) = -\left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx}\right)\right)(x) \dot{T}(y)$. We then compute

$$\begin{aligned}
\dot{L} f_0(x) &= \int_0^1 \dot{k}(x,y) f_0(y) dy \\
&= \int_0^1 - \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right)(x) \dot{T}(y) f_0(y) dy \\
&= -\mathcal{G}^* \left[\dot{T} f_0 \right](x) \\
&= \mathcal{G}^* \left[\frac{\mathcal{G}\left[(\mathrm{Id} - L_0^*)^{-1}c\right] f_0}{\| \mathcal{G}\left[(\mathrm{Id} - L_0^*)^{-1}c\right] f_0 \|_2} f_0 \right](x).
\end{aligned}$$

Thus, the linear response is

$$(\mathrm{Id} - L_0)^{-1} \dot{L} f_0 = (\mathrm{Id} - L_0)^{-1} \mathcal{G}^* \left[\frac{\mathcal{G}\left[(\mathrm{Id} - L_0^*)^{-1}c\right] f_0}{\| \mathcal{G}\left[(\mathrm{Id} - L_0^*)^{-1}c\right] f_0 \|_2} f_0 \right].$$

□

3.5.3 Approximation of the Optimal Response

In this section we will obtain a result similar to that of Proposition 3.3.13 for the solution (3.5.7) of the optimisation problem (3.5.4)–(3.5.5).

Proposition 3.5.5. *Let (T_0, ρ) be a deterministic system with additive noise satisfying $(T1)$ and $(T2)$. Suppose the associated transfer operator L_0, with the kernel k_0 as in (3.4.5), satisfies $(A1)$ of Theorem 3.1.2. Let $\{L_n\} \subset \mathcal{B}(L^2)$ be a sequence of Hilbert-Schmidt integral operators with stochastic kernels $\{k_n\} \subset L^\infty([0,1]^2)$ such that $\lim_{n\to\infty} \|k_n - k_0\|_{L^\infty([0,1]^2)} = 0$. Then, there exists $n_0 > 0$ such that for each $n \geq n_0$, L_n satisfies assumption $(A1)$ of Theorem 3.1.2 and there exists a unique probability density $f_n \in L^\infty$ such that $L_n f_n = f_n$. Let $\{c_n\} \subset L^2$ be such that $c_n \in span\{f_n\}^\perp$ and $\lim_{n\to\infty} \|c_n - c\|_2 = 0$. Suppose there exists a $\kappa > 0$ such that $\|k_n\|_{L^\infty([0,1]^2)} \leq \kappa$. Then, the sequence of perturbations*

$$\dot{T}_n(y) := \begin{cases} -\|f_n \mathcal{G}((Id - L_n^*)^{-1} c_n) \mathbf{1}_{\widetilde{F}_\delta}\|_2^{-1} f_n(y) \mathcal{G}((Id - L_n^*)^{-1} c_n)(y) & y \in \widetilde{F}_\delta, \\ 0 & otherwise, \end{cases} \tag{3.5.13}$$

converges to the optimal perturbation $\dot{T}$ in L^∞ as $n \to \infty$.

Proof. We can apply the argument at the beginning of the proof of Proposition 3.3.13 to conclude that there exists $n_0 > 0$ such that for each $n \geq n_0$, L_n satisfies $(A1)$ and there exists unique probability densities $f_n \in L^\infty$ such that $L_n f_n = f_n$.

To simplify presentation, let $h(x,y) := \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx}\right)\right)(x)$, $Q_0 := (\mathrm{Id} - L_0^*)^{-1}$ and $Q_n := (\mathrm{Id} - L_n^*)^{-1}$. We note the following estimate

$$\begin{aligned} &\left| f_n(y) \mathcal{G}(Q_n c_n)(y) - f_0(y) \mathcal{G}(Q_0 c)(y) \right| \\ &\leq |f_0(y) - f_n(y)| \left| \mathcal{G}(Q_0 c)(x) \right| + |f_n(y)| \left| \mathcal{G}\left(Q_0 c - Q_n c_n\right)(x) \right| \\ &\leq \|h\|_{L^\infty([0,1]^2)} \left(|f_0(y) - f_n(y)| \|Q_0 c\|_1 + (|f_n(y) - f_0(y)| + |f_0(y)|) \|Q_0 c - Q_n c_n\|_1 \right). \end{aligned}$$

Thus, to show that $\|\dot{T}_n - \dot{T}\|_\infty \to 0$, we need to show that $\|Q_n c_n - Q_0 c\|_1 \to 0$. We can analogously apply the argument used to show $\|Q_n c_n - Q_0 c\|_\infty \to 0$ in the proof

of Proposition 3.3.13, but in L^2 instead of L^∞, to conclude that $\|Q_n c_n - Q_0 c\|_1 \leq \|Q_n c_n - Q_0 c\|_2 \to 0$. □

3.5.4 Explicit Formula for the Optimal Perturbation to Increase the Mixing Rate

In this section, we will obtain the results of Section 3.3.4 for deterministic systems with additive noise. We being with setting up the optimisation problem to enhance mixing. We then obtain an explicit formula for the optimal perturbation.

We recall that to enhance mixing in Section 3.3.4, we considered perturbing k_0 so that the logarithm of the real part of the perturbed second eigenvalue decreases. From Lemma 3.3.16, we had the formula

$$\frac{d}{d\varepsilon}\Re(\log \lambda_\varepsilon)\bigg|_{\varepsilon=0} = \frac{\langle \dot{k}, E\rangle_{L^2([0,1]^2,\mathbb{R})}}{|\lambda_0|^2},$$

where λ_ε denotes the second largest eigenvalue in magnitude of the integral operator L_ε with the kernel $k_\varepsilon = k_0 + \varepsilon \dot{k} + o(\varepsilon)$. Since we want to perturb T_0 by $\dot{T}$, we will reformulate the above inner product to a term involving $\dot{T}$.

Proposition 3.5.6. *Let L_0 and $\mathcal{I}$ be as in Proposition 3.4.5. Let e and $\hat{e}$ be the eigenvectors of L_0 and L_0^*, respectively, corresponding to an eigenvalue $\lambda_0 \in \mathcal{I}$. Let $E(x,y) = \big(\Re(\hat{e})(x)\Re(e)(y) + \Im(\hat{e})(x)\Im(e)(y)\big)\Re(\lambda_0) + \big(\Im(\hat{e})(x)\Re(e)(y) - \Re(\hat{e})(x)\Im(e)(y)\big)\Im(\lambda_0)$. Then*

$$\langle \dot{k}, E\rangle_{L^2([0,1]^2,\mathbb{R})} = \langle \dot{T}, \widehat{E}\rangle_{L^2([0,1],\mathbb{R})},$$

where

$$\widehat{E}(y) = -\int_0^1 \left(\mathscr{P}_\pi\left(\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x)E(x,y)dx \tag{3.5.14}$$

and $\widehat{E} \in L^\infty([0,1],\mathbb{R})$.

Proof. We first show that $\widehat{E} \in L^\infty([0,1],\mathbb{R})$. We can write

$$\begin{aligned}
&-\int_0^1 \left(\mathscr{P}_\pi\left(\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x)E(x,y)dx \\
&\qquad = -\sum_{i=1}^4 \beta_i h_i(y)\int_0^1 \left(\mathscr{P}_\pi\left(\tau_{-T_0(y)}\frac{d\rho}{dx}\right)\right)(x)g_i(x)dx
\end{aligned}$$

$$= -\sum_{i=1}^{4} \beta_i h_i(y)(\mathcal{G}g_i)(y),$$

where $\beta_1 = \beta_2 = \Re(\lambda_0)$, $\beta_3 = -\beta_4 = \Im(\lambda_0), g_1 = g_4 = \Re(\hat{e}), g_2 = g_3 = \Im(\hat{e})$, $h_1 = h_3 = \Re(e), h_2 = h_4 = \Im(e)$. From the proof of Theorem 3.5.3, we have $\mathcal{G}g_i \in L^\infty([0,1],\mathbb{R})$. Also, from Lemma 3.4.1, we have that $k_0 \in L^\infty([0,1]^2)$ and therefore $g_i, h_i \in L^\infty([0,1],\mathbb{R})$; thus, $\widehat{E} \in L^\infty([0,1],\mathbb{R})$.

Finally, we compute

$$\begin{aligned}
&\left\langle \dot{k}, E \right\rangle_{L^2([0,1]^2,\mathbb{R})} \\
&\quad = \int_0^1 \int_0^1 \dot{k}(x,y)E(x,y)dxdy \\
&\quad = -\int_0^1 \int_0^1 \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right)(x)\dot{T}(y)E(x,y)dxdy \\
&\quad = \int_0^1 \dot{T}(y)\widehat{E}(y)dy = \left\langle \dot{T}, \widehat{E} \right\rangle_{L^2([0,1],\mathbb{R})}.
\end{aligned}$$

□

Using the result of Proposition 3.5.6, we have the following formulation, and result, for the optimisation problem of enhancing mixing for systems with additive noise.

Proposition 3.5.7. *Let P_δ be the set in (3.5.2). Then, the problem of finding $\dot{T} \in P_\delta$ such that*

$$\left\langle \dot{T}, \widehat{E} \right\rangle_{L^2([0,1],\mathbb{R})} = \min_{\dot{h} \in P_\delta} \left\langle \dot{h}, \widehat{E} \right\rangle_{L^2([0,1],\mathbb{R})} \tag{3.5.15}$$

has a unique solution.

Proof. Since $S(\dot{h}) := -\langle \dot{h}, \widehat{E} \rangle_{L^2([0,1],\mathbb{R})}$ is linear and continuous, and since P_δ is strictly convex, we apply Propositions 3.3.1 and 3.3.3 to obtain the result. □

Since the objective function in (3.5.15) is linear, the solution will be in $S_{T_0,\delta} \cap \partial B_1$. Hence, we consider the following optimisation problem:

$$\min_{\dot{T} \in S_{T_0,\delta}} \quad \left\langle \dot{T}, \widehat{E} \right\rangle_{L^2([0,1],\mathbb{R})} \tag{3.5.16}$$

$$\text{such that} \quad \|\dot{T}\|_2^2 - 1 = 0. \tag{3.5.17}$$

Theorem 3.5.8. *Let (T_0, ρ) be a deterministic system with additive noise satisfying $(T1)$ and $(T2)$. Suppose the associated transfer operator $L_0 : L^2([0,1], \mathbb{C}) \to L^2([0,1], \mathbb{C})$, with the kernel k_0 as in (3.4.5), satisfies $(A1)$ of Theorem 3.1.2. Suppose $\lambda_0 \in \mathcal{G}$, where $\mathcal{G}$ is as in Proposition 3.4.5, is geometrically simple. Then, the unique solution to the optimisation (3.5.16)–(3.5.17) is*

$$\dot{T}(y) = \begin{cases} \frac{1}{\alpha} \int_0^1 \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx} \right) \right)(x) E(x,y) dx & y \in \widetilde{F}_\delta, \\ 0 & \text{otherwise}, \end{cases} \tag{3.5.18}$$

where

$$\begin{aligned} E(x,y) = &\big(\Re(\hat{e})(x)\Re(e)(y) + \Im(\hat{e})(x)\Im(e)(y)\big)\Re(\lambda_0) \\ &+ \big(\Im(\hat{e})(x)\Re(e)(y) - \Re(\hat{e})(x)\Im(e)(y)\big)\Im(\lambda_0) \end{aligned}$$

and α is selected so that $\|\dot{T}\|_2 = 1$. Furthermore, $\dot{T} \in L^\infty$.

Proof. The result is obtained via Lagrange multipliers. Hence, we will refer to the arguments in the proofs of Theorems 3.5.3 and 3.3.18 for the proof of this result with the following computations needed to obtain equation (3.5.18): First, let $\widehat{E}$ be as in (3.5.14). For the necessary conditions, we will need that

$$\langle \tilde{T}, \widehat{E} + 2\mu \dot{T} \rangle_{L^2([0,1],\mathbb{R})} = 0 \tag{3.5.19}$$

for all $\tilde{T} \in S_{T_0,\delta}$ and

$$\|\dot{T}\|_2^2 = 1. \tag{3.5.20}$$

Thus, from (3.5.19), and the fact that $\dot{T}$ should be in $S_{T_0,\delta}$, we have that $\dot{T} = -\mathbf{1}_{\widetilde{F}_\delta} \frac{\widehat{E}}{2\mu}$; from (3.5.20) we have that $\dot{T} = \mp \mathbf{1}_{\widetilde{F}_\delta} \frac{\widehat{E}}{\left\|\widehat{E}\right\|_2}$ (i.e. $2\mu = \pm \|\widehat{E}\|_2$). For the sufficient conditions, which will be the same as that in the proof of Theorem 3.5.3 since the objective is linear, we require that $\mu > 0$; thus, we conclude that (3.5.18) is the unique solution. The essential boundedness of $\dot{T}$ follows from that of $\widehat{E}$ (see Proposition 3.5.6). □

Corollary 3.5.9. *If $e, \hat{e}$ and λ_0 are real, then*

$$\dot{T}(y) = \begin{cases} sgn(\lambda_0)\frac{e(y)(\mathcal{G}\hat{e})(y)}{\|e\mathcal{G}\hat{e}\mathbf{1}_{\widetilde{F}_\mathcal{b}}\|_2} & y \in \widetilde{F}_\mathcal{b}, \\ 0 & \text{otherwise}, \end{cases}$$

where $\mathcal{G}$ is the operator in (3.5.6). Furthermore, if there exists an $\mathcal{b} > 0$ such that $\mathcal{b} \leq T_0(x) \leq 1 - \mathcal{b}$ for $x \in [0,1]$, then

$$\dot{T} = sgn(\lambda_0)\frac{e\ \mathcal{G}\hat{e}}{\|e\ \mathcal{G}\hat{e}\|_2}. \tag{3.5.21}$$

Proof. When $e, \hat{e}$ and λ_0 are real, we have $E(x,y) = \hat{e}(x)e(y)\lambda_0$ and the expression for $\dot{T}$ follows from (3.5.18). Finally, if $\mathcal{b} \leq T_0(x) \leq 1 - \mathcal{b}$, then $\widetilde{F}_\mathcal{b} = [0,1]$ and we have (3.5.21). □

3.5.5 Approximation of the Optimal Response

We conclude our analysis of deterministic systems with additive noise by obtaining the following convergence result for the optimisation problem (3.5.16)–(3.5.17).

Proposition 3.5.10. *Let (T_0, ρ) be a deterministic system with additive noise satisfying $(T1)$ and $(T2)$. Suppose the associated transfer operator $L_0 : L^2([0,1],\mathbb{C}) \to L^2([0,1],\mathbb{C})$, with the kernel k_0 as in (3.4.5), satisfies $(A1)$ of Theorem 3.1.2 and λ_0 is geometrically simple. Let $\{L_n\} \subset \mathcal{B}(L^2([0,1],\mathbb{C}))$ be a sequence of Hilbert-Schmidt integral operators with stochastic kernels $\{k_n\} \subset L^\infty([0,1]^2,\mathbb{R})$ such that $\lim_{n\to\infty}\|k_n - k_0\|_{L^\infty([0,1]^2)} = 0$. Then, there exists $n_0 > 0$ such that for each $n \geq n_0$, L_n satisfies $(A1)$ of Theorem 3.1.2 and there exists $\lambda_n \in \mathbb{C}$ and functions $e_n, \hat{e}_n \in L^\infty([0,1],\mathbb{C})$, with $\|e_n\|_2 = 1 = \|\hat{e}\|_2$, such that $L_n e_n = \lambda_n e_n$, $L_n^* \hat{e}_n = \lambda_n \hat{e}_n, \lim_{n\to\infty}|\lambda_n - \lambda_0| = 0, \lim_{n\to\infty}\|e_n - e\|_\infty = 0$ and $\lim_{n\to\infty}\|\hat{e}_n - \hat{e}\|_\infty$. Let*

$$\begin{aligned} E_n(x,y) := &\left(\Re(\hat{e}_n)(x)\Re(e_n)(y) + \Im(\hat{e}_n)(x)\Im(e_n)(y)\right)\Re(\lambda_n) \\ &+ \left(\Im(\hat{e}_n)(x)\Re(e_n)(y) - \Re(\hat{e}_n)(x)\Im(e_n)(y)\right)\Im(\lambda_n). \end{aligned}$$

Then, the sequence of perturbations

$$\dot{T}_n(y) := \begin{cases} \frac{1}{\alpha_n} \int_0^1 \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx}\right)\right)(x) E_n(x,y) dx & y \in \widetilde{F}_\delta \\ 0 & \text{otherwise,} \end{cases} \tag{3.5.22}$$

where $\alpha_n > 0$ is selected so that $\|\dot{T}_n\|_2 = 1$, converges to the optimal $\dot{T}$ in L^∞ as $n \to \infty$.

Proof. From $\|k_n - k_0\|_{L^2([0,1]^2,\mathbb{R})} \to 0$ (which follows from $\|k_n - k_0\|_{L^\infty([0,1]^2,\mathbb{R})} \to 0$), we have $\|L_n - L_0\|_{L^2 \to L^2} \to 0$. Thus, from the argument in the proof of Proposition 3.3.21, we have the convergence of the eigenvalues and the eigenvectors in L^∞; we also have $\lim_{n\to\infty} \|E_n - E\|_{L^\infty([0,1]^2,\mathbb{R})} = 0$. If we let $C := \operatorname{esssup}_{(x,y)\in[0,1]^2} \left| \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx}\right)\right)(x) \right|$, we then have

$$\begin{aligned} |\dot{T}_n(y) - \dot{T}(y)| \leq C \Bigg(& \left| \frac{1}{\alpha_n} - \frac{1}{\alpha} \right| \|E_n - E\|_{L^\infty([0,1]^2,\mathbb{R})} + \left| \frac{1}{\alpha} \right| \|E_n - E\|_{L^\infty([0,1]^2,\mathbb{R})} \\ & + \left| \frac{1}{\alpha} - \frac{1}{\alpha_n} \right| \|E\|_{L^\infty([0,1]^2,\mathbb{R})} \Bigg). \end{aligned}$$

Noting that α_n is the L^2 norm of $\int_0^1 \left(\mathscr{P}_\pi \left(\tau_{-T_0(y)} \frac{d\rho}{dx}\right)\right)(x) E_n(x,y) dx$, the convergence $\lim_{n\to\infty} \|E_n - E\|_{L^\infty([0,1]^2,\mathbb{R})} = 0$, with the reverse triangle inequality, implies $\lim_{n\to\infty} \alpha_n = \alpha$. Thus, $\lim_{n\to\infty} \|\dot{T}_n - \dot{T}\|_\infty = 0$. □

The following result immediately follows from the above proposition.

Corollary 3.5.11. *Suppose there exists an $\delta > 0$ such that $\delta < T_0(y) < 1 - \delta$ for all $y \in [0,1]$. If $e, \hat{e}$ and λ_0 are real, and there exists an $\tilde{n}_0 > 0$ such that $e_n, \hat{e}_n$ and λ_n are real for all $n \geq \tilde{n}_0$, then the sequence*

$$\dot{T}_n = sgn(\lambda_n) \frac{e_n \mathcal{G} \hat{e}_n}{\|e_n \mathcal{G} \hat{e}_n\|_2}, \tag{3.5.23}$$

where $\mathcal{G}$ is the operator in (3.5.6), converges to (3.5.21) in L^∞ as $n \to \infty$.

3.6 Applications and Numerical Experiments

In this section we will consider two stochastically perturbed systems, namely the Pomeau-Manneville map and a weakly mixing interval exchange map. For each of these maps we numerically estimate:

1. The unique kernel perturbation that maximises the change in expectation of a prescribed observation function. An expression for this optimal kernel is given by (3.3.5).
2. The unique kernel perturbation that maximally increases the mixing rate. An expression for this optimal kernel is given by (3.3.21) and (3.3.25).
3. The unique map perturbation that maximises the change in expectation of a prescribed observation function. An expression for this optimal kernel is given by (3.5.7).
4. The unique map perturbation that maximally increases the mixing rate. An expression for this optimal kernel is given by (3.5.18) and (3.5.21).

The numerical methodology will be explained as we proceed through these four optimisation problems.

3.6.1 Pomeau-Manneville Map

We consider the Pomeau-Manneville map [64]

$$T_0(x) = \begin{cases} x(1+(2x)^\alpha), & x \in [0, 1/2); \\ 2x - 1, & x \in [1/2, 1] \end{cases}, \tag{3.6.1}$$

with parameter value $\alpha = 1/2$. For this parameter choice it is known that the map T_0 admits a unique absolutely continuous invariant probability measure, but only algebraic decay of correlations [64]. With the addition of noise as per (3.4.1), the transfer operator defined by (3.4.4) and (3.4.5) for $\varepsilon = 0$ becomes compact as an operator on L^2. In our numerical experiments we will use the smooth noise kernel $\rho_\delta : [-\delta, \delta] \to \mathbb{R}$, defined by namely $\rho_\delta(x) = N(\delta)\exp(-\delta^2/(\delta^2 - x^2))$, where $N(\delta)$ is a normalisation factor ensuring $\int \rho_\delta(x)\, dx = 1$.

We now begin to set up our numerical procedure for estimating L_0, which is a standard application of Ulam's method [80]. Let $B_n = \{I_1, \ldots, I_n\}$ denote an

equipartition of $[0,1]$ into n subintervals, and set $\mathcal{B}_n = \text{span}\{\mathbf{1}_{I_1}, \ldots, \mathbf{1}_{I_n}\}$. Define the (Ulam) projection $\pi_n : L^2([0,1]) \to \mathcal{B}_n$ by $\pi_n(g) = \sum_{i=1}^n \left(\frac{1}{\ell(I_i)} \int_{I_i} g(x)dx\right) \mathbf{1}_{I_i}$. The finite-rank transfer operator $L_n := \pi_n L_0 : L^2([0,1]) \to \mathcal{B}_n$ can be computed numerically. We use MATLAB's built-in functions `integral.m` and `integral2.m` to perform the ρ-convolution (using an explicit form of ρ_δ) and the Ulam projections, respectively.

To apply the theory discussed in the earlier sections, we make the following remarks. First note that the kernel k_n of the operator L_n is given by

$$k_n(z,y) = \sum_{i=1}^n \frac{1}{\ell(I_i)} \int_{I_i} k_0(x,y)dx \mathbf{1}_{I_i}(z),$$

where k_0 is the kernel in (3.4.5) with $\varepsilon = 0$. Since $k_0 \in L^\infty([0,1]^2)$, we have that $\|k_n\|_{L^\infty([0,1]^2)} \leq \|k_0\|_{L^\infty([0,1]^2)} =: \kappa$. Furthermore, since k_0 is a stochastic kernel, then k_n is also a stochastic kernel. We also have that $\lim_{n\to\infty} \|k_n - k_0\|_{L^\infty([0,1]^2)} = 0$ since k_0 is uniformly Lipschitz in the first variable. Next, we note that if $c \in Lip([0,1])$ then, with $c_n := \pi_n(c)$, $\lim_{n\to\infty} \|c_n - c\|_\infty = 0$. Hence, if c is uniformly Lipschitz and since k_0 is uniformly Lipschitz in the first variable then, from Propositions 3.3.13 and 3.3.21, the approximate $\dot{k}_n$ (in Propositions 3.3.13 and 3.3.21) converge in L^∞ to the optimal $\dot{k}$ (in (3.3.5) and (3.3.21), respectively). Also, the assumptions for Propositions 3.5.5 and 3.5.10 follow from the points above and the fact that T_0 and ρ_δ satisfy assumptions $(T1)$ and $(T2)$.

Figure 3.2 shows the column-stochastic matrix corresponding to L_n for $\delta = 0.1$. Approximations to the invariant probability densities for our stochastic dynamics are displayed in Figure 3.3 (left) for large and small noise supports. A lower level of noise permits greater concentration of invariant probability mass near the fixed point $x = 0$ of the map T_0. Also shown in Figure 3.3 (right) are the estimated eigenfunctions corresponding to the second-largest eigenvalue of L_n. The signs of these second eigenfunctions split the interval $[0,1]$ into left and right hand portions, broadly indicating that the slow mixing is due to positive mass near $x = 0$ and negative mass away from $x = 0$ [20]; see [36] for further discussion of this point in the Pomeau-Manneville setting.

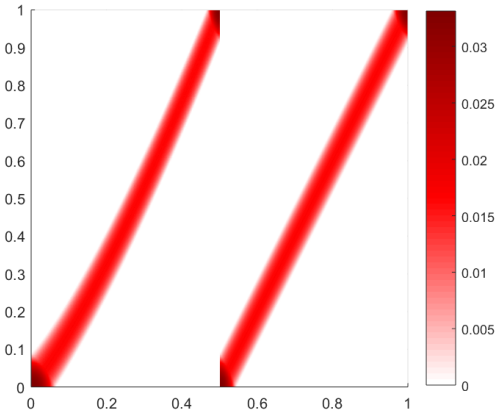


Figure 3.2: Transition matrix for the system (3.4.1) generated by the Pomeau-Manneville map T_0 (3.6.1). The additive noise in (3.4.1) is drawn according to ρ_δ with $\delta = 1/10$.

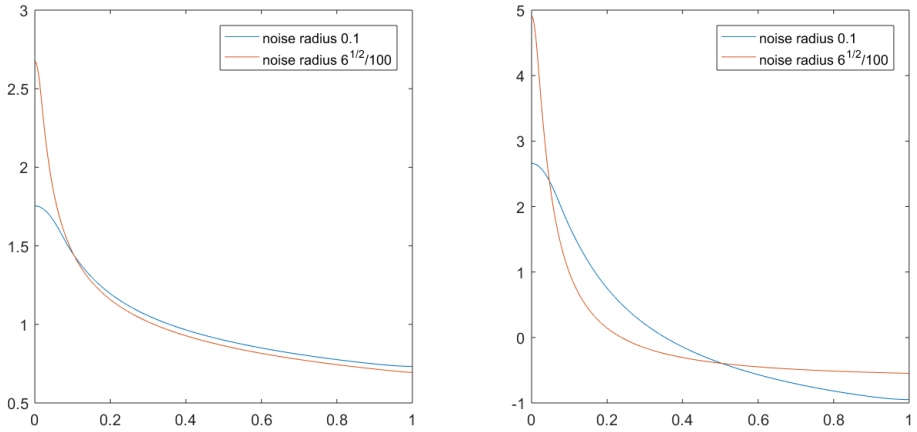


Figure 3.3: Approximate invariant densities (left) and eigenfunctions corresponding to the 2nd largest eigenvalue of L_0 (right) for the system (3.4.1) with T_0 given by the Pomeau-Manneville map (3.6.1). The additive noise $\{\omega_n\}$ is drawn according to ρ_δ with δ taking the values $1/10$ (blue) and $\sqrt{6}/100$ (red).

Kernel Perturbations

We use the monotonically increasing observation function $c(x) = -\cos(x)$. In order to estimate $\dot{k}$ as given in (3.3.5) we use the approximate version $\dot{k}_n$ from (3.3.12), with the ingredients f_n (obtained as the leading eigenvector of L_n), c_n (obtained as $\pi_n(c)$), and $(\mathrm{Id} - L_n^*)^{-1}c_n$ (obtained as a vector $y \in \mathbb{R}^n$ by numerically solving the linear system $(\mathrm{Id} - L_n^*)y = c_n, f_n^\top y = 0$). Figure 3.4 shows the optimal kernel perturbations $\dot{k}_n$ arising from (3.3.12) with $n = 500$. Because c is an increasing

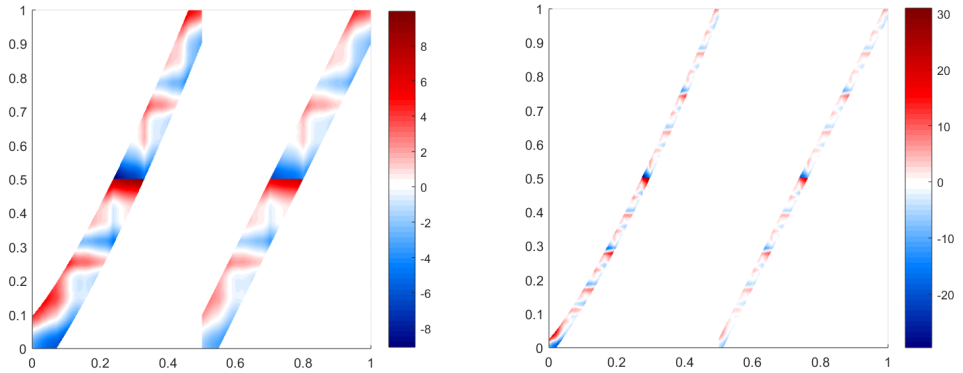


Figure 3.4: Optimal kernel perturbations for the Pomeau-Manneville map to maximise the change in expectation of $c(x) = -\cos(x)$, computed using (3.3.12) with $n = 500$ subintervals. Left: $\delta = 1/10$, Right: $\delta = \sqrt{6}/100$.

function, intuitively one might expect the kernel perturbation to try to shift mass in the invariant density from left to right. Broadly speaking, this is what one sees in the high-noise case in Figure 3.4 (left): vertical strips typically have red above blue, corresponding to a shift of mass to the right in $[0, 1]$. The main exception to this is around the y-axis value of $1/2$, where red is strongly below blue along vertical strips. This is because at the next iteration, these red regions will be mapped near $x = 1$ and achieve the highest value of c. In the low-noise case of Figure 3.4 (right), we see a similar solution with higher spatial frequencies, and strong perturbations near the critical values of $x = 0$ and $T_0(x) = 1/2$.

To investigate the optimal kernel perturbation to maximally increase the rate of mixing in the stochastic system, we use the expression $\dot{k}$ in (3.3.21). The approximate version $\dot{k}_n$ in (3.3.26) requires estimates of the left and right eigenfunctions of L_0 corresponding to the second largest eigenvalue λ; these are obtained directly as eigenvectors of L_n. Figure 3.5 shows the resulting optimal kernel perturbations. Because the fixed point at $x = 0$ is responsible for the slow algebraic decay of correlations for the deterministic dynamics of T_0, the fixed point will also play a dominant role in the mixing rate of the stochastic system for low to moderate levels of noise. Indeed, Figure 3.5 shows that the optimal perturbation concentrates its effort in a neighbourhood of the fixed point, and pushes mass away from the fixed point as much as possible. This is particularly extreme in the low noise case of

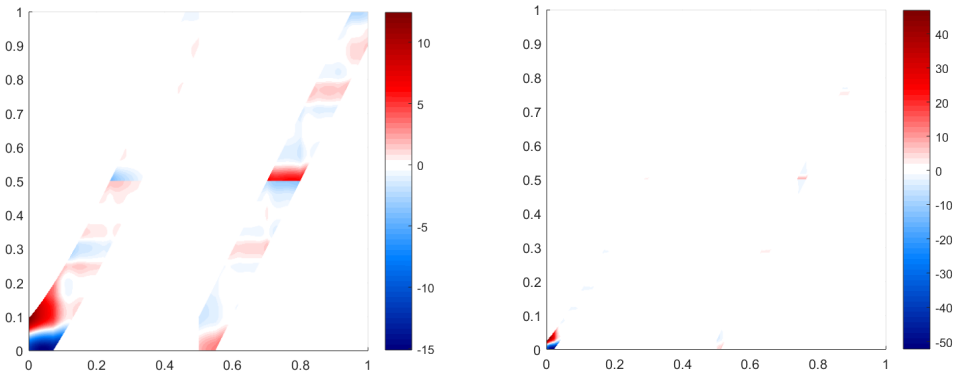


Figure 3.5: Optimal kernel perturbation for the Pomeau-Manneville map to maximally increase the mixing rate, computed with $n = 500$ subintervals. Left: $\delta = 1/10$, Right: $\delta = \sqrt{6}/100$.

Figure 3.5 (right) with the perturbation almost exclusively concentrated in a small neighbourhood of $x = 0$.

Map Perturbations

We now turn to the problem of finding the unique map perturbation $\dot{T}$ that maximises the change in expectation of the observation $c(x) = -\cos(x)$. We use the expression[4] (3.5.7) and its approximate counterpart (3.5.13). The objects f_n and $(\mathrm{Id} - L_n^*)^{-1} c_n$ are computed exactly as before in Section 3.6.1. The action of the operator $\mathcal{G}$ in (3.5.7) is computed using MATLAB's built-in function `integral.m` using an explicit form of $d\rho_\delta/dx$ for $d\rho/dx$ in (3.5.7).

Figure 3.6 (left) shows the optimal $\dot{T}$ for the two noise amplitudes $\delta = 1/10$ and $\delta = \sqrt{6}/100$. Figure 3.6 (right) illustrates the Pomeau-Manneville map (black) with perturbed maps $T_0 + \dot{T}/100$. We have chosen a scale factor of $1/100$ for visualisation purposes; one should keep in mind we are optimising for an infinitesimal change in the map. Figure 3.7 shows the kernel derivatives $\dot{k}$ corresponding to the optimal map derivatives $\dot{T}$ for the two noise levels. These kernel derivatives have a restricted form because they arise purely from a derivative in the map. One may compare Figure 3.7 with Figure 3.4 and note that the kernel derivative in Figure 3.7 (left) attempts

[4]Note that since $T_0^{-1}(\{0,1\})$ is a finite set, we may take $\ell > 0$ as small as we like. In the computations we set $\ell = 0$, so that $\widetilde{F}_\ell = [0,1] \bmod \ell$.

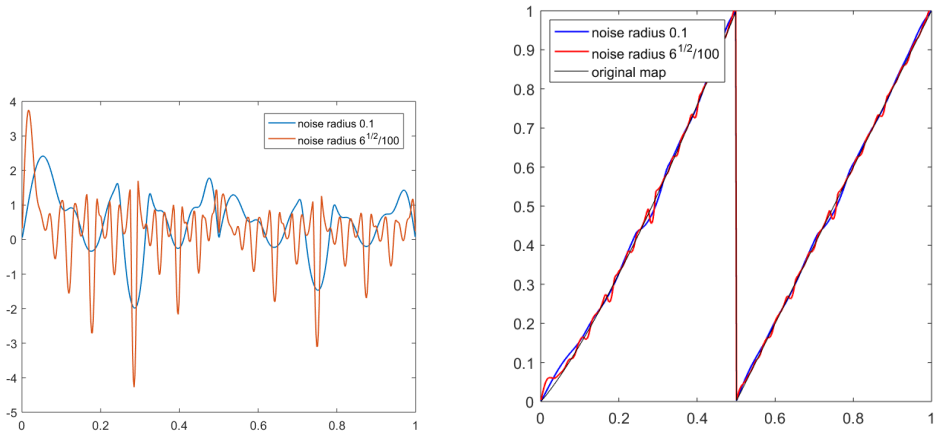


Figure 3.6: Left: Optimal map perturbation $\dot{T}$ for the Pomeau-Manneville map to maximise the change in expectation of $c(x) = -\cos(x)$, computed using (3.5.13) with $n = 500$. Right: Illustration of $T_0 + \dot{T}/100$.

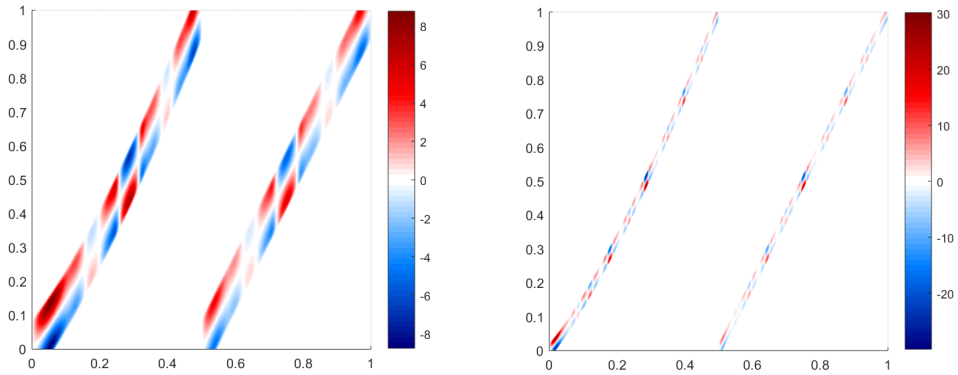


Figure 3.7: Kernel perturbations corresponding to the optimal map perturbations in Figure 3.6. Left: $\delta = 1/10$, Right: $\delta = \sqrt{6}/100$.

to follow the general structure of the kernel derivative in Figure 3.4 (left), while obeying its structural restrictions arising from the less flexible *map* perturbation.

The map perturbation that maximally increases the rate of mixing is a particularly interesting question. Our computations use (3.5.21) and its approximate counterpart (3.5.23). The computations follow as in Section 3.6.1 with the action of $\mathcal{G}$ computed as above. Figure 3.8 (left) shows the optimal $\dot{T}$ for the two noise amplitudes $\delta = 1/10$ and $\delta = \sqrt{6}/100$. A sharp map perturbation away from $x = 0$ is seen for both noise levels, with the perturbation sharper for the lower

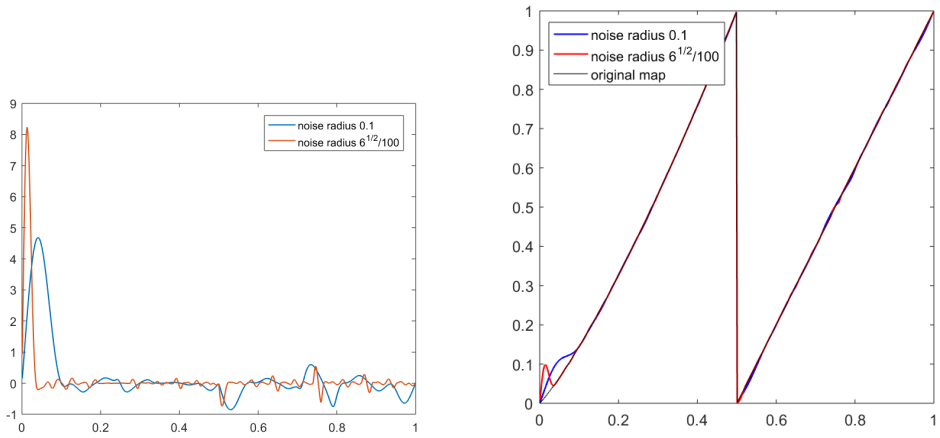


Figure 3.8: Left: Optimal map perturbation $\dot{T}$ for the Pomeau-Manneville map to maximise the change in the mixing rate, computed using (3.5.23) with $n = 500$. Right: Illustration of $T_0 + \dot{T}/100$.

noise case. This result corresponds well with the results seen for the optimal kernel perturbations in Figure 3.5, where probability mass was primarily moved away from $x = 0$. Figure 3.8 (right) illustrates the Pomeau-Manneville map (black) with perturbed maps $T_0 + \dot{T}/100$, where again the factor $1/100$ is just for illustrative purposes. When inspecting the kernel derivatives $\dot{k}$ corresponding to the optimal map perturbations $\dot{T}$ in Figure 3.9, we see similar behaviour to those in Figure 3.8.

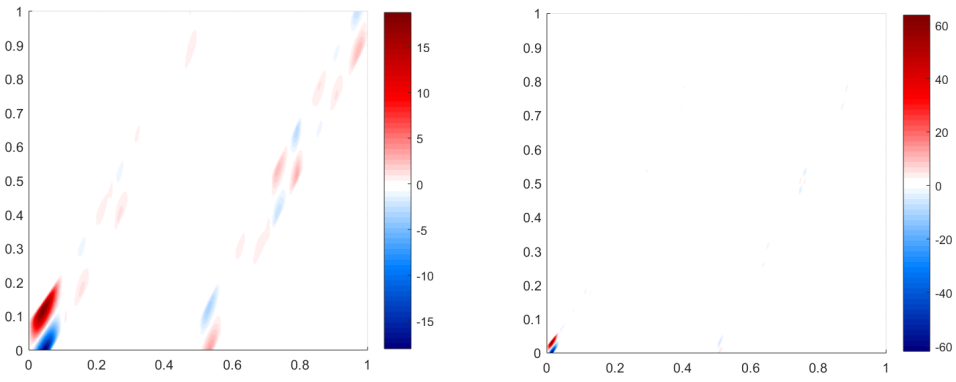


Figure 3.9: Kernel perturbations corresponding to the optimal map perturbations in Figure 3.8. Left: $\delta = 1/10$, Right: $\delta = \sqrt{6}/100$.

3.6.2 Interval Exchange Map

In our second example, we consider a weakly mixing interval exchange map because of an existing literature in mixing optimisation for these classes of maps with the addition of noise. Avila and Forni [5] prove that a typical interval exchange is either weak mixing or an irrational rotation. We use a specific weak-mixing [78] interval exchange map T_0 with interval permutation $(1234) \mapsto (4321)$ and interval lengths given by the normalised entries of the leading eigenvector of the matrix $\begin{pmatrix} 13 & 37 & 77 & 47 \\ 10 & 30 & 60 & 37 \\ 3 & 10 & 24 & 14 \\ 4 & 10 & 19 & 12 \end{pmatrix}$; see equation (51) in [78]. We again form a stochastic system using the same noise kernels as for the Pomeau-Manneville map in Section 3.6.1; we also note that the theoretical justification for the convergence of $\dot{k}_n$ to $\dot{k}$ in Propositions 3.3.13 and 3.3.21 is as discussed in Section 3.6.1. The mixing properties of this map have been studied in [29]. Figure 3.10 shows the column-stochastic matrix corresponding to L_n for $n = 500$ and $\delta = 0.1$.

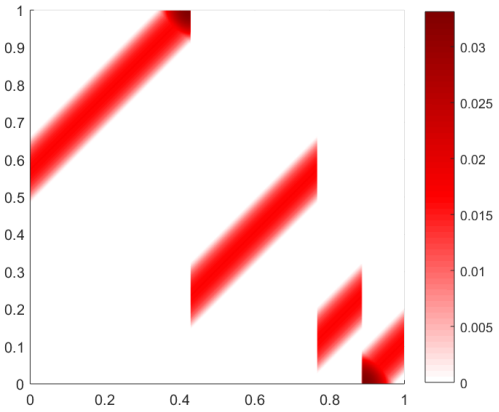


Figure 3.10: Transition matrix for the system (3.4.1) for $\varepsilon = 0$ and T_0 given by the interval exchange map above using $n = 500$ subintervals. The additive noise is drawn from the density ρ_δ with $\delta = 1/10$.

Kernel Perturbations

We use the same observation function $c(x) = -\cos(x)$ as in the Pomeau-Manneville case study, and estimate the optimal kernel perturbation $\dot{k}$ that maximally increases the expectation of c in an identical fashion. In broad terms, one again sees that

$\dot{k}$ attempts to shift invariant probability mass to the right in $[0, 1]$. In the low

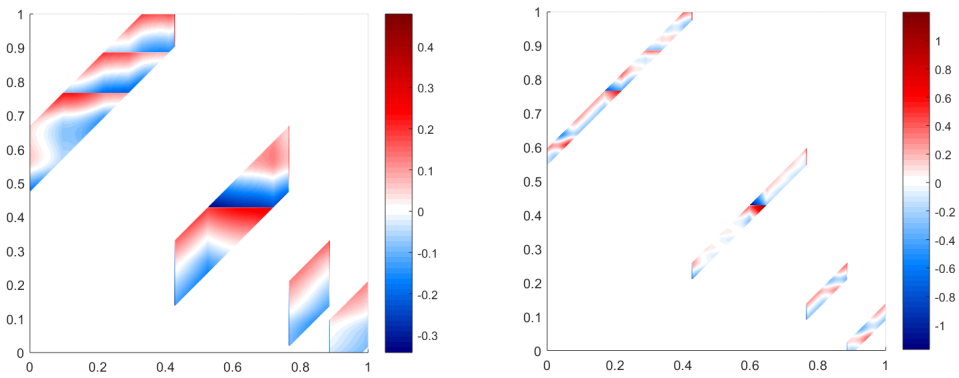


Figure 3.11: Optimal kernel perturbation for the interval exchange map to maximise the change in expectation of $c(x) = -\cos(x)$, computed using (3.3.12) with $n = 500$ subintervals. Left: $\delta = 1/10$, Right: $\delta = \sqrt{6}/100$.

noise case, Figure 3.11 (right), displays similar behaviour to the higher noise case of Figure 3.11 (left) but with lower noise, the deterministic dynamics plays a greater role and additional preimages are taken into account, leading to a more oscillatory optimal $\dot{k}$.

To investigate the optimal kernel perturbation to maximally increase the rate of mixing in the stochastic system, we use the expression $\dot{k}$ in (3.3.21). The method of numerical approximate is identical to that used for the Pomeau-Manneville map. Figure 3.12 shows the signed distribution of mass that is responsible for the slowest real[5] exponential rate of decay in the stochastic system. The second eigenfunctions become more oscillatory as the level of noise decreases, and as must be the case, the magnitude of the second eigenvalue increases from $\lambda \approx -0.7476$ to $\lambda \approx -0.9574$. Because the sign of these eigenvalues is negative, one expects a pair of almost-2-cyclic sets, consisting of three subintervals each, given by the positive and negative supports of the eigenfunctions. Figure 3.13 shows the approximate optimal kernel perturbations. For the high noise situation (Figure 3.13 (left)) it is difficult to interpret exactly why the solution looks as it does, however the sharp horizontal changes are clearly present at preimages of the deterministic dynamics. For the

[5]In our numerical experiments the largest magnitude real eigenvalue appears as the sixth (resp. fourth) eigenvector of L_{500} for $\delta = 1/10$ (resp. $\delta = \sqrt{6}/100$). Slightly larger complex eigenvalues are present, but we do not investigate these in order to make the dynamic interpretation more straightforward.

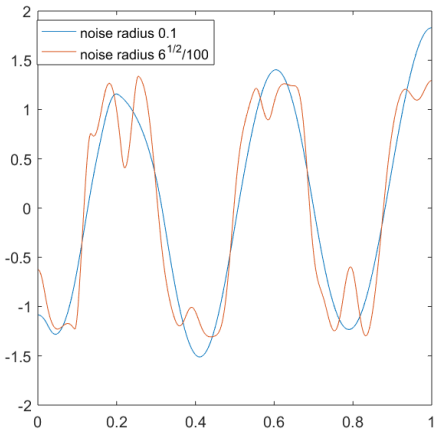


Figure 3.12: Approximate second eigenfunctions of the transfer operator L_0 of the system (3.4.1) with T_0 given by the interval exchange map above. The additive noise $\{\omega_n\}$ is drawn from the density ρ_δ with δ taking the values 1/10 (blue) and $\sqrt{6}/100$ (red).

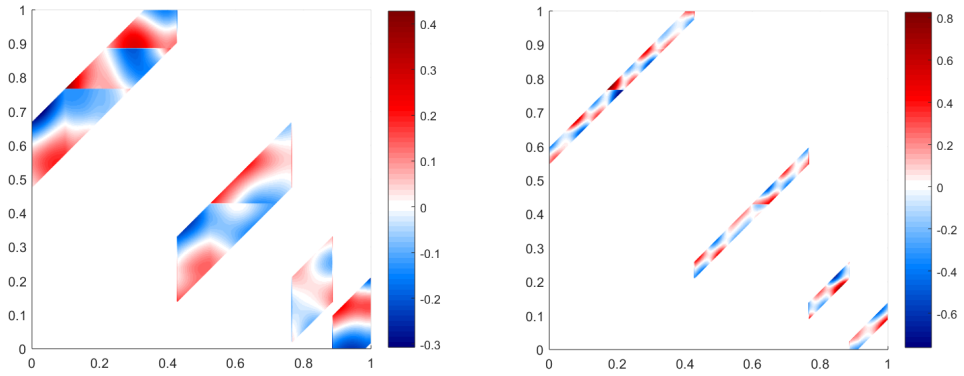


Figure 3.13: Optimal kernel perturbation for the interval exchange map to maximally increase the mixing rate, computed with $n = 500$ subintervals. Left: $\delta = 1/10$, Right: $\delta = \sqrt{6}/100$.

low noise case (Figure 3.13 (right)) it appears that there is an alternating shifting of mass left and right with alternating "red above blue" and "blue above red". This leads to greater mixing at smaller spatial scales than is possible in a single iteration of the deterministic interval exchange. We anticipate that decreasing the noise amplitude further will result in more rapid alternation of "red above blue" and "blue above red". This is because diffusion mixes at small scales, but as this mixing effect is decreased, small scale mixing now has to be accessed by increasing oscillation in the kernel.

Map Perturbations

The computations in this section follow those of Section 3.6.1 for map perturbations. Figure 3.14 (left) shows the optimal map perturbations $\dot{T}$ at two different noise levels. Figure 3.14 (right) illustrates $T_0 + \dot{T}/100$ for the two different levels of

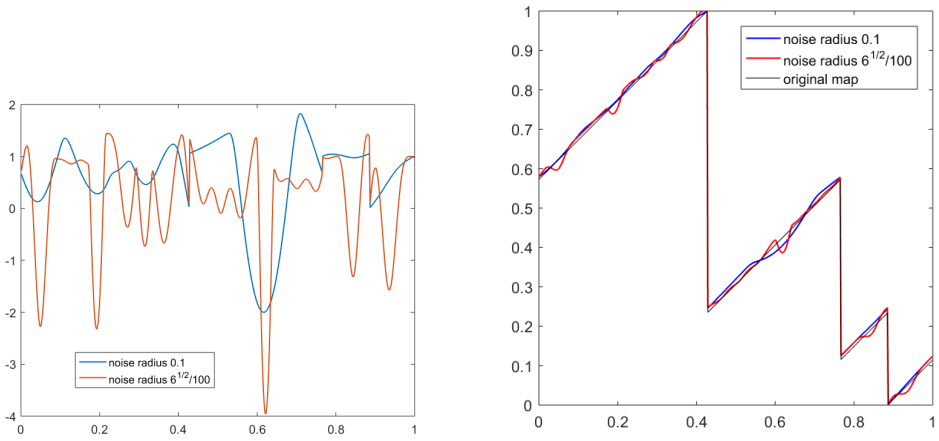


Figure 3.14: Left: Optimal map perturbation $\dot{T}$ for the interval exchange map to maximise the change in expectation of $c(x) = -\cos(x)$, computed using (3.5.13) with $n = 500$. Right: Illustration of $T_0 + \dot{T}/100$.

noise. The kernel perturbations generated by these optimal map perturbations are displayed in Figure 3.15. If one compares the kernel perturbations in Figure 3.15

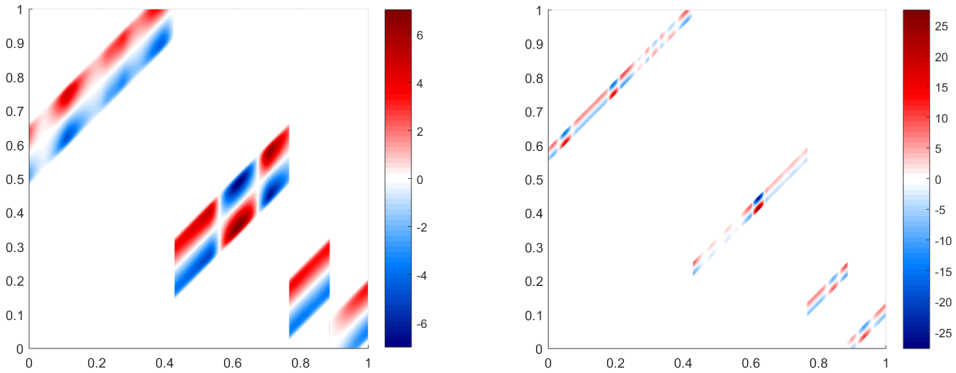


Figure 3.15: Kernel perturbations corresponding to the optimal map perturbations in Figure 3.14. Left: $\delta = 1/10$, Right: $\delta = \sqrt{6}/100$.

with those more flexible kernel perturbations in Figure 3.11, one sees that the two sets of kernel perturbations are broadly equivalent with one another in terms of the relative positions of the positive and negative (red and blue) perturbations.

The question of perturbing noisy interval exchange maps to increase the mixing rate has been studied by a number of authors [4, 29, 79]. The original interval exchange T_0 cuts and shuffles the unit interval into an increasing number of smaller pieces, assisting the small scale mixing of diffusion. Our results in Figure 3.16 (left) show an oscillatory $\dot{T}$, with increasing oscillations as the noise amplitude decreases. Thus, the optimisation attempts to include some additional mixing by

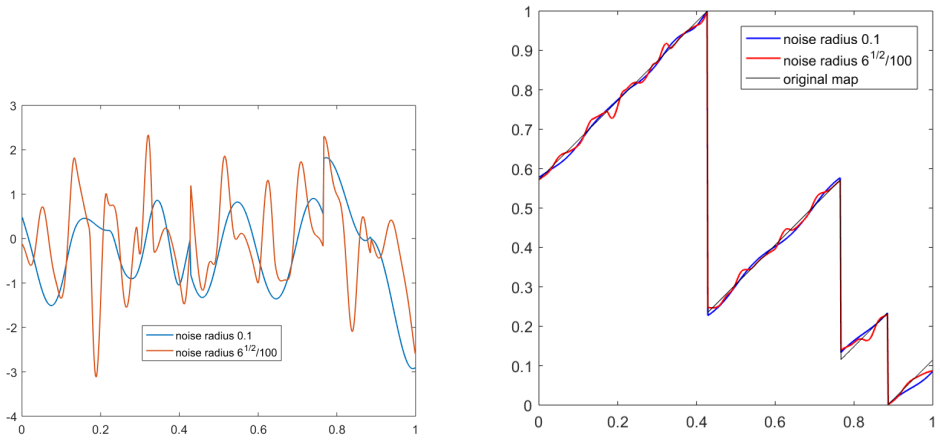


Figure 3.16: Left: Optimal map perturbation $\dot{T}$ for the interval exchange map to maximise the change in the mixing rate, computed using (3.5.23) with $n = 500$. Right: Illustration of $T_0 + \dot{T}/100$.

rapid local warping of the phase space. It is plausible that this additional warping effect enhances mixing beyond the rigid shuffling of the interval exchange. An illustration of $T_0+\dot{T}/100$ is given in Figure 3.16. We emphasise that the factor $1/100$

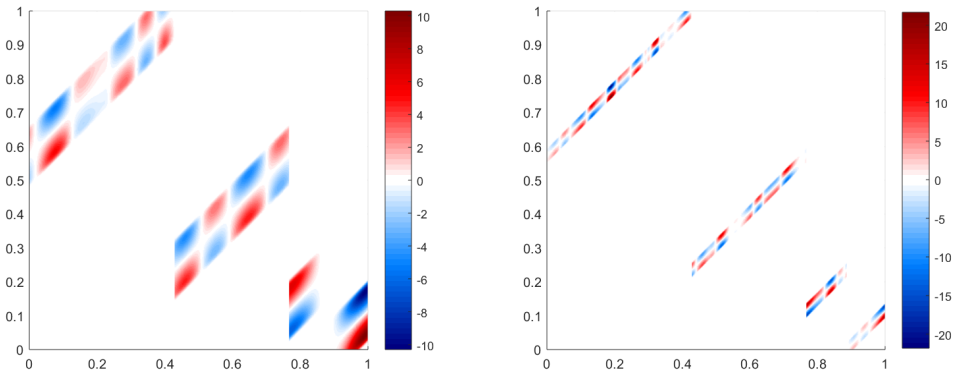


Figure 3.17: Kernel perturbations corresponding to the optimal map perturbations in Figure 3.16. Left: $\delta = 1/10$, Right: $\delta = \sqrt{6}/100$.

is only for visualisation purposes and for smaller factors, the perturbed map would remain a piecewise homeomorphism (modulo small overshoots at the boundaries, which are taken care of by the reflecting boundary conditions on the noise). This type of general map optimisation has not been attempted before and we believe opens up interesting new directions in the field of mixing optimisation.

Chapter 4

Linear Response for the Dynamic Laplacian and Finite-Time Coherent Sets

In this final chapter, we will apply the idea of linear response to quantify the response of finite-time mixing properties in dynamical systesm by developing theory to describe the response of finite-time coherent sets. In Section 4.1 we introduce differentiability hypotheses on the dynamics. In Section 4.2 we define the dynamic Laplacian, coherent sets, and the linear response problem. Section 4.3 contains the proof of the weak differentiability of the dynamic Laplacian with respect to the perturbing parameter, and the proof of the existence of linear response of eigenfunctions in the case when we have Dirichlet boundary conditions. In Section 4.4 we derive a linear system to compute the linear response, and demonstrate that the linear response results obtained for Dirichlet boundary conditions also hold for Neumann boundary conditions. Section 4.5 develops FEM-based approaches to compute the linear response, and we conclude in Section 4.6 with numerical experiments.

4.1 Perturbations

Let $\Omega \subset \mathbb{R}^n$ be a smooth compact subset of $\mathbb{R}^n$ that is either boundaryless or has a smooth boundary. For $\varepsilon_0 > 0$ small, using a parameter $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, define a family of maps $\{T_\varepsilon\}_{\varepsilon\in(-\varepsilon_0,\varepsilon_0)}$, where $T_\varepsilon : \Omega \to T_\varepsilon(\Omega)$. We think of T_0 as governing the original, unperturbed dynamics.

Before we specify the precise relationship between the unperturbed and perturbed maps, we note some special families of perturbations we have in mind:

1. T_ε is given by the flow map $\varphi_\varepsilon^{t_0,t_1}$ of some ordinary differential equation

$$\partial_t x = v(t, x, \varepsilon),$$

where the vector field v depends on a parameter ε. In this case,

$$T_\varepsilon(x) := \varphi_\varepsilon^{t_0,t_1}(x) = \varphi_0^{t_0,t_1}(x) + \varepsilon \partial_\varepsilon \varphi_\varepsilon^{t_0,t_1}(x)|_{\varepsilon=0} + o(\varepsilon),$$

where $t_0, t_1 \in \mathbb{R}$ are chosen such that the flow map is defined for all x. Under appropriate assumptions on v we have $T_\varepsilon = T_0 + \varepsilon \dot{T} + o(\varepsilon)$, where $\dot{T}(x) := \partial_\varepsilon \varphi_\varepsilon^{t_0,t_1}(x)|_{\varepsilon=0}$ satisfies the variational equation

$$\partial_t \dot{T}(x) = \partial_x v(t, T_0(x), 0)\dot{T}(x) + \partial_\varepsilon v(t, T_0(x), 0).$$

2. As a further specialisation of 1. we interpret the time t itself as the parameter ε, i.e. we consider

$$\partial_t x = v(x, t)$$

with the flow map φ^{t_0,t_1}. In this case we have that

$$\begin{aligned} T_\varepsilon(x) &:= \varphi^{t_0,t_1+\varepsilon}(x) \\ &= \varphi^{t_0,t_1}(x) + \varepsilon \frac{\partial}{\partial \tau} \varphi^{t_0,\tau}\Big|_{\tau=t_1}(x) + o(\varepsilon) \\ &= T_0(x) + \varepsilon \dot{T}(x) + o(\varepsilon), \end{aligned}$$

where

$$\dot{T}(\cdot) := \frac{\partial}{\partial \tau} \varphi^{t_0,\tau}\Big|_{\tau=t_1}(\cdot) = v(\cdot, t_1).$$

The precise setting we consider is the following: Let $\mathrm{Diff}^2(\overline{\Omega}, \mathbb{R}^n)$ be the space of C^2-diffeomorphisms from $\overline{\Omega}$ to $\mathbb{R}^n$ which is endowed with the C^2-norm

$$\|f\|_{C^2(\overline{\Omega},\mathbb{R}^n)} = \sum_{\alpha_j, |\alpha| \leq 2} \max_{x \in \overline{\Omega}} \left| \left(\frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}} f \right)(x) \right|_{\mathbb{R}^n},$$

where $\alpha = (\alpha_1, \ldots, \alpha_n), 0 \leq \alpha_j$ for $1 \leq j \leq n, |\alpha| := \sum_{j=1}^{n} \alpha_j, (x_i)$ are the coordinates on $\overline{\Omega}$ and $\frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \ldots \partial x_n^{\alpha_n}} f = \left(\frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \ldots \partial x_n^{\alpha_n}} f_1, \ldots, \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \ldots \partial x_n^{\alpha_n}} f_n \right)$, where $f_i : \mathbb{R}^n \to \mathbb{R}$. We then assume that the map $\varepsilon \mapsto T_\varepsilon$ is in $C^1((-\varepsilon_0, \varepsilon_0), \mathrm{Diff}^2(\overline{\Omega}, \mathbb{R}^n))$. From Taylor's theorem (see [61], XIII §6) for sufficiently small $\varepsilon_0 > 0$, one has

$$T_\varepsilon = T_0 + \varepsilon \dot{T} + R_\varepsilon \tag{4.1.1}$$

for $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, where the maps $x \mapsto \dot{T}(x)$ and $x \mapsto R_\varepsilon(x)$ are in $\mathrm{Diff}^2(\overline{\Omega}, \mathbb{R}^n)$, and $\|R_\varepsilon\|_{C^2(\overline{\Omega}, \mathbb{R}^n)} = o(\varepsilon)$.

4.2 Coherent Sets Via Dynamic Isoperimetry and the Linear Response Problem

We are interested in analysing the response of coherent sets to perturbations of the dynamics. Finite-time coherent sets can be obtained using the dynamic Laplacian. In this section (following the descriptions in [28] and [33]) we will discuss the method of dynamic isoperimetry and present the required set up to define the dynamic Laplacian and coherent sets. We consider the simple setting of T_ε volume-preserving and one application of T_ε, however, the methods we propose are easily extendible to non-volume-preserving T_ε and multiple applications of T_ε.

In [28], the following dynamic isoperimetric problem was considered: Given a manifold Ω, how can it be disconnected by a codimension 1 manifold Γ so that the evolved size of Γ is minimal relative to the volume of the two disconnected pieces Ω_1, Ω_2 of Ω. To address this, consider the dynamic Cheeger constant

$$\mathbf{h}(\Gamma) := \frac{\frac{1}{2}(\ell_{n-1}(\Gamma) + \ell_{n-1}(T_0(\Gamma)))}{\min\{\ell(\Omega_1), \ell(\Omega_2)\}}, \tag{4.2.1}$$

where ℓ_{n-1} is the codimension 1 volume and ℓ is the $n-$dimensional volume. If we can solve the problem

$$\mathbf{h} := \min\{\mathbf{h}(\Gamma) : \Gamma \text{ is a } C^\infty \text{ codimension 1 manifold disconnecting } \Omega\}, \tag{4.2.2}$$

then the Γ achieving the minimum generates material disconnectors in the phase space that remain coherent since they resist filamentation under the dynamics. In [28], the following dynamic Federer-Fleming theorem was proved:

$$\mathbf{h} = \mathbf{s},$$

where

$$\mathbf{s} := \inf_{f \in C^\infty(\Omega,\mathbb{R})} \frac{\frac{1}{2}(\|\nabla f\|_1 + \|\nabla T_{0,*} f\|_1)}{\inf_{\alpha\in\mathbb{R}} \|f-\alpha\|_1} \tag{4.2.3}$$

is the dynamic Sobolev constant and $T_{0,*}f := f \circ T_0^{-1}$. Note that with this result we are able to address the geometric problem of finding Γ by analytical methods. By considering the L^2 optimisation in (4.2.3), the problem can be solved exactly by considering the following eigenproblem:

$$\Delta_0^D v = \lambda v \qquad \text{on } \operatorname{int}(\Omega), \tag{4.2.4}$$

$$\nabla v \bullet A^0 \nu = 0 \qquad \text{on } \partial\Omega, \tag{4.2.5}$$

where $\Delta_0^D := \frac{1}{2}\left(\Delta_\Omega + T_0^* \Delta_{T_0(\Omega)} T_{0,*}\right), T_0^* f := f \circ T_0$, Δ_Ω is the Laplacian[1] on Ω, ν is the unit outward normal to $\partial\Omega$ and $A^0 := \frac{1}{2}\left(\mathrm{Id} + (DT_0^\top DT_0)^{-1}\right)$. The eigenfunction corresponding to the second eigenvalue of the eigenproblem (4.2.4)–(4.2.5) is the function achieving the minimum of an L^2 version of the optimisation problem in (4.2.3). We note that in the proof of the Federer-Fleming theorem, the set Γ minimising $\mathbf{h}(\Gamma)$ is obtained from a level set of the function achieving the infimum in the definition of the Sobolev constant. Thus, the level sets of the eigenfunctions of the eigenvalue problem (4.2.4)–(4.2.5) provide candidates for coherent sets (see [28, 32, 33, 35, 37] for more on extracting coherent sets from the eigenfunctions).

Following the approach in [33], we consider the following weak formulation of the eigenvalue problem (4.2.4)–(4.2.5):

$$-\frac{1}{2}\left(\int_\Omega \nabla u_0 \bullet \nabla\varphi \, d\ell + \int_{T_0(\Omega)} \nabla(T_{0,*}u_0) \bullet \nabla(T_{0,*}\varphi)\, d\ell\right) = \lambda_0 \int_\Omega u_0\varphi \, d\ell \tag{4.2.6}$$

[1] We restrict ourselves to the Euclidean metric here and write $\Delta = \Delta_\Omega = \Delta_{T_0(\Omega)} = \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2}$.

for all $\varphi \in V$, where $V = H^1(\Omega)$ or $H_0^1(\Omega)$, depending on the boundary condition. Note that if we let $\varphi = u_0$ in (4.2.6), the right hand side is positive and so is the bracket on the left hand side; thus, the eigenvalues λ_0 are negative (or 0). Note further that for $\varphi \in V$ we have

$$\begin{aligned} -\int_{T_0(\Omega)} \nabla(T_{0,*}u_0) \bullet \nabla(T_{0,*}\varphi)\, d\ell &= -\int_\Omega (DT_0^\top DT_0)^{-1}\nabla u_0 \bullet \nabla\varphi\, d\ell \\ &= \int_\Omega \operatorname{div}((DT_0^\top DT_0)^{-1}\nabla u_0)\cdot\varphi\, d\ell, \end{aligned}$$

where DT_0 is the Jacobian matrix of T_0; we note that in the equations immediately above, the first equality is obtained in [33] and the second one follows from the divergence theorem and, for the Dirichlet boundary conditions, the fact that φ is zero on the boundary. Hence, we have that

$$\int_\Omega \Delta_0^D u_0 \cdot \varphi\, d\ell = \int_\Omega \operatorname{div}\left(A^0 \nabla u_0\right)\cdot\varphi\, d\ell. \tag{4.2.7}$$

Viewing the dynamic Laplacian in divergence form (right hand side above) simplifies the perturbation analysis we will require.

Similarly to the above discussion, we compute coherent sets of T_ε, for $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, via the computation of the eigenfunction u_ε of the dynamic Laplacian

$$\Delta_\varepsilon^D := \frac{1}{2}\left(\Delta + T_\varepsilon^* \Delta T_{\varepsilon,*}\right)$$

at the leading eigenvalue $\lambda_\varepsilon \neq 0$. Thus, to answer the question of how coherent sets of T_ε depend on ε, we are going to show that the map $\varepsilon \mapsto u_\varepsilon$ is differentiable at 0 as a map from $(-\varepsilon_0, \varepsilon_0)$ to $H_0^1(\Omega)$ (or $H^1(\Omega)$) and devise a method for computing the *linear response* $\dot{u} := \frac{d}{d\varepsilon} u_\varepsilon|_{\varepsilon=0}$ of u_ε.

4.3 Existence of Linear Response

In this section we show that the map $\varepsilon \mapsto u_\varepsilon$ is differentiable with respect to ε by considering the dynamic Laplacian Δ_ε^D as a second order elliptic operator. We begin with a lemma about the regularity of the coefficient functions of the dynamic Laplacian. Using this result, we show in Theorem 4.3.2 that we can differentiate

the perturbed dynamic Laplacian with respect to ε. Finally, we state a regularity theorem for the spectral data of elliptic operators and use it to obtain the regularity of the map $\varepsilon \mapsto u_\varepsilon$.

Let $a^0 := (a^0_{11}, \dots, a^0_{nn})$ and $a^\varepsilon := (a^\varepsilon_{11}, \dots, a^\varepsilon_{nn})$ be the n^2-tuple of coefficients of the elliptic operators Δ_0^D and Δ_ε^D (see [28] for proof of uniform ellipticity). We let

$$Q^{\mathrm{sym}} = \frac{1}{2}(Q + Q^\top)$$

denote the symmetric part of some matrix Q and we denote by $\mathcal{B}(X, Y)$ the space of bounded linear maps from the Banach space X to Y (thus, $\mathcal{B}(\mathbb{R}^n) = \mathcal{B}(\mathbb{R}^n, \mathbb{R}^n)$ denotes the bounded linear maps from $\mathbb{R}^n$ to $\mathbb{R}^n$).

Lemma 4.3.1. *Let $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$. Then, the function $x \mapsto a^\varepsilon(x)$ is in $C^1(\overline{\Omega}, \mathbb{R})^{n^2}$. Furthermore, there exists a function $x \mapsto \dot{a}(x)$ in $C^1(\overline{\Omega}, \mathbb{R})^{n^2}$ such that*

$$\lim_{\varepsilon \to 0} \left\| \frac{a^\varepsilon - a^0}{\varepsilon} - \dot{a} \right\|_{C^1(\overline{\Omega}, \mathbb{R})^{n^2}} = 0, \tag{4.3.1}$$

where the matrix of coefficients $\dot{A} := (\dot{a}_{ij})$ is given by

$$\dot{A} = -\left((DT_0)^{-1} (D\dot{T}) (DT_0)^{-1} (DT_0)^{-\top} \right)^{\mathrm{sym}}. \tag{4.3.2}$$

Proof. The coefficient matrix of Δ_ε^D is $A^\varepsilon = \frac{1}{2}\left(\mathrm{Id} + (DT_\varepsilon^\top DT_\varepsilon)^{-1}\right)$ (see derivation of (4.2.7)). Since $\varepsilon \mapsto T_\varepsilon$ is in $C^1((-\varepsilon_0, \varepsilon_0), \mathrm{Diff}^2(\overline{\Omega}, \mathbb{R}^n))$, we have that for any $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$ the map $x \mapsto T_\varepsilon(x)$ is in $\mathrm{Diff}^2(\overline{\Omega}, \mathbb{R}^n)$; thus, the maps $x \mapsto DT_\varepsilon(x)$ and $x \mapsto DT_\varepsilon^{-1}(x)$ are in $C^1(\overline{\Omega}, \mathcal{B}(\mathbb{R}^n))$. From $(DT_\varepsilon^\top DT_\varepsilon)^{-1} = DT_\varepsilon^{-1} DT_\varepsilon^{-\top}$ and the product rule, the map $x \mapsto A^\varepsilon(x) = \frac{1}{2}\left(\mathrm{Id} + DT_\varepsilon^{-1}(x) DT_\varepsilon^{-\top}(x)\right)$ is in $C^1(\overline{\Omega}, \mathcal{B}(\mathbb{R}^n))$; equivalently, a^ε, the collection of functions forming the elements of the square matrix A^ε, is in $C^1(\overline{\Omega}, \mathbb{R})^{n^2}$.

Next, we recall from (4.1.1) that for sufficiently small $\varepsilon_0 > 0$, we have that $T_\varepsilon = T_0 + \varepsilon \dot{T} + R_\varepsilon$ for $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, where $\|R_\varepsilon\|_{C^2(\overline{\Omega}, \mathbb{R}^n)} = o(\varepsilon)$. Also, we have

$$\begin{aligned}
(DT_\varepsilon)^{-1} &= \left(DT_0 + \varepsilon D\dot{T} + DR_\varepsilon \right)^{-1} \\
&= \left(DT_0(\mathrm{Id} + (DT_0)^{-1}(\varepsilon D\dot{T} + DR_\varepsilon))) \right)^{-1}
\end{aligned}$$

$$= \left(\mathrm{Id} + (DT_0)^{-1}(\varepsilon D\dot{T} + DR_\varepsilon)\right)^{-1} (DT_0)^{-1}.$$

Using the fact that $\|R_\varepsilon\|_{C^2(\overline{\Omega},\mathbb{R}^n)} = o(\varepsilon)$, we have that $\|DR_\varepsilon\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} = o(\varepsilon)$ and so there exists $C < \infty$, that is independent of ε, such that

$$\begin{aligned}
&\|(DT_0)^{-1}(\varepsilon D\dot{T} + DR_\varepsilon)\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} \\
&\leq \|(DT_0)^{-1}\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} \left(|\varepsilon|\|D\dot{T}\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} + \|DR_\varepsilon\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))}\right) \\
&\leq |\varepsilon|\|(DT_0)^{-1}\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} \left(\|D\dot{T}\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} + C\right).
\end{aligned}$$

Since ε is small, we have that

$$|\varepsilon| < \left(\|(DT_0)^{-1}\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} \left(\|D\dot{T}\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} + C\right)\right)^{-1}$$

and therefore $\|(DT_0)^{-1}(\varepsilon D\dot{T} + DR_\varepsilon)\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} < 1$. Thus, we can use the Neumann series representation to obtain

$$\begin{aligned}
&(DT_\varepsilon)^{-1} \\
&= \left(\mathrm{Id} - (DT_0)^{-1}(\varepsilon D\dot{T} + DR_\varepsilon) + \left((DT_0)^{-1}(\varepsilon D\dot{T} + DR_\varepsilon)\right)^2 - \cdots\right)(DT_0)^{-1} \\
&= \left(\mathrm{Id} - \varepsilon(DT_0)^{-1}D\dot{T} + \widehat{R}_\varepsilon\right)(DT_0)^{-1} \\
&= (DT_0)^{-1} - \varepsilon(DT_0)^{-1}(D\dot{T})(DT_0)^{-1} + \widehat{R}_\varepsilon(DT_0)^{-1},
\end{aligned}$$

where $\widehat{R}_\varepsilon = (DT_0)^{-1}DR_\varepsilon + \sum_{i\geq 2}(-1)^i \left((DT_0)^{-1}(\varepsilon D\dot{T} + DR_\varepsilon)\right)^i$. Noting that

$$\begin{aligned}
\|\widehat{R}_\varepsilon\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} &\leq \|(DT_0)^{-1}\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))}\|DR_\varepsilon\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} \\
&\quad + \sum_{i\geq 2} \|(DT_0)^{-1}\|^i_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} \left(\varepsilon\|D\dot{T}\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} + \|DR_\varepsilon\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))}\right)^i,
\end{aligned}$$

and using the fact that $\|DR_\varepsilon\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} = o(\varepsilon)$, we have that $\|\widehat{R}_\varepsilon\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} = o(\varepsilon)$. Hence, we have

$$(DT_\varepsilon)^{-1}(DT_\varepsilon)^{-\top}$$

$$
\begin{aligned}
&= (DT_0)^{-1}(DT_0)^{-\top} \\
&\quad - \varepsilon \left((DT_0)^{-1}(D\dot{T})(DT_0)^{-1}(DT_0)^{-\top} + (DT_0)^{-1}(DT_0)^{-\top}(D\dot{T})^{\top}(DT_0)^{-\top} \right) + \widetilde{R}_\varepsilon \\
&= (DT_0)^{-1}(DT_0)^{-\top} + 2\varepsilon \dot{A} + \widetilde{R}_\varepsilon,
\end{aligned}
$$

where $\|\widetilde{R}_\varepsilon\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} = o(\varepsilon)$. From $(DT_\varepsilon^{\top} DT_\varepsilon)^{-1} = (DT_\varepsilon)^{-1}(DT_\varepsilon)^{-\top}$, we conclude that $\|A^0 - A^\varepsilon - \varepsilon\dot{A}\|_{C^1(\overline{\Omega},\mathcal{B}(\mathbb{R}^n))} = o(\varepsilon)$ and therefore $\|a^\varepsilon - a^0 - \varepsilon\dot{a}\|_{C^1(\overline{\Omega},\mathbb{R})^{n^2}} = o(\varepsilon)$. □

We will soon use the lemma above to state a result about the differentiability of the dynamic Laplace operator in a suitable setting. Let

$$
L_b := \sum_{i,j=1}^{n} \partial_i (b_{ij} \partial_j) \tag{4.3.3}
$$

be a second order differential operator, where $b := (b_{11}, \ldots, b_{nn}) \in C^k(\overline{\Omega}, \mathbb{R})^{n^2}$, for $k \geq 1$. We denote by $\Lambda(L_b)$ the set of pairs $(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega)$ that satisfy

$$
\begin{aligned}
L_b u &= \lambda u \quad \text{in } \Omega, \\
u &= 0 \quad \text{on } \partial\Omega
\end{aligned} \tag{4.3.4}
$$

in a weak sense; that is

$$
-\int_\Omega B\nabla u \bullet \nabla\varphi d\ell = \lambda \int_\Omega u \cdot \varphi d\ell \text{ for all } \varphi \in H_0^1(\Omega),
$$

where $B = (b_{ij})$ is the coefficient matrix. Note that if we let $b = a^\varepsilon$, then $L_b = \Delta_\varepsilon^D$.

Theorem 4.3.2. *Let $\dot{\Delta} := \sum_{i,j=1}^n \partial_i(\dot{a}_{ij}\partial_j)$, where $(\dot{a}_{11}, \ldots, \dot{a}_{nn}) = \dot{a}$ is as in Lemma 4.3.1. Then, $\dot{\Delta}$ is a weak derivative of Δ_ε^D with respect to ε; that is, for $\psi, \varphi \in H_0^1(\Omega)$*

$$
\lim_{\varepsilon \to 0} \left| \int_\Omega \left(\frac{(\Delta_\varepsilon^D - \Delta_0^D)\psi}{\varepsilon} - \dot{\Delta}\psi \right) \cdot \varphi d\ell \right| = 0. \tag{4.3.5}
$$

Proof. We note that from Lemma 4.3.1 we can write $a_{ij}^{\varepsilon} = a_{ij}^{0} + \varepsilon \dot{a}_{ij} + r_{ij}^{\varepsilon}$, where ε is small and $\|r_{ij}^{\varepsilon}\|_{C^1(\overline{\Omega},\mathbb{R})} = o(\varepsilon)$. We compute

$$\begin{aligned}
\left| \int_{\Omega} \left(\Delta_{\varepsilon}^{D} - \Delta_{0}^{D} - \varepsilon \dot{\Delta} \right) \psi \cdot \varphi d\ell \right| &= \left| \int_{\Omega} \sum_{i,j=1}^{n} (a_{ij}^{\varepsilon} - a_{ij}^{0} - \varepsilon \dot{a}_{ij}) \partial_j \psi \ \partial_i \varphi d\ell \right| \\
&= \left| \int_{\Omega} \sum_{i,j=1}^{n} r_{ij}^{\varepsilon} \partial_j \psi \ \partial_i \varphi d\ell \right| \\
&\leq \sum_{i,j=1}^{n} \|r_{ij}^{\varepsilon}\|_{C^0(\overline{\Omega},\mathbb{R})} \|\nabla \psi\|_{L^2(\Omega)} \|\nabla \varphi\|_{L^2(\Omega)} \\
&= o(\varepsilon).
\end{aligned} \tag{4.3.6}$$

□

Having established the appropriate setting and conditions required for the differentiability of the dynamic Laplacian, we next state, and then immediately apply, the theorem we require to obtain the differentiability of the spectral data with respect to the parameter ε.

Theorem 4.3.3 ([48]). *Let $\Omega \subset \mathbb{R}^n$ be a bounded domain and $a^0 \in C^k(\overline{\Omega},\mathbb{R})^{n^2}$, where $k \geq 1$, be coefficients of the uniformly elliptic operator L_{a^0}. Let $(\lambda_0, u_0) \in \Lambda(L_{a^0})$ and assume λ_0 is algebraically simple. Then there exists a neighbourhood $\mathcal{U} \subset C^k(\overline{\Omega},\mathbb{R})^{n^2}$ of a^0 and functions of C^k class $\boldsymbol{\lambda} : \mathcal{U} \to \mathbb{R}$ and $\mathbf{u} : \mathcal{U} \to H_0^1(\Omega)$ such that:*

1. *$\boldsymbol{\lambda}(a^0) = \lambda_0$ and $\mathbf{u}(a^0) = u_0$;*
2. *$(\boldsymbol{\lambda}(a), \mathbf{u}(a)) \in \Lambda(L_a)$ for every $a \in \mathcal{U}$.*

Theorem 4.3.4. *Let $(\lambda_\varepsilon, u_\varepsilon) \in \Lambda(L_{a^\varepsilon})$, where $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, a^ε be the coefficient functions of Δ_ε^D and λ_0 be algebraically simple. Then there exists a function $\dot{u} \in H_0^1(\Omega)$ such that*

$$\lim_{\varepsilon \to 0} \left\| \frac{u_\varepsilon - u_0}{\varepsilon} - \dot{u} \right\|_{H_0^1(\Omega)} = 0.$$

Furthermore, there exists $\dot{\lambda} \in \mathbb{R}$ such that

$$\lim_{\varepsilon \to 0} \left| \frac{\lambda_\varepsilon - \lambda_0}{\varepsilon} - \dot{\lambda} \right| = 0.$$

Proof. From Lemma 4.3.1, we have $a^0 \in C^1(\overline{\Omega}, \mathbb{R})^{n^2}$; hence, we can apply Theorem 4.3.3 since L_{a^0} is uniformly elliptic (see [28]) and λ_0 is assumed simple. Thus, there exists a neighbourhood $\mathcal{U} \ni a^0$ such that the maps $\mathbf{u} : \mathcal{U} \to H_0^1(\Omega)$ and $\boldsymbol{\lambda} : \mathcal{U} \to \mathbb{R}$ are C^1. Specifically, there exists bounded linear maps $B_1 : C^1(\overline{\Omega}, \mathbb{R})^{n^2} \to H_0^1(\Omega)$ and $B_2 : C^1(\overline{\Omega}, \mathbb{R})^{n^2} \to \mathbb{R}$ satisfying

$$\lim_{\|a^\varepsilon - a^0\|_{C^1(\overline{\Omega},\mathbb{R})^{n^2}} \to 0} \frac{\|\mathbf{u}(a^\varepsilon) - \mathbf{u}(a^0) - B_1(a^\varepsilon - a^0)\|_{H_0^1(\Omega)}}{\|a^\varepsilon - a^0\|_{C^1(\overline{\Omega},\mathbb{R})^{n^2}}} = 0$$

and

$$\lim_{\|a^\varepsilon - a^0\|_{C^1(\overline{\Omega},\mathbb{R})^{n^2}} \to 0} \frac{|\boldsymbol{\lambda}(a^\varepsilon) - \boldsymbol{\lambda}(a^0) - B_2(a^\varepsilon - a^0)|}{\|a^\varepsilon - a^0\|_{C^1(\overline{\Omega},\mathbb{R})^{n^2}}} = 0.$$

Furthermore, from Taylor's theorem (see [61], XIII, §6), we have that

$$\mathbf{u}(a^\varepsilon) = \mathbf{u}(a^0) + B_1(a^\varepsilon - a^0) + U_\varepsilon, \tag{4.3.7}$$

where $\|U_\varepsilon\|_{H_0^1(\Omega)} = o(\|a^\varepsilon - a^0\|_{C^1(\overline{\Omega},\mathbb{R})^{n^2}})$, and

$$\boldsymbol{\lambda}(a^\varepsilon) = \boldsymbol{\lambda}(a^0) + B_2(a^\varepsilon - a^0) + l_\varepsilon, \tag{4.3.8}$$

where $|l_\varepsilon| = o(\|a^\varepsilon - a^0\|_{C^1(\overline{\Omega},\mathbb{R})^{n^2}})$.

Let $\dot{u} := B_1(\dot{a}) \in H_0^1(\Omega)$ and $\dot{\lambda} := B_2(\dot{a})$. Using the fact that we can write $a_{ij}^\varepsilon = a_{ij}^0 + \varepsilon \dot{a}_{ij} + r_{ij}^\varepsilon$, where $\|r_{ij}^\varepsilon\|_{C^1(\overline{\Omega},\mathbb{R})} = o(\varepsilon)$, and equations (4.3.7) and (4.3.8), the results follow. □

4.4 Derivation of the Linear Response Formula

Having established the existence of the linear response $\dot{u}$, in this section we will derive the linear response formula for computing $\dot{u}$ (this will be in the form of a linear system); we also obtain the formula for $\dot{\lambda}$. We will do this for Dirichlet boundary conditions first and in Section 4.4.1 we will consider Neumann boundary conditions.

Theorem 4.4.1. *Let $\dot{\lambda}$ and $\dot{u}$ be as in Theorem 4.3.4 and $\dot{\Delta}$ be as in Theorem 4.3.2. Then,*

$$\dot{\lambda} = \frac{\int_\Omega \dot{\Delta} u_0 \cdot u_0 d\ell}{\int_\Omega u_0 \cdot u_0 d\ell} \tag{4.4.1}$$

and the linear response $\dot{u} \in H_0^1(\Omega)$ is a solution to the weak form of the linear system

$$\begin{cases} (\Delta_0^D - \lambda_0 I)\dot{u} = (\dot{\lambda} I - \dot{\Delta})u_0 & \text{in } \Omega \\ \dot{u} = 0 & \text{on } \partial\Omega; \end{cases} \tag{4.4.2}$$

that is, for all $\varphi \in H_0^1(\Omega)$,

$$-\int_\Omega A^0 \nabla \dot{u} \bullet \nabla \varphi \, d\ell - \lambda_0 \int_\Omega \dot{u} \cdot \varphi \, d\ell = \dot{\lambda} \int_\Omega u_0 \cdot \varphi \, d\ell + \int_\Omega \dot{A} \nabla u_0 \bullet \nabla \varphi \, d\ell. \tag{4.4.3}$$

Furthermore, if we restrict the linear response to $V_0 := span\{u_0\}^\perp \subset H_0^1(\Omega)$, then $\dot{u}^* = \dot{u} - \langle \dot{u}, u_0 \rangle_{H_0^1(\Omega)} u_0 \in V_0$, where $\dot{u}$ is a solution to (4.4.3), is the unique solution.

Proof. We show the result in two steps. In the first step, we compute the weak derivative of $\lambda_\varepsilon u_\varepsilon$ with respect to ε and in the second step we compute the weak derivative of $\Delta_\varepsilon^D u_\varepsilon$ with respect to ε. Since these are equal, because u_ε is the eigenfunction associated to the eigenvalue λ_ε, we show that the result follows. Before proceeding, we note that for all $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, we normalise the eigenfunctions u_ε as follows: $\|u_\varepsilon\|_{H_0^1(\Omega)} = 1$.

Sublemma 4.4.2. *For $\varphi \in H_0^1(\Omega)$,*

$$\lim_{\varepsilon \to 0} \int_\Omega \left(\frac{\lambda_\varepsilon u_\varepsilon - \lambda_0 u_0}{\varepsilon} \right) \cdot \varphi d\ell = \int_\Omega \left(\lambda_0 \dot{u} + \dot{\lambda} u_0 \right) \cdot \varphi d\ell.$$

Proof. From Theorem 4.3.4 we have that $u_\varepsilon = u_0 + \varepsilon \dot{u} + g^\varepsilon$ and $\lambda_\varepsilon = \lambda_0 + \varepsilon \dot{\lambda} + \mu^\varepsilon$, where $\|g^\varepsilon\|_{H_0^1(\Omega)} = o(\varepsilon)$ and $|\mu^\varepsilon| = o(\varepsilon)$. Hence, we have

$$\lambda_\varepsilon u_\varepsilon = \lambda_0 u_0 + \varepsilon(\lambda_0 \dot{u} + \dot{\lambda} u_0) + f^\varepsilon,$$

where $f^\varepsilon = u_0 \mu^\varepsilon + \varepsilon^2 \dot{u} \dot{\lambda} + \varepsilon \dot{u} \mu^\varepsilon + g^\varepsilon \cdot (\lambda_0 + \varepsilon \dot{\lambda} + \mu^\varepsilon)$. Noting that g^ε and μ^ε are $o(\varepsilon)$, we apply Holder's inequality to obtain $\left| \int_\Omega f^\varepsilon \cdot \varphi d\ell \right| = o(\varepsilon)$; the result then follows. □

Sublemma 4.4.3. *For $\varphi \in H_0^1(\Omega)$,*

$$\lim_{\varepsilon\to 0}\int_\Omega \left(\frac{\Delta_\varepsilon^D u_\varepsilon - \Delta_0^D u_0}{\varepsilon}\right)\cdot\varphi d\ell = \int_\Omega \left(\Delta_0^D \dot{u} + \dot{\Delta} u_0\right)\cdot\varphi d\ell.$$

Proof. From Theorem 4.3.4, $u_\varepsilon = u_0 + \varepsilon\dot{u} + g^\varepsilon$, where $\|g^\varepsilon\|_{H_0^1(\Omega)} = o(\varepsilon)$. Also, from Lemma 4.3.1, $a_{ij}^\varepsilon = a_{ij}^0 + \varepsilon\dot{a}_{ij} + r_{ij}^\varepsilon$, where $\|r_{ij}^\varepsilon\|_{C^1(\overline{\Omega},\mathbb{R})} = o(\varepsilon)$. Hence, by considering the expansion $\Delta_\varepsilon^D = \Delta_0^D + \varepsilon\dot{\Delta} + G^\varepsilon$, where $G^\varepsilon := \sum_{i,j=1}^n \partial_i(r_{ij}^\varepsilon\partial_i)$, we obtain

$$\begin{aligned}
\int \Delta_\varepsilon^D u_\varepsilon\cdot\varphi d\ell &= \int \Delta_\varepsilon^D(u_0+\varepsilon\dot{u}+g^\varepsilon)\cdot\varphi d\ell\\
&= \int(\Delta_0^D u_0 + \varepsilon\dot{\Delta}u_0 + G^\varepsilon u_0)\cdot\varphi d\ell + \varepsilon\int(\Delta_0^D\dot{u} + \varepsilon\dot{\Delta}\dot{u} + G^\varepsilon\dot{u})\cdot\varphi d\ell\\
&\quad + \int \Delta_\varepsilon^D g^\varepsilon\cdot\varphi d\ell\\
&= \int \Delta_0^D u_0\cdot\varphi d\ell + \varepsilon\int\left(\dot{\Delta}u_0 + \Delta_0^D\dot{u}\right)\cdot\varphi d\ell\\
&\quad + \int\left(G^\varepsilon u_0 + \varepsilon^2\dot{\Delta}\dot{u} + \varepsilon G^\varepsilon\dot{u} + \Delta_\varepsilon^D g^\varepsilon\right)\cdot\varphi d\ell.
\end{aligned}$$

If we show that

$$\underbrace{\left|\int\left(G^\varepsilon u_0 + \varepsilon^2\dot{\Delta}\dot{u} + \varepsilon G^\varepsilon\dot{u} + \Delta_\varepsilon^D g^\varepsilon\right)\cdot\varphi d\ell\right|}_{I} = o(\varepsilon)$$

then the result follows. We have

$$\begin{aligned}
I &\le \left|\int G^\varepsilon u_0\cdot\varphi d\ell\right| + \varepsilon^2\left|\int\dot{\Delta}\dot{u}\cdot\varphi d\ell\right| + |\varepsilon|\left|\int G^\varepsilon\dot{u}\cdot\varphi d\ell\right| + \left|\int\Delta_\varepsilon^D g^\varepsilon\cdot\varphi d\ell\right|\\
&= o(\varepsilon) + \underbrace{\varepsilon^2\left|\int\dot{\Delta}\dot{u}\cdot\varphi d\ell\right|}_{I'} + o(\varepsilon) + \underbrace{\left|\int\Delta_\varepsilon^D g^\varepsilon\cdot\varphi d\ell\right|}_{II'},
\end{aligned}$$

where we obtained the last line by using (4.3.6) with $\psi = u_0$ and $\psi = \dot{u}$. From Theorem 4.3.2, we have that $\left|\int\dot{\Delta}\dot{u}\cdot\varphi d\ell\right|$ is bounded since $\dot{u}, \varphi \in H_0^1(\Omega)$; hence, $I' = o(\varepsilon)$.

We also have

$$II' \leq \underbrace{\left| \int \Delta_0^D g^\varepsilon \cdot \varphi d\ell \right|}_{I''} + \underbrace{|\varepsilon| \left| \int \dot{\Delta} g^\varepsilon \cdot \varphi d\ell \right|}_{II''} + \underbrace{\left| \int G^\varepsilon g^\varepsilon \cdot \varphi d\ell \right|}_{III''}.$$

Using the fact that $\|g^\varepsilon\|_{H_0^1(\Omega)} = o(\varepsilon)$, we can use the argument in (4.3.6) with Δ_0^D and $\dot{\Delta}$ (instead of $\Delta_\varepsilon^D - \Delta_0^D - \varepsilon\dot{\Delta}$), to conclude that $I'' = o(\varepsilon) = II''$. Furthermore, using the fact that $\|r_{ij}^\varepsilon\|_{C^1(\overline{\Omega},\mathbb{R})} = o(\varepsilon)$, we can again use the argument in (4.3.6) to obtain $III'' = o(\varepsilon)$; thus, $I = o(\varepsilon)$. □

From Sublemmas 4.4.2 and 4.4.3, we immediately have that for $\varphi \in H_0^1(\Omega)$,

$$\int_\Omega \left(\Delta_0^D \dot{u} + \dot{\Delta} u_0 \right) \cdot \varphi d\ell = \int_\Omega \left(\lambda_0 \dot{u} + \dot{\lambda} u_0 \right) \cdot \varphi d\ell. \tag{4.4.4}$$

Substituting $\varphi = u_0$ into (4.4.4), the left hand side becomes

$$\int_\Omega \dot{u} \cdot \Delta_0^D u_0 d\ell + \int_\Omega \dot{\Delta} u_0 \cdot u_0 d\ell = \int_\Omega \dot{u} \cdot \lambda_0 u_0 d\ell + \int_\Omega \dot{\Delta} u_0 \cdot u_0 d\ell,$$

while the right hand side becomes

$$\int_\Omega \lambda_0 \dot{u} \cdot u_0 d\ell + \int_\Omega \dot{\lambda} u_0 \cdot u_0;$$

from these observations we obtain (4.4.1). By Green's theorem, (4.4.4) implies (4.4.3), which is the weak formulation of the problem (4.4.2).

Finally, we note that $(\dot{\lambda} I - \dot{\Delta}) u_0 \in L^2(\Omega)$ and, by (4.4.1), we have that $\langle (\dot{\lambda} I - \dot{\Delta}) u_0, u_0 \rangle_{L^2} = \dot{\lambda} \langle u_0, u_0 \rangle_{L^2} - \langle \dot{\Delta} u_0, u_0 \rangle_{L^2} = 0$. Hence, by Theorem 1.2.16 [51], there exists a solution $\dot{u} \in H_0^1(\Omega)$. All other solutions are of the form $\dot{u} + cu_0$ for $c \in \mathbb{R}$; thus, if we restrict $\dot{u}$ to $V_0 = \text{span}\{u_0\}^\perp$, there is a unique solution $\dot{u}^* \in V_0$, which is the projection of a solution $\dot{u}$ of (4.4.3) onto the space V_0. □

4.4.1 Neumann Boundary Conditions

In this section we will present the required modifications to the previous theory which allows us to conclude that linear response exists when considering Neumann

boundary conditions. Furthermore, we will also obtain a linear system, the weak form of which we can use to compute the linear response.

Let $W = \{f \in H^1(\Omega) : \int_\Omega f d\ell = 0\}$ and $\Lambda_N(L_b)$ be the set of pairs $(\lambda, u) \in \mathbb{R} \times W$ that, in a weak sense, satisfy

$$\begin{aligned} L_b u &= \lambda u \quad \text{in } \Omega, \\ \nabla u \bullet B\nu &= 0 \quad \text{on } \partial\Omega, \end{aligned} \tag{4.4.5}$$

where $B = (b_{ij})$ is the matrix of coefficient functions of the operator L_b, considered in the form (4.3.3), and ν is the unit outward normal to $\partial\Omega$.

Theorem 4.4.4. *Let $(\lambda_\varepsilon, u_\varepsilon) \in \Lambda_N(L_{a^\varepsilon})$, where $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, a^ε be the coefficient functions of Δ_ε^D and λ_0 be algebraically simple. Then there exists a function $\dot{u} \in W$ such that*

$$\lim_{\varepsilon \to 0} \left\| \frac{u_\varepsilon - u_0}{\varepsilon} - \dot{u} \right\|_{H^1(\Omega)} = 0.$$

Furthermore, there exists $\dot{\lambda} \in \mathbb{R}$ such that

$$\lim_{\varepsilon \to 0} \left| \frac{\lambda_\varepsilon - \lambda_0}{\varepsilon} - \dot{\lambda} \right| = 0.$$

Proof. On W we have the result of Theorem 4.3.3; that is, there existence a neighbourhood $\mathcal{U} \subset C^k(\overline{\Omega}, \mathbb{R})^{n^2}$ and C^k functions $\boldsymbol{\lambda} : \mathcal{U} \to \mathbb{R}$ and $\mathbf{u} : \mathcal{U} \to W$ such that $(\boldsymbol{\lambda}(a), \mathbf{u}(a)) \in \Lambda_N(L_a)$ for all $a \in \mathcal{U}$ (this follows by noting that the isomorphism from the Lax-Milgram theorem, which is required in the proof of Theorem 4.3.3 for elliptic operators of the form (4.3.3), exists when restricted to the subspace W of $H^1(\Omega)$). Hence, the arguments in Theorem 4.3.4 hold in this setting; thus, the eigenfunction $u_\varepsilon \in W$ and the eigenvalue λ_ε are differentiable with respect to ε. □

Furthermore, we have the following analogue to Theorem 4.4.1 for the Neumann boundary setting.

Theorem 4.4.5. *Let $\dot{\lambda}$ and $\dot{u}$ be as in Theorem 4.4.4 and $\dot{\Delta}$ be as in Theorem 4.3.2. Then,*

$$\dot{\lambda} = \frac{\int_\Omega \dot{\Delta} u_0 \cdot u_0 d\ell}{\int_\Omega u_0 \cdot u_0 d\ell} \tag{4.4.6}$$

and the linear response $\dot{u} \in W$ is a solution to the weak form of the linear system

$$\begin{cases} (\Delta_0^D - \lambda_0 I)\dot{u} = (\dot{\lambda} I - \dot{\Delta})u_0 & \text{in } \Omega \\ \nabla \dot{u} \bullet A^0 \nu = 0 & \text{on } \partial\Omega; \end{cases} \tag{4.4.7}$$

that is, for all $\varphi \in W$,

$$-\int_\Omega A^0 \nabla \dot{u} \bullet \nabla \varphi \, d\ell - \lambda_0 \int_\Omega \dot{u} \cdot \varphi \, d\ell = \dot{\lambda} \int_\Omega u_0 \cdot \varphi \, d\ell + \int_\Omega \dot{A} \nabla u_0 \bullet \nabla \varphi \, d\ell. \tag{4.4.8}$$

Furthermore, if we restrict the linear response to $W_0 := (\text{span}\{u_0\})^\perp \cap W$, then $\dot{u}^* = \dot{u} - \langle \dot{u}, u_0 \rangle_{H^1(\Omega)} u_0 \in W_0$, where $\dot{u}$ is a solution to (4.4.8), is the unique solution.

Before we prove this theorem, we note the following result.

Lemma 4.4.6. *If for a sufficiently small $\varepsilon_0 > 0$, $\nabla u_\varepsilon \bullet A^\varepsilon \nu = 0$ on $\partial\Omega$ for all $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, then $\dot{A} \nabla u_0 \bullet \nu + A^0 \nabla \dot{u} \bullet \nu = 0$.*

Proof. Since A^ε is symmetric, $A^\varepsilon \nabla u_\varepsilon \bullet \nu = \nabla u_\varepsilon \bullet A^\varepsilon \nu = 0$ for all $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$ and thus

$$A^0 \nabla u_0 \bullet \nu + \varepsilon \left(\dot{A} \nabla u_0 \bullet \nu + A^0 \nabla \dot{u} \bullet \nu \right) + o(\varepsilon) = 0 \quad \text{for all } \varepsilon \in (-\varepsilon_0, \varepsilon_0).$$

Using the fact that $A^0 \nabla u_0 \bullet \nu = 0$, we can conclude that $\dot{A} \nabla u_0 \bullet \nu + A^0 \nabla \dot{u} \bullet \nu = 0$. □

Proof of Theorem 4.4.5. The result is obtained similarly to the setting in Theorem 4.4.1 if we obtain (4.4.4) for the Neumann setting. Thus, we first show that for $\psi, \varphi \in W$,

$$\lim_{\varepsilon \to 0} \left| \int_\Omega \left(\frac{(\Delta_\varepsilon^D - \Delta_0^D)\psi}{\varepsilon} - \dot{\Delta}\psi \right) \cdot \varphi d\ell \right| = 0.$$

Let $\text{Tr} : H^1(\Omega) \to L^2(\partial\Omega; \ell_{n-1})$ be the trace operator; note that Tr is a bounded linear operator since $\partial\Omega$ is C^1 (Theorem 1 §5.5, [24]). If we write $A^\varepsilon = A^0 + \varepsilon \dot{A} + \bar{R}^\varepsilon$,

where $\bar{R}^\varepsilon = (r_{ij}^\varepsilon)$ and $\|r_{ij}^\varepsilon\|_{C^1(\overline{\Omega},\mathbb{R})} = o(\varepsilon)$, we obtain

$$\begin{aligned}\left|\int_\Omega (\Delta_\varepsilon^D\psi - \Delta_0^D\psi - \varepsilon\dot{\Delta}\psi)\cdot\varphi d\ell\right| &\le \left|\int_\Omega \bar{R}^\varepsilon\nabla\psi\bullet\nabla\varphi d\ell\right| + \left|\int_{\partial\Omega}(\bar{R}^\varepsilon\nabla\psi\bullet\nu)\mathrm{Tr}\varphi d\ell_{n-1}\right| \\ &\le o(\varepsilon) + \sum_{i,j=1}^n \int_{\partial\Omega}\left|r_{ij}^\varepsilon\partial_j\psi\nu_i\ \mathrm{Tr}\varphi\right| d\ell_{n-1},\end{aligned}$$

where the first bound follows from the argument in (4.3.6). From the fact that $\|r_{ij}^\varepsilon\|_{C^0(\overline{\Omega},\mathbb{R})} = o(\varepsilon)$, ν is the unit outward normal and Tr is bounded, we have

$$\begin{aligned}\sum_{i,j=1}^n \int_{\partial\Omega}\left|r_{ij}^\varepsilon\partial_j\psi\nu_i\ \mathrm{Tr}\varphi\right| d\ell_{n-1} &\le \sum_{i,j=1}^n \|r_{ij}^\varepsilon\|_{C^0(\overline{\Omega},\mathbb{R})}\int_{\partial\Omega}\left|\partial_j\psi\mathrm{Tr}\varphi\right| d\ell_{n-1} \\ &\le \sum_{i,j=1}^n \|r_{ij}^\varepsilon\|_{C^0(\overline{\Omega},\mathbb{R})}\|\partial_j\psi\|_{L^2(\partial\Omega)}\|\mathrm{Tr}\varphi\|_{L^2(\partial\Omega)} \\ &\le \sum_{i,j=1}^n \|r_{ij}^\varepsilon\|_{C^0(\overline{\Omega},\mathbb{R})}\|\nabla\psi\|_{L^2(\Omega)}\|\varphi\|_{H^1(\Omega)} \\ &= o(\varepsilon).\end{aligned}$$

Thus, we can use a similar argument to that in Theorem 4.4.1 to obtain (4.4.4) for the Neumann setting; that is, for all $\varphi \in W$, we have

$$\begin{aligned}-\int_\Omega A^0\nabla\dot{u}\bullet\nabla\varphi\, d\ell + \int_{\partial\Omega}\varphi\cdot A^0\nabla\dot{u}\bullet\nu\, d\ell_{n-1} - \lambda_0\int_\Omega \dot{u}\cdot\varphi\, d\ell \\ = \dot{\lambda}\int_\Omega u_0\cdot\varphi\, d\ell + \int_\Omega \dot{A}\nabla u_0\bullet\nabla\varphi\, d\ell - \int_{\partial\Omega}\varphi\cdot\dot{A}\nabla u_0\bullet\nu\, d\ell_{n-1}.\end{aligned}$$

Using Lemma 4.4.6, the above equation implies (4.4.8), which is a weak form of problem (4.4.7). Finally, the uniqueness of the solution on W_0 follows as in the Dirichlet setting. □

4.5 Numerical Approach to Computing $\dot{u}$

We now describe how to compute the linear response vector $\dot{u}$ numerically. To this end, we approximately solve the weak form (4.4.3), respectively (4.4.8), using the method described in [33]. That is, we consider (4.4.3), respectively (4.4.8), on a finite-dimensional approximation space $V_N \subset H_0^1(\Omega)$ or W, respectively. Note that while we needed to restrict to $W \subset H^1(\Omega)$ in order to obtain the content in

Section 4.4.1, numerically we can still work with $V_N \subset H^1(\Omega)$ since the eigenvectors at eigenvalues $\neq 0$ will be orthogonal to the constant function. In practice, the approximation space will be realised as a finite element space, typically using linear triangular Lagrange elements.

In [33], two different variants of a finite-element discretisation of the basic eigenproblem for the dynamic Laplacian have been proposed, one based on the evaluation of the right Cauchy Green deformation tensor (the *CG method*) and one based on an explicit approximation of the transfer operator associated to T_ε (the *TO method*). We now describe how to use both variants in order to compute $\dot{u}$.

4.5.1 The CG Method

Let $\varphi_1, \dots, \varphi_N$ be a basis for V_N. As usual, we define the Galerkin approximation $\dot{\tilde{u}} = \sum_{j=1}^N \dot{v}_j \varphi_j$ of $\dot{u}$ in (4.4.3), respectively (4.4.8), by requiring it to satisfy

$$-\int_\Omega A^0 \nabla \dot{\tilde{u}} \bullet \nabla \varphi_j d\ell - \lambda_0 \int_\Omega \dot{\tilde{u}} \cdot \varphi_j d\ell = \dot{\lambda} \int_\Omega \tilde{u}_0 \cdot \varphi_j d\ell + \int_\Omega \dot{A} \nabla \tilde{u}_0 \bullet \nabla \varphi_j d\ell$$

for $j = 1, \dots, N$, where $\tilde{u}_0 = \sum_{j=1}^N v_{0,j} \varphi_j$ is the Galerkin approximation of u_0. Plugging in the linear combinations for $\tilde{u}_0$ and $\dot{\tilde{u}}$, this immediately yields the linear system

$$(K - \lambda_0 M)\dot{v} = (\dot{\lambda} M - L) v_0, \tag{4.5.1}$$

for the coefficient vectors v_0 and $\dot{v}$. Here,

$$\begin{gathered} M = \left(\int_\Omega \varphi_j \bullet \varphi_\ell \, d\ell \right)_{j,\ell}, \quad K = -\left(\int_\Omega A^0 \nabla \varphi_j \bullet \nabla \varphi_\ell \, d\ell \right)_{j,\ell}, \\ L = -\left(\int_\Omega \dot{A} \nabla \varphi_j \bullet \nabla \varphi_\ell \, d\ell \right)_{j,\ell} \end{gathered} \tag{4.5.2}$$

are the mass, the stiffness and the "linear response" matrix, respectively. Note that due to Theorem 4.4.1, we need to solve (4.5.1) on V_0. We implement this by adding the corresponding orthogonality constraint as an additional equation to the linear system so that in fact we solve

$$\begin{bmatrix} K - \lambda_0 M & v_0 \\ v_0^\top & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ \alpha \end{bmatrix} = \begin{bmatrix} (\dot{\lambda} M - L) v_0 + v_0 \\ 0 \end{bmatrix} \tag{4.5.3}$$

for $\dot{v}$ in order to obtain $\dot{u}^*$. A corresponding Matlab code is given in the FEMDL package.

4.5.2 The TO Method

As shown in [33], the matrices M and K from (4.5.2) can be computed without having to evaluate A^0 (which is numerically expensive and potentially unstable). Instead, the action of the transfer operator is approximated explicitly. Similarly, the matrix L can be constructed without having to evaluate $\dot{A}$, as we will now show.

Proposition 4.5.1. *For $f, g \in H^1(\Omega)$,*

$$-\int_\Omega \dot{A}\nabla f \bullet \nabla g \; d\ell = \int_{T_0(\Omega)} (\nabla T_{0,*} g)^\top D(T_{0,*}\dot{T})^{sym}(\nabla T_{0,*} f) \; d\ell.$$

Proof. We recall from (4.3.2) that

$$\begin{aligned}\dot{A} &= -\left((DT_0)^{-1}(D\dot{T})(DT_0)^{-1}(DT_0)^{-\top}\right)^{\mathrm{sym}} \\ &= -\frac{1}{2}\left((DT_0)^{-1}(D\dot{T})(DT_0)^{-1}(DT_0)^{-\top} + \left((DT_0)^{-1}(D\dot{T})(DT_0)^{-1}(DT_0)^{-\top}\right)^\top\right).\end{aligned}$$

Next, we compute

$$\begin{aligned}&\int_\Omega (DT_0)^{-1}(D\dot{T})(DT_0)^{-1}(DT_0)^{-\top}\nabla f \bullet \nabla g \; d\ell \\ &= \int_\Omega (D\dot{T})(DT_0)^{-1}(DT_0)^{-\top}\nabla f \bullet (DT_0)^{-\top}\nabla g \; d\ell \\ &= \int_\Omega (D\dot{T})(DT_0)^{-1}(\nabla T_{0,*} f)\circ T_0 \bullet (\nabla T_{0,*} g)\circ T_0 \; d\ell \\ &= \int_{T_0(\Omega)} [((D\dot{T})\circ T_0^{-1})\ (DT_0)^{-1}\circ T_0^{-1}](\nabla T_{0,*} f)\bullet \nabla T_{0,*} g \; d\ell \\ &= \int_{T_0(\Omega)} [((D\dot{T})\circ T_0^{-1})\ (DT_0^{-1})]\nabla T_{0,*} f \bullet \nabla T_{0,*} g \; d\ell \\ &= \int_{T_0(\Omega)} [D(T_{0,*}\dot{T})]\nabla T_{0,*} f \bullet \nabla T_{0,*} g \; d\ell \\ &= \int_{T_0(\Omega)} (\nabla T_{0,*} g)^\top D(T_{0,*}\dot{T})(\nabla T_{0,*} f) \; d\ell.\end{aligned}$$

Similarly, we have

$$\int_\Omega \left((DT_0)^{-1}(D\dot{T})(DT_0)^{-1}(DT_0)^{-\top}\right)^\top \nabla f \bullet \nabla g \; d\ell$$

$$= \int_{T_0(\Omega)} (\nabla T_{0,*} g)^\top (D(T_{0,*}\dot{T}))^\top (\nabla T_{0,*} f)\, d\ell.$$

We thus obtain

$$\begin{aligned} -\int_\Omega \dot{A}\nabla f \bullet \nabla g d\ell &= \int_\Omega \left((DT_0)^{-1}(D\dot{T})(DT_0)^{-1}(DT_0)^{-\top}\right)^{\text{sym}} \nabla f \bullet \nabla g d\ell \\ &= \int_{T_0(\Omega)} (\nabla T_{0,*} g)^\top D(T_{0,*}\dot{T})^{sym} (\nabla T_{0,*} f)\, d\ell. \end{aligned}$$

□

If we want to use the integral on the right hand side in Proposition 4.5.1 to compute the matrix L, we need to approximate the action of the transfer operator $T_{0,*} : H^1(\Omega) \to H^1(T_0(\Omega))$. To this end, we work with two different approximation spaces, $V_N^0 \subset H^1(\Omega)$ and $V_N^1 \subset H^1(T_0(\Omega))$. Let $\varphi_1^0, \ldots, \varphi_N^0$ be a basis of V_N^0 and $\varphi_1^1, \ldots, \varphi_N^1$ of V_N^1. Suppose we know how to approximate the push forward of some function $g \in H^1(\Omega)$ by some function in V_N^1, i.e.

$$T_{0,*} g \approx \sum_k g_k \varphi_k^1,$$

where $g_k \in \mathbb{R}$; then, we can use $\sum_k g_k \nabla \varphi_k^1$ as an approximation for $\nabla(T_{0,*} g)$. We denote by $\dot{T}_1, \ldots, \dot{T}_n$ the component functions of $\dot{T}$. Correspondingly,

$$T_{0,*}\dot{T} = \dot{T} \circ T_0^{-1} = (\dot{T}_1 \circ T_0^{-1}, \ldots, \dot{T}_n \circ T_0^{-1}) = (T_{0,*}\dot{T}_1, \ldots, T_{0,*}\dot{T}_n).$$

We write $\nabla(T_{0,*}\dot{T}_i) \approx \sum_s w_s^i \nabla \varphi_s^1$, where $w_s^i \in \mathbb{R}$, so that

$$D(T_{0,*}\dot{T}) = \begin{bmatrix} (\nabla T_{0,*}\dot{T}_1)^\top \\ \vdots \\ (\nabla T_{0,*}\dot{T}_n)^\top \end{bmatrix} \approx \begin{bmatrix} \sum_s w_s^1 \partial_1 \varphi_s^1 & \ldots & \sum_s w_s^1 \partial_n \varphi_s^1 \\ \vdots & & \vdots \\ \sum_s w_s^n \partial_1 \varphi_s^1 & \ldots & \sum_s w_s^n \partial_n \varphi_s^1 \end{bmatrix}.$$

We then obtain the approximation

$$(\nabla T_{0,*} g)^\top D(T_{0,*}\dot{T}) \nabla T_{0,*} f$$

$$
\begin{aligned}
&\approx \left[\sum_k g_k \partial_1 \varphi_k^1, \ldots, \sum_k g_k \partial_n \varphi_k^1\right] \begin{bmatrix} \sum_s w_s^1 \partial_1 \varphi_s^1 & \ldots & \sum_s w_s^1 \partial_n \varphi_s^1 \\ \vdots & & \vdots \\ \sum_s w_s^n \partial_1 \varphi_s^1 & \ldots & \sum_s w_s^n \partial_n \varphi_s^1 \end{bmatrix} \begin{bmatrix} \sum_l f_l \partial_1 \varphi_l^1 \\ \vdots \\ \sum_l f_l \partial_n \varphi_l^1 \end{bmatrix} \\
&= \sum_{kl} g_k \underbrace{\left(\sum_s \left[\left(\sum_{i=1}^n w_s^i \partial_i \varphi_k^1\right)\left(\sum_{i=1}^n \partial_i \varphi_s^1 \partial_i \varphi_l^1\right)\right]\right)}_{=:B} f_l \\
&= \mathbf{g}^\top B \mathbf{f}.
\end{aligned}
$$

Similarly, one obtains $(\nabla T_{0,*} g)^\top (D(T_{0,*}\dot{T}))^\top (\nabla T_{0,*} f) \approx \mathbf{g}^\top B^\top \mathbf{f}$, and therefore

$$
\begin{aligned}
-\int_\Omega \dot{A} \nabla f \bullet \nabla g \, d\ell &= \int_{T_0(\Omega)} (\nabla T_{0,*} g)^\top D(T_{0,*}\dot{T})^{sym} (\nabla T_{0,*} f) \, d\ell \\
&\approx \int_{T_0(\Omega)} \mathbf{g}^\top B^{sym} \mathbf{f} \, d\ell.
\end{aligned}
$$

Remark 4.5.2. *We note that $B = (B_{kl})$ is a function of $x \in \Omega$ and for $n = 2$ we have*

$$
\begin{aligned}
&B_{kl}(x) \\
&= \sum_s \left(w_s^1 (\partial_1 \varphi_k^1)(x) + w_s^2 (\partial_2 \varphi_k^1)(x)\right)\left((\partial_1 \varphi_s^1)(x)(\partial_1 \varphi_l^1)(x) + (\partial_2 \varphi_s^1)(x)(\partial_2 \varphi_l^1)(x)\right).
\end{aligned}
$$

We will conclude this section by describing how to compute the g_k in the approximation $T_{0,*} g \approx \sum_k g_k \varphi_k^1$ using the two methods presented in [33]. Let $\{x_i\}_{i=1}^N$ be the nodes of the mesh of Ω at the initial time and suppose that $g \approx \sum_k \tilde{g}_k \varphi_k^0$, where $\varphi_k^0 \in V_N^0$ for $k = 1, \ldots, N$. We then have

$$
\begin{aligned}
T_{0,*} g &\approx \sum_k \tilde{g}_k T_{0,*} \varphi_k^0 \\
&\approx \sum_k \tilde{g}_k \sum_i \alpha_i^k \varphi_k^1 \\
&= \sum_k g_k \varphi_k^1,
\end{aligned}
$$

where $g_k = \tilde{g}_k \sum_i \alpha_i^k$. The method of *collocation on nonadapted meshes* can be used to obtain $\alpha_i^k = \varphi_k(T_0^{-1}(x_i))$ (see Section 3.2.2 in [33]). Alternatively, the method of

collocation on adapted meshes can instead be used to obtain $\alpha_i^k = \varphi_k(T_0^{-1}(x_i)) = \varphi_k^0(x_i) = \delta_{k,i}$, where $\delta_{k,i}$ is the Kronecker delta (see Section 3.2.3 in [33]).

4.6 Experiments

Since we identify coherent sets as level sets of eigenfunctions, and are interested in the evolution of coherent sets, we will begin this section with a small note about the evolution of level sets.

4.6.1 Level Set Evolution

We are interested in the change of the level sets of u_ε as we perturb the parameter ε. From the level-set method [72], we note the following. Let $\Gamma_\varepsilon = \{x \in \Omega : u_\varepsilon(x) = 0\}$ be a closed curve in Ω. If the curve Γ_0 moves in the outward normal direction with speed s, we have the following level-set equation

$$\dot{u} + s|\nabla u_0| = 0. \tag{4.6.1}$$

Since we know u_0 and $\dot{u}$, we can solve for s and thus, we know the evolution of the level set Γ_0; the curve Γ_0 evolves in the direction ∇u_0 with speed s, i.e. it evolves according to the vector field $\frac{-\dot{u}}{|\nabla u_0|}\nabla u_0$. In the following experiments, we will use this vector field to verify that the coherent sets change as expected (see for example Figures 4.2 and 4.4).

4.6.2 The Standard Map

We start with the standard map on the flat 2-torus, given by

$$T(x, y) = (x + y + a\sin x, y + a\sin x) \pmod{2\pi}. \tag{4.6.2}$$

In Figure 4.1 (left) we show the second eigenvector u_0 of the dynamic Laplacian for the nominal parameter value $a = 0.98$, which identifies two coherent sets in the upper and lower half of the domain. Interestingly, even for a rather large linear extrapolation, the vector $u_0 + \frac{1}{2}\dot{u}$ is quite similar to the exact second eigenvector u_ε (right) at $a + \varepsilon = 0.98 + 0.5 = 1.48$. Figure 4.2 shows the (normalised) velocity field of the level set curves at $\varepsilon = 0$. Clearly, the change in the level contour from

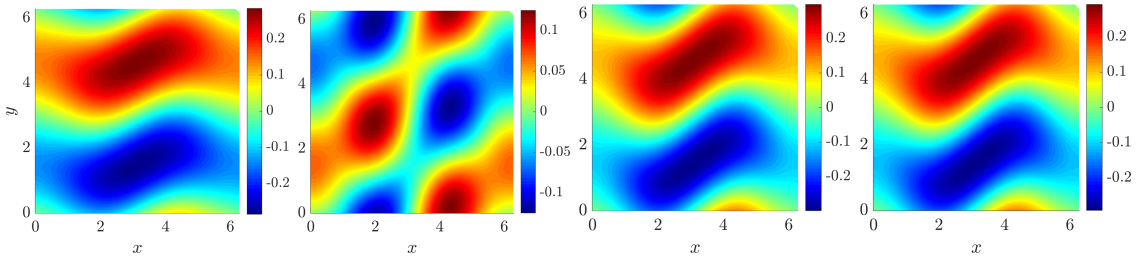


Figure 4.1: Standard map (left to right): u_0, $\dot{u}$, $u_0 + \frac{1}{2}\dot{u}$ and u_ε.

$\varepsilon = 0$ (solid line) to $\varepsilon = 0.5$ is consistent with the prediction by the velocity field (obtained as per Section 4.6.1). Note that we obtain predictions for the perturbed level contours very cheaply by computing level contours for $u_0 + \varepsilon\dot{u}$, $\varepsilon \in [0, 0.5]$.

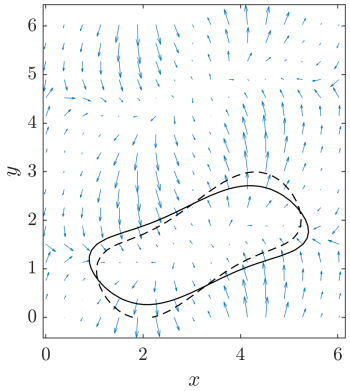


Figure 4.2: Standard map: velocity of level contour, level contours for $\varepsilon = 0$ (solid) and $\varepsilon = 0.5$ (dashed).

4.6.3 The Rotating Double Gyre

As a second experiment, we consider the rotating double gyre flow [70]. This is a non-periodic time-variant Hamiltonian system with Hamiltonian $H = -\psi$, where ψ is the stream function

$$\psi(x, y, t) = (1 - s(t))\psi_P(x, y) + s(t)\psi_F(x, y)$$
$$\psi_P(x, y) = \sin(2\pi x)\sin(\pi y)$$
$$\psi_F(x, y) = \sin(\pi x)\sin(2\pi y)$$

and $s(t)$ is the transition function

$$s(t) = \begin{cases} 0 & \text{for } t < 0, \\ t^2(3-2t) & \text{for } t \in [0,1], \\ 1 & \text{for } t > 1. \end{cases}$$

On the square $\Omega = [0,1]^2$, the vector field initially (at $t = 0$) exhibits two gyres, with centers at $(\frac{1}{2}, \frac{1}{2})$ and $(\frac{3}{2}, \frac{1}{2})$, which rotate by $\pi/2$ during the flow time $T = 1$. We view the flow time T as the parameter.

In Figure 4.3 (left) we show the second eigenvector u_0 of the dynamic Laplacian for $T = 0.6$ (corresponding to $\varepsilon = 0$) which identifies two coherent sets in the left and right half of the domain. Again, even for a rather large linear extrapolation, the vector $u_0 + 0.2\dot{u}$ is quite similar to the exact second eigenvector u_ε (right) at $T + \varepsilon = 0.6 + 0.2 = 0.8$. Figure 4.4 shows the (normalised) velocity field of the

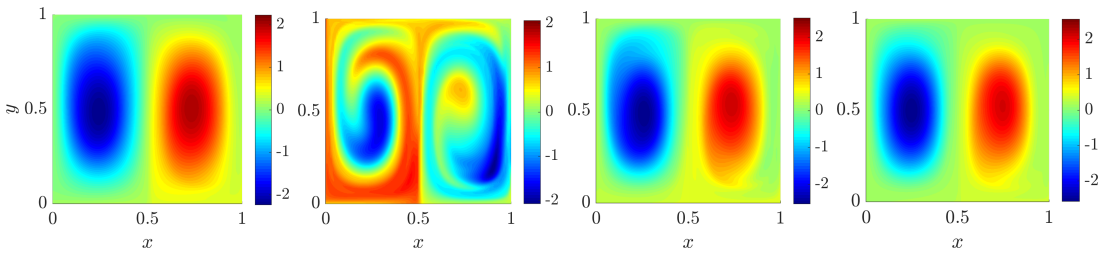


Figure 4.3: Rotating double gyre (left to right): u_0, $\dot{u}$, $u_0 + 0.2\dot{u}$ and u_ε.

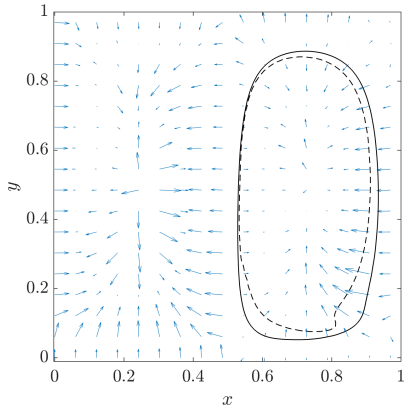


Figure 4.4: Rotating double gyre: velocity of level contour, level contours for $\varepsilon = 0$ (solid) and $\varepsilon = 0.2$ (dashed).

level set curves at $\varepsilon = 0$. Again, the change in the level contour from $\varepsilon = 0$ (solid line) to $\varepsilon = 0.2$ is consistent with the prediction by the velocity field.

Chapter 5

Conclusion

In this thesis we applied the concept of linear response to investigate two problems in dynamical systems. The first was concerned with optimising linear response, a question that has not been explicitly addressed in the literature. In Chapter 2 we considered the problems of finding stochastic perturbations that (i) maximise the ℓ^2 norm of the linear response, (ii) maximise the expectation of a specified observable, and (iii) maximise the rate of convergence to the equilibrium. The solution to (i) involved solving an eigenvalue problem. We obtained closed form solutions for (ii) and (iii). We then addressed (i) and (ii) for the non-homogeneous case. In the final section, we applied the theory to an Ulam discretisation of stochastically perturbed one-dimensional chaotic maps.

In Chapter 3 we extended the research above by working with Hilbert-Schmidt integral operators to address the optimisation problems (ii) and (iii). We first obtained linear response formulae for the invariant density and the second eigenvalue of integral preserving compact operators. By considering infinitesimal additive perturbations to the kernel of the Hilbert-Schmidt integral operator, we were able to express the linear response formulae in terms of the derivative of the kernel with respect to the perturbing parameter. From this, we used the idea in Chapter 2 of applying the Lagrange multiplier method to obtain explicit formulae for the optimal kernel perturbations. We also proved approximation results, which validate numerical computations of the optimal kernels. In the setting of deterministic systems with additive noise, we considered optimal map perturbations addressing (ii) and (iii). By reformulating the map perturbation as a kernel perturbation, we used

the theory developed in earlier sections to obtain explicit formulae for the optimal map perturbations and the corresponding approximation results. In the final section we numerically computed optimal kernel and map perturbations of stochastically perturbed deterministic systems. Future work could tackle problem (i) for Hilbert-Schmidt integral operators.

The second question we considered was about the response of finite-time coherent sets to a parameter change. Following the work in [28] and [33], we also wanted to obtain a computationally feasible method to analyse the response. When the dynamics depend smoothly on a perturbing parameter, we proved the differentiability, with respect to the perturbing parameter, of the eigenfunctions and eigenvalues of the dynamic Laplacian. We then obtained linear response formulae for the eigendata with respect to the perturbing parameter. Since the coherent sets can be obtained from the eigenfunctions of the dynamic Laplacian, the linear response formulae can be used to analyse perturbations of coherent sets. We demonstrated the use of the numerical schemes we developed on two dynamical systems. These numerical results showed that even for large parameter perturbations the level sets of the perturbed eigenfunctions were very close to the level sets obtained from the linear response approximation. We are currently implementing the numerical methods on real ocean data.

Appendix A

Chapter 2 Appendix

A.1 Algorithms and Code for Computing m^*

A.1.1 Optimisation Problem (2.2.2)–(2.2.4)

Algorithm 1

1. Compute $\mathbf{f}$ as the invariant probability vector of the stochastic matrix M.
2. Construct the matrix B from Section 2.2.3. We use the specific basis defined in (2.2.19) and (2.2.20).
3. Compute $QB = (\mathrm{Id}_n - M + \mathbf{f}\mathbf{1}^\top)^{-1}B$.
4. Compute the singular vector $\mathbf{y}$ corresponding to the largest singular value of QB (this is the eigenvector corresponding to the (assumed simple) largest eigenvalue of $B^\top Q^\top QB$ discussed in Section 2.2.3). Normalise $\mathbf{y}$ so that $\|\mathbf{y}\|_2^2 = \frac{1}{\|\mathbf{f}\|_2}$ (see (2.2.24)).
5. Form the matrix $m^* = B\mathbf{y}\mathbf{f}^\top$ (see (2.2.23)).

Matlab Code

```
function [m,f] = lin_resp(M)
n=length(M);
%Step 1
[V,D] = eigs(M,1);
f = V;
f = f/sum(f);
%Step 2
B = triu(ones(n))-diag([1:n-1],-1);%Step 5
B(:,n) = [];
B = sparse(normc(B));
%Step 3
QB = inv(eye(n)-M+f*ones(1,n))*B;
%Step 4
[U2,D2,V2] = svds(QB,1);
y = 1/(norm(f)*norm(V2))*V2;
```

```
m = B*y*f';                                    end
```

A.1.2 Optimisation Problem (2.2.26)–(2.2.29)

Algorithm 2

1. Compute $\mathbf{f}$ as the invariant probability vector of the stochastic matrix M.
2. Construct the matrix B from Section 2.2.3. We use the specific basis defined in (2.2.19) and (2.2.20).
3. Define the matrix $\widetilde{U} \in \mathbb{R}^{n\times\ell}$, where $\ell = n^2 - (n + n_1)$ (with n_1 equal the number of zeroes in M) is the nullity of the matrix A in Lemma 2.2.4. For $Q = (\mathrm{Id}_n - M + \mathbf{f}\mathbf{1}^\top)^{-1}$ and using (2.2.37) we compute $\widetilde{U} = Q(f_1B_1|\dots|f_nB_n)$, where B_i is given in Proposition 2.2.6. (Note that the j1 and j2 in the code for this step provide the column index range used to determine where f_iB_i belongs in $(f_1B_1|\dots|f_nB_n)$)
4. Compute the singular vector $\boldsymbol{\alpha}^*$ corresponding to the largest singular value of $\widetilde{U}$ (the eigenvector corresponding to the (assumed simple) largest eigenvalue of $\widetilde{U}^\top\widetilde{U}$).
5. Calculate $m^* = [\widehat{m}_1^*|\dots|\widehat{m}_1^*]$ where

$$\begin{pmatrix} \widehat{m}_1^* \\ \vdots \\ \widehat{m}_n^* \end{pmatrix} = \widehat{m}^* = E\boldsymbol{\alpha}^* = \begin{pmatrix} B_1\boldsymbol{\alpha}_1^* \\ \vdots \\ B_n\boldsymbol{\alpha}_n^* \end{pmatrix},$$

$\boldsymbol{\alpha}^* = \begin{pmatrix} \boldsymbol{\alpha}_1^* \\ \vdots \\ \boldsymbol{\alpha}_n^* \end{pmatrix}$ and B_i is given in Proposition 2.2.6. In the second and third equality above, we used (2.2.18) and Proposition 2.2.5 respectively. (Note that in the code for this step, j1 and j2 track the length of the vectors $\boldsymbol{\alpha}_i^*$ for $i = 1, \dots, n$)

Matlab Code

```
function [m,f] = lin_resp(M)
n=length(M);
%Step 1
[V,D] = eigs(M,1);
f = V;
f = f/sum(f);
%Step 2
B = triu(ones(n))-diag([1:n-1],-1);
B(:,n) = [];
B = sparse(normc(B));
%Step 3
n1 = length(find(M==0));
l =n^2-(n+n1);
U = zeros(n,l);
j1 = 1; j2 = 0;
for i=1:n
   R = find(M(:,i)==0);
   r = length(R);
       if r~= n-1
       B_i=zeros(n,n-r-1);
       R2=setdiff([1:n],R);
       r2=length(R2);
       B_i(R2,:)=B(1:r2,1:(r2-1));
       j2=j2+n-r-1;
       U(:,j1:j2)=f(i)*B_i;
       j1=j2+1;
   end
end
M_inf = f*ones(1,n);
Q = inv(eye(n)-M+M_inf); U = Q*U;
%Step 4
[U2,D2,V2] = svds(U,1);
%Step 5
m = sparse(n,n); j1=1; j2=0;
for i=1:n
    R = find(M(:,i)==0);
    r=length(R);
    j2=n-r-1+j2;
    if r~= n-1
       B_i = zeros(n,n-r-1);
       R2=setdiff([1:n],R);
       r2=length(R2);
       B_i(R2,:)=B(1:r2,1:(r2-1));
       m(:,i) = B_i*V2(j1:j2);
    else
       m(:,i) = sparse(n,1);
    end
    j1=j2+1;
end
end
```

A.1.3 Optimisation Problem (2.3.1)–(2.3.4)

Algorithm 3

1. Compute the invariant probability vector $\mathbf{f}$ of the stochastic matrix M.

2. Solve $\left(\mathrm{Id}_n - M + \mathbf{f}\mathbf{1}^\top\right)^\top \mathbf{w} = \mathbf{c}$ for $\mathbf{w}$.

3. Calculate m^*_{ij} according to (2.3.8), where $\nu = \|m^*\|_F$.

Matlab Code

```
function m = lin_resp_fun(M,c)
n=length(M);

%Step 1
[V,D] = eigs(M,1);
f = V;
f = f/sum(f);

%Step 2
Z = eye(n)-M+f*ones(1,n);
w = Z'\c;

%Step 3
m = zeros(n);
for j=1:n
   N_j = find(M(:,j)>10^-7);
   if(length(N_j) > 1)
      m(N_j,j)=f(j)*(w(N_j)-mean(w(N_j)));
   end
end
m = m./(norm(m,'fro'));
end
```

Remark A.1.1. *When M is large, but sparse, to avoid creating the full matrix $\mathbf{f}\mathbf{1}^\top$ in Step 2 above, one can replace Step 2 with: Solve the following (sparse) linear system for* $\mathbf{w}$

$$\begin{pmatrix} Id_n - M^\top \\ \mathbf{f}^\top \end{pmatrix} \mathbf{w} = \begin{pmatrix} \mathbf{c} - (\mathbf{f}^\top \mathbf{c})\mathbf{1} \\ \mathbf{f}^\top \mathbf{c} \end{pmatrix}. \tag{A.1.1}$$

A.1.4 Optimisation Problem (2.4.3)–(2.4.6)

Algorithm 4

1. Compute $\mathbf{r}_2$ and $\mathbf{l}_2$, the right and left eigenvectors corresponding to the second largest eigenvalue of M, normalised as $\mathbf{r}_2^*\mathbf{r}_2 = 1$ and $\mathbf{l}_2^*\mathbf{r}_2 = 1$.

2. Construct the matrix S from (2.4.8).

3. Calculate m^*_{ij} according to (2.4.9), where $\nu = -\|m^*\|_F$.

Matlab Code

```
function m = lin_resp_eval2(M)

%Step 1
[V,D] = eigs(M,2);
if abs(D(2,2))>abs(D(1,1))
    V(:,[1,2]) = V(:,[2,1]);
    D(:,[1,2]) = D(:,[2,1]);
end
r = V(:,2);
[V1,D1] = eigs(M',2);
if abs(D1(2,2))>abs(D1(1,1))
    V1(:,[1,2]) = V1(:,[2,1]);
    D1(:,[1,2]) = D1(:,[2,1]);
end
l = V1(:,2);
l = (1/(conj(l)'*r))*V1(:,2);

%Step 2
d = D(2,2);
S=real(d)*(real(l)*real(r)')...
    +real(d)*(imag(l)*imag(r)')...
    +imag(d)*(real(l)*imag(r)')...
    -imag(d)*(imag(l)*real(r)');
%Step 3
n=length(M);
m = zeros(n);
for i=1:n
    K = find(M(:,i)>10^-7);
    if(length(K) > 1)
       m(K,i) = (S(K,i)- mean(S(K,i)));
    end
end
m = -m./(norm(m,'fro'));
end
```

A.2 Proof of the LICQ Condition from Section 2.3

Proof. Let $J = \{j : \exists i \text{ with } (i,j) \notin N\}$. For $j \in J$, let $f_j(m) = \sum_{i=1}^{n} m_{ij}$. For $(i,j) \in N$, let $g_{ij}(m)$ denote the left hand side of the equality in (2.3.4). Finally, let $f(m)$ denote the left hand side of the equality in (2.3.3). For $j \in J$ we have $\frac{\partial f_j}{\partial m_{kl}}(m) = \delta_{jl}$. For $(i,j) \in N$ we have $\frac{\partial g_{ij}}{\partial m_{kl}}(m) = \delta_{ik}\delta_{jl}$, and lastly $\frac{\partial f}{\partial m_{kl}}(m) = 2m_{kl}$. The condition LICQ (Definition 12.4 [71]) is satisfied if

$$\sum_{j\in J} a_j \frac{\partial f_j}{\partial m_{kl}}(m) + \sum_{(i,j)\in N} a_{ij} \frac{\partial g_{ij}}{\partial m_{kl}}(m) + a\frac{\partial f}{\partial m_{kl}}(m) = 0, \text{ for } 1 \le k,l \le n, \quad \text{(A.2.1)}$$

implies $a_j = 0$ for $j \in J$, $a_{ij} = 0$ for $(i,j) \in N$, and $a = 0$.

1. Let $l \in J$. Let $k \in \{1, \ldots, n\}$ satisfy $(k,l) \notin N$. For such (k,l), equation (A.2.1) becomes $a_l + 2am_{kl} = 0$. Since m satisfies (2.3.2), one has that $\sum_{k:(k,l)\notin N}(a_l + 2am_{kl}) = \sum_{k:(k,l)\notin N} a_l + \sum_{k=1}^{n} 2am_{kl} = \sum_{k:(k,l)\notin N} a_l = 0$, because $m_{kl} = 0$ for $(k,l) \in N$. Thus $a_l = 0$ for all $l \in J$.
2. By (2.3.3), there exists $k, l \in \{1, \ldots, n\}$ such that $m_{kl} \neq 0$. Thus $(k,l) \notin N$ and so $l \in J$. For such (k,l), using part 1. we know $2am_{kl} = 0$ and thus $a = 0$.
3. Using part 2. for $(k,l) \in N$, (A.2.1) becomes either $a_{kl} = 0$ if $l \notin J$, or $a_l + a_{kl} = 0$ if $l \in J$. For the latter case, using part 1. we have $a_l = 0$ and so $a_{kl} = 0$. Thus $a_{kl} = 0$ for all $(k,l) \in N$.

□

Appendix B

Chapter 3 Appendix

B.1 Upper Bound for the Reflecting Boundary Operator

Lemma B.1.1. *Let $\mathscr{P}_\pi$ be as in (3.4.3) and $f \in L^2([-1,2])$. Then, $\|\mathscr{P}_\pi f\|_{L^2([0,1])} \leq \sqrt{7}\|f\|_{L^2([-1,2])}$.*

Proof. For $f \in L^2([-1,2])$, we have

$$
\begin{aligned}
&\left| \int_0^1 \mathscr{P}_\pi f(x)^2 dx \right| \\
&= \left| \int_0^1 (f(x) + f(-x) + f(2-x))^2 dx \right| \\
&= \Bigg| \int_0^1 f(x)^2 + f(-x)^2 + f(2-x)^2 + \\
&\quad 2\left[f(x)f(-x) + f(x)f(2-x) + f(-x)f(2-x)\right] dx \Bigg| \\
&= \Bigg| \int_0^1 f(x)^2 dx + \int_{-1}^0 f(x)^2 dx + \int_1^2 f(x)^2 dx \\
&\qquad + 2\left[\int_0^1 f(x)f(-x)dx + \int_0^1 f(x)f(2-x)dx + \int_0^1 f(-x)f(2-x)dx\right] \Bigg| \\
&\leq \|f\|^2_{L^2([-1,2])} \\
&\qquad + 2\left[\sqrt{\int_0^1 |f(x)|^2 dx}\sqrt{\int_0^1 |f(-x)|^2 dx} + \sqrt{\int_0^1 |f(x)|^2 dx}\sqrt{\int_0^1 |f(2-x)|^2 dx}\right. \\
&\qquad \left. + \sqrt{\int_0^1 |f(-x)|^2 dx}\sqrt{\int_0^1 |f(2-x)|^2 dx}\right] \\
&\leq \|f\|^2_{L^2([-1,2])} \\
&\quad + 2[\|f\|_{L^2([-1,2])}\|f\|_{L^2([-1,2])} + \|f\|_{L^2([-1,2])}\|f\|_{L^2([-1,2])} + \|f\|_{L^2([-1,2])}\|f\|_{L^2([-1,2])}] \\
&= 7\|f\|^2_{L^2([-1,2])};
\end{aligned}
$$

thus, $\|\mathscr{P}_\pi f\|_{L^2([0,1])} \leq \sqrt{7}\|f\|_{L^2([-1,2])}$. $\square$

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