Prediction in Projection: A new paradigm in delay-coordinate reconstruction

by

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Prediction in Projection: A new paradigm in delay-coordinate reconstruction

Thesis directed by Prof. Elizabeth Bradley

Delay-coordinate embedding is a powerful, time-tested mathematical framework for reconstructing the dynamics of a system from a series of scalar observations. Most of the associated theory and heuristics are overly stringent for real-world data, however, and real-time use is out of the question due to the expert human intuition needed to use these heuristics correctly. The approach outlined in this thesis represents a paradigm shift away from that traditional approach. I argue that perfect reconstructions are not only unnecessary for the purposes of delay-coordinate based forecasting, but that they can often be less effective than reduced-order versions of those same models. I demonstrate this using a range of low- and high-dimensional dynamical systems, showing that forecast models that employ *imperfect* reconstructions of the dynamics—*i.e.*, models that are not necessarily true embeddings—can produce surprisingly accurate predictions of the future state of these systems. I develop a theoretical framework for understanding why this is so. This framework, which combines information theory and computational topology, also allows one to quantify the amount of predictive structure in a given time series, and even to choose which forecast method will be the most effective for those data.

Dedication

To Mom.

This dissertation—and my entire academic journey—would have been abandoned multiple times, and likely never would have begun, if it were not for your endless love and support.

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Chapter 1

Overview and Motivation

Complicated nonlinear dynamics are ubiquitous in natural and engineered systems. Methods that capture and use the state-space structure of a dynamical system are a proven strategy for forecasting the behavior of systems like this, but use of these methods is not always straightforward. The governing equations and the state variables are rarely known; rather, one has a single (or perhaps a few) series of scalar measurements that can be observed from the system. It can be a challenge to model the full dynamics from data like this, especially in the case of *forecast* models, which are only really useful if they can be constructed and applied on faster time scales than those of the target system. While the traditional state-space reconstruction machinery is a good way to accomplish the task of modeling the dynamics, it is problematic in real-time forecasting because it generally requires input from and interpretation by a human expert. This thesis argues that that roadblock can be sidestepped by using a reduced-order variant of delay-coordinate embedding to build forecast models: I show that the resulting forecasts can be as good as—or better than—those obtained using complete embeddings, and with far less computational and human effort. I then explore the underlying reasons for this using a novel combination of techniques from computational topology and information theory.

Modern approaches to modeling a time series for forecasting arguably began with Yule's work on predicting the annual number of sunspots [122] through what is now known as *autoregression*. Before this, time-series forecasting was done mostly through simple global extrapolation [119]. Global linear methods, of course, are rarely adequate when one is working with nonlinear dynamical systems; rather, one needs to model the details of the state-space dynamics in order to make accurate predictions. The usual first step in this process is to reconstruct that dynamical structure from the observed data. The state-space reconstruction techniques proposed by Packard *et al.* [89] in 1980 were a critical breakthrough in this regard. In 1981, Takens showed that this method, *delay-coordinate embedding*, provides a topologically correct representation of a nonlinear dynamical system if a specific set of theoretical assumptions are satisfied. I discuss this in detail in Section 2.1.1 alongside the appropriate citations.

A large number of creative strategies have been developed for using the state-space structure of a dynamical system to generate predictions, as discussed in depth in Section 2.3.3. Perhaps the most simple of these is the "Lorenz Method of Analogues" (LMA), which is essentially nearestneighbor prediction [72]. Even this simple strategy, which builds predictions by looking for the nearest neighbor of a given point and taking that neighbor's observed path as the forecast—works quite well for forecasting nonlinear dynamical systems. LMA and similar methods have been used successfully to forecast measles and chickenpox outbreaks [112], marine phytoplankton populations [112], performance dynamics of a running computer(e.g., [36,37]), the fluctuations in a far-infrared laser [98, 119], and many more.

The reconstruction step that is necessary before any of these methods can be applied to scalar time-series data, however, can be problematic. Delay-coordinate embedding is a powerful piece of machinery, but estimating good values for its two free parameters, the time delay τ and the dimension m, is not trivial. A large number of heuristics have been proposed for this task, but these methods, which I cover in depth in Sections 2.1.2 and 2.1.3, are computationally intensive and they require input from—and interpretation by—a human expert. This can be a real problem in a prediction context: a millisecond-scale forecast is not useful if it takes seconds or minutes to produce. If effective forecast models are to be constructed and applied in a manner that outpaces the dynamics of the target system, then, one may not be able to use the full, traditional delay-coordinate embedding machinery to reconstruct the dynamics. And the hurdles of delay-coordinate reconstruction are even more of a problem in nonstationary systems, since the reconstruction machinery is only guaranteed to work for an infinitely long noise-free observation of a single dynamical system. This means that no matter how much effort and human intuition is put into estimating m, or how precise a heuristic is developed for that process, the theoretical constraints of delay-coordinate embedding can never be satisfied in practice. This means that an experimentalist can never guarantee, on any theoretical basis, the correctness of their embedding, no matter their choice of m. In Section 2.1, I provide an in-depth discussion of these issues.

The conjecture that forms the basis for this thesis is that a formal embedding, although mandatory for detailed dynamical analysis, *is not necessary for the purposes of prediction*—in particular, that reduced-order variants of delay-coordinate reconstructions are adequate for the purposes of forecasting, even though they are not true embeddings [38]. As a first step towards validating that conjecture, I construct two-dimensional time-delay reconstructions from a number of different time-series data sets, both simulated and experimental, and then build forecast models in those spaces. I find that forecasts produced using the Lorenz method of analogues on these reduced-order models of the dynamics are roughly as accurate as—and often even *more* accurate than—forecasts produced by the same method working in the complete embedding space of the corresponding system. This exploration is detailed in Chapter 4.

Figure 1.1 shows a quick proof-of-concept example: a pair of forecasts of the so-called "Dataset A," a time series from a far-infrared laser from the Santa Fe Institute prediction competition [119]. Even though the low-dimensional reconstruction used to generate the forecast in the right panel of the figure is not completely faithful to the underlying dynamics of this system, it appears to be good enough to support accurate short-term forecast models of nonlinear dynamics. While this example is encouraging, Dataset A is only one time series and it was drawn from a comparatively simple system—one that is well-described by a first-return map (or, equivalently, a one-dimensional surface of section). The examples presented in Chapter 4 offer a broader validation of this thesis's central claim by constructing forecasts using two-dimensional delay reconstructions of ensembles of data sets from a number of different systems whose dynamics are far more complex than the time series in Figure 1.1. Uniformly, the results indicate that the full complexity (and



(a) LMA on a complete embedding

(b) LMA on a two-dimensional delay reconstruction

Figure 1.1: Forecasts of SFI Dataset A using Lorenz's method of analogues in (a) a delay-coordinate embedding of the state-space dynamics and (b) a 2D delay reconstruction of those dynamics. Blue os are the true continuation c_j of the time series and red xs (p_j) are the forecasts; black error bars are provided if there is a discrepancy between the two. Reconstruction parameter values for (a) were estimated using standard techniques: the first minimum of the average mutual information [33] for the delay in both images and the false-near neighbor (FNN) method of Kennel *et al.* [62], with a threshold of 10%, for the dimension in the left-hand image. Even though the 2D reconstruction used in (b) is not faithful to the underlying topology, it enables successful forecasting of the time series.

effort) of the delay-coordinate 'unfolding' process may not be strictly necessary to the success of forecast models of real-world nonlinear dynamical systems. Finally, I want to emphasize that this reduced-order strategy is intended as a *short*-term forecasting scheme. Dimensional reduction is a double-edged sword; it enables on-the-fly forecasting by eliminating a difficult estimation step, but it effects a guaranteed memory loss in the model. I explore this limitation experimentally in Section 4.3 and theoretically in Section 5.1.3.

While the results in Chapter 4 are interesting from a practical perspective, in that they allow delay-coordinate reconstruction to be used in real time, they are perhaps even more interesting from a theoretical perspective. The central premise of this thesis is a heresy, according to the dogma of delay-coordinate embedding, but regardless, it works. This naturally leads to the need for a deeper exploration into why such a deviation from theory provides so much practical traction.

That exploration is precisely the focus of Chapter 5, where I provide two disjoint explanations of why prediction in projection—my reduced-order strategy—works. The first is from an information theoretic perspective; the second utilizes computational topology. These two disjoint branches of mathematics offer two very different, but quite complementary, tools for exploring this discontinuity between theory and practice. The prior, the subject of Section 5.1, provides a framework for understanding how information is stored and transmitted from past to future in delay-coordinate reconstructions. Building upon ideas from this field, I develop a novel method called time-delayed active information storage (\mathcal{A}_{τ}) that can be used to select forecast-optimal parameters for delay-coordinate reconstructions [42]. Using \mathcal{A}_{τ} , I show that for noisy finite length time series, a two-dimensional projection (*i.e.*, m = 2) often provides as much—or more—information about the future than a traditional embedding. This further corroborates the central premise of this thesis. This counter-intuitive result, its source, and its implications are discussed in depth in Section 5.1.3. Section 5.2 offers an alternative view of the reconstruction process—one based on topology. As I discuss in Section 2.1.1, the theoretical restrictions of delay-coordinate embedding are intended to ensure a *diffeomorphic* reconstruction, something that is required for analysis of dynamical invariants but that is excessive for reconstruction of topology. I conjecture that one of the reasons prediction in projection works is that topology (which is preserved by a homeomorphism) becomes correct at much lower embedding dimensions than what one would expect from the associated theorems. The results in Section 5.2 confirm this, providing insight into the mechanics of prediction in projection, explaining why this approach exhibits so much accuracy while being theoretically wrong, and offering a deeper understanding into delay-coordinate reconstruction theory in general.

Of course, no forecast model will be ideal for *every* task. In fact, as a corollary of the undecidability of the halting problem [117], no single forecasting schema is ideal for all noise-free deterministic signals [119]—let alone all real-world time-series data sets. I do not want to give the impression that this reduced-order model will be effective for *every* time series, but I have shown that it is effective for a broad spectrum of signals. Following this line of reasoning, it is important to be able to determine when prediction is possible at all, and, if so, what forecast model is the best one to use. To this end, I have developed a Shannon information-theory based heuristic for

quantifying precisely when a given time-series is predictable given the correct model [41]. This heuristic—the focus of Chapter 6—allows for *a priori* evaluation of when prediction in projection will be effective.

The rest of this thesis is organized as follows. Chapter 2 reviews all the necessary background and related work, including the theory and practice of delay-coordinate embedding, information theory, and the forecast methods, as well as the figure of merit that I use for assessing forecast accuracy. In Chapter 3, I introduce the case studies used in this thesis. In Chapter 4, I demonstrate the effectiveness of this reduced order forecast strategy on a range of different examples, comparing it to traditional linear and nonlinear forecasting strategies, and exploring some of its limitations. In Chapter 5, I provide a mathematical foundation for *why* prediction in projection works. In Chapter 6, I describe a measure for quantifying time-series predictability to understand *when* my reduced-order method—or any forecasting strategy—will be effective. At the end of Chapters 4-6 I discuss specialized avenues of future research directly associated with the specific contribution of that chapter. In Chapter 7, I conclude and outline the next frontier of this work: developing strategies for grappling with nonstationary time series in the context of delay coordinate based forecasting—which, I believe, will require a combination of all aspects of this thesis to solve.

Chapter 2

Background and Related Work

2.1 Reconstructing Nonlinear Deterministic Dynamics

The term nonlinear deterministic dynamical system describes a set X combined with a deterministic nonlinear evolution or update rule Φ , also called the generating equations. The set X could be as simple as \mathbb{R}^n or a similar geometric manifold, or as abstract as a set of symbols [79]. Elements of the set X are referred to as *states* of the dynamical system; the set X is generally referred to as the *state space*. The update or evolution rule is a fixed mapping that gives a unique image to any particular element of the set. In the problems treated in this thesis, this update rule is deterministic and fixed: given a particular state, the next state of the system is completely determined. The theory of dynamical systems is both vast and rich. This section of this dissertation is intended to review the subset of this field that is needed to understand the core ideas of my thesis. It is not intended as a general review of this field. For more complete reviews, see [14, 59, 79].

Dynamical systems can be viewed as falling into one of two categories: those that are discrete in time and those that are continuous in time. The former are referred to as maps and denoted by

$$\vec{y}_{n+1} = \Phi(\vec{y}_n), n \in \mathbb{N} \tag{2.1}$$

The latter are referred to as flows and are represented by a system of first-order ordinary differential equations

$$\frac{d}{dt}\vec{y}(t) = \Phi(\vec{y}(t)), t \in \mathbb{R}^+$$
(2.2)

When the generating equations Φ of a dynamical system are known, the future state of any particular initial condition can be completely determined. Unfortunately, knowledge of the generating equations (or even the state space) is a luxury that is very rarely afforded to an experimentalist. In practice, the dynamical system under study is a black box that is observed at regular time intervals. In such a situation, one can reconstruct the underlying dynamics using so-called *delay-coordinate embedding*, the topic of the following section.

2.1.1 Delay-Coordinate Embedding

The process of collecting a time series $\{x_j\}_{j=1}^N$ or trace is formally the evaluation of an observation function [99] $h : \mathbb{X} \to \mathbb{R}$ at the true system state $\vec{y}(t_j)$ at time t_j for j = 1, ..., N, *i.e.*, $x_j = h(\vec{y}(t_j))$ for j = 1, ..., N. Specifically, h smoothly observes the path of the dynamical system through state space at regular time intervals, *e.g.*, measuring the angular position of a pendulum every 0.01 seconds or measuring the average number of instructions executed by a computer per cycle [6,83]. Provided that the underlying dynamics Φ and the observation function h—are both smooth and generic, Takens [113] formally proves that the delay coordinate map

$$F(h, \Phi, \tau, m)(\vec{y}(t_j)) = ([x_j \ x_{j-\tau} \ \dots \ x_{j-(m-1)\tau}]) = \vec{x}_j$$
(2.3)

from an *d*-dimensional smooth compact manifold M to \mathbb{R}^m is almost always a diffeomorphism on M whenever $\tau > 0$ and m is large enough, *i.e.*, m > 2d.

Definition (Diffeomorphism, Diffeomorphic). A function $f : M \to N$ is said to be a diffeomorphism if it is a C^1 bijective correspondence whose inverse is also C^1 . Two manifolds M and N are said to be diffeomorphic if there exists a diffeomorphism F that maps M onto N.

What all of this means is that, given an observable deterministic dynamical system—a computer for example, a highly complex nonlinear dynamical system [83] with no obvious (\mathbb{X}, Φ) —I can measure a single quantity (*e.g.*, instructions executed per cycle or L2 cache misses) and use that time series to faithfully reconstruct the underlying dynamics *up to diffeomorphism*. In other words, the true unknown dynamics (X, Φ) and the dynamics reconstructed from this scalar time series *have the same topology*. Though this is less information than one might like, it is still very useful, since many important dynamical properties (*e.g.*, the Lyapunov exponent that parametrizes chaos) are invariant under diffeomorphism. It is also useful for the purposes of prediction—the goal of this thesis.

The delay-coordinate embedding process involves two parameters: the time delay τ and the embedding dimension m. For notational convenience, I denote the embedding space with dimension m and time delay τ as $\mathbb{E}[m, \tau]$. To assure topological conjugacy, the Takens proof [113] requires that the embedding dimension m must be at least twice the dimension d of the ambient space; a tighter bound of $m > 2d_{cap}$, the capacity dimension of the original dynamics, was later established by Sauer *et al.* [99].

Definition (Capacity Dimension [79]). Let $N(\epsilon)$ denote the minimum number of open sets (ϵ -balls) of diameter less than or equal to ϵ that form a finite cover of a compact metric space X. Then the capacity dimension of X is a real number d_{cap} such that: $N(\epsilon) \approx \epsilon^{-d_{cap}}$ as $\epsilon \to 0$, explicitly

$$d_{cap} \equiv -\lim_{\epsilon \to 0^+} \frac{\ln N(\epsilon)}{\ln \epsilon}$$
(2.4)

if this limit exists.

Operationalizing either of these theoretical constraints can be a real challenge. d is not known and accurate d_{cap} calculations are not easy with experimental data. And besides, one must first embed the data before performing those calculations.

Apropos of the central claim of this thesis, it is worth considering the intention behind these bounds on m. The worst-case bound of $m > 2d_{cap}$ is intended to eliminate *all* projection-induced trajectory crossings in the reconstructed dynamics. For most systems, and most projections, the dimensions of the subspaces occupied by these false crossings are far smaller than those of the original systems [99]; often, they are sets of measure zero. For the delay-coordinate map to be a diffeomorphism, all of these crossings must be unfolded by the embedding process. This is necessary if one is interested in calculating dynamical invariants like Lyapunov exponents. However, the near-neighbor relationships that most state-space forecast methods use in making their predictions are *not* invariant under diffeomorphism, so it does not make sense to place that strict condition on a model that one is using for those purposes. False crossings will, of course, cause incorrect predictions, but that is not a serious problem in practice if the measure of that set is near zero, particularly when one is working with noisy, real-world data.

My reduced-order strategy explicitly fixes m = 2. This choice takes care of one of the two free parameters in the delay-coordinate reconstruction process, but selection of a value for the delay, τ , is still an issue. The theoretical constraints in this regard are less stringent: τ must be greater than zero and not a multiple of the period of any orbit [99,113]. In practice, however, the noisy and finite-precision nature of digital data and floating-point arithmetic combine to make the choice of τ much more delicate [59]. It is to this issue that I will turn next.

2.1.2 Traditional Methods for Estimating the Embedding Delay τ

The τ parameter defines the amount of time separating each coordinate of the delay vectors: $\vec{x}_j = [x_j, x_{j-\tau}, \dots, x_{j-(m-1)\tau}]^T$. The theoretical constraints on the time delay are far from stringent and this parameter does not—in theory [99,113]—play a role in the correctness of the embedding. However, that assumes an infinitely long noise-free time series [99,113], a luxury that is rare in practice. As a result of this practical limitation, the time delay τ plays a crucial role in the *usefulness*¹ of the embedding [17,18,33,59,67,68,95].

The fact that the time delay does not play into the underlying mathematical framework is a double-edged sword. Because there are no theoretical constraints, there is no practical way to derive an "optimal" lag or even know what criterion an "optimal" lag would satisfy [59]. Casdagli *et al.* [24] provide a theoretical discussion of this, together with some treatment of the impacts of τ on reconstructing an attractor using a noisy observation function. Unfortunately no practi-

¹ Here by *usefulness* I mean that not only are the dynamical invariants (*e.g.*, Lyapunov exponents and fractal dimension) and topological properties, (*e.g.*, neighborhood relations) preserves, but also that those quantities are attainable from the reconstructed dynamics.

cal methods for estimating τ came from that discussion, but it does nicely outline a range of τ between *redundancy* and *irrelevance*. For very small τ , especially with noisy observations, x_j and $x_{j-\tau}$ are effectively indistinguishable. In this situation, the reconstruction coordinates are highly *redundant* [24, 46], *i.e.*, they contain nearly the same information about the system.² This is not a good choice for τ because additional coordinates add almost nothing new to the model. Choosing an arbitrarily *large* τ is undesirable as well. On this end of the spectrum, the coordinates of the reconstruction become causally unrelated, *i.e.*, the measurement of $x_{j-\tau}$ is *irrelevant* in understanding x_j [24]. Useful τ values lie somewhere between these two extrema. In practice, selecting useful τ values can be quite challenging, as demonstrated in the following example.

Example 1. To explore the effects of τ on an embedding, I first construct an artificial time series by integrating the Rössler system [96]

$$\dot{x} = -y - z \tag{2.5}$$

$$\dot{y} = x + ay \tag{2.6}$$

$$\dot{z} = b + z(x - c) \tag{2.7}$$

with a = 0.15, b = 0.20, and c = 10.0, using a standard fourth-order Runge-Kutta integrator starting from $[x(0), y(0), z(0)]^T = [10, 0, 0]^T$ for 100,000 time steps with a time step of $\pi/100$. This results in a trajectory of the form $\vec{y}(t_j) = [x(t_j), y(t_j), z(t_j)]^T$, where $t_j = j(\pi/100)$ for j = 1, ..., 100, 000. This trajectory is plotted in Figure 2.1(a). To discard transient behavior, I remove the first 1,000 points of this trajectory. I define the observation function as $h(\vec{y}(t_j)) = x(t_j) = x_j$, resulting in the time series: $\{x_j\}_{j=1001}^{100,000}$. The first 5,000 points of this time series can be seen in Figure 2.1(b).

To illustrate the role of τ in the delay-coordinate embedding process, I embed $\{x_j\}_{j=1001}^{100,000}$ using m = 2 and several different choices of τ . These embeddings are shown in Figure 2.2. In theory, each of the choices of τ in Figure 2.2 should yield correct, topologically equivalent embeddings—given the right choice of m. In practice, however, that is not the case.

First consider the top-left panel of Figure 2.2 where $\tau = 1$. Here, the axes are spread apart so little that the embedding appears to be a noisy line. This is because x_j and $x_{j-\tau}$ are effectively

 $^{^{2}}$ This is made more rigorous in Section 2.2, where I discuss information theory.



Figure 2.1: The Rössler attractor and a segment of the time series of its x coordinate.

indistinguishable at this small τ . In the embedding in the bottom-right panel of Figure 2.2, the reconstruction appears to be a ball of noise with only traces of underlying structure. At this large τ , the coordinates of the reconstruction are causally unrelated. This is known as "overfolding." To visualize this concept, consider the progression in Figure 2.2 from $\tau = 30$ to $\tau = 341$. As τ increases, the reconstruction expands away from the diagonal and begins to resemble the original attractor. However, as τ increases past this point, the top corner of the reconstruction is slightly folded over.

This "melting" effect is called folding in the literature. "Overfolding" occurs when the reconstructed attractor folds back on itself, completely collapsing back to the diagonal, (as can be seen for $\tau = 101$) and then re-expanding away from the diagonal, (as can be seen for $\tau = 341$). Overfolding produces an unnecessarily (and in the case of noise, often incorrect) reconstruction [24, 59, 95]. Compare, for example, the bottom-left panel of Figure 2.2 with the actual attractor in Figure 2.1(a). From a theoretical standpoint, given the right choice of m, these two objects are topologically equivalent; from a practical standpoint, however, the embedding is overly complex.

If the time series were noisy, this overfolding would likely introduce additional error. With knowledge of the true attractor, it is easy to say that the $\tau = 30$ and $\tau = 46$ embeddings most closely match its shape; without that knowledge, however, the choice is not obvious. The situation



Figure 2.2: Delay-coordinate reconstruction of the Rössler time series in Figure 2.1(b) with m = 2 and varying τ .

is even more delicate than this. If one knew, somehow, that $\tau = 30$ and $\tau = 46$ were both good reconstructions, how would one know which of these two choices was optimal? With $\tau = 30$, no folding has occurred, which is beneficial because with noisy or projected dynamics (choosing m too small), foldings may cause false crossings.³ But the trajectory in $\mathbb{E}[m, 30]$ is not as "space filling" as $\tau = 46$ or as spread apart from the diagonal, so the coordinates are most likely more redundant. Weighing the importance of these kinds of criteria is non-trivial and, I believe, application specific. In the rest of this section, I review heuristics aimed at optimizing the estimation of τ by weighing these different attributes against one another.

There are dozens of methods for estimating τ —e.g., [17,18,33,42,46,59,67,68,88,95]. This is a central issue in my thesis, so the following section surveys this literature in some depth. Choice of τ is application- and system-specific [17,59,95]; a τ that works well for Lyapunov exponent calculation may not work well for forecasting. For this reason, Kantz & Schreiber [59] suggest that it may be necessary to perform additional system- and application-specific tuning of τ after using any generic selection heuristic. In my first set of examples, I use the method of *mutual information* [33,68]—described below in detail. While this is the standard τ -selection method, I will show in Section 4.3.1 that this choice is almost always *suboptimal* for forecasting. In Section 5.1, I provide a solution to this: an alternative τ selection method that leverages "active information storage" to select a τ that is optimal for forecasting specific reconstructions [42].

2.1.2.1 Linear Independence and Autocorrelation

A naïve strategy for selecting the time delay would be to choose a τ that forces the coordinates of the delay vectors to be *linearly* independent. This is equivalent to choosing the first zero of the autocorrelation function $R(\tau)$

$$R(\tau) = \frac{1}{N - \tau} \frac{\sum_{j} (x_j - \mu_x) (x_{j - \tau} - \mu_x)}{\sigma_x^2}$$
(2.8)

where N, μ_x and σ_x are respectively the length, average and standard deviation of the time series [33, 59]. Several other methods have been proposed that suggest instead choosing τ where the autocorrelation function first drops to a particular fraction of its initial value, or at the first

 $^{^{3}}$ A *false crossing* is when two trajectories intersect due to projection or measurement error, a phenomenon that cannot happen in a theoretical deterministic dynamical system.

inflection point of that function [59,95].

An advantage to this class of methods is that its members are extremely computationally efficient; the autocorrelation function, for instance, can be calculated with the fast Fourier transform [95]. However, autocorrelation is a linear statistic that ignores nonlinear correlations. This often yields τ values that work well for some systems and not well for others [33, 59, 95].

2.1.2.2 General Independence and Mutual Information

Instead of seeking linear independence between delay coordinates, it may be more appropriate to seek general independence—*i.e.*, coordinates that share the least amount of *information* (also called "redundancy") with one another. The following discussion requires some methods from information theory; for a review of these concepts, please refer to Section 2.2. Fraser & Swinney argue that selecting the first minimum of the *time-delayed mutual information* will minimize the redundancy of the embedding coordinates, maximizing the information content of the overall delay vector [33]. In that approach, one obtains generally independent delay coordinates by symbolizing the two time series $X_j = \{x_j\}_{j=1}^N$ and $X_{j-\tau} = \{x_{j-\tau}\}_{j=1+\tau}^N$ by binning, discussed in Section 2.2.5.1, and then computes the mutual information between X_j and $X_{j-\tau}$ for a range of τ , call this $I[X_j, X_{j-\tau}; \tau]$. Then for each τ , $I[X_j, X_{j-\tau}; \tau]$ is the amount of information shared between the coordinates x_j and $x_{j-\tau}$, *i.e.*, $I[X_j, X_{j-\tau}]$ quantifies how redundant the second axis is [33]. According to [33], choosing a τ that minimizes $I[X_j, X_{j-\tau}]$, results in generally independent delay coordinates that are minimally redundant.

The argument for choosing τ in this way applies *strictly* to two-dimensional embeddings [33, 59], but was extended to work in m dimensions in [68]. To accomplish this, Liebert & Schuster rewrote mutual information in terms of second-order Renyí entropies. This transformation allowed them to show that the minima of $I[X_j, X_{j-\tau}; \tau]$ agreed with the minima of the correlation sum [49], $C(\epsilon; m, \tau)$, defined as

$$C(\epsilon; m, \tau) = \frac{1}{N^2} \sum_{\substack{i,j=1\\i \neq j}}^{N} \Theta[\epsilon - ||\vec{x_i} - \vec{x_j}||]$$
(2.9)

where N is the length of the time series, Θ is the Heavyside function, and $\vec{x_i}, \vec{x_j}$ are the i^{th} and j^{th} delay vectors in $\mathbb{E}[m, \tau]$. In addition to extending the argument of [33] to m dimensions, the modification of [68] allowed for much faster approximations of τ by simply finding the minimum of $C(\epsilon; m, \tau)$, which can be done quickly with the Grassberger-Procaccia algorithm [49,68].

The choice of the *first* minimum of $I[X_j, X_{j-\tau}; \tau]$ is intended to avoid the kind of overfolding of the reconstructed attractor and irrelevance between coordinates that was demonstrated in Figure 2.2. This choice is discussed and empirically verified in [68] by showing that the first minimum of $C(\epsilon; m, \tau)$ (so in turn $I[X_j, X_{j-\tau}; \tau]$) corresponded to the most reliable calculations of the *correlation dimension* [49].

Definition (Correlation Dimension). If the correlation sum, $C(\epsilon)$, decreases like a power law, $C(\epsilon) \sim \epsilon^D$, then D is called the <u>correlation dimension</u>. Formally

$$D = \lim_{\epsilon \to 0} \frac{\log C(\epsilon)}{\log \epsilon}$$
(2.10)

if this limit exists. The Grassberger-Procaccia algorithm⁴ [49] allows the correlation dimension to be approximated for $\mathbb{E}[m, \tau]$ as

$$D = \lim_{\epsilon \to 0} \frac{\log C(\epsilon; m, \tau)}{\log \epsilon}$$
(2.11)

It was not shown in [68], however, that this choice corresponds to the best choice of τ for the purposes of forecasting. In Section 4.3.1 I show that this is in fact not the case for all time series. Even so, it is a reasonable starting point, as this method is the gold standard in the associated literature. In my first round of experiments, and as a point of comparison, I select τ at the first minimum of the mutual information [33, 68] as calculated by mutual in the TISEAN package [53].

⁴ The term Grassberger-Procaccia algorithm is used generically for any algorithm that estimates the correlation dimension (and more generally the correlation integral) from the small- ϵ behavior of the correlation sum $C(\epsilon; m, \tau)$.

There are a few possible drawbacks to this method. For example, there is no guarantee that $I[X_j, X_{j-\tau}; \tau]$ will ever achieve a minimum; a first-order autoregressive process, for example, does not [59]. Rosenstein *et al.* [95] argue that calculating mutual information is too computationally expensive. Several papers [51,75] have argued that mutual information can give inconsistent results, especially with noisy data.

2.1.2.3 Geometric and Topological Methods

There are several geometric and topological methods for approximating τ that address some of the shortcomings of mutual information, including: wavering product [67], fill factor, integral local deformation [18], and displacement from diagonal [95], among others. Most of these methods have the distinct advantage of attempting to solve for both m and τ simultaneously, albeit at the cost of being more complicated and less computationally efficient. (This additional computational overhead is not a factor in my reduced-order framework as I explicitly fix m = 2.)

2.1.2.4 Wavering Product

The wavering product of Liebert *et al.* [67] is a topological method for simultaneously determining embedding dimension and time delay. This approach focused on detecting when the attractor is properly unfolded, *i.e.*, the situation in which projection-induced overlap disappears.

Liebert *et al.* focused on preserving neighborhood relations of points in $\mathbb{E}[m, \tau]$. When transitioning from $\mathbb{E}[m, \tau]$ to $\mathbb{E}[m + 1, \tau]$, an embedding preserves neighborhood relations of every point in $\mathbb{E}[m, \tau]$, *i.e.*, inner points remain inner points, and analogously with the boundary points. If these neighborhood relations are preserved, then *m* is a sufficient embedding dimension. The so-called "direction of projection" [67] that mitigates false crossings is associated with the best choice of τ , *i.e.*, the τ that yields (for a fixed dimension) the smallest amount of overlap. To this end, they defined two quantities

$$Q_1(i,k,m,\tau) = \frac{dist_{m+1}^{\tau}(i,j(k,m))}{dist_{m+1}^{\tau}(i,j(k,m+1))}, \quad Q_2(i,k,m,\tau) = \frac{dist_m^{\tau}(i,j(k,m))}{dist_m^{\tau}(i,j(k,m+1))}$$
(2.12)

where, $dist_{m+1}^{\tau}(i, j(k, m))$ is the standard Euclidean distance measured in $\mathbb{E}[m+1, \tau]$ between an i^{th} reference point $\vec{x_i}$ in $\mathbb{E}[m, \tau]$ and its k^{th} nearest neighbor $\vec{x}_{j(k,m)}$ in $\mathbb{E}[m, \tau]$ or similarly for $dist_{m+1}^{\tau}(i, j(k, m+1))$, the k^{th} nearest neighbor of $\vec{x_i}$ in $\mathbb{E}[m+1, \tau]$. To determine if the neighborhood relations are preserved in the embedding, they defined the wavering product

$$W_i(m,\tau) = \left(\left(\prod_{k=1}^{N_{nb}} Q_1(i,k,m,\tau) Q_2(i,k,m,\tau) \right)^{1/(2N_{nb})} \right)^{1/(2N_{nb})}$$
(2.13)

where N_{nb} is the number of neighbors used in each neighborhood. If $W_i(m, \tau) \approx 1$, then the topological properties are preserved *locally* by the embedding [67]. In order to compute this *globally*, Liebert *et al.* defined the average wavering product as

$$\overline{W}(m,\tau) = \ln\left[\frac{1}{N_{ref}}\sum_{i=1}^{N_{ref}}W_i(m,\tau)\right]$$
(2.14)

where N_{ref} is the number of reference points, typically chosen to be about 10% of the signal. A minimum of $\overline{W}(m,\tau)/\tau$ as a function of τ yields an optimal τ for that choice of m. They also showed that a sufficient embedding dimension can be found when $\overline{W}(m,\tau)/\tau$ converged to zero. Choosing the embedding parameters in this way guarantees that the embedding faithfully preserves neighborhood relations. This is particularly important when forecasting based on neighbor relations.

This technique works very well on many systems, including the Rössler system and the Mackey-Glass system. In particular, Liebert *et al.* showed that choosing m and τ in this way allowed for accurate estimation of the information dimension [49]. Noise, however, is a serious challenge for this heuristic [62], so it may not be useful for real-world datasets.

2.1.2.5 Integral Local Deformation

Integral local deformation, introduced by Buzug & Pfister in [18], attempts to maintain continuity of the dynamics on the reconstructed attractor: *viz.*, neighboring trajectories remain close for small evolution times. The underlying rationale is that false crossings will cause what look like neighboring trajectories to separate exponentially in very short evolution time. Integral local deformation quantifies this. Buzug & Pfister show that choosing m and τ to minimize this quantity gives an approximation of τ that minimizes false crossings created by projection.

In my work, I rely strongly on the continuity of the reconstructed dynamics, since I use the image of neighboring trajectories for forecasting. Integral local deformation seems useful at first glance for choosing a τ that helps to preserve the continuity of the underlying dynamics in the face of projection. However, the computational complexity of this measure makes it ineffective for on-the-fly adaptation or selection of τ .

2.1.2.6 Fill Factor

In [18], Buzug & Pfister introduced a purely geometric heuristic for estimating τ . This method attempts to maximally fill the embedding space by *spatially* spreading out the points as far as possible. To accomplish this, Buzug & Pfister calculate the average volume of a large number of *m*-dimensional parallelepipeds, spanned by a set of m + 1 arbitrarily chosen *m*-dimensional delay vectors. They then show that the first maximum of the average of these volumes as a function of τ (for a fixed *m*) maximizes the distance between trajectories. This method is computationally efficient, as no near-neighbor searching is required. However, for any attractor with multiple unstable foci, there is no significant maximum of the fill factor as a function of τ [18,95]. In addition, this method cannot take into account overfolding, as an overfolded embedding may be more spacefilling than the "properly" unfolded counterpart [95]. This consideration is corrected (at the cost of additional computational complexity) in the method described next.

2.1.2.7 Average Displacement / Displacement from Diagonal

The average displacement method introduced by Rosenstein *et al.* [95], which is also known as the displacement from diagonal method [59], also seeks a τ that causes the embedded attractor to fill the space as much as possible, while mitigating error caused by overfolding and also addressing some other concerns [18]. Rosenstein *et al.* define the average displacement (from diagonal) for
$\mathbb{E}[m,\tau]$ as

$$\langle S_m(\tau) \rangle = \frac{1}{N} \sum_{i=1}^N \sqrt{\sum_{j=1}^{m-1} (x_{i+j\tau} - x_i)^2}$$
 (2.15)

For a fixed m, $\langle S_m(\tau) \rangle$ increases with increasing τ (at least initially; the attractor may collapse for large τ due to overfolding). Rosenstein *et al.* suggest choosing τ and m where the slope between successive $\langle S_m(\tau_i) \rangle$ drops to around 40% of the slope between $\langle S_m(\tau_1) \rangle$ and $\langle S_m(\tau_2) \rangle$, where τ_1 and τ_2 are the first and second choices of τ . In noisy data sets, this leads to consistent and accurate computation of the correlation dimension. However, this—like most heuristics—was developed to correctly approximate dynamical invariants (*e.g.*, correlation dimension), and comes with no guarantees about forecast accuracy.

Remark. Several papers (e.g., [64, 77, 85, 95, 105]) have claimed that the emphasis should be placed on the window size $\tau_w = \tau m$ rather than τ or m independently. The basic premise behind this idea is that it is more important to choose τ_w to span an important time segment (e.g., mean orbital period) than the actual choice of either τ or m independently. This is something I have not found to be the case when choosing parameters for delay reconstruction-based forecasting.

2.1.3 Traditional Methods for Estimating the Embedding Dimension m

As the embedding dimension m is not a parameter in my reduced-order algorithm, I only review a few important methods for estimating it. This discussion is important mainly because these conventions are the point of departure (and comparison) for my work.

A scalar time series $\{x_j\}_{j=1}^N$ measured from a dynamical system is a projection of the original state space onto a one-dimensional sub-manifold. A fundamental concern in the theoretical embedding dimension requirement $m > 2d_{cap}$ is to ensure that the embedding has enough dimensions to "spread out" and thus avoid false crossings. Such crossings violate several properties of deterministic dynamical systems, *e.g.*, determinism, uniqueness and continuity. In Figure 2.3(a), for example, the $\mathbb{E}[2, 45]$ embedding of the *x*-coordinate of the Rössler system contains trajectory



Figure 2.3: An illustration of the utility of higher embedding dimensions to eliminate false crossings in the dynamics.

crossings. In Figure 2.3(b), however, the top-right region of Figure 2.3(a) has folded under the attractor and the intersections on the top left of Figure 2.3 have become a "tunnel." The issue here is that the dynamics do not have enough space to spread apart in two dimensions. However when this dimension is increased, the attractor can spread out and the intersections disappear. According to [99], choosing $m > 2d_{cap}$ ensures that the attractor has enough space to spread out and false crossings will not occur. More precisely, the probability of a crossing occurring in a ball of size ϵ is $p_c \propto \epsilon^{m-2d_{cap}}$. Recall from Section 2.1.1, however, that this is for an infinitely long noise free time series and may not hold in practice, as noise can easily cause false crossings and violate the assumptions that went into this estimation. It should also be noted that, even if I knew the capacity dimension d_{cap} of the system—which is generally not the case—I do not necessarily want to choose m to be $2d_{cap} + 1$. This is a (generally loose) sufficient bound that should ensure the correctness of the embedding. But it is often the case that the embedding unfolds completely before $m = 2d_{cap} + 1$. The Lorenz system [71] has $d_{cap} = 2.06 \pm 0.01$, for example. [99] would suggest using m = 5, but in fact this system can be embedded properly using m = 3 [62].

Naïvely, it may seem that simply choosing an "extremely large" m would be a simpler and completely reasonable choice. This is not true, in practice. First, the complexity of many of the algorithms that deduce information about dynamical systems scale exponentially with m [68]. Worse yet, each noisy data point creates m noisy embedding points in the reconstruction [24]. This amplification of noise quickly destroys the usefulness of an embedding. In light of both of these concerns, good values for the *minimal* m are highly sought after. For a noisy real-valued time series, this is still an open problem, but there exist several heuristic approximations (*e.g.*, [18,20,53,59,62,64,67]). Recall, too, that several of the methods presented in the previous section for estimating τ —*e.g.*, *wavering product* [67] and *integral local deformation* [18]—simultaneously estimate both the delay and the dimension, m—the other free parameter in the embedding process.

There are two standard classes of methods for estimating the minimal m, the method of dynamical invariants and the method of false neighbors. In the following sections, I review the basics of these two families.

2.1.3.1 Method of Dynamical Invariants

Dynamical invariants, such as correlation dimension, are topological measures of a system that persist under diffeomorphism. In theory, this means that once a particular choice of embedding dimension, say \hat{m} , yields a topologically valid reconstruction, increasing m should have no impact on these dynamical invariants. This is the case because in theory every $\mathbb{E}[m > \hat{m}, \tau]$ will be topologically conjugate, to one another and to the original dynamics. This implies that dynamical invariants will become *persistent* for increasing m, once \hat{m} has been reached. Hence, choosing the first m for which dynamical invariants stop changing is a good way to estimate the minimal dimension needed to obtain a topologically valid reconstruction. The class of methods that is the topic of this section follows directly from this logic: to choose m, one approximates some dynamical invariant (*e.g.*, dominant Lyapunov exponent or correlation dimension) for a range of embedding dimensions, choosing the first embedding dimension for which it becomes persistent, and then corroborates with other dynamical invariants.

For example, one can approximate the correlation dimension for a range of embedding dimensions using the Grassberger & Procaccia algorithm [49], choosing the first m for which that approximation stops changing. Then one corroborates this choice by approximating the dominant Lyapunov exponent for a range of m (using for example the algorithm in [120]), then choosing the first m where this result stops changing. Finally, one ensures these two estimates of m are consistent with each other.

Recall, though, that noise in the data can impact any dynamical invariant calculation, and that that impact increases with m [24]. It is more often the case that there is a range of embedding dimensions for which the dynamical invariant being approximated stays "fairly consistent." Ascertaining this is computationally expensive and requires time-intensive post processing and human interpretation. For these reasons, it is common to use an alternative heuristic, such as those covered in the next section, to narrow down the search to a smaller range of embedding dimensions and then select from this range using the method of dynamical invariants.

2.1.3.2 The Method of False Neighbors

The method of false neighbors was proposed by Kennel *et al.* in [62]. This heuristic searches for points that appear close only because the embedding dimension is too small. Consider a point on the top of the tunnel in Figure 2.3(b) and a point directly below this point on the planar part of the Rössler attractor. These two points are near neighbors in $\mathbb{E}[2, 45]$ because the tunnel collapses down on the planar region; however, they are not near neighbors in $\mathbb{E}[3, 45]$ because the embedded attractor inflates, separating points on the top of the tunnel from the points on the planar region. Since these two points are neighbors in $\mathbb{E}[2, 45]$ and *not* neighbors in $\mathbb{E}[3, 45]$, they are *false near(est) neighbors* at m = 2. Consider, in contrast, two neighboring points on the top of the tunnel in $\mathbb{E}[3, 45]$. If the space is projected down to $\mathbb{E}[2, 45]$, these points would still be neighbors.

More formally, Kennel *et al.* define the k^{th} nearest neighbor $\vec{x}_{j(k,m)} \in \mathbb{E}[m,\tau]$ of $\vec{x}_i \in \mathbb{E}[m,\tau]$ as a *false near(est) neighbor* if

$$\left(\frac{dist_{m+1}^{\tau}(i,j(k,m))^2 - dist_m^{\tau}(i,j(k,m))^2}{dist_m^{\tau}(i,j(k,m))^2}\right)^{1/2} > R_{tol}$$
(2.16)

where R_{tol} is some tolerance. Recall that the $dist_m^{\tau}(i, j(k, m))$ is the distance between the i^{th} point

 $\vec{x}_i \in \mathbb{E}[m, \tau]$ and its k^{th} nearest neighbor $\vec{x}_{j(k,m)} \in \mathbb{E}[m, \tau]$. But notice for delay vectors that $dist_{m+1}^{\tau}(i, j(k, m))^2 = |x_{i-m\tau} - x_{j(k,m)-m\tau}|^2 + dist_m^{\tau}(i, j(k, m))^2$, so this condition simplifies to

$$\frac{|x_{i-m\tau} - x_{j(k,m)-m\tau}|}{dist_m^{\tau}(i,j(k,m))} > R_{tol}$$

$$(2.17)$$

In particular, a neighbor is a false neighbor if the distance between the two points in $\mathbb{E}[m + 1, \tau]$ is significantly more (*viz.*, R_{tol}) than the distance between the two neighbors in $\mathbb{E}[m, \tau]$. Kennel *et al.* claim that choosing a single nearest neighbor is sufficient (*i.e.*, k = 1) [62]. In addition, they claim that empirically $R_{tol} \ge 10$ seems to give robust results. This tolerance can be interpreted as defining false neighbors as points that are 10 times farther apart in $\mathbb{E}[m + 1, \tau]$ than in $\mathbb{E}[m, \tau]$.

This heuristic alone is not enough to distinguish chaos from uniform noise and can incorrectly classify time series constructed from a uniform distribution as having low-dimensional dynamics. Kennel *et al.* found that for a uniformly distributed random time series, on average, the nearest neighbor of a point is not near at all. Rather, $dist_m^{\tau}(i, j(k, m)) \approx R_A$, where $R_A = \sqrt{\frac{1}{N} \sum_{j=1}^{N} (x_j - \mu_x)^2}$. That is, the average distance to the nearest neighbor is the size of the attractor. To handle this, they defined a secondary heuristic $\frac{dist_{m+1}^{\tau}(i, j(k, m))}{R_A} > A_{tol}$, where A_{tol} is another free parameter chosen as 2.0 without justification. I want to note that this heuristic is added to distinguish pure-uniform noise from chaotic dynamics, *not* to aid in estimating embedding dimension for noisy observations of a chaotic system.

For a time series with noise, near-neighbor relations—which are the basis for this class of heuristics—can cause serious problems in practice. For well-sampled, noise-free data, it makes sense to choose m as the first embedding dimension for which the ratio of true to false neighbors goes to zero [62]. For noisy data however, this is unrealistic; in practice, the standard approach is to choose the first m for which the percentage of false near(est) neighbors drops below 10%. If topological correctness is vitally important for the application, a range of embedding dimensions for which the percentage of false near(est) neighbors to around $\approx 10\%$ is typically chosen and then this range is refined using the method of dynamical invariants described above. This 10% is an arbitrary threshold, however; depending on the magnitude of noise present in the data, it may need to be adjusted, as may R_{tol} and A_{tol} . For example, in the computer performance data presented in Section 3.2.1.2, the percentage of false near(est) neighbors rarely dropped below even 20%.

Recently an extension of the false near(est) neighbor method was proposed by Cao [20], which attempts to get around the three different tolerances (R_{tol} , A_{tol} and the percentage of false neighbors) in [62]. Cao points out that the tolerances—in particular, R_{tol} —need to be specified on a per-time-series and even per-dimension basis. Assigning these tolerances universally is inadvisable and in many cases will lead to inconsistent estimates. In [20], he illustrates that different choices of these three tolerances result in very different estimates for m. To get around this, he defines an alternative heuristic that is tolerance free

$$E(m) = \frac{1}{N - m\tau} \sum_{i=1}^{N - m\tau} \frac{dist_{m+1}^{\tau}(i, j(k, m))}{dist_{m}^{\tau}(i, j(k, m))}$$
(2.18)

While the inside of the sum is very similar to Equation 2.17 of [62], the numerator is slightly different: $dist_{m+1}^{\tau}(i, j(k, m))$ instead of $|x_{i-m\tau} - x_{j(k,m)-m\tau}|$. That is, the former measures the distance between an element and its k^{th} -nearest neighbor in $\mathbb{E}[m, \tau]$ measured in $\mathbb{E}[m + 1, \tau]$, whereas the latter measures the *change* in distance between $\vec{x}_i, \vec{x}_{j(k,m)} \in \mathbb{E}[m, \tau]$, and the same vectors extended in $\mathbb{E}[m + 1, \tau]$. Cao then defines $E1(m) = \frac{E(m+1)}{E(m)}$ and shows that when E1(m)stops changing, a sufficient embedding dimension has been found. He also claims that if E1(m)does not stop changing, then one is observing noise and not deterministic dynamics [20]. Cao does admit that it is sometimes hard to determine if the E1(m) curve is just slowly growing but will plateau eventually (in the case of high dimensional dynamics) or just constantly growing (in the case of noise). To deal with this, he defines a secondary heuristic to help distinguish these two cases. As this method has been shown to give more consistent m, I hoped that this method could provide a more accurate comparison point. However, I was never able to successfully replicate the results in [20] on any experimental data, so I chose to use the traditional version of this algorithm proposed by Kennel *et al.* in [62].

The astute reader may have noticed a similarity between the method of false neighbors [62],

the method of wavering products [67], and the methods of Cao [20]. It is true that these methods are quite similar. In fact, almost all the methods for determining minimum embedding dimension [18,20,53,59,62,64,67] are based in some way on minimizing the number of false crossings. As this parameter is not important in my work, I do not go into all of these nuances but simply use the standard false near(est) neighbor approach to which the rest of these methods are fundamentally related. In particular, I use the TISEAN [53] implementation of this algorithm (false_nearest) to choose m with a $\approx 20\%$ threshold on the percentage of neighbors and the R_{tol} and A_{tol} selected by the TISEAN implementation. In my later discussion, I refer to the reconstruction produced in this manner as an embedding of the data. This is by no means perfect, but since it is the most widely used method for estimating m, it is the most useful for the purposes of comparison.

2.1.4 Delay-Coordinate Embedding Reality Check

As discussed in Section 2.1.1, the theory of delay-coordinate embedding [99, 113] outlines beautiful machinery to reconstruct—up to diffeomorphism—the dynamics of a system from a scalar observation. Unfortunately this theoretical machinery requires both infinitely-long and noise-free observations of the dynamical system: luxuries that are never afforded to a time-series analyst in practice. While there has been a tremendous amount of informative literature on estimating the free parameters of delay-coordinate embedding, at the end of the day these heuristics are just that: empirical estimates with no theoretical guarantees. This means that, even if the most careful rigorous in-depth analysis is used to estimate τ and m, there is no way to guarantee, in the experimental context, that the reconstructed dynamics are in fact diffeomorphic to the observed dynamics.

Even worse, overestimating m has drastic impacts on the usefulness of the embedding, as it exponentially amplifies the noise present in the reconstruction. If little usable structure is present in a time series in the first place, perverting this precious structure by amplifying noise is something a practitioner can ill afford to do. Moreover, the methods that are most commonly used for estimating m are based on neighbor relations, which are easily corrupted by noisy data. As a result, these heuristics tend to overestimate m.

In addition to noise amplification concerns and the lack of theoretical guarantees, the methods for estimating minimal embedding dimension are highly subjective, dependent on the estimate of τ , and require a great deal of human intuition to interpret correctly. This time-consuming, errorprone human-intensive process makes it effectively impossible to use delay-coordinate embedding for automated or 'on-the-fly' forecasting. As stated in Chapter 1, this is unfortunate because delaycoordinate embedding is such a powerful modeling framework. My reduced-order framework—the foundation of this thesis—will, I hope, at least partially rectify this shortcoming.

2.2 Information Theory Primer

In this section, I provide a basic overview of notation and concepts from Shannon information theory [103], as well as a review of some more-advanced topics that are utilized throughout the thesis. I will first cover the basics; an expert in this field can easily skip this part. I will then move on to non-traditional topics *viz.*, multivariate information theory (Section 2.2.3), methods for computing information measures on real-valued time series (Section 2.2.5), and measures to quantify the predictability of a real-valued time series (Section 2.2.6).

2.2.1 Entropy

Perhaps the most fundamental concept or building block in information theory is the concept of Shannon Entropy.

Definition ((Shannon) Entropy [103]). Let Q be a discrete random variable with support $\{q_1, ..., q_n\}$ and a probability mass function p that maps a possible symbol to the probability of that symbol occurring, e.g., $p(q_i) = p_i$, where p_i is the probability that an observation q is measured to be q_i . The average amount of information gained by taking a measurement of Q and thereby specifying an observation q is the Shannon Entropy (or simply entropy) H of Q, defined by

$$H[Q] = -\sum_{i=1}^{n} p(q_i) \log(p(q_i))$$
(2.19)

Throughout this thesis, log is calculated with base two, so that the information is in bits. The entropy H[Q] can be interpreted as the amount of "surprise" in observing a measurement of a discrete random variable Q, or equivalently the average uncertainty in the outcome of a process, or the amount of "information" in each observation of a process.

Example 2 (Entropy of fair and biased coins). First consider a fair coin: $Q = \{h, t\}$ and p(h) = p(t) = 1/2.

$$H[Q] = -[p(h)\log(p(h)) + p(t)\log(p(t))]$$
(2.20)

$$= -\left[\frac{1}{2}\log(\frac{1}{2}) + \frac{1}{2}\log(\frac{1}{2})\right]$$
(2.21)

$$= -\left(\frac{-1}{2} + \frac{-1}{2}\right) = 1 \tag{2.22}$$

At every flip of the coin there is one bit of "new" information, or one bit of surprise. In contrast, consider an extremely biased coin with heads on both sides: $Q = \{h, t\}$ and p(h) = 1, p(t) = 0. Then H[Q] = 0, i.e., there are zero bits of "new" information at each toss, as the coin always gives heads.

To gain an intuitive understanding of what phrases like 'one bit of "new" information', or 'one bit of surprise' mean, it is sometimes easier to interpret Equation (2.19) as the average number of (optimal) yes-no questions one needs to ask in order to determine what the outcome of observing a system will be. Returning to the coin-flip example above, since the fair coin had H[Q] = 1, on average, one (optimal) question needs to be asked to determine the outcome of the coin flip: "Was the coin a head?" With the biased coin, however, the entropy was zero, which means on average no questions were needed in order to infer the observation was a head (it always is!). The following example clarifies this.

Example 3 (Entropy of Animal-Vegetable-Mineral [28]). You may have, at some point during your childhood, played the game "Animal-Vegetable-Mineral." If not, the rules are simple: player

one thinks of an object, and by a series of yes-no questions, and the other players attempt to guess the object. "Is it bigger than a breadbox?" No. "Does it have fur?" Yes. "Is it a mammal?" No. This continues until the players can guess the object.

As anyone who has played this game will attest, some questions are better than others—for example, you usually try to focus on general categories first (hence, the name of the game itself is it an animal?) then get more specific within that category. Asking on the first round "is it a dissertation?" is likely to waste time—unless, perhaps, you are playing with a graduate student who is about to defend.

If a game lasts too long, you may begin to wonder if there exists an optimal set of questions to ask. "Could I have gotten the answer sooner, if I had skipped that useless question about the fur?" A moment's reflection shows that, in fact, the optimal set of questions depends upon the player: if someone is biased towards automobiles, it would be sensible to focus on questions that specify make, model, year, etc. You could then imagine writing down a script for this player: "first ask if it is a car; then if yes, ask if it is domestic, if no, ask if it is a Honda...;" or for my nieces: "first ask if it's Elsa from Frozen." (It almost always is.)

For each player and their preferences (i.e., for every probability distribution over the things that player might choose), there is an optimal script. And for each optimal script for a given person, the game will last five rounds, or ten rounds, or seven, or twenty, depending on what they choose that time. Profoundly, the number of questions you have to ask on average for a particular person and optimal script pair is given by Equation (2.19). In particular, we are measuring information (and uncertainty): the average number of yes-no questions we'll need to ask to find out an answer.

Understanding entropy is important to the rest of the discussion in this chapter as it is the fundamental building block of all other information-theoretic quantities.

2.2.2 Mutual Information

It is often interesting to consider how knowledge about something informs us about something else. People carrying umbrellas, for example, tells us something about the weather; it is not perfect but (informally) if you tell me something about the weather, you also reduce my uncertainty about umbrella-carrying [28]. To constructively introduce the so-called *mutual information*, I will adapt the next example from [28].

How can we quantify the information between the weather W and umbrella-carrying U? For simplicity, I will assume you only get to see one person—who is either carrying (u_1) or not carrying (u_2) an umbrella, *i.e.*, $U = \{u_1, u_2\}$ with probability $p(u_i)$.

Now assume that there are some finite number of weather types (say "rain", "cloudy", "windy" etc., labeled with w_j), each with a probability of occurring, $p(w_j)$. Then from Section 2.2.1, the uncertainty in the weather is simply

$$H[W] = -\sum_{i=1}^{N} p(w_j) \log(p(w_j))$$
(2.23)

We are interested in the probability of seeing a particular weather type given that we see the person carrying an umbrella. For this, consider the conditional probability of weather type i given that you see someone carrying an umbrella— $p(w_i|u_1)$. Generally, $p(w_i|u_1)$ will be higher than $p(w_j|u_1)$ when i is labeling weather with precipitation and j is not, so the uncertainty of the weather given that someone is carrying an umbrella is then

$$H[W|u_1] = -p(u_1) \sum_{j} p(w_j|u_1) \log(p(w_j|u_1))$$
(2.24)

or in words, "the uncertainty about the weather, given that the person who walked in was carrying an umbrella." Similarly, for the reverse case, we could compute the associated uncertainty $H[W|u_2]$, to determine "the uncertainty about the weather, given that the person who walked in was not carrying an umbrella." Combining (summing) these two we get the *conditional entropy* between two variables (weather type and state of umbrella-carrying in this example).

Definition (Conditional Entropy [103]). Define Q and R to be discrete random variables with support $\{q_1, ..., q_n\}$ and $\{r_1, ..., r_m\}$ respectively. Then the <u>conditional entropy</u> is defined as

$$H[Q|R] = -\sum_{i} p(r_i) \sum_{j} p(q_j|r_i) \log(p(q_j|r_i))$$
(2.25)

where $p(q_j|r_i)$ is the conditional probability of q_j given r_i .

_

We can then quantify the "reduction in uncertainty" in the weather given that someone is carrying an umbrella by $H[W] - H[W|u_1]$, and the reverse with $H[W] - H[W|u_2]$. Note that the reduction can be positive or negative—in some climates, seeing your colleague not carrying an umbrella will make you more uncertain about the weather. Consider, for example, an extremely rainy climate; it is either sunny, cloudy, or rainy, but most often rainy. You are generally quite certain about the weather before you see your colleague (it is raining). So when they walk through the door without their umbrella, you think it is less likely to be raining, and so you are more uncertain (the options sunny, cloudy, or rainy are now more evenly balanced).

Now consider the "average reduction in uncertainty" of the weather given the state of umbrella carrying

$$I[W,U] = p(u_1)(H[W] - H[W|u_1]) + p(u_2)(H[W] - H[W|u_2])$$
(2.26)

$$= H[W] - (p(u_1)H[W|u_1] + p(u_2)H[W|u_2])$$
(2.27)

$$= H[W] - H[W|U]$$
 (2.28)

This is called the *mutual information*; it tells us how much less uncertain we are, on average, about W given that we know U.

Definition (Mutual Information). Define Q and R to be discrete random variables with support $\{q_1, ..., q_n\}$ and $\{r_1, ..., r_m\}$ respectively, and let H(Q) be the entropy of Q and H(Q|R) be the conditional entropy. Then the mutual information I between Q and R is defined as

$$I[Q,R] = -\sum_{i,j} p(q_j, r_i) \log \frac{p(q_j, r_i)}{p(q_j)p(r_i)}$$
(2.29)

$$= H[Q] - H[Q|R]$$
 (2.30)

Note: I[Q, R] = I[R, Q] [33].

In the next section, I extend this discussion to information shared between *more than* two variables. In the language of *this* section, that is equivalent to the situation where I have two or more colleagues with umbrellas U_{C1} and U_{C2} and I want to know the average reduction in uncertainty of the weather given the state of U_{C1} and U_{C2} , *i.e.*, $I[W, U_{C1}, U_{C2}]$. This is unfortunately not a straightforward generalization and there is little agreement in the literature about interpreting or even defining multivariate mutual information.

2.2.3 *I*-Diagrams and Multivariate Mutual Information

The mathematical definitions of multivariate mutual information can get quite confusing to interpret, especially when comparing and contrasting the difference in these definitions. To clarify this discussion, I will use *I*-Diagrams of Yeung [121]—a highly useful visualization technique for interpreting information theoretic quantities.

2.2.3.1 *I*-Diagrams

Figure 2.4 shows *I*-diagrams of some of the important quantities introduced in Sections 2.2.1 and 2.2.2: (a) entropy H[Q], (b) joint entropy H[Q, R] (c) conditional entropy H[Q|R] and (d) mutual information I[Q, R]. In *I*-Diagrams, each circle represents the uncertainty in a particular variable and the shaded region is the information quantity of interest, *e.g.*, in (a) we are interested in H[Q]—the uncertainty in Q—so the entire circle is shaded. Figure 2.4(b) introduces a new measure: joint entropy $H[Q, R] = \sum_{q,r} p(q, r) \log(p(q, r))$. H[Q, R] is uncertainty about processes Q and R; this is easily depicted in an *I*-Diagram by simply shading both circles.

The real magic of *I*-Diagrams comes from their ability to depict more-complex information theoretic measures by simply manipulating shaded regions. For example, recall from Section 2.2.2 that conditional entropy H[Q|R]—Figure 2.4(b)—is the uncertainty about process Q given knowledge of R. One way of writing this is H[Q|R] = H[Q, R] - H[Q]: *i.e.*, subtracting the shaded regions in (a) and (b) produces the shaded region in (c). The same can be done with mutual information. Recall from Section 2.2.2 that I[Q, R] is the shared uncertainty between Q and R or I[Q, R] = H[Q] - H[Q|R]: *i.e.*, subtracting the shaded region in (a) from the shaded region in (c) produces the shaded region in (d). While obviously not a proof, this kind of approach allows us to easily build intuition about more complicated identities, *e.g.*, symmetry of mutual information:



Figure 2.4: *I*-Diagrams of H[Q], H[Q,R], H[Q|R] and I[Q,R]

I[Q, R] = H[Q] - H[Q|R] = H[R] - H[R|Q] = I[R, Q].

In the next section, I will use *I*-diagrams to explore three common interpretations of multivariate mutual information, interaction information [76] (also commonly called the co-information [10]), the binding information [87] (also called the dual total correlation [50]), and total correlation [118] (also commonly called multi-information [111]).

2.2.4 Multivariate Mutual Information

When interpreting I[Q, R] using *I*-Diagrams, the situation is quite simple, as there is exactly one region of "shared uncertainty;" when generalizing even to three variables I[Q, R, S], the situation becomes much more confusing—and this is reflected in the mathematical uncertainties as well. Consider the generic three-variable *I*-Diagram in Figure 2.5. Instead of having one region of overlap as in Figure 2.4(d), there are now four. There are three standard ways of shading each





(b) The interaction information (or coinformation), C[Q, R, S].



(c) The binding information, $\mathcal{B}[Q,R,S]$ (or dual total correlation).



(d) The total correlation (or multi-information), $\mathcal{M}[Q, R; S]$. The centermost region is more darkly shaded here to reflect the extra weight that that region carries in the calculation.

Figure 2.5: Generalizations of the mutual information to the multivariate case.

these regions to quantify I[Q, R, S].

One interpretation is the so-called *interaction information* [10,76]

$$C[Q, R, S] \equiv I[Q, R, S] \equiv -(H[Q] + H[R] + H[S]) + (H[Q, R] + H[Q, S] + H[R, S]) - H[Q, R, S]$$
(2.31)

As depicted in Figure 2.5(b), this is the intersection of H[Q], H[R] and H[S]. It describes the reduction in uncertainty that any two processes (e.g., Q and R), together, provide regarding the third process (e.g., Q and R). While this may seem like the natural extension of mutual information, it does not take into account the information that is shared between the two process but not with the third. One common criticism of this interpretation is that C[Q, R, S] is quite often negative. For example, when the shared information between $\{Q, R\}$ is due entirely to information in S, the interaction information can be negative as well as positive. Many interpretations of negative information have been provided—e.g., that the variable S inhibits (*i.e.*, accounts for or explains some of) the correlation between $\{Q, R\}$ —but in general negative information is frowned upon [1].

The next obvious step is to take into account the information that is shared between any two process but *not shared with the third*, as well as the information shared between all three processes. This is called the binding information [50, 87]

$$\mathcal{B}[Q,R,S] \equiv I[Q,R,S] \equiv H[Q,R,S] + \left[\sum_{i=1}^{3} H[X_{(i-1)\%3}, X_{(i+1)\%3}]) - H[Q,R,S]\right]$$
(2.32)

where $X_0 = Q$, $X_1 = R$, and $X_2 = S$, and % is the modulus operator. This quantity is depicted in Figure 2.5(c). $\mathcal{B}[Q, R, S]$ has the nice feature that it is always positive, but it equally weights information contained in two variables as information contained in all three. The total correlation [111, 118]

$$\mathcal{M}[Q,R,S] \equiv I[Q,R,S] \equiv I[X_0,X_1,X_2] \equiv \sum_{i=0}^{2} \left(H[X_i]\right) - H[X_0,X_1,X_2]$$
(2.33)

depicted in Figure 2.5(d) addresses this shortcoming, but is equally criticized for over emphasizing information that is shared by all three variables.

The total correlation and binding information are both always positive but their relative merits are a subject of contention. For a nice comparison of these and discussion of the associated issues, please see [1]. The takeaway of this section should be that extending mutual information as defined in Section 2.2.2 to even the three-variable case, let alone beyond that, is non-trivial and not well understood at all. This will become very important in Section 5.1, where I propose a new information-theoretic method for selecting delay reconstruction parameters.

2.2.5 Estimating Information from Real-Valued Time-Series Data

Note that all the information theory discussed thus far has been on *discrete* random variables. The topic of this thesis, however, involves *real-valued* time series. To compute any information measure on *real-valued* time series, one must "symbolize" that data, *i.e.*, map the real values to a set of discrete symbols. Ideally, this symbolization should preserve the information and/or dynamics of the original time series, but this can be hard to accomplish in practice. The processes by which this is accomplished, and the issues that make it difficult, are the focus of this section.

2.2.5.1 Simple Binning

A common (and by far the simplest) symbolization method is *binning*. To symbolize a realvalued time series $\{x_j\}_{j=1}^N$ by binning, one breaks the time series support into n bins, which need not be equally spaced. Then one defines a discrete random variable Q to have a symbol for each bin b_i , *i.e.*, Q has support $\{b_i\}_{i=1}^n$. The associated probability mass function is then computed using

$$p(b_i) = \frac{|\{j|x_j \in b_i\}|}{N}$$
(2.34)

For example, consider a time series with support on [0, 1] and bins $b_1 = [0, 0.5)$ and $b_2 = [0.5, 1]$. Then one simply estimates the probability mass function associated with b_1 and b_2 by counting the number of time-series elements that appear in each subinterval [0, 0.5) and [0.5, 1].

This method is extremely simple, but simplicity is often a double-edged sword. Binning is a very fast and efficient symbolization, but it is known to introduce severe biasing and spurious dynamics if the bin boundaries do not happen to create a so called *generating partition* of the dynamics [13,63].

Definition (Generating Partition). Given a dynamical system $f : \mathcal{M} \to \mathcal{M}$ on a measure space (\mathcal{M}, F, μ) , a finite partition $P = \{b_i\}_{i=1}^n$ is said to be generating if the union of all images and

preimages of P gives the set of all μ -measurable sets F. In other words, the "natural" tree of partitions always generates some sub- σ -algebra, but if it gives the full σ -algebra of all measurable sets F, then P is called generating [97].

Unfortunately, even for most canonical dynamical systems, let alone all real-valued time series, the generating partition is not known or computable. Even when the partition is known it can be fractal, as is the case with the Hénon map, for example, and thus useless for creating a *finite* partition. For a good review of the difficulties in finding a generating partition see [26]. I review this in more detail in Section 2.2.6.

2.2.5.2 Kernel estimation methods

A useful alternative to simple binning is a class of methods known as *kernel estimation* [34, 100], in which the relevant probability density functions are estimated via a function Θ with a resolution or bandwidth ρ that measures the similarity between two points in $Q \times R$ space.⁵ Given points $\{q_i, r_i\}$ and $\{q'_i, r'_i\}$ in $Q \times R$, one can define

$$\hat{p}_{\rho}(q_i, r_i) = \frac{1}{N} \sum_{i'=1}^{N} \Theta\left(\left| \begin{array}{c} q_i - q'_i \\ r_i - r'_i \end{array} \right| - \rho \right)$$
(2.35)

where $\Theta(x > 0) = 0$ and $\Theta(x \le 0) = 1$. That is, $\hat{p}_{\rho}(q_i, r_i)$ is the proportion of the N pairs of points in $Q \times R$ space that fall within the kernel bandwidth ρ of $\{q_i, r_i\}$, i.e., the proportion of points similar to $\{q_i, r_i\}$. When $|\cdot|$ is the max norm, this is the so-called box kernel. This too, however, can introduce bias [70] and is obviously dependent on the choice of bandwidth ρ . After these estimates, and/or the analogous estimates for $\hat{p}(q)$, are produced, they are then used directly to compute local estimates of entropy or mutual information for each point in space, which are then averaged over all samples to produce the entropy or mutual information of the time series. For more details on this procedure, see [70].

A less biased method to perform kernel estimation when one is interested in computing mutual information is the Kraskov-Stügbauer-Grassberger (KSG) estimator [63]. This approach

 $^{^5}$ In the case of delay-coordinate reconstruction, $Q\times R = X_j\times X_{j-\tau}$

dynamically alters the kernel bandwidth to match the density of the data, thereby smoothing out errors in the probability density function estimation process. In this approach, one first finds the k^{th} nearest neighbor for each sample $\{q, r\}$ (using max norms to compute distances in q and r), then sets kernel widths ρ_q and ρ_r accordingly and performs the pdf estimation. There are two algorithms for computing I[Q, R] with the KSG estimator [70]. The first is more accurate for small sample sizes but more biased; the second is more accurate for larger sample sizes. I use the second of the two in the results reported in this dissertation, as I have fairly long time series. This algorithm sets ρ_q and ρ_r to the q and r distances to the k^{th} nearest neighbor. One then counts the number of neighbors within and on the boundaries of these kernels in each marginal space, calling these sums n_q and n_r , and finally calculates

$$I[Q,R] = \psi(k) - \frac{1}{k} - \langle \psi(n_q) + \psi(n_r) \rangle + \psi(n)$$

$$(2.36)$$

where ψ is the digamma function⁶. This estimator has been demonstrated to be robust to variations in k as long as $k \ge 4$ [70].

In this thesis, I employ the Java Information Dynamics Toolkit (JIDT) implementation of the KSG estimator [70]. The computational complexity of this implementation is $\mathcal{O}(kN \log N)$, where N is the length of the time series and k is the number of neighbors being used in the estimate. While this is more expensive than traditional binning ($\mathcal{O}(N)$), it is bias corrected, allows for adaptive kernel bandwidth to adjust for under- and over-sampled regions of space, and is both model and parameter free (aside from k, to which it is very robust).

2.2.6 Estimating Structural Complexity and Predictability

An understanding of the predictive capacity of a real-valued time series—i.e., whether or not it is even predictable—is essential to any forecasting strategy. In joint work with Ryan James, I propose to quantify the complexity of a signal by approximating the entropy production of the system that generated it. In general, estimating the entropy (production) of an arbitrary, real-

⁶ The formula for the other KSG estimation algorithm is subtly different; it sets ρ_q and ρ_r to the maxima of the q and r distances to the k nearest neighbors.

valued time series is a challenging problem, as discussed above, but recent advances in Shannon information theory—in particular, permutation entropy [9, 32]—have reduced this challenge. I review this class of methods in this section.

For the purposes of this thesis, I view the Shannon entropy—in particular, its growth rate with respect to word length (the Shannon entropy rate)—as a measure of the complexity and hence the predictability for a time series. Time-series data consisting of i.i.d. random variables, such as white noise, have high entropy rates, whereas highly structured time-series—for example, those that are periodic—have very low (or zero) entropy rates. A time series with a high entropy rate is almost completely unpredictable, and conversely. This can be made more rigorous: Pesin's relation [91] states that in chaotic dynamical systems, the Kolmogorov-Sinai (KS) entropy is equal to the sum of the positive Lyapunov exponents λ_i . These exponents directly quantify the rate at which nearby states of the system diverge with time: $|\Delta x(t)| \approx e^{\lambda t} |\Delta x(0)|$. The faster the divergence, the larger the entropy. The KS entropy is defined as the supremum of the Shannon entropy rates of all partitions—*i.e.*, all possible choices for binning [92]. As an aside, an alternative definition of the generating partition defined above is a partition that achieves this supremum.

From a different point of view, I can consider the information (as measured by the Shannon entropy) contained in a single observable of the system at a given point in time. This information can be partitioned into two components: the information shared with past observations—*i.e.*, the mutual information between the past and present—and the information in the present that is not contained in the past (*viz.*, "the conditional entropy of the present given the past"). The first part is known as the *redundancy*; the second is the aforementioned *Shannon entropy rate*. Again working with R. G. James, I establish that the more redundancy in a signal, the more predictable it is [40,41]. This is discussed in more detail in Chapter 6.

Previous approaches to measuring temporal complexity via the Shannon entropy rate [74,102] required categorical data: $x_i \in S$ for some finite or countably infinite *alphabet* S. Data taken from real-world systems are, however, effectively⁷ real-valued. So for this reason I need to symbolize

⁷ Measurements from finite-precision sensors are discrete, but data from modern high-resolution sensors are, for

the time series, as discussed above. The methods discussed above however, are generally biased or fragile in the face of noise.

Bandt and Pompe introduced the *permutation entropy* (PE) as a "natural complexity measure for time series" [9]. Permutation entropy involves a method for symbolizing real-valued time series that follows the intrinsic behavior of the system under examination. This method has many advantages, including robustness to observational noise, and its application does not require any knowledge of the underlying mechanisms of the system. Rather than looking at the statistics of sequences of values, as is done when computing the Shannon entropy, permutation entropy looks at the statistics of the *orderings* of sequences of values using ordinal analysis. Ordinal analysis of a time series is the process of mapping successive time-ordered elements of a time series to their value-ordered permutation of the same size. By way of example, if $(x_1, x_2, x_3) = (9, 1, 7)$ then its *ordinal pattern*, $\phi(x_1, x_2, x_3)$, is 231 since $x_2 \leq x_3 \leq x_1$. The ordinal pattern of the permutation $(x_1, x_2, x_3) = (9, 7, 1)$ is 321.

Definition (Permutation Entropy). Given a time series $\{x_i\}_{i=1,...,N}$, define S_{ℓ} as all ℓ ! permutations π of order ℓ . For each $\pi \in S_{\ell}$, define the relative frequency of that permutation occurring in $\{x_i\}_{i=1,...,N}$

$$p(\pi) = \frac{|\{i|i \le N - \ell, \phi(x_{i+1}, \dots, x_{i+\ell}) = \pi\}|}{N - \ell + 1}$$
(2.37)

where $p(\pi)$ quantifies the probability of an ordinal and $|\cdot|$ is set cardinality. The <u>permutation entropy</u> of order $\ell \geq 2$ is defined as

$$PE(\ell) = -\sum_{\pi \in \mathcal{S}_{\ell}} p(\pi) \log_2 p(\pi)$$
(2.38)

Notice that $0 \leq PE(\ell) \leq \log_2(\ell!)$ [9]. With this in mind, it is common in the literature to normalize permutation entropy as follows: $\frac{PE(\ell)}{\log_2(\ell!)}$. With this convention, "low" PE is close to 0 and "high" PE is close to 1. Finally, it should be noted that the permutation entropy has been shown to be identical to the Kolmogorov-Sinai entropy for many large classes of systems [7], as long as the purposes of entropy calculations, effectively continuous. observational noise is sufficiently small. As mentioned before, PE is equal to the Shannon entropy rate of a generating partition of the system. This transitive chain of equalities, from permutation entropy to Shannon entropy rate via the KS entropy, allows one to approximate the redundancy of a signal—being the dual of the Shannon entropy rate—by $1 - \frac{PE(\ell)}{\log_2(\ell!)}$.

In this thesis, I utilize a variation of the basic permutation entropy technique, the weighted permutation entropy (WPE), which was introduced in [32]. The intent behind the weighting is to correct for observational noise that is larger than the trends in the data, but smaller than the larger-scale features. Consider, for example, a signal that switches between two fixed points and contains some additive noise. The PE is dominated by the noise about the fixed points, driving it to ≈ 1 , which in some sense hides the fact that the signal is actually quite structured. To correct for this, the weight of a permutation is taken into account

$$w(x_{i+1}^{\ell}) = \frac{1}{\ell} \sum_{j=i}^{i+\ell} \left(x_j - \bar{x}_{i+1}^{\ell} \right)^2$$
(2.39)

where x_{i+1}^{ℓ} is a sequence of values $x_{i+1}, \ldots, x_{i+\ell}$, and \bar{x}_{i+1}^{ℓ} is the arithmetic mean of those values. The weighted probability of a permutation is defined as

$$p_w(\pi) = \frac{\sum_{i \le N-\ell} w(x_{i+1}^{\ell}) \cdot \delta(\phi(x_{i+1}^{\ell}), \pi)}{\sum_{i \le N-\ell} w(x_{i+1}^{\ell})}$$
(2.40)

where $\delta(x, y)$ is 1 if x = y and 0 otherwise. Effectively, this weighted probability emphasizes permutations that are involved in "large" features and de-emphasizes permutations that are small in amplitude, relative to the features of the time series. The standard form of weighted permutation entropy is

$$WPE(\ell) = -\sum_{\pi \in \mathcal{S}_{\ell}} p_w(\pi) \log_2 p_w(\pi), \qquad (2.41)$$

which can also be normalized by dividing by $\log(\ell!)$, to make $0 \leq WPE(\ell) \leq 1$.

In practice, calculating permutation entropy and weighted permutation entropy involves choosing a good value for the word length ℓ . The primary consideration in that choice is that the value be large enough that forbidden ordinals are discovered, yet small enough that reasonable statistics over the ordinals are gathered. If an average of 100 counts per ordinal is considered to be sufficient, for instance, then $\ell = \operatorname{argmax}_{\hat{\ell}}\{N \gtrsim 100\hat{\ell}!\}$. In the literature, $3 \leq \ell \leq 6$ is a standard choice—generally without any formal justification. In theory, the permutation entropy should reach an asymptote with increasing ℓ , but that can require an arbitrarily long time series. In practice, what one should do is calculate the *persistent* permutation entropy by increasing ℓ until the result converges, but data length issues can intrude before that convergence is reached. I use this approach to choose $\ell = 6$ for the experiments presented in this thesis. This value represents a good balance between accurate ordinal statistics and finite-data effects.

2.3 Forecast Methods

Any discussion of new prediction technology is incomplete, of course, without a solid comparison to traditional techniques. In this section, I describe the four different forecasting methods used in my thesis as points of comparison. These forecast methods include:

- The *random-walk* method, which uses the previous value in the observed signal as the forecast,
- The *naïve* method, which uses the mean of the observed signal as the forecast,
- The ARIMA (auto-regressive integrated moving average) method, a common linear forecast strategy for scalar time-series data, instantiated via the ARIMA procedure [56], and
- The *LMA* (Lorenz method of analogues) method, which uses a near-neighbor forecast strategy on a delay-coordinate reconstruction of the signal.

ARIMA, as its name suggests, is based on standard autoregressive techniques. LMA, introduced in Chapter 1, is designed to capture and exploit the deterministic structure of a signal from a nonlinear dynamical system. The naïve and random-walk methods, somewhat surprisingly, often outperform these more-sophisticated prediction strategies in the case of highly complex signals, as discussed briefly below and in depth in Chapter 6.

2.3.1 Simple Prediction Strategies

A random-walk predictor simply uses the last observed measurement as the forecast: that is, the predicted value p_i at time *i* is calculated using the relation

$$p_i \equiv x_{i-1} \tag{2.42}$$

where $\{x_j\}_{j=1}^N$ is the time-series data. The prediction strategy that I refer to using the term "naïve" averages all prior observations to generate the forecast

$$p_i \equiv \mu_{x,i-1} = \sum_{j=1}^{i-1} \frac{x_j}{i-1}$$
(2.43)

While both of these methods are simplistic, they are not without merit. For a time series that possess very little predictive structure (WPE \approx 1), these two methods can actually be the best choice. In forecasting currency exchange rates, for instance, sophisticated econometrics-based prediction models fail to consistently outperform the random-walk method [78,82]. These signals are constantly changing, subject to jump processes, noisy, and possess very little predictive structure, but their variations are not—aside from jump processes—very large, so the random-walk method's strategy of simply guessing the last known value is not a bad choice. If a signal has a unimodal distribution with low variance, the naïve prediction strategy will perform quite well, even if the signal is highly complex, simply because the mean is a good approximation of the future behavior. Moreover, the naïve prediction strategy's temporal average effects a low-pass filtering operation, which mitigates the complexity in signals with very little predictive structure.

Both of these methods have significant weaknesses, however. Because they do not model the temporal patterns in the data, or even the distribution of its values, they cannot track changes in that structure. This causes them to fail in a number of important situations. Random-walk strategies are a particularly bad choice for time series that change significantly at every time step. In the worst case—a large-amplitude square wave whose period is equivalent to twice the sample time—a random-walk prediction would be exactly 180 degrees out of phase with the true continuation. The naïve method would be a better choice in this situation, since it would always predict the mean. It would, however, perform poorly when a signal had a number of long-lived regimes that have significantly different means. In this situation, the inertia of the naïve method's accumulating mean is a liability and the agility of the random-walk method is an advantage, since it can respond quickly to regime shifts.

Of course, methods that can capture and exploit the geometry of the data, or its temporal patterns, can be far more effective in the situations described in the previous two paragraphs. The ARIMA and LMA methods covered in the following sections are designed to do exactly that. However, if a signal contains little predictive structure, forecast strategies like ARIMA and LMA have nothing to work with and thus will often be outperformed by the two simple strategies described in this section. This contrast is explored further in Sections 2.4 and 4.2.

2.3.2 (ARIMA) A Regression-Based Prediction Strategy

A simple and yet powerful way to capture and exploit the structure of data is to fit a hyperplane to the dataset and then use it to make predictions. The roots of this approach date back to the original autoregressive schema of Yule [122], which forecasts the value at the next time step through a weighted average of the past q observations

$$p_i \equiv \sum_{j=i-q}^{i-1} a_j x_j \tag{2.44}$$

The weighting coefficients a_j are generally computed using either an ordinary least-squares approach, or with the method of moments using the Yule-Walker equations. To account for noise in the data, one can add a so-called "moving average" term to the model; to remove nonstationarities, one can detrend the data using a differencing operation. A strategy that incorporates all three of these features is called a *nonseasonal ARIMA model*. If evidence of periodic structure is present in the data, a *seasonal ARIMA model*, which adds a sampling operation that filters out periodicities,

can be a good choice.

There is a vast amount of theory and literature regarding the construction and use of models of this type; please see [15] for an in-depth exploration. For the purposes of this thesis, I choose seasonal ARIMA models to serve as a good exemplar for a broad class of linear predictors and a useful point of comparison for my work. Fitting such a model to a time series involves choosing values for the various free parameters in the autoregressive, detrending, moving average, and filtering terms. I employ the automated fitting techniques described in [56] to accomplish this. This procedure uses sophisticated methods—KPSS unit-root tests [65], a customization of the Canova-Hansen test [19], and the Akaike information criterion [2], conditioned on the maximum likelihood of the model fitted to the detrended data—to select good values for these free parameters.

ARIMA forecasting is a common and time-tested procedure. Its adjustments for seasonality, nonstationarity, and noise make it an appropriate choice for short-term predictions of time-series data generated by a wide range of processes. If information is being generated and/or transmitted in a nonlinear way, however, a global linear fit is inappropriate and ARIMA forecasts can be inaccurate. Another weakness of this method is prediction horizon: an ARIMA forecast is guaranteed to converge to a constant or linear trend after some number of predictions, depending on model order. To sidestep this issue, and make the comparison as fair as possible, I build ARIMA forecasts in a stepwise fashion: *i.e.*, fit the model to the existing data, use that model to perform a one-step prediction, rebuild it using the latest observations, and iterate until the desired prediction horizon is reached. For consistency, I take the same approach with the other models in this proposal as well, even though doing so amounts to artificially hobbling LMA, the method that is the topic of the next section.

2.3.3 Lorenz Method of Analogues

The dynamical systems community has developed a number of methods that leverage delaycoordinate reconstruction for the purposes of forecasting dynamical systems (*e.g.*, [23,72,93,107,112, 119]). Since the goal of this thesis is to show that incomplete reconstructions—those that are not true embeddings—can give these kinds of methods enough traction to generate useful predictions, I choose one of the oldest and simplest members of that family to use in my analysis: Lorenz's method of analogues (LMA), which is essentially nearest-neighbor forecasting in reconstruction space.

To apply LMA to a scalar time-series data set $\{x_j\}_{j=1}^n$, one begins by performing a delaycoordinate reconstruction to produce a trajectory of the form

$$\{\vec{x}_j = [x_j \ x_{j-\tau} \ \dots \ x_{j-(m-1)\tau}]^T\}_{j=1-(m-1)\tau}^n$$
(2.45)

using one or more of the heuristics presented in Sections 2.1.2 and 2.1.3 to choose m and τ . Forecasting the next point in the time series, x_{n+1} , amounts to reconstructing the next delay vector \vec{x}_{n+1} in the trajectory. Note that, by the form of delay-coordinate vectors, all but the first coordinate of \vec{x}_{n+1} are known. To choose that first coordinate, LMA finds the nearest neighbor of \vec{x}_n in the reconstructed space⁸ —namely $\vec{x}_{j(1,m)}$ —and maps that vector forward using the delay map, obtaining

$$\vec{x}_{j(1,m)+1} = [x_{j(1,m)+1} \ x_{j(1,m)+1-\tau} \ \dots \ x_{j(1,m)+1-(m-1)\tau}]^T$$
(2.46)

Using the image of the neighbor, one defines

$$\vec{p}_{n+1} \equiv [x_{j(1,m)+1} \ x_{n+1-\tau} \ \dots \ x_{n+1-(m-1)\tau}]^T$$
 (2.47)

The LMA forecast of x_{n+1} is then $p_{n+1} \equiv x_{j(1,m)+1}$. If performing multi-step forecasts, one appends the new delay vector

$$\vec{p}_{n+1} = [x_{j(1,m)+1} \ x_{n+1-\tau} \ \dots \ x_{n+1-(m-1)\tau}]^T$$
(2.48)

to the end of the trajectory and repeats this process as needed.

In my work, I use the LMA algorithm in two ways: first—as a baseline for comparison purposes—on an embedding of each time series, with m chosen using the false near(est) neighbor

⁸ \vec{x}_n should not be chosen as its own neighbor as it has no forward image. In some cases, a longer Theiler exclusion may be useful [115].

method [62]; second, with m fixed at 2. In the rest of this thesis, I will refer to these as fnn-LMA and ro-LMA, respectively. The experiments reported in Chapter 4, unless stated otherwise, use the same τ value for both fnn-LMA and ro-LMA, choosing it at the first minimum of the time-delayed mutual information of the time series [33]. In Section 4.3, I explore the effects of varying τ on the accuracy of both methods. In Section 5.1, I show that a time-delayed version of the so-called *active information storage* is a highly effective method for selecting τ , and m as well, when forecasting is the end goal.

Dozens—indeed, hundreds—of more-complicated variants of the LMA algorithm have appeared in the literature (e.g., [23, 107, 112, 119]), most of which involve building some flavor of local-linear model around each delay vector and then using it to make the prediction of the next point. For the purposes of this thesis, I chose to use the basic original LMA because it is dynamically the most straightforward and thus provides a good baseline assessment. While I believe that the claims stated here extend to other state space-based forecast methods, the pre-processing steps involved in some of those methods make a careful analysis of the results somewhat problematic. One can use GHKSS-based techniques, for instance, to project the full dynamics onto linear submanifolds [48] and then use those manifolds to build predictions. While it might be useful to apply a method like that to an incomplete reconstruction, the results would be some nonlinear conflation of the effects of the two different projections and it would be difficult to untangle and understand the individual effects. (Note that the careful study of the effects of projection in forecasting that are undertaken in this thesis may suggest why GHKSS-based techniques work so well; this point is discussed further in Chapter 4.)

Since LMA does not rest on an assumption of linearity (as ARIMA models do), it can handle both linear and nonlinear processes. If the underlying generating process is nondeterministic, however, it can perform poorly. For an arbitrary real-valued time series, without any knowledge of the generating process and with all of the attendant problems (noise, sampling issues, and so on), answers to the question as to which forecast model is best should, ideally, be derived from the data, but that is a difficult task. By quantifying the balance between redundancy, predictive structure, and entropy for these real-valued time series—as I describe in Chapter 6—I can begin to answer these questions in an effective and practical manner.

2.4 Assessing Forecast Accuracy

To assess and compare the prediction methods studied here, I calculate a figure of merit in the following way. I split each N-point time series into two pieces: the first 90%, referred to as the "initial training" signal and denoted $\{x_j\}_{j=1}^n$, and the last 10%, known as the "test" signal $\{c_j\}_{j=n+1}^{(k+n+1)=N}$. Following the procedures described in Section 2.3, I build a model from the initial training signal, use that model to generate a prediction p_{n+1} of the value of x_{n+1} , and compare p_{n+1} to the true continuation, c_{n+1} . I then rebuild the model using $\{c_{n+1}\} \cup \{x_j\}_{j=1}^n$ and repeat the process k times, out to the end of the observed time series. This "one step prediction" process is not technically necessary in the fnn-LMA or ro-LMA methods, which can generate arbitrary-length⁹ predictions, but the performance of the other three methods used here will degrade severely if the associated models are not periodically rebuilt. In order to make the comparison fair, I use the iterative one-step prediction schema for all five methods. This has the slightly confusing effect of causing the "test" signal to be used both to assess the accuracy of each model and for periodic refitting.

As a numerical measure of prediction accuracy, for each h-step forecast, I calculate the h-step mean absolute scaled error (h-MASE) between the true and predicted signals, defined as

$$h - \text{MASE} = \sum_{j=n+1}^{k+n+1} \frac{|p_j - c_j|}{\frac{k}{n-h} \sum_{i=1}^n \sqrt{\frac{\sum_{\ell=1}^h (x_i - x_{i+\ell})^2}{h}}}$$
(2.49)

h-MASE is a normalized measure: the scaling term in the denominator is the average *h*-step insample forecast error for a random-walk prediction over the initial training signal $\{x_i\}_{i=1}^n$. That is, *h*-MASE< 1 means that the prediction error in question was, on the average, smaller than the error of an *h*-step random-walk forecast on the same data. Analogously, *h*-MASE> 1 means that the

⁹ Although the accuracy of these predictions will degrade with prediction horizon, in the presence of positive Lyapunov exponents.

corresponding prediction method did *worse*, on average, than the random-walk method. I choose this error metric because it allows for fair comparison across varying methods, prediction horizons, and signal scales, and is a standard error measure in the forecasting literature [57].

To provide insight into interpreting *h*-MASE values, I will refer back to the proof-of-concept example presented in Chapter 1. The one-step forecasts in Figure 1.1, for instance, had 1-MASE values of 0.117 and 0.148—*i.e.*, the fnn-LMA and ro-LMA forecasts of the SFI dataset A were, respectively $\frac{1}{0.117} = 8.5$ and $\frac{1}{0.148} = 6.5$ times better than a one-step random-walk forecast of the initial training portion of the same signal.

For any non-constant signal, h-step forecasting with random walk will degrade as h increases. In general, then, it is to be expected that h-MASE will decrease drastically with increasing prediction horizon. Thus, h-MASE scores should not be compared for different h. For example, 10-MASE can be compared to 10-MASE for two different methods or signals but should not be compared to 1-MASE or 100-MASE, even on the same signal. While its comparative nature may seem odd, this error metric allows for fair comparison across varying methods, prediction horizons, and signal scales, making it a standard error measure in the forecasting literature—and a good choice for this thesis, which involves a number of very different signals.

Chapter 3

Case Studies

I use several different dynamical systems as case studies throughout this thesis, both real and synthetic. Two of them—the Lorenz 96 model and sensor data from a laboratory experiment on computer performance dynamics—persist across all chapters of this document; I use a number of others as well to drive home different points in different chapters. Each is described in more depth in the following sections.

3.1 Synthetic Case Studies

When developing any new mathematical theory or method it is important to first explore it in the context of well-understood synthetic examples. This gives me a controlled environment where I can test the boundaries of my theory, *e.g.*, increasing data length or adding a (controlled) signal-to-noise ratio.

3.1.1 The Lorenz-96 Model

The Lorenz-96 model was introduced by Edward Lorenz in [73] to study atmospheric predictability. Lorenz-96 is defined by a set of K first-order differential equations relating the K state variables $\xi_1 \dots \xi_K$

$$\dot{\xi}_k = (\xi_{k+1} - \xi_{k-2})(\xi_{k-1}) - \xi_k + F \tag{3.1}$$

for k = 1, ..., K, where $F \in \mathbb{R}$ is a constant forcing term that is independent of k. In this model,

each ξ_k is some atmospheric quantity (such as temperature or vorticity) at a discrete location on a periodic lattice representing a latitude circle of the earth. Following standard practice [61], I enforce periodic boundary conditions and solve Equation (3.1) from several randomly chosen initial conditions using a standard fourth-order Runge-Kutta solver for 60,000 steps with a step size of $\frac{1}{64}$ normalized time units. I then discard the first 10,000 points of each trajectory in order to eliminate transient behavior. Finally, I create scalar time-series traces by individually "observing" each of the K state variables of the trajectory: *i.e.*, $h_i(\xi_i(t_j)) = x_{j,i}$ for $j \in \{10, 000, \dots, 60, 000\}$ and for $i \in \{1, \dots, K\}$. I repeat all of this from a number of different initial conditions—seven for the K = 47 Lorenz-96 system and 15 for the K = 22 case—producing a total of 659 traces for my forecasting study.

In [61], Karimi & Paul studied this model extensively, performing and analyzing numerous parameter sweeps showing that it exhibits a vast array of possible dynamics: everything from fixed points and periodic attractors to low- and high-dimensional chaos. One particularly interesting feature of this dynamical system is the relationship between state-space dimension and how much



Figure 3.1: The Lorenz 96 attractor (F = 5) with (left) K = 22 and (right) K = 47. Since 22 and 47 dimensional plots are not possible, I plot 3D projections of these systems. In particular, each differently colored trajectory represents different projections or equivalently choices of k: k=2 is aqua, k = 6 is blue and k = 18 is red.

Grid Points	<i>m</i> -fnn	au	m-Embedology	m-Takens
K = 22	8	26	pprox 7	45
K = 47	10	31	≈ 41	95

Table 3.1: Estimated and theoretical embedding parameter values for the Lorenz-96 model. m-fnn is the embedding dimension produced by the false-nearest neighbor method. τ is chosen as the first minimum of the mutual information curve. m-Embedology is derived following [99] and m-Takens is derived from [113].

of that space is occupied by dynamics. For different choices of the parameter values, the Lorenz-96 system yields dynamics with low fractal dimensions in large state spaces as well as large fractal dimensions in large state spaces. All of these features make this model an ideal candidate for testing and evaluating ro-LMA. For my initial investigation, I fix F = 5 and choose K = 22 and K = 47—choices that yield chaotic trajectories with low and high [61] Kaplan-Yorke (Lyapunov) dimension [60] respectively: $d_{KY} \leq 3$ for the K = 22 dynamics and $d_{KY} \approx 19$ for K = 47. Projections of trajectories on these attractors can be seen in Figure 3.1.

For each of these time series, I use the procedures outlined in Section 2.1.1 to estimate values for the free parameters of the embedding process, obtaining m = 8 and $\tau = 26$ for all traces in the K = 22 case, and m = 10 and $\tau = 31$ for the K = 47 traces. Table 3.1 tabulates the estimated and theoretical embedding parameter values for these two test cases, derived using the methodologies described in Sections 2.1.1-2.1.3.

It has been shown in [109] that $d_{KY} \approx d_{cap}$ for typical chaotic systems. This suggests that embeddings of the K = 22 and K = 47 time series would require $m \gtrsim 6$ and $m \gtrsim 38$, respectively. The values suggested by the false-near neighbor method for the K = 22 traces are in line with this, but the K = 47 false-near neighbor values are far smaller than $2d_{KY}$. For K = 47 there are two potential causes for this disparity. First, the false-near neighbor method does not guarantee $m > 2d_{KY}$, it is simply a heuristic to mitigate false crossings in the dynamics. Second $m > 2d_{KY}$ is a *sufficient* bound—it could very well be the case that false crossings are eliminated before this bound is reached.



Figure 3.2: Classic Lorenz attractor ($\sigma = 10$, $\rho = 28$, $\beta = 8/3$): (a) A 50,000-point trajectory in \mathbb{R}^3 generated using fourth-order Runga-Kutta with a time step of $\frac{1}{64}$. (b) A time-series trace of the *x* coordinate of that trajectory. (c) A 3*D* projection of a delay-coordinate embedding of the trajectory in (b) with dimension m = 5 and delay $\tau = 12$.

3.1.2 Lorenz 63

The now canonical Lorenz-63 model was introduced by Lorenz in 1963 as a first example of "Deterministic Nonperiodic Flow," what is now known as *chaos.*¹ Lorenz 63 is defined by a set of three first-order differential equations system [71]

$$\dot{x} = \sigma(y - x) \tag{3.2}$$

$$\dot{y} = x(\rho - z) - y \tag{3.3}$$

$$\dot{z} = xy - \beta z \tag{3.4}$$

with the typical chaotic parameter selections: $\sigma = 10$, $\rho = 28$, and $\beta = 8/3$. Figure 3.2(a) shows a 50,000-point trajectory in \mathbb{R}^3 generated using fourth-order Runga-Kutta on those equations with a time step of $T = \frac{1}{64}$, as well as a time-series trace of the *x* coordinate of that trajectory— Figure 3.2(b)—and a 3*D* projection of a delay-coordinate embedding of that trace with dimension m = 5 and delay $\tau = 12$, Figure 3.2(c). This canonical example is used in Chapter 5 to establish an explanation of why ro-LMA is able to get traction even though it works with a reconstruction that does not meet the theoretical conditions of an embedding. Table 3.2 tabulates the estimated and theoretical embedding parameter values for this system.

¹ Although Lorenz did not coin this term.

<i>m</i> -fnn	au	m-Embedology	m-Takens
5	174	≈ 5	7

Table 3.2: Estimated and theoretical embedding parameter values for the Lorenz 63 model, chosen as described in the caption of Table 3.1.

3.2 Experimental Case Studies

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Validation with synthetic data is an important first step in evaluating any new theory, as it provides a controlled, well-defined and well-understood environment. However, these are luxuries, rarely if ever afforded to an experimentalist. Furthermore, experimental data often misbehaves more—and in different ways—than synthetic data. For these reasons, it is vital to test a method with experimental time-series data if one is interested in real-world applications.

3.2.1 Computer Performance

As has been established in prior work by our group, it is highly effective to treat computers as nonlinear dynamical systems [6,36–38,40–42,83,84]. In this view, register and memory contents and physical variables like the temperature of different regions of the processor chip define the state of the system. The logic hardwired into the computer, combined with the software executing on that hardware, defines the dynamics of the system. Under the influence of these dynamics, the state of the processor moves on a trajectory through its high-dimensional state space as the clock cycles progress and the program executes. Like Lorenz-96, this system has been shown to exhibit a range of interesting deterministic dynamical behavior, from periodic orbits to low- and high-dimensional chaos [6,83], making it a good test case for this thesis. It also has important practical implications; these dynamics, which arise from the deterministic, nonlinear interactions between the hardware and the software, have profound effects on execution time and memory use.

3.2.1.1 Theoretical Description

For the purposes of this thesis, I will consider a "stored-program computer," *i.e.*, a standard von Neumann architecture, as a deterministic nonlinear dynamical system. In a stored-program computer, the current state—both instructions and data—are stored in some form of addressable memory. The contents of this memory are, as established in [83], the state space X of the computer. Other components of the computer, such as external memory and video cards, also play roles in its state. Those roles depend on the decisions made by the computer designers—how things are implemented and connected—almost all of which are proprietary. In order to distinguish known and unknown effects, I follow [83] and define the state space X as a composition of the addressable memory elements \vec{m} and the unknown implementation variables \vec{u} :

$$\mathbb{X} = \{ \vec{\xi} \mid \vec{\xi} = [\vec{m}, \ \vec{u}] \}$$
(3.5)

The distinction between \vec{m} and \vec{u} is important because the dynamics of a running computer have two distinct sources: a map \vec{F}_{code} that acts on the addressable memory \vec{m} directly, as dictated by the program instructions, and a map \vec{F}_{impl} that captures how the implementation affects the evolution of the computer state. The overall dynamics of the computer—that is, the mapping from its state at the j^{th} clock cycle to its state at the $j + 1^{st}$ clock cycle—is a composition of these two maps:

$$\vec{\xi}(t_{j+1}) = \Phi(\vec{\xi}(t_j)) = \vec{F}_P(\vec{\xi}(t_j)) = \vec{F}_{impl} \circ \vec{F}_{code}(\vec{\xi}(t_j))$$
(3.6)

where \vec{F}_P is the performance dynamics of the computer. An improved design for the processor, for instance—that is, a "better" \vec{F}_P —is a change in \vec{F}_{impl} . The form of the map \vec{F}_{code} is dictated by the combination of the computer's formal specification (x86_64, for the Intel i7 used in the experiments here) and the software that it is running. Both \vec{F}_{impl} and \vec{F}_{code} are nonlinear and deterministic, and their composed dynamics must be modeled together in order to predict future computer performance.

The framework outlined in the previous paragraph lets me use the methods of nonlinear
dynamics—in particular, delay-coordinate embedding—to model \vec{F}_P , as long as I observe those dynamics in a way that satisfies the associated theorems (see Section 2.1.1). The hardware performance monitor registers (HPMs) that are built into modern processors can be programmed to count events on the chip: the total number of instructions executed per cycle (IPC), for instance, or the total number of references to the data cache. These are some of the most widely used and salient metrics in the computer performance analysis literature [3, 66, 81, 86, 104]. IPC is a good proxy for processor efficiency because most modern microprocessors can execute more than one instruction per clock cycle. While this metric may not be an element of the state vector $\vec{\xi}$, the fundamental theorems of delay-coordinate embedding only require that one measures a quantity that is a smooth, generic function of at least one state variable. It was shown in [6] that the transformation performed by the HPMs in sampling the state² $\vec{\xi}$ is indeed smooth and generic unless those registers overflow—an unlikely event, given that they are 64 bits long and that I read them every 100,000 instructions.

The choice of that sample interval is important for another reason as well. The HPMs are part of the system under study, so accessing them can disturb the very dynamics that they are sampling. This potential *observer problem* was addressed in [84] by varying the sample interval and testing to make sure that the sampling was not affecting the dynamics. To further reduce perturbation, the measurement infrastructure used to gather the data for the experiments reported here only monitors events when the target program is running, and not when the operating system (or the monitoring tool itself) have control of the microprocessor. I have completed a careful examination of the impact of interrupt rate on prediction results that corroborates the discussion above; these results are reported in [37]. Finally, I follow best practices from the computer performance analysis community [43] when measuring the system: I only use local disks and limit the number of other processes that are running on the machine (*i.e.*, Linux init level 1).

The next section describes the experimental observation of this system and the different choices of \vec{F}_{code} . For an in-depth description of this custom-measurement infrastructure, including

 $^{^{2}}$ This process entails subtracting successive HPM readings, checking for overflow and adjusting accordingly.



Figure 3.3: (Left) Time-series data from a computer performance experiment: processor load traces, in the form of instructions executed per cycle (IPC) of a simple program (col_major) that repeatedly initializes a 256×256 matrix. Each point is the average IPC over a 100,000 instruction period. (Right) A 3D projection of a 12D embedding of this time series.

a deeper discussion of the implications of the sampling interval, please see [6, 37, 83, 84].

3.2.1.2 Experimental methods

The computer performance time-series data sets for the experiments presented in this thesis were collected on an Intel Core[®] i7-2600-based machine running the 2.6.38-8 Linux kernel. I also carried out experiments on an Intel Core2 Duo. Those Core2 results, reported in [36] but omitted here, are consistent with the results reported in this dissertation. This i7 microprocessor chip has eight processing units, a clock rate of 3.40 GHz, and a cache size of 8192 KB. The experiments in this thesis involve performance traces gathered during the execution of several different programs, beginning with the simple col_major loop whose performance is depicted in the left panel of Figure 3.3, as well as a more-complex program from the SPEC 2006CPU benchmark suite (403.gcc) [54]. In addition, I also carried out careful analysis of standard computer performance benchmarks programs such as 482.sphinx [54], linear algebra software from LAPACK (Linear Algebra PACKage) such as dgesdd and dgeev [8] and row_major (the row-major analogue of col_major). Many of these experiments are omitted here for brevity; please see [36,37,40,41] for these companion results. I select col_major and 403.gcc from this larger constellation of experiments for the discussion in my thesis because they are informative in their own right and representative of the other results I encountered; col_major is a simple highly-structured chaotic time series, while 403.gcc is a chaotic time series where almost all structure has been consumed by noise.

In all of these experiments, the scalar observation x_j is a measurement of the processor performance at time j during the execution of each program. To record these measurements, I use the libpfm4 library, via PAPI (Performance Application Programming Interface) 5.2 [16], to stop program execution at 100,000-instruction intervals—the unit of time in these experiments—and read off the contents of the CPU's onboard hardware performance monitors, which I programmed to count how many instructions are executed in each clock cycle(IPC). I also recorded and analyzed other metrics including total L2 cache misses, missed branch predictions, and L2 instruction cache hits. Description of these metrics, as well as corresponding analysis, are published in [36, 37]. In this thesis, I only report results on IPC, as it is representative of all of these results. For statistical validation, I collect 15 performance traces from each of the programs. These traces, and the processes that generated them, are described in more depth in the rest of this section.

col_major is a simple C program that repeatedly initializes the upper triangle of a 2048 \times 2048 matrix in column-major order by looping over the following three lines of code:

for
$$(i=0; i < 2048; i++)$$

for $(j=i; j < 2048; j++)$
data $[j][i] = 0;$

As mentioned in Chapter 1 and shown in Figure 3.3, this simple program exhibits surprisingly complicated behavior. I also collected data from the row-major analogue to col_major. These time series were very different than col_major, but the forecasting results were largely the same, so they are omitted here but can be found in [36, 40].

The SPEC CPU2006 benchmark suite [54] is a collection of complicated programs that are used in the computer-science community to assess and compare the performance of different computers. 403.gcc is a member of that suite. It is a *compiler*: a program that translates code written in a high-level language (C, in the case of 403.gcc) into a lower-level format that can be executed



Figure 3.4: Processor load traces (IPC) of the SPEC benchmark 403.gcc. Each point is the average IPC in a 100,000 instruction period.

by the processor chip. Its behavior is far more complicated than that of col_major, as is clear from Figure 3.4. Unlike col_major, where the processor utilization is quite structured, the performance of 403.gcc appears almost random. In addition to 403.gcc, I also studied 482.sphinx from this benchmark suite: a speech-recognition tool [54]. 482.sphinx and the associated results are covered in more depth in [37, 40].

Table 3.3 tabulates the estimated embedding parameters for col_major and 403.gcc. Notice that because these dynamical systems are not understood from a theoretical perspective, *i.e.*, the governing equations or knowledge of the state space dimension are unknown, I must rely on the heuristics presented in Section 2.1.3. I should note that it has been estimated that the state space of these systems is at least 2^{32} dimensions [83], which would mean that *m*-Takens> 2^{33} . However, the same paper suggests the actual fractal dimension of these dynamics are much smaller, due in part to standard programming and design principles, which have the effect of reducing the dimension of the dynamics, and that *m*-Embedology is probably less that ten.

	m-fnn	au	m-Embedology	m-Takens
col_major	12	2	**	**
403.gcc	13	10	**	**

Table 3.3: Estimated embedding parameter values for the computer performance experiments. τ and *m*-fnn chosen as in Table 3.1. *m*-Embedology and *m*-Takens are not provided as these dimensions are unknown for a experimental system like this one.

Chapter 4

Prediction in Projection

In this chapter, I demonstrate that the accuracies of forecasts produced by ro-LMA—Lorenz's method of analogues, operating on a two-dimensional time-delay reconstruction of a trajectory from a dynamical system—are similar to, and often better than, forecasts produced by fnn-LMA, which operates on an embedding of the same dynamics. While the brief example in Chapter 1 is a useful first validation of that statement, it does not support the kind of exploration that is necessary to properly evaluate a new forecast method, especially one that violates the basic tenets of delay-coordinate embedding. The SFI dataset A is a single trace from a single system—and a low dimensional system at that. My goal in this chapter is to show that ro-LMA is comparable to or better than fnn-LMA for a range of systems and parameter values—and to repeat each experiment for a number of different trajectories from each system. This exploration serves as an experimental validation of the central premise of this thesis. And of course, any discussion of new forecasting strategies is incomplete without a solid comparison with traditional methods. To this end, I present results for two dynamical systems, one simulated and one real: the Lorenz-96 model and sensor data from a laboratory experiment on computer performance dynamics. I produce ro-LMA forecasts of these systems and compare them to forecasts using the four traditional strategies presented in Section 2.3.

4.1 A Synthetic Example: Lorenz-96

In this example, I perform two sets of forecasting experiments with ensembles of traces from the Lorenz-96 model [73], introduced in Section 3.1.1: one with K = 22 and the other with K = 47.

4.1.1 Comparing ro-LMA and fnn-LMA

As I will illustrate in the following discussion, both ro-LMA and fnn-LMA worked quite well for the K = 22 dynamics. See Figure 4.1(a) for a time-domain plot of an ro-LMA forecast of a representative trace from this system and Figures 4.1(b) and (c) for graphical representations of the forecast accuracy on that trace for both methods. In Figures 4.1(b) and (c), the vertical axis is the prediction p_j and the horizontal axis is the true continuation c_j . On this type of plot, a perfect prediction would lie on the diagonal. The diagonal structure on the p_j vs. c_j plots in the Figure indicates that both of these LMA-based methods perform very well on this trace. More importantly—from the standpoint of evaluation of my primary claim—the LMA forecasting strategy worked *better* on a two-dimensional reconstruction of these dynamics than on a full embedding, and by a statistically significant margin: the 1-MASE scores¹ of ro-LMA and fnn-LMA forecasts, computed following the procedures described in Section 2.4, are 0.391 ± 0.016 and 0.441 ± 0.033 , respectively, across the 330 traces at this parameter value. This is somewhat startling, given that the two-dimensional delay reconstruction used by ro-LMA falls far short of the requirement for topological conjugacy [99] in this system. Clearly, though, it captures *enough* structure to allow LMA to generate good predictions.

The K = 47 case is a slightly different story: here, ro-LMA still outperforms fnn-LMA, but not by a statistically significant margin. The 1-MASE scores across all 329 traces were 0.985 ± 0.047 and 1.007 ± 0.043 for ro-LMA and fnn-LMA, respectively. In view of the higher complexity of the state-space structure of the K = 47 version of the Lorenz-96 system, the overall increase in 1-MASE scores over the K = 22 case makes sense. Recall that d_{KY} is far higher for the K = 47 case:

¹ one-step ahead Mean Absolute Scaled Error



(a) 2,500-point forecast using the reduced-order forecast method ro-LMA. Blue circles and red \times s are the true and predicted values, respectively; vertical bars show where these values differ.



Figure 4.1: ro-LMA and fnn-LMA forecasts of a representative trace from the Lorenz-96 system with K = 22 and F = 5. Top: a time-domain plot of the first 2,500 points of the ro-LMA forecast. Bottom: the predicted (p_j) vs true (c_j) values for forecasts of that trace generated by (b) ro-LMA and (c) fnn-LMA. On such a plot, a perfect prediction would lie on the diagonal. The 1-MASE scores of the forecasts in (b) and (c) were 0.392 and 0.461, respectively.

this attractor fills more of the state space and has many more manifolds that are associated with positive Lyapunov exponents. This has obvious implications for predictability. Since I use the same traces for both methods, one might be tempted to think that the better performance or ro-LMA is a predictable consequence of data length—simply because filling out a higher-dimensional object like the reconstruction used by the fnn-LMA model requires more data. When I re-run the experiments with longer traces, the 1-MASE scores for ro-LMA and fnn-LMA did converge, but not until the traces are over 10⁶ points long, and at the (significant) cost of near-neighbor searches in a space with many more dimensions. Note, too, that the longer delay vectors used by fnn-LMA span far more of the training set, which at first glance would seem to be a serious advantage from an information-theoretic standpoint (although, as shown later in Section 5.1, this is not always an advantage). In view of this, the comparable performance of ro-LMA is quite impressive. All of these issues are explored at more length in Section 4.3.

4.1.2 Comparing ro-LMA with Traditional Linear Methods

For the K = 22 time series, the LMA-based methods do significantly better than the naïve and ARIMA methods and about twice as well as the random walk method and this makes sense. Each point in the time series of Figure 4.1(a) is very close to its predecessor and successor, which plays to the strengths of random walk. In contrast, the oscillations of the signal and the inertia of the mean make the naïve method ineffective. The fact that the LMA-based methods outperform the random walk at all, let alone twice as well, is quite impressive. Successive points of this signal are so close together that it is really an ideal candidate for random walk forecasting, leaving little room for another method to be more successful. However, both of the LMA-based techniques successfully meet this challenge: about 2.5 times and 1.8 times better than random walk, respectively, for **ro-LMA** and **fnn-LMA**. See Figures 4.1(b) and 4.1(c) for a visual comparison.

K = 47 is a very similar story; all of the LMA-based methods outperform naïve and ARIMA by several orders of magnitude for the same reasons discussed in the previous paragraph. The comparison between the LMA methods and random walk is more interesting. Both ro-LMA and fnn-LMA MASE scores are almost identical to those of random walk forecasts. For the reasons

Parameters	ro-LMA	fnn-LMA	ARIMA	naïve
$\{K = 22, F = 5\}$	0.391 ± 0.016	0.441 ± 0.033	17.031 ± 0.310	17.006 ± 0.233
$\{K = 47, F = 5\}$	0.985 ± 0.047	1.007 ± 0.043	18.330 ± 0.583	17.768 ± 0.765

Table 4.1: The average 1-MASE scores of all four forecast methods for the two ensembles of Lorenz-96 time series.

discussed above, this is not surprising; random walk is very well suited for this signal leaving a very small margin to be outperformed. Table 4.1 compares the forecast accuracy of all Lorenz-96 time series with each of the methods discussed above.

4.2 Experimental Data: Computer Performance Dynamics

Validation with synthetic data is an important first step in evaluating any new forecast strategy, but experimental time-series data are the acid test if one is interested in real-world applications. My second set of tests of ro-LMA, and comparisons of its accuracy to that of traditional forecast strategies, involves data from the laboratory experiment on computer performance dynamics that was introduced in Section 3.2.1.

I have tested **ro-LMA** on traces of many different processor and memory performance metrics gathered during the execution of a variety of programs on several different computers (see *e.g.*, [35–37,40,41]). Here, for conciseness, I focus on *processor* performance traces from two different programs, one simple (**col_major**) and one complex (403.gcc), running on the same Intel i7-based computer. As discussed in Section 3.2.1, computer performance dynamics result from a composition of hardware and software. These two programs represent two different dynamical systems, even though they are running on the same computer. The dynamical differences are visually apparent from the traces in Figures 3.3 and 3.4; they are also mathematically apparent from nonlinear time-series analysis of embeddings of those data [83], as well as in calculations of the information content of the two signals. Among other things, 403.gcc has much less predictive structure than **col_major** and is thus much harder to forecast [41]. These attributes make this a useful pair of experiments



Figure 4.2: Predicted (p_j) versus true values (c_j) for col_major and 403.gcc generated with four of the forecast methods considered in this thesis.

for an exploration of the utility of reduced-order forecasting.

For statistical validation, I collect 15 performance traces from the computer as it ran each program, calculated embedding parameters as described in Section 2.1.1, and generated forecasts of each trace using ro-LMA and the traditional methods outlined in Section 2.3. Figure 4.2 shows some representative examples. Recall that on such a plot, a perfect prediction would lie on the diagonal. Horizontal lines result when a constant predictor (*e.g.*, naïve) is used on a non-constant signal. In the case of Figure 4.2, fnn-LMA and ro-LMA both generate very accurate predictions of the col_major trace, while ARIMA does not. Note that the shape of Figure 4.2(b) (ARIMA on col_major) is reminiscent of the projected embedding in the right panel of Figure 3.3. This structure is also present in a p_j vs. c_j plot of a random-walk forecast (not shown) on this same signal. Indeed, for a random-walk predictor, a p_j vs. c_j plot is technically equivalent to a two-dimensional embedding with $\tau = 1$. For ARIMA, the correspondence is not quite as simple, since the p_j values are linear combinations of a number of past values of the c_j , but the effect is largely the same.

The 1-MASE scores for ro-LMA and fnn-LMA across all 15 trials in this set of experiments

Signal	fnn-LMA $MASE$	ro-LMA $MASE$	ARIMA MASE	naïve MASE	
col_major	0.050 ± 0.002	0.0625 ± 0.0032	0.599 ± 0.211	0.571 ± 0.002	
403.gcc	1.530 ± 0.021	1.4877 ± 0.016	1.837 ± 0.016	0.951 ± 0.001	

Table 4.2: The average 1-MASE scores of all four forecast methods for the 15 trials of col_major and 403.gcc.

were 0.050 ± 0.002 and 0.063 ± 0.003 , respectively; ARIMA scored much worse (0.599 ± 0.211) . This difference in performance is not surprising; the col_major time series contains plenty of nonlinear structure that the LMA-based methods can capture and utilize, whereas ARIMA can not. These 1-MASE scores mean that both fnn-LMA and ro-LMA perform roughly 20 times better on col_major than a random-walk predictor, while ARIMA only outperform random walk by a factor of 1.7. This is in accordance with the visual appearance of the corresponding images in Figure 4.2. For 403.gcc, however, ro-LMA is somewhat more accurate: 1-MASE scores of 1.488 ± 0.016 versus fnn-LMA's 1.530 ± 0.021 . Note that the 403.gcc 1-MASE scores are higher for both forecast methods than for col_major, simply because the 403.gcc signal contains less predictive structure [41]. This actually makes the comparison somewhat problematic, as discussed at more length in Section 4.3.

Comparing ro-LMA to the the naïve method is illustrative. ro-LMA does significantly better on all signals but 403.gcc. This is reassuring as 403.gcc has very high complexity, almost no redundancy, and very little predictive structure [41]. With signals like this, simple forecast methods that do not rely on predictive structure tend to do very well; this is discussed in more depth in Chapter 6.

Table 4.2 summarizes all of the computer performance experiments presented in this discussion. Overall, these results are consistent with the Lorenz-96 example in the previous section: prediction accuracies of ro-LMA and fnn-LMA are quite similar on all traces, despite the former's use of a theoretically incomplete reconstruction. This amounts to a validation of the conjecture on which this thesis is based. And in both numerical and experimental examples, ro-LMA actually *outperform* fnn-LMA on the more-complex traces (403.gcc, K = 47). I believe that this is due to the noise mitigation that is naturally effected by a lower-dimensional reconstruction.

4.3 Time Scales, Data Length and Prediction Horizons

In this Section, I explore the effects of the values of the τ parameter (Section 4.3.1), prediction horizon (Section 4.3.2) and data length (Section 4.3.3) on ro-LMA. For the remainder of this chapter, I discontinue comparing ro-LMA to traditional linear methods, as that comparison would not add anything to the discussion, and instead focus on the direct comparison between ro-LMA and fnn-LMA.

4.3.1 The τ Parameter

The embedding theorems require only that τ be greater than zero and not a multiple of any period of the dynamics. In practice, however, τ can play a critical role in the success of delaycoordinate reconstruction—and any nonlinear time-series analysis that follows [33, 38, 59, 95]. It follows naturally, then, that τ might affect the accuracy of an LMA-based method that uses the structure of a time-delay reconstruction to make forecasts.

Figure 4.3 explores this effect in more detail. Across all τ values, the 1-MASE of col_major was generally lower than the other three experiments—again, simply because this time series has more predictive structure. The K = 22 curve is generally lower than the K = 47 one for the same reason, as discussed at the end of the previous section. For both Lorenz-96 traces, prediction accuracy increases monotonically with τ . It is known that increasing τ can be beneficial for longer prediction horizons [59]. The situation in Figure 4.3 involves short prediction horizons, so it makes sense that my observations are consistent with the contrapositive of that result.

For the experimental traces, the relationship between τ and 1-MASE score is less simple. There is only a slight upward overall trend (not visible at the scale of the Figure) and the curves are nonmonotonic. This latter effect is likely due to periodicities in the dynamics, which are very strong in the col_major signal (*viz.*, a dominant unstable period-three orbit in the dynamics, which traces out the top, bottom, and middle bands in Figure 3.3). Periodicities can cause obvious problems for delay reconstructions—and forecast methods that employ them—if the delay is a



Figure 4.3: The effect of τ on ro-LMA forecast accuracy. The blue dashed curves are the average 1-MASE of the ro-LMA forecasts; the red dotted lines show \pm the standard deviation. The black vertical dashed lines mark the τ that is the first minimum of the mutual information curve for each time series.

harmonic or subharmonic of their frequencies, simply because the coordinates of the delay vector are not independent samples of the dynamics. It is for this reason that Takens mentions this condition in his original paper. Here, the effect of this is an oscillation in the forecast accuracy vs. τ curve: low when it is an integer multiple of the period of the dominant unstable periodic orbit in the col_major dynamics, for instance, then increasing with τ as more independence is introduced into the coordinates, then falling again as τ reaches the next integer multiple of the period, and so on.

This naturally leads to the issue of choosing a good value for the delay parameter. Recall that all of the experiments reported so far used a τ value chosen at the first minimum of the mutual information curve for the corresponding time series. These values are indicated by the black vertical dashed lines in Figure 4.3. This estimation strategy was simply a starting point, chosen here because it is arguably the most common heuristic used in the nonlinear time-series



Figure 4.4: Time-domain plots of ro-LMA forecasts of a K = 47 Lorenz-96 trace with default and best-case τ values: (a) the first minimum of the time-delayed average mutual information and (b) the minimum of Figure 4.3(b).

analysis community. As is clear from Figure 4.3, though, it is *not* the best way to choose τ for reduced-order forecast strategies. Only in the case of col_major is the τ value suggested by the mutual-information calculation optimal for ro-LMA—that is, does it fall at the lowest point on the 1-MASE vs. τ curve.

This suggests that one can often improve the performance of ro-LMA simply by choosing a different τ —i.e., by adjusting the one free parameter of that reduced-order forecast method. In all cases (aside from col_major, where the default τ was the optimal value), adjusting τ allow ro-LMA to outperform fnn-LMA. The improvement can be quite striking: for visual comparison, Figure 4.4 shows ro-LMA forecasts of a representative K = 47 Lorenz-96 trace using default and best-case values of τ . However, that comparison is not really fair. Recall that the embedding that is used by fnn-LMA, as defined so far, fixes τ at the first minimum of the average mutual information for the corresponding trace. It may well be the case that that τ value is suboptimal for *that* method as well—as it was for ro-LMA. To test this, I perform an additional set of experiments to find the optimal τ for fnn-LMA. Table 4.3 shows the numerical values of the 1-MASE scores, for forecasts made with default and best-case τ values, for both methods and all traces. In the two simulated examples, best-case fnn-LMA is better, but not by a huge margin. That is, even if one

Signal	ro-LMA	ro-LMA	fnn-LMA	fnn-LMA
	(default τ)	(best-case τ)	(default τ)	(best-case τ)
Lorenz-96 $K = 22$	0.391 ± 0.016	0.073 ± 0.002	0.441 ± 0.033	0.137 ± 0.006
Lorenz-96 $K = 47$	0.985 ± 0.047	0.115 ± 0.006	1.007 ± 0.043	0.325 ± 0.020
col_major	0.063 ± 0.003	0.063 ± 0.003	0.050 ± 0.002	0.049 ± 0.002
403.gcc	1.488 ± 0.016	1.471 ± 0.014	1.530 ± 0.021	1.239 ± 0.020

Table 4.3: The effects of the τ parameter. The "default" value is fixed, for both ro-LMA and fnn-LMA, at the first minimum of the average mutual information for that trace; the "best case" value is chosen individually, for each method and each trace, from plots like the ones in Figure 4.3.

optimizes τ individually for these two methods, ro-LMA keeps up with, and sometimes outperforms, fnn-LMA. Again, this supports the main point of this thesis: forecast methods based on incomplete reconstructions of time-series data can be very effective—and much less work than those that require a full embedding.

In view of my claim that part of the advantage of ro-LMA stems from the natural noise mitigation effects of a low-dimensional reconstruction, it may appear somewhat odd that fnn-LMA works better on the experimental time-series data, which certainly contain noise. Comparisons of large 1-MASE scores are somewhat problematic, however. Recall that 1-MASE > 1 means that the forecast is worse than an in-sample random-walk forecast of the same trace. The bottom row of numbers in Table 4.3, then, indicate that both LMA-based methods—no matter the τ values generate poor predictions for 403.gcc: 24-53% worse, on the average, than simply predicting that the next value will be equal to the previous value. There could be a number of reasons for this poor performance. This signal has almost no predictive structure [41] and fnn-LMA's extra axes may add to its ability to capture that structure—in a manner that outweighs the potential noise effects of those extra axes. The dynamics of col_major, on the other hand, are fairly low dimensional and dominated by a single unstable periodic orbit; it could be that the embedding of these dynamics used in fnn-LMA captures its structure so well that fnn-LMA is basically perfect and ro-LMA cannot do any better.

While the plots and 1-MASE scores in this section suggest that ro-LMA forecasts are quite

good—better than traditional linear methods, and as good or better than LMA upon true embeddings it is important to note that both "default" and "best-case" τ values were chosen after the fact in all of those experiments. This is not useful in practice. A significant advantage of a reduced-order forecast strategy like **ro-LMA** is its ability to work 'on the fly' in situations where one may not have the leisure to run an average mutual information calculation on a long segment of the trace and find a clear minimum—let alone construct a plot like Figure 4.3 and choose an optimal τ from it. (Producing that plot required 3,000 runs involving a total of 22,010,700 forecasted points, which took approximately 44.5 hours on an Intel Core i7.)

The results that I report in Section 5.1 and in [42], however, suggest that it is possible to estimate optimal τ values for delay reconstruction-based forecasting by calculating the value that maximizes the information shared between each delay vector and the future state of the system. For all of the examples in this thesis, that strategy produces the same τ value as found with the exhaustive search mentioned above. This is a fairly efficient calculation: $\mathcal{O}(n \log n)$ time where nis the length of the time series. Even so, it can be onerous if n is very large. However, this measure can be calculated on very small subsets of the time series and still produce accurate results, which could allow τ to be selected *adaptively* for the purposes of forecasting nonstationary systems with **ro-LMA**.

4.3.2 Prediction Horizon

There are fundamental limits on the prediction of chaotic systems. Positive Lyapunov exponents make long-term forecasts a difficult prospect beyond a certain point for even the most sophisticated methods [41, 59, 119]. Note that the coordinates of points in higher-dimensional delay-reconstruction spaces sample wider temporal spans of the time series. In theory, this means that one should be able to forecast further into the future with a higher-dimensional reconstruction without losing memory of the initial condition. This raises an important concern about ro-LMA: whether its accuracy will degrade with increasing prediction horizon more rapidly than that of fnn-LMA.

Table 4.4: The *h*-step mean absolute scaled error (*h*-MASE) scores for different forecast horizons (*h*). As explained in Section 2.4, *h*-MASE scores should not be compared for different h (*i.e.*, down the columns of this table).

Signal	h ro-LMA		ro-LMA	fnn-LMA	fnn-LMA
		(default τ)	(best-case τ)	(default τ)	(best-case τ)
Lorenz-96 $K = 22$	1	0.391 ± 0.016	0.073 ± 0.002	0.441 ± 0.003	0.137 ± 0.006
Lorenz-96 $K = 22$	10	0.101 ± 0.008	0.066 ± 0.003	0.062 ± 0.011	0.033 ± 0.002
Lorenz-96 $K = 22$	50	0.084 ± 0.007	0.074 ± 0.008	0.005 ± 0.002	0.004 ± 0.001
Lorenz-96 $K = 22$	100	0.057 ± 0.005	0.050 ± 0.004	0.003 ± 0.001	0.003 ± 0.001
Lorenz-96 $K = 47$	1	0.985 ± 0.047	0.115 ± 0.006	0.995 ± 0.053	0.325 ± 0.020
Lorenz-96 $K = 47$	10	0.223 ± 0.011	0.116 ± 0.005	0.488 ± 0.042	0.218 ± 0.012
Lorenz-96 $K = 47$	50	0.117 ± 0.011	0.112 ± 0.010	0.127 ± 0.011	0.119 ± 0.010
Lorenz-96 $K = 47$	100	0.075 ± 0.006	0.068 ± 0.005	0.079 ± 0.005	0.075 ± 0.004
col_major	1	0.063 ± 0.003	0.063 ± 0.003	0.050 ± 0.002	0.049 ± 0.002
col_major	10	0.054 ± 0.006	0.046 ± 0.003	0.021 ± 0.001	0.018 ± 0.001
col_major	50	0.059 ± 0.009	0.037 ± 0.003	0.012 ± 0.003	0.009 ± 0.001
col_major	100	0.044 ± 0.004	0.028 ± 0.006	0.010 ± 0.003	0.007 ± 0.001
403.gcc	1	1.488 ± 0.016	1.471 ± 0.014	1.530 ± 0.021	1.239 ± 0.020
403.gcc	10	0.403 ± 0.009	0.396 ± 0.009	0.384 ± 0.007	0.369 ± 0.010
403.gcc	50	0.154 ± 0.003	0.151 ± 0.005	0.143 ± 0.003	0.141 ± 0.003
403.gcc	100	0.101 ± 0.002	0.101 ± 0.003	0.095 ± 0.002	0.093 ± 0.002

Recall that the formulations of both methods, as described and deployed in the previous sections of this chapter, assume that measurements of the target system are available in real time: they "rebuild" the LMA models after each step, adding new time-series points to the embeddings or reconstructions as they arrive. Both ro-LMA and fnn-LMA can easily be modified to produce longer forecasts, however—say, h steps at a time, only updating the model with new observations at h-step intervals. Naturally, one would expect forecast accuracy to suffer as h increased for any non-constant signal. The question at issue in this section is whether the greater temporal span of the data points used by fnn-LMA mitigates that degradation, and to what extent.

In Table 4.4, I provide *h*-MASE scores—with $h \ge 1$ to reflect the increased prediction horizons I am considering—for *h*-step versions of the different forecast experiments² from Sections 4.1 and 4.2. The important comparisons here are, as mentioned above, across the rows of the table. The

² For an explanation of h-MASE see Section 2.4.

different methods "reach" different distances back into the time series to build the models that produce those forecasts, of course, depending on their delay and dimension. At first glance, this might appear to make it hard to sensibly compare, say, default- τ ro-LMA and best-case- τ fnn-LMA, since they use different τ s and different values of the reconstruction dimension and thus are spanning different ranges of the time series. Because *h* is measured in units of the sample interval of the time series, however, comparing one *h*-step forecast to another (for the same *h*) does make sense.

There are a number of interesting questions to ask about the patterns in this table, beginning with the one that set off these experiments: how do fnn-LMA and ro-LMA compare if one individually optimizes τ for each method? The numbers indicate that ro-LMA beats fnn-LMA for h = 1 on the K = 22 traces, but then loses progressively badly (*i.e.*, by more σ s) as h grows. col_major follows the same pattern except that ro-LMA is worse even at h = 1. For 403.gcc, fnn-LMA performs better at both τ s and all values of h, but the disparity between the accuracy of the two methods does not systematically worsen with increasing h. For K = 47, ro-LMA consistently beats fnn-LMA for both τ s for $h \leq 10$ but the accuracy of the two methods is comparable for longer prediction horizons. These results suggest that optimizing τ can improve both fnn-LMA and ro-LMA and that, depending on the signal, this optimization can change the relative accuracy of the two methods. This finding catalyzed the development of the forecast-specific parameter selection framework that is outlined in Section 5.1 and [42].

Another interesting question is whether the assertions in the previous section stand up to increasing prediction horizon. Those assertions are based on the results that appear in the h = 1rows of Table 4.4: ro-LMA was better than fnn-LMA on the K = 22 Lorenz-96 experiments, for instance, for both τ values. This pattern does not persist for longer prediction horizons: rather, fnn-LMA generally outperforms ro-LMA on the K = 22 traces for h = 10, 50, and 100. The h = 1comparisons for K = 47 and col_major do generally persist for higher h, however. As mentioned before, 403.gcc is problematic because its 1-MASE scores are so high, but the accuracies of the two methods are similar for all h > 1.

The fact that fnn-LMA generally outperforms ro-LMA for longer prediction horizons makes



Figure 4.5: A best-case- τ ro-LMA forecast of a K = 47 Lorenz-96 trace for h = 50. The forecast (red) follows the true trajectory (blue) for a while, falls off onto a shadow trajectory, then gets recorrected when a new set of observations are incorporated into the model after h time steps.

sense simply because ro-LMA samples less of the time series and therefore has less 'memory' about the dynamics. This is a well-known effect [119]. In view of the fundamental limits on prediction of chaotic dynamics, however, it is worth considering whether *either* method is really making correct long-term forecasts. Indeed, time-domain plots of long-term forecasts (e.g., Figure 4.5) reveal that both fnn-LMA and ro-LMA forecasts have fallen off the true trajectory and onto shadow trajectories—another well-known phenomenon when forecasting chaotic dynamics [98].

In other words, it appears that even a 50-step forecast of these chaotic trajectories is a tall order: *i.e.*, that I am running up against the fundamental bounds imposed by the Lyapunov exponents. In view of this, it is promising that **ro-LMA** generally keeps up with **fnn-LMA** in many cases—even when both methods are struggling with the prediction horizon, and even though the model that **ro-LMA** uses has much less memory about the past history of the trajectory. An important aspect of my future research on this topic will be developing efficient methods for deriving bounds on reasonable prediction horizons purely from the time series, *i.e.*, without using traditional methods such as Lyapunov exponents, which are difficult to estimate from experimental data. See [42] for some of my preliminary results on this line of research.

4.3.3 Data Length

Most real-world data sets are fixed in length and some are quite short. Moreover, many of the dynamical systems that one might like to predict are nonstationary. For these reasons, it is important to understand the effects of data length upon forecast methods that employ delay reconstructions. For the reconstruction to be an actual embedding that supports accurate calculations of dynamical invariants, the data requirements are fairly dire. Traditional estimates (*e.g.*, by Smith [106] and by Tsonis *et al.* [116]) suggest that $\approx 10^{17}$ data points would be required to embed the Lorenz-96 K = 47 data in Section 4.1, where the known d_{KY} values [61] indicate that one might need at least m = 38 dimensions to properly unfold the dynamics. As described in Section 2.1.1, however, that is only truly necessary if one is interested in preserving the diffeomorphism between true and reconstructed dynamics, down to the last detail. For the purposes of prediction, thankfully, one can make progress with far less data. For example, Sauer [98] successfully forecasted the continuation of a 16,000-point time series using a 16-dimensional embedding; Sugihara & May [112] used delay-coordinate embedding with m as large as seven to successfully forecast biological and epidemiological time-series data as short as 266 points.

While the results in the previous sections are based on far longer traces than the examples mentioned at the end of the previous paragraph, it is still worth exploring whether data-length issues are affecting those results—and evaluating whether those effects differentially impact ro-LMA because of its lower-dimensional model. This kind of test can be problematic in practice, of course, since it requires varying the length of the data set. In a synthetic example like Lorenz-96, that is not a problem, since one can just run the ODE solver for more steps.

Figure 4.6 shows 1-MASE scores for ro-LMA and fnn-LMA forecasts of the Lorenz-96 system as a function of data length. For both K = 22 and K = 47, the fnn-LMA error is higher than the ro-LMA error, corroborating the results in the previous sections. Both generally improve with data length, as one would expect—but only up to a point. The 1-MASE scores of the ro-LMA forecasts, in particular, reach a plateau at about 350,000 points in the K = 22 case and 150,000



(a) 1-MASE as a function of data length for predic- (b) 1-MASE as a function of data length for predictions of the Lorenz-96 K = 22, F = 5 traces. tions of the Lorenz-96 K = 47, F = 5 traces.

Figure 4.6: The effects of data length on forecast error for fixed prediction horizon h = 1. The dashed lines show the mean forecast error for each method; the dotted lines indicate the range of the standard deviation.

in the K = 47 case. fnn-LMA, on the other hand, keeps improving out to the end of the Figure. Eventually, there is a crossover for K = 22, but not until 1.6 million points. For K = 47, the curves are still converging out to 4 million points. The difference in crossover points is not surprising, given that the dimension of the K = 47 dynamics is so much higher: $d_{KY} \ll 3$, versus ≈ 19 . What is surprising, and useful, is that for traces with 1 million points—far more data than a practitioner can generally hope for—ro-LMA is still outperforming fnn-LMA. Moreover, it is doing so using fewer dimensions, which makes it computationally efficient.

Plateaus in curves like the ones in Figure 4.6 suggest that the corresponding forecast method has captured all of the information that it can use, so that adding data does not improve the forecast. This effect, which is described at more length in Section 5.1, depends on dimension for the obvious reason that filling out a higher-dimensional object requires more data. This suggests another piece of forecasting strategy: when one is data-rich, it may be wise to choose fnn-LMA over ro-LMA. In making this choice, though, one should also consider the added computational complexity, which will be magnified by the longer data length. When data are not plentiful, though, or the system is nonstationary, my results suggest that it is advantageous to ignore the theoretical bounds of [99] and use low-dimensional reconstructions in forecast models.

4.4 Summary

In summary, it appears that incomplete embeddings—time-delay reconstructions that do not satisfy the formal conditions of the embedding theorems—are indeed adequate for the purposes of forecasting dynamical systems. Indeed, they appear to offer simple state-space based methods *even more* traction on this prediction task than full embeddings, with greatly reduced computational effort.

The study in this thesis specifically focuses on the 2D instantiation of the claim above, for two reasons. First, that is the extreme that, in a sense, most seriously violates the basic tenets of the delay-coordinate embedding machinery; second, working in 2D enables the largest reduction in the cost of the near-neighbor searches that are the bulk of the computational effort in most state space-based forecast methods. A number of other issues arise when one considers increasing the reconstruction dimension beyond two, besides raw computational complexity. Among other things, that would introduce another free parameter into the method, thereby requiring some sort of principled strategy for choosing its value (a choice that ro-LMA completely avoids by fixing m = 2). In general, one would expect forecast accuracy to improve with the number of dimensions in the reconstruction, but not without limit. Among other things, noise effects grow with that dimension (simply because every noisy data point affects m points in the reconstructed trajectory). And from an information-theoretic standpoint, one would expect diminishing returns when the span of the delay vector $(m \times \tau)$ exceeds the "memory" of the system. For all of those reasons, it would seem that there should be a plateau beyond which increasing the reconstruction dimension does not improve the accuracy of a forecast methods that use the resulting models. I explore that issue further in [42] and synopsize the relevant material in Section 5.1. In that discussion, I use the measure mentioned in the last paragraph of Section 4.3.1 to derive optimal reconstruction dimensions for near-neighbor forecasting for a broad range of systems, noise levels, and forecast horizons—all of which turn out to be m = 2. In the bulk of the dynamical systems literature on forecasting, however, the optimal reconstruction dimension for the purposes of forecasting was thought to be near the value that provides a true embedding of the data. The results in this thesis suggest, again, that this is not the case.

I chose the classic Lorenz method of analogues as a good exemplar of the class of state spacebased forecast methods, but I believe that my results will hold for other members of that class (e.g., [23, 93, 98, 107, 112, 119]). Working with a low-dimensional reconstruction could potentially reduce the computational search and storage costs of any such method, while also avoiding the so-called "curse of dimensionality" and mitigating noise multipliers caused by extra embedding dimensions [24]. Reduced-order reconstructions also reduces data requirements, since fewer points are required to fill out a lower-dimensional object. And when one fixes m = 2, there is only a single free parameter τ in the method—one that can be estimated effectively from a short sample of the data set, allowing the reduced-order method to adapt to nonstationary dynamics. There may be some limitations on the class of methods for which these claims hold, of course; matters may get more complicated, and the results less clear, for forecast methods that perform other kinds of projections. On the flip side, however, my results can be viewed as explaining why those methods work so well.

Again, no forecast model will be ideal for all noise-free deterministic signals, let alone all realworld time-series data sets. However, the proof of concept offered in this section is encouraging: prediction in projection—a simple yet powerful reduction of a time-tested method—appears to work remarkably well, even though the models that it uses are not necessarily topologically faithful to the true dynamics.

Chapter 5

Why it Works: A Deeper Understanding of Delay-Coordinate Reconstruction

The experimental validation of ro-LMA provided in Chapter 4 is promising but that analysis gave rise to several unanswered questions, *e.g.*,

- Why does ro-LMA work when it is effectively a heresy?,
- If m = 2 works so well, why not m = 3?,
- How much data is necessary before m > 2 is the clear winner over higher-dimensional reconstructions?,
- If one wants to forecast two or three steps into the future, is m = 2 still efficient, or should m be increased?,
- Can τ be chosen a priori to optimize the accuracy of ro-LMA?, and
- Can all of these questions be answered strictly by analyzing the data?

This chapter provides a two-part analysis that answers many of these questions. The first part leverages information theory to select forecast-optimal parameters for delay-coordinate reconstruction. The second borrows methods from computational topology to gain new insight into the delay-coordinate embedding theory and machinery.

These two theoretical frameworks—information theory and computational topology—are mathematically disjoint but complementary in terms of developing a complete theory of reconstructionbased forecasting. In particular, the combination of these two tools allows, for the construction of a new paradigm in delay-coordinate reconstruction. Section 5.1 offers a novel method, developed in collaboration with R. G. James, for leveraging the information that is stored in delay vectors to perform parameter selection that is tailored to the exact stipulations of the data set at hand (*e.g.*, data length, signal-to-noise ratio and desired forecast horizon). The traditional approach to this is based on the assumption that the diffeomorphism instantiated by the delay-coordinate map, which is essential for dynamical invariant calculations, is also optimal for forecasting. As the results in Chapter 4 suggest, however, this may not be the best approach. Section 5.1 further corroborates these findings and suggests a reason why. Section 5.2 provides a deeper theoretical understanding of delay-coordinate reconstruction through computational topology, offering yet another reason why **ro-LMA** works. This exploration is based on the assumption that, when forecasting, one might only require knowledge of the topology of the invariant set; in collaboration with J. D. Meiss, I conjecture that the reconstructed dynamics might be *homeomorphic* to the original dynamics at a lower dimension than that needed for a diffeomorphically correct embedding. This suggests why **ro-LMA** gets traction despite its use of an incomplete reconstruction.

The combination of these powerful mathematical tools—information theory and computational topology—allows me to construct a deeper and more complete story of reduced-order forecasting with delay-coordinate reconstruction.

5.1 Leveraging Information Storage to Select Reconstruction Parameters

As has been discussed throughout this thesis, the task of choosing good values for the free parameters in delay-coordinate reconstruction has been the subject of a large and active body of literature over the past few decades. The majority of these techniques focus on the *geometry* of the reconstruction, which is appropriate when one is interested in quantities like fractal dimension and Lyapunov exponents. It is not necessarily the best approach when one is building a delay reconstruction for the purposes of prediction, however, as I showed in Section 4.3.1. That issue, which is the focus of this section, has received comparatively little attention in the extensive literature on delay reconstruction-based prediction [23, 72, 93, 107, 112, 119].

In this section, I propose a robust, computationally efficient method that I call *time delayed* active information storage, \mathcal{A}_{τ} , which can be used to select parameter values that maximize the information shared between the past and the future—or, equivalently, that maximize the reduction in uncertainty about the future given the current model of the past [42]. The implementation details, and a complexity analysis of the algorithm, are covered in Section 5.1.1. In Section 5.1.2, I show that simple prediction methods working with \mathcal{A}_{τ} -optimal reconstructions—*i.e.*, constructions using parameter values that follow from the \mathcal{A}_{τ} calculations—perform better, on both real and synthetic examples, than those same forecast methods working with reconstructions that are built using the traditional parameter selection heuristics (time-delayed mutual information for τ and false-near neighbors for m). Finally, in Section 5.1.3 I explore the utility of \mathcal{A}_{τ} in the face of different data lengths and prediction horizons.

5.1.1 Shared Information and Delay Reconstructions

The information shared between the past and the future is known as the excess entropy [25]. I will denote it here by $E = I[\overleftarrow{X}, \overrightarrow{X}]$, where I is the mutual information [121] and \overleftarrow{X} and \overrightarrow{X} represent the infinite past and the infinite future, respectively. E is often difficult to estimate from data due to the need to calculate statistics over potentially infinite random variables [58]. While this is possible in principle, it is too difficult in practice for all but the simplest of dynamics [110]. In any case, the excess entropy is not exactly what one needs for the purposes of prediction, since it is not realistic to expect to have the infinite past or to predict infinitely far into the future. For my purposes, it is more productive to consider the information contained in the *recent* past and determine how much that explains about the not-too-distant future. To that end, I define the *state active information storage*

$$\mathcal{A}_{\mathcal{S}} \equiv I[\mathcal{S}_j, \ X_{j+h}] \tag{5.1}$$

where S_j is an estimate of the state of the system at time j and X_{j+h} is the state of the system h steps in the future. In the special case where the state estimate S takes the form of a standard

m-dimensional delay vector, I will refer to $\mathcal{A}_{\mathcal{S}}$ as the time delayed active information storage

$$\mathcal{A}_{\tau} \equiv I[[X_j, X_{j-\tau}, \dots, X_{j-(m-1)\tau}], X_{j+h}]$$

$$(5.2)$$

 \mathcal{A}_{τ} can be nicely visualized—and compared to traditional methods like time-delayed mutual information—using the I-diagrams of Yeung, introduced in Section 2.2.3. Figure 5.1(a) shows an I-diagram of time-delayed mutual information for a specific τ . Recall that in a diagram like this, each circle represents the uncertainty in a particular variable. The left circle in Figure 5.1(a), for instance, represents the average uncertainty in observing $X_{j-\tau}$ (*i.e.*, $H[X_{j-\tau}]$); similarly, the top circle represents $H[X_{j+h}]$, the uncertainty in the h^{th} future observation. Also recall that each of the overlapping regions represents shared uncertainty: e.g., in Figure 5.1(a), the shaded region represents the shared uncertainty between X_j and $X_{j-\tau}$ —more precisely, the quantity $I[X_j, X_{j-\tau}]$. Notice that minimizing the shaded region in Figure 5.1(a)—that is, rendering X_j and $X_{j-\tau}$ as independent as possible—maximizes the total uncertainty that is explained by the combined model $[X_j, X_{j-\tau}]$ (the sum of the area of the two circles). This is precisely the argument made by Fraser and Swinney in [33]; see Section 2.1.2 for a full explanation. However, it is easy to see from the I-diagram that choosing τ in this way does not explicitly take into account explanations of the *future*—that is, it does not reduce the uncertainty about X_{t+h} . Moreover, this approach to selecting τ does not automatically extend to higher dimensional embeddings, e.g., minimizing $I[X_j, X_{j-\tau}]$, may or may not minimize $I[X_j, X_{j-\tau}, X_{j-2\tau}]$ and in fact this extension is non-trivial; see Section 2.2.3 for a full discussion of why this is so. The obvious next step would be to explicitly include the future in the estimation procedure. As I discussed in Section 2.2.3, however, explicitly including the future in the calculation *i.e.*, $I[X_j, X_{j-\tau}, X_{j+h}]$, is not straightforward. The rest of this section discusses some of the common interpretations of this quantity and why they are not appropriate for the task at hand.

The interaction information [10,76] is one such interpretation of $I[X_j, X_{j-\tau}, X_{j+h}]$ depicted in Figure 2.5(b); this is the intersection of $H[X_j]$, $H[X_{j-\tau}]$ and $H[X_{j+h}]$. It describes the reduction in uncertainty that the *two* past states, together, provide regarding the future. While this is obviously



Figure 5.1: (a) An I-diagram of the time-delayed mutual information. The circles represent uncertainties (*H*) in different variables; the shaded region represents $I[X_j; X_{j-\tau}]$, the time-delayed mutual information between the current state X_j and the state τ time units in the past, $X_{j-\tau}$. Notice that the shaded region is indifferent to $H[X_{j+h}]$, the uncertainty about the future. (b) An I-diagram of \mathcal{A}_{τ} , the quantity proposed in this section: $I[[X_j, X_{j-\tau}]; X_{j+h}]$. This quantity captures the shared information between the past, present, and future independently, as well as the information that the past and present, together, share with the future.

an improvement over the time-delayed mutual information of Figure 5.1(a), it does not take into account the information that is shared between X_j and the future but not shared with the past (i.e., $X_{j-\tau}$), and vice versa. The binding information and total correlation, depicted in Figures 2.5(c) and (d), address this shortcoming, but both also include information that is shared between the past and the present, but not with the future. This is not terribly useful for the purposes of prediction. Moreover, the total correlation overweights information that is shared between all three circles—past, present, and future—thereby artificially over-valuing information that is shared in all delay coordinates. In the context of predicting X_{t+h} , the provenance of the information is irrelevant and so the total correlation also seems ill-suited to the task at hand.

Note that the total correlation has been used in a similar manner to the time-delayed mutual information method in estimating τ [33]: *e.g.*, minimizing $\mathcal{M}[X_j; X_{j-\tau}; X_{j-2\tau}]$ for a threedimensional embedding. Minimizing the total correlation is equivalent to maximizing the entropy, making the delay vectors maximally informative because dependencies among the dimensions have been minimized. While on the surface this may seem a boon to prediction, consider the issue of predicting the state of the system at time $j + \tau$: if the coordinates of the delay vector are maximally independent, they will also be independent of the value being predicted. In light of this, the minimal total correlation approach is not well aligned with the goal of prediction.

Time-delayed active information storage addresses all of the issues raised in the previous paragraphs. By treating the generic delay vector as a joint variable, rather than a series of single variables, \mathcal{A}_{τ} captures the shared information between the past, present, and future independently—the left and right colored wedges in Figure 5.1(b)—as well as the information that the past and present, together, share with the future (the center wedge). By choosing delay-reconstruction parameters that maximize \mathcal{A}_{τ} , then, one can explicitly maximize the amount of information that each delay vector contains about the future [42].

That property means that \mathcal{A}_{τ} can be used to select τ for ro-LMA. Specifically, to estimate a "forecast-optimal" τ value for ro-LMA using \mathcal{A}_{τ} , one would simply calculate $\mathcal{A}_{\tau} = I[[X_j, X_{j-\tau}], X_{t+h}]$ for a range of τ , choosing the first maximum (*i.e.*, minimizing the uncertainty about the h^{th} future observation). In Section 5.1.2, I explore that claim using ro-LMA and fnn-LMA, but that exploration can be easily extended to any time-delayed state estimator—such as the methods used in [23,107,112,119]—by using the general form of \mathcal{A}_{τ} , *viz.*, the state active information storage, \mathcal{A}_{S} . For example, if the time series is pre-processed (*e.g.*, via a Kalman filter [108], a low-pass filter and an inverse Fourier transform [98], or some other local-linear transformation [23,59,107,112,119],) the state estimator simply becomes $\mathcal{S}_j = \hat{\vec{x}}_j$ where $\hat{\vec{x}}_j$ is the processed *m*-dimensional delay vector.

5.1.2 Selecting "Forecast-Optimal" Reconstruction Parameters

This section demonstrates how to use \mathcal{A}_{τ} to choose parameter values for delay-coordinate reconstructions constructed specifically for the purposes of forecasting, using several of the case studies presented in Chapter 3. For the discussion that follows, the term " \mathcal{A}_{τ} -optimal" is used to refer to the parameter values (m and τ) that maximize \mathcal{A}_{τ} over a range of m and τ . The general parameter selection framework is presented at first, not assuming the use of either fnn-LMA or ro-LMA, and then the \mathcal{A}_{τ} -optimal reconstructions are compared to fnn-LMA and ro-LMA. For simplicity, in this initial discussion, forecast horizons are fixed at h = 1 for each experiment. For the \mathcal{A}_{τ} calculations, this means that $\mathcal{A}_{\tau} = I[\mathcal{S}_j, X_{j+1}]$, with $\mathcal{S}_j = [X_j, X_{j-\tau}, \dots, X_{j-(m-1)\tau})]^T$. Recall that with one-step forecasts, 1-MASE is the figure of merit. Section 5.1.3.2 considers increasing the prediction horizon using h-MASE, with h > 1, to assess accuracy. Section 5.1.3.1 considers the effects of the length of the traces.

5.1.2.1 Synthetic Examples

The first step in this demonstration uses some standard synthetic examples, both maps (Hénon, logistic) and flows: the classic Lorenz 63 system [71] and the Lorenz 96 atmospheric model [73]. The dynamics of each of these systems are reconstructed from the traces described in Chapter 3 using different values m and τ . \mathcal{A}_{τ} is computed for each of those reconstructed trajectories using a Kraskov-Stügbauer-Grassberger (KSG) estimator [63], as described in Section 2.2.5.2. LMA is then used to generate forecasts of every trace using each $\{m, \tau\}$ pair, their 1-MASE scores are computed as described in Section 2.4, and the relationship between the 1-MASE scores and the \mathcal{A}_{τ} values for the corresponding time series are discussed.

Flow Examples

Figure 5.2(a) shows a heatmap of the \mathcal{A}_{τ} values for reconstructions of a representative trajectory from the Lorenz 96 system with $\{K = 22, F = 5\}$, for a range of m and τ . Not surprisingly, this image reveals a strong dependency between the values of the reconstruction parameters and the reduction in uncertainty about the near future that is provided by the reconstruction. Very low τ values, for instance, produce delay vectors that have highly redundant coordinates, and so provide substantial information about the immediate future. Again, the standard heuristics only focus on minimizing redundancy between coordinates, choosing the τ value that minimizes the mutual information between the first two coordinates in the delay vector. For this Lorenz 96 trajectory, that approach [33] yields $\tau = 26$, while standard dimension-estimation heuristics [62] suggest m = 8.



Figure 5.2: The effects of reconstruction parameter values on \mathcal{A}_{τ} and forecast accuracy for the Lorenz 96 system. (a) \mathcal{A}_{τ} values for different delay reconstructions of a representative trace from that system with $\{K = 22, F = 5\}$. (b) 1-MASE scores for LMA forecasts on different delay reconstructions of that trace.

The \mathcal{A}_{τ} value for a delay reconstruction built with those parameter values is 3.471 ± 0.051 . This is *not*, however, the \mathcal{A}_{τ} -optimal reconstruction; choosing m = 2 and $\tau = 1$, for instance, results in a higher value ($\mathcal{A}_{\tau} = 5.301 \pm 0.019$)—*i.e.*, significantly more reduction in uncertainty about the future. This may be somewhat counter-intuitive, since each of the delay vectors in the \mathcal{A}_{τ} -optimal reconstruction spans far less of the data set and thus one would expect points in that space to contain *less* information about the future. Figure 5.2(a) suggests, however, that this in fact not the case; rather, the uncertainty *increases* with both dimension and time delay.

The question at issue in this section is whether that reduction in uncertainty about the future correlates with improved accuracy of an LMA forecast built from that reconstruction. Since the \mathcal{A}_{τ} optimal choices maximize the shared information between the state estimator and X_{j+1} , one would expect a delay reconstruction model built with those choices to afford LMA the most leverage. To test that conjecture, I perform an exhaustive search with $m = 2, \ldots, 15$ and $\tau = 1, \ldots, 50$. For each $\{m, \tau\}$ pair, I use LMA to generate forecasts from the corresponding reconstruction, compute their 1-MASE scores, and plot the results in a heatmap similar to the one in Figure 5.2(a). As one would expect, the 1-MASE and \mathcal{A}_{τ} heatmaps are generally antisymmetric. This antisymmetry breaks down somewhat for low m and high τ , where the forecast accuracy is low even though the reconstruction contains a lot of information about the future.

I suspect that this breakdown is due to a combination of overfolding (too-large values of τ) and projection (low m). Even though each point in an overfolded reconstruction may contain a lot of information about the future, the false crossings created by this combination of effects pose problems for a near-neighbor forecast strategy like LMA. The improvement that occurs if one adds another dimension is consistent with this explanation. Notice, too, that this effect only occurs far from the maximum in the A_{τ} surface—the area that is of interest if one is using A_{τ} to choose parameter values for reconstruction models.

In general, though, maximizing the redundancy between the state estimator and the future does appear to minimize the resulting forecast error of LMA. Indeed, the maximum on the surface of Figure 5.2(b) ($m = 2, \tau = 1$) is exactly the minimum on the surface of Figure 5.2(a). The accuracy of this forecast is almost six times higher (1-MASE = 0.074 ± 0.002) than that of a forecast constructed with the parameter values suggested by the standard heuristics (0.441 ± 0.033). Note that the optima of these surfaces may be broad: *i.e.*, there may be *ranges* of m and τ for which A_{τ} and 1-MASE are optimal, and roughly constant. In these cases, it makes sense to choose the lowest m on the plateau, since that minimizes computational effort, data requirements, and noise effects. Notice that in this experiment, m = 2 was actually the A_{τ} -optimal reconstruction dimension, and that correspondence let me calculate the forecast optimal τ for **ro-LMA** without exhaustive search.

While the results discussed in the previous paragraph do provide a preliminary validation of the claim that one can use \mathcal{A}_{τ} to select good parameter values for delay reconstruction-based forecast strategies, they only involve a single example system. Similar experiments on traces from the Lorenz 96 system with different parameter values {K = 47, F = 5} (not shown) demonstrate identical results—indeed, the heatmaps are visually indistinguishable from the ones in Figure 5.2. Furthermore, for {K = 47, F = 5}, m = 2 is again the \mathcal{A}_{τ} -optimal reconstruction dimension,



Figure 5.3: The effects of reconstruction parameter values on \mathcal{A}_{τ} and forecast accuracy for the Lorenz 63 system. (a) \mathcal{A}_{τ} values for different delay reconstructions of a representative trace from that system. (b) 1-MASE scores for LMA forecasts on different delay reconstructions of that trace.

and \mathcal{A}_{τ} again estimates the forecast optimal τ for ro-LMA—quickly, without exhaustive search. Figure 5.3 shows heatmaps of \mathcal{A}_{τ} and 1-MASE for similar experiments on the canonical Lorenz 63 system [71]. As in the Lorenz 96 case, the heatmaps are generally antisymmetric, confirming that maximizing \mathcal{A}_{τ} is roughly equivalent to minimizing 1-MASE. Again, though, the antisymmetry is not perfect; for high τ and low m, the effects of projecting an overfolded attractor cause false crossings that trip up LMA. As before, adding a dimension mitigates this effect by removing these false crossings. Both the Lorenz 63 and Lorenz 96 plots show a general decrease in predictability for large m and high τ , with roughly hyperbolic equipotentials dividing the colored¹ regions. The locations and heights of these equipotentials differ because the two signals are not equally easy to predict. This matter is discussed further at the end of this section.

Numerical \mathcal{A}_{τ} and 1-MASE values for LMA forecasts on different reconstructions of both Lorenz systems are tabulated in the top three rows of Table 5.1, along with the reconstruction parameter values that produced those results. These results bring out two important points. First,

¹ Note that the color map scales are not identical across all heatmap figures in this thesis; rather, they are chosen individually, to bring out the details of the structure of each experiment.

Table 5.1: 1-MASE values for various delay reconstructions of the different examples studied here. 1-MASE_H is the representative accuracy of LMA forecasts that use delay reconstructions with parameter values (m_H and τ_H) chosen via standard heuristics for the corresponding traces. Similarly, 1-MASE_{A_{τ}} is the accuracy of LMA forecasts that use reconstructions built with the m and τ values that maximize A_{τ} , and 1-MASE_E is the error of the best forecasts for each case, found via exhaustive search over the m, τ parameter space. **: on these signals the standard heuristics failed.

Signal	1-MASE_H	$1\text{-MASE}_{\mathcal{A}_{\tau}}$	1-MASE_E
Parameters	$\{m_H, \tau_H\}$	$\{m_{\mathcal{A}_{\tau}}, \tau_{\mathcal{A}_{\tau}}\}$	$\{m_E, au_E\}$
Lorenz 96 $K = 22$	0.441 ± 0.033	0.074 ± 0.002	0.074 ± 0.002
$101012-50 \ \mathrm{M} = 22$	$\{8, 26\}$	$\{2,1\}$	$\{2,1\}$
Lorenz-96 $K = 47$	1.007 ± 0.043	0.115 ± 0.006	0.115 ± 0.006
	$\{10, 31\}$	$\{2,1\}$	$\{2,1\}$
Lorenz 63	0.144 ± 0.008	0.062 ± 0.006	0.058 ± 0.005
LOTENZ 05	$\{5, 12\}$	$\{3,1\}$	$\{2, 1\}$
Hénon Man	**	$4.46 \times 10^{-4} \pm 2.63 \times 10^{-5}$	$4.46 \times 10^{-4} \pm 2.63 \times 10^{-5}$
Henon Map	{ ** , ** }	$\{2,1\}$	$\{2,1\}$
Logistic Mon	**	$2.19 \times 10^{-5} \pm 2.72 \times 10^{-6}$	$2.19 \times 10^{-5} \pm 2.72 \times 10^{-6}$
Logistic map	{ ** , ** }	$\{1, 1\}$	$\{1, 1\}$

as suggested by the heatmaps, the m and τ values that maximize \mathcal{A}_{τ} (termed $m_{\mathcal{A}_{\tau}}$ and $\tau_{\mathcal{A}_{\tau}}$ in the table) are close, or identical, to the values that minimize 1-MASE (m_E and τ_E) for all three Lorenz systems. This is notable because—as discussed in Section 5.1.3.1—the former can be estimated quite reliably from a small sample of the trajectory in only a few seconds of compute time, whereas the exhaustive search that is involved in computing m_E and τ_E for Table 5.1 required close to 30 hours of CPU time per system/parameter set ensemble. A second important point that is apparent from Table 5.1 is that delay reconstructions built using the traditional heuristics—the values with the H subscript—are comparatively ineffective for the purposes of LMA-based forecasting. This is notable because that is the default approach in the literature on state-space based forecasting methods for dynamical systems. Moreover, in all cases m_E and $m_{\mathcal{A}_{\tau}}$ are far lower than what the embedding theory would suggest, further corroborating the basic premise of this thesis.



Figure 5.4: Histograms of A_{τ} and 1-MASE values for all traces from the Lorenz 96 {K = 22, F = 5} and {K = 47, F = 5} systems for all { m, τ } values in Figures 5.2 and 5.3: (a) A_{τ} (b) 1-MASE.

A close comparison of Figures 5.2 and 5.3 brings up another important point: some time series are harder to forecast than others. Figure 5.4 breaks down the details of the two suites of Lorenz 96 experiments, showing the distribution of \mathcal{A}_{τ} and 1-MASE values for all of the reconstructions. Although there is some overlap in the K = 22 and K = 47 histograms—*i.e.*, best-case forecasts of the former are better than most of the forecasts of the latter—the K = 47 traces generally contain less information about the future and thus are harder to forecast accurately. As discussed in Section 4.1, this is to be expected.

Map Examples

Delay reconstruction of discrete-time dynamical systems, while possible in theory, can be problematic in practice. Although the embedding theorems do apply in these cases, the heuristics for estimating m and τ often fail. The time-delayed mutual information of [33], for example, may decay exponentially, without showing any clear minimum. And the lack of spatial continuity of the orbit of a map violates the underlying idea behind the method of [62]. State space-based forecasting methods can, however, be very useful in generating predictions of trajectories from systems like this—*if* one selects the two free parameters properly.

In view of this, it would be particularly useful if one could use \mathcal{A}_{τ} to choose embedding parameter values for maps. This section explores that notion using two canonical examples, shown in the bottom two rows of Table 5.1. For the Hénon map

$$x_{n+1} = 1 - ax_n^2 + y_n \tag{5.3}$$

$$y_{n+1} = bx_n \tag{5.4}$$

with a = 1.4 and b = 0.3, the \mathcal{A}_{τ} -optimal parameter values, m = 2 and $\tau = 1$, occur at $\mathcal{A}_{\tau} = 6.617 \pm 0.011$, over the 15 trajectories generated from randomly-chosen initial conditions. As in the flow examples, these are identical to the values that minimized 1-MASE $(4.46 \times 10^{-4} \pm 2.63 \times 10^{-5})$. These parameter values make sense, of course; a first-return map of the x coordinate is effectively the Hénon map, so $[x_j, x_{j-1}]$ is a perfect state estimator (up to a scaling term). But in practice, of course, one rarely knows the underlying dynamics of the system that generated a time series, so the fact that one can choose good reconstruction parameter values by maximizing \mathcal{A}_{τ} is notable—especially since standard heuristics for that purpose fail for this system.

The same pattern holds for the logistic map, $x_{n+1} = rx_n(1 - x_n)$, with r = 3.65. Again, for validation, I generate 15 trajectories from randomly-chosen initial conditions. For this ensemble of experiments, the \mathcal{A}_{τ} -optimal parameter values, which occur at $\mathcal{A}_{\tau} = 9.057 \pm 0.001$, coincided with the minimum of the 1-MASE surface $(2.19 \times 10^{-5} \pm 2.72 \times 10^{-6})$. As in the Hénon example, these values (m = 1 and $\tau = 1$) make complete sense, given the form of the map. But again, one does not always know the form of the system that generated a given time series. In both of these map examples, the standard heuristics fail, but \mathcal{A}_{τ} clearly indicates that one does not actually need to reconstruct these dynamics—rather, that near-neighbor forecasting on the time series itself is the best approach.

5.1.2.2 Selecting Reconstruction Parameters of Experimental Time Series

The previous section provided a preliminary verification of the conjecture that parameters that maximize \mathcal{A}_{τ} also maximize forecast accuracy for LMA, for both maps and flows. While experiments with synthetic examples are useful, it is important to show that \mathcal{A}_{τ} is also a useful way to choose parameter values for delay reconstruction-based forecasting of real-world data, where the time series are noisy and perhaps short, and one does not know the dimension of the underlying


Figure 5.5: The effects of reconstruction parameter values on \mathcal{A}_{τ} and forecast accuracy for SFI dataset A. (a) \mathcal{A}_{τ} values for different delay reconstructions of that signal. (b) 1-MASE scores for LMA forecasts of those reconstructions.

system—let alone its governing equations. This section extends the exploration in the previous section, using experimental data from two different dynamical systems: a far-infrared laser and a laboratory computer-performance experiment.

A Far-Infrared Laser

I begin this discussion by returning to the canonical test case from Chapter 1, SFI dataset A [119], which was gathered from a far-infrared laser. As in the synthetic examples in Section 5.1.2.1, the \mathcal{A}_{τ} and 1-MASE heatmaps (Figure 5.5) are largely antisymmetric for this signal. Again, there is a band across the bottom of each image because of the combined effects of overfolding and projection. Note the similarity between Figures 5.5 and 5.3: the latter resemble "smoothed" versions of the former. It is well known [119] that the SFI dataset A is well described by the Lorenz 63 system with some added noise, so this similarity is reassuring. An LMA forecast using the \mathcal{A}_{τ} -optimal reconstruction of this trace was more accurate² than similar forecasts using reconstruc-

 $^{^{2}}$ Note that the SFI dataset A 1-MASE values are not averages as there is only one trace.

tions built using traditional heuristics—1-MASE_{A_{τ}} = 0.0592 versus 1-MASE_H = 0.0733—and only slightly worse than the optimal value 1-MASE_E = 0.0538. However, the values of { $m_{A_{\tau}}, \tau_{A_{\tau}}$ } and { m_E, τ_E } are not identical for this signal. This is because the optima in the heatmaps in Figure 5.5 are bands, rather than unique points—as was the case in the synthetic examples in Section 5.1.2.1. In a situation like this, a range of { m, τ } values are statistically indistinguishable, from the standpoint of the forecast accuracy afforded by the corresponding reconstruction. The values suggested by the A_{τ} calculation ($m_{A_{\tau}} = 9$ and $\tau_{A_{\tau}} = 1$) and by the exhaustive search ($m_E = 7, \tau_E = 1$) are all on this plateau, those suggested by the traditional heuristics ($m_H = 7, \tau_H = 3$) however are not. Again, these results suggest that one can use A_{τ} to choose good parameter values for delay reconstruction-based forecasting, but SFI dataset A is only a single trace from a fairly simple system.

Computer Performance Dynamics

Finally, I will return to the computer performance dynamics of col_major and 403.gcc: experiments that involve multiple traces from each system, which allows for statistical analysis. As in the previous examples (Lorenz 63, Lorenz 96, Hénon Map, Logistic Map, SFI dataset A), heatmaps of 1-MASE and \mathcal{A}_{τ} for a representative col_major time series—Figure 5.6(b)—are largely antisymmetric. And again, reconstructions using the \mathcal{A}_{τ} -optimal parameter values allowed LMA to produce highly accurate forecasts of this signal: 1-MASE_{\mathcal{A}_{τ}} = 0.050 ± 0.002, compared to the optimal 1-MASE_E = 0.049 ± 0.002. There are several major differences between these plots and the previous ones, though, beginning with the vertical stripes. These are due to the dominant unstable periodic orbit of period 3 in the chaotic attractor in the col_major dynamics. When τ is a multiple of this period ($\tau = 3\kappa$), the coordinates of the delay vector are not independent, which lowers \mathcal{A}_{τ} and makes forecasting more difficult. (There is a nice theoretical discussion of this effect in [99].) Conversely, \mathcal{A}_{τ} spikes and 1-MASE plummets when $\tau = 3\kappa - 1$, since the coordinates in such a delay vector cannot share any prime factors with the period of the orbit. The band along the bottom of both images is, again, due to a combination of overfolding and projection. The other 14 traces in this experiment yield structurally identical heatmaps and the variance between these



Figure 5.6: The effects of reconstruction parameter values on \mathcal{A}_{τ} and forecast accuracy for a representative trace of col_major. (a) \mathcal{A}_{τ} values for different delay reconstructions of that trace. (b) 1-MASE scores for LMA forecasts on those reconstructions.

trials were only ± 0.037 on average.

Another difference between the col_major heatmaps and the ones in Figures 5.2, 5.3, and 5.5 is the apparent overall trend: the "good" regions (low 1-MASE and high \mathcal{A}_{τ}) are in the lower-left quadrants of those heatmaps, but in the upper-right quadrants of Figure 5.6. This is partly an artifact of the difference in the color-map scale, which is chosen here to bring out some important details of the structure, and partly due to that structure itself. Specifically, the optima of the col_major heatmaps—the large dark red and blue regions in Figures 5.7(a) and (b), respectively are much broader than the ones in the earlier discussion of this section, perhaps because the signal is so close to periodic. (This is also the case to some extent in the SFI Dataset A example, for the same reason.) This geometry makes precise comparisons of \mathcal{A}_{τ} -optimal and 1-MASE-optimal parameter values somewhat problematic, as the exact optima on two almost-flat but slightly noisy landscapes may not be in the same place. Indeed, the \mathcal{A}_{τ} values at $\{m_{\mathcal{A}_{\tau}}, \tau_{\mathcal{A}_{\tau}}\}$ and $\{m_E, \tau_E\}$ are within a standard error across all 15 traces of col_major.

And that brings up an interesting tradeoff. For practical purposes, what one wants is



Figure 5.7: 1-MASE and \mathcal{A}_{τ} for ro-LMA forecasts of all 15 col_major traces, plotted as a function of τ . The blue dashed curves show the averages across all trials; the red dotted lines are that average \pm the standard deviation. (a) \mathcal{A}_{τ} values for delay reconstructions of these traces with m = 2 and a range of values of τ . (b) 1-MASE scores for ro-LMA forecasts of those reconstructions.

 $\{m_{\mathcal{A}_{\tau}}, \tau_{\mathcal{A}_{\tau}}\}$ values that produce a 1-MASE value that is *close to* the optimum 1-MASE_E. However, the algorithmic complexity of most nonlinear time-series analysis and prediction methods scales badly with m. In cases where the \mathcal{A}_{τ} maximum is broad, then, one might want to choose the lowest value of m on that plateau—or even a value that is on the *shoulder* of that plateau, if one needs to balance efficiency over accuracy. As I showed in Chapter 4, using **ro-LMA** does just that, and that appears to work quite well for the **col_major** data. This amounts to marginalizing the heatmaps in Figure 5.6 with m = 2, which produces cross sections like the ones shown in Figure 5.7. The antisymmetry between \mathcal{A}_{τ} and 1-MASE is quite apparent in these plots; the global maximum of the former coincides with the global minimum (0.0649 \pm 0.003) of the latter, at $\tau = 2$. This is not much higher than the overall optimum of 0.0496 \pm 0.002—a value from forecasts whose free parameters requires almost six orders of magnitude more CPU time to compute. This result not only corroborates the main premise of this thesis, but also suggests a more effective way to calculate \mathcal{A}_{τ} one simply fixes m = 2, as is done with ro-LMA, then selects τ by calculating \mathcal{A}_{τ} across a range of τ s, rather than across a 2D $\{m, \tau\}$ space.

The correspondence between 1-MASE and \mathcal{A}_{τ} also holds true for other marginalizations: *i.e.*, the minimum 1-MASE and the maximum \mathcal{A}_{τ} occur at the same τ value for all *m*-wise slices of the col_major heatmaps, to within statistical fluctuations. The methods of [33] and [62], incidentally, suggest $\tau_H = 2$ and $m_H = 12$ for these traces; the average 1-MASE of an LMA forecast on such a reconstruction is 0.0530 ± 0.002 , which is somewhat better than the best result from the m = 2marginalization, although still short of the overall optimum. The correspondence between τ_H and $\tau_{\mathcal{A}_{\tau}}$ is coincidence; for this particular signal, maximizing the independence of the coordinates happens to maximize the information about the future that is contained in each delay vector. This is most likely due to the strength of the unstable three cycle present in these dynamics. In this case, the coordinates would be maximally independent *and* contain the most information about the future when $\tau = \rho - 1$, where ρ is the period of the dynamics. The m = 12 result is not coincidence—and quite interesting, in view of the fact that the m = 2 forecast is so good. It is also surprising in view of the huge number of transistors—potential state variables—in a modern computer. As described in [83], however, the hardware and software constraints in these systems confine the dynamics to a much lower-dimensional manifold.

The col_major program is what is known in the computer-performance literature as a "microkernel"—a extremely simple example that is used in proof-of-concept testing. The fact that its dynamics are so rich speaks to the complexity of the hardware (and the hardware-software interactions) in modern computers; again, see [83,84] for a much deeper discussion of these issues. Modern computer programs are far more complex than this simple micro-kernel, of course, which begs the question: what does \mathcal{A}_{τ} tell us about the dynamics of truly complex systems like the memory or processor usage patterns of sophisticated programs—which the computer performance community models as stochastic systems?



Figure 5.8: The effects of reconstruction parameter values on \mathcal{A}_{τ} and forecast accuracy for a representative trace from a computer-performance dynamics experiment using the 403.gcc benchmark. (a) \mathcal{A}_{τ} values for different delay reconstructions of this trace. (b) 1-MASE scores for LMA forecasts on those reconstructions.

For 403.gcc, the answer is, again, that \mathcal{A}_{τ} appears to be an effective and efficient way to assess predictability. As shown in [41] and synopsized in Chapter 6, this time series shares little to no information with the future: *i.e.*, it *cannot* be predicted using delay reconstruction-based forecasting methods, regardless of τ and m values. The experiments in [41] required dozens of hours of CPU time to establish that conclusion; \mathcal{A}_{τ} gives the same results in a few seconds, using much less data. The structure of the heatmaps for this experiment, as shown in Figure 5.8, is radically different. The patterns visible in the previous 1-MASE plots, and the antisymmetry between \mathcal{A}_{τ} and 1-MASE plots, are absent from this pair of images, reflecting the lack of predictive content in this signal. Note, too, that the color map scales are different in this figure. This reflects the much-lower values of \mathcal{A}_{τ} for this signal: over all 15 experiments of 403.gcc, for the parameter range in Figure 5.8, \mathcal{A}_{τ} reached an absolute maximum of 0.7722, compared to the absolute maximum of 5.3026 for all experiments of the Lorenz 96 with K = 22. Indeed, the 1-MASE surface in Figure 5.8(b) never dips below 1.0, Figure 5.2, in contrast, never exceeds ≈ 0.6 and generally stays below 0.3. These results are consistent across all traces in these experiments, *i.e.*, for all 15 traces of 403.gcc, 1-MASE never drops below 1.0. That is, regardless of parameter choice, LMA forecasts of 403.gcc are no better than simply using the prior value of this scalar time series as the prediction. In comparison, with every experiment with Lorenz 96 K = 22—regardless of parameter choice—the 1-MASE for LMA generally stays below 0.3—more than twice as good as a random walk. The uniformly low \mathcal{A}_{τ} values in Figure 5.8(a) are an effective indicator of this—and, again, they can be calculated quickly, from a relatively small sample of the data. It is to that issue that I turn next.

5.1.3 Data Requirements and Prediction Horizons

In some real-world situations, it may be impractical to rebuild forecast models at every step, as I have done in the previous sections of this thesis—because of computational expense, for instance, or because the data rate is very high. In these situations, one may wish to predict h time steps into the future, then stop and rebuild the model to incorporate the h points that have arrived during that period, and repeat.

In chaotic systems, of course, there are fundamental limits on prediction horizon even if one is working with infinitely long traces of all state variables. A key question at issue in this section is how that effect plays out in forecast models that use delay reconstructions from scalar time-series data. I explore that issue in Section 5.1.3.2. And since real-world data sets are not infinitely long, it is also important to understand the effects of data length on the estimation of \mathcal{A}_{τ} . I explore this question in the following section, using one-step-ahead forecasts so that I can compare the results to those in the previous sections.

5.1.3.1 Data Requirements for A_{τ} Estimation

The quantity of data used in a delay reconstruction directly impacts the usefulness of that reconstruction. If one is interested in approximating the correlation dimension via the Grassberger-Procaccia algorithm, for instance, it has been shown that one needs $10^{(2+0.4m)}$ data points [106,116]. Those bounds are overly pessimistic for forecasting, however, as mentioned in Section 4.3.3. A key challenge, then, is to determine whether one's time series *really* calls for as many dimensions and data points as the theoretical results require, or whether one can get away with fewer dimensions—and how much data one needs in order to figure all of that out.

 \mathcal{A}_{τ} is a useful solution to those challenges. As established in the previous sections, calculations of this quantity can reveal what dimension is required for delay reconstruction-based forecasting of dynamical systems. And, as alluded to there, \mathcal{A}_{τ} can be estimated accurately from a surprisingly small number of points. The experiments in this section explore that intertwined pair of claims in more depth by increasing the length of the Lorenz 96 traces and testing whether the information content of the state estimator derived from standard heuristics converges to the \mathcal{A}_{τ} -optimal estimator. (This kind of experiment is not possible in practice, of course, when the time series is fixed, but can be done in the context of this synthetic example.)

Figure 5.9 shows the results. When the data length is short, the m = 2 state estimator has the most information about the future. This makes perfect sense; a short time series cannot fully sample a complicated object, and when an ill-sampled high-dimensional manifold is projected into a low-dimensional space, infrequently visited regions of that manifold can act effectively like noise. From an information-theoretic standpoint, this would increase the effective Shannon entropy rate of each of the variables in the delay vector. In the *I*-diagram in Figure 5.1(b), this would manifest as drifting apart of the two circles, decreasing the size of the shaded region that one needs to maximize for effective forecasting.

If that reasoning is correct, longer data lengths should fill out the attractor, thereby mitigating the spurious increase in the Shannon entropy rate and allowing higher-dimensional reconstructions to outperform lower-dimensional ones. This is indeed what happens, as shown in Figure 5.9. For both the K = 22 and K = 47 traces, once the signal is 2 million points long, the four-dimensional estimator stores more information about the future than the two-dimensional case. Note, though, that the optimal A_{τ} of the m = 8 reconstruction model is still lower than in the m = 2 or m = 4cases, even at the right-hand limit of the plots in Figure 5.9. That is, even with a time series that contains 4×10^6 points, it is more effective to use a lower-dimensional reconstruction to make an LMA forecast. But the really important message here is that \mathcal{A}_{τ} allows one to determine the best reconstruction parameters for the available data, which is an important part of the answer to the challenges outlined at the beginning of this chapter.

Something very interesting happens in the m = 2 results for Lorenz 96 model with K = 47: the \mathcal{A}_{τ} curve reaches a maximum value around 100,000 points and stops increasing, regardless of data length. What this means is that this two-dimensional reconstruction contains as much information about the future as can be ascertained from the **ro-LMA** state estimator, suggesting



(b) Lorenz-96 $\{K = 47, F = 5\}$ system

Figure 5.9: Average optimal \mathcal{A}_{τ} versus data length for all 15 traces from the Lorenz-96 system using $\tau = 1$ in all cases. Blue circles corresponds to m = 2, purple diamonds to m = 4, and red xs to m = 8. (a) Optimal \mathcal{A}_{τ} for traces from the $\{K = 22, F = 5\}$ system. (b) Optimal \mathcal{A}_{τ} for traces from the $\{K = 47, F = 5\}$ system. that increasing the length of the training set would not improve forecast accuracy. To explore this, I construct LMA forecasts of different-length traces (100,000–2.2 million points) from this system, then reconstruct their dynamics with different m values and the appropriate $\tau_{A_{\tau}}$ for each case, and—again—repeat this full experiment 15 times for statistical validation. For m = 2, both A_{τ} and 1-MASE results did indeed plateau at 200,000 points—at 5.736 \pm 0.0156 and 0.0809 \pm 0.0016, respectively. As before, more data does afford higher-dimensional reconstructions more traction on the prediction problem: the m = 4 forecast accuracy surpassed m = 2 at around 2 million points. In neither case, by the way, did m = 8 catch up to either m = 2 or m = 4, even at 4 million data points. Of course, one must consider the cost of storing the additional variables in a higher-dimensional model, particularly in data sets this long, so it may be worthwhile in practice to settle for the m = 2 forecast—which is only slightly less accurate and requires only 200,000 points. This has another major advantage as well. If the time series is non-stationary, a forecast strategy that requires fewer points is particularly useful because it can adapt more quickly.

5.1.3.2 Choosing reconstruction parameters for increased prediction horizons.

So far in this section, I have considered forecasts that were constructed one step at a time and studied the correspondence of their accuracy with one-step-ahead calculations of \mathcal{A}_{τ} . Here, I consider longer prediction horizons (*h*) and explore whether one can use a *h*-step-ahead version of \mathcal{A}_{τ} —i.e., $I[\mathcal{S}_j, X_{j+h}]$, with h > 1—to choose parameter values that maximize the information that each delay vector contains about the value of the time series *h* steps in the future.

Of course, one would expect the \mathcal{A}_{τ} -optimal $\{m, \tau\}$ values for a given time series to depend on the prediction horizon. It has been shown, for instance, that longer-term forecasts generally do better with larger τ [59], and conversely [38]. It also makes sense that one might need to reach different distances into the past (via the span of the delay vector) in order to reduce the uncertainty about events that are further into the future [119]. All of these effects are corroborated by \mathcal{A}_{τ} . Figure 5.10 demonstrates this with a representative trace of the K = 22 Lorenz 96 system, focusing on m = 2 for simplicity. The topmost dashed curve in this figure is for the h = 1 case—*i.e.*, a



Figure 5.10: The effects of prediction horizon (h) on \mathcal{A}_{τ} for a representative time series of the K = 22 Lorenz 96 system for a fixed reconstruction dimension (m = 2). The curves in the image, from top to bottom, correspond to prediction horizons of h = 1 to h = 100.

horizontal slice of Figure 5.2(a) made at m = 2. The maximum of this curve is the optimal τ value $(\tau_{\mathcal{A}_{\tau}})$ for this reconstruction. The overall shape of this curve reflects the monotonic increase in the uncertainty about the future with τ that is noted on page 86. The other curves in Figure 5.10 show \mathcal{A}_{τ} as a function of τ for $h = 2, 3, \ldots$, down to h = 100. Note that the lower curves do not decrease monotonically; rather, there is a slight initial rise. This is due to the issue raised above about the span of the delay vector: if one is predicting further into the future, it may be useful to reach further into the past. In general, this causes the optimal τ to shift to the right as prediction horizon increases, going down the plot—*i.e.*, longer prediction horizons require larger τ_{S} (*cf.* [59]). For very long horizons, the choice of τ appears to matter very little. In particular, \mathcal{A}_{τ} is fairly constant (and quite low) for $5 < \tau < 50$ when h > 30—*i.e.*, regardless of the choice of τ , there is very little information about the *h*-distant future in any delay reconstruction of this signal for h > 30. This effect should not be surprising, and is well corroborated in the literature. However, it can be hard to know a *priori*, when one is confronted with a data set from an unknown system, what prediction horizon makes sense. \mathcal{A}_{τ} offers a computationally efficient way to answer that question from not very much data.

Figure 5.11 shows a similar exploration but considers the effects of the reconstruction dimen-



Figure 5.11: The effects of prediction horizon (h) on average \mathcal{A}_{τ} (over 22 trials) of the K = 22Lorenz 96 system for a fixed time delay ($\tau = 1$) and two different reconstructions of the system. The red line represents m = 2; the blue represents $m_H = 8$, the value suggested for this signal by the technique of false neighbors.

sion on \mathcal{A}_{τ} as forecast horizon increases, this time fixing $\tau = 1$ for simplicity. These results indicate that the m = 2 state estimator contains more information about the future for short prediction horizons. This ties back to a central theme of this thesis: low-dimensional reconstructions can work quite well. Unsurprisingly, that does not always hold for arbitrary prediction horizons, Figure 5.11 shows that the full reconstruction is better for longer horizons. This is to be expected, since a higher reconstruction dimension allows the state estimator to capture more information about the past. Finally, note that \mathcal{A}_{τ} decreases monotonically with prediction horizon for both m = 2 and m_H . This, too, is unsurprising. Pesin's relation [91] says that the sum of the positive Lyapunov exponents is equal to the entropy rate, and if there is a non-zero entropy rate, then generically observations will become increasingly independent the further apart they are. This explanation also applies to Figure 5.10, of course, but it does *not* hold for signals that are wholly (or nearly) periodic.

Recall that the col_major dynamics in Section 5.1.2.2 are chaotic, but with a dominant unstable periodic orbit—which have a variety of interesting effects on the results. Figure 5.12 explores the effects of prediction horizon on those results. Not surprisingly, there is some periodicity in the \mathcal{A}_{τ} versus *h* relationships, but not for the same reasons that caused the stripes in Figure 5.6(b). Here, the *peaks* in \mathcal{A}_{τ} do occur at multiples of the period. That is, the m = 2 state estimator can



Figure 5.12: The effects of prediction horizon (h) on average \mathcal{A}_{τ} over the 15 trials of col_major for a fixed time delay $(\tau = 1)$ and two different reconstruction dimensions. The red line represents m = 2; the blue represents $m_H = 12$, the value suggested for this signal by the technique of false neighbors.

forecast with the most success when the value being predicted is in phase with the delay vector. Note that this effect is far stronger for m = 2 than m_H , simply because of the instability of that periodic orbit; the visits made to it by the chaotic trajectory are more likely to be short than long. As expected, \mathcal{A}_{τ} decays with prediction horizon—but only at first, after which it begins to rise again, peaking at h = 69 and h = 71. This may be due to a second higher-order unstable periodic orbit in the col_major dynamics.

In theory, one can derive rigorous bounds on prediction horizon. The time at which S_j will no longer have any information about the future can be determined by considering:

$$R(h) = \frac{I[S_j, X_{j+h}]}{H[X_{j+h}]}$$
(5.5)

i.e., the percentage of the uncertainty in X_{j+h} that can be reduced by the delay vector. Generically, this will limit to some small value equal to the amount of information that the delay vector contains about any arbitrary point on the attractor. Given some criteria regarding how much information above the "background" is required of the state estimator, one could use an R(h) versus h curve to determine the maximum practical horizon.

In practice, one can select parameters for delay reconstruction-based forecasting by explicitly including the prediction horizon in the A_{τ} function, fixing the horizon h at the required value,

performing the same search as I did in earlier sections over a range of m and τ , and then choosing a point on (or near) the optimum of that \mathcal{A}_{τ} surface. The computational and data requirements of this calculation, as shown in Section 5.1.3.1, are far superior to those of the standard heuristics used in delay reconstructions.

5.1.4 Summary

 \mathcal{A}_{τ} is a novel metric for quantifying how much information about the future is contained in a delay reconstruction. Using a number of different dynamical systems, I demonstrated a direct correspondence between the \mathcal{A}_{τ} value for different delay reconstructions and the accuracy of forecasts made with Lorenz's method of analogues on those reconstructions. Since \mathcal{A}_{τ} can be calculated quickly and reliably from a relatively small amount of data, without any knowledge about the governing equations or the state space dynamics of the system, that correspondence is a major advantage, in that it allows one to choose parameter values for delay reconstruction-based forecast models without doing an exhaustive search on the parameter space. Significantly, \mathcal{A}_{τ} optimal reconstructions are better, for the purposes of forecasting, than reconstructions built using standard heuristics like mutual information and the method of false neighbors, which can require large amounts of data, significant computational effort, and expert human interpretation. Perhaps, most importantly \mathcal{A}_{τ} allows one to answer other questions regarding forecasting with theoretically unsound models—e.g., why it is possible to obtain a better forecast using a low-dimensional reconstruction than with a true embedding. It also allows one to understand bounds on prediction horizon without having to estimate Lyapunov spectra or Shannon entropy rates, both of which are difficult to obtain for arbitrary real-valued time series. That, in turn, allows one to tailor one's reconstruction parameters to the amount of available data and the desired prediction horizon—and to know if a given prediction task is just not possible.

The experiments reported in this section involved a simple near-neighbor forecast strategy and state estimators that are basic delay reconstructions of raw time-series data. The definition and calculation of \mathcal{A}_{τ} do not involve any assumptions about the state estimator, though, so the results presented here should also hold for other state estimators. For example, it is common in forecasting applications to pre-process the time series: for example, low-pass filtering or interpolating to produce additional points. Calculating \mathcal{A}_{τ} after performing such an operation will accurately reflect the amount of information in that new time series—indeed, it would reveal if that pre-processing step *destroyed* information. And I believe that the basic conclusions in this section extend to other statespace based forecast schemas besides LMA, such as those used in [23, 98, 107, 112, 119]—although \mathcal{A}_{τ} may not accurately select optimal parameter values for strategies that involve *post*-processing the data (e.g., GHKSS [48]).

There are many other interesting potential ways to leverage \mathcal{A}_{τ} in the practice of forecasting. If the \mathcal{A}_{τ} -optimal $\tau = 1$, that may be a signal that the time series is undersampling the dynamics and that one should increase the sample rate. One could use the more general form $\mathcal{A}_{\mathcal{S}}$ at a finer grain to optimizing τ individually for each dimension, as suggested in [85, 90, 105], where optimal values are selected based on criteria that are not directly related to prediction. To do this, one could define $\mathcal{S}_j = [X_j, X_{j-\tau_1}, X_{j-\tau_2}, \dots, X_{j-\tau_{m-1}}]$ and then simply maximize $\mathcal{A}_{\mathcal{S}}$ using that state estimator constrained over $\{\tau_i\}_{i=1}^{m-1}$.

5.2 Exploring the Topology of Dynamical Reconstructions

Topology is of particular interest in forecasting dynamics, since many properties—the existence of periodic orbits, recurrence, entropy, etc.—depend only upon topology. However, computing topology from time series can be a real challenge—even with the aid of delay-coordinate reconstruction. As I have mentioned repeatedly throughout this thesis, success of this reconstruction procedure depends heavily on the choice of the two free parameters, but the embedding theorems provide little guidance regarding how to choose good values for these parameters. The delay-coordinate reconstruction machinery (both theorems and heuristics) targets the computation of dynamical invariants like the correlation dimension and the Lyapunov exponent. However, if one just wants to extract the topological structure of an invariant set—as is the case with forecasting—a scaled-back version of that machinery may be sufficient. In the following discussion, I adopt the philosophy that one might only desire knowledge of the topology of the invariant set. In collaboration with J. D. Meiss, I conjecture that this might be possible with a lower reconstruction dimension than that needed to obtain a true embedding. That is, the reconstructed dynamics might be *homeomorphic* to the original dynamics at a lower dimension than that needed for a diffeomorphically correct embedding [39]. This is an alternative validation of the central premise of my thesis.

To compute topology from data, one can use a simplicial complex–e.g., the witness complex of [27]. To construct such a complex, one chooses a set of "landmarks," typically a subset of the data, that become the vertices of the complex. The connections between the landmarks are determined by their nearness to the rest of the data—the "witnesses." Two landmarks in the complex are joined by an edge, for instance, if they share at least one witness.

My initial work on this approach [39] suggests that the witness complex correctly resolves the homology of the underlying invariant set—*viz.*, its Betti numbers—even if the reconstruction dimension is well below the thresholds for which the embedding theorems assure smooth conjugacy between the true and reconstructed dynamics. This means that some features of the large-scale topology are present even if the reconstruction dimension does not satisfy the associated theorems. I conjecture that this structure affords ro-LMA the means necessary to generate accurate forecasts. The witness complex is covered in more depth in Section 5.2.1, which also describes the notion of *persistence* and demonstrates how that idea is used to choose scale parameters for a complex built from reconstructed time-series data. In Section 5.2.2, I explore how the homology of such a complex changes with reconstruction dimension.

5.2.1 Witness Complexes for Dynamical Systems

To compute the topology of data that sample an invariant set of a dynamical system, one needs a complex that captures the shape of the data but is robust with respect to noise and other sampling issues. A witness complex is an ideal choice for these purposes. Such a complex is determined by the reconstructed time-series data, $W \subset \mathbb{R}^m$ —the *witnesses*—and an associated set $L \subset \mathbb{R}^m$, the *landmarks*, which can (but need not) be chosen from among the witnesses. The landmarks form the vertex set of the complex; the connections between them are dictated by the geometric relationships between W and L. In a general sense, a witness complex can be defined through a relation $R(W,L) \subset W \times L$. As Dowker noted [29], any relation gives rise to a pair of simplicial complexes. In the one used here, a point $w \in W$ is a witness to an abstract k-dimensional simplex $\sigma = \langle l_{i_1}, l_{i_2}, \ldots, l_{i_{k+1}} \rangle \subset L$ whenever $\{w\} \times \sigma \subset R(W,L)$. The collection of simplices that have witnesses is a complex relative to the relation R. For example, two landmarks are connected if they have a common witness—this is a one-simplex. Similarly, if three landmarks have a common witness, they form a two-simplex, and so on.

There are many possible definitions for a witness relation R; see [39] for a discussion. A relation that is particularly useful for analyzing noisy real data [4,39] is the ε -weak witness [21], or what is called a "fuzzy" witness [4]: a point witnesses a simplex if all the landmarks in that simplex are within ε of the closest landmark to the witness:

Definition (Fuzzy Witness). The fuzzy witness set for a point $l \in L$ is the set of witnesses

$$\mathcal{W}_{\varepsilon}(l) = \{ w \in W : \|w - l\| \le \min_{l' \in L} \|w - l'\| + \varepsilon \}$$
(5.6)

In this case, the relation consists of the collections $R = \bigcup_{l \in L} (\mathcal{W}_{\varepsilon}(l) \times \{l\})$ and a simplex σ is in the complex whenever $\bigcap_{l \in \sigma} \mathcal{W}_{\varepsilon}(l) \neq \emptyset$ —that is, when all of its vertices share a witness. This relation is illustrated in Figure 5.13.

The fuzzy witness complex reduces to the "strong witness complex" of de Silva and Carlsson [27] when $\varepsilon = 0$. In such a complex, an edge exists between two landmarks *iff* there exists a witness that is exactly equidistant from those landmarks. This is not a practical notion of shared closeness for finite noisy data sets. In this case, ε in Equation (5.6) allows for some amount of immunity to finite data and noise effects, but must be chosen correctly as I discuss in the next paragraph. A simpler implementation of the fuzzy witness complex consists of simplices whose pairs of vertices have a common witness; this implementation gives a "clique" or "flag" complex, analogous to the Rips complex [45]. This is called a "lazy" complex in [27] and instantiated as the



Figure 5.13: Illustration of the fuzzy witness relation Equation (5.6). The closest landmark to witness w_a is l_1 , and since $||w_a - l_2|| < D_{a1} + \varepsilon$, the simplex $\langle l_1, l_2 \rangle$ is in the complex. Similarly w_b witnesses the edge $\langle l_2, l_3 \rangle$.

LazyWitnessStream class in the javaPlex [114] software. In the notation introduced above, the complex is

$$\mathcal{K}_{\varepsilon}(W,L) = \{ \sigma \subset L : \mathcal{W}_{\varepsilon}(l) \cap \mathcal{W}_{\varepsilon}(l') \neq \emptyset, \ \forall l, l' \in \sigma \}$$
(5.7)

Following [4], I will use this particular construction in the following discussion. My goal is to study the topology of witness complexes of delay-coordinate reconstructions and determine whether the topology is resolved correctly when the reconstruction dimension is low.

Figure 5.14 shows four witness complexes built from the 100,000-point trajectory of the Lorenz 63 system that is shown in Figure 3.2(a) for varying values of the fuzziness parameter, ϵ . The landmarks (red dots) consist of $\ell = 201$ points equally spaced along the trajectory, *i.e.*, every $\Delta t = 500^{th}$ point of the time series. There are many ways to choose³ landmarks; this particular strategy distributes them according to the invariant measure of the attractor. One could also choose landmarks randomly from the trajectory or using the "max-min" selector⁴ of [27]; each of these gives results similar to those shown. When ε is small, very few witnesses fall in the thin regions required by Equation (5.6), so the resulting complex does not have many edges and is thus not a good representation of the shape of the data. As ε grows, more witnesses fall in the "shared" regions

 $^{^{3}}$ For a deeper discussion of the number of landmarks to use and landmark selection choice see [39].

 $^{^4}$ Choose the first landmark at random, and given a set of landmarks, choose the next to be the data point farthest away from the current set.



Figure 5.14: "One-skeletons" of witness complexes constructed from the trajectory of Figure 3.2(a) using the fuzzy witness relation depicted in Figure 5.13. In each one-skeleton, the red dots are the $\ell = 201$ equally-spaced landmarks. A black edge between two landmarks l_i and l_j signifies the existence of a one simplex $\langle l_i, l_j \rangle$ in the complex, *i.e.*, l_i and l_j shared at least one witness. As ϵ increases, more landmarks will satisfy $||w_a - l_k|| < D_{a1} + \varepsilon$ for each w_a and the one complex will fill in.

and the complex fills in, revealing the basic homology of the attractor of which the trajectory is a sample. There is an obvious limit to this, however: when ε is very large, even the largest holes in the complex are obscured.

In order to evaluate the topology of incomplete reconstructions, one needs to ensure the correctness of the topology. However, as Figure 5.14 illustrates, the simplex, from which one estimates the topology, depends on the choice of ϵ , and choosing the right ϵ for that job is non-trivial. One can do so using the progression of images in Figure 5.14 and the notion of *persistence*. Studying the change in homology under changing scale parameters is a well-established notion in computational topology. The underlying idea of persistence [30,94,123] is that any topological property of physical interest should be (relatively) independent of parameter choices in the associated algorithms.

One useful way to represent information about the changing topology of a complex is the barcode persistence diagram [45]. Figure 5.15 shows barcodes of the first two Betti numbers for the witness complexes of Figure 5.14. Each horizontal line in the barcode is the interval in ε for which there exists a particular non-bounding cycle, thus the number of such lines is the rank of the homology group—a Betti number. The values for β_0 and β_1 are computed using javaPlex [114] over the range $0.017 \le \varepsilon \le 1.7$, using the ExplicitMetricSpace to choose the equally spaced points and the LazyWitnessStream to obtain a clique complex from the $\ell = 201$ landmarks. There are no three-dimensional voids in the results, *i.e.*, β_2 was always zero for this range of ε —a reasonable implication for this 2.06-dimensional attractor. When ε is very small, as in Figure 5.14(a), the witness complex has many components and the β_0 barcode shows a large number of entries. As ε grows, the spurious gaps between these components disappear, leaving a single component that persists above $\varepsilon \approx 0.014$. That is, witness complexes constructed with $\varepsilon > 0.014$ correctly capture the connectedness of the underlying attractor. The β_1 barcode plot shows a similar pattern: there are many holes for small ε that are successively filled in as that parameter grows, leaving the two main holes (*i.e.*, $\beta_1 = 2$) for $\varepsilon > 1.01$. Above $\varepsilon > 3.2$ (not shown in Figure 5.15), one of those holes disappears; eventually, for $\varepsilon > 4.05$, the complex becomes topologically trivial. Above this value, the resulting complexes—recall Figure 5.14(d)—have no non-contractible loops and are homologous to a point (acyclic).

As alluded to above, this notion of persistence can be turned around and used to select good values for the parameters that play a role in topological data analysis—e.g., looking for the ε value at which the homology stabilizes or selecting the number of landmarks that are necessary to construct a topologically faithful complex. However, definitions of what constitutes stabilization are subjective and can be problematic. Even so, persistence is a powerful technique and I make use of it in a number of ways in the rest of this section.

The examples in Figures 5.14 and 5.15 involve a full trajectory from a dynamical system. This thesis focuses on reconstructions of scalar time-series data—structures whose topology is guaranteed to be identical to that of the underlying dynamics if the reconstruction process is carried



Figure 5.15: Persistence barcodes computed using javaPlex for a $\ell = 201$ witness complex of the trajectory of Figure 3.2(a). Each plot tabulates the two lowest Betti numbers of the complex for 100 values of the scale parameter ε . The left panel shows the behavior when $0.001 \le \varepsilon \le 0.1$, the right panel zooms out to the range $0.017 \le \varepsilon \le 1.7$.

out properly. But what if the dimension *m* does *not* satisfy the requirements off the theorems? Can one still obtain useful results about the *topology* of that underlying system, even if those dynamics are not properly unfolded in the sense of [89,99,113]? Throughout this thesis, I have argued that in the context of forecasting, the answer to that question is yes. In the next section, I take a step away from forecasting and examine whether the answer is also yes in the case of *topology*—specifically homology—and discuss the implications of that answer for the central theme of this thesis.

5.2.2 Topologies of Reconstructions

As discussed in Section 2.1.1, a scalar time series of a dynamical system is a projection of the *d*-dimensional dynamics onto \mathbb{R}^1 —an action that does not automatically preserve the topology of the object. Delay-coordinate embedding allows one to reconstruct the underlying dynamics, up to diffeomorphism, if the reconstruction dimension is large enough. The question at issue in this section is whether one can use the witness complex to obtain a useful, coarse-grained description of the topology from lower-dimensional reconstructions, namely the homology—e.g., the basic connectivity of the invariant set, or the number of holes in it that are larger than a certain scale. The answer to this question can provide a deeper understanding of the mechanics of **ro-LMA**.



Figure 5.16: One-skeletons of the witness complexes (top row) and barcode diagrams for β_1 (bottom row) of the Lorenz system. The plots in the left-hand column are computed from the threedimensional (x, y, z) trajectory of Figure 3.2(a); those in the right-hand column are computed from a two-dimensional (m = 2) delay-coordinate reconstruction from the x coordinate of that trajectory with $\tau = 174$. In both cases, $\ell = 201$ equally spaced landmarks (red ×s) are used. Both complexes have two persistent nonbounding cycles (green and blue edges) but the 2D reconstruction requires only ≈ 1900 simplices to resolve those cycles (at $\varepsilon = 0.2$), while the full 3D trajectory requires ≈ 7000 simplices (at $\varepsilon = 1.2$) to eliminate spurious loops.

The short answer is yes. Figure 5.16 shows a side-by-side comparison of witness complexes and barcode diagrams for the Lorenz 63 trajectory of Figure 3.2(a) and a two-dimensional reconstruction (m = 2) using the x coordinate of that trajectory. The full 3D trajectory on the left and the 2D reconstruction on the right have the same homology. In other words, the correct large-scale homology is accessible from a witness complex of a 2D reconstruction, even though the reconstruction does not satisfy the conditions of the associated theorems.

And that leads to a fundamental question for this thesis: how does the homology of a delaycoordinate reconstruction change with the dimension m? The standard answer to this in the delaycoordinate embedding literature is that the topology should change at first, then stabilize when m became large enough⁵ to correctly unfold the topology of the underlying attractor. In practice, however, a too-large m will invoke the curse of dimensionality and destroy the fidelity of the reconstruction. Moreover, increasing m exacerbates both noise effects and computational expense. For all of these reasons, it would be a major advantage if one could obtain useful information about the homology of the underlying attractor—even if not the full topology—from a low-dimensional delay-coordinate reconstruction.

Again, it appears that this is possible. Figure 5.17 shows witness complexes for m = 2and m = 3 reconstructions of the Lorenz time series of Figure 3.2(b). The barcodes for the first two Betti numbers of these two complexes, as computed using javaPlex, have similar structure: the complexes become connected ($\beta_0 = 1$) at a small value of ε , and the dominant, persistent homology corresponds to the two primary holes ($\beta_1 = 2$) in the attractor. Note, by the way, that Figure 5.17(a) is not simply a 2D projection of Figure 5.17(b); the edges in each complex reflect the geometry of the witness relationships in different spaces, and so may differ. Higher-dimensional reconstructions—not easily displayed—have the same homology for suitable choices of ε , though for m > 5, it is necessary to increase the number of landmarks to obtain a persistent $\beta_1 = 2$.

That brings up an important point: if one wants to sensibly compare witness complexes constructed from different reconstructions of a single data set, one has to think carefully about the ℓ and ε parameters. Here, I use persistence to choose a good value of ℓ . I find that the results are robust with respect to changes in that value, across all reconstruction dimension values in this study, so I fix $\ell \approx 200$ for all the experiments reported in this section.⁶

In the experiments in the previous section, the scale parameter ε was given in absolute units. To generalize this approach across different examples and different reconstruction dimensions, it makes sense to compare reconstructions with ε chosen to be a fixed fraction of the diameter,

⁵ For example, recall the method of dynamical invariants.

⁶ The precise value varies slightly because the length of a trajectory reconstructed from a fixed-length data set decreases with increasing m (since one needs a full span of $m \times (\tau)$ data points to construct a point in the reconstruction space).



Figure 5.17: The effects of reconstruction dimension: One-skeletons of witness complexes of different reconstructions of the scalar time series of Figure 3.2(b). Both reconstructions use $\tau = 174$, the first minimum of the average time-delayed mutual information, $\ell = 198$ equally spaced landmarks (red dots), and $\xi = 0.54\%$, as defined in Equation (5.8).

 $\operatorname{diam}(W)$, of the set W

$$\varepsilon = \xi \operatorname{diam}(W) \tag{5.8}$$

For example, for the full 3D attractor in Figure 3.2(a)

$$\operatorname{diam}(W_{xyz}) = \sqrt{(x_{max} - x_{min})^2 + (y_{max} - y_{min})^2 + (z_{max} - z_{min})^2} = 75.3$$
(5.9)

so the ε values used in Figure 5.15—0.017 $\leq \varepsilon \leq 1.7$ in absolute units—translate to $2.3 \times 10^{-4} \leq \xi \leq 0.023$ in this diameter-scaled measure.

The diameter of the reconstruction varies in a natural way with the dimension m. Since delay-coordinate reconstruction of scalar data unfolds the full range of those data along every added dimension, the diameter of an m-dimensional reconstruction will be

diam
$$(W_m) = \sqrt{m(x_{max} - x_{min})^2} = 37.0\sqrt{m}$$
 (5.10)

for this dataset, where x represents the scalar time-series data. Since this unfolding will change the geometry of the reconstruction, I need to scale ε accordingly. The witness complexes in Figure 5.17 are constructed with a fixed value of $\xi = 0.54\%$. That is, for Figure 5.17(a), $\varepsilon = 37.0\sqrt{2}(0.0054) = 0.283$ in absolute units, while for Figure 3.2(b), diam $(W_3) = 37.0\sqrt{3}$ and $\varepsilon = 0.346$. This scaling

of ε —which is used throughout the rest of this section—should allow the witness complex to adapt appropriately to the effects of changing reconstruction dimension and finite data.

To formalize the exploration of the reconstruction homology and extend that study across multiple dimensions, one can use a variant of the classic barcode diagram that shows, for each simplex, the reconstruction dimension values at which it appears in and vanishes from the complex. Figure 5.18(a) shows such a plot for edges that involve l_0 , the first landmark on the reconstructed trajectory. A number of interesting features are apparent in this image. Unsurprisingly, most of the one-simplices that exist in the m = 1 witness complex—many of which are likely due to the strong effects of the projection of the underlying \mathbb{R}^d trajectory onto \mathbb{R}^1 —vanish when one moves to m = 2. There are other short-lived edges in the complex as well: e.g., the edge from l_0 to l_{120} that is born at m = 2 and dies at m = 3. The sketch in Figure 5.18(b) demonstrates how edges can be born as the dimension increases: in the m = 2 reconstruction, ℓ_1 and ℓ_3 share a witness (the green square); when one moves to m = 3, spreading all of the points out along the added dimension, that witness is moved far from ℓ_3 —and into the shared region between ℓ_1 and ℓ_2 . There are also long-lived edges in the complex of Figure 5.18(a). The one between l_0 and l_{140} that persists from m = 1 to m = 8 is particularly interesting: this pair of landmarks has shared witnesses in the scalar data and in all reconstructions. Possible causes for this are explored in more depth below. All of these effects depend on ξ , of course; lowering ξ will decrease both the number and average length of the edge persistence bars.

While this Δm barcode image is interesting, the amount of detail that it contains makes it somewhat unwieldy. To study the *m*-persistence of all of $\ell \times \ell$ edges in a witness complex, one would need to examine ℓ of these plots—or condense them into a single plot with ℓ^2 entries on the vertical axis. Instead, one can plot what I call an *edge lifespan diagram*: an $\ell \times \ell$ matrix whose $(i, j)^{th}$ pixel is colored according to the maximum range of *m* for which an edge exists in the complex between the *i*th and *j*th landmarks; see Figure 5.19. If the edge $\{l_i, l_j\}$ existed in the complex for $2 \leq m < 3$ and $5 \leq m < 8$, for instance, Δm would be three and the *i*, *j*th pixel would be coded in cyan. Edges that do not exist for any dimension are coded white.



Figure 5.18: (a) Dimension barcode for edges in the witness complex of the reconstructed scalar time series of Figure 3.2(b) that involve l_0 , the first landmark, for reconstructions with $m = 1, \ldots, 8$. The vertical axis is labeled with the indices of the remaining 197 landmarks in the complex; a circle at the $m-1 \rightarrow m$ tickmark on the horizontal axis indicates the transition at which an edge between l_0 and l_i is born; a square indicates the transition at which that edge vanishes from the complex. An arrow at the right-hand edge of the plot indicates an edge that was still stable when the algorithm completed. For all reconstructions, $\tau = 174$, $\ell = 198$, and $\xi = 0.54\%$. (b) Sketch of the birth and death of edges at the $m = 2 \rightarrow 3$ transition.



Figure 5.19: Edge lifespan diagram: pixel i, j on this image is color-coded according to the maximum range Δm of dimension for which an edge exists between landmarks l_i and l_j in the witness complex of the reconstructed scalar time series of Figure 3.2(b) for $m = 1, \ldots, 8$. For all reconstructions, $\tau = 174, \ell = 198$, and $\xi = 0.54\%$.

A prominent feature of Figure 5.19 is a large number (683) of edges with a lifespan 1 (blue). Of these edges, 463 exist for m = 1, but not for m = 2, and thus reflect the anomalous behavior of projecting a 2.06 dimensional object onto a line. This is also seen, as described above, in the barcode of Figure 5.18.

Another interesting set of features in the lifespan diagram is the diagonal line segments. Note that the *color* of the pixels in these segments varies, though most of them correspond to edges with longer lifespans. These segments indicate the existence of Δm -persistent edges $\{l_i, l_j\}, \{l_{i+1}, l_{j+1}\}, \{l_{i+2}, l_{j+2}\}, \dots$ This is likely due to the continuity of the dynamics [5]. Recall that the landmarks are evenly spaced in time, so l_{i+1} is the Δt -forward image of l_i . Thus a diagonal segment may indicate that the Δt -forward images of (at least one) witness that is shared between l_i and l_j is shared between l_{i+1} and l_{j+1} , and so on. The lengths of the longer line segments suggest that that continuity fails after 5-10 Δt steps, probably because of the positive Lyapunov exponents on the attractor. As a simple check on this reasoning, one can compute an edge lifespan diagram for a dynamical system with a limit cycle. The structure of such a plot (not shown) is dominated by diagonal lines of high Δm -persistence, with a few other scattered one-persistent edges.

The rationale behind studying the maximal m-lifespan goes back to one of the basic premises of persistence: that features that persist for a wide range of parameter values are in some sense meaningful. To explore this, Figure 5.20 shows the witness complex of Figure 5.17(a), highlighting the $\Delta m \geq 2$ -persistent edges: those that exist at m = 2 and persist at least to m = 4. There exists a fundamental core to the complex that persists as the dimension grows and thus is robust to geometric distortion, but there are also short-lived edges that fill in the complex in accord with the local geometric structure of the reconstruction. Indeed, when m = 2, the projection artificially compresses near the origin; small simplicies fill in this region due to the landmark clustering there. However, in the transition to m = 3—viz., Figure 5.17(b)—this region stretches away from the origin, spreading the landmarks out. There is a similar cluster of "fragile" edges near the lower left corner of the complex.

Even though geometric evolution with increasing reconstruction dimension leads to the death of many local edges, the large-scale homology is correct in both complexes of Figure 5.17, although the fine-scale topology is resolved differently by the dimension-dependent geometry. So while the



Figure 5.20: Witness complex of Figure 5.17(a) with $\Delta m \geq 2$ -persistent edges shown as thick (black) lines, and the $\Delta m = 1$ edges as (red) dashed lines.

edges with longer lifespan are indeed more important to the core structure, the short-lived edges are also important because they allow the complex to adapt to the geometric evolution of the attractor and fill in the details of the skeleton that are necessary and meaningful in that dimension.

In the spirit of the false near-neighbor method [62], one might be tempted to take the shortlived edges as an indication that the reconstruction dimension is inadequate. However, one computes homology from the overall complex. As the example above shows, homology is relatively robust with respect to individual edges. The moral of this story is that the lifespan of an edge is not necessarily an obvious indication of its importance to the homology of the complex; Δm persistence plays a different role here than the abscissa of traditional barcode persistence plots.

The results in this section show that it is possible to compute the homology of an invariant set of a dynamical system using a simplicial complex built from a low-dimensional reconstruction of a scalar time series. These results have a number of interesting implications. Among other things, they suggest that the traditional delay-coordinate reconstruction process may be excessive if one is only interested in large-scale topological structure such as the homology. This is directly apropos of the central claim of this thesis, as it explains why it is possible to construct accurate predictions of the future state of a high-dimensional dynamical system using a two-dimensional delaycoordinate reconstruction. The delay-coordinate machinery strives to obtain a diffeomorphism—not a homeomorphism—between the true and reconstructed attractors. However, many of the properties of attractors that are important for forecasting (continuity, recurrence, entropy, etc.) are topological, so requiring only a homeomorphism is not only natural, but also more efficient [80].

This section uses a single example—the Lorenz 63 system—but I believe that the approach will work on other dynamical systems and I plan in the future to do a careful exploration of additional systems, both maps and flows.

5.3 Summary

Chapter 4 offered experimental validation of my proposed paradigm shift in the practice of delay-coordinate reconstruction, but left many unanswered questions about the theoretical underpinnings (and implications) of this approach. This chapter answered those questions by drawing on the complementary theoretical frameworks of information theory and computational topology. The novel computationally-efficient metric (\mathcal{A}_{τ}) explicitly leveraged information stored in a delay vector to select forecast-optimal parameters for delay coordinate reconstruction. This metric allowed for tailoring of reconstruction parameters to available data length, the signal-to-noise ratio in the time series, and the desired prediction horizon. In addition, this information-theoretic approach gave me the language and methods to answer difficult questions like the ones posed on page 79. Perhaps most importantly, the results in Section 5.1 validated that the state estimator of **ro-LMA** often has more information about the near future than a traditional embedding—a fact that is completely counter to all the current theory.

Section 5.2 deviated significantly from the tone of the rest of this thesis. Instead of discussing

delay-coordinate reconstruction purely from a forecasting perspective, it turned a critical eye toward the theoretical foundation and assumptions of this powerful framework, which is the basis for all of nonlinear time-series analysis. The consistent story throughout the previous chapters is that the theoretical requirements of delay-coordinate reconstruction are not necessary—and can indeed be overkill—when one wishes to use it for the purposes of short-term forecasting. But, why is this the case? Is it simply because more information is present in lower-dimensional state estimators, as established in Section 5.1, or is there something deeper underpinning this method from a theoretical perspective? In Section 5.2, I used the canonical Lorenz 63 system to argue that large-scale homology can be attainable at much lower dimensions than the theory might suggest. I believe this in turn suggests that a homeomorphism, in the form of the delay-coordinate map, can be achieved at lower dimensions than what is needed for a diffeomorphism. This insight suggested an alternative explanation as to why ro-LMA gets traction before it should: specifically, that a homeomorphic reconstruction of a dynamical system may be sufficient for short-term forecasting of dynamical systems. However, further work will be required to rigorously prove this broader claim.

Chapter 6

Model-Free Quantification of Time-Series Predictability

Time-series data can span a wide range of complexities and no *single* forecast algorithm can be expected to handle this entire spectrum effectively. This poses an interesting problem when one is developing any new forecasting technology, such as the reduced order framework outlined in this thesis. In particular, given an arbitrary time series—with an undefined level of complexity—can one expect that method to be effective? The first step to answering this question is to define a spectrum of predictive complexity [41].

On the low end of this spectrum are time series that exhibit perfect predictive structure, *i.e.*, signals whose future values can be perfectly predicted from past values. Signals like this can be viewed as the product of an underlying process that generates information and/or transmits it from the past to the future in a perfectly predictable fashion. Constant or periodic signals, for example, fall in this class. On the opposite end of this spectrum are signals that are—from a forecasting perspective—*fully complex*, where the underlying generating process transmits no information at all from the past to the future. White noise processes fall in this class. In fully complex signals, knowledge of the past gives no insight into the future, regardless of what model one chooses to use. Signals in the midrange of this spectrum, *e.g.*, deterministic chaos, pose interesting challenges from a modeling perspective. In these signals, enough information is being transmitted from the past to the future that an *ideal* model—one that captures the generating process—can forecast the future behavior of the observed system with high accuracy.

This leads naturally to an important and challenging question to which I alluded in the first

paragraph of this chapter: given a noisy real-valued time series from an unknown system, does there exist any forecast model that can leverage the information (if any) that is being transmitted forward in time by the underlying generating process? A first step in answering this question is to reliably quantify where on the complexity spectrum a given time series falls; a second step is to determine how complexity and predictability are related in these kinds of data sets. With these answers in hand, one can develop a practical strategy for assessing appropriateness of forecast methods for a given time series. If the forecast produced by **ro-LMA** is poor, for example, but the time series contains a significant amount of predictive structure, one can reasonably conclude that **ro-LMA** is inadequate to the task and that one should seek another method.

The goal of this chapter is to develop effective heuristics to put that strategy into practice. Recall that Chapter 4 of this thesis demonstrated that ro-LMA *can* be effective, and Chapter 5 provided reasons *why* and *how* this is the case. The heuristic proposed in this chapter goes one step further and addresses *when* ro-LMA—and indeed any forecast algorithm—can be expected to be effective.

The information in an observation can be partitioned into two pieces: redundancy and entropy generation [25]. The approach exploits this decomposition in order to assess how much predictive structure is present in a signal—*i.e.*, where it falls on the complexity spectrum mentioned above. I define *complexity* as a particular approximation of Kolmogorov-Sinai entropy [69]. That is, I view a random-walk time series (which exhibits high entropy) as purely complex, whereas a low-entropy periodic signal is on the low end of the complexity spectrum. This differs from the notion of complexity used by *e.g.*, [101], which would consider a time series without any statistical regularities to be non-complex. In collaboration with R. G. James, I argue that an extension of *permutation entropy* [9]—a method for approximating the entropy through ordinal analysis—is an effective way to assess the complexity of a given time series. Permutation entropy, introduced in Section 2.2.6, is ideal for this purpose because it works with real-valued data and is known to converge to the true entropy value. Other existing techniques either require specific knowledge of the generating process or produce biased values of the entropy [13].

I focus on real-valued, scalar, time-series data from physical experiments. I do not assume any knowledge of the generating process or its properties: whether it is linear, nonlinear, deterministic, stochastic, etc. To explore the relationship between complexity, predictive structure, and actual predictability, I generate forecasts for several experimental computer performance time-series datasets using the five different prediction strategies discussed in this thesis, then compare the accuracy of those predictions to the permutation entropy of the associated signals. This results in two primary findings:

- (1) The permutation entropy of a noisy real-valued time series from an unknown system is correlated with the accuracy of an appropriate predictor.
- (2) The relationship between permutation entropy and prediction accuracy is a useful empirical heuristic for identifying mismatches between prediction models and time-series data.

There has, of course, been a great deal of good work on different ways to measure the complexity of data, and previous explorations have confirmed repeatedly that complexity is a challenge to prediction. It is well known that the way information is generated and processed internally by a system plays a critical role in the success of different forecasting methods—and in the choice of which method is appropriate for a given time series. This constellation of issues has not been properly explored, however, in the context of noisy, poorly sampled, real-world data from unknown systems. That exploration, and the development of strategies for putting its results into effective practice, is the primary contribution of this chapter. The empirical results in Section 6.2 not only elucidate the relationship between complexity and predictability, but also provide a practical strategy to aid practitioners in assessing the appropriateness of a prediction model for a given real-world noisy time series from an unknown system—a challenging task for which little guidance is currently available. In the context of this thesis, the value of this is that it provides a general framework for assessing whether or not ro-LMA is an appropriate choice for a given time series, or if a more sophisticated or even a *simpler* strategy is required.

The rest of this chapter is organized as follows. Section 6.1 discusses previous results on

generating partitions, local modeling, and error distribution analysis, and situates this work in that context. In Section 6.2, I estimate the complexity of a number of time-series traces and compare that complexity to the accuracy of various predictions models operating on that time series. In Section 6.3, I discuss these results and their implications, and consider future areas of research.

6.1 Traditional Methods for Predicting Predictability

Hundreds, if not thousands, of strategies have been developed for a wide variety of prediction tasks. The purpose of this chapter is not to add a new weapon to this arsenal, nor to do any sort of theoretical assessment or comparison of existing methods. In the spirit of this thesis, the goals here are focused more on the *practice* of prediction: (i) to empirically quantify the predictive structure that is present in a real-valued scalar time series and (ii) to explore how the performance of prediction methods is related to that inherent complexity. It would, of course, be neither practical nor interesting to report results for every existing forecast strategy; instead, I use the same representative set of methods that appear throughout this thesis, as described in Section 2.3.

Quantifying predictability, which is sometimes called "predicting predictability," is not a new problem. Most of the corresponding solutions fall into two categories that I call model-based error analysis and model-free information analysis. The first class focuses on errors produced by a specific forecasting schema. This analysis can proceed locally or globally. The local version approximates error distributions for different regions of a time-series model using local ensemble in-sample¹ forecasting. These distributions are then used as estimates of out-of-sample forecast errors in those regions. For example, Smith *et al.* make in-sample forecasts using ensembles around selected points in order to predict the local predictability of a time series [107]. This approach can be used to show that different portions of a time series exhibit varying levels of local predictive

¹ The terms "in sample" and "out of sample" are used in different ways in the forecasting community. Here, I distinguish those terms by the part of the time series that is the focus of the prediction: the observed data for the former and the unknown future for the latter. In-sample forecasts—comparisons of predictions generated from *part* of the observed time series—are useful for assessing model error and prediction horizons, among other things.

uncertainty.

Local model-based error analysis works quite well, but it only approximates the *local* predictive uncertainty *in relation to a fixed model*. It cannot quantify the *inherent* predictability of a time series and thus cannot be used to draw conclusions about predictive structure that other forecast methods may be able to leverage. Global model-based error analysis moves in this direction. It uses out-of-sample error distributions, computed *post facto* from a class of models, to determine which of those models was best. After building an autoregressive model, for example, it is common to calculate forecast errors and verify that they are normally distributed. If they are not, that suggests that there is structure in the time series that the model-building process was unable to recognize, capture, and exploit. The problem with this approach is lack of generality. Normally distributed errors indicate that a model has captured the structure in the data insofar as is possible, *given the formulation of that particular model (viz.,* the best possible linear fit to a nonlinear dataset). This gives no indication as to whether another modeling strategy might do better.

A practice known as deterministic vs. stochastic modeling [22, 44] bridges the gap between local and global approaches to model-based error analysis. The basic idea is to construct a series of local linear fits, beginning with a few points and working up to a global linear fit that includes all known points, and then analyze how the average out-of-sample forecast error changes as a function of number of points in the fit. The shape of such a "DVS" graph indicates the amounts of determinism and stochasticity present in a time series.

The model-based error analysis methods described in the previous three paragraphs are based on specific assumptions about the underlying generating process and knowledge about what will happen to the error if those assumptions hold or fail. Model-*free* information analysis moves away from those restrictions. My approach falls into this class: I wish to measure the inherent complexity of an arbitrary empirical time series, then study the correlation of that complexity with the predictive accuracy of forecasts made using a number of different methods.

I build on the notion of *redundancy* that was introduced on page 123, which formally quantifies how information propagates forward through a time series: *i.e.*, the mutual information between the past n observations and the current one. The redundancy of i.i.d. random processes, for instance, is zero, since all observations in such a process are independent of one another. On the other hand, deterministic systems, including chaotic ones, have high redundancy—in fact, maximal redundancy in the infinite limit—and thus they can be perfectly predicted if observed for long enough [44]. In practice, it is quite difficult to estimate the redundancy of an arbitrary, real-valued time series. Doing so requires knowing either the Kolmogorov-Sinai entropy or the values of all positive Lyapunov exponents of the system. Both of these calculations are difficult, the latter particularly so if the data are very noisy or the generating system is stochastic.

Using entropy and redundancy to quantify the inherent predictability of a time series is not a new idea. Past methods for this, however, (e.g., [74, 102]) have hinged on knowledge of the generating partition of the underlying process, which lets one transform real-valued observations into symbols in a way that preserves the underlying dynamics [69]. Using a partition that is not a generating partition—e.g., simply binning the data—can introduce spurious complexity into the resulting symbolic sequence and thus misrepresent the entropy of the underlying system [13]. Generating partitions are luxuries that are rarely, if ever, afforded to an analyst, since one needs to know the underlying dynamics in order to construct one. And even if the dynamics are known, these partitions are difficult to compute and often have fractal boundaries [31]. (See Section 2.2.5.1 for a review of these issues.)

In the development described in the following section, I sidestep these issues by using a variant of the *permutation entropy* of Bandt and Pompe [9] to estimate the value of the Kolmogorov-Sinai entropy of a real-valued time series—and thus the redundancy in that data, which my results confirm to be an effective proxy for predictability. This differs from existing approaches in a number of ways. It does not rely on generating partitions—and thus does not introduce bias into the results if one does not know the dynamics or cannot compute the partition. Permutation entropy makes no assumptions about, and requires no knowledge of, the underlying generating process: whether it is linear or nonlinear, what its Lyapunov spectrum is, etc. These features make my approach applicable to noisy real-valued time series from all classes of systems, deterministic and stochastic.
6.2 Predictability, Complexity, and Permutation Entropy

In this section, I offer an empirical validation of the two findings introduced on page 124, namely:

- (1) The weighted permutation entropy (WPE) of a noisy real-valued time series from an unknown system is correlated with prediction accuracy—*i.e.*, the predictable structure in an empirical time-series data set can be quantified by its WPE.
- (2) The relationship between WPE and mean absolute scaled error (1-MASE) is a useful empirical heuristic for identifying mismatches between prediction models and time-series data *i.e.*, when there is structure in the data that the model is unable to exploit.

The experiments below involve four different prediction methods: fnn-LMA, naïve, ARIMA and random walk, applied to time-series data from eight different experimental systems: col_major, 403.gcc, and six different segments of a computer performance experiment that I have not yet discussed in this thesis called dgesdd, a Fortran program from the LAPACK linear algebra package [8] that calculates the singular value decomposition of a rectangular M by N matrix with real-valued entries. For my experiments, I choose M = 750 and N = 1000 and generate the matrix entries randomly.

The behavior of this program as it computes the singular values of this matrix is complex and interesting, as is clearly visible in Figure 6.1. As the code moves though its different phases diagonalizing the matrix, computing its transpose, multiplying, etc.—the processor utilization patterns change quite radically. For the first $\sim 21,000$ (in units of 100,000 instructions) measurements, roughly 1.8 instructions are executed per cycle, on the average, by the eight processing units on this chip. After that, the IPC moves through a number of different oscillatory regimes, which I have color-coded in the figure in order to make textual cross-references easy to track.

The wide range of behaviors in Figure 6.1 provides a distinct advantage, for the purposes of this chapter, in that a number of different generating processes—with a wide range of complexities—



Figure 6.1: A processor performance trace of instructions per cycle (IPC) during the execution of dgesdd. The colors (also separated by vertical dashed lines) identify the different *segments* of the signal that are discussed in the text.

are at work in different phases of a single time series. The col_major and 403.gcc traces in Figures 3.3 and 3.4, in contrast, appear to be far more consistent over time—probably the result of a single generating process with consistent complexity. dgesdd, has multiple regimes, each probably the result of different generating processes. To take advantage of this rich experimental data set, I split the signal into six different segments, thereby obtaining an array of examples for the analyses in the following sections. For notational convenience, I refer to these 90 time-series data sets² as dgesdd_i, with $i \in \{1...6\}$ where *i* corresponds to one of the six segments of the signal, ordered from left to right. These segments, which were determined visually, are shown in different colors in Figure 6.1. Visual decomposition is subjective, of course, particularly since the regimes exhibit some fractal structure. Thus, it may be the case that more than one generating process is at work in each of our segments. This is a factor in the discussion that follows.

The objective of these experiments is to explore how prediction accuracy is related to WPE. Working from the first 90% of each signal, I generate a prediction of the last 10% using all four

 $^{^{2}}$ 15 runs, each with six regimes



Figure 6.2: Weighted permutation entropy versus 1-MASE of the best prediction of a number of different time series. The solid curve is a least-squares log fit of these points. The dashed curves reflect the standard deviation of the model in its parameter space. Points that lie below and to the right of the shaded region indicate that the time series has more predictive structure than the forecast strategy is able to utilize.

prediction methods, then calculate the 1-MASE value of those predictions. I also calculate the WPE of each time series using a wordlength chosen via the procedure described at the end of Section 2.2.6. In order to assess the run-to-run variability of these results, I repeat all of these calculations on 15 separate trials: *i.e.*, 15 different runs of each program.

Figure 6.2 plots the WPE values versus the corresponding 1-MASE values of the *best* prediction for each of the 120 time series in this study. The obvious upward trend is consistent with the notion that there is a pattern in the WPE-MASE relationship. However, a simple linear fit is a bad idea here. First, any signal with zero entropy should be perfectly predictable (*i.e.*, 1-MASE \approx 0), so any curve fitted to these data should pass through the origin. Moreover, WPE does not grow without bound, so one would expect the patterns in the WPE-MASE pairs to reach some sort of asymptote. For these reasons, I choose to fit a function³ of the form $y = a \log(bx + 1)$ to these points, with y = WPE and x = 1-MASE. The solid curve in the figure shows this fit; the dashed curves show the standard deviation of this model in its parameter space: *i.e.*, $y = a \log(bx + 1)$ with \pm one standard deviation on each of the two parameters. Points that fall within this deviation volume (light grey) correspond to predictions that are comparable to the best ones found in this study; points that fall *above* that volume (dark grey) are better still. I choose to truncate the shaded region because of a subtle point regarding the 1-MASE of an ideal predictor, which should not be larger than 1 unless the training and test signals are different. This is discussed at more length below.

The curves and regions in Figure 6.2 are a graphical representation of the first finding introduced on page 124. This representation is, I believe, a useful heuristic for determining whether a given prediction method is well matched to a particular time series. If your point is outside the grey region, then that particular model is not capturing all the available structure of the time series. This is not, of course, a formal result. The forecast methods and data sets used here were chosen to span the space of standard prediction strategies and the range of dynamical behaviors, but they do not cover those spaces exhaustively. My goal here is an *empirical* assessment of the relationship between predictability and complexity, not formal results about a "best" predictor for a given time series. There may be other methods that produce lower 1-MASE values than those in Figure 6.2, but the sparseness of the points above and below the one- σ region about the dashed curve in this plot strongly suggests a pattern of correlation between the underlying predictability of a time series and its WPE. The rest of this section describes these results and claims in more detail—including the measures taken to assure meaningful comparisons across methods, trials, and programs—elaborates on the meaning of the different curves and limits in the figure, and ties these results into the overall thesis goals.

Figure 6.3 shows WPE vs. 1-MASE plots for the full set of experiments; Table 6.1 contains all the associated numerical values. There are 15 points in each cluster, one for each trial. (The

³ The specific values of the coefficients are $a = 7.97 \times 10^{-2}$ and $b = 1.52 \times 10^{3}$.

Table 6.1:	1-MASE	scores and	l weighted	permutation	entropies f	for all	eight	examples	studied $\$	in
this chapter	r. LMA =	- Lorenz m	nethod of a	analogues; RW	V = random	n-walk	predi	ction.		

· 1 /

Signal	RW 1-MASE	naïve 1-MASE	ARIMA 1-MASE	fnn-LMA 1 -MASE	WPE
col_major	1.001 ± 0.002	0.571 ± 0.002	0.599 ± 0.211	0.050 ± 0.002	0.513
403.gcc	1.138 ± 0.011	1.797 ± 0.010	1.837 ± 0.016	1.530 ± 0.021	0.943
$dgesdd_1$	0.933 ± 0.095	2.676 ± 4.328	0.714 ± 0.075	0.827 ± 0.076	0.957
$dgesdd_2$	1.125 ± 0.012	3.054 ± 0.040	2.163 ± 0.027	1.279 ± 0.020	0.846
$dgesdd_3$	0.707 ± 0.009	31.386 ± 0.282	0.713 ± 0.010	0.619 ± 0.021	0.716
$dgesdd_4$	1.034 ± 0.035	2.661 ± 0.074	0.979 ± 0.032	0.779 ± 0.036	0.825
$dgesdd_5$	1.001 ± 0.047	20.870 ± 0.192	2.370 ± 0.051	0.718 ± 0.048	0.678
$dgesdd_6$	1.060 ± 0.055	2.197 ± 0.083	1.438 ± 0.061	0.739 ± 0.068	0.748

points in Figure 6.2 are the leftmost of the points for the corresponding trace in any of the four plots in Figure 6.3.) The WPE values do not vary very much across trials. For most traces, the variance in 1-MASE scores is low as well, resulting in small, tight clusters. In some cases— ARIMA predictions of col_major, for instance—the 1-MASE variance is larger, which spreads out the clusters horizontally. The mean 1-MASE scores of predictions generated with fnn-LMA are generally closer to the dashed curve; the ARIMA method clusters are more widely spread, the naïve clusters even more so. A few of the clusters have very high variance; these are discussed later in this section.

The main thing to note here, however, is not the details of the shapes of the clusters, but rather their positions in the four plots: specifically, the fact that many of them are to the right of and/or below the dashed curve that identifies the boundary of the shaded region. These predictions are not as good as my heuristic suggests they could be. Focusing in on any single signal makes this clear: fnn-LMA works best for dgesdd₆, for instance, followed by the random-walk prediction method, then ARIMA and naïve. Again, this provides some practical leverage: if one calculates an WPE vs. 1-MASE value that is outside the shaded region, that suggests that the prediction method is not well matched to the task at hand—that is, the time series has more predictive structure than the method is able to use. The results of ARIMA on dgesdd₆, for instance, suggest that one should try



Figure 6.3: WPE vs. 1-MASE for all trials, methods, and systems—with the exception of $dgesdd_1$, $dgesdd_3$, and $dgesdd_5$, which are omitted from the top-right plot for scale reasons, as described in the text. Numerical values, including means and standard deviations of the errors, can be found in Table 6.1. The curves and shaded regions are the same as in the previous figure.

a different method. The position of the fnn-LMA cluster for $dgesdd_6$, on the other hand, reflects the ability of that method to capture and exploit the structure that is present in this signal. WPE vs. 1-MASE values like this, which fall in the shaded region, indicate to the practitioner that the prediction method is well-suited to the task. The following discussion uses a number of examples to lay out the details that underlie these claims.

Though col_major is a very simple program, its dynamics are actually quite complicated,

as discussed in Section 3.2.1.2. Recall from Figure 4.2 and Table 4.2 that the naïve, ARIMA, and (especially) random-walk prediction methods do not perform very well on this signal. The 1-MASE scores of these predictions are 0.571 ± 0.002 , 1.001 ± 0.002 , and 0.599 ± 0.211 , respectively, across all 15 trials. That is, naïve and ARIMA perform only ≈ 1.7 times better than the random-walk method, a primitive strategy that simply uses the current value as the prediction. However, the WPE value for the col_major trials is 0.513 ± 0.003 , which is in the center of the complexity spectrum described on page 122.

This disparity—WPE values that suggest a high rate of forward information transfer in the signal, but predictions with comparatively poor 1-MASE scores—is obvious in the geometry of three of the four images in Figure 6.3, where the col_major clusters are far to the right of and/or below the dashed curve. Again, this indicates that these methods are not leveraging the available information in the signal. The dynamics of col_major may be complicated, but they are not unstructured. This signal is nonlinear and deterministic [83], and if one uses a prediction technique that is based a nonlinear model (fnn-LMA)—rather than a method that simply predicts the running mean (naïve) or the previous value (random walk), or one that uses a linear model (ARIMA)—the 1-MASE score is much improved: 0.050 ± 0.001 . This prediction is 20 times more accurate than a random-walk forecast, which is more in line with the level of predictive structure that the low WPE value suggests is present in the col_major signal. The 1-MASE scores of random-walk predictions of this signal are all ≈ 1 —as one would expect—pushing those points well below the shaded region. Clearly the stationarity assumption on which that method is based does not hold for this signal.

The col_major example also brings out some of the shortcomings of automated modelbuilding processes. Note that the + points are clustered very tightly in the lower left quadrant of the naïve, random-walk, and fnn-LMA plots in Figure 6.3, but spread out horizontally in the ARIMA plot. This is because of the way the auto.arima process—the fitting procedure that I use for ARIMA models—works [56]. If a KPSS test⁴ of the time series in question indicates that it is

⁴ A Kwiatkowski-Phillips-Schmidt-Shin (KPSS) test [65]—one of many tests performed by auto.arima to chose the ARIMA parameters—is used for testing that an observable time series is stationary around a deterministic trend.

nonstationary, the ARIMA recipe adds an integration term to the model. This test gives mixed results in the case of the col_major process, flagging five of the 15 trials as stationary and ten as nonstationary. I conjectured that ARIMA models without an integration term perform more poorly on these five signals, which increases the error and thereby spreads out the points. I tested this hypothesis by forcing the inclusion of an integration term in the five cases where a KPSS test indicated that such a term was not needed. This action removes the spread, pushing all 15 of the col_major ARIMA points in Figure 6.3 into a tight cluster.

The discussion in the previous paragraph highlights the second finding of this chapter: the ability of the graphical heuristic of Figure 6.2 to flag inappropriate models. auto.arima is an automated, mechanical procedure for choosing modeling parameters for a given data set. While the tests and criteria employed by this algorithm (Section 2.3.2) are sophisticated, the results can still be sub-optimal—if the initial space of models being searched is not broad enough, for instance, or if one of the preliminary tests gives an erroneous result. Moreover, auto.arima always returns a model, and it can be very hard to detect when that model is bad. The results discussed in this chapter suggest a way to do so: if the 1-MASE score of an auto-fitted model like an auto.arima result is out of line with the WPE value of the data, that can be an indication of inappropriateness in the order selection and parameter estimation procedure.

The WPE of dgesdd₅ (0.677 ± 0.006) is higher than that of col_major. This indicates that the rate of forward information transfer of the underlying process is lower, but that observations from this system still contain a significant amount of structure that can, in theory, be used to predict the future course of the time series. The 1-MASE scores of the naïve and ARIMA predictions for this system are 20.870 ± 0.192 and 2.370 ± 0.051 , respectively: that is, 20.87 and 2.37 times worse than a simple random-walk forecast⁵ of the training set portions of the same signals. As before, the positions of these points on a WPE vs. 1-MASE plot—significantly below and to the right of the shaded region—should suggest to a practitioner that a different method might do better. Indeed,

⁵ The naïve 1-MASE score is large because of the bimodal nature of the distribution of the values of the signal, which makes guessing the mean a particularly bad strategy. The same thing is true of the $dgesdd_3$ signal.

for dgesdd₅, fnn-LMA produces a 1-MASE score of 0.718 ± 0.048 and a cluster of results that largely within the shaded region on the WPE-MASE plot. This is consistent with the second finding of this chapter: the fnn-LMA method can capture and reproduce the way in which the dgesdd₅ system processes information, but the naïve and ARIMA prediction methods cannot.

The WPE of 403.gcc is higher still: 0.943 ± 0.001 . This system transmits very little information forward in time and provides almost no structure for prediction methods to work with. Here, the random-walk predictor is the best of the methods used here. This makes sense; in a fully complex signal, where there is no predictive structure to utilize, methods that depend on exploiting that structure—like ARIMA and fnn-LMA—cannot get any traction. Since fitting a hyperplane using least squares should filter out some of the noise in the signal, the fact that fnn-LMA outperforms ARIMA (1.530 \pm 0.021 vs. 1.837 \pm 0.016) may be somewhat counterintuitive. However, the small amount of predictive structure that is present in this signal is nonlinear (*cf.*, [83]), and fnn-LMA is designed to capture and exploit that kind of structure. Note that all four 403.gcc clusters in Figure 6.3 are outside the shaded region; in the case of the random-walk prediction, for instance, the 1-MASE value is 1.1381 \pm 0.011. This is due to nonstationarity in the signal: in particular, differences between the training and test signals. The same effect is at work in the dgesdd₂ results, for the same reasons—and visibly so, judging by the red segment of Figure 6.1, where the period and amplitude of the oscillations are decreasing.

dgesdd₁—the dark blue (first) segment of Figure 6.1—behaves very differently than the other seven systems in this study. Though its weighted permutation entropy is very high (0.957 ± 0.016) , three of the four prediction methods do quite well on this signal, yielding mean 1-MASE scores of 0.714 ± 0.075 (ARIMA), 0.827 ± 0.076 (fnn-LMA), and 0.933 ± 0.095 (random walk). This pushes the corresponding clusters of points in Figure 6.3 well above the trend followed by the other seven signals. The reasons for this are discussed below. The 1-MASE scores of the predictions that are produced by the naïve method for this system, however, are highly inconsistent. The majority of the blue diamond-shaped points on the top-right plot in Figure 6.3 are clustered near a 1-MASE score of 0.6, which is better than the other three methods. In five of the 15 dgesdd₁ trials, however, there



Figure 6.4: A small portion of the $dgesdd_1$ time series

are step changes in the signal. This is a different nonstationarity than in the case of col_major large jump discontinuities rather than small shifts in the baseline—and not one that I am able to handle by simply forcing the ARIMA model to include a particular term. The naïve method has a very difficult time with signals like this, particularly if there are multiple step changes. That raised the 1-MASE scores of these trials, pushing the corresponding points⁶ to the right, and in turn raising both the mean and variance of this set of trials.

The effects described in the previous paragraph are also exacerbated by the way 1-MASE is calculated. Recall that 1-MASE scores are scaled *relative to a random-walk forecast*. This creates several issues. Since random-walk prediction works very badly on signals with frequent, large, rapid transitions (even simple periodic signals) this class of signals can exhibit low WPE, and high 1-MASE. This is because the random-walk forecast of this signal will be 180 degrees out of phase with the true continuation. This effect can shift points leftwards on a WPE vs. 1-MASE plot, and that is exactly why the dgesdd₁ clusters in Figure 6.3 are above the dashed curve. This time series, part of which is shown in closeup in Figure 6.4, is not quite the worst-case signal for a random-walk prediction, but it still poses a serious challenge. It is dominated by a noisy regime (between

⁶ This includes the cluster of three points near 1-MASE ≈ 2.5 , as well as two points that are beyond the domain of the graph, at 1-MASE $\approx 11.2 - 14.8$.

 \approx 1.86 and \approx 1.88 on the vertical scale in Figure 6.4), punctuated by short excursions above 1.9. In the former regime, which makes up more than 80% of the signal, there are frequent dips to 1.82 and occasional larger dips below 1.8. These single-point dips are the bane of random-walk forecasting. In this particular case, roughly 40% of the forecasted points are off by the width of the associated dip, which skews the associated 1-MASE scores. Signals like this are also problematic for the naïve prediction strategy, since the outliers have significant influence on the mean. This compounds the effect of the skew in the scaling factor and exacerbates the spread in the dgesdd₁ 1-MASE values.

The second effect that can skew 1-MASE scores is nonstationarity. Since this metric is normalized by the error of a random-walk forecast on the training signal, differences between the test signal and training signal can create issues. This is why the 1-MASE values in Table 6.1 are not identically one for every random-walk forecast of every time series: the last 10% of these signals is significantly different from the first 90%. The deviation from 1.00 will depend on the process that generated the data—whether it has multiple regimes, what those regimes look like, and how it switches between them—as well as the experimental setup (e.g., sensor precision and data length). For the processes studied here, these effects do not cause the 1-MASE values to exceed 1.15, but pathological situations (e.g., a huge switch in scale right at the training/test signal boundary, or a signal that simply grows exponentially) could produce higher values. This suggests another potentially useful heuristic: if the 1-MASE of a random-walk prediction of a time series is significantly different from 1, it could be an indication that the signal is nonstationary.

The curves in Figures 6.2 and 6.3 are determined from finite sets of methods and data. I put a lot of thought and effort into making these sets representative and comprehensive. The forecast methods involved ranged from the simple to the sophisticated; the time-series data analyzed in this section are sampled from systems whose behavior spans the dynamical behavior space. While I am cautiously optimistic about the generality of my conclusions, more exploration will be required before I can make definitive or general conclusions. However, my preliminary exploration shows that data from the Hénon map [55], the Lorenz 63 system [71], the SFI dataset A [119], and a random-walk process all fall within the one- σ volume of the fit in Figures 6.2 and 6.3 region, as do various nonlinear transformations of dgesdd₂, dgesdd₅ and dgesdd₆, so I am optimistic.

In this chapter I strictly used fnn-LMA as the nonlinear exemplar to explore how prediction accuracy is related to WPE. With this relationship established, applying this heuristic to assessing the appropriateness of ro-LMA for a given signal is quite trivial: one simply compares the accuracy of ro-LMA, tabulated in Tables 4.1 and 4.2, with the WPE of that signal, given in Table 6.1, using the graphical heuristic in Figure 6.2.

Note that there has been prior work under a very similar title to our paper on this topic [41], but there are only superficial similarities between the two research projects. Haven *et al.* [52] utilize the relative entropy to quantify the difference in predictability between two distributions: one evolved from a small ensemble of past states using the known dynamical system, and the other the observed distribution. My work quantifies the predictability of a single observed time series using weighted permutation entropy and makes no assumptions about the generating process.

More closely related is the work of Boffetta *et al.* [12], who investigated the scaling behavior of finite-size Lyapunov exponents (FSLE) and ϵ -entropy for a wide variety of deterministic systems with known dynamics and additive noise. While the scaling of these measures acts as a general proxy for predictability bounds, this approach differs from my work in a number of fundamental ways. First, [12] is a theoretical study that does not involve any actual predictions. I focus on real-world time-series data, where one does not necessarily have the ability to perturb or otherwise interact with the system of interest, nor can one obtain or manufacture the (possibly large) number of points that might be needed to estimate the ϵ -entropy for small ϵ . Second, I do not require *a priori* knowledge about the noise and its interaction with the system. Third, I tie information—in the form of the weighted permutation entropy—directly to prediction error via calculated values of a specific error metric. Though FSLE and ϵ -entropy allow for the comparison of predictability between systems, they do not directly provide an estimate of prediction error. Finally, my approach also holds for stochastic systems, where neither the FLSEs nor their relationship to predictability are well defined.

6.3 Summary

Forecast strategies that are designed to capture predictive structure are ineffective when signal complexity outweighs information redundancy. This poses a number of serious challenges in practice. Without knowing anything about the generating process, it is difficult to determine how much predictive structure is present in a noisy, real-world time series. And even if predictive structure exists, a given forecast method may not work, simply because it cannot exploit the structure that is present (*e.g.*, a linear model of a nonlinear process). If a forecast model is not producing good results, a practitioner needs to know why: is the reason that the data contain no predictive structure—*i.e.*, that no model will work—or is the model that s/he is using simply not good enough?

In this chapter, I have argued that redundancy is a useful proxy for the inherent predictability of an empirical time series. To operationalize that relationship, I used an approximation of the Kolmogorov-Sinai entropy, estimated using a weighted version of the permutation entropy of [9]. This WPE technique—an ordinal calculation of forward information transfer in a time series—is ideal for my purposes because it works with real-valued data and is known to converge to the true entropy value. Using a variety of forecast models and more than 150 time-series data sets from experiments and simulations, I have shown that prediction accuracy is indeed correlated with weighted permutation entropy: the higher the WPE, in general, the higher the prediction error. The relationship is roughly logarithmic, which makes theoretical sense, given the nature of WPE, predictability, and 1-MASE.

An important practical corollary to this empirical correlation of predictability and WPE is a practical strategy for assessing appropriateness of forecast methods. If the forecast produced by a particular method is poor but the time series contains a significant amount of predictive structure, one can reasonably conclude that that method is inadequate to the task and that one should seek another method. fnn-LMA, for instance, performed better in most cases because it is more general. (This is particularly apparent in the col_major and dgesdd₅ examples.) The naïve method, which

simply predicts the mean, can work very well on noisy signals because it effects a filtering operation. The simple random-walk strategy outperforms fnn-LMA, ARIMA, and the naïve method on the 403.gcc signal, which is extremely complex—*i.e.*, extremely low redundancy.

The curves and shaded regions in Figures 6.2 and 6.3 operationalize the discussion in the previous paragraph. These geometric features are a preliminary, but potentially useful, heuristic for knowing when a model is not well-matched to the task at hand: a point that is below and/or to the right of the shaded regions on a plot like Figure 6.3 indicates that the time series has more predictive structure than the forecast model can capture and exploit—and that one would be well advised to try another method. In the context of this thesis, this heuristic allows a practitioner to know if ro-LMA is capturing all the available predictive structure in a time series or if another method such as fnn-LMA should be used instead.

These curves were determined empirically using a specific error metric and a finite set of forecast methods and time-series traces. If one uses a different error metric, the geometry of the heuristic may be different—and may not even make sense, if one uses a metric that does not support comparison across different time series. And while the methods and traces used in this study were chosen to be representative of the practice, they are of course not completely comprehensive. It is certainly possible, for instance, that the nonlinear dynamics of computer performance is subtly different from the nonlinear dynamics of other systems. My preliminary results on other systems, not shown here, *e.g.*, Hénon, Lorenz 63, a random-walk process, SFI dataset A, and more, lead me to believe that the results of this chapter will generalize beyond the examples presented.

Chapter 7

Conclusion and Future Directions

Delay-coordinate embedding, the bedrock of nonlinear time-series analysis, has been the foundation of forecasting techniques for nonlinear dynamical systems. A significant hurdle in the application of these techniques in a real-time fashion or for nonstationary systems is proper estimation of the embedding dimension. The source of this difficulty is rooted in trying to obtain a diffeomorphic reconstruction of the observed system, *i.e.*, a topologically perfect representation. This thesis presented a paradigm shift away from that traditional approach, showing that for short-term delay-coordinate based forecasting of limited noisy data, *perfection is not necessary, and can even be detrimental.*

As a first step along this path, I introduced a novel forecasting schema, ro-LMA, that sidesteps the difficult parameter estimation step by simply fixing m = 2. For a range of low- and highdimensional synthetic and experimental systems, I showed that ro-LMA produced short-term predictions on par with or exceeding the accuracy of traditional embeddings even though ro-LMAemployed *incomplete* reconstructions of the dynamics—*i.e.*, models that are not necessarily true embeddings. This effected an experimental validation of the central premise of this thesis, *viz.*, the current paradigm in delay-coordinate embedding may be overly stringent for short-term forecasts of real-world data.

The utility of incomplete reconstructions is in stark contrast to traditional views of delaycoordinate embedding, so experimental validation of this bold claim is insufficient. In order to present a complete validation of this methodology, I provided two complementary theoretical frameworks, based in information theory and computational topology, to explain *why* and *how* this reduced-order modeling strategy works.

The information-theoretic analysis focused on understanding how information about the future is stored in delay-coordinate vectors. Leveraging this knowledge, in collaboration with R. G. James, I constructed a novel metric, time-delayed active information storage (\mathcal{A}_{τ}) , for selecting forecast-specific reconstruction parameters. This approach to parameter selection is drastically different than standard approaches. Instead of focusing on the calculation of dynamical invariants as the end goal, \mathcal{A}_{τ} maximizes the information about the future stored in each delay vector explicitly optimizing the reconstruction for the purposes of forecasting. A_{τ} allows one to select parameter values that are tailored specifically to the quantity of data available, the signal-to-noise ratio of the time series and the required forecast horizon—and does so quickly, efficiently and directly from the data. A_{τ} independently corroborated the central claims of this thesis, showing that for noisy, limited datasets, often the state estimator used in ro-LMA contained as much—or more information about the near future as a full embedding. This result is counter-intuitive; one would think, up to some limit, each new dimension would add information to the model. The fact that more information is not necessarily gained in each new dimension changes the way delay-coordinate based forecasting should be approached, and offers a fundamental explanation of why prediction in projection is effective in practice.

The topological analysis in Section 5.2 questioned the fundamental need for a *diffeomorphic* reconstruction—especially when one is not interested in calculating dynamical invariants. In collaboration with J. D. Meiss, I conjectured that it may be possible to ascertain information about the large-scale topology of the invariant set—specifically, the homology—with a lower reconstruction dimension than that needed to obtain an embedding. Using a simple canonical example, I showed that the witness complex correctly resolved the homology of the underlying invariant set, *viz.*, its Betti numbers, even if the reconstruction dimension was well below the thresholds for which the embedding theorems assure smooth conjugacy between the true and reconstructed dynamics. Since many properties that one cares about for forecasting—the existence of periodic orbits, re-

currence, entropy, etc.—depend only upon topology, the stabilization of large-scale topology at low dimensions effects an alternative validation of the central premise of this thesis. I further conjectured—but did not prove—that this unexpected resolution of large-scale topology at low dimensions may be due to the existence of a *homeomorphism* between the original and reconstructed dynamics. Proving the broader claim that the delay-coordinate map is a homeomorphism at lower embedding dimensions than required for a diffeomorphism and that a homeomorphic reconstruction is sufficient for short-term forecasting will be a key future direction of research.

While I illustrated that ro-LMA works for a broad spectrum of signals and provided sound theoretical evidence supporting why it works, it is important to remember that ro-LMA—or any forecast model for that matter—will not be ideal for all tasks. Following this line of reasoning it was vital to understand *when* ro-LMA would be effective. In this capacity, again in collaboration with R. G. James, I developed a model-free framework for quantifying when a time-series exhibits predictable features, *viz.*, bounded information production. This heuristic allows one to know *a priori* whether ro-LMA—or any forecast method—is appropriate for forecasting a given time series.

There are a number of important avenues for future work associated with each topic proposed in this thesis; those avenues were all discussed individually in their respective chapters. However, the next frontier of this work, which draws upon all aspects of the research described in this dissertation, is developing strategies for grappling with nonstationary time series—a serious challenge in any time-series modeling problem—in the context of delay coordinate based forecasting. We live in a nonlinear *and* nonstationary world. Real-world systems change over time: bearings break down, computer systems get updated, transistors wear out, the climate moves between glacial and interglacial periods, etc. The nonlinear and nonstationary nature of systems like these highlights the need for adaptive models, built on the fly, that require little to no human interaction.

My first experience with nonstationarity involved a performance trace of row_major running on an Intel Core Duo that exhibited an interesting phenomenon termed "ghost triangles" (as can be seen in Figure 7.1) [5]. After a routine (automatic) operating system update, not only were the "ghost triangles" gone, but the entire triangular structure present in the two-dimensional



Figure 7.1: A two-dimensional reconstruction of L2 cache-misses of row_major on an Intel Core Duo with $\tau = 100,000$ instructions.

reconstruction had been lost. I thought I had learned my lesson the hard way with unforeseen change, but the dynamics were even more sensitive than I originally thought. As a result of the auto-update fiasco, our group purchased a new computer and disabled its update scheduler. However, I soon learned this was not enough. When I went back to repeat some experiments, the computer crashed with a standard kernel **panic()** halt. After this, the traces were never the same: the system halt caused a bifurcation in the performance dynamics. Figure 7.2 shows a before-and-after example involving another SPEC benchmark, 482.sphinx. According to computer design theory, this halt should *not* have changed anything. Nonetheless, it actually caused a fundamental shift in the performance and a change in the dynamical structure.

These examples drive home the fact that real-world nonlinear systems routinely undergo bifurcations in their dynamics. This means that a forecast model should not be trained once and then used for all time. Instead, it should be constantly adapted to the current dynamics. For the fnn-LMA method, this is next to impossible due to the human-intensive parameter selection process. The agility of ro-LMA (no need to estimate m) should make it possible to tackle delay-coordinate based forecasting of nonstationary time series. Detecting regime shifts—and adapting the time delay accordingly—is the first step in this important area of future work.



Figure 7.2: Processor load (IPC) traces [Top] and 3D projections of the respective reconstructed dynamics [Bottom] of 482.sphinx before [(a),(c)] and after [(b,d)] a kernel panic() halt.

To accomplish this, I plan to study whether the methods described in this thesis can signal regime shifts in a time series. Fuzzy witness complexes may be a useful strategy in this vein of research by detecting and characterizing bifurcations [11]. Suppose that, for example, the first part of the data set corresponds trivially to an equilibrium—that is, to a set with $\beta_k = 0$ for all k > 0—but that this equilibrium undergoes a bifurcation to an oscillatory regime midway through the data set. In this case, a shift in β_1 signals a regime change.

Not all regime shifts are the result of a bifurcation, however. In cases like that, a change in information mechanics, *e.g.*, information storage (A_{τ}) or information production (WPE), could signal a regime shift—even if the topology of the new regime was too similar (or identical) to the old regime. My WPE vs. 1-MASE results could be particularly powerful in this scenario, as their values could not only help with regime-shift detection, but also suggest what kind of model might work well in each new regime. Similarly, changes in information storage could also be quite useful. A change in \mathcal{A}_{τ} suggests a regime shift has occurred and simultaneously suggests a forecast-optimal parameter set for the new regime. Even more importantly, it indicates whether new parameter values are even necessary in the new regime!

Of particular interest in this new frontier of research will be the class of so-called hybrid systems [47], which exhibit discrete transitions between different continuous regimes—e.g., a lathe that has an intermittent instability or traffic at an internet router, whose characteristic normal traffic patterns shift radically during an attack. Traded financial markets, too, are highly susceptible to jump processes. Effective modeling and prediction of these kinds of systems is quite difficult; doing so adaptively and automatically is an important and interesting challenge.

The elements of this thesis could be combined to form a complete nonstationary forecasting framework that could address that challenge. The method would work as follows: use \mathcal{A}_{τ} to select forecast-optimal parameters and start forecasting using **ro-LMA**. While forecasting on a small buffer of new data, monitor information production (WPE), information propagation and storage (\mathcal{A}_{τ}) and the homology (witness complex). If any of these drastically change, a regime shift has occurred and the model should be rebuilt. Nicely, as \mathcal{A}_{τ} and WPE are already being monitored on the new data buffer, the new regime is already modeled and forecasting can begin immediately.

This thesis bridged the gap between rigorous nonlinear mathematical models—which are ineffective in real-time—and naïve methods that are agile enough for adaptive modeling of nonstationary processes. This in and of itself has real practical utility for a wide spectrum of forecasting tasks as a simple, agile, noise-resilient, forecasting strategy for nonlinear systems, but this thesis went far beyond practical optimizations at the sacrifice of theoretical rigor. Specifically, the theoretical analysis outlined here offered a deeper understanding of delay-coordinate embedding—an understanding that suggests (and justifies) the need for a new paradigm in delay-reconstruction theory that was the overall goal of this research project.

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