METASTABLE SETS IN OPEN DYNAMICAL SYSTEMS
AND SUBSTOCHASTIC MARKOV CHAINS

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Doctor of Philosophy

By

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Abstract 350 words maximum: (PLEASE TYPE)

In this thesis we look at dynamical systems in which typical trajectories (1) have some probability of exiting the state space and (2) before exiting, tend to remain in one subset of the state space for a long time. The first property defines an open dynamical system and the second property is called metastability. Sets in which trajectories remain for a long time are called metastable or almost-invariant sets. The major contribution of this thesis is the development of techniques to locate and characterise metastable sets in open dynamical systems.

In closed dynamical systems, there are well-established connections between the spectrum of the Perron-Frobenius transfer operator and the metastability properties of the system. One can use the eigenfunctions of the transfer operator to locate metastable sets, and one can derive bounds on the maximal invariance ratio in terms of the second largest eigenvalue of a discretised version of the Perron-Frobenius operator. In Chapters 3 and 4 we extend these techniques to open dynamical systems.

Chapter 3 introduces a new closing operation for open systems that has a minimal effect on the metastability properties, and allows us to apply existing results for closed systems to locate metastable sets, and to derive bounds on the maximal invariance ratio in terms of the second largest eigenvalue of the new operator. In Chapter 4 we derive bounds on the metastability and the conductance of subslochastic Markov chains, which can be related to discretised transfer operators for open dynamical systems. Both conductance and metastability quantify how well subsets of states interact and mix. In Chapter 5 we apply some of the techniques to a global ocean model, and characterise the connectivity of the surface ocean using both absorption probabilities and eigenvectors.

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Abstract

In this thesis we look at dynamical systems in which typical trajectories (1) have a non-zero probability of exiting the state space and (2) before exiting, tend to remain in one proper subset of the state space for a long time. The first property defines an open dynamical system and the second property is called metastability. Sets in which trajectories remain for a long time are called metastable or almost-invariant sets. The major contribution of this thesis is the development of techniques to locate and characterise metastable sets in open dynamical systems.

In closed dynamical systems, there are well-established connections between the spectrum of the Perron-Frobenius operator and the metastability properties of the system. After introducing the research aims in Chapter 1, we review the existing literature and establish notation in Chapter 2. One can use the eigenfunctions of the transfer operator to locate metastable sets, and one can derive bounds on the maximal invariance ratio of a set in terms of the second largest eigenvalue of a discretised version of the Perron-Frobenius operator. In Chapters 3 and 4 we extend these techniques to open dynamical systems. Chapter 3 introduces a new closing operation for open systems that has a minimal effect on the metastability properties, and allows us to apply existing techniques for
closed systems to locate metastable sets, and to derive bounds on the maximal invariance ratio in terms of the second largest eigenvalue of the new operator. In Chapter 4 we derive bounds on the metastability and the conductance of substochastic Markov chains, which can be related to discretised transfer operators for open dynamical systems. Both conductance and metastability quantify how well subsets of states interact and mix. In Chapter 5 we apply some of the techniques developed in previous chapters to a global ocean model, and characterise the connectivity of the surface of the ocean using both absorption probabilities and eigenvector methods.
Undoubtedly the most important person who helped bring this thesis into existence is my supervisor, Gary Froyland. I really can’t overstate how grateful I am for the time, energy and dedication that he spent helping me over the past three and a half years. His care for detail, patience and boundless enthusiasm taught me to be careful, patient and enthusiastic myself, and even though I found things tough at the beginning, with Gary’s encouragement I ended up enjoying my research very much.

I also wish to thank Phil Pollett and Erik van Sebille, with whom I worked on projects that resulted in Chapters 3 and 5 respectively. It was wonderful to be able to collaborate with them both.

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Finally, lots of love and thanks to my family and to Nick for being the best.
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Frequently Used Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$\bar{X}$</td>
<td>State space</td>
</tr>
<tr>
<td>$X$</td>
<td>Transient part of the state space</td>
</tr>
<tr>
<td>$H$</td>
<td>Absorbing part of the state space; hole or sink</td>
</tr>
<tr>
<td>$\mathbb{1}_A(x)$</td>
<td>Characteristic function defined as $\mathbb{1}_A(x) = 1$ if $x \in A$, and 0 otherwise.</td>
</tr>
<tr>
<td>$\mathcal{B}(\cdot)$</td>
<td>$\sigma$-algebra</td>
</tr>
<tr>
<td>$m, \bar{m}, m_X$</td>
<td>Reference measure, sometimes specified to $(\bar{X}, \mathcal{B}(\bar{X}))$ or $(X, \mathcal{B}(X))$</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Invariant measure</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Conditionally invariant measure</td>
</tr>
<tr>
<td>$\bar{T}, T$</td>
<td>Closed, open map</td>
</tr>
<tr>
<td>$\bar{P}, P$</td>
<td>Frobenius-Perron operator, conditional Frobenius-Perron operator</td>
</tr>
<tr>
<td>$\bar{P}, P$</td>
<td>Stochastic, substochastic transition matrix</td>
</tr>
<tr>
<td>$\lambda_{L,i}$</td>
<td>The $ith$ largest eigenvalue for a given matrix or operator $L$</td>
</tr>
<tr>
<td>$\bar{p}, p, v$</td>
<td>Leading left eigenvector of $\bar{P}, P$, leading right eigenvector of $P$</td>
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</table>
Chapter 1

Introduction

In this thesis we are concerned with the related properties of ergodicity in dynamical systems and irreducibility in Markov chains. Our focus is on dynamical systems that are close to non-ergodic and transition matrices that are close to reducible; in both cases, the process is said to exhibit metastable behaviour. Metastability implies that a process operates on different timescales. Typically there are fast processes that locally mix the state space and there are slow processes that control switching between different (larger) parts of the state space.

For dynamical systems, metastability implies that typical trajectories remain in one subset of the state space for a long time, exhibiting quasi-stable behaviour, before eventually switching to a different subset. Quasi-stable behaviour also occurs in open dynamical systems. The distinguishing feature of open systems is the presence of a hole, with the stipulation that trajectories cannot re-enter the remainder of the state space once they have fallen through the hole, whereas in metastable systems, the state space consists of different subsets that trajectories can exit and re-enter with some small probability.

In Chapter 2 we review the existing literature on open and closed dynamical systems and metastability, and establish notation used throughout the thesis. In Chapter 3 we
study the metastability properties of dynamical systems in the presence of holes and specifically to develop techniques to identify and characterise metastable sets in open systems. A frequently-used technique known as Ulam’s method [127] allows one to study dynamical systems using Markov chains, and the presence of a hole in a dynamical system translates to the presence of an absorbing state in the Markov chain. A substochastic transition probability matrix may be defined over the transient states, and in Chapter 4 we study the property of metastability and the related property of conductance for substochastic Markov chains. We give a quantification of metastability in terms of a maximal conditional probability ratio, and we derive new bounds on this ratio in terms of the spectrum of the substochastic transition matrix and a second related matrix.

Finally, in Chapter 5 we study a particular example of an open, metastable dynamical system in detail. The dynamics of the ocean surface circulation is known to contain attracting regions such as the great oceanic gyres and the associated garbage patches [133, 78, 92, 91, 88, 130]. Less well-known are the extents of the basins of attractions of these regions and how the strongly attracting they are. Understanding the basins of attraction sheds light onto the question of how well connected different regions of the ocean are. Using short flow time trajectory data from a global ocean model, we create a Markov chain model of the surface ocean dynamics. Surface upwelling and downwelling is simply computed and compares well with the observed pattern of upwelling and downwelling in the real ocean. We analyse the Markov chain to determine multiple attracting regions and their absorption probabilities. The analysis is complicated by the fact that the surface ocean is not a conservative dynamical system. Analysing the Markov chain also enables
us to separate the ocean into regions with minimal surface mixing; each of these regions contains a major oceanic gyre.
Chapter 2

Preliminaries and Literature Review

In this chapter we present a review of dynamical systems and the probabilistic methods used to study them. The focus of this thesis will be on open dynamical systems, and these are introduced in Section 2.1 along with their better-understood closed counterparts. Section 2.2 presents relevant background on the operators used to analyse dynamical systems, and introduces the discretised versions that enable numerical experiments. The discretised operators can be related to transition probability matrices of Markov chains. Markov chains underscore much of the methodology that we shall use throughout the thesis, and so Section 2.3 presents a thorough review of relevant Markov chain theory.

This chapter should serve as a general guide to the notation, language and relevant background material used throughout the remainder of the thesis. We also give informal motivation for the problems that are addressed in the following chapters.

2.1 Closed and Open Dynamical Systems

The classical setting for dynamical systems is one in which a transformation $\bar{T} : X \rightarrow X$ is iterated to generate forward trajectories $(x, \bar{T}(x), \bar{T}^2(x), \ldots)$ of infinite length. Dynamical systems provide a means to understand a wide range of physical phenomena. An
overview of some of the fundamental concepts is provided in Section 2.1.1. In this thesis we will be more concerned with transformations of densities and sets than transformations of individual points. We therefore devote Section 2.1.2 to an overview of ergodic theory, which allows us to consider transformations of densities. We will be particularly interested in so-called metastable sets $B$ for which $\bar{T}(B) \approx B$, and these are introduced in Section 2.1.3.

2.1.1 Transformations on measure spaces

We begin with a transformation $\bar{T} : \bar{X} \circlearrowleft$. In order to discuss the probability or mass transported by $\bar{T}$ we endow $\bar{X}$ with a $\sigma$-algebra $\mathcal{B}(\bar{X})$ to create the measurable space $(\bar{X}, \mathcal{B}(\bar{X}))$. Let $\gamma$ be a natural finite reference measure on $(\bar{X}, \mathcal{B}(\bar{X}))$. Often in this thesis $\bar{X}$ will be a Euclidean space, in which case $\gamma$ is naturally given by Lebesgue measure over $\bar{X}$, and we denote it by $\bar{m}$.

**Definition 2.1.** A transformation $\bar{T} : \bar{X} \circlearrowleft$ is called measurable if $\bar{T}^{-1}(B) \in \mathcal{B}(\bar{X})$ for all $B \in \mathcal{B}(\bar{X})$.

**Definition 2.2.** We refer to $(\bar{X}, \mathcal{B}(\bar{X}), \bar{T})$, where $\bar{T} : \bar{X} \circlearrowleft$ is measurable, as a closed dynamical system. The bar notation $(\bar{X}, \bar{T},$ etc) will usually be used to indicate a closed system, to differentiate it from an open system.

The texts of Robinson [111], Alligood, Sauer and Yorke [77] and Brin and Stuck [12] provide standard introductions to closed dynamical systems. Lasota and Mackey [80] and Ding and Zhou [35] give treatments of closed dynamical systems with greater focus on probabilistic methodologies and ergodic theory.

Much of the focus of this thesis will be on open dynamical systems. A common way to obtain an open dynamical system is to begin with a closed dynamical system
Let any trajectory that enters $H$ be immediately terminated. Throughout the literature on open dynamical systems, $H$ is variously referred to as a hole, a sink, a coffin state or an absorbing state. We will generally refer to $H$ as a hole.

**Definition 2.3.** Suppose $(\bar{X}, \mathcal{B}(\bar{X}), \bar{T})$ is a closed dynamical system, and $\bar{X} = X \cup H$ with $\bar{T}^{-1}H \cap X \neq \emptyset$. Restricting the domain to $X$ and letting $\mathcal{B}(X) = \mathcal{B}(\bar{X}) \cap X$, $T := \bar{T}|_{X}$, we obtain an open dynamical system, denoted by $(X, \mathcal{B}(X), T)$.

As before, $T : X \circlearrowleft$ is called measurable if $T^{-1}(B) \in \mathcal{B}(X)$ for all $B \in \mathcal{B}(X)$, and we define $\gamma$ to be a natural finite reference measure over $X$. When $X$ is a Euclidean space, $\gamma$ is naturally Lebesgue measure $m$ over $X$.

Definition 2.3 describes a method for constructing an open dynamical system. This is not the only possible way to construct an open dynamical system – here we have followed the set-up given in the survey paper [29]. The crucial part of the definition is that the pre-images of $B \subset X$ under $\bar{T}$ are contained in $X$, but there is at least one set $B \subset X$ whose image under $\bar{T}$ is not contained in $X$; hence there is some possibility of exit through the hole. In this sense, open dynamical systems are examples of systems defined on domains that are not invariant under the dynamics (see the discussion in [29]).

The field of open dynamical systems is a relatively recent one for which there does not yet exist a standard textbook (although some material is contained in [37, 19]). Many of the methods used to analyse open dynamical systems are adapted from the closed setting.

### 2.1.2 Invariant measures

We will now present some results from ergodic theory for both closed and open dynamical systems. A general introduction to ergodic theory is given in Walters [131].
**Definition 2.4.** For a closed dynamical system \((\bar{X}, \mathcal{B}(\bar{X}), \bar{T})\) a \(\bar{T}\)-invariant measure \(\mu\) is a measure that satisfies

\[
\mu(B) = \mu(\bar{T}^{-1}B) \quad \text{for all } B \in \mathcal{B}(\bar{X}).
\]  

(2.1)

The transformation \(\bar{T}\) is called \(\mu\)-preserving, and the system \((\bar{X}, \mathcal{B}(\bar{X}), \bar{T}, \mu)\) is called measure preserving. If \(\mu\) is absolutely continuous with respect to \(\bar{\gamma}\) (ie. \(\mu(A) = 0\) whenever \(\bar{\gamma}(A) = 0\)), then \(\mu\) is called an absolutely continuous invariant measure, or ACIM.

Early results due to Renyi [110], Krzyzewski and Szlenk [76] and Lasota and Yorke [81] demonstrated the existence of an ACIM for piecewise monotonic transformations of the interval, and existence theorems have since been generalised to a wide class of transformations and spaces (see e.g. [35] for discussion). Existence of an ACIM generally requires some expansivity and regularity conditions on \(\bar{T}\) (eg. \(\bar{T}\) is piecewise \(C^2\) and \(|\bar{T}| > 1\)).

There is a version of invariance for measures defined on open dynamical systems, but the notion of invariance must be conditional on non-escape through the hole.

**Definition 2.5.** For an open dynamical system \((X, \mathcal{B}(X), T)\) a conditionally invariant measure \(\nu\) is a probability measure over \(X\) which satisfies

\[
\nu(T^{-1}B) = \nu(B) \cdot \nu(T^{-1}X) \quad \text{for all } B \in \mathcal{B}(X).
\]  

(2.2)

The transformation \(T\) is called conditionally \(\nu\)-preserving, and the system \((X, \mathcal{B}(X), T, \nu)\) is called conditionally measure preserving. If \(\nu\) is absolutely continuous with respect to \(\gamma\) (ie. \(\nu(B) = 0\) whenever \(\gamma(B) = 0\)), then \(\nu\) is called an absolutely continuous conditionally invariant measure, or ACCIM.
We denote \( \lambda_1 = \nu(T^{-1}X) < 1 \) so that (2.2) is succinctly written as \( \nu(T^{-1}(B)) = \lambda_1 \nu(B) \), and there is an obvious analogy with (2.1).

Early work on the existence for ACCIMs in one-dimensional dynamics was carried out by Pianigiani and Yorke in 1979 [106]. Sufficient conditions for existence of an ACCIM were given in Collet et al in the early 2000s [18, 101]. ACCIMs have been studied in the context of open maps of the interval endowed with ‘sufficiently small’ holes [20, 21, 128, 85, 28, 59]. A survey paper by Demers and Young [29] gives several examples to demonstrate that even in cases where an ACCIM exists, it may not be unique or physically relevant in the sense that densities converge to it under iteration of \( T \). Conditions necessary for a unique ACCIM are discussed in [85, 29].

A key concept for the study of mass transported by a dynamical systems is that of ergodicity.

**Definition 2.6.** A closed measure preserving dynamical system \( (\bar{X}, \mathfrak{B}(\bar{X}), \bar{T}, \mu) \) is said to be **ergodic** if the only sets \( B \in \mathfrak{B}(\bar{X}) \) for which \( B = \bar{T}^{-1}B \) satisfy \( \mu(B) = 0 \) or \( \mu(B) = 1 \).

The assumption of ergodicity underlies several key theorems in the study of dynamical systems. For example, we state without proof the following corollary of the Birkhoff Individual Ergodic Theorem [8], which equates time and space averages of integrable functions.

**Theorem 2.7.** Let \( (\bar{X}, \mathfrak{B}(\bar{X}), \bar{T}, \mu) \) be a measure preserving and ergodic closed dynamical system. Then, for any \( \mu \)-integrable function \( f \) defined over \( \bar{X} \),

\[
\lim_{n \to \infty} \frac{1}{n} \sum_{k=0}^{n-1} f(\bar{T}^k(x)) = \frac{1}{\mu(\bar{X})} \int_{\bar{X}} f(x) \, d\mu \quad \mu\text{-a.e.}
\]
Setting \( f = 1_B \) (where \( 1 \) denotes the characteristic function of \( B \)), Theorem 2.7 implies that the fraction of points \( \bar{T}^k(x) \) in \( B \) as \( k \to \infty \) is \( \mu(B)/\mu(\bar{X}) \). In light of Birkhoff’s Ergodic Theorem, a natural way to approximate the invariant measure \( \mu \) numerically seems to suggest itself: one could generate an orbit of length \( n \) (\( n \) very large) of a point \( x \in \bar{X} \) and approximate \( \mu(B) \) by \( \frac{\#\{ k < n : \bar{T}^k x \in B \}}{n} \). However, problems can arise because the \( k \to \infty \) limit of the fraction of points \( \bar{T}^k(x) \) in \( B \) only equals \( \mu(B)/\mu(\bar{X}) \) for \( \mu \)-almost-all \( x \), and one does not know a priori whether it will hold for the particular \( x \) selected. The theorem also requires that the trajectories are calculated exactly, which is not possible with finite-precision computer arithmetic, and furthermore, the rate of convergence is often very slow; see the discussion in [93].

It is common to assume ergodicity when studying dynamical systems. In principle this is not a restrictive assumption, because if a system is non-ergodic it may be decomposed into parts that are ergodic, and the ergodic components can be studied separately. In practice, however, it is not always clear how to determine whether a given system is ergodic, or how to find its ergodic components. The following simple example demonstrates a decomposition into ergodic components.

**Example 2.8.** Let \( \bar{T} : \bar{X} \to \bar{X} \) be the map whose graph is depicted in Figure 2.1. Each interval \( X_j, j = 1, 2 \) is equal to its own pre-image, so \( X_1 \) and \( X_2 \) represent two ergodic components of the map. The map \( \bar{T} \) preserves normalised Lebesgue measure over the entire interval, but it also preserves normalised Lebesgue measure over each \( X_j, j = 1, 2 \). The action of the restriction of \( \bar{T} \) to each \( X_j, j = 1, 2 \) is identical to the action of \( \bar{T} \) over the entire space \( \bar{X} \).
2.1.3 Metastability and closed dynamical systems

In this thesis we will be concerned with systems that are close to non-ergodic. Typical trajectories of these systems remain in one of its components for a long time before eventually switching to a different component.

A closed dynamical system that is close to non-ergodic can be obtained by fractionally perturbing a non-ergodic system, as demonstrated in the next example.

**Example 2.9.** Consider a small perturbation of the non-ergodic closed dynamical system depicted in Figure 2.1 to the map $\tilde{T}$ whose graph is depicted in Figure 2.2a. The perturbation consists of an upward shift of the middle branch by an amount $\alpha$. Specifically, we will consider the closed measure preserving dynamical system $([0, 1], \mathcal{B}([0, 1]), \tilde{T}, \tilde{m}),$
where $\bar{T}$ is defined by

$$
\bar{T}(x) = \begin{cases} 
2x, & \text{if } 0 < x < 1/4; \\
2x - \frac{1}{2} + \alpha, & \text{if } 1/4 < x < \frac{3/2 - \alpha}{4}; \\
2x - \frac{3}{2} + \alpha, & \text{if } \frac{3/2 - \alpha}{4} < x < 3/4; \\
2x - 1, & \text{if } x > 3/4.
\end{cases}
$$

The parameter $\alpha$ can be varied between 0 and $\frac{1}{2}$, and for every value of $\alpha$, Lebesgue measure $\bar{m}$ on the unit interval is a $\bar{T}$-invariant probability measure. When $\alpha = 0$, there are two invariant sets of positive $\bar{m}$-measure, $X_1 = [0, 1/2]$ and $X_2 = [1/2, 1]$. This is the situation described in Example 2.8 and shown in Figure 2.1. When $0 < \alpha \leq 1/2$, $([0, 1], \mathcal{B}(0, 1), \bar{T}, \bar{m})$ is exact and thus mixing, and there are no nontrivial invariant sets (see eg. [131], Remark 1, p40). To emphasise the relationship between this map and the usual doubling map, we call this the $\alpha$-shifted doubling map. For ‘small’ values of $\alpha$, one can coarse-grain the state space into the two shaded squares, which are ‘almost-invariant’ under the dynamics.

Roughly speaking, a closed dynamical system may be thought of as close to non-ergodic, or metastable if there is some $B \in \mathcal{B}(\bar{X})$ such that $B \approx \bar{T}^{-1}B$, with $0 < \mu(B) < 1$ (compare with Definition 2.6). We develop this idea in Definitions 2.10-2.11. The study of metastability has foundations in both dynamical systems, where it is also called almost-invariance [26, 27, 49], and in Markov chain theory [82].

**Definition 2.10.** Consider a closed measure preserving dynamical system $(\bar{X}, \mathcal{B}(\bar{X}), \bar{T}, \mu)$. The conditional probability of points in $B$ remaining in $B$ under $\bar{T}$ is given by the $\mu$-
invariance ratio of $B$, defined as

$$
\Psi_{\bar{T},\mu}(B) := \frac{\mu(B \cap \bar{T}^{-1}B)}{\mu(B)}.
$$

We call $\Psi_{\bar{T},\mu}(B)$ the $\mu$-invariance ratio of $B$.

**Definition 2.11.** We will refer to the maximal $\mu$-invariance ratio under $\bar{T}$ as the metastability of $(\bar{T}, \mu)$, defined as

$$
\Psi_{\bar{T},\mu} := \max_{B: \mu(B) \leq 1/2} \Psi_{\bar{T},\mu}(B).
$$

A justification for the restriction $\mu(B) \leq 1/2$ is given in Corollary 1 of [51].

Early work on invariance and metastability was carried out in [27]. The maximal $\mu$-invariance ratio $\Psi_{\bar{T},\mu}$ was studied in [48], building on the earlier work in [49] that looked at the maximal $\bar{m}$-invariance ratio $\Psi_{\bar{T},\bar{m}}$ (the latter being defined using Lebesgue measure $\bar{m}$ instead of the invariant measure $\mu$ in (2.3)-(2.4)). For metastable systems, we expect to find a partition of $\bar{X}$ into $B, B^c := \bar{X} \setminus B$ such that $\Psi_{\bar{T},\mu}(B) \approx 1$ and $\Psi_{\bar{T},\mu}(B^c) \approx 1$. 

Figure 2.2: The map given in Example 2.9
We call a set $B$ almost-invariant if $\Psi_{T,\mu}(B) \approx 1$, and we will sometimes use the term metastable (dynamical) system to refer to a dynamical system for which there is an $B$ such that $\Psi_{T,\mu}(B) \approx 1$.

**Remark 1.** It is possible to consider a more restrictive definition of metastability, where one additionally requires that $\mu(B)/\mu(B^c) \approx 1$. This additional criteria excludes maps such as a Poumeau-Manneville type map with an indifferent fixed point with tangency of type $x^{1+\alpha}$ near $x = 0$ and $B = [0, \epsilon]$. In this case, one has $\Psi_{T,\mu}(B) \approx 1$ and $\Psi_{T,\mu}(B^c) \approx 1$ but $\mu(B)/\mu(B^c) \approx 0$. Maps of this type were studied in [56].

**Example 2.12.** In Example 2.9 depicted in Figure 2.2, we set $\alpha = 1/16$. Then

$$\frac{\bar{m}((T)^{-1}X_1 \cap X_1)}{\bar{m}(X_1)} = \frac{\bar{m}((T)^{-1}X_2 \cap X_2)}{\bar{m}(X_2)} = 15/16.$$ 

By determining the sets $B \in \mathcal{B}(\tilde{X})$ that return large values of $\Psi_{T,\mu}(B)$ we learn about the finite-time transport properties of $T$. In smooth dynamics in dimensions $\geq 2$, the dynamical creation of almost-invariant sets may be due to co-dimension 1 stable and unstable manifolds, for example, as in lobe dynamics [113, 112, 132], and there is numerical evidence that there is a relationship between the geometry of invariant manifolds of low period orbits and dominant almost-invariant sets [51]. However, in general, determining the location of almost-invariant regions is a difficult problem. Even in the simple case of Example 2.12, there may well be a set $B \subset [0, 1]$ with $\bar{m}(B) \leq 1/2$ and $\Psi_{T,\mu}(B) > 15/16$. Often, almost-invariant regions have very irregular boundaries; see the discussion in [54].
2.1.4  Metastability and open dynamical systems

There is a clear similarity between open and metastable dynamical systems: both systems give rise to quasi-stable behaviour on a subset of the state space before trajectories eventually leave that subset. The similarity between the two characterisations has been exploited recently in [70, 58], both of which treated metastable systems as perturbations of non-ergodic systems, and in [54], which uses an approach originally created to identify almost-invariant sets to partition closed systems into two open systems with slow escape rates. Antecedents for current characterisations of metastability can be traced back to Lorenz [86] and Pianigiani and Yorke [106]. The distinguishing feature of open systems is that the trajectories cannot re-enter the subset $X$ once they have fallen through the hole, whereas in metastable systems, trajectories can exit and re-enter $X_1$ or $X_2$ with some small probability. For open systems one refers to the “escape rate” from $X$ to $H$, whereas in metastable systems one refers to the “exchange rate” between $X_1$ and $X_2$.

Example 2.13. Consider the map $\bar{T}$ defined in Example 2.9 and depicted in Figure 2.2. Suppose we let $X = [0, 0.45) \cup (0.55, 1]$, ie. we define a hole $H = [0.45, 0.55]$ and consider the open map $\bar{T}|_X : [0, 0.45) \cup (0.55, 1] \circlearrowleft$. A schematic representation of the dynamics is presented in Figure 2.3. As well as the exchange between between $X_1$ and $X_2$, there is escape to the hole $H$ from both sets.

A physical example of an open metastable system is a billiard table with a partition containing a small gap in the centre of the table. Balls may fall into the pockets (holes) and rarely transition from one half of the table to the other. In geophysical models of the ocean or atmosphere, typically one does not consider the entire global ocean or atmosphere (for computational reasons), but rather considers much smaller subdomains,
the boundaries of which leak water or air over time (the holes). Thus, one may consider the almost-invariant sets in these systems, such as oceanic gyres, as part of an open system.

**Definition 2.14.** For an open measure preserving dynamical system \((X, \mathcal{B}(X), T, \nu)\), the conditional probability of points in \(B \in \mathcal{B}(X)\) remaining in \(B\) under \(T\) is given by the \(\nu\)-invariance ratio of \(B\), defined as

\[
\Psi_{T,\nu}(B) := \frac{\nu(B \cap T^{-1}B)}{\nu(B)}. \quad (2.5)
\]

We call \(\Psi_{T,\nu}(B)\) the \(\nu\)-invariance ratio of \(B\).

**Definition 2.15.** We will refer to the maximal \(\nu\)-invariance ratio under \(T\) as the metastability of \((T, \nu)\), defined as

\[
\Psi_{T,\nu} := \max_{B : \nu(B) \leq 1/2} \Psi_{T,\nu}(B). \quad (2.6)
\]

Definitions 2.14-2.15 are formulated so as to be analogous to Definitions 2.10-2.11 for closed dynamical systems.
Proposition 2.16. For an open, conditionally measure preserving system \((X, \mathcal{B}(X), T, \nu)\) with \(\nu(T^{-1}X) = \lambda_1\) and \(\Psi_{T,\nu}(B)\) defined by (2.5), we have

\[
\Psi_{T,\nu}(B) = \frac{\nu(B \cap T^{-1}B)}{\nu(B)} \leq \frac{\nu(T^{-1}B)}{\nu(B)} = \nu(T^{-1}X) = \lambda_1, \tag{2.7}
\]

Proof. The first inequality follows from set inclusion and the following equality follows by Equation (2.2).

When \(\Psi_{T,\nu}(B) = \lambda_1\) the only mass that leaves \(B\) in one iteration immediately falls in the hole; there is no transmission to \(X \setminus B\). We will call a set \(B\) almost-invariant if \(\Psi_{T,\nu} \approx \lambda_1\).

2.2 Perron-Frobenius Operators

A typical approach taken in the literature is to use the transfer or Perron-Frobenius operator to study a particular class of transformations known as non-singular transformations.

Definition 2.17. A transformation \(\bar{T}\) is called non-singular with respect to \(\bar{\gamma}\) if \(\bar{\gamma}(B) = 0 \Rightarrow \bar{\gamma}(\bar{T}^{-1}B) = 0\) for all \(B \in \mathcal{B}(\bar{X})\).

Definition 2.18. For a closed dynamical system \((\bar{X}, \mathcal{B}(\bar{X}), \bar{T})\), the Perron-Frobenius operator \(\bar{\mathcal{P}} : L^1(\bar{\gamma}) \ominus\) is defined as

\[
\int_B \bar{\mathcal{P}} g \, d\bar{\gamma} = \int_{\bar{T}^{-1}(B)} g \, d\bar{\gamma} \quad \text{for all } B \in \mathcal{B}(\bar{X}).
\]

Definition 2.19. If \(\bar{\mathcal{P}} f = f\) for some \(f \in L^1(\bar{\gamma})\) with \(\|f\|_1 = 1\) and \(f \geq 0\) then we call \(f\) a \(\bar{\mathcal{P}}\)-invariant density, or simply an invariant density.
There is a well-understood connection between $T$-invariant measures and $\overline{P}$-invariant densities. If $\mu$ is an ACIM for $\overline{T}$ (i.e. Equation (2.1) holds) and $\mu$ is also absolutely continuous with respect to $\overline{\gamma}$ then the Radon-Nikodym derivative $f = d\mu/d\overline{\gamma}$ satisfies $\overline{P}f = f$. Conversely, if $\overline{P}f = f$ then the measure $\mu$ given by $\mu(A) = \int_A f \, d\overline{\gamma}$ is $\overline{T}$-invariant, and if $f$ is the unique function in $L^1$ satisfying $\overline{P}f = f$, $\|f\|_1 = 1$ and $f \geq 0$ then the corresponding measure $\mu$ is ergodic; see e.g. [80].

**Definition 2.20.** For an open dynamical system $(X, \mathcal{B}(X), T)$ the *conditional Perron-Frobenius operator* $\mathcal{P} : L^1(\overline{\gamma}) \circ$ is defined as

$$
\int_B \mathcal{P}g \, d\overline{\gamma} = \int_{T^{-1}(B)} g \, d\overline{\gamma} \quad \text{for all } B \in \mathcal{B}(X).
$$

One may also write $\mathcal{P}(g) = \overline{\mathcal{P}}(1_X \cdot g)$.

**Definition 2.21.** If $\mathcal{P}f = \lambda f$ for some $f \in L^1(\overline{\gamma})$ with $\|f\|_1 = 1$, $f \geq 0$ and $\lambda > 0$ then we call $f$ a *conditionally invariant density*.

As with closed dynamical systems, the eigenfunctions of the conditional Frobenius-Perron operator correspond to densities of ACCIMs. Specifically, if $f \in L^1(\overline{\gamma})$ satisfies $\mathcal{P}f = \lambda f$ for some $\lambda \in (0, 1]$ with $\|f\|_1 = 1$ and $f \geq 0$, then $\nu = f \cdot \overline{\gamma}$ is a conditionally invariant measure, i.e. Equation (2.2) holds with $\lambda_1 = \lambda$. A proof of this can be found in eg. [106]. Demers and Young [29] demonstrate that there may be many ACCIMs with overlapping support for a fairly general class of transformations.

#### 2.2.1 Perron-Frobenius operators and invariance ratios

Using $\overline{\mathcal{P}}$ and $\mathcal{P}$ allows us to rewrite the definitions of the invariance ratios that were given in Definitions 2.10-2.15.
Proposition 2.22. Let \((\bar{X}, \mathcal{B}(\bar{X}), \bar{T}, \mu)\) be a closed measure preserving dynamical system with Perron-Frobenius operator \(\bar{P}\), and let \(f = \frac{d\mu}{d\gamma}\) be the invariant density corresponding to the ACIM \(\mu\). Assume \(f > 0\). Let \(\langle g_1, g_2 \rangle_\mu\) denote the scalar product \(\int g_1 \cdot g_2 \, d\mu\) for \(g_1 \in L^1(\mu), g_2 \in L^\infty(\mu)\). One has

\[
\mu(B \cap \bar{T}^{-1}B) = \langle \bar{P}_\mu 1_B, 1_B \rangle_\mu,
\]

where \(\bar{P}_\mu(g) := \bar{P}(f \cdot g)/f\).

Proof. One has

\[
\mu(B \cap \bar{T}^{-1}B) = \int_{\bar{T}^{-1}(B)} 1_B \, d\mu = \int_{\bar{X}} (f 1_B) 1_B \circ T \, d\mu = \int_B \bar{P}_\mu 1_B \, d\mu = \int_{\bar{X}} \bar{P}_\mu 1_B \cdot 1_B \, d\mu = \langle \bar{P}_\mu 1_B, 1_B \rangle_\mu,
\]

noting that \(1_B \in L^\infty(\mu)\) and \(\bar{P}_\mu 1_B \in L^1(\mu)\).

Proposition 2.23. Let \((X, \mathcal{B}(X), T, \nu)\) be an open measure preserving dynamical system with conditional Perron-Frobenius operator \(P\), with \(f = \frac{d\nu}{d\gamma}\) the conditionally invariant density corresponding to the ACCIM \(\nu\), and suppose that \(f > 0\). Let \(\langle g_1, g_2 \rangle_\nu\) denote the scalar product. If \(f > 0\), one has

\[
\nu(B \cap T^{-1}B) = \langle P_\nu 1_B, 1_B \rangle_\nu,
\]

noting that \(1_B \in L^\infty(\nu)\) and \(P_\nu 1_B \in L^1(\nu)\).
where $\mathcal{P}_\nu(g) := \mathcal{P}(f \cdot g)/f$.

**Proof.** Identical to the proof of Proposition 2.22.

Using Propositions 2.22-2.23 we can write

$$
\Psi_{\bar{T},\bar{\mu}}(B) \triangleq \Psi_{\bar{\mathcal{P}},\bar{\mu}}(B) = \frac{\langle 1_B, \bar{\mathcal{P}} \bar{1}_B \rangle_{\bar{\mu}}}{\mu(B)} \tag{2.8}
$$

for the closed system, and

$$
\Psi_{T,\nu}(B) \triangleq \Psi_{\mathcal{P},\nu}(B) = \frac{\langle 1_B, \mathcal{P} \nu 1_B \rangle_{\nu}}{\nu(B)} \tag{2.9}
$$

for the open system.

**Remark 2.** The quotients on the RHS of both (2.8) and (2.9) are essentially Rayleigh quotients (see [63], p176). We will make use of this equivalence later.

**Notation for invariance ratios**

We will tend to use the operator-based definitions of the invariance ratios given in Equations (2.8, 2.9) more than the map-based definitions given in Equations (2.3, 2.5). We favour the $\Psi_{\mathcal{P},\mu}, \Psi_{\mathcal{P},\nu}$ notation because it provides a clearer connection with concepts in Markov chain theory (see Section 2.3), and it will allow us more flexibility later to define invariance ratios for arbitrary operators that may not directly correspond to maps.

### 2.3 Markov processes

As we saw in Section 3.1.2, the Perron-Frobenius operators encode a great deal of information about the dynamics of a given system. In Chapter 3 we will discuss how to
extract that information by considering “discretised” Perron-Frobenius operators acting on “discretised” densities. As we shall see, the action of the discretised Perron-Frobenius operators can be represented by Markov chain transition matrices (making a density-measure replacement). In anticipation of this result, we will dedicate this section to an overview of the relevant background and theory of Markov chains. The contents of this section also serve as background material for Chapter 4, in which we study the metastability and conductance of Markov chains. In Section 2.3.1 we introduce some useful definitions, leading to the very important Perron-Frobenius theorem. Section 2.3.2 defines stochastic and substochastic Markov processes and Section 2.3.3 introduces stationary and quasi-stationary distributions. Section 2.3.4 introduces the concept of metastability in the context of Markov chains, and the related concept of conductance.

2.3.1 The Perron-Frobenius theorem

The Perron-Frobenius theorem is a far-reaching result concerning the spectral properties of non-negative matrices. The definitions in this section and the theorem itself are standard fare in textbooks on Markov chains and linear algebra; see for example [6, 63, 89, 34].

Definition 2.24. For non-negative $A \in \mathbb{R}^{n \times n}$, state $j$ is said to be accessible from state $i$ if $A_{ij}^m > 0$ for some $m \geq 1$, and $i$ and $j$ are said to communicate if $i$ is accessible from $j$ and vice versa.

Definition 2.25. A state $i$ is called essential if $i$ is accessible from all states $j$ accessible from $i$. A state $i$ is called inessential if it is not essential [83].

Definition 2.26. A set of states that all communicate with one another is called a communicating class [6]. The states in a single communicating class are all either essential or inessential, and we classify communicating classes as essential or inessential accordingly.
Definition 2.27. A communicating class $S$ is called closed if, for non-negative $A \in \mathbb{R}^{n \times n}$, $A_{ij} = 0$ for all $i \in S, j \notin S$, i.e. states $j \notin S$ are not accessible from states $i \in S$.

Definition 2.28. A non-negative matrix $A \in \mathbb{R}^{n \times n}$ is called irreducible if all its states lie in a single communicating class [6].

Definition 2.29. A non-negative matrix $A \in \mathbb{R}^{n \times n}$ is called periodic if $A = A^k$ for some $k > 1$, called the period of $A$. A matrix which is not periodic is called aperiodic.

Theorem 2.30 (Perron-Frobenius Theorem [105, 45]). Suppose that $A \in \mathbb{R}^{n \times n}$ is non-negative, irreducible and aperiodic. Then there exists a unique largest real eigenvalue $\lambda_{A,1} > 0$ associated with one-dimensional left and right eigenspaces, i.e. there are unique vectors $x, y \geq 0$ such that

$$xA = \lambda_{A,1}x \quad \text{and} \quad Ay = \lambda_{A,1}y.$$ (2.10)

2.3.2 Stochastic and substochastic transition matrices

Consider a finite set of states $\tilde{X}_n := \{x_i\}_{i=1}^n$, and let $P$ be the transition matrix for a discrete-time Markov chain taking values in $\tilde{X}_n$.\(^1\)

Suppose that $\tilde{X}_n$ is partitioned as $X_n \cup H$ and

$$(P^m)_{ij} = 0 \quad \text{for all } i \in H, j \in X_n, \text{ and } m \geq 1 $$ (2.11)

so that states in $X_n$ are inaccessible from states in $H$, as per Definition 2.24. The subscript $n$ refers to the cardinality of the subset $X_n$; clearly, $n < \tilde{n}$. We think of $H$\(^1\)Formally, let $\{Z_t\}_{t \in \mathbb{N}}$ be a sequence of $\tilde{X}_n$-valued random variables defined on some probability space $(\Omega, \mathcal{F}, P)$, and define $P_{ij} = P(Z_t = j | Z_{t-1} = i)$.

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as a set of absorbing states or a “hole” from which trajectories never leave. We assume that all the states in $X_n$ communicate, in which case $P|_{X_n}$ is an irreducible matrix as per Definition 2.28. By Theorem 2.30, there are unique left and right eigenvectors for $P|_{X_n}$, and we denote these by $p, v$.

**Remark 3.** Irreducibility of $P|_{X_n}$ ensures uniqueness of $p$ and $v$. In reducible systems, the eigenspace corresponding to the leading eigenvalue may be multi-dimensional. We address this situation in Chapter 5, where we relax the condition of irreducibility.

In the sequel, we assume that $p$ and $v$ have $\ell^1$-norm 1. We denote the $p$-probability measure of $B \subset X_n$ by $p(B) := \sum_{i \in B} p_i$. We consider two cases:

**Stochastic case:** In addition to (2.11), one has $P_{ij} = 0$ for all $i \in X_n, j \in H$. The stochastic process on $X_n$ governed by $P|_{X_n}$ operates as a standard (closed) Markov chain, and a process that begins in $X_n$ never enters the hole $H$. One has $\sum_{j \in X} P_{ij} = 1$ for all $i \in X_n$, and $P|_{X_n}$ is stochastic. We will henceforth signify stochastic matrices over $X_n$ with a bar: $P|_{X_n} := \bar{P}$.

**Substochastic case:** In addition to (2.11), there is at least one pair $(i, j), i \in X_n, j \in H$ for which $P_{ij} > 0$. There is a positive probability of a process in $X_n$ entering the hole $H$. One has $\sum_{j \in X_n} P_{ij} < 1$ for at least one $i \in X_n$. We call the matrix $P|_{X_n}$ substochastic and from now on denote it by $P$.

In the substochastic setting, the states belonging to $H$ are referred to as **absorbing**, **coffin** or **cemetery** states, and states in $X_n$ are referred to as **transient** states.

2.3.3 Stationary and quasi-stationary distributions

In the stochastic case, $\lambda_{P,1} = 1$ and the unique right eigenvector $v$ associated with $\lambda_{P,1} = 1$ is $1$. We denote the unique left eigenvector associated with $\lambda_{P,1}$ by $\bar{p}$. The prob-
ability distribution \( \hat{\rho} \) satisfying the eigenvector condition \( \hat{\rho} \hat{P} = \hat{\rho} \) is called the \textit{stationary} distribution of the Markov chain generated by \( \hat{P} \) (see [118], Theorem 4.1). We defer to e.g. [11, 118] for discussions of stochastic Markov processes.

In the substochastic case, the condition that \( \sum_{j \in X_n} P_{ij} < 1 \) for at least one \( i \) implies \( \lambda_{P,1} < 1 \). We denote the unique left eigenvector associated with \( \lambda_{P,1} \) by \( \rho \). In this case, \( \rho \) is called the \textit{quasi-stationary distribution} of the Markov chain on \( X_n \).

The notion of modelling long-term behaviour for a substochastic Markov process was first explored by Bartlett [5] and Ewans [38, 39] in the context of population modelling. Subsequent work showed conditions under which the quasi-stationary distribution is equal to the limiting conditional distribution of the process, where the latter is defined as the \( t \to \infty \) limiting probability of the Markov process generated by \( P \) being in state \( i \) at time \( t \), conditioned on the fact that the process has remained in \( X_n \) until time \( t \) (see eg. [22]). The equivalence of the quasi-stationary distribution and the limiting conditional distribution has been developed in the discrete-time, finite-state setting [22, 73, 71, 72], and for countable-state processes [119, 126]. The continuous-time setting has been analysed in [43, 97, 104, 23]. Other settings that have been considered include semi-Markov processes [2, 15, 44], continuous-state processes [123], and settings where \( P \) may be reducible [108, 129]. Applications of substochastic Markov chains include biological, environmental, and financial models, where frequently a path terminates when it enters a death or valueless state.

\subsection*{2.3.4 Metastability and conductance}

We will develop the relevant objects for stochastic and substochastic Markov chains in parallel. Suppose that we have a random walk over a state space \( X_n \) governed by a
transition matrix $M$. We do not specify whether $M$ is stochastic or substochastic. We let $\ell$ be the stationary (resp. quasi-stationary) distribution of the random walk governed by the stochastic (resp. substochastic) $M$. We define a cut to be a division of $X_n$ into complementary sets $B$ and $B^c := X_n \setminus B$.

Given subsets $B, C \subset X$, the $\ell$-flux from $B$ to $C$ under $M$ is the probability, according to $\ell$, that the process is in $B$ at time $t$ and in $C$ at time $t + 1$:

$$Q_{M,\ell}(B, C) = \sum_{i \in B, j \in C} \ell_i M_{ij}.$$  \hspace{1cm} (2.12)

We also define the $\ell$-flux ratio from $B$ to $C$ under $M$, as

$$\frac{Q_{M,\ell}(B, C)}{\ell(B)}.$$  \hspace{1cm} (2.13)

If $C = B$ in (2.13) then (2.13) gives the conditional probability of the process remaining in $B$ for one time-step. We call this the $\ell$-invariance ratio of $B$ under $M$, and denote it by

$$\psi_{M,\ell}(B) := \frac{Q_{M,\ell}(B, B)}{\ell(B)}.$$  \hspace{1cm} (2.14)

Similarly, if $C = B^c$ in (2.13) then (2.13) gives the conditional probability of the process transitioning out of $B$ in one time-step. We call this the $\ell$-flux ratio of $B$ under $M$, and denote it by

$$\phi_{M,\ell}(B) := \frac{Q_{M,\ell}(B, B^c)}{\ell(B)}.$$  \hspace{1cm} (2.15)
The maximal $\ell$-invariance ratio under $M$ is called the *metastability* of $M$, defined by

$$
\psi_{M,\ell} := \max_{B \in X, \ell(B) \leq 1/2} \psi_{M,\ell}(B).
$$

(2.16)

There is a clear connection between the metastability defined in (2.16) for discrete-time Markov chains and the invariance ratios defined in (2.8)-(2.9) for Perron-Frobenious operators. The minimal $\ell$-flux ratio under $M$ is called the *conductance* of $M$:

$$
\phi_{M,\ell} := \min_{B \subset X, \ell(B) \leq 1/2} \phi_{M,\ell}(B).
$$

(2.17)

The conductance has many other names within the literature, such as the *Cheeger constant* [14], the *isoperimetric constant* [82] or the *bottleneck ratio* [83].

**Definition 2.31.** We say that $M$ is $\ell$-reversible if $\ell_i M_{ij} = \ell_j M_{ji}$.

When $M \equiv \bar{P}$ is stochastic, Definition 2.31 is called the detailed balance condition, and it implies that the underlying random walk is identical if the time-direction of the walk is reversed (see eg. [71]). This corresponds to the usual definition of reversibility for Markov chains, but we use the terminology $\ell$-reversible so that it is clear that we mean reversible with respect to the probability distribution $\ell$. When $M \equiv P$ is substochastic, satisfying the detailed balance condition does not imply that the random walk is identical when reversed. Indeed there are several possibilities for what a “reversed process” might mean (see eg. [23, 107]). Hence, our use of the terminology $\ell$-reversible only implies that $\ell_i M_{ij} = \ell_j M_{ji}$ is satisfied, and does not necessarily correspond to a statement about the distribution of the underlying random walk.
For $\bar{p}$-reversible stochastic matrices (corresponding to symmetry of the matrix in an inner product space weighted by $\bar{p}$), the conductance and metastability can be bound by expressions involving the second eigenvalue of $\bar{P}$ [121, 82]. For stochastic matrices that are not time-reversible, the similar bounds have been derived in terms of a matrix derived from $\bar{P}$ [48, 16]. These ideas have also been extended to lower eigenvalues [66]. Hence, examining the spectrum of $\bar{P}$ is a simple way to gather information about the metastability and conductance of a process. Moreover, the second and lower eigenvectors contain valuable information concerning the sets $B \subset X$ that minimise the conductance and maximise the metastability [30, 49, 66, 48, 51].
A closing scheme for finding almost-invariant sets in open dynamical systems

In this chapter we study the metastability properties of dynamical systems in the presence of holes. Specifically, our goal is to develop techniques to identify and characterise almost-invariant sets in open systems, and to derive rigorous bounds on the maximal almost-invariance ratio. Our methods extend the methodology of [48] by applying a “closing operation” to an open system, resulting in an “induced closed system” whose metastability properties are very similar to those of the original open system.

We state here our main result linking the metastability of a set $B \subset X$ under the induced closed system, denoted by $\Psi_{\tilde{P},\nu}(B)$ and defined in Definition 3.8, with the metastability of a set $B \subset X$ under the original open system, denoted by $\Psi_{P,\nu}(B)$ and defined in Definition 2.9.

**Theorem 3.1.** Consider an open, conditionally measure preserving system $(X, \mathcal{B}(X), \nu, T)$. Under mild conditions on $\nu$, the following relationship holds:

$$\Psi_{\tilde{P},\nu}(B) = \Psi_{P,\nu}(B) + \nu(B \cap H^1),$$
where \( H^1 = X \cap T^{-1}H \) is the set of points in \( X \) that will fall into \( H \) in one step.

Thus, for holes where the \( \nu \)-measure of \( H^1 \) is small, the difference between the invariance ratios (or metastability) of the original open and induced closed systems is also small.

An outline of the chapter is as follows. We begin in Section 3.1 by describing how to discretise the dynamics to get a Markov chain representation of the dynamics. We also summarise the relevant results of [48]. Section 3.2 contains our main results. We introduce the closing operator for converting an open system into a closed system. Formulae for the discretised Perron-Frobenius operators describing this induced closed system are developed and we prove relevant quantitative relationships between the original open system and the induced closed system, such as Theorem 3.1. An illustrative example will be discussed throughout the chapter. Section 3.3 describes the algorithm to locate almost-invariant sets, and Section 3.4 contains numerical experiments for a two-dimensional system.

The contents of this chapter have appeared as a publication [53].

3.1 Discretising the dynamics

We briefly recap the concepts outlined in Chapter 2 that we will use. Consider a closed dynamical system \((\bar{X}, \mathcal{B}(\bar{X}), \bar{m}, \bar{T})\), where \( \bar{T} \) is non-singular (Definition 2.17) and ergodic (Definition 2.6), and \( \bar{m} \) represents normalised Lebesgue measure over \( \bar{X} \). Form an open dynamical system \((X, \mathcal{B}(X), m, T)\) by introducing a hole \( H \) into the state space \( \bar{X} \) and defining \( X := \bar{X} \setminus H, T := T|_X \), as described in Definition 2.3. Suppose that the open dynamical system admits an ACCIM \( \nu \) (Definition 2.5). Corresponding to the dynamics of the closed system we have the Frobenius Perron operator \( \bar{P} \) (Definition 2.18) and
corresponding to the open system we have the conditional Frobenius-Perron operator \( \mathcal{P} \) (Definition 2.20).

As \( \bar{\mathcal{P}} \) and \( \mathcal{P} \) capture a significant amount of dynamical information we employ numerical methods to extract this information. We use a Galerkin-based procedure known as Ulam’s method [127]; see also [93, 47, 10, 35].

Given the compact metric space \( (\bar{X}, \mathcal{B}(\bar{X}), \bar{m}) \), we partition \( \bar{X} \) into \( \bar{n} \) disjoint connected sets \( \{B_i\}_{i=1}^{\bar{n}} \) of small diameter. In practical computations, if \( \bar{X} \subset \mathbb{R}^d \) then the sets \( B_i, i = 1, \ldots, \bar{n} \) are often \( d \)-dimensional cubes and henceforth we refer to them as boxes. We assume that the hole \( H \) is an exact union of boxes from this partition. We also let \( \bar{I} = \{1, 2, \ldots, \bar{n}\} \), \( I = \{i \in \bar{I} : B_i \subset X\} \) with \( n := \text{card}(I) \). Also, \( \mathcal{H} = \{i \in \bar{I} : B_i \subset H\} \). Write \( \bar{X}_n := \{B_i : i \in \bar{I}\} \) and \( X_n := \{B_i : i \in I\} \). We refer to \( \bar{X}_n \) and \( X_n \) as the discretised state space for the closed and open system, respectively. We form \textit{discretised} \( \sigma \)-algebras for the closed and open dynamical systems by defining the collection of all sets that are unions of boxes in \( \bar{X}_n \) by \( \mathcal{B}_n \), and similarly, the collection of all sets that are unions of boxes in \( X_n \) by \( \mathcal{B}_n \). Hence \( (\bar{X}_n, \mathcal{B}_n) \) and \( (X_n, \mathcal{B}_n) \) are the discretised measurable spaces for the closed and open dynamical systems.

\subsection{Discretised densities}

The collection of densities over \( \bar{X}_n \) consists of elements \( f_n \in \text{span}\{\mathbbm{1}_{B_i} : i \in \bar{I}\} \) such that \( f_n \geq 0 \). Similarly, the collection of densities over \( X_n \) consists of \( f_n \in \text{span}\{\mathbbm{1}_{B_i} : i \in I\} \) such that \( f_n \geq 0 \). For the closed dynamics we define a projection \( \Pi_n : L^1(\bar{m}) \to \text{span}\{\mathbbm{1}_{B_i} : i \in \bar{I}\} \) by

\[ \Pi_n g(x) = \sum_{i \in \bar{I}} \left( \frac{1}{\bar{m}(B_i)} \int_{B_i} g \ d\bar{m} \right) \mathbbm{1}_{B_i} \]  \hfill (3.1)
For the open dynamics we similarly define $\Pi_n : L^1(m) \to \text{span}\{1_{B_i} : i \in I\}$ by

$$
\Pi_n g(x) = \sum_{i \in I} \left( \frac{1}{m(B_i)} \int_{B_i} g \, dm \right) 1_{B_i}.
$$

(3.2)

3.1.2 Discretised Perron-Frobenius operators

**Definition 3.2.** Define $\bar{Q}_{\bar{n}} : \text{span}\{1_{B_i} : i \in \bar{I}\} \to \text{span}\{1_{B_i} : i \in \bar{I}\}$ by $\bar{Q}_{\bar{n}} = \Pi_{\bar{n}} \circ \bar{P}$ and $Q_n : \text{span}\{1_{B_i} : i \in I\} \to \text{span}\{1_{B_i} : i \in I\}$ by $Q_n = \Pi_n \circ \mathcal{P}$.

The matrix representations of $\bar{Q}_{\bar{n}}$ and $Q_n$ (under multiplication on the left) acting on $\text{span}\{1_{B_i} : i \in \bar{I}\}$ and $\text{span}\{1_{B_i} : i \in I\}$ respectively are:

$$(Q_{\bar{n}})_{ij} = \frac{m(B_i \cap \bar{T}^{-1} B_j)}{m(B_j)}$$

and

$$(Q_n)_{ij} = \frac{m(B_i \cap T^{-1} B_j)}{m(B_j)} = \frac{\bar{m}(B_i \cap T^{-1} B_j)}{\bar{m}(X)} = \frac{\bar{m}(B_i \cap \bar{T}^{-1} B_j)}{\bar{m}(B_j)}$$

where $\bar{T}$ and $T$ are diagonal matrices with diagonal elements $\bar{m}_{ii} = m(\bar{B}_i)$, $i \in \bar{I}$ and $m_{ii} = m(B_i)$, $i \in I$, respectively. The matrix $\bar{P}_{\bar{n}}$ is row stochastic and may be interpreted as a transition matrix; the entry

$$(\bar{P}_{\bar{n}})_{ij} = \frac{\bar{m}(B_i \cap \bar{T}^{-1} B_j)}{\bar{m}(B_i)}$$

(3.5)
is the conditional probability of a randomly chosen (with respect to the uniform distribution) point in box \(i\) moving to box \(j\) after one iteration of the map \(\bar{T}\). Similarly, the matrix \(P_n = (P_{ij})\) is defined with entries

\[
(P_n)_{ij} = \frac{m(B_i \cap T^{-1}B_j)}{m(B_i)} = \frac{\bar{m}(B_i \cap T^{-1}B_j)/\bar{m}(X)}{\bar{m}(B_i)/\bar{m}(X)} = \frac{\bar{m}(B_i \cap T^{-1}B_j)}{\bar{m}(B_i)}. \tag{3.6}
\]

This matrix is row sub-stochastic and may be interpreted as a transition matrix for a transient Markov chain approximation of the open dynamical system \(T\). The matrices \(\bar{P}_n\) and \(P_n\) are irreducible (Definition 2.28) as a consequence of the ergodicity of \(\bar{T}\). Note that \(\bar{P}_n\) and \(P_n\) are identical over \(i, j \in \mathcal{I}\). Consequently, an easy way to obtain \(P_n\) is to remove the rows and columns of \(\bar{P}_n\) that correspond to the hole \(H\) (recalling that \(H\) is assumed to consist of a finite number of boxes). Henceforward, we suppress the \(\bar{n}, n\) dependency for these matrices and simply write \(\bar{P}, P\).

### 3.1.3 Discretised measures

Because \(\bar{P}\) is non-negative and irreducible, the Perron-Frobenius Theorem (Theorem 2.30) guarantees there is a unique left eigenvector \(\bar{p} \geq 0\) (normalised so that \(\sum_{i \in \mathcal{I}} \bar{p}_i = 1\)) of \(\bar{P}\) satisfying \(\bar{p}\bar{P} = \bar{p}\). We can define an approximation to the ACIM for \(\bar{T}\) as:

\[
\mu_{\bar{n}}(B) = \sum_{i \in \mathcal{I}} \frac{\bar{m}(B_i \cap B)}{\bar{m}(B_i)} \bar{p}_i, \quad B \subset \bar{X}. \tag{3.7}
\]

Similarly, because \(P\) is non-negative and irreducible, there is a unique left eigenvector \(p \geq 0\) (normalised so that \(\sum_{i \in \mathcal{I}} p_i = 1\)) of \(P\) satisfying \(pP = \lambda_{\mathcal{P}, \mathcal{F}} p\). We can define an
approximation to the ACCIM for $T$ as:

$$
\nu_n(B) = \sum_{i \in I} \frac{m(B_i \cap B)}{m(B_i)} p_i = \sum_{i \in I} \frac{\bar{m}(B_i \cap B)/\bar{m}(X)}{\bar{m}(B_i)/\bar{m}(X)} p_i = \sum_{i \in I} \frac{\bar{m}(B_i \cap B)}{\bar{m}(B_i)} p_i, \quad B \subset X.
$$

(3.8)

**Remark 4.** A rigorous justification for the strong ($L^1$) approximation $\mu_n$ goes back to Li [84] who considered expanding, piecewise $C^2$ maps $T$ of the unit interval. Since then, similar results have been developed for various classes of maps (see [50, 33, 46, 94], among many others). In the open setting, Ulam’s method has been applied to estimate escape rates [4], and the approximation of $\nu_n$ has been rigorously justified for Lasota-Yorke maps with holes [9].

### 3.1.4 Discretised invariance ratios

Having formulated discretised versions of Perron-Frobenius operators as transition matrices whose stationary (resp. quasi-stationary) distributions approximate the ACIM (resp. ACCIM) of the closed (resp. open) dynamical system, we can access discretised invariance ratios for our dynamical systems by simply applying the invariance ratios defined for Markov chains, given in Equations (2.12)-(2.14) and (2.16). Denote the index set of boxes that make up a set $B \in \mathcal{B}_n$ by $\tilde{I}_B = \{ i \in \tilde{I} : B_i \cap B \neq \emptyset \}$, and similarly, denote the index set of boxes that make up a set $B \in \mathcal{B}_n$ by $\mathcal{I}_B = \{ i \in \mathcal{I} : B_i \cap B \neq \emptyset \}$.

The discrete version of $\Psi_{P,\mu}$ (see (2.8)) is given by

$$
\psi_{P,\mu}(B) = \frac{\sum_{i,j \in \tilde{I}_B} \tilde{p}_i \bar{P}_{ij}}{\sum_{i \in \tilde{I}_B} \tilde{p}_i}, \quad B \in \mathcal{B}_n.
$$

(3.9)
The discrete version of $\Psi_{P,\nu}$ (see (2.9)) is given by

$$
\psi_{P,p}(B) = \sum_{i,j \in I_B} \frac{p_i P_{ij}}{\sum_{i \in I_B} p_i}, \quad B \in B_n.
$$

(3.10)

We refer the reader to [49] for rigorous results concerning convergence of $\psi_{\bar{P},\bar{\nu}}$ to $\Psi_{\bar{P},\mu}$ as the box diameters go to zero.

### 3.1.5 An application of discretisation to an interval map

We will introduce a hole into the $\alpha$-shifted doubling map discussed in Example 2.9, and depicted in Figure 2.2, and then calculate the discretised conditional Frobenius-Perron operator, the discretised conditionally invariant measure and discretised invariance ratios.

We fix $H = [0, 0.0468]$, and compute the invariance ratio for all intervals of measure $1/2$.

We partition the unit interval into $\bar{n} = 10000$ boxes each of width $10^{-4}$, so the interval $[0.0468, 1]$ is covered by $n = 9532$ boxes. We compute the transition matrix $P$, and plot the left eigenvector, corresponding to the approximation of the ACCIM, in Figure 3.1.

The leading eigenvalue of $P$ is approximately 0.9639.

**Remark 5.** To select the location of the hole we carried out several experiments, in which we varied the location and size of the hole and calculated the ACCIM of the resulting open systems. Our aim in doing this was to find a location for the hole that would have a significant impact on the long term dynamics: in particular, we sought a hole location that resulted in an ACCIM that was very different to Lebesgue measure (the ACIM for the closed system). Ensuring that $\bar{p}$ and $p$ are different means that both the numerator and the denominator of the invariance ratios differ.
Figure 3.1: The approximate accim for the 1/16-shifted doubling map with a hole \( H = [0, 0.0468] \), computed using \( n = 9532 \).

We will now compute the invariance ratios for the closed system for intervals of the form \([x, x + 0.5]\), where the left end point \( x \in [0, 0.5] \). This will enable us to compare the invariance ratios for all possible intervals of \( \mu \)-measure 1/2. Since the unit interval is partitioned into \( \tilde{n} = 10000 \) boxes, we begin by computing the invariance ratio for the closed system with \( x = 0 \), increment \( x \) by 0.0001, and repeat the calculations, stopping when \( x = 0.5 \). The resulting invariance ratios are shown in Figure 3.2a. We find that the maximum value of \( \psi_{P,\tilde{p}}(B) \) for \( B \) in the class of intervals described above is \( \psi_{P,\tilde{p}}([0, 1/2]) = \psi_{P,\tilde{p}}([1/2, 1]) = 0.9375 \).

To repeat this exercise for the open system, we discard the boxes corresponding to the hole \( H = [0, 0.0468] \), which leaves \( n = 9532 \). For comparability with the closed system, we take intervals of the form \( l(x) = [x, y(x)] \), where \( \nu_n(l(x)) = 1/2 \). We set \( x = 0.0468 \) and calculate \( y(0.0468), \psi_{P,\tilde{p}}(l(0.0468)) \). We then increment \( x \) by 0.0001 and...
repeat, stopping when \( x = 0.6840 \) because \( \nu_n([0.6840,1]) = 1/2 \). The results are shown in Figure 3.2b. The maximum value of \( \psi_{P,p}(l(x)) \) is \( \psi_{P,p}(l(0.5001)) = 0.6821 \).

![Figure 3.2](image)

Figure 3.2: The invariance ratios for the closed system and the open system, for all intervals of invariant measure 1/2 for the 1/16-shifted doubling map. The dashed lines in the second panel indicates the preimage of the hole. The graph of \( T \) is overlaid onto the second panel.

For this particular example we find that the invariance ratio for the closed system is always greater than that for the open system for this particular class of intervals. This is at least in part because the interval for the open system contains the preimage of the hole \( H^1 = [0.7188,0.7421] \) whenever \( x > 0.1562 \). However, it is also because of the dynamics of \( T \) and the difference between the measures \( \mu \) and \( \nu \). To see why, consider the graph of the map, overlaid in Figure 3.2b, and as an illustrative example, consider the set \( l(0.0468) \). The set of points which will leave the interval (the ‘exchange set’) under iteration of \( T \) are those between \([0.5608,0.6840]\), i.e., those whose image is outside of the original interval. But this exchange set has higher \( \nu \)-measure than the rest of the interval (see Figure 3.1), and consequently the invariance ratio is lower. By contrast, the closed system has Lebesgue as its invariant measure, so it will never give additional weight to
the exchange set. Note that this argument is particular to the example under discussion here, and holds because the denominators of the invariance ratios $\psi_{\bar{P},\bar{p}}(B)$ and $\psi_{P,p}(B)$ are the same, and we need only compare the numerators.

In this section we considered only intervals of invariant measure $1/2$. The next section describes a heuristic to find subsets of the unit interval of measure no greater than $1/2$ with high invariance ratios.

3.1.6 Time-reversal symmetry

The invariance ratio $\psi_{\bar{P},\bar{p}}(B)$ for the discretised closed system is time-symmetric even if the original dynamics given by $\bar{T}$ or the discrete dynamics given by $\bar{P}$ are not. Mathematically, $\psi_{\bar{P},\bar{p}} = \psi_{\hat{\bar{P}},\bar{p}}$, where $\hat{\bar{P}}_{ij} := \bar{p}_j \bar{P}_{ji}/\bar{p}_i$ is the transition matrix governing the Markov chain $\bar{P}$ in backward time. Thus, one can define $\bar{R} = (\bar{P} + \hat{\bar{P}})/2$, a reversible Markov chain with invariant measure $\bar{p}$, and obtain $\psi_{\bar{R},\bar{p}}$, and it is a simple matter to show that $\psi_{\bar{R},\bar{p}} = \psi_{\bar{P},\bar{p}}$. Utilising bounds due to [67], this construction yields rigorous upper and lower bounds on the invariance ratio of sets in $B_n$:

$$1 - \sqrt{2(1 - \lambda_{\bar{R},2})} \leq \max_{B \in B_n, \mu_n(B) \leq 1/2} \psi_{\bar{P},\bar{p}}(B) \leq \frac{1 + \lambda_{\bar{R},2}}{2},$$  (3.11)

where $\lambda_{\bar{R},2}$ denotes the second largest eigenvalue of $\bar{R}$. The corresponding right eigenvector $v$ of $\bar{R}$ is used in a heuristic procedure to construct sets $B$ with high values of $\psi_{\bar{P},\bar{p}}(B)$.

One chooses a “threshold value” $c$ and defines sets $B_1(c) = \bigcup_{i : v_i \leq c} B_i$ and $B_2(c) = \bigcup_{i : v_i > c} B_i$. The threshold $c$ may then be varied to maximise $\psi_{\bar{P},\bar{p}}(B_1(c))$ or $\psi_{\bar{P},\bar{p}}(B_2(c))$ while maintaining $\mu_n(B_1(c)), \mu_n(B_2(c)) \leq 1/2$. For further details, we refer the reader to [48] or [51].

We wish to apply this methodology based on the reversible transition matrix $\bar{R}$, as this
approach has found success in physical oceanography [52, 24], epidemic models [7], and 3D fluid mixers [124]. Furthermore, connections between almost-invariant sets, which are probabilistic notions of transport barriers, have been connected with geometric concepts of barriers to transport such as invariant manifolds [51].

It is not clear how to directly apply the methodology of [48] in the absence of a closed system as there is no obvious candidate for $\hat{P}$. We therefore will construct a “closed version” of $P$ which approximately maintains the metastability of properties of $P$. We then derive its time-reversed counterpart.

3.2 The ‘Closure’ of the Open System

Define $H^1 = X \cap T^{-1}(H)$, the set of points in $X$ that are about to fall into the hole. Further, define a functional $\tau : L^1(m) \to \mathbb{R}$ to be the total signed probability mass of $g : X \to \mathbb{R}$ on $H^1$ with respect to $m$:

$$\tau(g) = \int_{H^1} g \, dm. \quad (3.12)$$

We will now construct new Markov operators for the original and the discretised spaces.

**Definition 3.3.** A Markov operator on $X$ is a linear operator $\mathcal{M} : L^1(m) \to L^1(m)$ satisfying $\mathcal{M}g \geq 0$ and $\int \mathcal{M}g \, dm = \int g \, dm$ for $g \geq 0, g \in L^1(m)$.

**Definition 3.4.** Let $\tau$ be given by (3.12), and let $(X, \mathcal{B}(X), \nu, T)$ be an open conditionally measure preserving dynamical system with conditional Perron-Frobenius operator $P$ and $f = d\nu/dm$ the (normalised) conditionally invariant density corresponding to the
ACCIM \nu. Define the operator \( \tilde{\mathcal{P}} : L^1(m) \to \) by

\[
\tilde{\mathcal{P}} g = \mathcal{P}(g) + \tau(g) \cdot f.
\]

(3.13)

We call \( \tilde{\mathcal{P}} \) the closure of \( \mathcal{P} \). The action of \( \tilde{\mathcal{P}} \) is the same as that of \( \mathcal{P} \), except that the part of the density \( g \) that is about to fall into \( H \) is redistributed over all of \( X \) according to the conditionally invariant density \( f \), scaled by the amount of mass about to fall into \( H \).

**Lemma 3.5.** \( \tilde{\mathcal{P}} \) is a Markov operator with fixed point \( f \).

**Proof.** Note that \( X = H^1 \cup T^{-1}X \) and \( H^1 \cap T^{-1}X = \emptyset \). Firstly, we show that \( \tilde{\mathcal{P}} \) is a Markov operator. The fact that \( \tilde{\mathcal{P}} g \geq 0 \) whenever \( g \geq 0 \) is clear, so we only need to show that \( \int \tilde{\mathcal{P}} g \, dm = \int g \, dm \). One has

\[
\int_X \tilde{\mathcal{P}} g \, dm = \int_X \mathcal{P} g \, dm + \int_{H^1} g \, dm \int_X f \, dm
\]

\[
= \int_{T^{-1}X} g \, dm + \int_{H^1} g \, dm
\]

\[
= \int_X g \, dm,
\]

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as required. Secondly, we show that \( f \) is a fixed point of \( \hat{P} \). We note

\[
\int_{H^1} f \, dm = \int_X f \, dm - \int_{T^{-1}(X)} f \, dm = 1 - \int_X P f \, dm = 1 - \lambda P_{\cdot, 1} f = 1 - \lambda P_{\cdot, 1},
\]

which shows that \( f \) is a fixed point of \( \hat{P} \).

We will define an Ulam-type approximation \( \tilde{Q}_n : \text{span}\{1_{B_i} : i \in \mathcal{I}\} \) by \( \tilde{Q}_n := \Pi_n \hat{P} \).

**Lemma 3.6.** The matrix representation of \( \hat{P} \) on \( \text{span}\{1_{B_i} : i \in \mathcal{I}\} \) is

\[
\tilde{Q}_{n,ij} = Q_{n,ij} + \frac{\int_{B_i} f \, dm}{m(B_j)} \cdot m(B_i)(1 - \sum_{j \in \mathcal{X}} P_{ij}),
\]

where \( m(B_i)(1 - \sum_{j \in \mathcal{I}} P_{ij}) \) is the matrix representation of \( \tau \) on \( \text{span}\{1_{B_i} : i \in \mathcal{I}\} \).

**Proof.** As \( \tilde{Q}_n = \Pi_n \hat{P} = \Pi_n (P + \tau \cdot f) \), our main task is to construct the matrix representation for \( \Pi_n (\tau(g) \cdot f) \) when \( g \in \text{span}\{1_{B_i} : i \in \mathcal{I}\} \). We write \( g = \sum_{i \in \mathcal{I}} g_i 1_{B_i} \), where
each \( g_i \in \mathbb{R} \). One has

\[
\Pi_n(\tau(g) \cdot f) = \sum_{j \in I} \frac{1}{m(B_j)} \left( \int_{B_j} \tau(g) \cdot f \, dm \right) \mathbb{1}_{B_j}
\]

\[
= \sum_{j \in I} \frac{1}{m(B_j)} \left( \int_{B_j} f \, dm \cdot \tau(g) \right) \mathbb{1}_{B_j}
\]

\[
= \sum_{j \in I} \frac{\int_{B_j} f \, dm}{m(B_j)} \tau(g) \mathbb{1}_{B_j}
\]

\[
= \sum_{j \in I} \frac{\int_{B_j} f \, dm}{m(B_j)} \left( \int_{H^1} g \, dm \right) \mathbb{1}_{B_j} \tag{3.16}
\]

\[
= \sum_{j \in I} \frac{\int_{B_j} f \, dm}{m(B_j)} \left( \int_{H^1} \left( \sum_{i \in X} g_i \mathbb{1}_{B_i} \right) \, dm \right) \mathbb{1}_{B_j}
\]

\[
= \sum_{j \in I} \frac{\int_{B_j} f \, dm}{m(B_j)} \left( \sum_{i \in X} g_i m(B_i \cap H^1) \right) \mathbb{1}_{B_j}
\]

\[
= \sum_{j \in I} \left( \sum_{i \in \bar{I}} g_i \left( \frac{\int_{B_j} f \, dm}{m(B_j)} m(B_i \cap H^1) \right) \right) \mathbb{1}_{B_j}.
\]

We now examine the term \( m(B_i \cap H^1) \), which is the matrix representation of \( \tau \) on \( \text{span}\{ \mathbb{1}_{B_i} : i \in I \} \). The expression \( m(B_i \cap H^1) \) can be written as

\[
m(B_i \cap H^1) = \sum_{j \in \mathcal{H}} m(B_i) m(B_i \cap T^{-1}B_j) \]

\[
= m(B_i) \sum_{j \in \mathcal{H}} \frac{m(B_i \cap T^{-1}B_j)/\bar{m}(X)}{m(B_i)/\bar{m}(X)}
\]

\[
= m(B_i) \sum_{j \in \mathcal{H}} \frac{\bar{m}(B_i \cap T^{-1}B_j)}{\bar{m}(B_i)}
\]

\[
= m(B_i) \sum_{j \in \mathcal{H}} \bar{P}_{ij}
\]

\[
= m(B_i) \left( \sum_{j \in I} \bar{P}_{ij} - \sum_{j \in I} P_{ij} \right)
\]

\[
= m(B_i) \left( 1 - \sum_{j \in I} P_{ij} \right).
\]
Thus,
\[
\tilde{Q}_{n,ij} = Q_{n,ij} + \frac{\int_{B_j} f \, dm}{m(B_j)} \cdot m(B_i) \left( 1 - \sum_{j \in I} P_{ij} \right),
\]
as required. \qed

In light of the fact that \( m(B_i)(1 - \sum_{j \in I} P_{ij}) \) is the matrix representation of \( \tau \) on \( \text{span}\{1_{B_i} : i \in I\} \), we let \( 1 - \sum_{j \in I} P_{ij} =: \tau_{n,i} \). We note that \( \int_{B_j} f \, dm \) is not known, however, Remark 4 on page 32 justifies in certain cases (and in practice, most cases) the replacement of \( \int_{B_j} f \, dm \) with \( p_j \). Making this replacement, we henceforth define

\[
\tilde{P} = M^{-1} \tilde{Q}_n M.
\]

**Lemma 3.7.** The matrix \( \tilde{P} \) is row stochastic, has \( p \) as a fixed left eigenvector and satisfies

\[
\tilde{P} = P + \tau_n p,
\]

where \( \tau_n \) is a column vector with elements \( \tau_{n,i} = 1 - \sum_{j \in I} P_{ij} \) and \( p \) is a row vector.

**Proof.** We make the replacement \( p_j \) for \( \int_{B_j} f \, dm \) and so

\[
\tilde{P}_{ij} = \frac{1}{m(B_i)} \left( Q_{n,ij} + \frac{p_j}{m(B_j)} \cdot m(B_i) \left( 1 - \sum_{j \in I} P_{ij} \right) \right) m(B_j)
\]

\[= P_{ij} + \left( 1 - \sum_{j \in I} P_{ij} \right) \cdot p_j = P_{ij} + \tau_i \cdot p_j,
\]
which shows that \( \tilde{P} \) indeed can be written in the form given in Equation 3.18. It then follows that \( \tilde{P} \) is stochastic since

\[
\sum_{j \in I} \tilde{P}_{ij} = \sum_{j \in I} P_{ij} + \sum_{j \in I} \tau_{i} p_{j} = \sum_{j \in I} P_{ij} + \tau_{i} = \sum_{j \in I} P_{ij} + 1 - \sum_{j \in I} P_{ij} = 1. \tag{3.20}
\]

Finally, \( \tilde{P} \) has \( p \) as a fixed left eigenvector since

\[
\sum_{i \in I} p_{i} \tilde{P}_{ij} = \sum_{i \in I} p_{i} P_{ij} + \sum_{i \in I} p_{i} \tau_{i} p_{j} = \lambda_{P,1} p_{j} + p_{j} \sum_{i \in I} p_{i} (1 - \sum_{j \in I} P_{ij}) = \lambda_{P,1} p_{j} + p_{j} - p_{j} \sum_{i \in I} \sum_{k \in I} p_{i} P_{ik} = \lambda_{P,1} p_{j} + p_{j} (1 - \lambda_{P,1}) = p_{j}.
\]

We call \( \tilde{P} \) the closure of \( P \). The idea of resurrecting a Markov chain at the time it leaves a particular set goes back to [5], but only recently has the idea been exploited fully (see for example [40, 17]). In this case, since \( p \) is the leading fixed left eigenvector, it follows that \( \nu_{n} \), the accim for the open system, is an invariant measure for the discrete closure system.

We would now like to define invariance ratios in terms of the closure operators \( \tilde{P} \) and \( \tilde{P} \). We firstly recall the definitions of the invariance ratios for the open and closed
dynamical systems, given in Equations (2.9) and (2.8):

\[ \Psi_{P,\nu}(B) = \frac{\langle 1_B, \mathcal{P}_\nu 1_B \rangle_\nu}{\nu(B)} \quad \text{and} \quad \Psi_{\bar{P},\mu}(B) = \frac{\langle 1_B, \bar{\mathcal{P}}_\mu 1_B \rangle_\mu}{\mu(B)} \]

This permits a natural definition for the invariance ratios under the closure operators.

**Definition 3.8.** For \( B \in \mathcal{B}(X) \) and \( \bar{\mathcal{P}}_\nu(g) := \bar{\mathcal{P}}(f \cdot g)/f, \ g \in L^1(m) \), we define

\[
\Psi_{\bar{P},\nu}(B) := \frac{\langle 1_B, \bar{\mathcal{P}}_\nu 1_B\rangle_\nu}{\nu(B)} \tag{3.21}
\]

Note that there is no equivalent formulation of \( \Psi_{\bar{P},\nu} \) in terms of a transformation, as there is for \( \Psi_{P,\mu} \) and \( \Psi_{P,\nu} \) (see the discussion in Section 2.2.1). This is because there is no deterministic transformation that corresponds to the closure operators.

The following theorem shows that the metastability properties of the system induced by the closure operation are closely related to those of the open system.

**Theorem 3.9.** For an \((X, \mathcal{B}(X), \nu, T)\) open conditionally measure preserving dynamical system with \( f = d\nu/dm \) the (normalised) conditionally invariant density corresponding to the ACCIM \( \nu \), assume in addition that \( f > 0 \). With \( \Psi_{\bar{P},\nu} \) defined as Definition 3.8, one has

\[
\Psi_{\bar{P},\nu}(B) = \Psi_{P,\nu}(B) + \nu(B \cap H^1) \quad \text{for} \ B \in \mathcal{B}(X). \tag{3.22}
\]
Proof. Firstly note that the operator $\tilde{P}_\nu : L^1(\nu) \ominus$, defined by $\tilde{P}_\nu(g) := \tilde{P}(f \cdot g)/f$ can be written as

$$\tilde{P}_\nu(g) = \frac{\mathcal{P}(f \cdot g)}{f} + \frac{\tau(f \cdot g)}{f \cdot f}$$

$$= \mathcal{P}_\nu(g) + \int_{H^1} \frac{g \cdot f}{m}$$

$$= \mathcal{P}_\nu(g) + \int_{H^1} g \cdot \nu$$

It is a simple matter to show that $\tilde{P}_\nu$ is also a Markov operator, with fixed point $1_X$.

From Definition 3.8,

$$\Psi_{\tilde{P}_\nu}(B) = \frac{\langle 1_B, \tilde{P}_\nu 1_B \rangle_\nu}{\nu(B)}$$

$$= \frac{\langle 1_B, (\mathcal{P}_\nu 1_B + \int_{H^1} 1_B \, d\nu) \rangle_\nu}{\nu(B)}$$

$$= \frac{\langle 1_B, \mathcal{P}_\nu 1_B \rangle_\nu + \left( \int_{H^1} 1_B \, d\nu \right) \nu(B)}{\nu(B)}$$

$$= \Psi_{\mathcal{P}_\nu}(B) + \frac{\nu(B) \int_{H^1} 1_B \, d\nu}{\nu(B)}$$

$$= \Psi_{\mathcal{P}_\nu}(B) + \nu(B \cap H^1)$$.

The above theorem shows that the invariance ratio for the closure of the open system is equal to the invariance ratio of the open system, plus an adjustment term of at most $\nu(H^1) = 1 - \lambda_{P, 1}$. In particular, if $B \cap H^1 = \emptyset$, $\Psi_{\tilde{P}_\nu} = \Psi_{\mathcal{P}_\nu}$. In analogy to Definition 3.8, we define a discretised version of $\Psi_{\tilde{P}_\nu}(B)$ for sets $B \in B_n$:
Definition 3.10. For $B \in \mathbb{B}_n$, we set

$$\psi_{\tilde{P},p}(B) := \frac{\sum_{i,j \in I_B} p_i \tilde{P}_{ij}}{\sum_{i \in I_B} p_i}.$$ (3.23)

In analogy to Theorem 3.9, one has

Lemma 3.11. For $B \in \mathbb{B}_n$,

$$\psi_{\tilde{P},p}(B) = \psi_{P,p}(B) + \nu_n(B \cap H^1).$$ (3.24)

Proof. We have

$$\psi_{\tilde{P},p}(B) := \frac{\sum_{i,j \in I_B} p_i \tilde{P}_{ij}}{\sum_{i \in I_B} p_i}$$

$$= \frac{\sum_{i,j \in I_B} p_i (P_{ij} + \tau_i \tau_j)}{\sum_{i \in I_B} p_i}$$

$$= \frac{\sum_{i,j \in I_B} p_i P_{ij}}{\sum_{i \in I_B} p_i} + \frac{\sum_{i \in I_B} p_i \tau_i \sum_{j \in I_B} p_j}{\sum_{i \in I_B} p_i}$$ (3.25)

$$= \psi_{P,p}(B) + \sum_{i \in I_B} \tau_i p_i$$

$$= \psi_{P,p}(B) + \sum_{i \in I_B} \frac{m(B \cap H^1)}{m(B_i)} p_i$$

$$= \psi_{P,p}(B) + \nu_n(B \cap H^1).$$

$\Box$
3.2.1 An application of closure to an interval map

We return to the $1/16$-shifted doubling map with $H = [0, 0.0468]$ example discussed in Section 3.1.5. We again calculate the invariance ratios for all intervals of the form $l(x) = [x, y(x)]$, where $\nu_n(l(x)) = 1/2$ and the left end point $x$ is between $[0.0468, 0.6839]$. The interval $[0.0468, 1]$ is partitioned into $n = 9532$ boxes of width $10^{-4}$, we set $x = 0.0468$, compute $y(0.0468), \psi_{P,p}(l(0.0468))$ and $\psi_{\tilde{P},p}(l(0.0468))$, advance $x$ by $0.0001$, and repeat. Figure 3.3 shows that $\psi_{P,p}(B)$ is equal to $\psi_{\tilde{P},p}(B)$ when the set $B$ does not overlap the preimage of the hole $H^1 = [0.7188, 0.7421]$, as per Lemma 3.11. This is the case when $x < 0.1562$. Lemma 3.11 also dictates that the discrepancy between $\psi_{\tilde{P},p}(B)$ and $\psi_{P,p}(B)$ is bounded above by $1 - \lambda_{P,1} = 0.0361$.

![Figure 3.3: The difference $\psi_{\tilde{P},p}(B) - \psi_{P,p}(B)$ for intervals of $\nu$-measure 1/2 for the 1/16-shifted doubling map. The difference is zero when the interval does not include the preimage of the hole (which is demarcated with dashed lines), and is bounded from above by $1 - \lambda_{n,1} = 0.0361.\)
3.3 Using eigenvector maximality properties of $\tilde{R}$

Now that we have a stochastic matrix $\tilde{P}$ (Lemma 3.7) and a relationship between $\psi_{P,p}$ and $\psi_{\tilde{P},p}$ (Lemma 3.11), we may apply the methodology of [48] to find almost-invariant sets for the induced closed system.

Let $\hat{P}_{ij} = p_j \tilde{P}_{ji} / p_i$, $i, j \in I$ denote the transition matrix for the Markov chain $\tilde{P}$ in backward time. The invariance ratio $\psi_{\tilde{P},p}(B)$ is time-symmetric:

**Lemma 3.12.** For $B \in B_n$,

$$\psi_{\tilde{P},p}(B) = \frac{\sum_{i,j \in I_B} p_i \hat{P}_{ij}}{\sum_{i \in I_B} p_i}.$$ 

*Proof.* Straightforward to verify. \hfill \Box

We define a time-symmetrised version of $\tilde{P}$ as

$$\tilde{R}_{ij} = (\hat{P}_{ij} + \tilde{P}_{ij}) / 2, \quad i, j \in I.$$

The Markov chain with transition matrix $\tilde{R}$ is reversible and preserves the measure $p$.

Using the matrix $\tilde{R}$ and the relationship between $\psi_{P,p}$ and $\psi_{\tilde{P},p}$ given in Lemma 3.11 we can produce rigorous bounds for almost-invariant ratios for the original open system.

**Theorem 3.13.** One has the following bounds for the maximum invariance ratio in an open system:

$$1 - \sqrt{2(1 - \lambda_{\tilde{R},2})} - (1 - \lambda_{P,1}) \leq \max_{B \in B_n, \nu_n(B) \leq 1/2} \psi_{P,p}(B) \leq \frac{1 + \lambda_{\tilde{R},2}}{2}.$$
Proof. Apply (3.11) to the matrix $\tilde{R}$ and invariant measure $\nu_n$. Theorem 3.9 yields the result.

Furthermore, we may apply the heuristic from [48] to the induced closed system to find sets with high invariance ratios for the original open system.

**Example 3.14.** To the $\alpha$-shifted map with $\alpha = 1/16$ we have introduced a hole $H = [0, 0.0468]$, and computed $P$ with $n = 9532$ boxes. The leading two eigenvalues of $P$ are $\{0.9639, 0.8920\}$ and the leading two eigenvalues of $\tilde{P}$ are $\{1, 0.8920\}$.

We then form $\tilde{R}$ and compute its second eigenvalue as 0.9736 and corresponding right eigenvector $v_2(\tilde{R})$. We are also now able to compute the bounds in Theorem 3.13, and state that the maximal invariance ratio $\psi_{P,p}(B)$ must be in the interval $[0.7343, 0.9868]$.

We now wish to apply the thresholding algorithm described in Section 3.1, or in greater detail in Steps 6-7 of Algorithm 1 in Section 3.4 (see also [48] or [51]). Briefly summarising, we select a value $c$ to maximise $\psi_{P,p}(B^{opt}) := \max(\psi_{P,p}(B_1(c)), \psi_{P,p}(B_2(c)))$, subject to $\nu_n(B^{opt}) \leq 1/2$, where $B_1(c) = \bigcup_{i: v_i \leq c} B_i$ and $B_2(c) = \bigcup_{i: v_i > c} B_i$ for some candidate eigenvector $v$. Our suggested approach is to take $v$ to be the second right eigenvector of $\tilde{R}$. However, we will also compare this result with sets obtained from three other candidate methods that one might use in the absence of our new approach. Our goal in doing so is to see whether the new matrix $\tilde{R}$ is an improvement over existing alternatives.

**Method 1** Threshold the second right eigenvector of $\tilde{R}$ (Figures 3.4a, 3.4b).

**Method 2** Consider the closed $\alpha$-shifted map, which preserves Lebesgue measure on $[0,1]$. Compute $\bar{P}$ and form the matrix $\bar{R}$ as described in Section 3.3. Truncate the
second right eigenvector of $\tilde{R}$ to $[1/16, 1]$ and threshold it (Figures 3.4c, 3.4d)\(^1\).

**Method 3** Threshold the second left eigenvector of $P$ (Figures 3.4e, 3.4f)\(^2\).

**Method 4** Compute $\tilde{P}$ for the closed $\alpha$-shifted map. Truncate the the second left eigenvector of $\tilde{P}$ to $[1/16, 1]$ and threshold it (Figures 3.4g, 3.4h).

The values of $\psi_{P,p}(B^{\text{opt}})$ and $\nu_n(B^{\text{opt}})$ resulting from Methods 1-4 are summarised in Table 3.1. In this particular example, using the right eigenvectors of $\tilde{R}$ or $\tilde{R}$, as per Methods 1 and 2 produced higher invariance ratios than using the left eigenvectors of $P$ or $\tilde{P}$, as per Methods 3 and 4. Whilst Method 2 finds a set with a slightly higher invariance ratio than Method 1, both methods deliver comparable results. Recall that in Section 3.1.5, where we exhaustively searched for sets $A^{\text{opt}}$ comprised of single intervals of $\nu$-measure 1/2, the best invariance ratio we found was 0.6821, much lower than any set found by Methods 1–4.

### 3.3.1 Computational issues

While the matrix $P$ is typically very sparse, the matrix $\tilde{P}$ is typically dense. However, by exploiting the “sparse plus rank-one” structure of $\tilde{P}$ we can still efficiently compute eigenvectors of $\tilde{R}$.

---

\(^1\)We use the right eigenvectors of $\tilde{R}$ and $\tilde{R}$ because one has $v_{2}^{\text{right}} \perp p$ (recall $p$ is the leading left eigenvector) by a standard result of linear algebra. Thus we think of the entries in $v_{2}^{\text{right}}$ as relaxations of $\pm 1$, where the value $+1$ corresponds to membership in one almost-invariant set and $-1$ corresponds to membership in the complementary almost-invariant set.

\(^2\)For non-invertible maps the right eigenvectors of $P$ are typically highly irregular and one instead uses left eigenvectors, which are smoother. This approach has been taken for closed systems in e.g. [27].
Note that

\[
\sum_{j=1}^{n} \tilde{R}_{ij} x_j = (1/2) \sum_{j=1}^{n} (\tilde{P}_{ij} + p_j \tilde{P}_{ji}/p_i) x_j
\]

\[
= (1/2) \sum_{j=1}^{n} (P_{ij} + \tau_{ni} p_j + (p_j/p_i) \cdot (P_{ji} + p_i \tau_{nj})) x_j
\]

\[
= (1/2) \left( \sum_{j=1}^{n} (P_{ij} + p_j \tilde{P}_{ji}/p_i) x_j + \left( \sum_{j=1}^{n} p_j x_j \right) \tau_{ni} + \left( \sum_{j=1}^{n} p_j \tau_{nj} x_j \right) 1_i \right).
\]

The matrix \( P_{ij} + p_j \tilde{P}_{ji}/p_i \) is sparse and can be stored in memory for fast sparse matrix-vector multiplication in eg. MATLAB. The other two terms involving \( x \) are very fast to compute. Thus, we may use iterative solvers to rapidly compute eigenvalues and eigenvectors of high-dimensional matrices formed from high resolution grids (large \( n \)).

The following sample MATLAB code takes as input the matrix \( P \) and calculates the top \( k \) eigenvalues and right eigenvectors of \( \tilde{R} \).

```matlab
function [v,lambda]=Rhat_eigs(P,k),
[p,1]=eigs(P',1); %compute \( p \) (leading left eigenvector of \( P \))

p=p/sum(p); %normalise sum of \( p \) to 1
pdiag=diag(sparse(p));
pdiaginv=diag(sparse(1./p));
Phat=pdiaginv*P'*pdiag; %create \( \hat{P} \) in sparse form

tau=(1-sum(P'))'; %create \( \tau \)

%find eigenvectors of \( \tilde{R} \)
[v,lambda]=eigs(@matrix_closure_mult,size(P,1),k);

function y=matrix_closure_mult(x),
%calculates \((1/2)\cdot(\tilde{P}+\hat{\tilde{P}})\cdot x=\tilde{R}\cdot x\)

y=(P*x+Phat*x+(p'*x)*tau+sum(x.*tau.*p))/2;
end
end
```

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3.4 Examples

We demonstrate the ideas from the previous sections using a more complex numerical example. For clarity, we first outline the steps to carry out this process in the following algorithm. Steps 1 and 2 are easily carried out using MATLAB and the purpose-built software GAIO [25].

Algorithm 1.

1. Partition the state space $X$ into connected sets $\{B_1, B_2, \ldots, B_n\}$. This can be achieved relatively easily using eg. GAIO via MATLAB. GAIO [25] integrates the partitioning process with the construction of the transition matrix.

2. Construct the transition matrix corresponding to the open system, $P = (P)_{ij} = \frac{m(B_i \cap T^{-1}B_j)}{m(B_j)}$. The matrix $P$ can be quickly estimated using images of sample points within each box, see eg. [25].

3. Compute the vector $p$ as the leading left eigenvector of $P$, normalised to sum to 1. This is fast using eg. MATLAB as $P$ is sparse.

4. Construct $\tau = 1 - \sum_j P_{ij}$, and $\tilde{P} = P + \tau(p)'$.

5. Form $\hat{P}_{ij} = p_j \tilde{P}_{ji}/p_i$ and $\hat{R} = (\hat{P} + \hat{P})/2$, and compute the second largest eigenvalue $\lambda_{R,2}$ and corresponding right eigenvector $v$ of $\hat{R}$.

6. For $c \in [\min_i v_i, \max_i v_i]$ define $B_1(c) = \bigcup_{i : v_i \leq c} B_i$ and $B_2(c) = \bigcup_{i : v_i > c} B_i$. By incrementing $c$, find $c_1 = \arg\max_c \{\psi_{P,p}(B_1(c)) : \nu_n(B_1(c)) \leq 1/2\}$ and $c_2 = \arg\max_c \{\psi_{P,p}(B_2(c)) : \nu_n(B_2(c)) \leq 1/2\}$.

7. Return $\max\{\psi_{P,p}(B_1(c_1)), \psi_{P,p}(B_2(c_2))\}$ as the maximal almost-invariance ratio found for the open system and set $B^{opt}$ to be whichever of $B_1(c_1)$ or $B_2(c_2)$ achieves this maximum.
We will now apply Algorithm 1 to a periodically forced two-dimensional system of ODEs defined on $X = [0, 2] \times [0, 1]$ by:

\begin{align}
\dot{x} &= -\pi A \sin(\pi f(x, t)) \cos(\pi y) \\
\dot{y} &= \pi A \cos(\pi f(x, t)) \sin(\pi y) \frac{df}{dx}(x, t) \\
f(x, t) &= \epsilon \sin(\omega t)x^2 + (1 - 2\epsilon \sin(\omega t))x
\end{align}

(3.26a, 3.26b, 3.26c)

Lebesgue measure is preserved by the corresponding flow. This flow, known as the “Double Gyre” has studied in several recent papers including [120, 51]. Following [51], we set $A = 0.25$, $\epsilon = 0.25$ and $\omega = 2\pi$ so that the period of the flow equals 1. Let $\phi(x; s, t)$ be the time $(t - s)$ evolution of an orbit beginning at $x$ at time $s$. We divide the state space $\tilde{X}$ into a $2^8 \times 2^7$ grid, so that $n = 2^{15}$. The matrix $\tilde{P}$ is then formed by considering 625 uniformly distributed test points in each box, and integrating from initial time $t = 0$ over one period. $P$ is formed by removing the rectangles $H_1 = [0.15, 0.85] \times [0.15, 0.85]$ and $H_2 = [1.2, 1.85] \times [0.15, 0.85]$, to form $X = \tilde{X} \setminus (H_1 \cup H_2)$. Hence, this construction discards orbits for which $\phi(x; 0, 1) \in H_1 \cup H_2$, but not orbits for which $\phi(x; 0, t) \in H_1 \cup H_2$ for some $t \in (0, 1)$ and $\phi(x; 0, 1) \in X$.

After removing these holes we have $n = 17198$ boxes covering the restricted state space $X$. The leading eigenvalues of $P$ are $\lambda_{P, 1} = 0.9740$ and $\lambda_{P, 2} = 0.8679$. The leading left eigenvector $p$ is then computed (see Figure 3.5), and we use this to remove all boxes with $\nu_n$-measure of less than $10^{-9}$. This leaves us $n = 12843$ boxes. We recompute $P$, and construct $\tilde{P}, \tilde{R}$ and $v_2$ as described in Steps 4-5 (see Figure 3.6). We then perform the thresholding process described in Steps 6-7 with the second right eigenvector of $\tilde{R}$. 

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Table 3.2: Summary of results for periodically forced double gyre.

<table>
<thead>
<tr>
<th>Eigenvector used for thresholding</th>
<th>$\psi_{P,p}(B^{opt})$</th>
<th>$\nu_n(B^{opt})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Left 2nd eigenvector of $P$</td>
<td>0.8527</td>
<td>0.4866</td>
</tr>
<tr>
<td>Right 2nd eigenvector of $R$</td>
<td>0.9305</td>
<td>0.4565</td>
</tr>
</tbody>
</table>

We do not compute thresholding results with $\bar{P}$ or its time-reversed counterpart $\bar{R}$, as we did in Methods 2 and 4 of Example 3.14, because in this example we wish to focus on methods applicable to situations when only the open system is available. The invariance ratios $\psi_{P,p}(B_1(c))$ and $\psi_{P,p}(B_2(c))$ obtained for different threshold values $c$ are plotted in Figure 3.7. The maximal invariance ratio for a set of $\nu_n$-measure less than 1/2 is found when $c^* = 0.001805$, and then we have

$$B^{opt} = B_2 = \bigcup_{i: v_i \geq c^*} B_i,$$

where $v$ is the second right eigenvector of $\bar{R}$. This set has $\nu_n$-measure 0.4565 and an invariance ratio $\psi_{P,p}(B_1) = 0.9305$, and is shown in Figure 3.8. For comparison, we also repeat Steps 6-7 using the second left eigenvector of $P$, and find a set $B^{opt}$, shown in Figure 3.9. The results are compared in Table 3.2; we once again find a higher invariance ratio by thresholding the second right eigenvector of $\bar{R}$ than any other candidate eigenvector.

We note that the separation seen in Figure 3.8 is similar to the separation seen in the closed system (Figure 16 in [51]), despite the significantly different asymptotic behaviour; the conditionally invariant measure shown in Figure 3.5 is significantly different to the area-preservation of the closed system. As the separation seen in [51] appears to be strongly related to the stable and unstable manifolds of the hyperbolic periodic points on
the top and bottom of the rectangle, and at least part of these manifolds are contained in the support of the conditionally invariant measure in Figure 3.5, it may be that transport related to lobe dynamics still plays a dominant transmission role in the open system. We refer the reader to [51] for further discussion of the lobes.

3.5 Conclusion

The determination of almost-invariant or metastable regions in dynamical systems provides important information on the transport of mass at a macroscopic level. The most successful methods to study almost-invariance in closed systems are based on the Perron-Frobenius operator $P$. While considerable research has been done on almost-invariance in closed systems, little if any attention has been paid to open systems, where trajectories terminate when entering a hole, and the time-asymptotic dynamics occur on a survivor set.

We have introduced the notion of almost-invariance in open systems and developed a new closing operation to construct a Markov operator $\tilde{P}$ from the conditional Perron-Frobenius operator $P$ corresponding to the open system. Existing techniques for almost-invariant sets, such as those in [48], may now be applied to this Markov operator. We showed that the invariance ratios of sets according to the (i) the conditional Perron-Frobenius operator $P$ and (ii) the Markov operator $\tilde{P}$, differ by an amount equal to the conditionally invariant measure of the set in question intersected with the hole. We further developed rigorous upper and lower bounds for the maximum possible invariance ratios of discretised sets based on the second eigenvalue of a matrix constructed from the closing operation, and applied our new methodology to an interval map and a two-dimensional flow. In the case of the interval map, we assumed we had access to the closed
system, and we found that our method delivered a comparable, although slightly lower, invariance ratio than that found using standard methods applied to the closed system. In the case of the two-dimensional flow, we did not have access to the closed system, and our method was superior to the alternative considered. More work is needed to determine whether the methodology proposed in this chapter is consistently superior to alternative approaches for open dynamical systems. We also showed how to compute eigenvectors of the dense matrix $\tilde{R}$ by exploiting its “sparse plus rank-one” structure.
Figure 3.4: The graphs in the left column depict the eigenvector that was used for thresholding, together with the optimal set $B^{opt}$. The graphs in the right hand column show the thresholding process. The red lines corresponds to $\psi_{P,p}(B_1(c))$ and the blue dashed line to $\psi_{P,p}(B_2(c))$. The black vertical line represents the value for which $\nu_n(B_1(c)) = \nu_n(B_2(c)) = 1/2$. The value of $c^*$corresponding to the $\psi_{P,p}(B^{opt})$ is indicated.
Figure 3.5: The conditionally invariant measure of the double gyre defined on $X = \bar{X} \setminus (H_1 \cup H_2)$.

Figure 3.6: The second eigenvector $v_2$ of $\tilde{R}$. 
Figure 3.7: Thresholding for the double gyre: using the second right eigenvector of $\tilde{R}$, we compute $\psi_{P,P}(B_1(c))$ (red solid line) and $\psi_{P,P}(B_2(c))$ (blue dashed line) for each threshold value $c$. The black vertical line indicates the value for which $\nu(B_1) = \nu(B_2) = 1/2$, and the optimal $c^*$ which gives $\psi_{P,P}(B_1(c^*)) = 0.9305$ is indicated.

Figure 3.8: For the periodically forced double gyre defined on $X$, the set with the highest invariance ratio of 0.9305 is shown in orange, and the complementary set is shown in dark brown.
Figure 3.9: For the periodically forced double gyre defined on $X$, the partition into optimally almost-invariant sets found by thresholding with the second left eigenvector of $P$. The set with the highest invariance ratio of 0.8527 is shown in orange, and the complementary set is shown in dark brown.
Chapter 4

Bounds on the conductance and metastability of substochastic Markov chains

In this chapter we derive new bounds on the conductance and metastability of substochastic reversible and non-reversible Markov chains. Section 4.1 recaps the relevant definitions that were given in Section 2.3, and foreshadows the main theorems of the chapter. Section 4.2 discusses the derivation of bounds on the conductance and metastability in the stochastic setting, paving the way for the main contribution of this chapter: bounds on the conductance and metastability in the substochastic setting, which are introduced in Section 4.3. Concluding remarks are contained in Section 4.4, and proofs in Section 4.5.

4.1 Preliminaries

We recall the definitions of the metastability and conductance associated with a transition matrix $M$, which were established in Section 2.3 in (2.16) and (2.17). For ease of reference we repeat the definitions here: the minimal $\ell$-flux (conductance) and maximal $\ell$-invariance
(metastability) under $M$, respectively, are given by:

$$
\phi_{M,\ell} := \min_{B: \ell(B) \leq 1/2} \frac{Q_{M,\ell}(B, B^c)}{\ell(B)}, \quad \psi_{M,\ell} := \max_{B: \ell(B) \leq 1/2} \frac{Q_{M,\ell}(B, B)}{\ell(B)}.
$$

(4.1)

These definitions are to be understood here in terms of a generic $(M, \ell)$ pair, where $M$ is a transition matrix and $\ell$ some measure associated with a Markov process. Our goal in this chapter is to construct bounds on $\phi_{M,\ell}$ and $\psi_{M,\ell}$ under different specifications of $\ell$ and $M$. The simplest situation is when $M$ is an irreducible (Definition 2.28) transition matrix of a stochastic Markov chain and $\ell$ the unique stationary distribution; in this case we denote $M, \ell$ by $\bar{P}, \bar{p}$ for consistency with Chapter 3. Bounds on $\phi_{\bar{P},\bar{p}}$ and $\psi_{\bar{P},\bar{p}}$ have already been constructed for the case when $\bar{P}$ is $\bar{p}$-reversible (Definition 2.31) [82, 67] and not $\bar{p}$-reversible [16, 48]. Our contribution is bounds for the case when $M$ is substochastic; in this case we denote $M$ by $P$. We assume throughout that $P$ is irreducible. For substochastic $P$ there may not be a unique or best choice for the measure $\ell$, as there are several probability distributions used to describe the long- or medium-term behaviour of substochastic Markov chains [107, 22, 23]. We let $m = p$, where $p$ is the unique\(^1\) quasi-stationary distribution, defined by the eigenvector condition

$$
pP = \lambda_{P,1}p.
$$

(4.2)

We formulate bounds both with and without the condition that $P$ is $p$-reversible.

\(^1\)Uniqueness is guaranteed by irreducibility of $P$
Remark 6. We may consider $P$ as an operator on the inner product space $(\mathbb{R}^n, \langle x, y \rangle_p)$, where $\langle x, y \rangle_p = \sum_{i \in X} x_i y_i p_i$ for $x, y \in \mathbb{R}$. The statement that $P$ is $p$-reversible is equivalent to the statement that $P$ is self-adjoint with respect to the inner product space weighted by $p$. Indeed, we introduce the concept of $p$-reversibility precisely because it is equivalent to self-adjointness, and the bounds that we demonstrate rely on some theoretical results pertaining to self-adjoint operators.

We state here our main results on these bounds in terms of the spectrum of $P$, firstly in the case when $P$ satisfies a generalised ‘detailed balance’ condition and secondly for general substochastic $P$.

**Theorem 4.1.** Let $P$ be irreducible and substochastic with quasi-stationary distribution $p$, and suppose $p_i P_{ij} = p_j P_{ji}$ for all $i, j \in X$. Let $\lambda_{P,1}, \lambda_{P,2} \in \mathbb{R}$ be the leading and second largest eigenvalues of $P$ respectively. Denote by $\phi_{P,p}$ the conductance and by $\psi_{P,p}$ the metastability of $P$ (see (4.1)). Then

$$\frac{\lambda_{P,1} - \lambda_{P,2}}{2} \leq \phi_{P,p} \leq \sqrt{2(\lambda_{P,1} - \lambda_{P,2})} \quad (4.3)$$

and

$$\lambda_{P,1} - \sqrt{2(\lambda_{P,1} - \lambda_{P,2})} \leq \psi_{P,p} \leq \frac{\lambda_{P,1} + \lambda_{P,2}}{2}. \quad (4.4)$$

**Theorem 4.2.** For an irreducible and substochastic matrix $P$ with quasi-stationary distribution $p$, define $\hat{P}$ by $\hat{P}_{ij} = p_j P_{ji}/p_i$ and let $R = (P + \hat{P})/2$. Let $\lambda_{P,1} \in \mathbb{R}$ be the leading eigenvalue of $P$, $\lambda_{R,2} \in \mathbb{R}$ the second largest eigenvalue for $R$, $\rho = \min_i \sum_{j \in X} P_{ij}$.
and $\bar{\rho} = \max_i \sum_{j \in X} P_{ij}$. Assuming $\lambda_{P,1} > \lambda_{R,2}$, one has

$$\frac{2\rho - \bar{\rho} - \lambda_{R,2}}{2} - \frac{(\lambda_{P,1} - \bar{\rho})^2}{8(\lambda_{P,1} - \lambda_{R,2})} \leq \phi_{P,\bar{\rho}} \leq \sqrt{\bar{\rho} + \lambda_{P,1} - 2\lambda_{R,2}} + \frac{\bar{\rho} - \lambda_{P,1}}{2} \tag{4.5}$$

and

$$\max \left( \frac{\lambda_{P,1} + 2\rho - \bar{\rho}}{2}, \lambda_{R,2} \right) - \sqrt{\bar{\rho} + \lambda_{P,1} - 2\lambda_{R,2}} \leq \psi_{P,\bar{\rho}} \leq \frac{\bar{\rho} + \lambda_{R,2}}{2} + \frac{(\bar{\rho} - \lambda_{P,1})^2}{8(\lambda_{P,1} - \lambda_{R,2})}. \tag{4.6}$$

**Remark 7.** (a) Note that if $\lambda_{P,1} = 1$ in Theorem 4.1 (so $P$ is stochastic) then (4.3) and (4.4) reduce to the following bounds on the conductance [121] and metastability [48] of stochastic Markov chains:

$$\frac{1 - \lambda_{P,2}}{2} \leq \phi_{P,\bar{\rho}} \leq \sqrt{2(1 - \lambda_{P,2})} \tag{4.7}$$

and

$$1 - \sqrt{2(1 - \lambda_{P,2})} \leq \psi_{P,\bar{\rho}} \leq \frac{1 + \lambda_{P,2}}{2}. \tag{4.8}$$

(b) Under the hypotheses of Theorem 4.2, if one additionally has $p_i P_{ij} = p_j P_{ji}$ then we can show (see (4.16b)) that $\rho = \lambda_{P,1} = \bar{\rho}$, and so (4.5) and (4.6) reduce to (4.3) and (4.4).

(c) The bounds (4.7) have historically been expressed as bounds on the spectral gap $1 - \lambda_{P,2}$ in terms of the conductance $\phi_{P,\bar{\rho}}$, rather than bounds on $\phi_{P,\bar{\rho}}$ in terms of $1 - \lambda_{P,2}$. The spectral gap determines the *mixing rate* of the chain, an important quantity in applications such as Markov Chain Monte Carlo methods (see discussion in [11]). As well as the conductance-based bounds on the spectral gap that we
discuss, an alternative type of bound on the spectral gap can be shown using the path method [67, 32, 109, 31], which relies on finding sequences of transitions such that every pair of states communicates, but no transition is ‘overused’.

4.2 Stochastic transition matrices

In this section we briefly discuss the derivation of bounds (4.7) and (4.8) on the conductance and metastability in the stochastic setting. We firstly note some basic properties of the $\bar{p}$-flux and $\bar{p}$-invariance that hold when $\bar{P}$ is stochastic.

**Lemma 4.3.** For a stochastic transition matrix $\bar{P}$, the following properties hold.

1. $Q_{\bar{P},\bar{p}}(X, X) = 1$.

2. $Q_{\bar{P},\bar{p}}(B, B) = \bar{p}(B) - Q_{\bar{P},\bar{p}}(B^c, B)$ for all $B \subset X$.

3. $Q_{\bar{P},\bar{p}}(B, B^c) = Q_{\bar{P},\bar{p}}(B^c, B)$ for all $B \subset X$.

4. $\psi_{\bar{P},\bar{p}} = 1 - \phi_{\bar{P},\bar{p}}$.

**Proof.** Part (1) is obvious. For part (2), write $Q_{\bar{P},\bar{p}}(B, B)$ as

$$\sum_{i \in X, j \in B} \bar{p}_i \bar{P}_{ij} - \sum_{i \notin B, j \in B} \bar{p}_i \bar{P}_{ij} = \bar{p}(B) - Q_{\bar{P},\bar{p}}(B^c, B).$$

For part (3), note that

$$\sum_{i \in B, j \in X} \bar{p}_i \bar{P}_{ij} = \bar{p}(B)$$

because 1 is a right eigenvector of $\bar{P}$, and

$$\sum_{i \in X, j \in B} \bar{p}_i \bar{P}_{ij} = \bar{p}(B)$$
because $\bar{p}$ is a left eigenvector. Thus

$$\sum_{i \in B, j \in X} \bar{p}_i \bar{P}_{ij} = \sum_{i \in X, j \in B} \bar{p}_i \bar{P}_{ij},$$

and subtracting $\sum_{i,j \in B} \bar{p}_i \bar{P}_{ij}$ from each side completes the proof. The final part of the Lemma can be derived by dividing both sides of the identity in Part (2) by $\bar{p}(B)$ and then taking the minimum of both sides over all sets $B \subset X$ such that $\bar{p}(B) \leq 1/2$.

4.2.1 Bounds on $\phi_{\bar{P},\bar{p}}$ and $\psi_{\bar{P},\bar{p}}$ when $\bar{P}$ is $\bar{p}$-reversible

We state here existing results for stochastic transition matrices.

**Theorem 4.4** ([121]). For a stochastic, irreducible, $\bar{p}$-reversible matrix $\bar{P}$ with second largest eigenvalue $\lambda_{\bar{P},2}$, one has

$$\frac{1 - \lambda_{\bar{P},2}}{2} \leq \phi_{\bar{P},\bar{p}} \leq \sqrt{2(1 - \lambda_{\bar{P},2})}. \quad (4.9)$$

Bounds for $\psi_{\bar{P},\bar{p}}$ are trivially obtained from (4.9) using Part (4) of Lemma 4.3:

$$1 - \sqrt{2(1 - \lambda_{\bar{P},2})} \leq \psi_{\bar{P},\bar{p}} \leq \frac{1 + \lambda_{\bar{P},2}}{2}. \quad (4.10)$$

**Remark 8.** Following Donath and Hoffman [36] and Fiedler [41], eigenvectors with eigenvalues close to 1 have been used to construct subsets $B$ with high $\bar{p}$-invariance ratios. For example, one can set $B = \bigcup_{v_{2,i} > c} \{i\}$ or $B = \bigcup_{v_{2,i} < c} \{i\}$, where $v_2$ is the right eigenvector corresponding to $\lambda_{\bar{P},2}$. This approach has been used to spectrally partition graphs, e.g. [62] and more recently to identify almost-invariant sets in dynamical systems [49, 48].

We illustrate this heuristic in the following examples.
Example 4.5. A walk on an undirected graph $G(X, E)$ is a bi-infinite sequence of vertices \{\ldots, i_{s-1}, i_s, i_{s+1}, \ldots\} such that each pair $(i_s, i_{s+1}) \in E$. The degree of a vertex $i$ is defined as $\text{deg}_i := \# \{j \in X : (i, j) \in E\}$. A random walk on $G$ can be defined by assigning conditional transition probabilities $\bar{P}_{ij}$ of moving from $i$ to $j$. Suppose that $\bar{P}$ is the transition probability matrix corresponding to the graph $G$ shown in Figure 4.1, where the conditional transition probabilities are defined according to

$$
\bar{P}_{ij} = \begin{cases} 
\frac{1}{\text{deg}_i}, & \text{if } \text{deg}_i \neq 0; \\
0, & \text{otherwise.}
\end{cases} \tag{4.11}
$$

It is easy to verify that $\bar{p}_i = \text{deg}_i / \sum_{j \in X} \text{deg}_j$ (see Section 9.1 of [83]) and that $\bar{P}$ is $\bar{p}$-reversible. The first and second eigenvalues for $\bar{P}$ are 1 and 0.9274, and the bounds of Theorem 4.4 state that $\phi_{\bar{P}, \bar{p}} \in [0.0363, 0.3811]$ and $\psi_{\bar{P}, \bar{p}} \in [0.6189, 0.9637]$. The right eigenvector $v_2$ corresponding to $\lambda_{\bar{P}, 2}$ is

$$v_2 = (-0.3332, -0.3332, -0.3332, -0.3332, -0.3332, 0.2364, 0.2364, 0.3332, 0.3332, 0.3332).$$

Constructing $B = \bigcup_{v_2, > 0} \{i\}$ or $B = \bigcup_{v_2, < 0} \{i\}$, as described in Remark 8, gives the sets $B = \{1, 2, 3, 4, 5\}$ or $B = \{6, 7, 8, 9, 10\}$. An exhaustive calculation of (2.17) and (2.16) shows that these are the sets that attain $\phi_{\bar{P}, \bar{p}} = 0.0476$ and $\psi_{\bar{P}, \bar{p}} = 0.9524$. 

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4.2.2 Bounds on $\phi_{\bar{P},\bar{p}}$ and $\psi_{\bar{P},\bar{p}}$ when $\bar{P}$ is not $\bar{p}$-reversible

If $\bar{P}$ is not $\bar{p}$-reversible one can define the adjoint of $\bar{P}$ in $(\mathbb{R}^{[X]}, \langle \cdot, \cdot \rangle_{\bar{p}})$ by $\tilde{P}_{ij} = \bar{p}_j \bar{P}_{ji}/\bar{p}_i$.

One has

$$Q_{\tilde{P},\bar{p}}(B, B^c) = \sum_{i \in B, j \notin B} \bar{p}_i \tilde{P}_{ij} = \sum_{i \in B, j \notin B} \bar{p}_j \bar{P}_{ji} = Q_{\bar{P},\bar{p}}(B^c, B). \quad (4.12)$$

One can define $\bar{R} = (\bar{P} + \tilde{P})/2$; it is obvious that $\bar{R}$ is stochastic and that $\bar{p} \bar{R} = \bar{p}$. By (4.12) one has

$$Q_{\bar{R},\bar{p}}(B, B^c) = 1/2(Q_{\bar{P},\bar{p}}(B, B^c) + Q_{\bar{P},\bar{p}}(B^c, B)), \quad (4.13)$$

and applying part (3) of Lemma 4.3, one has $Q_{\bar{R},\bar{p}}(B, B^c) = Q_{\bar{P},\bar{p}}(B, B^c)$. Thus, applying Theorem 4.4, one obtains an analogous result for the non-$\bar{p}$-reversible case:

**Theorem 4.6** ([48, 16]). For an irreducible and stochastic matrix $\bar{P}$ and $\bar{R} = (\bar{P} + \tilde{P})/2$

with second largest eigenvalue $\lambda_{R,2}$, one has

$$1 - \frac{\lambda_{R,2}}{2} \leq \phi_{\bar{P},\bar{p}} \leq \sqrt{2(1 - \lambda_{R,2})} \quad (4.14)$$

and

$$1 - \sqrt{2(1 - \lambda_{R,2})} \leq \psi_{\bar{P},\bar{p}} \leq \frac{1 + \lambda_{R,2}}{2}. \quad (4.15)$$

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The bounds on $\phi_{\bar{P}, \bar{p}}$ given in (4.14) are a rearrangement of Theorem 5.1 in [16], while the bounds on $\psi_{\bar{P}, \bar{p}}$ in (4.15) are from [48]. The spectral heuristic for identifying high $\bar{p}$-invariant ratio subsets (see Remark 8) uses the second right eigenvector $v_2$ of $R$; see [48] for details.

4.3 Substochastic transition matrices

In this section, we construct bounds analogous to those given by Theorems 4.4 and 4.6 for substochastic Markov chains. Define $\rho_i := \sum_{j \in X} P_{ij}$ and $\rho := \min_i \rho_i \leq \rho_i \leq \max_i \rho_i =: \bar{\rho}$. We have

$$\rho \leq \lambda_{P,1} \leq \bar{\rho} \quad \text{in the general case, and} \quad (4.16a)$$

$$\rho = \lambda_{P,1} = \bar{\rho} \quad \text{iff } P1 = \lambda_{P,1}1 \quad (4.16b)$$

both elementary results of linear algebra (see eg. [89]). Further, let $p_\rho(B) := \sum_{i \in B} p_i \rho_i$ and as a direct consequence of (4.16a) we have, for all $B \subset X$,

$$p_\rho(B) \leq p_{\rho}(B) \leq \bar{p}_p(B) \quad \text{in the general case, and} \quad (4.17a)$$

$$p_{\rho}(B) = \lambda_{P,1} p(B) \quad \text{iff } P1 = \lambda_{P,1}1. \quad (4.17b)$$

We next note some properties of $P$, analogous to those given in Lemma 4.3 for the stochastic case.

**Lemma 4.7.** For a substochastic irreducible transition matrix $P$ with unique quasi-stationary distribution $p$, the following facts hold.

1. $Q_{P,p}(X, X) = \lambda_{P,1}$. 

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2. \( Q_{P,P}(B,B) = \lambda_{P,1} p(B) - Q_{P,P}(B^c, B) \) for all \( B \subset X \).

3. \( Q_{P,P}(B, B^c) = Q_{P,P}(B^c, B) + p_p(B) - \lambda_{P,1} p(B) \) for all \( B \subset X \); if \( P1 = \lambda_{P,1} 1 \),
\[
Q_{P,P}(B, B^c) = Q_{P,P}(B^c, B)
\]
for all \( B \subset X \).

4. \( \rho - \phi_{P,p} \leq \psi_{P,p} \leq \bar{\rho} - \phi_{P,p} \); if \( P1 = \lambda_{P,1} 1 \), \( \psi_{P,p} = \lambda_{P,1} - \phi_{P,p} \).

**Proof.** Part (1) is obvious. For part (2), write

\[
Q_{P,P}(B, B) = \sum_{i \in X, j \in B} p_i P_{ij} - \sum_{i \notin B, j \in B} p_i P_{ij} = \lambda_{P,1} p(B) - Q_{P,P}(B^c, B).
\]

To show the general case of part (3), note that

\[
Q_{P,P}(B, B^c) = \sum_{i \in B, j \in X} p_i P_{ij} - \sum_{i,j \in B} p_i P_{ij}
\]
\[
= p_p(B) - Q_{P,P}(B, B)
\]
\[
= p_p(B) - \lambda_{P,1} p(B) + Q_{P,P}(B^c, B),
\]

where the last equality follows by using part (2). If \( P1 = \lambda_{P,1} 1 \) then \( p_p(B) = \lambda_{P,1} p(B) \)
by (4.17b), so the general case reduces to \( Q_{P,P}(B, B^c) = Q_{P,P}(B^c, B) \). Part (4) of the Lemma follows by combining parts (2) and (3) to obtain:

\[
Q_{P,P}(B, B) = p_p(B) - Q_{P,P}(B, B^c),
\]

(4.18)

which implies

\[
\bar{p} p(B) - Q_{P,P}(B, B^c) \leq Q_{P,P}(B, B) \leq \bar{p} p(B) - Q_{P,P}(B, B^c).
\]

(4.19)
If \( P \mathbf{1} = \lambda_{P,1} \mathbf{1} \), then by (4.17b) one obtains

\[
Q_{P,p}(B,B) = \lambda_{P,1} p(B) - Q_{P,p}(B,B^c).
\] (4.20)

In the general (resp. \( P \mathbf{1} = \lambda_{P,1} \mathbf{1} \)) case, dividing (4.19) (resp. (4.20)) by \( p(B) \) and then taking the minimum of both sides over all sets \( B \subset X \) such that \( p(B) \leq 1/2 \) yields the result.

We would like to calculate the minimal \( p \)-flux ratio and maximal \( p \)-invariance ratio under \( P \). As with the stochastic case, we treat the cases where \( P \) is \( p \)-reversible and not \( p \)-reversible separately.

4.3.1 **Bounds on \( \phi_{P,p} \) and \( \psi_{P,p} \) when \( P \) is \( p \)-reversible**

We begin with a Lemma demonstrating that \( p \)-reversibility guarantees that \( P \mathbf{1} = \lambda_{P,1} \mathbf{1} \).

**Lemma 4.8.** Consider a substochastic irreducible transition matrix \( P \) with non-zero eigenvector \( p \). If \( p_i P_{ij} = p_j P_{ji} \) for all \( i, j \in X \), then \( P \mathbf{1} = \lambda_{P,1} \mathbf{1} \).

**Proof.** Summing \( p_i P_{ij} = p_j P_{ji} \) over \( i \in X \) we get \( \lambda_{P,1} p_j \) on the left hand side and \( p_j \sum_{i \in X} P_{ji} \) on the right hand side. This implies that \( \sum_{i \in X} P_{ji} = \lambda_{P,1} \) for all \( j \), or that \( P \mathbf{1} = \lambda_{P,1} \mathbf{1} \). \( \square \)

**Remark 9.** The converse of Lemma 4.8 is not true; consider for example the matrix given by

\[
P = \begin{pmatrix}
b - a & 0 & a \\
b - a & a & 0 \\
a & a & b - 2a
\end{pmatrix}.
\] (4.21)

where \( a > 0 \) and \( b > 2a \). Clearly \( P \mathbf{1} = b \mathbf{1} \). Positivity of \( P^2 \) implies \( p_i > 0 \) for \( i = 1, 2, 3 \) by the Perron-Frobenius Theorem. We have \( p_1 P_{12} = 0 \) while \( p_2 P_{21} > 0 \).
We now state and discuss the first of our main results.

**Theorem 4.9.** For an irreducible, substochastic, $p$-reversible matrix $P$ with leading eigenvalues $\lambda_{P,1} > \lambda_{P,2}$, one has

\[
\frac{\lambda_{P,1} - \lambda_{P,2}}{2} \leq \phi_{P,p} \leq \sqrt{2(\lambda_{P,1} - \lambda_{P,2})}.
\]

(4.22)

and

\[
\lambda_{P,1} - \sqrt{2(\lambda_{P,1} - \lambda_{P,2})} \leq \psi_{P,p} \leq \lambda_{P,1} + \lambda_{P,2}.
\]

(4.23)

**Proof.** See Section 4.5.1.

**Example 4.10.** We modify Example 4.5 to create a substochastic, irreducible, $p$-reversible matrix. Suppose that $P$ is the transition probability matrix corresponding to the graph $G$ shown in Figure 4.2, with a 1/16 conditional probability of transitioning from each state to an unlabelled state $H$, and the conditional transition probabilities over $X$ defined according to

\[
P = \begin{pmatrix}
0 & \frac{15}{64} & \frac{15}{64} & \frac{15}{64} & \frac{15}{64} & 0 & 0 & 0 & 0 & 0 \\
\frac{15}{64} & 0 & \frac{15}{64} & \frac{15}{64} & \frac{15}{64} & 0 & 0 & 0 & 0 & 0 \\
\frac{15}{64} & \frac{15}{64} & 0 & \frac{15}{64} & \frac{15}{64} & 0 & 0 & 0 & 0 & 0 \\
\frac{15}{64} & \frac{15}{64} & \frac{15}{64} & 0 & \frac{15}{64} & 0 & 0 & 0 & 0 & 0 \\
\frac{15}{80} & \frac{15}{80} & \frac{15}{80} & \frac{15}{80} & 0 & \frac{15}{80} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{15}{80} & 0 & \frac{15}{80} & \frac{15}{80} & \frac{15}{80} & \frac{15}{80} \\
0 & 0 & 0 & 0 & 0 & \frac{15}{64} & 0 & \frac{15}{64} & 15/64 & 15/64 \\
0 & 0 & 0 & 0 & 0 & \frac{15}{64} & \frac{15}{64} & 0 & 15/64 & 15/64 \\
0 & 0 & 0 & 0 & 0 & \frac{15}{64} & \frac{15}{64} & 15/64 & 0 & 15/64 \\
0 & 0 & 0 & 0 & 0 & 15/64 & 15/64 & 15/64 & 0 & 15/64 \\
0 & 0 & 0 & 0 & 0 & 15/64 & 15/64 & 15/64 & 15/64 & 0
\end{pmatrix}.
\]

One can check that $p_i = \deg_i / \sum_{j \in X} \deg_j$, where \(\deg_i = \# \{ j \in X : (i,j) \in E \} \) for $i \in X$, so $p_i P_{ij} = p_j P_{ji}$. Furthermore, $\lambda_{P,1} = 15/16, \lambda_{P,2} = 0.8694$, and the bounds of
Figure 4.2: A graph with a bottleneck between highly connected subsets of vertices.

Theorem 4.9 apply to give \( \phi_{P,p} \in [0.0340, 0.3690] \) and \( \psi_{P,p} \in [0.5685, 0.9035] \). The right eigenvector \( v_2 \) corresponding to \( \lambda_{P,2} \) is

\[
v_2 = (-0.3332, -0.3332, -0.3332, -0.3332, -0.2364, 0.2364, 0.3332, 0.3332, 0.3332, 0.3332).
\]

Constructing \( B = \bigcup_{v_2, >0} \{i\} \) or \( B = \bigcup_{v_2, <0} \{i\} \) (see Remark 8), we obtain the sets \( B = \{1, 2, 3, 4, 5\} \) or \( B = \{6, 7, 8, 9, 10\} \), which we can show, via exhaustive calculation of (2.17) and (2.16), are the sets that attain \( \phi_{P,p} = 0.0476 \) and \( \psi_{P,p} = 0.9524 \).

**Example 4.11.** Let \( X \subset \mathbb{C} \) be the \( n \)-th roots of unity, ie. \( X := \{z^k\}_{k=1}^n \) where \( z = e^{i2\pi k/n} \). Suppose there are undirected edges leading from each \( z^k \) to its adjacent node, forming an \( n \)-cycle with edge set \( E(\to) := (z^k, z^{k+1}) \) for \( k = \{1, \ldots, n\} \). We suppose that there are edges leading from each \( z^k \) to \( H = \{0\} \), ie. \( E(\to) = (z^k, 0) \) for all \( k = 1, \ldots, n \) with conditional probability \( \epsilon \). Consider a random walk on \( X := \{z^k\}_{k=1}^n \) with substochastic transition probability matrix \( P \) defined over \( X \) by

\[
P_{jk} = \begin{cases} 
1/2, & \text{if } j = k \\
(1 - 2\epsilon)/4, & \text{if } k = j \pm 1 \text{ mod } n; \\
0, & \text{otherwise,}
\end{cases}
\]

(4.24)
for $1 \leq j, k \leq n$. This scenario is depicted in Figure 4.3 for $n = 5$.

![Random walk defined on $\{z^k\}_{k=1}^5 \cup \{0\} \subset \mathbb{C}$, $z^5 = 1$.](image)

Figure 4.3: Random walk defined on $\{z^k\}_{k=1}^5 \cup \{0\} \subset \mathbb{C}$, $z^5 = 1$.

Since there are edges leading from $X$ to $H$, $P$ is substochastic. Further, $P$ is symmetric and hence $p$-reversible with $p = 1$. The collection of vectors $z := \{z_r\}_{r=1}^n$ whose elements are $(z_r)_j = z^{j(r-1)}$ are eigenvectors of $P$ since

$$
(Pz_r)_j = \frac{2z^{j(r-1)} + (1 - 2\epsilon)(z^{(r-1)(j+1)} + z^{(r-1)(j-1)})}{4}
= z^{j(r-1)}2 + (1 - 2\epsilon)(z^{r-1} + z^{-(r-1)})
= \lambda_{P,r}(z_r)_j,
$$

where $\lambda_{P,r} = \frac{1+(1-2\epsilon)\cos(2\pi(r-1)/n)}{2}$; see [83]. Evaluating $\lambda_{P,r}$ at $r = 1, 2$, one has $\lambda_{P,1} = 1-\epsilon$, $\lambda_{P,2} = 1/2(1 + (1 - 2\epsilon)\cos(2\pi/n))$. Hence, the bounds for $\phi_{P,p}$, as given in Theorem 4.9 are equal to

$$
\frac{(1 - 2\epsilon)(1 - \cos(2\pi/n))}{4} \leq \phi_{P,p} \leq \sqrt{(1 - 2\epsilon)(1 - \cos(2\pi/n))},
$$

(4.25)

and the bounds for $\psi_{P,p}$ are:

$$
1 - \epsilon - \sqrt{(1 - 2\epsilon)(1 - \cos(2\pi/n))} \leq \psi_{P,p} \leq \frac{3 - 2\epsilon + (1 - 2\epsilon)\cos(2\pi/n)}{4}.
$$

(4.26)
Table 4.1: Bounds on $\phi_{P,p}$ and $\psi_{P,p}$ for the substochastic reversible $n$-cycle, $\epsilon = 1/16$

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<th>$n$</th>
<th>$\lambda_{P,1}$</th>
<th>$\lambda_{P,2}$</th>
<th>Range for $\phi_{P,p}$</th>
<th>Range for $\psi_{P,p}$</th>
<th>Value of $\phi_{P,p}$</th>
<th>Value of $\psi_{P,p}$</th>
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<td>[0.1599,0.7863]</td>
<td>0.2188</td>
<td>0.7188</td>
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<td>[0.1094,0.6614]</td>
<td>[0.2761,0.8281]</td>
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</tr>
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<td>[0.0824,0.5740]</td>
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<td>0.7917</td>
</tr>
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<td>0.8500</td>
</tr>
</tbody>
</table>

The set with minimal $p$-flux for this system is found by taking a segment of length $\lfloor n/2 \rfloor$, which gives a minimal $p$-flux ratio of $(1 - 2\epsilon)/(2\lfloor n/2 \rfloor)$. Taking a segment of length $\lfloor n/2 \rfloor$ also returns the maximal $p$-invariance ratio, of $(\lfloor n/2 \rfloor + (1 - 2\epsilon)(\lfloor n/2 \rfloor - 1))/(2\lfloor n/2 \rfloor)$.

A comparison of the bounds in (4.25) and (4.26) with the values of $\phi_{P,p}$ and $\psi_{P,p}$ for different values of $n$ is given in Table 4.1. The left and right eigenvectors corresponding to $\lambda_{P,2}$ are equal (because $P$ is symmetric) and have entries $(z_2)_j = z^j$.

**Remark 10.** We contrast our results with the spectral conductance bounds for Markov processes with killing investigated by Lawler and Sokal [82] for continuous time Markov processes defined on a measurable (not necessarily finite) state space. Here we briefly recap their results, translated to a finite state space $X$. Consider a continuous time Markov process with transition rate matrix $\bar{A}_{ij} = \eta_{ij}$, where

$$\eta_{ii} := -\sum_{j \neq i} \eta_{ij}.$$ 

Lawler and Sokal consider processes that are positive-recurrent and irreducible; these two conditions ensure there is a unique finite invariant probability measure for the process [71], denoted here by $\bar{\rho}$. Next suppose that the process at state $i$ is killed (ie. exits the state space permanently) at rate $k_i \geq 0$, and define the killing matrix $K$ with entries $k_i$ on
the diagonal and 0 elsewhere. The rate matrix $A = \tilde{A} - K$ for the process with killing is given by

$$A_{ij} = \begin{cases} 
\eta_{ii} - k_i, & \text{if } i = j; \\
\eta_{ij}, & \text{otherwise},
\end{cases}$$

for $1 \leq i, j \leq n$. The definition of the minimal $\bar{p}$-flux rate under $A$ for the process with killing is given in (3.3) and (3.4) of [82], as

$$\phi_{A,\bar{p}} := \min_{B \in \mathcal{X}, \bar{p}(B) > 0} \phi_{A,\bar{p}}(B),$$

where

$$\phi_{A,\bar{p}}(B) = \frac{\sum_{i \in B, j \notin B} \bar{p}_i \eta_{ij} + \sum_{i \in B} \bar{p}_i k_i}{\bar{p}(B)} = -\frac{\sum_{i, j \in B} \bar{p}_i \eta_{ij} + \sum_{i \in B} \bar{p}_i k_i}{\bar{p}(B)} = -\frac{\sum_{i, j \in B} \bar{p}_i A_{ij}}{\bar{p}(B)}.$$  \hfill (4.27)

The numerator in (4.27) measures both the rate of flow to $B^c := X \setminus B$ and the rate of killing. Bounds on $\phi_{A,\bar{p}}$ in terms of the largest eigenvalue of $A$ are given by Theorem 3.1 of Lawler and Sokal [82]:

**Theorem 4.12** ([82]). Let $A = \tilde{A} - K$ and suppose the invariant probability measure $\bar{p}$ for the process without killing satisfies $\bar{p}_i \eta_{ij} = \bar{p}_j \eta_{ji}$ for all $i, j \in X$. Denote the largest eigenvalue of $A$ by $\lambda_{A,1}$. Choose $M$ so that $M \geq \frac{1}{\bar{p}_j} \left( \sum_{i \in X} \bar{p}_i \eta_{ij} + \frac{1}{2} k_j \right)$ for all $j \in X$. Then

$$\sqrt{-2M\lambda_{A,1}} \leq \phi_{A,\bar{p}} \leq -\lambda_{A,1}.$$  \hfill (4.28)

**Proof.** This is a simple rearrangement of Theorem 3.1 of [82]. \hfill \Box

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Our bounds in Theorem 4.9 differ from those of [82] in two ways. The bounds of Theorem 4.9 use information from the two leading eigenvalues \( \lambda_{P,1}, \lambda_{P,2} \); not only the leading eigenvalue \( \lambda_{A,1} \) as in (4.28). Furthermore, Theorem 4.12 considers the conditional probability of points leaving \( B \) according to \( \bar{p} \) (the stationary distribution for the process without killing), whereas Theorem 4.9 considers the conditional probabilities according to \( p \) (the quasi-stationary distribution for the process with killing).

4.3.2 Bounds on \( \phi_{P,p} \) and \( \psi_{P,p} \) when \( P \) is not \( p \)-reversible

Following the methodology used in the stochastic case, if a substochastic Markov chain \( P \) is not \( p \)-reversible, we construct the adjoint of \( P \) in \( (\mathbb{R}^{|X|}, \langle \cdot, \cdot \rangle_p) \), given by \( \hat{P}_{ij} = p_j P_{ji} / p_i \). Then \( R = (P + \hat{P})/2 \) is self-adjoint on \( (\mathbb{R}^{|X|}, \langle \cdot, \cdot \rangle_p) \). One can easily show that an analogue of (4.13), namely

\[
Q_{R,p}(B, B^c) = 1/2(Q_{P,p}(B, B^c) + Q_{P,p}(B^c, B)),
\]

holds for substochastic \( R \). Substituting \( Q_{P,p}(B^c, B) = Q_{P,p}(B, B^c) + \lambda_{P,1}p(B) - p_p(B) \) from Part (3) of Lemma 4.7 into (4.29), one can derive the relationship

\[
Q_{R,p}(B, B^c) = Q_{P,p}(B, B^c) + \frac{1}{2} (\lambda_{P,1}p(B) - p_p(B)).
\]

One has

\[
(pR)_j = 1/2(\rho_j + \lambda_{P,1})p_j, \quad j \in X,
\]

and

\[
(R1)_j = 1/2(\rho_j + \lambda_{P,1}), \quad j \in X.
\]
We present here a brief collection of some important results concerning the spectra of $P, \hat{P}$ and $R$. Denote the leading left and right eigenvectors of $R$ by $u_1, r$ respectively, and scale $r$ so that $\langle r, 1 \rangle_p = 1$. Denote the leading right eigenvector of $P$ by $v_1$, and form the vector $pv_1$ by elementwise multiplication, i.e. $(pv_1)_i = p_i v_{1,i}$.

The leading left and right eigenvector properties are presented in Table 4.2.

Table 4.2: Spectra of $P, \hat{P}$ and $R$

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Left Eigenvector Property</th>
<th>Right Eigenvector Property</th>
<th>Other Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P$</td>
<td>$pP = \lambda_{P,1}p$</td>
<td>$Pv_1 = \lambda_{P,1}v_1$</td>
<td>$(P1)_i = \rho_i$ and $\rho 1 \leq P1 \leq \bar{p}$</td>
</tr>
<tr>
<td>$\hat{P}$</td>
<td>$(pv_1)\hat{P} = \lambda_{P,1}(pv_1)$</td>
<td>$\hat{P}1 = \lambda_{P,1}1$</td>
<td>$(p\hat{P})_j = p_j \rho_j$ and $p\rho \leq p\hat{P} \leq p\bar{p}$</td>
</tr>
<tr>
<td>$R$</td>
<td>$u_1R = \lambda_{R,1}u_1$</td>
<td>$Rr = \lambda_{R,1}r$</td>
<td>$\frac{\rho + \lambda_{P,1}}{2}p \leq pR \leq \frac{\rho + \lambda_{P,1}}{2}p$</td>
</tr>
</tbody>
</table>

We also have the following lemma.

**Lemma 4.13.** For $P$ irreducible and substochastic with leading eigenvalue $\lambda_{P,1}$ and maximal row sum $\bar{p}$, and $R = (P + \hat{P})/2$ with largest two eigenvalues $\lambda_{R,1}, \lambda_{R,2}$, we have $\lambda_{P,1} + \bar{p} \geq 2\lambda_{R,1} > 2\lambda_{R,2}$.

**Proof.**

$$\lambda_{R,2} < \lambda_{R,1} = \lambda_{R,1} \sum_{i\in X} p_i r_i = \sum_{i,j\in X} p_i R_{ij} r_j \leq \sum_{i,j\in X} (\bar{p} + \lambda_{P,1})/2 p_j r_j = (\bar{p} + \lambda_{P,1})/2,$$  

where the second inequality follows from (4.31), also see Table 4.2.
**Theorem 4.14.** Let $P$ be an irreducible and substochastic matrix and $R = (P + \hat{P})/2$, with $\lambda_{P,1}$ the leading eigenvalue of $P$, $\lambda_{R,2}$ the second largest eigenvalue for $R$ and suppose $\lambda_{P,1} > \lambda_{R,2}$. Define $\underline{\rho} = \min_{i \in X} \sum_{j \in X} P_{ij}$ and $\bar{\rho} = \max_{i \in X} \sum_{j \in X} P_{ij}$. One has

$$\frac{2\rho - \bar{\rho} - \lambda_{R,2}}{2} - \frac{(\bar{\rho} - \lambda_{P,1})^2}{8(\lambda_{P,1} - \lambda_{R,2})} \leq \phi_{P,p} \leq \sqrt{\bar{\rho} + \lambda_{P,1} - 2\lambda_{R,2}} + \frac{\bar{\rho} - \lambda_{P,1}}{2} \leq \sqrt{\rho + \lambda_{P,1} - 2\lambda_{R,2}} + \frac{\rho - \lambda_{P,1}}{2}$$

(4.34)

and

$$\max \left( \lambda_{R,2}, \frac{2\rho - \bar{\rho} + \lambda_{P,1}}{2} \right) - \sqrt{\bar{\rho} + \lambda_{P,1} - 2\lambda_{R,2}} \leq \psi_{P,p} \leq \frac{\bar{\rho} + \lambda_{R,2}}{2} + \frac{(\bar{\rho} - \lambda_{P,1})^2}{8(\lambda_{P,1} - \lambda_{R,2})}$$

(4.35)

**Proof.** See Section 4.5.2.

**Remark 11.** When $p_{P,ij} = p_{j,P,ji}$ then $\underline{\rho} = \lambda_{P,1} = \bar{\rho}$ by (4.16b) and Lemma 4.8. Making this substitution into (4.34) and (4.35), noting $P = R$ and $\lambda_{R,2} = \lambda_{P,2}$, we recover the bounds given in Theorem 4.9 for the $p$-reversible case.

**Example 4.15.** To create a non-$p$-reversible substochastic example, we consider a random walk on the graph depicted in Figure 4.2, with conditional transition probability matrix given by

$$P = \begin{pmatrix}
0 & 1/5 & 1/5 & 1/5 & 1/5 & 0 & 0 & 0 & 0 & 0 \\
1/5 & 0 & 1/5 & 1/5 & 1/5 & 0 & 0 & 0 & 0 & 0 \\
1/5 & 1/5 & 0 & 1/5 & 1/5 & 0 & 0 & 0 & 0 & 0 \\
1/5 & 1/5 & 0 & 1/5 & 1/5 & 0 & 0 & 0 & 0 & 0 \\
1/6 & 1/6 & 1/6 & 1/6 & 1/6 & 0 & 1/6 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1/6 & 0 & 1/6 & 1/6 & 1/6 & 1/6 \\
0 & 0 & 0 & 0 & 0 & 1/5 & 0 & 1/5 & 1/5 & 1/5 \\
0 & 0 & 0 & 0 & 0 & 1/5 & 1/5 & 0 & 1/5 & 1/5 \\
0 & 0 & 0 & 0 & 0 & 1/5 & 1/5 & 1/5 & 0 & 1/5 \\
0 & 0 & 0 & 0 & 0 & 1/5 & 1/5 & 1/5 & 1/5 & 0
\end{pmatrix}.$$
The leading eigenvector of $P$ is given by

$$p = (0.0953, 0.0953, 0.0953, 0.0953, 0.1189, 0.1189, 0.0953, 0.0953, 0.1189, 0.0953).$$

The matrix $P$ is not $p$-reversible (for example $p_3 P_{35} = 0.0191$ while $p_5 P_{53} = 0.0198$). We calculate $\rho = 0.8$, $\bar{\rho} = 0.833$, $\lambda_{P,1} = 0.8079$, and $\lambda_{R,2} = 0.7461$. Calculating the bounds given in Theorem 4.14, we find that $\phi_{P,p} \in [0.0268, 0.3987]$, and $\psi_{P,p} \in [0.4180, 0.7907]$. One can calculate $\phi_{P,p} = 0.0396$ and $\psi_{P,p} = 0.7683$, with the set that attains these being $\{1, 2, 3, 4, 5\}$ or $\{6, 7, 8, 9, 10\}$.

**Example 4.16.** We modify Example 4.11 to create a substochastic, non-$p$-reversible matrix. We define a substochastic transition probability matrix $P$ over $X$ by

$$P_{jk} = \begin{cases} 
1/2, & \text{if } j = k; \\
1/4, & \text{if } j \neq n \text{ and } k = j \pm 1 \mod n; \\
(1 - 2\epsilon)/4, & \text{if } j = n \text{ and } k = j \pm 1 \mod n; \\
0, & \text{otherwise}.
\end{cases} \quad (4.36)$$

This scenario is depicted in Figure 4.4 for $n = 5$. There is no simple analytic expression

![Figure 4.4: Random walk defined on $\{z^k\}_{k=1}^5 \cup \{0\} \subset \mathbb{C}, z^5 = 1$](image)
for $\lambda_{P,1}$ or $p$ for general $n$. Because $P$ is not $p$-reversible, we form $R = (P + \hat{P})/2$.

For $n = 5$ and $\epsilon = 1/16$, the bounds (4.34) evaluate to $0.0686 \leq \phi_{P,p} \leq 0.8174$, while $Q_{p,P}(B^*,(B^*)^c)/p(B^*) = 0.2342$ with $B^* = \{z^0, z^1\}$ or $\{z^0, z^1\}$. The bounds of (4.35) evaluate to $0.1076 \leq \psi_{P,p} \leq 0.8273$, with $\psi_{P,p} = 0.75$ being attained by any pair $z^k, z^{k+1}$ for $k = 1, 2, 3$. The right eigenvector $v_2$ corresponding to $\lambda_{R,2}$ is given by

$$v_2 = (-0.6057, -0.3649, 0.3649, 0.6057, 0).$$

Constructing $B = \bigcup_{v_{2,i} > 0} \{i\}$ or $B = \bigcup_{v_{2,i} < 0} \{i\}$ (see Remark 8), we obtain the sets $\{z^1, z^2\}$ and $\{z^3, z^4\}$. A comparison of the bounds on $\phi_{P,p}$ and $\psi_{P,p}$ from Theorem 4.14 with the values of $\phi_{P,p}$ and $\psi_{P,p}$ for different values of $n$ is given in Table 4.3.

### 4.4 Conclusion

We derived new bounds on the conductance and metastability of substochastic Markov chains, in both the $p$-reversible and non-$p$-reversible cases. Our results extend existing analogous results for stochastic Markov chains, and are consistent with these well-known results in the stochastic case. Throughout the chapter two examples were presented: one example with a single transition between two highly-connected subsets of vertices, and one based on a standard $n$-cycle.
If $P$ is $p$-reversible, the bounds on the metastability and conductance (Theorem 4.9) rely only on the leading two eigenvalues of $P$. If $P$ is not $p$-reversible, the bounds (Theorem 4.14) are functions of the maximal and minimal row sums of $P$, the leading eigenvalue of $P$ and the second largest eigenvalue of $R$, the reversal of $P$. Since the maximal and minimal row sums of $P$ are equal to the leading eigenvalue of $P$ if $P$ is $p$-reversible, the bounds for the non-$p$-reversible case are consistent with the bounds for the $p$-reversible case. Additional work is needed to assess whether the new bounds that we have derived are tight.

The determination of metastable or minimally mixing subsets of a state space provides important information about the mixing properties of the system. The connection between the spectra of Markov chain transition probability matrices and the existence of metastable and minimally mixing subsets is well-established in the case of stochastic Markov chains; this chapter is a step in the direction of establishing similar connections in the case of substochastic Markov chains.

4.5 Proofs of the Theorems in Chapter 4

4.5.1 Proof of Theorem 4.9

The proof in this section closely follow the standard proof on Cheeger’s inequality. We include them here to show the applicability of these arguments to the substochastic setting.
Lower bound on $\phi_{P,p}$ of Theorem 4.9

We first show that $\frac{\lambda_{P,1} - \lambda_{P,2}}{2} \leq \phi_{p,P}$. Let

$$x_i = \begin{cases} p(B^c), & \text{if } i \in B; \\ -p(B), & \text{if } i \notin B. \end{cases}$$

One has $\langle x, 1 \rangle_p = 0$ and

$$\langle x, x \rangle_p = p(B)p(B^c)^2 + p(B^c)p(B)^2 = p(B)p(B^c)(p(B^c) + p(B)) = p(B)p(B^c).$$

Further note that for arbitrary $x \in \mathbb{R}^n$, one has

$$\langle Px, x \rangle_p = \sum_{i,j \in B} p_i P_{ij} x_i x_j + 2 \sum_{i \in B, j \notin B} p_i P_{ij} x_i x_j + \sum_{i,j \notin B} p_i P_{ij} x_i x_j, \quad (4.37)$$

by the self-adjointness of $P$ in $(X, \langle \cdot, \cdot \rangle_p)$. Substituting $x$ into (4.37) yields

$$\langle Px, x \rangle_p = p(B^c)^2 Q_{P,p}(B, B) - 2p(B^c)p(B)Q_{P,p}(B, B^c) + p(B)^2 Q_{P,p}(B^c, B^c)$$

$$= p(B^c)^2 (\lambda_{P,1} p(B) - Q_{P,p}(B, B^c)) - 2p(B^c)p(B)Q_{P,p}(B, B^c) + p(B)^2 (\lambda_{P,1} p(B^c) - Q_{P,p}(B, B^c))$$

$$= p(B^c)^2 \lambda_{P,1} p(B) + p(B)^2 \lambda_{P,1} p(B^c) - Q_{P,p}(B, B^c)(p(B^c)^2 + 2p(B^c)p(B) + p(B)^2)$$

$$= p(B^c)p(B)\lambda_{P,1} (p(B^c) + p(B)) - Q_{P,p}(B, B^c)(p(B^c) + p(B))^2$$

$$= p(B^c)p(B)\lambda_{P,1} - Q_{P,p}(B, B^c).$$

By Rayleigh’s Theorem, $\lambda_{P,2} \geq \langle Px, x \rangle_p / \langle x, x \rangle_p$, thus

$$\lambda_{P,2} \geq \frac{p(B^c)p(B)\lambda_{P,1} - Q_{P,p}(B, B^c)}{p(B)p(B^c)}.$$
Rearranging this gives
\[
\frac{Q_{P,p}(B, B^c)}{p(B)} \geq p(B^c)(\lambda_{P,1} - \lambda_{P,2}).
\]
Noting that \(p(B^c) \geq 1/2\), this becomes
\[
\frac{Q_{P,p}(B, B^c)}{p(B)} \geq \frac{\lambda_{P,1} - \lambda_{P,2}}{2}.
\]
This establishes the lower bound on \(\phi_{p,P}\).

**Upper bound on \(\phi_{P,p}\) of Theorem 4.9**

We now consider the upper bound and show that \(\phi_{p,P} \leq \sqrt{2(\lambda_{P,1} - \lambda_{P,2})}\). Denote the leading right eigenvector of \(P\) by \(v_1\) and the second left eigenvector of \(P\) be given by \(u_2\). Since \(\langle v_1, u_2 \rangle_p = 0\) and \(v_1 > 0\), \(u_2\) must have both positive and negative values. Define \(x\) by dividing \(u_2\) elementwise by \(p\), and order \(x\) as
\[
x_1 \geq x_2 \geq \ldots \geq x_k > 0 \geq x_{k+1} \geq \ldots \geq x_n
\]
for some \(k \in \{1 \ldots n\}\). Let \(B = \{1, \ldots, k\}\), and assume that \(\sum_{i \in B} p_i \leq 1/2\) (if not, switch the parity of \(u_2\)). Define \(y\) as
\[
y_i = \begin{cases} x_i, & \text{if } u_{2,i} \geq 0; \\ 0, & \text{otherwise.} \end{cases} \tag{4.38}
\]
We require two preliminary lemmas for the proof.
Lemma 4.17. For $y$ defined by (4.38), we have

$$\lambda_{P,1} - \lambda_{P,2} \geq \frac{\langle y, (\lambda_{P,1} - P)y \rangle_p}{\langle y, y \rangle_p}.$$ 

Proof. Since $u_2$ is an eigenvector of $P$, one has

$$u_2(\lambda_{P,1} - \lambda_{P,2})y = u_2(\lambda_{P,1} - P)y. \quad (4.39)$$

The left-hand side of (4.39) is

$$u_2(\lambda_{P,1} - \lambda_{P,2})y = (\lambda_{P,1} - \lambda_{P,2}) \sum_{i \in B} p_{i}y_{i}^2 = (\lambda_{P,1} - \lambda_{P,2})\langle y, y \rangle_p, \quad (4.40)$$

while the right-hand side is

$$u_2(\lambda_{P,1} - P)y = \lambda_{P,1} \sum_{i \in B} u_{2,i}y_{i} - \sum_{i \in X, j \in B} u_{2,i}P_{ij}y_j$$

$$= \lambda_{P,1}\langle y, y \rangle_p - \sum_{i \in X, j \in B} u_{2,i}P_{ij}y_j \quad (4.41)$$

$$\geq \lambda_{P,1}\langle y, y \rangle_p - \sum_{i \in B} u_{2,i}P_{ij}y_j \quad \text{since } u_{2,i} \leq 0 \text{ for } i \notin B$$

$$= \langle y, (\lambda_{P,1} - P)y \rangle_p.$$

Combining (4.39)-(4.41) yields the desired result. \qed

Lemma 4.18. For a substochastic, $p$-reversible transition matrix $P$ and arbitrary $z \in \mathbb{R}^n$,

$$\langle z, (\lambda_{P,1} - P)z \rangle_p = \frac{1}{2} \sum_{i,j \in X} p_{ij}(z_j - z_i)^2.$$
Proof.

$$\langle z, (\lambda P, 1 - P)z \rangle_p = \sum_{i \in X} z_i^2 \lambda P, 1 p_i - \sum_{i,j \in X} z_i p_{ij} z_j p_i$$

$$= \sum_{i,j \in X} z_i^2 P_{ji} p_j - \sum_{i,j \in X} z_i p_{ij} z_j p_i$$

$$= \sum_{i,j \in X} z_i^2 P_{ij} p_i - \sum_{i,j \in X} z_i p_{ij} z_j p_i \quad \text{since } P \text{ is } p\text{-reversible}$$

$$= \sum_{i,j \in X} z_i p_{ij} p_i (z_i - z_j)$$

$$= \sum_{i,j \in X} z_j p_{ji} p_j (z_j - z_i) \quad \text{interchanging } i \text{ and } j$$

$$= \sum_{i,j \in X} z_j p_{ij} p_i (z_j - z_i) \quad \text{since } P \text{ is } p\text{-reversible.}$$

Taking the average of the last and third-last lines yields,

$$\langle z, (\lambda P, 1 - P)z \rangle_p = \frac{1}{2} \sum_{i,j \in X} p_i P_{ij} (z_i - z_j)^2. \quad (4.43)$$

$$\square$$

We apply the result for general \( z \in \mathbb{R}^n \) from Lemma 4.18 to our specific vector \( y \) to re-express the inner product in the numerator of the RHS of the expression of Lemma 4.17, giving

$$\lambda_{P,1} - \lambda_{P,2} \geq \frac{1}{2} \sum_{i,j \in X} p_i P_{ij} (y_i - y_j)^2 \sum_{i \in B} p_i y_i^2$$

$$= \frac{\sum_{i < j} p_i P_{ij} (y_i - y_j)^2}{\sum_{i \in B} p_i y_i^2} \quad \text{by } p\text{-reversibility.} \quad (4.44)$$
Using the inequality \((a + b)^2 \leq 2(a^2 + b^2)\),

\[
\sum_{i<j} p_i P_{ij} (y_i + y_j)^2 \leq 2 \sum_{i<j} p_i P_{ij} (y_i^2 + y_j^2).
\]

\[
= 2 \sum_{i<j} p_i P_{ij} y_i^2 + 2 \sum_{i<j} p_i P_{ij} y_j^2 \quad \text{since } P \text{ is self-adjoint in } (X, \langle \cdot, \cdot \rangle_p)
\]

\[
= 2 \sum_{i \neq j} p_i P_{ij} y_i^2
\]

\[
\leq 2 \sum_{i \in B} p_i y_i^2.
\]

(4.45)

Hence,

\[
\frac{\sum_{i<j} p_i P_{ij} (y_i + y_j)^2}{2 \sum_{i \in B} p_i y_i^2} \leq 1.
\]

(4.46)

We multiply the RHS of (4.44) by this term; since it is \(\leq 1\) the direction of the inequality is preserved and we obtain

\[
\lambda_{P,1} - \lambda_{P,2} \geq \frac{\sum_{i<j} p_i P_{ij} (y_i - y_j)^2 \sum_{i<j} p_i P_{ij} (y_i + y_j)^2}{\sum_{i \in B} p_i y_i^2} \frac{1}{2 \sum_{i \in B} p_i y_i^2}.
\]

(4.47)

We note the following version of the Cauchy-Schwarz inequality,

\[
\left( \sum_{i<j} p_i P_{ij} (y_i^2 - y_j^2) \right)^2 \leq \left( \sum_{i<j} p_i P_{ij} (y_i - y_j)^2 \right) \left( \sum_{i<j} p_i P_{ij} (y_i + y_j)^2 \right)
\]

(4.48)

and so

\[
2(\lambda_{P,1} - \lambda_{P,2}) \geq \left( \frac{\sum_{i<j} p_i P_{ij} (y_i^2 - y_j^2)}{\sum_{i \in B} p_i y_i^2} \right)^2.
\]

(4.49)
Recall that $B = \{1, \ldots, k\}$. For $l \leq k$, we define a new set $B_l = \{1, \ldots, l\}$. Hence,

$$
\sum_{i<j} p_i P_{ij} (y_i^2 - y_j^2) = \sum_{i<j} p_i P_{ij} \left( \sum_{i \leq l < j} (y_i^2 - y_{i+1}^2) \right)
$$

(4.50)

$$
= \sum_{l=1}^{k} (y_l^2 - y_{l+1}^2) \sum_{i \in B_l, j \notin B_l} p_i P_{ij}.
$$

Since $l \leq k$, $p(B_l) \leq p(B) \leq \frac{1}{2}$. One therefore has $\phi_{P,p} \leq \phi_{P,p}(B_l)$, or $Q_{P,p}(B_l, B_l^c) \geq \phi_{P,p}(B_l)$.

$$
\sum_{i<j} p_i P_{ij} (y_i^2 - y_j^2) \geq \sum_{l=1}^{k} (y_l^2 - y_{l+1}^2) \phi_{P,p}(B_l)
$$

(4.51)

$$
= \phi_{P,p} \sum_{i=1}^{k} p_i \sum_{l=1}^{k} (y_i^2 - y_{l+1}^2)
$$

$$
= \phi_{P,p} \sum_{i \in B_l} p_i y_i^2.
$$

Therefore,

$$
2(\lambda_{P,1} - \lambda_{P,2}) \geq \phi_{P,p}^2
$$

(4.52)

Rearranging,

$$
\phi_{P,p} \leq \sqrt{2(\lambda_{P,1} - \lambda_{P,2})}
$$

(4.53)

as required.

**Bounds on $\psi_{P,p}$ of Theorem 4.9.**

By Part 4 of Lemma 4.7, we have $\psi_{P,p} = \lambda_{P,1} - \phi_{P,p}$, so we can write (4.22) as

$$
\frac{\lambda_{P,1} - \lambda_{P,2}}{2} \leq \lambda_{P,1} - \psi_{P,p} \leq \sqrt{2(\lambda_{P,1} - \lambda_{P,2})}.
$$

(4.54)
Rearranging, we obtain (4.23).

4.5.2 Proof of Theorem 4.14

Upper bound on $\psi_{P,p}$ of Theorem 4.14.

For arbitrary $x \in \mathbb{R}^n$, one has

$$\langle Rx, x \rangle_p = \sum_{i,j \in B} p_i R_{ij} x_i x_j + 2 \sum_{i \in B, j \in B^c} p_i R_{ij} x_i x_j + \sum_{i,j \in B^c} p_i R_{ij} x_i x_j. \quad (4.55)$$

Define $p_r(B) := \sum_{i \in B} p_i r_i$, and let

$$x_i = \begin{cases} 
    p_r(B^c), & \text{if } i \in B; \\
    -p_r(B), & \text{otherwise.}
\end{cases}$$

One has $\langle x, r \rangle_p = 0$ and $\langle x, x \rangle_p = p(B)p_r(B^c)^2 + p(B^c)p_r(B)^2$. Substituting this specific $x$ into (4.55), and noting that $Q_{R,p}(B, B^c) = Q_{R,p}(B^c, B)$, one obtains

$$\langle Rx, x \rangle_p = p_r(B^c)^2 Q_{R,p}(B, B) - 2p_r(B^c)p_r(B)Q_{R,p}(B, B^c) + p_r(B)^2 Q_{R,p}(B^c, B^c). \quad (4.56)$$

To derive an upper bound for $\psi_{P,p}$, we need to replace $Q_{R,p}(B, B^c)$ and $Q_{R,p}(B^c, B^c)$ with expressions involving $Q_{P,p}(B, B)$. We can derive an expression for $Q_{R,p}(B, B^c)$ by combining (4.30) with (4.18) to give:

$$Q_{R,p}(B, B^c) = Q_{P,p}(B, B^c) + \frac{1}{2} (\lambda_{P,1} p(B) - p_p(B))$$

$$= p_p(B) - Q_{P,p}(B, B) + \frac{1}{2} (\lambda_{P,1} p(B) - p_p(B))$$

$$= \frac{1}{2} (\lambda_{P,1} p(B) + p_p(B)) - Q_{P,p}(B, B). \quad (4.57)$$

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For $Q_{R,p}(B^c, B^c)$, we have

$$Q_{R,p}(B^c, B^c) = \sum_{i,j \in X} p_i R_{ij} - 2 \sum_{i \in B, j \notin B} p_i R_{ij} - \sum_{i,j \in B} p_i R_{ij}$$

by (4.55) with $x = 1$

$$= \lambda_{P,1} - 2Q_{R,p}(B, B^c) - Q_{R,p}(B, B)$$

(4.58)

$$= \lambda_{P,1} - (\lambda_{P,1} p(B) + p_p(B) - 2Q_{P,p}(B, B)) - Q_{P,p}(B, B)$$

by (4.57)

$$= \lambda_{P,1} + Q_{P,p}(B, B) - p_p(B) - \lambda_{P,1} p(B).$$

(4.59)

Substituting (4.59) and (4.57) into (4.56), we obtain

$$\langle Rx, x \rangle_p = p_r(B^c)^2 Q_{P,p}(B, B) - p_r(B^c) p_r(B) (\lambda_{P,1} p(B) + p_p(B) - 2Q_{P,p}(B, B))$$

$$+ p_r(B)^2 (\lambda_{P,1} + Q_{P,p}(B, B) - p_p(B) - \lambda_{P,1} p(B))$$

$$\geq p_r(B^c)^2 Q_{P,p}(B, B) - p_r(B^c) p_r(B) ((\bar{p} + \lambda_{P,1}) p(B) - 2Q_{P,p}(B, B))$$

$$+ p_r(B)^2 (\lambda_{P,1} + Q_{P,p}(B, B) - (\bar{p} + \lambda_{P,1}) p(B))$$

$$= Q_{P,p}(B, B) (p_r(B^c)^2 + 2p_r(B^c) p_r(B) + p_r(B)^2)$$

$$- (\bar{p} + \lambda_{P,1}) p_r(B) (p_r(B^c) + p_r(B)) + \lambda_{P,1} p_r(B)^2$$

$$= Q_{P,p}(B, B) - (\bar{p} + \lambda_{P,1}) p_r(B) p(B) + \lambda_{P,1} p_r(B)^2,$$

where the final step uses the equality $p_r(B^c)^2 + 2p_r(B^c) p_r(B) + p_r(B)^2 = 1$, a consequence of the normalisation $\langle r, 1 \rangle_p = 1$ (see Table 4.2). By Rayleigh’s Theorem, $\lambda_{R,2} \geq \langle Rx, x \rangle_p / \langle x, x \rangle_p$, thus

$$\lambda_{R,2} \geq \frac{Q_{P,p}(B, B) - (\bar{p} + \lambda_{P,1}) p_r(B) p(B) + \lambda_{P,1} p_r(B)^2}{p(B) p_r(B^c)^2 + p(B^c) p_r(B)^2}.$$
Rearranging,

\[ Q_{p_r}(B, B) \leq \lambda_{P,2}(p(B)p_r(B^c))^2 + p(B^c)p_r(B)^2 + (\bar{\rho} + \lambda_{P,1})p_r(B)p(B) - \lambda_{P,1}p_r(B)^2 \]

\[ = \lambda_{R,2}p(B)(p_r(B^c)^2 - p_r(B)^2) - (\lambda_{P,1} - \lambda_{R,2})p_r(B)^2 + (\lambda_{P,1} + \bar{\rho})p_r(B)p(B) \]

\[ = \lambda_{R,2}p(B)(p_r(B^c) - p_r(B)) - (\lambda_{P,1} - \lambda_{R,2})p_r(B)^2 + (\lambda_{P,1} + \bar{\rho})p_r(B)p(B). \]

Thus,

\[ \frac{Q_{p_r}(B, B)}{p(B)} \leq \lambda_{R,2}(p_r(B^c) - p_r(B)) - (\lambda_{P,1} - \lambda_{R,2})p_r(B)^2/p(B) + (\lambda_{P,1} + \bar{\rho})p_r(B) \]

\[ = \lambda_{R,2}(1 - 2p_r(B)) - (\lambda_{P,1} - \lambda_{R,2})p_r(B)^2/p(B) + (\lambda_{P,1} + \bar{\rho})p_r(B) \]

\[ = -((\lambda_{P,1} - \lambda_{R,2})p_r(B)^2/p(B) + (\lambda_{P,1} + \bar{\rho} - 2\lambda_{R,2})p_r(B) + \lambda_{R,2} \]

\[ \leq -(\lambda_{P,1} - \lambda_{R,2})p_r(B)^2 + (\lambda_{P,1} + \bar{\rho} - 2\lambda_{R,2})p_r(B) + \lambda_{R,2} \quad \text{if } p(B) \leq 1/2. \]

We now analyse the above quadratic equation in \( z = p_r(B) \), which varies between 0 and 1. Since \( \lambda_{P,1} - \lambda_{R,2} > 0 \), by differentiation the quadratic has a maximum at \( z^* = (\lambda_{P,1} + \bar{\rho} - 2\lambda_{R,2})/4(\lambda_{P,1} - \lambda_{R,2}) \). Thus,

\[ \frac{Q_{p_r}(B, B)}{p(B)} \leq \frac{(\lambda_{P,1} + \bar{\rho} - 2\lambda_{R,2})^2}{8(\lambda_{P,1} - \lambda_{R,2})} + \frac{(\lambda_{P,1} + \bar{\rho} - 2\lambda_{R,2})^2}{4(\lambda_{P,1} - \lambda_{R,2})} + \lambda_{R,2} \]

\[ = \frac{(\lambda_{P,1} + \bar{\rho} - 2\lambda_{R,2})^2}{8(\lambda_{P,1} - \lambda_{R,2})} + \lambda_{R,2} \]

\[ = \frac{(\lambda_{P,1}^2 + 2\bar{\rho}\lambda_{P,1} - 4\lambda_{P,1}\lambda_{R,2} - 4\bar{\rho}\lambda_{R,2} + \bar{\rho}^2 + 4\lambda_{R,2}^2) + 8\lambda_{R,2}(\lambda_{P,1} - \lambda_{R,2})}{8(\lambda_{P,1} - \lambda_{R,2})} \]

\[ = \frac{\lambda_{P,1}^2 - 2\bar{\rho}\lambda_{P,1} + \bar{\rho}^2 + 4\bar{\rho}(\lambda_{P,1} - \lambda_{R,2}) + 4\lambda_{R,2}(\lambda_{P,1} - \lambda_{R,2})}{8(\lambda_{P,1} - \lambda_{R,2})} \]

\[ = \frac{(\bar{\rho} - \lambda_{P,1})^2 + 4(\bar{\rho} + \lambda_{R,2})(\lambda_{P,1} - \lambda_{R,2})}{8(\lambda_{P,1} - \lambda_{R,2})} \]

\[ = \frac{\bar{\rho} + \lambda_{R,2}}{2} + \frac{(\bar{\rho} - \lambda_{P,1})^2}{8(\lambda_{P,1} - \lambda_{R,2})}. \]

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This completes the proof for the upper bound on $\psi_{P,p}$.

**Lower bound on $\phi_{P,p}$ of Theorem 4.14**

The proof follows the proof for the upper bound on $\psi_{P,p}$, so to avoid repetition we only provide a sketch of the proof.

First, from (4.18) we obtain

$$ Q_{P,p}(B, B) = p_p(B) - Q_{P,p}(B, B^c), \quad (4.60) $$

from (4.30),

$$ Q_{R,p}(B, B^c) = Q_{P,p}(B, B^c) + \frac{1}{2} (\lambda_{P,1}p(B) - p_p(B)), \quad (4.61) $$

and from (4.58),

$$ Q_{R,p}(B^c, B^c) = \lambda_{P,1} - 2Q_{R,p}(B, B^c) - Q_{R,p}(B, B) $$

$$ = \lambda_{P,1} - 2 \left( Q_{P,p}(B, B^c) + \frac{1}{2} (\lambda_{P,1}p(B) - p_p(B)) \right) - p_p(B) + Q_{P,p}(B, B^c) $$

$$ = \lambda_{P,1} - \lambda_{P,1}p(B) - Q_{P,p}(B, B^c), \quad (4.62) $$
where the second equality uses (4.60) and (4.61). Substituting (4.60), (4.61) and (4.62) into (4.56) we obtain

\[
\langle Rx, x \rangle_p = p_r(B^c)^2 (p_r(B) - Q_{P,p}(B, B^c)) \\
- p_r(B)p_r(B^c) (2Q_{P,p}(B, B^c) + \lambda_{P,1}p(B) - p_r(B)) \\
+ p_r(B)^2(\lambda_{P,1} - \lambda_{P,1}p(B) - Q_{P,p}(B, B^c)) \\
= -Q_{P,p}(B, B^c) - \lambda_{P,1}p(B)p_r(B) - p_r(B)p_r(B) + p_r(B)^2\lambda_{P,1} \\
\geq -Q_{P,p}(B, B^c) - p(B)p_r(B)(\lambda_{P,1} + \bar{\rho}) + \rho p(B) + p_r(B)^2\lambda_{P,1}.
\]

Applying Rayleigh’s theorem, dividing by \( p(B) \) and rearranging

\[
\frac{Q_{P,p}(B, B^c)}{p(B)} \geq p_r(B)^2(\lambda_{P,1} - \lambda_{R,2})/p(B) - (\lambda_{P,1} + \bar{\rho} - 2\lambda_{R,2})p_r(B) + (\bar{\rho} - \lambda_{R,2}) \\
\geq p_r(B)^2(\lambda_{P,1} - \lambda_{R,2}) - (\lambda_{P,1} + \bar{\rho} - 2\lambda_{R,2})p_r(B) + (\bar{\rho} - \lambda_{R,2}) \text{ if } p(B) \leq 1/2.
\]

We analyse the above quadratic equation in \( z = p_r(B) \). Since \( \lambda_{P,1} - \lambda_{R,2} > 0 \), by differentiation the quadratic has a minimum at \( z^* = (\lambda_{P,1} + \bar{\rho} - 2\lambda_{R,2})/4(\lambda_{P,1} - \lambda_{R,2}) \).

Substituting this in, grouping like terms and rearranging, one obtains

\[
\phi_{P,p} \geq \bar{\rho} - \bar{\rho} + \lambda_{R,2}/2 - (\lambda_{P,1} - \bar{\rho})^2/8(\lambda_{P,1} - \lambda_{R,2}).
\]

(4.63)

**Upper bound on \( \phi_{P,p} \) of Theorem 4.14**

Since \( R \) is self-adjoint in \((\mathbb{R}^{|X|}, \langle \cdot, \cdot \rangle_p)\), its top two left eigenvectors \( u_1, u_2 \) are orthogonal with respect to \( \langle \cdot, \cdot \rangle_{1/p} \). Since \( \langle u_1, u_2 \rangle_p = 0 \) and \( u_1 > 0 \), \( u_2 \) must have both positive and
negative values. Define \( x_i = u_{2,i}/p_i \) and order \( x \) as

\[ x_1 \geq x_2 \geq \ldots \geq x_k > 0 \geq x_{k+1} \geq \ldots \geq x_n. \]

Let \( B = \{1, \ldots, k\} \), and assume that \( \sum_{i \in B} p_i \leq 1/2 \) (if not, switch the parity of \( u_2 \)). Define \( y \) as

\[
y_i = \begin{cases} 
x_i, & \text{if } u_{2,i} \geq 0; \\
0, & \text{otherwise.}
\end{cases}
\] (4.64)

We now prove two preliminary lemmas, analogous to Lemmas 4.17 and 4.18 for the \( p \)-reversible case.

**Lemma 4.19.** For \( y \) defined by (4.64), we have

\[
\frac{\lambda_{P,1} + \bar{p}}{2} - \lambda_{R,2} \geq \frac{\langle ((\lambda_{P,1} + \bar{p})/2 - R) y, y \rangle_p}{\langle y, y \rangle_p}.
\]

**Proof.** Since \( u_2 \) is a left eigenvector of \( R \), one has

\[
u_2 \left( \frac{\lambda_{P,1} + \bar{p}}{2} - \lambda_{R,2} \right) y = u_2 \left( \frac{\lambda_{P,1} + \bar{p}}{2} - R \right) y.
\] (4.65)

The left-hand side of (4.65) is

\[
u_2 \left( \frac{\lambda_{P,1} + \bar{p}}{2} - \lambda_{R,2} \right) y = \left( \frac{\lambda_{P,1} + \bar{p}}{2} - \lambda_{R,2} \right) \sum_{i \in B} p_i y_i^2 = \left( \frac{\lambda_{P,1} + \bar{p}}{2} - \lambda_{R,2} \right) \langle y, y \rangle_p.
\] (4.66)
while the right-hand side is
\[
\begin{align*}
  u_2 \left( \frac{\lambda_{P,1} + \overline{\rho}}{2} - R \right) y &= \frac{\lambda_{P,1} + \overline{\rho}}{2} \sum_{i \in B} u_{2,i} y_i - \sum_{i \in X, j \in B} u_{2,i} R_{ij} y_j \\
  &= \frac{\lambda_{P,1} + \overline{\rho}}{2} \langle y, y \rangle_p - \sum_{i \in X, j \in B} u_{2,i} P_{ij} y_j \\
  &\geq \frac{\lambda_{P,1} + \overline{\rho}}{2} \langle y, y \rangle_p - \sum_{i, j \in B} u_{2,i} R_{ij} y_j \quad \text{since } u_{2,i} \leq 0 \text{ for } i \notin B \\
  &= \langle ((\lambda_{P,1} + \overline{\rho})/2 - R)y, y \rangle_p.
\end{align*}
\]

(4.67)

Combining (4.65)-(4.67) yields the desired result. \qed

Simplifying the statement of Lemma 4.19 one obtains the following obvious corollary, which we state here because we will use it in the final stages of the proofs of lower bound on $\phi_{P,p}$ from Theorem 4.14.

**Corollary 4.20.** For $y$ defined by (4.64), we have
\[
\lambda_{R,2} \langle y, y \rangle_p \leq \langle y, R y \rangle_p.
\]

**Lemma 4.21.** For arbitrary $z \in \mathbb{R}^n$, one has
\[
\langle z, ((\lambda_{P,1} + \overline{\rho})/2 - R)z \rangle_p \geq \frac{1}{2} \sum_{i,j \in X} p_i R_{ij} (z_i - z_j)^2.
\]
Proof.

\[
\langle z, \left( \frac{\lambda_{P,1}}{2} + \bar{\rho} - R \right) z \rangle_p = \sum_{i \in X} z_i^2 \left( \frac{\lambda_{P,1}}{2} + \bar{\rho} \right) p_i - \sum_{i,j \in X} z_i R_{ij} z_j p_i \\
\geq \sum_{i,j \in X} z_i^2 R_{ji} p_j - \sum_{i \in X} z_i R_{ij} z_j p_i \\
= \frac{1}{2} \sum_{i,j \in X} p_i R_{ij} (z_i - z_j)^2.
\]

Combining Lemmas 4.19 and 4.21, we obtain

\[
\bar{\rho} + \lambda_{P,1} - 2\lambda_{R,2} \geq \frac{2 \sum_{i<j} p_i R_{ij} (y_i - y_j)^2}{\langle y, y \rangle_p} = \frac{2 \sum_{i<j} p_i R_{ij} (y_i - y_j)^2}{\sum_{i \in B} p_i y_i^2}.
\]

(4.68)

To the right-hand side of (4.68) we now apply the same arguments as are laid out in Equations (4.46)-(4.48) in the proof of the upper bound on \( \phi_{P,p} \) in the case where \( P \) is \( p \)-reversible, to obtain

\[
\frac{2 \sum_{i<j} p_i R_{ij} (y_i - y_j)^2}{\sum_{i \in B} p_i y_i^2} \geq \left( \frac{\sum_{i<j} p_i R_{ij} (y_i^2 - y_j^2)}{\sum_{i \in B} p_i y_i^2} \right)^2.
\]

(4.69)

We now examine the numerator of the term being squared on the RHS of (4.69). Recall that \( B := \{1, \ldots, k\} \). For \( l \leq k \), we define a new set \( B_l = \{1, \ldots, l\} \). Then

\[
\sum_{i<j} p_i R_{ij} (y_i^2 - y_j^2) = \sum_{i<j} p_i R_{ij} \left( \sum_{i \leq l < j} (y_i^2 - y_{i+1}^2) \right)
\]

\[
= \sum_{l=1}^{k} (y_l^2 - y_{l+1}^2) \sum_{i \in B_l, j \in B_l^c} p_i R_{ij}.
\]

(4.70)
To show the upper bound on $\phi_{P,P}$, we make use of the expression for $Q_{R,P}(B,B^c)$ given in (4.30).

\[
\sum_{i<j} p_i R_{ij}(y_i^2 - y_j^2) \geq \sum_{l=1}^k (y_i^2 - y_{l+1}^2) \left( \sum_{i \in B_l, j \in B_{l'}^c} p_i P_{ij} - p(B_l)(\bar{\rho} - \lambda_{P,1})/2 \right).
\] (4.71)

Since $l \leq k$, $p(B_l) \leq \frac{1}{2}$, so $Q_{P,P}(B_l, B_{l'}^c) \geq \phi_{P,P} p(B_l)$. Therefore

\[
\sum_{i<j} p_i R_{ij}(y_i^2 - y_j^2) \geq \sum_{l=1}^k (y_i^2 - y_{l+1}^2) p(B_l) (\phi_{P,P} - (\bar{\rho} - \lambda_{P,1})/2)
= (\phi_{P,P} - (\bar{\rho} - \lambda_{P,1})/2) \sum_{l=1}^k (y_i^2 - y_{l+1}^2) \sum_{i=1}^k p_i
= (\phi_{P,P} - (\bar{\rho} - \lambda_{P,1})/2) \sum_{i=1}^k p_i (y_i^2 - y_{l+1}^2)
= (\phi_{P,P} - (\bar{\rho} - \lambda_{P,1})/2) \sum_{i=1}^k p_i y_i^2.
\] (4.72)

Therefore, combining (4.72) with (4.68),

\[
\bar{\rho} + \lambda_{P,1} - 2 \lambda_{R,2} \geq \left( \frac{(\phi_{P,P} - (\bar{\rho} - \lambda_{P,1})/2) \sum_{i \in B} p_i y_i^2}{\sum_{i \in B} p_i y_i^2} \right)^2
= (\phi_{P,P} - (\bar{\rho} - \lambda_{P,1})/2)^2.
\] (4.73)

Rearranging,

\[
\phi_{P,P} \leq \sqrt{\bar{\rho} + \lambda_{P,1} - 2 \lambda_{R,2} + (\bar{\rho} - \lambda_{P,1})/2}.
\] (4.74)
Lower bound on \( \psi_{p,p} \) of Theorem 4.14

Return to Equation 4.70 to give

\[
\sum_{i<j} p_i R_{ij} (y_i^2 - y_j^2) = \sum_{l=1}^{k} (y_l^2 - y_{l+1}^2) \sum_{i \in B_l, j \in B_l'} p_i R_{ij} \\
= \sum_{l=1}^{k} (y_l^2 - y_{l+1}^2) \left( \sum_{i \in B_l} p_i R_{ij} - \sum_{j \in B_l} p_i R_{ij} \right) \\
= \sum_{l=1}^{k} (y_l^2 - y_{l+1}^2) \left( \sum_{i \in B_l} \sum_{j \in X} R_{ij} - Q_{P,p}(B, B) \right).
\]

(4.75)

Since \( l \leq k \), \( p(B_l) \leq p(B) \leq \frac{1}{2} \), so \( Q_{P,p}(B_l, B_l) \leq \psi_{p,p}(B_l) \). Therefore

\[
\sum_{i<j} p_i R_{ij} (y_i^2 - y_j^2) \geq \sum_{l=1}^{k} (y_l^2 - y_{l+1}^2) \sum_{i \in B_l} p_i \left( \sum_{j \in X} R_{ij} - \psi_{p,p} \right) \\
= \sum_{l=1}^{k} (y_l^2 - y_{l+1}^2) \sum_{i=1}^{k} p_i \left( \sum_{j \in X} R_{ij} - \psi_{p,p} \right) \\
= \sum_{i=1}^{k} p_i \sum_{l=1}^{k} (y_l^2 - y_{l+1}^2) \left( \sum_{j \in X} R_{ij} - \psi_{p,p} \right) \\
= \sum \sum_{i \in B, j \in X} p_i y_i^2 R_{ij} - \psi_{p,p} \sum_{i \in B} p_i y_i^2 \\
= \sum_{i,j=1}^{n} p_i y_i^2 R_{ij} - \psi_{p,p} \sum_{i \in B} p_i y_i^2 \\
\geq \sum \sum_{i,j \in B} p_i y_i^2 R_{ij} - \psi_{p,p} \sum_{i \in B} p_i y_i^2.
\]

(4.76)
Since $y_i^2 \geq y_i y_j$, we have

$$
\sum_{i < j} p_i R_{ij} (y_i^2 - y_j^2) \geq \sum_{i,j \in B} p_i y_i y_j R_{ij} - \psi_{P,p} \sum_{i \in B} p_i y_i^2
$$

$$
= \langle y, Ry \rangle_p - \psi_{P,p} \sum_{i \in B} p_i y_i^2
$$

$$
\geq \lambda_{R,2} \langle y, y \rangle_p - \psi_{P,p} \sum_{i \in B} p_i y_i^2 \quad \text{using Corollary 4.20}
$$

$$
= \lambda_{R,2} \langle y, y \rangle_p - \psi_{P,p} \langle y, y \rangle_p.
$$

Therefore,

$$
\bar{p} + \lambda_{P,1} - 2\lambda_{R,2} \geq (\lambda_{R,2} - \psi_{P,p})^2.
$$

Rearranging,

$$
\psi_{P,p} \geq \lambda_{R,2} - \sqrt{\bar{p} + \lambda_{P,1} - 2\lambda_{R,2}}.
$$

(4.79)

Alternatively, we can combine the upper bound on $\phi_{P,p}$, with Part 4 of Lemma 4.7 ($\psi_{P,p} \geq \rho - \phi_{P,p}$), to obtain

$$
\psi_{P,p} \geq \rho - \sqrt{\bar{p} + \lambda_{P,1} - 2\lambda_{R,2}} - \frac{\bar{p} - \lambda_{P,1}}{2} = \frac{2\rho - \bar{p} + \lambda_{P,1}}{2} - \sqrt{\bar{p} + \lambda_{P,1} - 2\lambda_{R,2}}.
$$

(4.80)

Combining (4.79)-(4.80) we obtain

$$
\psi_{P,p} \geq \max \left( \lambda_{R,2}, \frac{2\rho - \bar{p} + \lambda_{P,1}}{2} \right) - \sqrt{\bar{p} + \lambda_{P,1} - 2\lambda_{R,2}}.
$$

This completes the proof of the lower bound on $\psi_{P,p}$.
Chapter 5

An analysis of the connectivity of the surface of the global ocean

Ocean dynamics operates on timescales of months to millennia. In this chapter we investigate phenomena on the ocean’s surface that manifest over very long time periods: we look for regions in which water, biomass and pollutants become trapped forever (which we refer to as attracting regions), or for long periods of time before eventually exiting (which we refer to as almost-invariant sets). While there have been several recent papers analysing almost-invariant sets in oceans [52, 24, 130], less attention has been devoted to analysing attracting regions and their basins of attraction. One study in this direction is Kazantsev [68, 69], who identified low-period orbits for a barotropic ocean model on a square. While attracting regions may be quite small in size or irregular in shape, they can nonetheless exert great influence on the dynamics globally if their basins of attraction are large. In this paper we use the basins of attraction to assess how well water mixes between different regions of the surface ocean. A better understanding of the surface ocean’s mixing properties might help us study the evolution of the so-called great ocean garbage patches [133, 78, 92, 91, 88, 130], which are regions in which plastics and other floating debris accumulate after being carried there by winds and currents.
Attracting regions have long been studied in dynamical systems \([116, 115, 90, 100]\), and a variety of different methods have been used to identify them. An intuitive method is to simulate trajectories to see whether they converge to some asymptotically stable set \([42]\). Another method \([57]\) employs Lyapunov functions \(L\), which attain local minima on periodic orbits and whose orbital derivatives are strictly negative in a neighbourhood \(U\) of periodic orbits; each sublevel set of \(L\) in \(U\) is a subset of the basin of attraction.

We will approach the problem using the set-oriented probabilistic approach that we used in Chapter 3, which is based on analysing a spatial discretisation of the flow dynamics. We take a set of short-run trajectories from a global ocean model and use these to construct a transition probability matrix, thereby representing the dynamics as a Markov chain. The transition probability matrix enables us to efficiently compute the evolution of densities and to calculate surface upwelling and downwelling. We are also able to make probabilistic statements about the flow; in particular, we can define the probability of eventual absorption into an attracting region from any other region of the surface ocean. This method has origins in cell-to-cell mapping \([64, 65]\), and was adapted to continuous-time systems in a recent paper \([75]\).

We identify attracting regions of the surface ocean and calculate the probability of being eventually absorbed into one of these. We use the absorption probabilities as a basis for partitioning the ocean into different non-overlapping regions, by calculating which attracting set a given particle is most likely to be eventually absorbed into. We compare the partitioning that we obtain using absorption probabilities with another, different method for partitioning the ocean, which is based on identifying regions that interact minimally with other regions using spectral methods developed in \([102, 26, 49, 48]\).
Our modelling framework allows for the possibility that particles of water may exit the ocean’s surface by washing up on coastlines or being absorbed into the polar ice caps. Dynamically speaking, we have an open dynamical system. Open dynamical systems theory can handle a wide variety of problems in which there is some probability of particles or trajectories exiting the computational domain, including billiards [106, 103, 13, 96, 1], wave scattering [79], lasers [60] and astronomy [95]. Our approach also allows us to determine the probability that a particle in any given location will eventually leave the computational domain.

An outline of the chapter is as follows. In Section 5.1 we describe the data and a method to discretise the dynamics. In Section 5.2 we define attracting sets, basins of attraction and absorption probabilities for the discretised dynamics, and explain how we will use these to analyse the connectivity of the ocean. In Section 5.3 we compare these results with a different method of analysing connectivity, based on a spectral method of constructing almost-invariant sets. Concluding remarks are contained in Section 5.4.

5.1 Data description, definitions and method

Let $\bar{X}$ be the entire surface of the ocean. Denote by $\bar{T}(x)$ the terminal point of a trajectory beginning at $x \in \bar{X}$ and integrated forward over 48 weeks using the (time-dependent) vector field implied by the Ocean General Circulation Model for the Earth Simulator (OFES model). OFES is a global high-resolution ocean-only model [87, 117] configured on a $1/10^\circ$ horizontal resolution grid with 54 vertical levels.

Our computational domain $X \subset \bar{X}$ consists of a 2D horizontal slice of the ocean at a depth of 15m over the region extending from $75^\circ S$ to $75^\circ N$. Forward orbits of $X$ may permanently leave $X$ via beaching or being frozen into the Arctic or Antarctic, so
$X \subset \tilde{T}(X)$. We form $T := \tilde{T}|_X : X \circlearrowleft$, the restriction of $\tilde{T}$ to $X$, and refer to $(X, T)$ as an open dynamical system, in contrast to the closed dynamical system $(\bar{X}, \bar{T})$.

In order to study the ocean’s connectivity, we first form a spatial discretisation of the dynamics using Ulam’s method, which was detailed in Section 3.1. Grid the space $X$ into boxes $\{B_i\}_{i=1}^N$. We use $2^6 \times 2^6$ boxes; discarding boxes $B_i \notin X$ leaves us with $N = 10234$ boxes. Let $\mathcal{I} := \{1, \ldots, N\}$, write $X_N := \{B_i : i \in \mathcal{I}\}$ and define the collection of all sets that are unions of boxes in $X_N$ by $\mathbf{B}_N$. Working on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with $\Omega$ being a set of events and $\mathcal{F}$ the $\sigma$-algebra corresponding to the set of measurable outcomes, we define a Markov chain $\{Z_t\}_{t \in \mathbb{N}}$ taking values on $\mathcal{I}$ whose conditional transition probabilities $\mathbb{P}(Z_{t+1} = j|Z_t = i)$ are equal to the Lebesgue proportion of mass from $B_i$ mapped to $B_j$ under one application of $T$,

$$\mathbb{P}(Z_{t+1} = j|Z_t = i) = \frac{m(B_i \cap T^{-1}(B_j))}{m(B_i)}, \quad i, j \in \mathcal{I}, \quad (5.1)$$

where $m$ is Lebesgue measure over $X$. Setting $P_{ij} := \mathbb{P}(Z_{t+1} = j|Z_t = i)$, we have a conditional transition probability matrix that satisfies

1. $P_{ij} \geq 0$ for all $i, j \in \mathcal{I}$,
2. $\sum_j P_{ij} \leq 1$ for all $i \in \mathcal{I}$, with $\sum_j P_{ij} < 1$ for at least one $i \in \mathcal{I}$.

Condition 2 is a result of the open dynamical system setting; we have

$$\sum_{j \in \mathcal{I}} P_{ij} = \sum_{j \in \mathcal{I}} \mathbb{P}(Z_{t+1} = j|Z_t = i) = \sum_{j \in \mathcal{I}} \frac{m(B_i \cap T^{-1}(B_j))}{m(B_i)} = \frac{m(B_i \cap T^{-1}(X_N))}{m(B_i)}, \quad (5.2)$$

with the final expression in (5.2) being less than 1 if there are particles in $B_i$ that exit the state space $X$ in 48 weeks under the nonrestricted map $\tilde{T}$. In practice, the entries
of \( P \) must be numerically approximated using ocean trajectory data. We initialise a set of particles on \( X \) at \( t = 1 \) Jan 2001, uniformly distributed over a \( 0.2^\circ \times 0.2^\circ \) grid (approx. 100 particles per box; there are fewer points in boxes that contain some land mass). We numerically estimate the entries of \( P \) by calculating

\[
P_{ij} = \frac{\# \{ x : x \in B_i \text{ and } T(x) \in B_j \}}{\# \{ x \in B_i \}}.
\]

A schematic description of the formation of \( P \) is given in Figure 5.1. In order to maintain a reasonably even sampling of points we reinitialise the uniform distribution of particles every 8 weeks to create 6 sets of consecutive 8 week trajectories and 6 transition matrices \( P(1), P(2), \ldots, P(6) \), as in [130]. We then form \( P = P(1) \cdot P(2) \cdot \ldots \cdot P(6) \).

In order to ensure that \( P \) is not unduly influenced by the number of seed particles per box, we recalculated \( P \) with 50 particles per box. The results presented in this section were substantially unchanged when recalculated with reduced seeding.

We can use \( P \) to visualise the forward evolution of a uniformly distributed set of points over the ocean’s surface. Let \( m_N \) be a vector with entries \( m_{N,i} = m(B_i) \), \( i \in \mathcal{I} \), and calculate \( m_N^{(k)} := m_N P^k \) for \( k \in \{0, 1, 2, \ldots\} \). These are depicted in Figure 5.2, and we can observe a divergence of mass from the Equator and a convergence toward the location of the gyres. Comparable results were obtained using a similar method in [88].

We can also calculate amounts of upwelling and downwelling over 48 weeks by imposing the restriction that the surface area of the ocean is preserved, so if \( m_{N,i}^{(1)} > m_{N,i} \) then the difference \( m_{N,i}^{(1)} - m_{N,i} \) must have been pushed down below the ocean’s surface (downwelled). Similarly, if \( m_{N,i} > m_{N,i}^{(1)} \) then the difference \( m_{N,i} - m_{N,i}^{(1)} \) must have emerged to the surface (upwelled). Ekman theory linearly relates the strength of the wind stress to
Figure 5.1: The top panel shows the configuration of a selection of particles over 4 boxes, at the time of initiation (left) and after 48 weeks (right). Note that some particles exit the box collection. In the bottom panel, the information about the movement of particles has been translated into a series of conditional probabilities of transitioning between boxes.

The mass flux in the upper 10 to 100 meters of the ocean. In our study, we assume that the thickness of the Ekman layer was a constant 50 metres over the entire ocean. We thus think of the ocean surface area as a horizontal layer of 50 metres depth. To calculate
Figure 5.2: Evolution of a uniform density under the action of $P$. The colour axes represent $m_N$, the horizontal and vertical axes represent the longitudinal and latitudinal coordinates, respectively.

Upwelling in the standard units of metres per day, we compute:

$$
\frac{50 \max\{m_{N,i} - m_{N,i}^{(1)}, 0\}}{(7 \times 48)m_{N,i}}
$$

where the factor $7 \times 48$ accounts for the number of days in 48 weeks. To calculate downwelling, we use $m_{N,i}^{(1)} - m_{N,i}$ in place of $m_{N,i} - m_{N,i}^{(1)}$ in the numerator.

In Figure 5.3a we observe a large amount of upwelling occurring around the equator, the Western coastal regions of North and South America, and the Western coastal regions of Africa, consistent with the standard observations and predictions of Ekman theory (see eg. [74]). Downwelling occurs in the North and South Pacific, the Indian, and the North and South Atlantic oceans (see Figure 5.3b), and is closely related to the regions of the
great garbage patches [130]. The numerical values of both upwelling and downwelling are consistent with recent studies; see Figure 2b of [114], for example.

![Map of upwelling and downwelling](image)

(a) Average rate of upwelling over 48 weeks (in m/day)

(b) Average rate of downwelling over 48 weeks (in m/day)

Figure 5.3: Amount of water upwelled to/downwelled from each box.

5.2 Attracting sets, basins of attraction and absorption probabilities

In this section we define the objects that we will use to analyse the connectivity of the surface ocean: attracting sets, basins of attraction and absorption probabilities.

5.2.1 Dynamical systems and attracting sets

We will use a definition of attracting sets and basins of attractions loosely based on [90].
Definition 5.1. Let \( C^c := X \setminus C \). A set \( C \) for which \( m(C \cap T^{-1}(C^c)) = 0 \) is called forward invariant, and a forward invariant set \( C \) for which \( m(C^c \cap T^{-1}(C)) > 0 \) is called attracting. For a metric space \( X \) with metric \( d \), and an attracting set \( C \), the basin of attraction \( D_C \subset X \) for \( C \) is defined as the set of points whose forward orbits tend toward \( C \).

\[
D_C := \{ x \in X : d(T^k(x), C) \to 0 \text{ as } k \to \infty \},
\]

where \( d(T^k(x), C) = \inf \{ d(T^k(x), y) : y \in C \} \).

Our definition of an attracting set, which requires a positive \( m \)-measure set of initial conditions to be attracted to \( C \), differs from classical topological definitions that require an open neighbourhood of \( C \) to be attracted; see [3, 116, 115, 90, 100].

5.2.2 Markov chains and absorption probabilities

In Definition 2.26 we introduced the idea of a closed communicating class, ie. a set of states \( S \subset I \) that communicate with all other states in \( S \) but don’t communicate with states outside of \( S \).\(^1\)

Definition 5.2. If \( S \) is a closed communicating class and we have \( P_{ij} > 0 \) for at least one \( i \notin S, j \in S \), then we will call \( S \) absorbing.

We suppose that there are \( K \) absorbing closed communicating classes \( \{S_k\}_{i=1, \ldots, K} \), and we define \( I_S := \bigcup_k S_k \). We also set \( I_T := I \setminus I_S \).

Definition 5.3. Conditional on beginning in state \( i \), the probability of eventually hitting an absorbing closed communicating class \( S_k \) is called the absorption probability into \( S_k \),

\(^1\)In graph theory applications, one can represent the states of the chain as vertices of a graph, with the transition probabilities being weighted edges between the vertices. A closed communicating class then corresponds to a strongly connected component.
and is given by

\[ h_{k,i} = \mathbb{P}\{Z_{t+r} \in S_k \text{ for some } r \geq 0 \mid Z_t = i\}. \]  

(5.5)

As each class \( \{S_k\}_{i=1,\ldots,K} \) is closed, clearly \( h_{k,i} = 0 \) for \( i \in \bigcup_{j=1,j\neq k}^K S_j \) so we are only interested in \( h_{k,i} \) for \( i \notin \bigcup_{j=1,j\neq k}^K S_j \). A result adapted from [99] gives a solution for \( h_k \).

We firstly define \( \{\hat{P}_k\}_{k \in \{1,\ldots,K\}} \) by

\[
\hat{P}_k = \begin{bmatrix}
\Pi_k P_k & 0 \\
R_k & Q_k
\end{bmatrix},
\]  

(5.6)

where \( P_{k,ij} = P_{ij} \) for \( i, j \in S_k \), \( \Pi_k \) is a diagonal matrix of size \( |S_k| \) with \( \Pi_{k,ii} = 1 / \sum_{j \in S_k} P_{ij} \) for \( i \in S_k \), \( R_{k,ij} = P_{ij} \) for \( j \in S_k, i \in I_T \) and \( Q_{k,ij} = P_{ij} \) for \( i, j \in I_T \).

**Theorem 5.4.** The vector of absorption probabilities \( h_k = (h_{k,i})_{i \in (I_T \cup S_k)} \) into an absorbing closed communicating class \( S \) is the minimal nonnegative solution to

\[
\hat{P}_k g = g
\]  

(5.7)

where \( g \) is a vector constrained to have \( g_i = 1 \) for \( i \in S_k \).
Proof. Firstly note that if \( i \in S_k \) then \( h_{k,i} = \mathbb{P}\{Z_{t+0} \in S_k \mid Z_t \in S_k\} = 1 \). Next we examine the case \( i \in I_T \). We have

\[
h_{k,i} = \mathbb{P}\{Z_{t+r} \in S_k \text{ for some } r \geq 1 \mid Z_t = i\}
\]

\[
= \mathbb{P}\{Z_{t+r} \in S_k \text{ for some } r \geq 2, Z_{t+1} \in I_T, Z_t = i\}/p_i + \mathbb{P}\{Z_{t+1} \in S_k \mid Z_t = i\}
\]

\[
= \sum_{j \in I_T} \mathbb{P}\{Z_{t+r} \in S_k \text{ for some } r \geq 2, Z_{t+1} = j, Z_t = i\}/p_i + \sum_{j \in S_k} P_{ij}
\]

\[
= \sum_{j \in I_T} \mathbb{P}\{Z_{t+r} \in S_k \text{ for some } r \geq 2 \mid Z_{t+1} = j\} \mathbb{P}\{Z_{t+1} = j, Z_t = i\}/p_i + \sum_{j \in S_k} P_{ij}
\]

\[
= \sum_{j \in I_T} \mathbb{P}\{Z_{t+r} \in S_k \text{ for some } r \geq 1 \mid Z_t = j\} P_{ij} + \sum_{j \in S_k} P_{ij}
\]

\[
= \sum_{j \in I_T} h_{k,j} P_{ij} + \sum_{j \in S_k} P_{ij}.
\]

\[\text{(5.8)}\]

Therefore, for \( i \in I_T \), we have shown that \( h_{k,i}, i \in I_T \) is a solution to the problem

\[
\sum_{j \in I_T \cup S_k} P_{ij} g_j = g_i \text{ subject to the constraint } g_j = 1 \text{ for } j \in S_k.
\]

\[\text{(5.9)}\]

Now we show that \( h_{k,i}, i \in I_T \) is the minimal solution to (5.9). Suppose that \( f \) is another solution, then \( f_i = 1 \) for \( i \in S_k \) and for \( i \in I_T \) we have

\[
f_i = \sum_{j \in I_T \cup S_k} P_{ij} f_j = \sum_{j \in S_k} P_{ij} f_j + \sum_{j \in I_T} P_{ij} f_j = \sum_{j \in S_k} P_{ij} + \sum_{j \in I_T} P_{ij} f_j.
\]

\[\text{(5.10)}\]
Substituting \( f_j = \sum_{l \in I_T \cup S_k} P_{jl} f_l \) in the final term,

\[
f_i = \sum_{j \in S_k} P_{ij} + \sum_{j \in I_T} P_{ij} \left( \sum_{l \in S_k} P_{jl} + \sum_{l \in I_T} P_{jl} f_l \right)
= \sum_{j \in S_k} P_{ij} + \sum_{j \in I_T, l \in S_k} P_{ij} P_{jl} + \sum_{j, l \in I_T} P_{ij} P_{jl} f_l
= \mathbb{P}\{Z_{t+1} \in S_k | Z_t = i\} + \mathbb{P}\{Z_{t+2} \in S_k | Z_t = i, Z_{t+1} \in I_T\} + \sum_{j, l \in I_T} P_{ij} P_{jl} f_l.
\]

(5.11)

After repeating the substitution for \( f \) in the final term \( n \) times, we obtain

\[
f_i = \mathbb{P}\{Z_{t+1} \in S_k | Z_t = i\} + \ldots + \mathbb{P}\{Z_{t+n} \in S_k | Z_t = i, Z_{t+1}, \ldots Z_{t+n-1} \in I_T\} + \sum_{j, l \in I_T} P_{ij} P_{jl} f_l.
\]

(5.12)

If \( f > 0 \) then the last term on the right is positive, and the remaining terms sum to \( \mathbb{P}\{Z_{t+n} \in S_k | Z_t = i\} \) (the probability of hitting \( S_k \) within \( n \) steps). So \( f_i \geq \mathbb{P}\{Z_{t+n} \in S_k | Z_t = i\} \), and

\[
f_i \geq \lim_{n \to \infty} \mathbb{P}\{Z_{t+n} \in S_k | Z_t = i\} = \mathbb{P}\{Z_{t+r} \in S_k \text{ for some } r \geq 0 | Z_t = i\} = h_{k,i}.
\]

(5.13)

Finally, we define the vector \( H = (H_i), i = I_T \) by

\[
H_i := \arg \max_k (h_{k,i})
\]

(5.14)

The entry \( H_i \) tells us the absorbing communicating class that a Markov chain beginning in state \( i \) will most likely hit. In the event that a single state \( i \) has an equally high probability
of hitting two different absorbing closed communicating classes (i.e. \( h_{k,i} = h_{l,i} > h_{m,i} \) for all \( m \in \{1, \ldots, K\}, m \neq k, l \)), we will set \( H_i \) to be the state with the smallest mean absorption time.\(^2\)

5.2.3 Relating attracting sets to Markov chains absorption probabilities

In Section 5.1 we defined a Markov chain representation of the dynamics, with the conditional transition probabilities defined by (5.1). We will now use this representation to relate attracting sets for dynamical systems to absorbing states for Markov chains.

**Lemma 5.5.** If \( S_k \) is an absorbing closed communicating class for the Markov chain defined by \( P \) in (5.1), then \( A_k := \bigcup_{i \in S_k} B_i \) is an attracting set for the open dynamical system \( T : X \to X \).

**Proof.** Suppose \( S_k \) is an absorbing closed communicating class for the Markov chain with conditional transition probabilities given by (5.1). Then by Definition 2.27 we have \( P_{ij} = 0 \) for \( i \in S_k, j \notin S_k \), which implies that \( m(A_k \cap T^{-1}B_j) = 0 \) for all \( j \notin S_k \), so \( A_k \) is a forward invariant set. Also, by Definition 5.2 we have \( P_{ij} > 0 \) for \( j \in S_k \) and at least one \( i \notin S_k \), which implies that \( m(B_i \cap T^{-1}(A_k)) > 0 \) for at least one \( i \notin S_k \), so \( A_k \) is an attracting set according to Definition 5.1. \( \square \)

We calculate \( h_{k,i} \) by solving (5.7). Using the numerical approximation of \( P_{ij} \) given in (5.3), \( h_{k,i} \) is equal to the proportion of particles beginning in \( B_i \) that eventually hit attracting state \( A_k \). Finally, we calculate \( H \) as per (5.14). The entry \( H_i \) is equal to the attracting set \( A_k \) that particles \( x \in B_i \) are most likely to hit when evolved by the Markov dynamics. Thus \( H \) is a natural way to identify ocean regions whose long-term behaviour is similar.

For ease of reference we summarise the steps to identify the attracting regions and the probabilities of particles hitting them in an algorithm.

**Algorithm 2.**

1. Partition the computational domain $X$ into connected sets $\{B_1, B_2, \ldots, B_N\}$.
2. Construct the transition matrix $P$ corresponding to the open system, following (5.3).
3. Determine the absorbing closed communicating classes of $P$. The communicating classes may be easily and quickly computed using eg. Tarjan’s algorithm [125].
4. Compute the vectors $h_k$ by solving (5.7) (this is simple to implement in e.g. MATLAB), and compute $H$ according to (5.14).

Applying Algorithm 2 to the global ocean’s surface, we identify 10 attracting regions: 5 in the North Pacific regions, 1 in the North Atlantic, 2 north of Alaska, 1 off the coast of Peru and 1 in the Southern Ocean. The absorption probabilities into each of these are depicted in Figure 5.4. There is a non-zero probability of absorption into the region $(106, 108) \times (-46, -42)$ off the coast of Peru (depicted in Figure 5.4b) over a large portion of the surface ocean, especially over the South Pacific, the South Atlantic and Indian oceanic regions. The absorption probability into the region at $(-144, -142) \times (62, 64)$ (depicted in Figure 5.4g) is close to 0.1 over the North Atlantic, indicating that around 10% of the water in this region will eventually be absorbed into this attracting region. Particles in the region around the North Sea have some positive probability of being absorbed into the attracting region $(-74, -70) \times (72, 74)$ (depicted in Figure 5.4j); likewise, particles in the Southern Ocean have some positive probability of being absorbed into the attracting region $(158, 160) \times (-76, -74)$ (Figure 5.4a). With the exception of the attracting region off the coast of Peru, the remainder of the regions that we identify
appear to be only very weakly attracting, with the probability of absorption being close
to zero over much of the surface ocean.

Figure 5.5 shows the vector $H$ defined by (5.14). Particles beginning anywhere in the
region shown in yellow (corresponding roughly to the North Atlantic) are all more likely
to be attracted to the attracting region in the North Atlantic (shown in Figure 5.4g) than
any other attracting set; particles beginning in a region near the Arctic shown in dark red
are more likely to be attracted to the attracting region in the Arctic (shown in Figure 5.4j)
than any other attracting set, and particle in the remainder of the ocean, encompassing
the North and South Pacific, the South Atlantic, the Indian and the Southern regions,
are more likely to be attracted to the attracting region near Peru (shown in Figure 5.4b)
than any other attracting set.

5.3 Almost-invariant sets

The definition of the absorption probabilities given in (5.7) gives the probability of hitting
an attracting set over an infinite time horizon. Often we are also interested in the dy-
namics over finite time horizons, which may be quite different to the infinite time horizon
dynamics. For example, Figure 5.4b shows that over infinitely long horizons, the proba-
bility of being absorbed into the attracting region near Peru is very high for particles in
the South Pacific region, but over time periods up to 1000 years or more, particles tend
towards the structures seen in Figure 5.2. In this section we discuss some methods to
quantify and locate almost-invariant sets in the global surface ocean.

In Section 2.1.4 we gave a definition of the $\nu$-invariance ratio for an open dynamical
system with conditionally invariant measure $\nu$. In Section 3.1.4 we went on to describe
how to construct a discretised approximation to the $\nu$-invariance ratio for the case where
Figure 5.4: Absorption probabilities into the attracting regions. Locations of the attracting regions are marked with pink crosses, and the coordinates of the crosses are given underneath each figure.
Figure 5.5: The vector $H$ defined by (5.14). Particles in the blue segment are most likely to be absorbed into the attracting set at $(106, 108) \times (-46, -42)$, which is indicated here by a blue-filled circle. Particles in the yellow segment are most likely to be absorbed into the attracting set at $(-144, -142) \times (62, 64)$, which is indicated here by a yellow-filled circle. Particles in the dark red segment are most likely to be absorbed into the attracting set at $(-74, -70) \times (72, 74)$, which is indicated here by a dark-red-filled circle. The locations of the remaining attracting sets are indicated with black crosses.

$P$ is irreducible, by using the unique left eigenvector $p$ of $P$ satisfying $\lambda P_1 P = pP$.

Irreducibility of $P$, by Definition 2.28, means that all states belong to a single communicating class. We identified ten separate absorbing closed communicating classes for $P$ in Section 5.2.1, so clearly $P$ is not irreducible, and it does not have a unique quasi-stationary distribution that we can use to construct a discretised invariance ratio. There may be several candidate measures that may be used to construct an invariance ratio.

We considered three possibilities:

Method 1: Calculate the leading eigenvector of the (substochastic) conditional transition probability matrix over the transient states $\mathcal{I}_T$.

Method 2: Use Lebesgue measure $m$. 

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Method 3: Use the $M$-year pushforward of $m$ for some choice of $M$.

Method 1 proved unsuccessful: the Markov chain restricted to $I_T$ may (and in our case does) contain absorbing closed communicating classes, so we still do not have an irreducible $P$ to work with. We therefore only consider Methods 2 and 3. For Method 3, we considered several different values of $M$, but the results did not change significantly for any choice of $M > 100$. We present results here for $M = 1000$, or $m_N^{(1000)} = m_N P^{1000}$, which is depicted in the final panel of Figure 5.2. For ease of notation we set $\eta := m_N^{(1000)}$.

We define our $\eta$-invariance ratio as:

$$
\psi_{P,\eta}(B) = \frac{\sum_{i,j \in I_B} \eta_i P_{ij}}{\sum_{i \in I_B} \eta_i},
$$

(5.15)

and our $m$-invariance ratio as:

$$
\psi_{P,m}(B) = \frac{\sum_{i,j \in I_B} m_i P_{ij}}{\sum_{i \in I_B} m_i},
$$

(5.16)

where $I_B = \{i \in I : B_i \cap B \neq \emptyset\}$ denotes the index set of boxes that make up a set $B \in B_N$. We write $\eta(B) = \sum_{i \in I_B} \eta_i$.

5.3.1 Eigenvector analysis

In this section we present alternative approaches for analysing the global dynamics of the OFES model. Our strategy is to compute eigenvectors of the matrix $P$ corresponding to real eigenvalues of $P$ close to 1. We use MATLAB’s iterative solver to rapidly compute eigenvalues and eigenvectors. Of the eigenvalues of $P$ close to 1, some correspond to eigenvectors associated with absorption to an absorbing state and some correspond to
exchange between large collections of boxes corresponding to the garbage patches [55].
The leading eigenvalues of $P$ are listed in Table 5.1. We visualise the eigenvectors in order
to determine their supports and associate them with the type of metastable behaviour
they correspond to. We are interested in those that demonstrate a concentration of mass
around the location of the five great ocean garbage patches, present in the North and
South Pacific, Indian, and North and South Atlantic Oceans [133, 78, 92, 91, 88, 130]. A
selection of the leading 15 left eigenvectors of $P$ that demonstrate these phenomena are
presented in Figure 5.6.

It is well known that the right eigenvectors of time-symmetric systems provide inform-
ation on almost-invariant sets (see Chapters 3 and 4, also [49, 48]). For Markov chains,
time-symmetry is implied by the detailed balance condition given in Definition 2.31. Our
Markov model of the dynamics of the surface ocean is not time-symmetric; the pres-
ence of the attracting sets is enough to guarantee this. Hence we will look at the right
eigenvectors of both $P$ and $\hat{P}$, where $\hat{P}_{ij} = \eta_j P_{ji}/\eta_i$ governs the dynamics under time
reversal\(^3\). The right eigenvectors of $\hat{P}$ contain information about the almost-invariant
sets for the forward flow, while the right eigenvectors of $P$ contain information about the
almost-invariant sets for the flow in backward time.

In Figure 5.7 we present two right eigenvectors of $\hat{P}$. The ones that we select, $v_{\hat{P},6}$
and $v_{\hat{P},9}$, were chosen because of the distinct level sets visible in their structure; this
structure is visible spatially in Figures 5.7a and 5.7b. The same level set structure was
repeated in some other eigenvectors, so to avoid repetition we do not show these, and
we also omit eigenvectors that only contain a very small number of non-zero terms. In

\[^3\text{If } P \text{ were irreducible, one would define } \hat{P}_{ij} = p_j P_{ji}/p_i \text{ where } p \text{ is the unique quasi stationary}
\text{distribution, as we did in Chapter 3 and 4. Our use of } \eta \text{ here means that our } \hat{P} \text{ is only an approximation}
\text{to the reversed-time dynamics.} \]
Figure 5.7a, one can identify a yellow triangular patch extending outwards from South America, and a blue patch extending from the west of Africa. The former is associated with the cold tongue of El Nino [61] and the latter correlates with the location of the Benguela upwelling area [98]. The Indonesian Throughflow (the phenomenon by which water from the Pacific shifts into the Indian Ocean via the Indonesian Archipelago [122]) is also visible in both Figure 5.7a and 5.7b, as is the movement of Pacific waters into the South Atlantic through Drake Passage at the Southern tip of South America.

In Figure 5.8 we show four right eigenvectors of $P$, again selected because of the distinct level sets visible in them. The differently-coloured patches in Figures 5.8a-5.8d can be related to the location of the garbage patches identified in Figure 5.2d and Figure 5.7. The set shown in dark blue in Figure 5.8a and dark red in Figure 5.8b contains the North Pacific garbage patch; the set shown in light blue in Figure 5.8a contains the South Atlantic garbage patch; the set shown in yellow in Figure 5.8a and dark red in Figure 5.8d contains the garbage patch between Australia and Africa; the set shown in dark red in Figure 5.8a and orange in Figure 5.8c contains the North Atlantic garbage patch; and the set shown in dark red in Figure 5.8a and blue in Figures 5.8b-5.8d contains the South Pacific patch.

The clearly-defined patterns visible in the depicted right eigenvectors of $\hat{P}$ and $P$ indicate that we may be able to successfully adapt the final steps of Algorithm 1 in Section 3.4 to an algorithm for locating almost-invariant sets in the surface ocean. Similar algorithms were used in [52, 24] to identify almost-invariant sets in the surface ocean and the three-dimensional ocean respectively. Our study differs from [52, 24] firstly because we consider a global ocean model rather than a subset of the ocean, and secondly because
we treat the ocean as an open dynamical system rather than a closed system as other studies have done.

**Algorithm 3.**

1. Form $\hat{P}_{ij} = \eta_j P_{ji} / \eta_i$ and $R = (P + \hat{P}) / 2$, and compute the 15 largest eigenvalues $\lambda_{R,r}, r = 1, \ldots, 15$, and corresponding right eigenvectors $v_{R,r}$ of $R$.

2. For $r \in \{1, \ldots, 15\}$, for $c_r \in [\min v_{R,r,i}, \max v_{R,r,i}]$ define $B_{r,1}(c_r) = \bigcup_{i : v_{R,r,i} \leq c_r} B_i$ and $B_{r,2}(c_r) = \bigcup_{i : v_{R,r,i} > c_r} B_i$. By incrementing $c_r$, find $c_{r,1} = \arg\max_{c_r} \{\psi_{P,\eta}(B_{r,1}(c_r)) : \eta(B_{r,1}(c_r)) \leq 1/2\}$ and $c_{r,2} = \arg\max_{c_r} \{\psi_{P,\eta}(B_{r,2}(c_r)) : \eta(B_{r,2}(c_r)) \leq 1/2\}$.

3. For each $r \in \{1, \ldots, 15\}$, return $\max\{\psi_{P,\eta}(B_{r,1}(c_{r,1})), \psi_{P,\eta}(B_{r,2}(c_{r,2}))\}$ as the maximal almost-invariance ratio found for the open system and set $B_{r,\text{opt}}$ to whichever of $B_{r,1}(c_{r,1})$ or $B_{r,2}(c_{r,2})$ achieves this maximum.

Applying Algorithm 3 we compute $R$ and the top 15 eigenvalues are tabulated in the last column of Table 5.1. After thresholding as per Step 2 of Algorithm 3, we find three interesting sets depicted in the right column of Figure 5.9, with invariance ratios given in Table 5.2.

The left column of 5.9 shows selected eigenvectors of $R$; we omit eigenvectors that only contain a very small number of non-zero terms, and do not add any information on the location of the almost-invariant sets, or which correspond the attracting sets that we identified in Section 5.2. The set identified in Figure 5.9b corresponds to the North Pacific Ocean. In Figure 5.9d we can identify the North Atlantic Ocean; Figure 5.9f appears to capture a highly invariant subset of the Indian Ocean.
Table 5.1: Top 15 eigenvalues for \( \hat{P}, P, R \).

<table>
<thead>
<tr>
<th>( \lambda )</th>
<th>( P )</th>
<th>( P )</th>
<th>( R )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda_1 )</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_2 )</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_3 )</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_4 )</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_5 )</td>
<td>1.0000</td>
<td>0.9999</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_6 )</td>
<td>0.9999</td>
<td>0.9999</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_7 )</td>
<td>0.9999</td>
<td>0.9996</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_8 )</td>
<td>0.9996</td>
<td>0.9991</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_9 )</td>
<td>0.9991</td>
<td>0.9975</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_{10} )</td>
<td>0.9975</td>
<td>0.9913</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_{11} )</td>
<td>0.9913</td>
<td>0.9852</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_{12} )</td>
<td>0.9852</td>
<td>0.9838</td>
<td>1.0000</td>
</tr>
<tr>
<td>( \lambda_{13} )</td>
<td>0.9838</td>
<td>0.9826</td>
<td>0.9999</td>
</tr>
<tr>
<td>( \lambda_{14} )</td>
<td>0.9826</td>
<td>0.9680</td>
<td>0.9997</td>
</tr>
<tr>
<td>( \lambda_{15} )</td>
<td>0.9680</td>
<td>0.9645</td>
<td>0.9994</td>
</tr>
</tbody>
</table>

Table 5.2: Summary of results for the surface ocean.

<table>
<thead>
<tr>
<th>Eigenvector used for thresholding</th>
<th>Eigenvector used for thresholding</th>
<th>Eigenvector used for thresholding</th>
<th>Eigenvector used for thresholding</th>
<th>Eigenvector used for thresholding</th>
<th>Eigenvector used for thresholding</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \psi_{P,\eta}(B_{opt}^c) )</td>
<td>( \eta(B_{opt}^c) )</td>
<td>( \psi_{P,m}(B_{opt}^c) )</td>
<td>( m(B_{opt}^c) )</td>
<td>( \psi_{P,m}(B_{opt}^c) )</td>
<td>( m(B_{opt}^c) )</td>
</tr>
<tr>
<td>Right 11th eigenvector of ( R )</td>
<td>0.9999</td>
<td>0.9999</td>
<td>0.2181</td>
<td>0.9804</td>
<td>0.4358</td>
</tr>
<tr>
<td>Right 12th eigenvector of ( R )</td>
<td>0.9999</td>
<td>0.9999</td>
<td>0.2281</td>
<td>0.9830</td>
<td>0.4996</td>
</tr>
<tr>
<td>Right 13th eigenvector of ( R )</td>
<td>0.9999</td>
<td>0.9975</td>
<td>0.1874</td>
<td>0.9902</td>
<td>0.5000</td>
</tr>
</tbody>
</table>

5.4 Conclusion

Ulam’s method, now a staple tool in many dynamical systems applications, enables one to use standard results from Markov chain theory to draw inferences about dynamical systems. In this chapter we built a Markov representation of the dynamics of the global surface ocean. We were then able to simply compute the evolution of densities and to calculate surface upwelling and downwelling, and to define the probability of eventual absorption into an attracting region from any other region of the surface ocean, exploiting a connection between attracting sets for dynamical systems and absorbing closed communicating classes of Markov chains. We used the absorption probabilities as a basis
for partitioning the ocean into different non-overlapping regions, by calculating which attracting set a given particle is most likely to be eventually absorbed into.

Upon examining the eigenvectors of both $P$ and $\hat{P}$, we were able to identify patterns that provide information about the almost-invariant sets of the Markov dynamics in both forward and backward time. Using the eigenvectors of the symmetrised conditional transition probability matrix, we identified three almost-invariant sets in the surface of the global ocean over a 48 week duration.
Figure 5.6: Selected left eigenvectors of $P$ showing the locations of the five great ocean garbage patches.

Figure 5.7: Right eigenvectors $\{v_{\hat{P},r}\}$ of $\hat{P}$.  

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Figure 5.8: Right eigenvectors $\{v_{P,r}\}$ of $P$. 
Figure 5.9: Left column: right eigenvectors of $R$. Right column: $B_{r}^{opt}$ obtained by applying Algorithm 3
The primary goal of this thesis was to investigate the property of metastability or almost-invariance in open dynamical systems. We sought to both locate almost-invariant sets and to derive bounds on the maximal almost-invariance ratio for a given open dynamical system. Our approach to achieve these aims was to discretise the open dynamical system, representing the dynamics via a substochastic Markov chain $P$ with (unique) quasi-stationary distribution $p$.

We began in Chapter 2 by surveying the extant research in open dynamical systems and metastability, and providing definitions of the objects that we used throughout the thesis. In particular, we quantified metastability for open systems by $\Psi_{\mathcal{P},\nu}$, and for discretised open systems by $\psi_{\mathcal{P},p}$.

In Chapter 3, we developed a new closing operation to construct a Markov operator $\hat{\mathcal{P}}$ from the conditional Perron-Frobenius operator $\mathcal{P}$. We related $\Psi_{\mathcal{P},\nu}(B)$ to $\Psi_{\hat{\mathcal{P}},p}(B)$, showing that they differ by an amount equal to the conditionally invariant measure of the set in question intersected with the hole. We developed $\hat{\mathcal{P}}$, the discretised counterpart to $\hat{\mathcal{P}}$ and developed rigorous upper and lower bounds for the maximum possible invariance ratios of discretised sets based on the second eigenvalue of a matrix $\tilde{R}$ constructed from
The eigenvectors of $\hat{R}$ were also used to locating almost-invariant sets, a method adapted from existing techniques for closed dynamical systems.

In Chapter 4, we focussed on deriving rigorous upper and lower bounds for the conductance and metastability of substochastic Markov chains, distinguishing two cases: one where $P$ satisfies a generalised detailed balance condition and one where it does not. In the former case, the bounds on the metastability and conductance (Theorem 4.9) rely only on the leading two eigenvalues of $P$. In the latter case, the bounds (Theorem 4.14) are functions of the maximal and minimal row sums of $P$, the leading eigenvalue of $P$ and the second largest eigenvalue of $R$, the reversal of $P$.

In Chapter 5, we turned our attention back to locating almost-invariant sets. We looked at ways to define the basin of attraction for open systems that additionally contain some internal sink, and used the absorption probabilities as a method to divide the ocean into separate regions. While we did not present rigorous results demonstrating the applicability of spectral methods in the context of the global surface ocean, we were nonetheless able to identify almost invariant sets using the eigenvectors of the symmetrised conditional transition probability matrix.

In conclusion, we have demonstrated a connection between the spectra of substochastic Markov chain transition matrices and the existence of metastable and minimally mixing subsets. This connection, while well-established for stochastic Markov chains and for closed dynamical systems, is a new contribution in the field of open dynamical systems.
References


