

# MODERN KOOPMAN THEORY FOR DYNAMICAL SYSTEMS\*

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**Abstract.** The field of dynamical systems is being transformed by the mathematical tools and algorithms emerging from modern computing and data science. First-principles derivations and asymptotic reductions are giving way to data-driven approaches that formulate models in operator theoretic or probabilistic frameworks. Koopman spectral theory has emerged as a dominant perspective over the past decade, in which nonlinear dynamics are represented in terms of an infinite-dimensional linear operator acting on the space of all possible measurement functions of the system. This linear representation of nonlinear dynamics has tremendous potential to enable the prediction, estimation, and control of nonlinear systems with standard textbook methods developed for linear systems. However, obtaining finite-dimensional coordinate systems and embeddings in which the dynamics appear approximately linear remains a central open challenge. The success of Koopman analysis is due primarily to three key factors: 1) there exists rigorous theory connecting it to classical geometric approaches for dynamical systems, 2) the approach is formulated in terms of measurements, making it ideal for leveraging big-data and machine learning techniques, and 3) simple, yet powerful numerical algorithms, such as the dynamic mode decomposition (DMD), have been developed and extended to reduce Koopman theory to practice in real-world applications. In this review, we provide an overview of modern Koopman operator theory, describing recent theoretical and algorithmic developments and highlighting these methods with a diverse range of applications. We also discuss key advances and challenges in the rapidly growing field of machine learning that are likely to drive future developments and significantly transform the theoretical landscape of dynamical systems.

**Key words.** Dynamical systems, Koopman operator, Data-driven discovery, Control theory, Spectral theory, Operator theory, Dynamic mode decomposition, Embeddings.

**AMS subject classifications.** 34A34, 37A30, 37C10, 37M10, 37M99, 37N35, 47A35, 47B33

**1. Introduction.** Nonlinearity is a central challenge in dynamical systems, resulting in diverse phenomena, from bifurcations to chaos, that manifest across a range of disciplines. However, there is currently no overarching mathematical framework for the explicit and general characterization of nonlinear systems. In contrast, linear systems are completely characterized by their spectral decomposition (i.e., eigenvalues and eigenvectors), leading to generic and computationally efficient algorithms for prediction, estimation, and control. Importantly, *linear superposition* fails for nonlinear dynamical systems, leading to a variety of interesting phenomenon including frequency shifts and the generation of harmonics. The Koopman operator theory of dynamical systems provides a promising alternative perspective, where it may be possible to enable linear superposition even for strongly nonlinear dynamics via the infinite-dimensional, but linear, Koopman operator. The Koopman operator is linear, advancing measurement functions of the system, and its spectral decomposition completely characterizes the behavior of the nonlinear system. Finding tractable *finite-dimensional* representations of the Koopman operator is closely related to finding effective coordinate transformations in which the nonlinear dynamics appear linear. Koopman analysis has recently gained renewed interest

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est [234, 231, 284, 57, 55, 232, 180], in large part because of its strong connections to data-driven modeling. In this review, we provide an overview of modern Koopman theory for dynamical systems, including an in-depth analysis of leading computational algorithms, such as the dynamic mode decomposition (DMD).

Koopman introduced his operator theoretic perspective of dynamical systems in 1931 to describe the evolution of measurements of Hamiltonian systems [170], and this theory was generalized by Koopman and von Neumann to systems with a continuous eigenvalue spectrum in 1932 [171]. Koopman's 1931 paper was central to the celebrated proofs of the ergodic theorem by von Neumann [248] and Birkhoff [28, 29]. The history of these developments is fraught with intrigue, as discussed by Moore [239]. In his original paper [170], Koopman drew connections between the Koopman eigenvalue spectrum and conserved quantities, integrability, and ergodicity. For Hamiltonian flows, the Koopman operator is unitary. It is no surprise then that DMD, the leading numerical algorithm for approximating the Koopman operator, is built on the discrete Fourier transform (DFT) and the singular value decomposition (SVD), which both provide unitary coordinate transformations [49].

The operator theoretic framework discussed here complements the traditional geometric and probabilistic perspectives on dynamical systems. For example, level sets of Koopman eigenfunctions form invariant partitions of the state-space of a dynamical system [55]; in particular, eigenfunctions of the Koopman operator may be used to analyze the ergodic partition [235, 54]. Koopman analysis has also been shown to generalize the Hartman–Grobman theorem to the entire basin of attraction of a stable or unstable equilibrium point or periodic orbit [185]. The Koopman operator is also known as the composition operator, which is formally the pull-back operator on the space of scalar observable functions [5], and it is the dual, or left-adjoint, of the Perron–Frobenius (PF) operator, or transfer operator, which is the push-forward operator on the space of probability density functions. When a polynomial basis is chosen to represent the Koopman operator, then it is closely related to Carleman linearization [63, 64, 65], which has been used extensively in nonlinear control [311, 177, 22, 328].

**1.1. An overview of Koopman theory.** In this review, we will consider dynamical systems of the form

$$(1.1) \quad \frac{d}{dt} \mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t)),$$

where  $\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^n$  is the state of the system and  $\mathbf{f}$  is a vector field describing the dynamics. In general, the dynamics may also depend on time  $t$ , parameters  $\beta$ , and external actuation or control  $\mathbf{u}(t)$ . Although we omit these here for simplicity, they will be considered in later sections.

A major goal of modern dynamical systems is to find a new vector of coordinates  $\mathbf{z}$  such that either

$$(1.2) \quad \mathbf{x} = \varphi(\mathbf{z}) \quad \text{or} \quad \mathbf{z} = \varphi(\mathbf{x})$$

where the dynamics are simplified, or ideally, linearized:

$$(1.3) \quad \frac{d}{dt} \mathbf{z} = \mathbf{L}\mathbf{z}.$$

While in geometric dynamics, one asks for homeomorphic (continuously invertible) or even diffeomorphic coordinate maps, which trivialize the choice between the two

options in (1.2), there is little hope for global coordinate maps of this sort. Rather, we contend with embeddings  $\varphi$  that lift the dynamics into a higher-dimensional space of  $\mathbf{z}$  variables, allowing for “unfolding” of nonlinearities.

In practice, we typically have access to *measurement data* of our system, discretely sampled in time. This data is governed by the discrete-time dynamical system

$$(1.4) \quad \mathbf{x}_{k+1} = \mathbf{F}(\mathbf{x}_k),$$

where  $\mathbf{x}_k = \mathbf{x}(t_k) = \mathbf{x}(k\Delta t)$ . Also known as a *flow map*, the discrete-time dynamics are more general than the continuous-time formulation in (1.1), encompassing discontinuous and hybrid systems as well. In this case, the goal is still to find a linearizing coordinate transform so that  $\mathbf{y}_{k+1} = \mathbf{K}\mathbf{y}_k$ . These coordinates are given by eigenfunctions of the discrete-time Koopman operator,  $\mathcal{K}$ , which advances a measurement function  $g(\mathbf{x})$  of the state forward in time through the dynamics:

$$(1.5) \quad \mathcal{K}g(\mathbf{x}_k) := g(\mathbf{F}(\mathbf{x}_k)) = g(\mathbf{x}_{k+1}).$$

For an eigenfunction  $\varphi$  of  $\mathcal{K}$ , corresponding to an eigenvalue  $\lambda$ , this becomes

$$(1.6) \quad \mathcal{K}\varphi(\mathbf{x}_k) = \lambda\varphi(\mathbf{x}_k) = \varphi(\mathbf{x}_{k+1}).$$

Thus, a tremendous amount of effort has gone into characterizing the Koopman operator and approximating its spectral decomposition from measurement data.

The coordinates  $\varphi$  and the linear operator  $\mathbf{L}$  are closely related to the continuous-time generator  $\mathcal{L}$  of the Koopman operator  $\mathcal{K}$ . In particular, eigenfunctions  $\varphi_j$  of  $\mathcal{L}$  provide such a linearizing coordinate system, and the operator  $\mathbf{L}$  is obtained by restricting the operator  $\mathcal{L}$  to the span of these functions. Spectral theory provides a complete description of the dynamics in terms of the eigenstructure of the linear operator  $\mathbf{L}$ . Thus, transforming the system into coordinates where the dynamics are linear dramatically simplifies all downstream analysis and control efforts.

**1.2. An illustrative example: The Duffing oscillator.** Although the objective of Koopman theory is easily expressed mathematically, it is helpful to explore its application on a simple dynamical system. Consider the nonlinear Duffing system  $\ddot{x} = x - x^3$  with state space representation

$$(1.7a) \quad \dot{x}_1 = x_2$$

$$(1.7b) \quad \dot{x}_2 = x_1 - x_1^3,$$

and the corresponding phase portrait in Figure 1.1. This example has three fixed points, a saddle at the origin with Jacobian eigenvalues  $\lambda_{\pm} = \pm 1$  and two centers at  $(x_1, x_2) = (\pm 1, 0)$  with eigenvalues  $\pm\sqrt{2}i$ . These results, shown in Figure 1.1(a), can be obtained by a local phase-plane analysis [36], and these local linearizations are valid in a small neighborhood of each fixed point, illustrated by the shaded regions.

There is no homeomorphic coordinate transformation that captures the global dynamics of this system with a linear operator, since any such linear operator  $\mathbf{L}$  has either one fixed point at the origin, or a subspace of infinitely many fixed points [48], but never three isolated fixed points. Instead, the Koopman operator can provide a system of coordinate transformations that extend the local neighborhoods where a linear model is valid to the full basin around them [185], as shown in Figure 1.1(b).

This interpretation may lead to seemingly unintuitive results, as even the most obvious observables, such as  $g(\mathbf{x}) = \mathbf{x}$ , may require different expansions in different

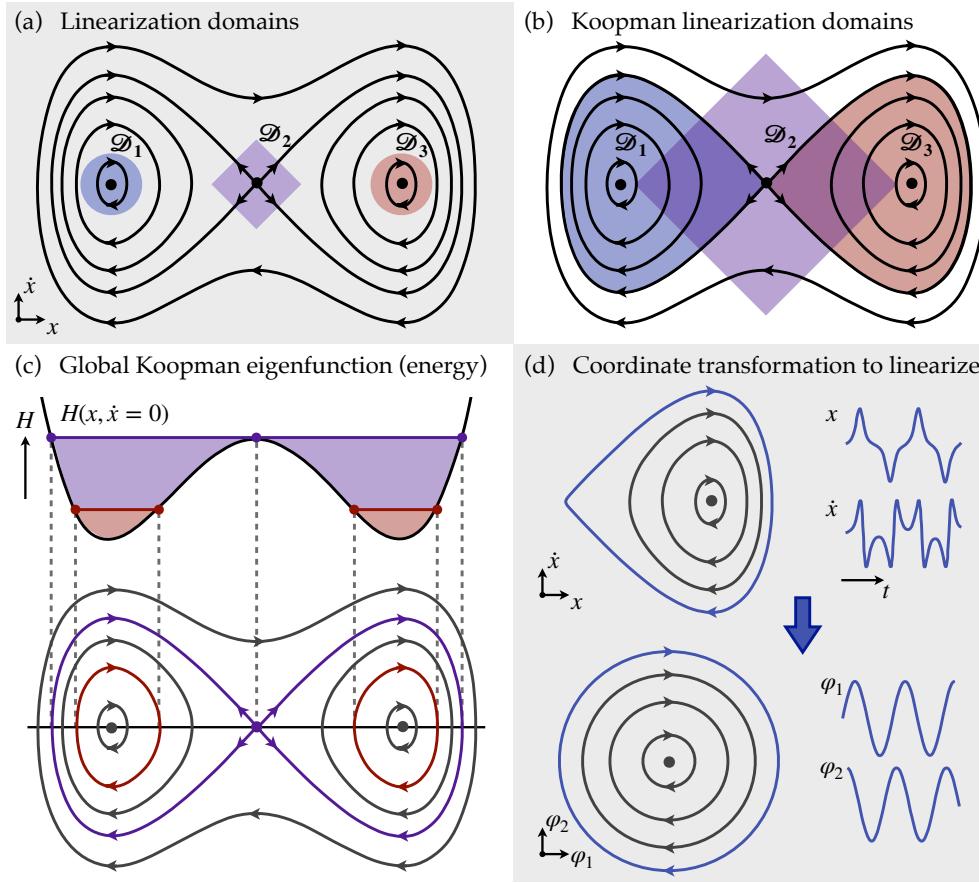


Fig. 1.1: Different Koopman perspectives for the Duffing oscillator,  $\ddot{x} = x - x^3$ , the equation for a particle in a double potential well. (a) Traditional linearization near the fixed points gives small regions where the system is approximately linear. (b) Koopman theory may extend the Hartman–Grobman theorem to enlarge the domain of linearity until the next fixed point [185]. (c) There are also global Koopman eigenfunctions, like the Hamiltonian energy, although these lose information about which basin the solution is in. (d) Yet a third perspective seeks a coordinate transformation to rescale space and time until dynamics live on a hypertoroid.

areas of the state space, as recently explored by Page and Kerswell [259]. Indeed, systems that possess multiple simple invariant solutions cannot be represented by a Koopman expansion that is globally uniformly convergent, implying that any choice of a representation of the Koopman operator  $\mathcal{K}$  in a system of coordinates may not hold everywhere, for any given observable of interest.

Even if there are no globally convergent linear Koopman representations, the Koopman eigenfunctions maybe be globally well defined, and even regular in the entire phase space. For example, the Hamiltonian energy function  $H = x_2^2 - x_1^2/2 + x_1^4/4$  is a Koopman eigenfunction for this conservative system, with eigenvalue  $\lambda = 0$ , as shown in Figure 1.1(c). In a sense, this global eigenfunction exploits symmetry in the dynamics to represent a global dynamic quantity, valid in all regions of phase space. This example establishes a connection between the Koopman operator and Noether’s theorem [251], as a symmetry in the dynamics gives rise to a new Koopman

eigenfunction with eigenvalue  $\lambda = 0$ . In addition, the constant function  $\varphi \equiv 1$  is a trivial eigenfunction corresponding to  $\lambda = 0$  for every dynamical system.

A final interpretation of Koopman theory is shown in [Figure 1.1\(d\)](#), related to [Figure 1.1\(b\)](#). In this case, we see that the Koopman operator establishes a change of coordinates, in space and time, in which the original nonlinear trajectories become linear. When obtaining these approximate coordinate systems from data, only approximately periodic dynamics will persist for long times. Rescaling space and time to make dynamics approximately periodic is the approach taken in [\[202, 186\]](#).

**1.3. Dynamics in the big data era.** The recent interest in Koopman operator theory is inherently linked to a growing wealth of data. Measurement technologies across every discipline of the engineering, biological, and physical sciences have revolutionized our ability to interrogate and extract quantities of interest from complex systems in real time with rich multi-modal and multi-fidelity time-series data. From broadband sensors that measure at exceptionally high sampling rates to high-resolution imaging, the front lines of modern science are being transformed by unprecedented quality and quantities of data. These advances are based on three foundational technologies: (i) improved sensors capable of measurement with higher quality and quantity, (ii) improved hardware for high-performance computing, data storage, and transfer, and (iii) improved algorithms for processing the data. Taken together, these advances form the underpinnings of the *big data* era and are driving the fourth paradigm of scientific discovery [\[135\]](#), whereby the data itself drives discovery.

Data science is now a targeted growth area across almost all academic disciplines. However, it has been almost six decades since John Tukey, co-developer of the *fast Fourier transform* with James Cooley, first advocated for data science as its own discipline [\[342, 89\]](#). Not surprisingly, the 1960s also coincided with pioneering developments of Gene Golub and co-workers on numerical algorithms for computing the *singular value decomposition* of a matrix [\[312\]](#), enabling one of the earliest data science exploration tools: *principal component analysis* (PCA). Thus the mathematical foundations for the *big data* era have been long in development. Indeed, its maturity is reflected in the emergence of the two cultures [\[37\]](#) of *statistical learning* and *machine learning*. In the former, the primary focus is on the development of interpretable models of data, while in the latter, accuracy is of paramount importance. Although accuracy and interpretability are not mutually exclusive, often the refinement of one comes at the expense of the other. For example, modern machine learning and artificial intelligence algorithms are revolutionizing computer vision and speech processing through deep neural network (DNN) architectures. DNNs have produced performance metrics in these fields far beyond any previous algorithms. Although individual components of DNNs may be interpretable, the integration across many layers with nonlinear activation functions typically render them opaque and uninterpretable. In contrast, sparsity promoting algorithms, such as the LASSO [\[336\]](#), are examples of statistical learning where interpretable variable selection is achieved. As will be highlighted throughout this review, Koopman theory is amenable to many of the diverse algorithms developed in both *statistical learning* and *machine learning*.

Dynamical systems theory has a long history of leveraging data for improving modeling insights, promoting parsimonious and interpretable models, and generating forecasting capabilities. In the 1960s, Kalman introduced a rigorous mathematical architecture [\[159, 160\]](#) whereby data and models could be combined through data assimilation techniques [\[102, 188\]](#), which is especially useful for forecasting and control. Thus the integration of streaming data and dynamical models has a nearly seven

decade history. In the modern era, it is increasingly common to build the dynamical models from the data directly. This is especially important in complex systems where first principles models are not available, or where it is not even known what the correct state-space variable should be. Biological systems, such as those that arise in neuronal recordings in the brain, are well suited for such data-driven model discovery techniques, as whole-brain imaging provides insight into how the microscale dynamics of individual neurons produces large scale patterns of spatio-temporal brain activity. Such systems are ideally suited for leveraging the modern data-driven modeling tools of machine learning to produce dynamical models characterizing the observed data.

**1.4. Koopman objectives and applications.** The ultimate promise of Koopman spectral theory is the ability analyze, predict, and control nonlinear systems with the wealth of powerful techniques from linear systems theory. This overarching goal may be broken into several specific goals:

*Diagnostics.* Spectral properties of the Koopman operator may be used effectively to characterize complex, high-dimensional dynamical systems. For example, in fluid mechanics, DMD is used to approximate the Koopman mode decomposition, resulting in an expansion of the flow as a linear combination of dominant coherent structures. Thus, Koopman mode decomposition can be used for dimensionality reduction and model reduction, generalizing the space-time separation of variables that is classically obtained via either Fourier transform or singular value decomposition [49].

*Prediction.* One of the major benefits of dynamical systems over other statistical models is that they provide a mechanistic understanding of how the future evolves, based on the current state of a system. Prediction is thus one of the central goals of any dynamical system framework. The prediction of a nonlinear system presents numerous challenges, such as sensitive dependence on initial conditions, parameter uncertainty, and bifurcations. Koopman operator theory provides insights into which observables are easier or harder to predict, and suggests robust numerical algorithms for such time-series prediction.

*Estimation and control.* In many systems, we not only seek to understand the dynamics, but also to modify, or *control*, their behavior for some engineering goal. In modern applications, it is rare to have complete measurements of a high-dimensional system, necessitating the *estimation* of these quantities from limited sensor measurements. By viewing the system through the linearizing lens of Koopman eigenfunctions, it is possible to leverage decades of results from linear estimation and control theory for the analysis of nonlinear systems. Indeed, linear systems are by far the most well studied and completely characterized class of dynamical systems for control.

*Uncertainty quantification and management.* Uncertainty is a hallmark feature of the real world, and dynamical systems provide us with a framework to forecast, quantify, and manage uncertainty. However, modeling uncertainty is challenging for strongly nonlinear and chaotic systems. Integrating uncertainty quantification into the Koopman operator framework is an important avenue of ongoing research.

*Understanding.* Beyond the practical goals value of prediction and control, dynamical systems provide a compelling framework with which to understand and model complex systems. Normal forms, for example, distill essential structural information about the dynamics, while remaining as simple as possible. For Koopman theory to be embraced, it will need to facilitate similar intuition and understanding.

Across a wide range of applications, researchers are developing and advancing Koopman operator theory to address these challenges. Some of these applications include fluid dynamics [294, 284, 232], epidemiology [277], neuroscience [45, 7], plasma

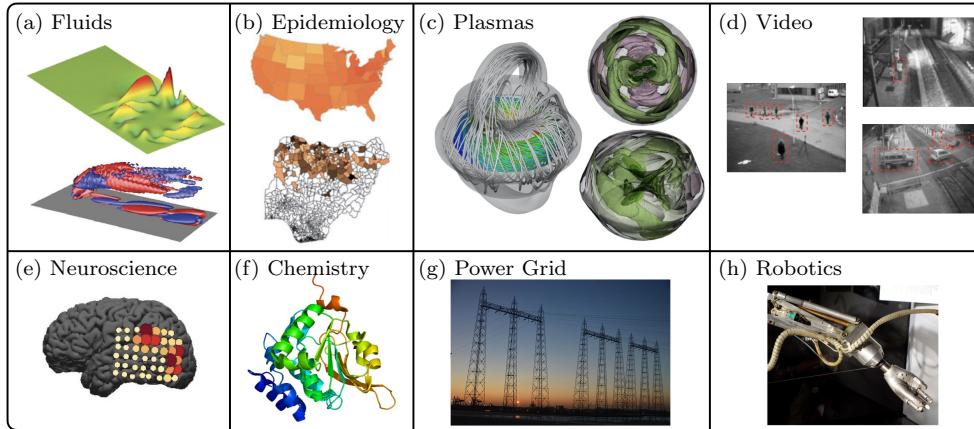


Fig. 1.2: Overview of applications of data-driven Koopman analysis via DMD. Figures reproduced with permission from: (a) top [294], bottom [284]; (b) [277]; (c) [162]; (d) [98]; (e) [45]; (f) from Emw [https://commons.wikimedia.org/wiki/File:Protein\\_PCMT1\\_PDB\\_1i1n.png](https://commons.wikimedia.org/wiki/File:Protein_PCMT1_PDB_1i1n.png); (g) from Henk Monster [https://commons.wikimedia.org/wiki/File:Power\\_grid\\_masts\\_besides\\_the\\_new\\_Waalbridge\\_Nijmegen\\_-\\_panoramio.jpg](https://commons.wikimedia.org/wiki/File:Power_grid_masts_besides_the_new_Waalbridge_Nijmegen_-_panoramio.jpg); (h) from Daderot [https://commons.wikimedia.org/wiki/File:Minsky\\_s\\_robot\\_arm,\\_late\\_1960s,\\_view\\_2\\_-\\_MIT\\_Museum\\_-\\_DSC03759.JPG](https://commons.wikimedia.org/wiki/File:Minsky_s_robot_arm,_late_1960s,_view_2_-_MIT_Museum_-_DSC03759.JPG).

physics [335, 162], finance [213], robotics [27, 4, 44, 43], and the power grid [325, 320]; a number of these are shown in Figure 1.2 and will be explored more in section 3.

**1.5. Organization and goals of review.** A primary goal of this review is to make modern Koopman operator theory accessible to researchers in many diverse fields. We seek to provide the reader with a big-picture overview of the state of the art, expediting the process of getting up to speed in this rapidly developing field. Further, we explore the dual theoretical and applied perspectives for understanding Koopman operator theory. To this end, each section will be approached from the perspective of providing a unified overview of major theoretical, methodological, numerical, and applied developments. Furthermore, we have compiled a number of striking success stories along with several outstanding challenges to help guide readers wishing to enter this field. Finally, it is our goal to highlight connections with existing and emerging methods from other fields, including geometric and probabilistic dynamical systems, computational science and engineering, and machine learning.

This review begins with relatively standard material and builds up to advanced concepts. Section 2 provides a practical introduction Koopman operator theory, including simple examples, the Koopman mode decomposition, and spectral theory. Similarly, section 3 provides an overview of dynamic mode decomposition, which is the most simple and widely used numerical algorithm to approximate the Koopman operator. Section 4 then introduces many of the most important concepts in *modern* Koopman theory. Advanced numerical and data-driven algorithms for representing the Koopman operator are presented in section 5. Thus, section 4 and section 5 provide advanced material extending section 2 and section 3, respectively. Section 6 investigates how Koopman theory is currently extended for advanced estimation and control. Section 7 provides a discussion and concluding remarks. This section also describes several ongoing challenges in the community, along with recent extensions and motivating applications. The goal here is to provide researchers with a quick sketch of the state of the art, so that they may quickly get to the frontier of research.

## 2. A practical introduction to the Koopman operator framework.

**2.1. Definitions and vocabulary.** The Koopman operator advances measurement functions of the state of a dynamical system with the flow of the dynamics. To explain the basic properties of the Koopman operator, we begin with an autonomous ordinary differential equation (1.1) on a finite-dimensional state space  $\mathcal{X} \subseteq \mathbb{R}^n$ . The flow map operator, or time- $t$  map,  $\mathbf{F}^t: \mathcal{X} \rightarrow \mathcal{X}$  advances initial conditions  $\mathbf{x}(0)$  forward along the trajectory by a time  $t$ , so that trajectories evolve according to

$$(2.1) \quad \mathbf{x}(t) = \mathbf{F}^t(\mathbf{x}(0)).$$

The family of Koopman operators  $\mathcal{K}^t: \mathcal{G}(\mathcal{X}) \rightarrow \mathcal{G}(\mathcal{X})$ , parameterized by  $t$ , are given by

$$(2.2) \quad \mathcal{K}^t g(\mathbf{x}) = g(\mathbf{F}^t(\mathbf{x})),$$

where  $\mathcal{G}(\mathcal{X})$  is a set of *measurement functions*  $g: \mathcal{X} \rightarrow \mathbb{C}$ . Another name for  $g$ , derived from this framework's origin in quantum mechanics, is an *observable* function, although this should not be confused with the unrelated *observability* from control theory. We can interpret (2.2) as defining a family of functions

$$(2.3) \quad g_t := \mathcal{K}^t g, \quad g_0 := g$$

that corresponds to the trajectory  $t \mapsto g_t$  in the set  $\mathcal{G}(\mathcal{X})$  of measurement functions.

In most applications, the set of functions  $\mathcal{G}(\mathcal{X})$  is not defined *a priori*, but is loosely specified by a set of properties it should satisfy, e.g., that it is a vector space, that it possesses an inner product, that it is complete, or that it contains certain functions of interest, such as continuous functions on  $\mathcal{X}$ . Hilbert spaces, such as  $L^2(\mathcal{X}, d\mu)$  or reproducing kernel Hilbert spaces (RKHS), are a common choice in modern applied mathematics, although historically other Banach spaces, such as integrable functions  $L^1$  or continuous functions  $C(\mathcal{X})$  have also been used. The choice of the space, whether explicit or implicit, can have consequences on the properties of the operator and its approximations. In all cases, however,  $\mathcal{G}(\mathcal{X})$  is of significantly higher dimension than  $\mathcal{X}$ , i.e., countably or uncountably infinite.

The most significant property of the Koopman operator is that it is linear when  $\mathcal{G}(\mathcal{X})$  is a linear (vector) space of functions:

$$(2.4) \quad \begin{aligned} \mathcal{K}^t (\alpha_1 g_1(\mathbf{x}) + \alpha_2 g_2(\mathbf{x})) &= \alpha_1 g_1(\mathbf{F}^t(\mathbf{x})) + \alpha_2 g_2(\mathbf{F}^t(\mathbf{x})) \\ &= \alpha_1 \mathcal{K}^t g_1(\mathbf{x}) + \alpha_2 \mathcal{K}^t g_2(\mathbf{x}). \end{aligned}$$

This property holds regardless of whether  $\mathbf{F}^t: \mathcal{X} \rightarrow \mathcal{X}$  is linear itself, as it is simply a consequence of definition (2.2), since the argument function  $g$  is on the “outside” of the composition, allowing linearity to carry over from the vector space of observables. In this sense, the Koopman framework obtains linearity of  $\mathcal{K}^t$  despite the nonlinearity of  $\mathbf{F}^t$  by trading the finite-dimensional state space  $\mathcal{X}$  for an infinite-dimensional function space  $\mathcal{G}(\mathcal{X})$ .

When time  $t$  is discrete,  $t \in \mathbb{N}$ , and the dynamics are autonomous, then  $\mathbf{F}^t$  is a repeated  $t$ -fold composition of  $\mathbf{F} \equiv \mathbf{F}^1$  given by  $\mathbf{F}^t(\mathbf{x}) = \mathbf{F}(\mathbf{F}(\cdots(\mathbf{F}(\mathbf{x}))))$ , so that  $\mathcal{K}^t g$  is likewise generated by repeated application of  $\mathcal{K} \equiv \mathcal{K}^1$ . The generator  $\mathcal{K}$  of the composition semigroup is then called *the* Koopman operator, which results in a dynamical system

$$(2.5) \quad g_{k+1} = \mathcal{K} g_k,$$

analogous to  $\mathbf{x}_{k+1} = \mathbf{F}(\mathbf{x}_k)$ , except that (2.5) is linear and infinite-dimensional.

When time  $t$  is continuous, the flow map family satisfies the *semigroup* property

$$(2.6) \quad \mathbf{F}^{t+s}(\mathbf{x}) = \mathbf{F}^t(\mathbf{F}^s(\mathbf{x})), \forall \mathbf{x}, t, s \geq 0,$$

which can be strengthened to a group property  $t, s \in \mathbb{R}$  if the flow map is invertible. The Koopman operator family  $\mathcal{K}^t$  inherits these properties as well. Given a continuous and sufficiently smooth dynamics, it is also possible to define the continuous-time infinitesimal generator of the Koopman operator family as

$$(2.7) \quad \mathcal{L}g := \lim_{t \rightarrow 0} \frac{\mathcal{K}_t g - g}{t} = \lim_{t \rightarrow 0} \frac{g \circ \mathbf{F}^t - g}{t}.$$

As our goal here is to provide an introduction, we omit the mathematical scaffolding that accompanies a careful definition of an operator derivative; all details in the context of Koopman operator theory are available in [187, §7.5].

The generator  $\mathcal{L}$  has been called the Lie operator [170], as it is the Lie derivative of  $g$  along the vector field  $\mathbf{f}(\mathbf{x})$  when the dynamics is given by (1.1) [5, 70]. This follows from applying the chain rule to the time derivative of  $g(\mathbf{x})$ :

$$(2.8) \quad \frac{d}{dt}g(\mathbf{x}(t)) = \nabla g \cdot \dot{\mathbf{x}}(t) = \nabla g \cdot \mathbf{f}(\mathbf{x}(t))$$

and equating with

$$(2.9) \quad \frac{d}{dt}g(\mathbf{x}(t)) = \lim_{\tau \rightarrow 0} \frac{g(\mathbf{x}(t + \tau)) - g(\mathbf{x}(t))}{\tau} = \mathcal{L}(g(\mathbf{x}(t))),$$

resulting in

$$(2.10) \quad \mathcal{L}g = \nabla g \cdot \mathbf{f}.$$

The adjoint of the Lie operator is called the Liouville operator, especially in Hamiltonian dynamics [115, 116], while the adjoint of the Koopman operator is the Perron–Frobenius operator [87, 84, 106, 107]. In many ways, the operator-theoretic framework for applied dynamical systems has two dual perspectives, corresponding either to the Koopman operator or the Perron–Frobenius operator. In subsection 4.3 we discuss these parallels in more detail.

Similar to (2.5),  $\mathcal{L}$  induces a linear dynamical system in continuous-time:

$$(2.11) \quad \frac{d}{dt}g = \mathcal{L}g.$$

The linear dynamical systems in (2.5) and (2.11) are analogous to the dynamical systems in (1.1) and (1.4), respectively.

An important special case of an observable function is the projection onto a component of the state  $g(\mathbf{x}) = x_i$  or, with a slight abuse of notation,  $g(\mathbf{x}) = \mathbf{x}$ . In this case, the left-hand side of (2.11) is plainly  $\dot{\mathbf{x}}$ , but the right hand side  $\mathcal{L}\mathbf{x}$  may not be simple to represent in a chosen basis for the space  $\mathcal{G}(\mathcal{X})$ . It is typical in real problems that representing  $\mathcal{L}\mathbf{x}$  will involve an infinite number of terms. For certain special structures, this may not be the case, as will be demonstrated in subsection 2.4.

In summary, the Koopman operator is linear, which is appealing, but is infinite dimensional, posing issues for representation and computation. Instead of capturing the evolution of all measurement functions in a function space, applied Koopman

analysis attempts to identify key measurement functions that evolve linearly with the flow of the dynamics. Eigenfunctions of the Koopman operator provide just such a set of special measurements that behave linearly in time. In fact, a primary motivation to adopt the Koopman framework is the ability to simplify the dynamics through the eigendecomposition of the operator.

**2.2. Eigenfunctions and the spectrum of eigenvalues.** A Koopman eigenfunction  $\varphi(\mathbf{x})$  corresponding to an eigenvalue  $\lambda$  satisfies

$$(2.12) \quad \varphi(\mathbf{x}_{k+1}) = \mathcal{K}\varphi(\mathbf{x}_k) = \lambda\varphi(\mathbf{x}_k).$$

In continuous-time, a Lie operator eigenfunction  $\varphi(\mathbf{x})$  satisfies

$$(2.13) \quad \frac{d}{dt}\varphi(\mathbf{x}) = \mathcal{L}\varphi(\mathbf{x}) = \mu\varphi(\mathbf{x}),$$

where  $\mu$  is a continuous-time eigenvalue. In general, eigenvalues and eigenvectors are complex-valued scalars and functions, respectively, even when the state space  $\mathcal{X}$  and dynamics  $\mathbf{F}(\mathbf{x})$  are real-valued.

It is simple to show that Koopman eigenfunctions  $\varphi(\mathbf{x})$  that satisfy (2.12) for  $\lambda \neq 0$  are also eigenfunctions of the Lie operator, although with a different eigenvalue. Applying the Lie operator (2.7) to such a  $\varphi$  leads to

$$(2.14) \quad \mathcal{K}^t\varphi = \lambda^t\varphi \implies \mathcal{L}\varphi = \lim_{t \rightarrow 0} \frac{\mathcal{K}^t\varphi - \varphi}{t} = \lim_{t \rightarrow 0} \frac{\lambda^t - 1}{t}\varphi = \log(\lambda)\varphi.$$

Conversely, the induced dynamics (2.11) applied to an eigenfunction of  $\mathcal{L}$  leads to

$$(2.15) \quad \mathcal{L}\varphi = \mu\varphi \implies \frac{d}{dt}\varphi = \mathcal{L}\varphi = \mu\varphi.$$

An eigenfunction  $\varphi$  of  $\mathcal{L}$  with eigenvalue  $\mu$  is then an eigenfunction of  $\mathcal{K}^t$  with eigenvalue  $\lambda^t = \exp(\mu t)$ . Thus, we will typically not make a distinction between Lie and Koopman eigenfunctions in the context of autonomous dynamical systems.

Eigenfunctions of  $\mathcal{K}, \mathcal{L}$  that are induced by already-linear dynamics further illustrate the connection between linear discrete dynamics  $\mathbf{x}_{n+1} = \mathbf{A}\mathbf{x}_n$  with analogous concepts for  $g_{n+1} = \mathcal{K}g_n$ . Given a left-eigenvector  $\boldsymbol{\xi}^\top \mathbf{A} = \lambda \boldsymbol{\xi}^\top$ , we form a corresponding Koopman eigenfunction as

$$(2.16) \quad \varphi(\mathbf{x}) := \boldsymbol{\xi}^\top \mathbf{x}$$

since

$$(2.17) \quad \mathcal{K}\varphi(\mathbf{x}) = \varphi(\mathbf{A}\mathbf{x}) = \boldsymbol{\xi}^\top \mathbf{A}\mathbf{x} = \lambda \boldsymbol{\xi}^\top \mathbf{x} = \lambda\varphi(\mathbf{x}).$$

In other words, while right-eigenvectors of  $\mathbf{A}$  give rise to time-invariant directions in the state space  $\mathcal{X}$ , the left-eigenvectors give rise to Koopman eigenfunctions, which are similarly time-invariant directions in the space of observables  $\mathcal{G}(\mathcal{X})$ .

In general systems, a set of Koopman eigenfunctions may be used to generate more eigenfunctions. In discrete time, we find that the product of two eigenfunctions  $\varphi_1(\mathbf{x})$  and  $\varphi_2(\mathbf{x})$  is also an eigenfunction:

$$(2.18) \quad \begin{aligned} \mathcal{K}(\varphi_1(\mathbf{x})\varphi_2(\mathbf{x})) &= \varphi_1(\mathbf{F}(\mathbf{x}))\varphi_2(\mathbf{F}(\mathbf{x})) \\ &= \lambda_1\lambda_2\varphi_1(\mathbf{x})\varphi_2(\mathbf{x}) \end{aligned}$$

with a new eigenvalue  $\lambda_1\lambda_2$  given by the product of the two eigenvalues of  $\varphi_1(\mathbf{x})$  and  $\varphi_2(\mathbf{x})$ . The corresponding relationship for  $\mathcal{L}$  can be found by applying (2.14),

$$(2.19) \quad \lambda_1\lambda_2 = e^{\mu_1}e^{\mu_2} = e^{\mu_1+\mu_2},$$

resulting in

$$(2.20) \quad \mathcal{L}(\varphi_1(\mathbf{x})\varphi_2(\mathbf{x})) = (\mu_1 + \mu_2)\varphi_1(\mathbf{x})\varphi_2(\mathbf{x}).$$

A simple consequence is that a complex conjugate pair of eigenfunctions of  $\mathcal{L}$ ,  $(\mu, \varphi)$ ,  $(\bar{\mu} \text{ and } \bar{\varphi})$ , additionally implies the existence of a real-valued eigenfunction  $|\varphi| = \sqrt{\varphi\bar{\varphi}}$  with an associated eigenvalue  $(\mu + \bar{\mu})/2 = \operatorname{Re} \mu$ , thus leading to a non-oscillatory growth/decay of the eigenvalue.

Algebraically, the set of Koopman eigenfunctions establishes a commutative monoid<sup>1</sup> under point-wise multiplication. Thus, depending on the dynamical system, there may be a finite set of *generator* eigenfunction elements that may be used to construct all other eigenfunctions. The corresponding Koopman eigenvalues form a multiplicative lattice, or an additive lattice for Lie eigenvalues due to (2.14).

Observables that can be formed as linear combinations of eigenfunctions, i.e.,  $g \in \operatorname{span}\{\varphi_k\}_{k=1}^K$  have a particularly simple evolution under the Koopman operator

$$(2.21) \quad g(\mathbf{x}) = \sum_k v_k \varphi_k \implies \mathcal{K}^t g(\mathbf{x}) = \sum_k v_k \lambda_k^t \varphi_k.$$

This implies that the subspace  $\operatorname{span}\{\varphi_k\}_{k=1}^K$  is invariant under the action of  $\mathcal{K}$ .

These simple relationships enable the analysis of the phase portrait of a dynamical system in terms of level sets, and they also enable the analysis of the evolution of general observables through the lens of their decomposition into eigenfunctions.

**2.2.1. Level sets of eigenfunctions.** Level sets of eigenfunctions can clarify the relationships between sets in the domain  $\mathcal{X}$ . In particular, (sub-)level sets associated with eigenfunctions map into each other. To see this, we write the eigenvalue and the eigenfunction in polar form

$$(2.22) \quad \varphi(\mathbf{x}) = R(\mathbf{x})e^{i\Theta(\mathbf{x})}$$

$$(2.23) \quad \lambda = re^{i\theta}$$

and define the associated sublevel sets to be

$$(2.24) \quad M_\varphi(C) := \{\mathbf{x} \in \mathcal{X}: R(\mathbf{x}) \leq C\},$$

$$(2.25) \quad A_\varphi(\alpha) := \{\mathbf{x} \in \mathcal{X}: \Theta(\mathbf{x}) \leq \alpha\}.$$

Given  $\mathbf{x} \in \mathcal{X}$ , we can evaluate the eigenfunction on its successor  $\mathbf{x}^+ = \mathbf{F}(\mathbf{x})$ , to find

$$(2.26) \quad \varphi(\mathbf{x}^+) = \mathcal{K}\varphi(\mathbf{x}) = \lambda\varphi(\mathbf{x}) = (rR(\mathbf{x}))e^{i(\theta+\Theta(\mathbf{x}))},$$

so that if  $\mathbf{x} \in M_\varphi(C)$  then  $\mathbf{x}^+ \in M_\varphi(rC)$  and if  $\mathbf{x} \in A_\varphi(\alpha)$  then  $\mathbf{x}^+ \in A_\varphi(\alpha + \theta)$ , or more succinctly

$$(2.27) \quad \mathbf{F}(M_\varphi(C)) = M_\varphi(rC), \quad \mathbf{F}(A_\varphi(\alpha)) = A_\varphi(\alpha + \theta).$$

---

<sup>1</sup>Monoids are groups without guaranteed inverses, or semigroups with an identity element.

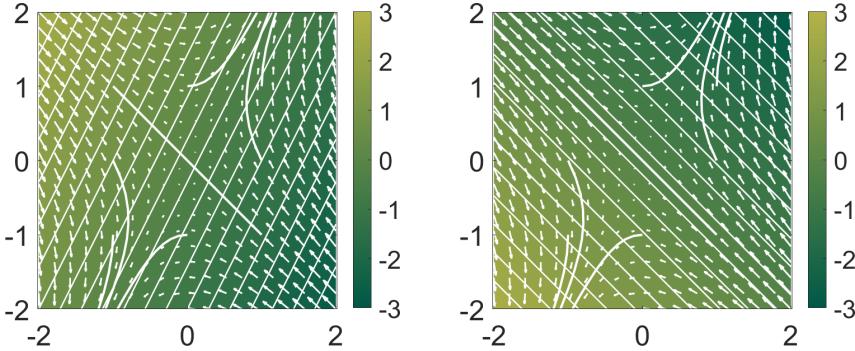


Fig. 2.1: Koopman eigenfunctions constructed as (2.16) for a linear matrix ODE  $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$  with a saddle-type fixed point at the origin. Velocity field and sample orbits are overlaid in white.

For the particular case of  $\lambda = 1$  these relationships simplify to

$$(2.28) \quad \mathbf{F}(M_\varphi(C)) = M_\varphi(C), \quad \mathbf{F}(A_\varphi(\alpha)) = A_\varphi(\alpha),$$

implying that level sets of invariant eigenfunctions are invariant sets.

When the eigenvalue is on the unit circle, with a phase  $\theta/2\pi = p/q \in \mathbb{Q}$ , then the level sets of phase satisfy

$$(2.29) \quad \mathbf{F}(A_\varphi(\alpha)) = A_\varphi\left(\alpha + \frac{2\pi p}{q}\right) \quad \mathbf{F}^q(A_\varphi(\alpha)) = A_\varphi(\alpha + 2\pi p) = A_\varphi(\alpha),$$

and, therefore, identify chains of  $q$ -periodic sets where the value of the phase indicates the order in which they are visited by a trajectory  $\mathbf{x}_k$ .

To illustrate these concepts, Figure 2.1 shows two eigenfunctions constructed from two left eigenvectors of a planar linear system  $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$  with saddle-type dynamics, as in (2.16). In contrast to right eigenvectors of  $\mathbf{A}$ , which act as invariant manifolds attracting/repelling the trajectories, Koopman eigenfunctions foliate the space into leaves (level sets), providing a time-ordering on the domain associated with each eigenvalue.

When system matrix  $\mathbf{A}$  has complex conjugate eigenvalues  $\lambda, \bar{\lambda}$ , the associated eigenfunctions  $\xi^\top \mathbf{x}$  and  $\bar{\xi}^\top \mathbf{x}$  are themselves complex conjugates. Visualizing the associated modulus  $R(\mathbf{x})$  and phase  $\Theta(\mathbf{x})$  (2.22) for planar dynamics with a focus equilibrium, as in Figure 2.2, demonstrates that the modulus acts as a Lyapunov function for the stable focus, as sub-level sets provide a time-ordering on the plane implying that trajectories converge to the origin. Indeed,  $|\xi^\top \mathbf{x}|$  is itself an eigenfunction of the Koopman operator  $\mathcal{K}^t$  associated with eigenvalues  $e^{t\Re\lambda}$ , therefore capturing the exponential envelope of oscillating trajectories. Level sets of  $|\xi^\top \mathbf{x}|$  are called *isostables* [225]. An analogous definition of an isostable for real-valued eigenvalues gives points that converge to the same trajectory in the stable/unstable manifold.

Level sets of the argument (angle) provide a cyclic foliation of the domain, acting as *isochrons* [225], i.e., collections of initial conditions that converge to the origin with a common phase. We will revisit the concepts of isochrons and isostables as tools for nonlinear reduction of order, in particular as a foundation for understanding the synchronization and control of oscillators, in subsection 4.1.

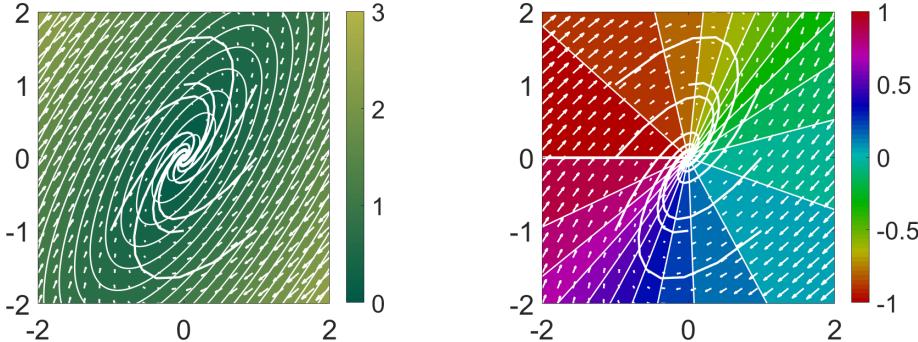


Fig. 2.2: Modulus  $R(\mathbf{x})$  and argument  $\Theta(\mathbf{x})$  of the Koopman eigenfunction constructed from a complex eigenvector of a linear matrix ODE  $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$  with a focus-type fixed point at the origin.

**2.2.2. Computing eigenfunctions.** There are several approaches to approximate Koopman eigenfunctions computationally. Given the evolution of an observable  $g(\mathbf{x}(t)) = g(\mathbf{F}^t(\mathbf{x}))$  it is possible to compute an eigenfunction associated with an eigenvalue  $e^{i\omega}$  by forming the following long-term *harmonic* or *Fourier average*

$$(2.30) \quad \tilde{g}_\omega(\mathbf{x}) := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T g(\mathbf{F}^t(\mathbf{x})) e^{-i\omega t} dt.$$

If  $\omega = 0$ , harmonic averages reduce to the trajectory (*ergodic*) average. When the space of observables  $\mathcal{G}(\mathcal{X})$  is taken as the  $L^1$  space of integrable functions with respect to a dynamically-preserved measure  $\mu$ , then pointwise convergence  $\mu$ -almost everywhere is guaranteed by the Birkhoff ergodic theorem [28].

More generally, Yosida's theorem [57] implies that in Banach spaces the limit not only exists, but that  $g \mapsto \tilde{g}_\omega$  is a projection onto the eigenspace associated with the eigenvalue  $e^{i\omega}$ . Said another way, eigenfunctions associated with eigenvalues on the unit circle  $|\lambda| = 1$  can be computationally approximated through (2.30), as employed in [234, 231, 55, 193]. Since such eigenvalues correspond to neutrally-stable steady-state behavior, they are of practical importance to analyze dynamics. This approach can, in principle, be extended to compute eigenfunctions associated with other eigenvalues as well, with conditions and restrictions given in [238]. Recently, [82] also provided an extension and reframing of such results to RKHS, including both theoretical and computational results.

Instead of the iteration (2.30) that requires simulating the evolution  $g_t$ , in certain cases it is possible to solve for eigenfunctions directly. The eigenfunction relation  $\mathcal{K}\varphi(\mathbf{x}) = \varphi(\mathbf{F}(\mathbf{x})) = \lambda\varphi(\mathbf{x})$  is a compositional algebraic equation that is challenging to solve directly. The relation (2.10) implies that the analogous relation for eigenfunctions of  $\mathcal{L}$  is the PDE

$$(2.31) \quad \nabla\varphi(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) = \lambda\varphi(\mathbf{x}).$$

With this PDE, it is possible to approximate eigenfunctions, either by solving for the Laurent series as in subsection 2.5 or with data via regression as in section 5. This formulation assumes that the dynamics are both continuous and differentiable.

**2.3. Koopman mode decomposition and finite representations.** Until now, we have considered scalar measurements of a system, and we explored special *eigen*-measurements (i.e., Koopman eigenfunctions) that evolve linearly in time. However, we often take multiple measurements of a system, which we will arrange in a vector  $\mathbf{g}$ :

$$(2.32) \quad \mathbf{g}(\mathbf{x}) = \begin{bmatrix} g_1(\mathbf{x}) \\ g_2(\mathbf{x}) \\ \vdots \\ g_p(\mathbf{x}) \end{bmatrix}.$$

Each of the individual measurements may be expanded in terms of a basis of eigenfunctions  $\varphi_j(\mathbf{x})$ :

$$(2.33) \quad g_i(\mathbf{x}) = \sum_{j=1}^{\infty} v_{ij} \varphi_j(\mathbf{x}).$$

Thus, the vector of observables,  $\mathbf{g}$ , may be similarly expanded:

$$(2.34) \quad \mathbf{g}(\mathbf{x}) = \begin{bmatrix} g_1(\mathbf{x}) \\ g_2(\mathbf{x}) \\ \vdots \\ g_p(\mathbf{x}) \end{bmatrix} = \sum_{j=1}^{\infty} \varphi_j(\mathbf{x}) \mathbf{v}_j,$$

where  $\mathbf{v}_j$  is the  $j$ -th *Koopman mode* associated with the eigenfunction  $\varphi_j$ .

For conservative dynamical systems, such as those governed by Hamiltonian dynamics, the Koopman operator is unitary on the space  $\mathcal{G}(\mathcal{X})$  of square-integrable functions with respect to the conserved measure. Thus, the Koopman eigenfunctions form an orthonormal basis for conservative systems, and it is possible to compute the Koopman modes  $\mathbf{v}_j$  directly by projection:

$$(2.35) \quad \mathbf{v}_j = \begin{bmatrix} \langle \varphi_j, g_1 \rangle \\ \langle \varphi_j, g_2 \rangle \\ \vdots \\ \langle \varphi_j, g_p \rangle \end{bmatrix},$$

where  $\langle \cdot, \cdot \rangle$  is the standard inner product of functions in  $\mathcal{G}(\mathcal{X})$ . These modes have a physical interpretation in the case of direct spatial measurements of a system,  $\mathbf{g}(\mathbf{x}) = \mathbf{x}$ , in which case the modes are coherent *spatial* modes that behave linearly with the same temporal dynamics (i.e., oscillations, possibly with linear growth or decay).

Given the decomposition in (2.34), it is possible to represent the dynamics of the measurements  $\mathbf{g}$  as follows:

$$(2.36a) \quad \mathbf{g}(\mathbf{x}(t)) = \mathcal{K}^t \mathbf{g}(\mathbf{x}_0) = \mathcal{K}^t \sum_{j=1}^{\infty} \varphi_j(\mathbf{x}_0) \mathbf{v}_j$$

$$(2.36b) \quad = \sum_{j=1}^{\infty} \mathcal{K}^t \varphi_j(\mathbf{x}_0) \mathbf{v}_j$$

$$(2.36c) \quad = \sum_{j=1}^{\infty} \lambda_j^t \varphi_j(\mathbf{x}_0) \mathbf{v}_j.$$

This sequence of triples  $\{(\lambda_j, \varphi_j, \mathbf{v}_j)\}_{j=1}^{\infty}$  is the *Koopman mode decomposition* and was introduced by Mezić in 2005 [231]. The Koopman mode decomposition was later connected to data-driven regression via the dynamic mode decomposition (DMD) [284], which is explored in [section 3](#), where the modes  $\mathbf{v}$  are called *dynamic modes*.

**2.3.1. Invariant eigenspaces and finite-dimensional models.** Instead of capturing the evolution of all measurement functions in a Hilbert space, applied Koopman analysis approximates the evolution on an invariant subspace spanned by a finite set of measurement functions. A *Koopman-invariant subspace* is defined as the span of a set of functions  $\{g_1, g_2, \dots, g_p\}$  if all functions  $g$  in this subspace

$$(2.37) \quad g = \alpha_1 g_1 + \alpha_2 g_2 + \dots + \alpha_p g_p$$

remain in this subspace after being acted on by the Koopman operator  $\mathcal{K}$ :

$$(2.38) \quad \mathcal{K}g = \beta_1 g_1 + \beta_2 g_2 + \dots + \beta_p g_p.$$

It is possible to obtain a finite-dimensional matrix representation of the Koopman operator by restricting it to an invariant subspace spanned by a finite number of functions  $\{g_j\}_{j=1}^p$ . The matrix representation  $\mathbf{K}$  acts on a vector space  $\mathbb{R}^p$ , with the coordinates given by the values of  $g_j(\mathbf{x})$ . This induces a finite-dimensional linear system.

Any finite set of eigenfunctions of the Koopman operator will span an invariant subspace. Discovering these eigenfunction coordinates is, therefore, a central challenge, as they provide intrinsic coordinates along which the dynamics behave linearly. In practice, it is more likely that we will identify an *approximately* invariant subspace, given by a set of functions  $\{g_j\}_{j=1}^p$ , where each of the functions  $g_j$  is well approximated by a finite sum of eigenfunctions:  $g_j \approx \sum_{k=1}^p v_{jk} \varphi_k$ .

**2.4. Example of a simple Koopman embedding.** Here, we consider an example system with a single fixed point from Tu et al. [341] that is explored in more detail in Brunton et al. [48], given by:

$$(2.39a) \quad \dot{x}_1 = \mu x_1$$

$$(2.39b) \quad \dot{x}_2 = \lambda(x_2 - x_1^2).$$

For  $\lambda < \mu < 0$ , the system exhibits a slow attracting manifold given by  $x_2 = x_1^2$ . It is possible to augment the state  $\mathbf{x}$  with the nonlinear measurement  $g = x_1^2$ , to define a three-dimensional Koopman invariant subspace. In these coordinates, the dynamics become linear:

$$(2.40a) \quad \frac{d}{dt} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} \mu & 0 & 0 \\ 0 & \lambda & -\lambda \\ 0 & 0 & 2\mu \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \quad \text{for} \quad \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_1^2 \end{bmatrix}.$$

The full three-dimensional Koopman observable vector space is visualized in [Figure 2.3](#). Trajectories that start on the invariant manifold  $y_3 = y_1^2$ , visualized by the blue surface, are constrained to stay on this manifold. There is a *slow* subspace, spanned by the eigenvectors corresponding to the slow eigenvalues  $\mu$  and  $2\mu$ ; this subspace is visualized by the green surface. Finally, there is the original asymptotically attracting manifold of the original system,  $y_2 = y_1^2$ , which is visualized as the red surface. The blue and red parabolic surfaces always intersect in a parabola that is

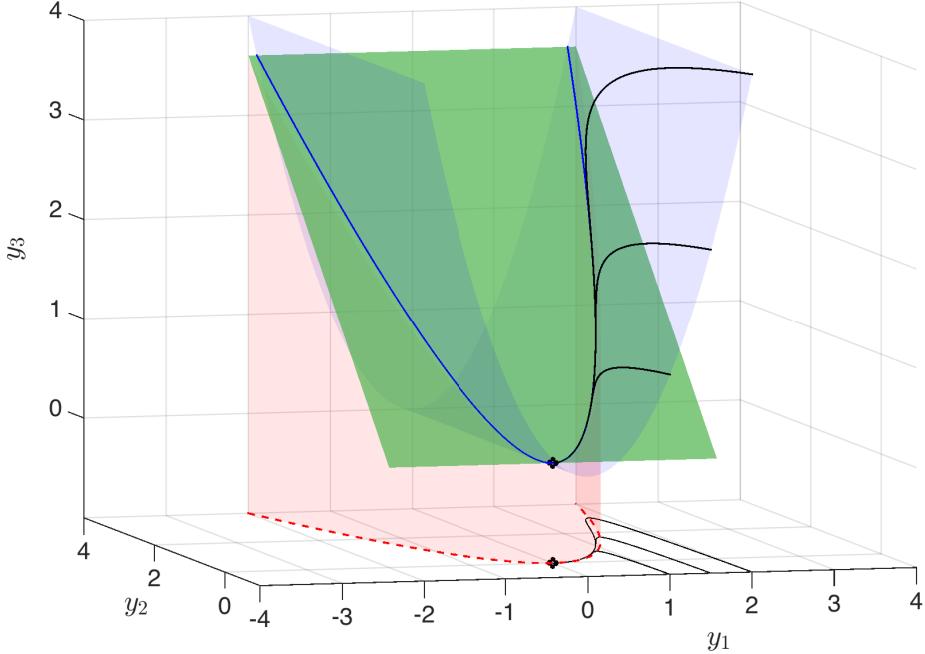


Fig. 2.3: Visualization of three-dimensional linear Koopman system from (2.40a) along with projection of dynamics onto the  $x_1$ - $x_2$  plane. The attracting slow manifold is shown in red, the constraint  $y_3 = y_1^2$  is shown in blue, and the slow unstable subspace of (2.40a) is shown in green. Black trajectories of the linear Koopman system in  $\mathbf{y}$  project onto trajectories of the full nonlinear system in  $\mathbf{x}$  in the  $y_1$ - $y_2$  plane. Here,  $\mu = -0.05$  and  $\lambda = 1$ . Reproduced from Brunton et al. [48].

inclined at a  $45^\circ$  angle in the  $y_2$ - $y_3$  direction. The green surface approaches this  $45^\circ$  inclination as the ratio of fast to slow dynamics become increasingly large. In the full three-dimensional Koopman observable space, the dynamics produce a single stable node, with trajectories rapidly attracting onto the green subspace and then slowly approaching the fixed point.

The left eigenvectors of the Koopman operator yield Koopman eigenfunctions. The Koopman eigenfunctions of (2.40a) corresponding to eigenvalues  $\mu$  and  $\lambda$  are:

$$(2.41) \quad \varphi_\mu = x_1, \quad \text{and} \quad \varphi_\lambda = x_2 - bx_1^2 \quad \text{with} \quad b = \frac{\lambda}{\lambda - 2\mu}.$$

The constant  $b$  in  $\varphi_\lambda$  captures the fact that for a finite ratio  $\lambda/\mu$ , the dynamics only shadow the asymptotically attracting slow manifold  $x_2 = x_1^2$ , but in fact follow neighboring parabolic trajectories. This is illustrated more clearly by the various surfaces in Figure 2.3 for different ratios  $\lambda/\mu$ .

In this way, a set of intrinsic coordinates may be determined from the observable functions defined by the left eigenvectors of the Koopman operator on an invariant subspace. Explicitly,

$$(2.42) \quad \varphi_\alpha(\mathbf{x}) = \boldsymbol{\xi}_\alpha^\top \mathbf{y}(\mathbf{x}), \quad \text{where} \quad \boldsymbol{\xi}_\alpha^\top \mathbf{K} = \alpha \boldsymbol{\xi}_\alpha^\top.$$

These eigen-observables define observable subspaces that remain invariant under the Koopman operator, even after coordinate transformations. As such, they may be regarded as intrinsic coordinates [352] on the Koopman-invariant subspace.

**2.5. Analytic series expansions for eigenfunctions.** Given the dynamics in (1.1), it is possible to solve the PDE in (2.31) using standard techniques, such as recursively solving for the terms in a Taylor or Laurent series. A number of simple examples are explored below.

**2.5.1. Linear dynamics.** Consider the simple linear dynamics

$$(2.43) \quad \frac{d}{dt}x = x.$$

Assuming a Taylor series expansion for  $\varphi(x)$ :

$$\varphi(x) = c_0 + c_1x + c_2x^2 + c_3x^3 + \dots$$

then the gradient and directional derivatives are given by:

$$\begin{aligned} \nabla\varphi &= c_1 + 2c_2x + 3c_3x^2 + 4c_4x^3 + \dots \\ \nabla\varphi \cdot f &= c_1x + 2c_2x^2 + 3c_3x^3 + 4c_4x^4 + \dots \end{aligned}$$

Solving for terms in the Koopman eigenfunction PDE (2.31), we see that  $c_0 = 0$  must hold. For any positive integer  $\lambda$  in (2.31), only one of the coefficients may be nonzero. Specifically, for  $\lambda = k \in \mathbb{Z}^+$ , then  $\varphi(x) = cx^k$  is an eigenfunction for any constant  $c$ . For instance, if  $\lambda = 1$ , then  $\varphi(x) = x$ .

**2.5.2. Quadratic nonlinear dynamics.** Consider a nonlinear dynamical system

$$(2.44) \quad \frac{d}{dt} = x^2.$$

There is no Taylor series that satisfies (2.31), except the trivial solution  $\varphi = 0$  for  $\lambda = 0$ . Instead, we assume a Laurent series:

$$\varphi(x) = \dots + c_{-3}x^{-3} + c_{-2}x^{-2} + c_{-1}x^{-1} + c_0 + c_1x + c_2x^2 + c_3x^3 + \dots$$

The gradient and directional derivatives are given by:

$$\begin{aligned} \nabla\varphi &= \dots - 3c_{-3}x^{-4} - 2c_{-2}x^{-3} - c_{-1}x^{-2} + c_1 + 2c_2x + 3c_3x^2 + 4c_4x^3 + \dots \\ \nabla\varphi \cdot f &= \dots - 3c_{-3}x^{-2} - 2c_{-2}x^{-1} - c_{-1} + c_1x^2 + 2c_2x^3 + 3c_3x^4 + 4c_4x^5 + \dots \end{aligned}$$

Solving for the coefficients of the Laurent series that satisfy (2.31), we find that all coefficients with positive index are zero, i.e.  $c_k = 0$  for all  $k \geq 1$ . However, the nonpositive index coefficients are given by the recursion  $\lambda c_{k+1} = kc_k$ , for negative  $k \leq -1$ . Thus, the Laurent series is

$$\varphi(x) = c_0 \left( 1 - \lambda x^{-1} + \frac{\lambda^2}{2} x^{-2} - \frac{\lambda^3}{3!} x^{-3} + \dots \right) = c_0 e^{-\lambda/x}.$$

This holds for all values of  $\lambda \in \mathbb{C}$ . There are also other Koopman eigenfunctions that can be identified from the Laurent series.

**2.5.3. Polynomial nonlinear dynamics.** For a more general nonlinear dynamical system

$$(2.45) \quad \frac{d}{dt} = ax^n,$$

$\varphi(x) = e^{\frac{\lambda}{(1-n)a}x^{1-n}}$  is an eigenfunction for all  $\lambda \in \mathbb{C}$ .

As mentioned in subsection 2.2, it is also possible to generate new eigenfunctions by taking powers of these primitive eigenfunctions; the resulting eigenvalues generate a lattice in the complex plane.

**3. Dynamic mode decomposition.** Dynamic mode decomposition, originally introduced by Schmid [295, 294] in the fluid dynamics community, has rapidly become the standard algorithm to approximate the Koopman operator from data [284, 341, 180]. Rowley et al. [284] established the first connection between DMD and the Koopman operator. The DMD algorithm was originally developed to identify spatio-temporal coherent structures from high-dimensional time-series data, as are commonly found in fluid dynamics. DMD is based on the computationally efficient singular value decomposition (SVD), also known as proper orthogonal decomposition (POD) in fluid dynamics, so that it provides scalable dimensionality reduction for high-dimensional data. The SVD orders modes hierarchically based on how much of the variance of the original data is captured by each mode; these modes remain invariant even when the order of the data is shuffled in time. In contrast, the DMD modes are linear combinations of the SVD modes that are chosen specifically to extract spatially correlated structures that have the same coherent linear behavior in time, given by oscillations at a fixed frequency with growth or decay. Thus, DMD provides dimensionality reduction in terms of a low-dimensional set of spatial modes along with a linear model for how the amplitudes of these modes evolve in time. In this way, DMD may be thought of as a combination of SVD/POD in space with the Fourier transform in time, combining the strengths of each approach [69, 180].

There are a number of factors that have led to the widespread adoption of DMD as a workhorse algorithm for processing high-dimensional spatiotemporal data. The DMD algorithm approximates the best-fit linear operator that advances high-dimensional measurements of a system forward in time [341]. Thus, DMD approximates the Koopman operator restricted to the measurement subspace given by direct measurements of the state of a system. DMD is valid for both experimental and simulated data, as it is based entirely on measurement data and does not require knowledge of the governing equations. In addition, DMD is highly extensible because of its simple formulation in terms of linear algebra, resulting in innovations related to control, compressed sensing, and multi-resolution, among others. Because of these strengths, DMD has been applied to a wide range of diverse applications beyond fluid mechanics, including neuroscience, disease modeling, robotics, video processing, power grids, financial markets, and plasma physics. Many of these extensions and applications will be discussed more here and in section 5.

**3.1. The DMD algorithm.** The DMD algorithm seeks a best fit linear operator  $\mathbf{A}$  that approximately advances the state of a system,  $\mathbf{x} \in \mathbb{R}^n$ , forward in time according to the linear dynamical system

$$(3.1) \quad \mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k,$$

where  $\mathbf{x}_k = \mathbf{x}(k\Delta t)$ , and  $\Delta t$  denotes a fixed time step that is small enough to resolve the highest frequencies in the dynamics. Thus, the operator  $\mathbf{A}$  is an approximation of the Koopman operator  $\mathcal{K}$  restricted to a measurement subspace spanned by direct measurements of the state  $\mathbf{x}$ .

DMD is fundamentally a data-driven algorithm, and the operator  $\mathbf{A}$  is approximated from a collection of snapshot pairs of the system,  $\{(\mathbf{x}(t_k), \mathbf{x}(t'_k))\}_{k=1}^m$ , where  $t'_k = t_k + \Delta t$ . A snapshot is typically a measurement of the full state of the system, such as a fluid velocity field sampled at a large number of spatially discretized locations, that is reshaped into a column vector of high dimension. The original formulation of Schmid [294] required data from a single trajectory with uniform sampling in time, so that  $t_k = k\Delta t$ . Here we present the *exact* DMD algorithm of Tu et al. [341], which

works for irregularly spaced data and data concatenated from multiple different time series. Thus, in exact DMD, the times  $t_k$  need not be sequential or evenly spaced, but for each snapshot  $\mathbf{x}(t_k)$  there is a corresponding snapshot  $\mathbf{x}(t'_k)$  one time step  $\Delta t$  in the future. These snapshots are arranged into two data matrices,  $\mathbf{X}$  and  $\mathbf{X}'$ :

$$(3.2a) \quad \mathbf{X} = \begin{bmatrix} | & | & & | \\ \mathbf{x}(t_1) & \mathbf{x}(t_2) & \cdots & \mathbf{x}(t_m) \\ | & | & & | \end{bmatrix}$$

$$(3.2b) \quad \mathbf{X}' = \begin{bmatrix} | & | & & | \\ \mathbf{x}(t'_1) & \mathbf{x}(t'_2) & \cdots & \mathbf{x}(t'_m) \\ | & | & & | \end{bmatrix}.$$

Equation (3.1) may be written in terms of these data matrices as

$$(3.3) \quad \mathbf{X}' \approx \mathbf{AX}.$$

The best fit operator  $\mathbf{A}$  establishes a linear dynamical system that approximately advances snapshot measurements forward in time, which may be formulated as an optimization problem

$$(3.4) \quad \mathbf{A} = \underset{\mathbf{A}}{\operatorname{argmin}} \|\mathbf{X}' - \mathbf{AX}\|_F = \mathbf{X}'\mathbf{X}^\dagger$$

where  $\|\cdot\|_F$  is the Frobenius norm and  $^\dagger$  denotes the pseudo-inverse. The pseudo-inverse may be computed using the SVD of  $\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^*$  as  $\mathbf{X}^\dagger = \mathbf{V}\Sigma^{-1}\mathbf{U}^*$ . The matrices  $\mathbf{U} \in \mathbb{C}^{n \times n}$  and  $\mathbf{V}^{m \times m}$  are unitary, so that  $\mathbf{U}^*\mathbf{U} = \mathbf{I}$  and  $\mathbf{V}^*\mathbf{V} = \mathbf{I}$ , where  $*$  denotes complex-conjugate transpose. The columns of  $\mathbf{U}$  are known as POD modes.

The matrix  $\mathbf{A}$  has  $n^2$  elements, so for high-dimensional data it may be intractable to represent this operator. Instead, the DMD algorithm seeks the leading spectral decomposition (i.e., eigenvalues and eigenvectors) of  $\mathbf{A}$  without ever explicitly constructing it. The data matrices  $\mathbf{X}$  and  $\mathbf{X}'$  typically have far more rows than columns, i.e.  $m \ll n$ , so that  $\mathbf{A}$  will have at most  $m$  nonzero eigenvalues and non-trivial eigenvectors. In practice, the effective rank of the data matrices, and hence the operator  $\mathbf{A}$ , may be even lower, given by  $r < m$ . Instead of computing  $\mathbf{A}$  in (3.4), we may project  $\mathbf{A}$  onto the first  $r$  POD modes in  $\mathbf{U}_r$  and approximate the pseudo-inverse using the rank- $r$  SVD approximation  $\mathbf{X} \approx \mathbf{U}_r\Sigma_r\mathbf{V}_r^*$ :

$$(3.5a) \quad \tilde{\mathbf{A}} = \mathbf{U}_r^*\mathbf{A}\mathbf{U}_r$$

$$(3.5b) \quad = \mathbf{U}_r^*\mathbf{X}'\mathbf{X}^\dagger\mathbf{U}_r$$

$$(3.5c) \quad = \mathbf{U}_r^*\mathbf{X}'\mathbf{V}_r\Sigma_r^{-1}\mathbf{U}_r^*\mathbf{U}_r$$

$$(3.5d) \quad = \mathbf{U}_r^*\mathbf{X}'\mathbf{V}_r\Sigma_r^{-1}.$$

The leading spectral decomposition of  $\mathbf{A}$  may be approximated from the spectral decomposition of the much smaller  $\tilde{\mathbf{A}}$ :

$$(3.6) \quad \tilde{\mathbf{A}}\mathbf{W} = \mathbf{W}\Lambda.$$

The diagonal matrix  $\Lambda$  contains the *DMD eigenvalues*, which correspond to eigenvalues of the high-dimensional matrix  $\mathbf{A}$ . The columns of  $\mathbf{W}$  are eigenvectors of  $\tilde{\mathbf{A}}$ , and provide a coordinate transformation that diagonalizes the matrix. These columns may be thought of as linear combinations of POD mode amplitudes that behave linearly with a single temporal pattern given by the corresponding eigenvalue  $\lambda$ .

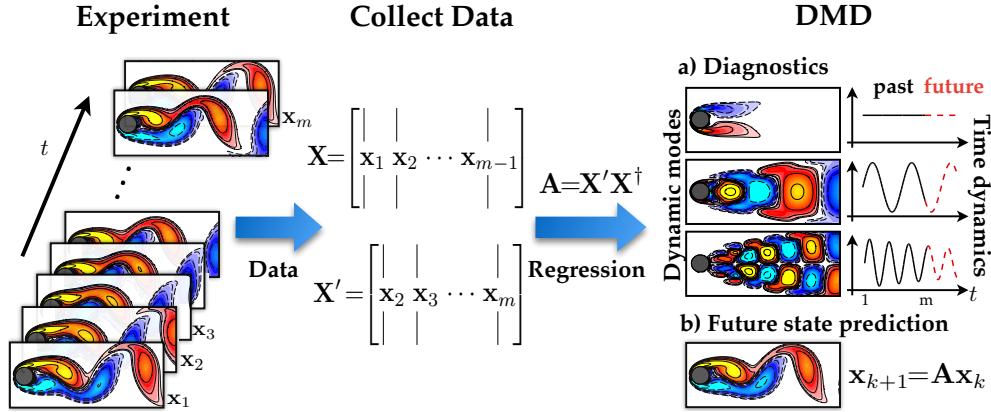


Fig. 3.1: Overview of DMD illustrated on the fluid flow past a circular cylinder at Reynolds number 100. *Reproduced from Kutz et al. [180].*

The eigenvectors of  $\mathbf{A}$  are the *DMD modes*  $\Phi$ , and they are reconstructed using the eigenvectors  $\mathbf{W}$  of the reduced system and the time-shifted data matrix  $\mathbf{X}'$ :

$$(3.7) \quad \Phi = \mathbf{X}'\tilde{\mathbf{V}}\tilde{\Sigma}^{-1}\mathbf{W}.$$

Tu et al. [341] proved that these DMD modes are eigenvectors of the full  $\mathbf{A}$  matrix under certain conditions. This approach is illustrated for a fluid flow in Figure 3.1. There are also several open-source DMD implementations [180, 88].

**3.1.1. Spectral decomposition and the DMD expansion.** Once the DMD modes and eigenvalues are computed, it is possible to represent the system state in terms of the DMD expansion:

$$(3.8) \quad \mathbf{x}_k = \sum_{j=1}^r \phi_j \lambda_j^{k-1} b_j = \Phi \Lambda^{k-1} \mathbf{b},$$

where  $\phi_j$  are eigenvectors of  $\mathbf{A}$  (DMD modes),  $\lambda_j$  are eigenvalues of  $\mathbf{A}$  (DMD eigenvalues), and  $b_j$  are the mode amplitudes. The amplitudes in  $\mathbf{b}$  are given by

$$(3.9) \quad \mathbf{b} = \Phi^\dagger \mathbf{x}_1.$$

Alternative approaches to compute  $\mathbf{b}$  [69, 150, 16] will be discussed in subsection 3.1.2.

The spectral expansion in (3.8) may be converted to continuous time by introducing the continuous eigenvalues  $\omega = \log(\lambda)/\Delta t$ :

$$(3.10) \quad \mathbf{x}(t) = \sum_{j=1}^r \phi_j e^{\omega_j t} b_j = \Phi \exp(\Omega t) \mathbf{b},$$

where  $\Omega$  is a diagonal matrix containing the continuous-time eigenvalues  $\omega_j$ . Thus, the data matrix  $\mathbf{X}$  may be represented as

$$(3.11) \quad \mathbf{X} \approx \begin{bmatrix} & & \\ \phi_1 & \cdots & \phi_r \\ & & \end{bmatrix} \begin{bmatrix} b_1 & & \\ & \ddots & \\ & & b_r \end{bmatrix} \begin{bmatrix} e^{\omega_1 t_1} & \cdots & e^{\omega_1 t_m} \\ \vdots & \ddots & \vdots \\ e^{\omega_r t_1} & \cdots & e^{\omega_r t_m} \end{bmatrix} = \Phi \text{diag}(\mathbf{b}) \mathbf{T}(\omega).$$

**3.1.2. Alternative optimizations for DMD.** The DMD algorithm is purely data-driven, and is thus equally applicable to experimental and numerical data. When characterizing experimental data with DMD, the effects of sensor noise and stochastic disturbances must be accounted for. Bagheri [19] showed that DMD is particularly sensitive to the effects of noisy data, and it has been shown that significant and systematic biases are introduced to the eigenvalue distribution [93, 18, 83, 131]. Although increased sampling decreases the variance of the eigenvalue distribution, it does not remove the bias [131]. This noise sensitivity has motivated several alternative optimization algorithms for DMD to improve the quality and performance of DMD over the standard optimization in (3.4), which is a least-square fitting procedure involving the Frobenius norm. These algorithms include the total least-squares DMD [131], forward-backward DMD [83], variable projection [16], and robust principal component analysis [292].

One of the simplest ways to remove the systematic bias of the DMD algorithm is by computing it both forward and backward in time and averaging the equivalent operator, as proposed by Dawson et al. [83]. Thus the two following approximations are considered

$$(3.12) \quad \mathbf{X}' \approx \mathbf{A}_1 \mathbf{X} \quad \text{and} \quad \mathbf{X} \approx \mathbf{A}_2 \mathbf{X}'$$

where  $\mathbf{A}_2^{-1} \approx \mathbf{A}_1$  for noise-free data. Thus the operator  $\mathbf{A}_2$  is the inverse, or backward time-step, mapping the snapshots from  $t_{k+1}$  to  $t_k$ . The forward and backward time operators are then averaged, removing the systematic bias from the measurement noise:

$$(3.13) \quad \mathbf{A} = \frac{1}{2} (\mathbf{A}_1 + \mathbf{A}_2^{-1})$$

where the optimization (3.4) can be used to compute both the forward and backward mapping  $\mathbf{A}_1$  and  $\mathbf{A}_2$ . This optimization can be formulated as

$$(3.14) \quad \mathbf{A} = \operatorname{argmin}_{\mathbf{A}} \frac{1}{2} (\|\mathbf{X}' - \mathbf{AX}\|_F + \|\mathbf{X} - \mathbf{A}^{-1}\mathbf{X}'\|_F),$$

which is highly nonlinear and non-convex due to the inverse  $\mathbf{A}^{-1}$ . An improved optimization framework was developed by Azencot et al. [17] which proposes

$$(3.15) \quad \mathbf{A} = \operatorname{argmin}_{\mathbf{A}_1, \mathbf{A}_2} \frac{1}{2} (\|\mathbf{X}' - \mathbf{A}_1 \mathbf{X}\|_F + \|\mathbf{X} - \mathbf{A}_2 \mathbf{X}'\|_F) \quad \text{s.t. } \mathbf{A}_1 \mathbf{A}_2 = \mathbf{I}, \mathbf{A}_2 \mathbf{A}_1 = \mathbf{I},$$

to circumvent some of the difficulties of the optimization in (3.14).

Hemati et al. [131] formulate another DMD algorithm, replacing the original least-squares regression with a total least-squares regression to account for the possibility of noisy measurements and disturbances to the state. This work also provides an excellent discussion on the sources of noise and a comparison of various denoising algorithms. The subspace DMD algorithm of Takeishi et al. [331] compensates for measurement noise by computing an orthogonal projection of future snapshots onto the space of previous snapshots and then constructing a linear model. Extensions that combine DMD with Bayesian approaches have also been developed [329].

Good approximations for the mode amplitudes  $\mathbf{b}$  in (3.11) have also proven to be difficult to achieve, with and without noise. Jovanović et al. [150] developed the first algorithm to improve the estimate of the modal amplitudes by promoting sparsity.

In this case, the underlying optimization algorithm is framed around improving the approximation (3.11) using the formulation

$$(3.16) \quad \underset{\mathbf{b}}{\operatorname{argmin}} (\|\mathbf{X} - \Phi \operatorname{diag}(\mathbf{b}) \mathbf{T}(\boldsymbol{\omega})\|_F + \gamma \|\mathbf{b}\|_1)$$

where  $\|\cdot\|_1$  denotes the  $\ell_1$ -norm penalization which promotes sparsity of the vector  $\mathbf{b}$ . More recently, Askham and Kutz [16] introduced the *optimized DMD* algorithm, which uses a variable projection method for nonlinear least squares to compute the DMD for unevenly timed samples, significantly mitigating the bias due to noise. The optimized DMD algorithm solves the exponential fitting problem directly:

$$(3.17) \quad \underset{\boldsymbol{\omega}, \Phi_{\mathbf{b}}}{\operatorname{argmin}} \|\mathbf{X} - \Phi_{\mathbf{b}} \mathbf{T}(\boldsymbol{\omega})\|_F.$$

This has been shown to provide a superior decomposition due to its ability to optimally suppress bias and handle snapshots collected at arbitrary times. The disadvantage of optimized DMD is that one must solve a nonlinear optimization problem.

**3.1.3. Krylov subspace perspective.** In the original formulation [294, 284], the matrices  $\mathbf{X}$  and  $\mathbf{X}'$  were formed from sequential snapshots, evenly spaced in time:

$$(3.18a) \quad \mathbf{X} = \begin{bmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_m \\ | & | & & | \end{bmatrix}$$

$$(3.18b) \quad \mathbf{X}' = \begin{bmatrix} | & | & & | \\ \mathbf{x}_2 & \mathbf{x}_3 & \cdots & \mathbf{x}_{m+1} \\ | & | & & | \end{bmatrix}.$$

The columns of  $\mathbf{X}$  belong to a Krylov subspace generated by  $\mathbf{A}$  and  $\mathbf{x}_1$ :

$$(3.19) \quad \mathbf{X} \approx \begin{bmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{A}\mathbf{x}_1 & \cdots & \mathbf{A}^{m-1}\mathbf{x}_1 \\ | & | & & | \end{bmatrix}.$$

Thus, DMD is related to Arnoldi iteration to find the dominant eigenvalues and eigenvectors of a matrix  $\mathbf{A}$ .

The matrices  $\mathbf{X}$  and  $\mathbf{X}'$  are also related through the *shift* operator  $\mathbf{S}$  by

$$(3.20) \quad \mathbf{X}' = \mathbf{X}\mathbf{S}.$$

Thus,  $\mathbf{S}$  acts on columns of  $\mathbf{X}$ , as opposed to  $\mathbf{A}$ , which acts on rows of  $\mathbf{X}$ . The shift operator  $\mathbf{S}$ , also known as a companion matrix, is given by

$$(3.21) \quad \mathbf{S} = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & a_1 \\ 1 & 0 & 0 & \cdots & 0 & a_2 \\ 0 & 1 & 0 & \cdots & 0 & a_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & a_m \end{bmatrix}.$$

In other words, the first  $m - 1$  columns of  $\mathbf{X}'$  are obtained by shifting the last  $m - 1$  columns of  $\mathbf{X}$ , and the last column is obtained as a best-fit combination of the  $m$  columns of  $\mathbf{X}$  that minimizes the residual. The shift operator may be viewed as a matrix representation of the Koopman operator, as it advances snapshots forward in time. The  $m \times m$  matrix  $\mathbf{S}$  has the same non-zero eigenvalues as  $\mathbf{A}$ , so that  $\mathbf{S}$  may be used to obtain dynamic modes and eigenvalues. However, computations based on  $\mathbf{S}$  are not as numerically stable as the DMD algorithm presented above.

**3.2. Methodological extensions.** The DMD algorithm has been successful in large part because of its simple formulation in terms of linear regression and because it does not require knowledge of governing equations. For these reasons, DMD has been extended to include several methodological innovations [180] presented here. Several of these extensions, including to nonlinear systems, delay measurements, and control, will be explored in much more detail in later sections. Algorithms to handle noisy data were already discussed in subsection 3.1.2.

**3.2.1. Including inputs and control.** Often, the goal of obtaining reduced-order models is to eventually design more effective controllers to manipulate the behavior of the system. Similarly, in many systems, such as the climate, there are external forcing variables that make it difficult to identify the underlying unforced dynamics. Proctor et al. [275] introduced the DMD with control (DMDc) algorithm to disambiguate the natural unforced dynamics and the effect of forcing or actuation given by the variable  $\mathbf{u}$ . This algorithm is based on

$$(3.22) \quad \mathbf{x}_{k+1} \approx \mathbf{A}\mathbf{x}_k + \mathbf{B}\mathbf{u}_k,$$

which results in another linear regression problem. This algorithm was motivated by epidemiological systems (e.g., malaria or polio), where it is not possible to stop intervention efforts, such as vaccinations and bed nets, in order to characterize the unforced dynamics [274]. DMDc will be explored extensively in subsection 6.2.1.

**3.2.2. Compression and randomized linear algebra.** The DMD algorithm is fundamentally based on the assumption that there are dominant low-dimensional patterns even in high-dimensional data, such as fluid flow fields. Randomized algorithms [124] are designed to exploit these patterns to accelerate numerical linear algebra. In the randomized DMD algorithm [30, 100] data is randomly project into a lower-dimensional subspace where computations may be performed more efficiently. The existence of patterns also facilitate more efficient measurement strategies based on principles of *sparsity* to reduce the number of measurements required in time [340] and space [52, 123, 98]. This has the broad potential to enable high-resolution characterization of systems from under-resolved measurements. In 2014, Jovanovic et al. [150] used sparsity promoting optimization to identify the fewest DMD modes required to describe a data set; the alternative, testing and comparing all subsets of DMD modes, is computationally intractable. Finally, libraries of DMD modes have also been used to identify dynamical regimes [178], based on the sparse representation for classification [358], which was used earlier to identify dynamical regimes using libraries of POD modes [38, 53].

**3.2.3. Nonlinear measurements and latent variables.** The connection between DMD and the Koopman operator [284, 341, 180] has motivated several extensions for strongly nonlinear systems. The standard DMD algorithm is able to accurately characterize periodic and quasi-periodic behavior, even in nonlinear systems. However, DMD models based on linear measurements of the system are generally not sufficient to characterize truly nonlinear phenomena, such as transients, intermittent phenomena, or broadband frequency cross-talk. In Williams et al. [352, 353], DMD measurements were augmented to include nonlinear measurements of the system, enriching the basis used to represent the Koopman operator. There are also important extensions of DMD to systems with latent variables. Although DMD was developed for high-dimensional data, it is often desirable to characterize systems with incomplete measurements. As an extreme example, consider a single measurement that

oscillates as a sinusoid,  $x(t) = \sin(\omega t)$ . Although this would appear to be a perfect candidate for DMD, the algorithm incorrectly identifies a real eigenvalue because the data does not have sufficient rank to extract a complex conjugate pair of eigenvalues  $\pm i\omega$ . This paradox was first explored by Tu et al. [341], where it was discovered that a solution is to stack delayed measurements into a larger matrix to augment the rank of the data and extract phase information. Delay coordinates have also been used effectively to extract coherent patterns in neural recordings [45]. The connections between delay DMD and Koopman were subsequently investigated [47, 14, 81, 161]. Nonlinear measurements and latent variable will both be explored extensively in section 5.

**3.2.4. Multiresolution.** DMD is often applied to complex, high-dimensional dynamical systems, such as fluid turbulence or epidemiological systems, that exhibit multiscale dynamics in both space and time. Many multiscale systems exhibit transient or intermittent phenomena, such as the El Niño observed in global climate data. These transient dynamics are not captured accurately by DMD, which seeks spatio-temporal modes that are globally coherent across the entire time series of data. To address this challenge, the multiresolution DMD (mrDMD) algorithm was introduced [181], which effectively decomposes the dynamics into different timescales, isolating transient and intermittent patterns. Multiresolution DMD modes were recently shown to be advantageous for sparse sensor placement by Manohar et al. [215].

**3.2.5. Streaming and parallelized codes.** Because of the computational burden of computing the DMD on high-resolution data, several advances have been made to accelerate DMD in streaming applications and with parallelized algorithms. DMD is often used in a streaming setting, where a moving window of snapshots are processed continuously, resulting in savings by eliminating redundant computations when new data becomes available. Several algorithms exist for streaming DMD, based on the incremental SVD [132], a streaming method of snapshots SVD [267], and rank-one updates to the DMD matrix [365]. The DMD algorithm is also readily parallelized, as it is based on the SVD. Several parallelized codes are available, based on the QR [290] and SVD [100, 101, 99].

**3.3. Domain applications.** DMD has been widely applied to a diverse range of applications. We will explore key applications in fluid dynamics, epidemiology, neuroscience, and video processing. In addition, DMD has been used for robotics [27, 4, 44, 111], finance [213], power grids [303, 324, 321, 326, 319, 322, 176], and plasma physics [335, 162].

**3.3.1. Fluid dynamics.** DMD originated in the fluid dynamics community [294], and has since been applied to a wide range of flow geometries (jets, cavity flow, wakes, channel flow, boundary layers, etc.), to study mixing, acoustics, and combustion, among other phenomena. In Schmid [295, 294], both a cavity flow and a jet were considered; the cavity flow example is shown in Figure 3.2. Rowley et al. [284] investigated a jet in cross-flow; modes are shown in Figure 3.3 with the corresponding eigenvalue spectrum. Thus, it is no surprise that DMD has subsequently been used broadly in both cavity flows [294, 203, 297, 24, 23] and jets [25, 298, 296, 293].

DMD has also been applied to wake flows, including to investigate frequency lock-on [339], the wake past a gurney flap [260], the cylinder wake [18], and dynamic stall [94]. Boundary layers have also been extensively studied with DMD [255, 291, 236]. In acoustics, DMD has been used to capture the near-field and far-field acoustics that result from instabilities observed in shear flows [308]. In combustion, DMD has been used to understand the coherent heat release in turbulent swirl flames [237] and

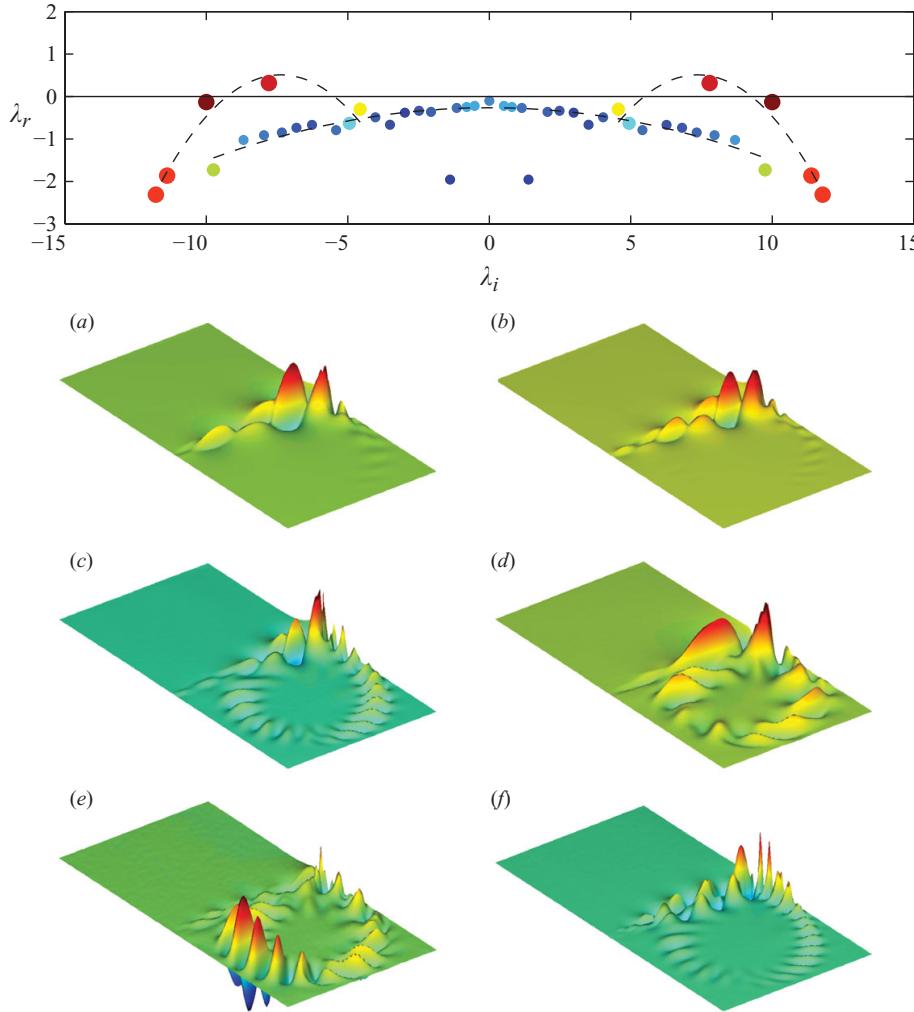


Fig. 3.2: (top) DMD eigenvalue spectrum for the cavity flow at Reynolds number  $Re = 4500$ . (bottom) Corresponding DMD modes, visualized by the streamwise velocity. (a) Most unstable dynamic mode, (b–d) DMD modes from the unstable branch, (e,f) DMD modes from the stable branch. *Modified with permission, from Schmid 2010 Journal of Fluid Mechanics [294].*

to analyze a rocket combustor [143]. DMD has also been used to analyze non-normal growth mechanisms in thermoacoustic interactions in a Rijke tube. DMD has been compared with POD for reacting flows [285]. DMD has also been used to analyze more exotic flows, including a simulated model of a high-speed train [242]. Shock turbulent boundary layer interaction (STBLI) has also been investigated with DMD to identify a pulsating separation bubble that is accompanied by shockwave motion [121]. DMD has also been used to study self-excited fluctuations in detonation waves [219]. Other problems include identifying hairpin vortices [333], decomposing the flow past a surface mounted cube [243], modeling shallow water equations [31], studying nano fluids past a square cylinder [289], and measuring the growth rate of instabilities in annular liquid sheets [92].

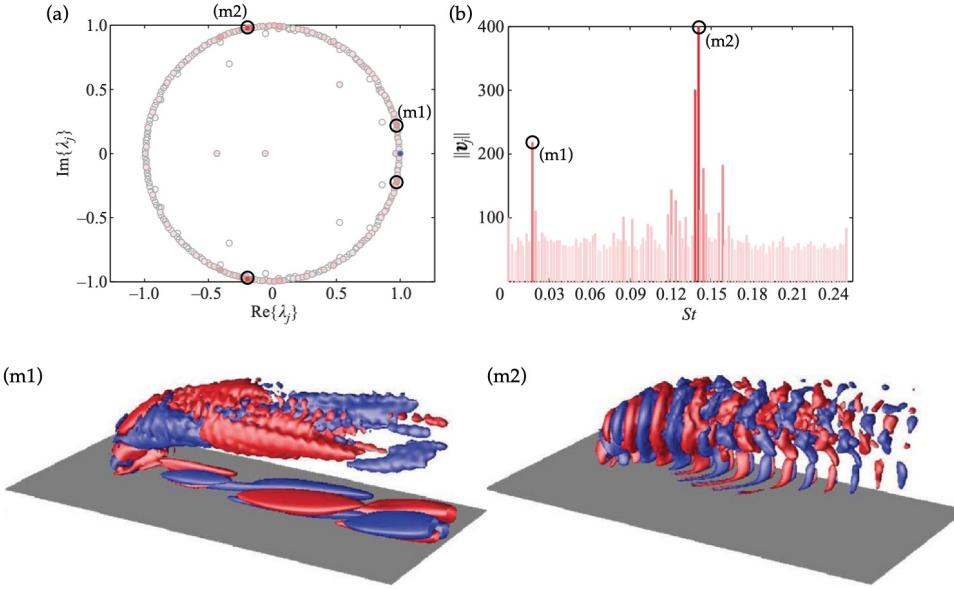


Fig. 3.3: DMD eigenvalues for jet-in-crossflow plotted on the unit circle (a) and as a power spectrum versus Strouhal number (b). Two DMD modes ( $m_1$ ) and ( $m_2$ ) are pictured below. *Modified with permission, from Rowley et al. 2009 Journal of Fluid Mechanics [284].*

It is interesting to note that the noise effects that were carefully analyzed by Bagheri [19] explain the eigenvalue spectrum observed earlier by Schmid et al. [293] for a turbulent jet. This comparison is shown in Figure 3.4.

**3.3.2. Epidemiology.** Epidemiological data often consists of high-dimensional spatiotemporal time series measurements, such as the number of infections in a given neighborhood or city. Thus, DMD provides particularly interpretable decompositions for these systems, as explored by Proctor and Eckhoff [277] and illustrated in Figure 3.5. Modal frequencies often correspond to yearly or seasonal fluctuations. Moreover, the phase of DMD modes gives insight into how disease fronts propagate spatially, potentially informing future intervention efforts. The application of DMD to disease systems also motivated the DMD with control algorithm [275], since it is infeasible to stop vaccinations in order to identify the unforced dynamics.

**3.3.3. Neuroscience.** Complex signals from neural recordings are increasingly high-fidelity and high dimensional, with advances in hardware pushing the frontiers of data collection. DMD has the potential to transform the analysis of such neural recordings, as evidenced in a recent study by B. Brunton et al. [45] that identified dynamically relevant features in ECOG data of sleeping patients, shown in Figure 3.6. Since then, several works have applied DMD to neural recordings or suggested possible implementation in hardware [6, 39, 337].

**3.3.4. Video processing.** DMD has also been used for segmentation in video processing, as a video may be thought of as a time-series of high-dimensional snapshots (images) evolving in time. Separating foreground and background objects in video is

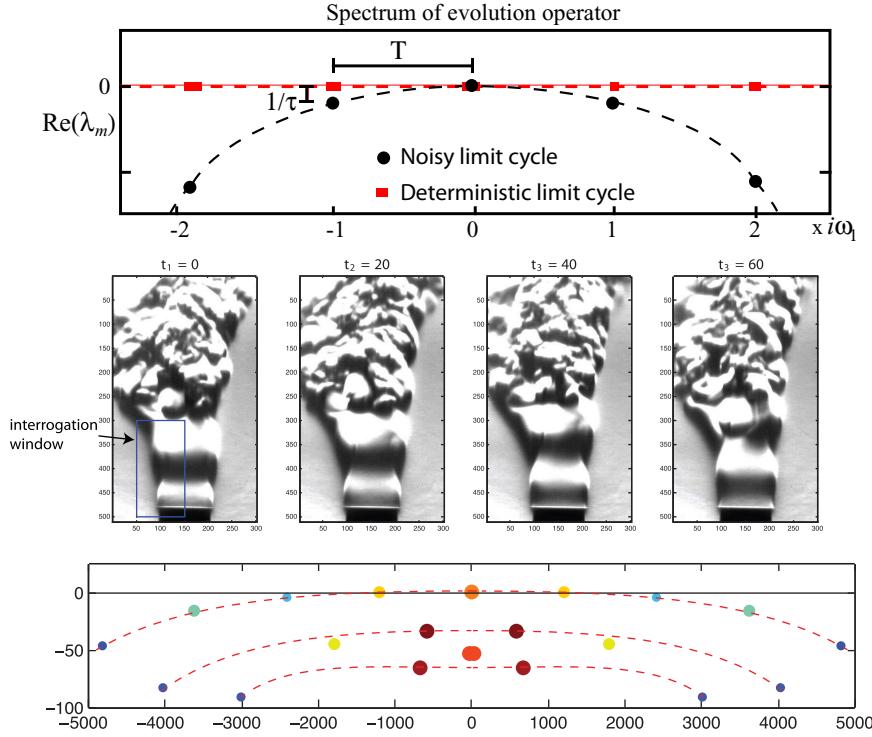


Fig. 3.4: (top) Koopman eigenvalue spectrum for oscillator with noise. (middle, bottom) DMD spectrum for jet flow, exhibiting similar noise pattern. *Reproduced with permission, from Bagheri 2014 Physics of Fluids [19]; (bottom, middle) panels originally from Schmid et al., 2011 Theoretical and Computational Fluid Dynamics [293].*

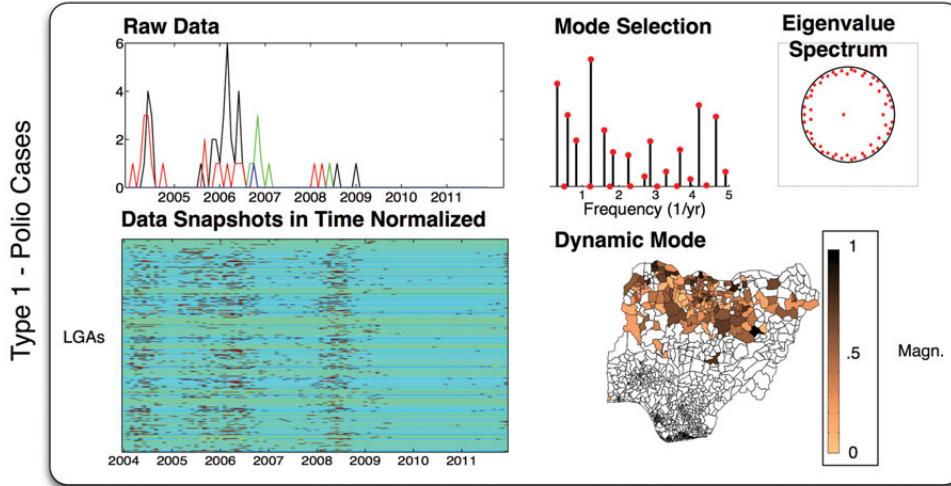


Fig. 3.5: Results of DMD analysis for Polio cases in Nigeria. *Reproduced with permission, from Proctor and Eckhoff 2014 International health [277].*

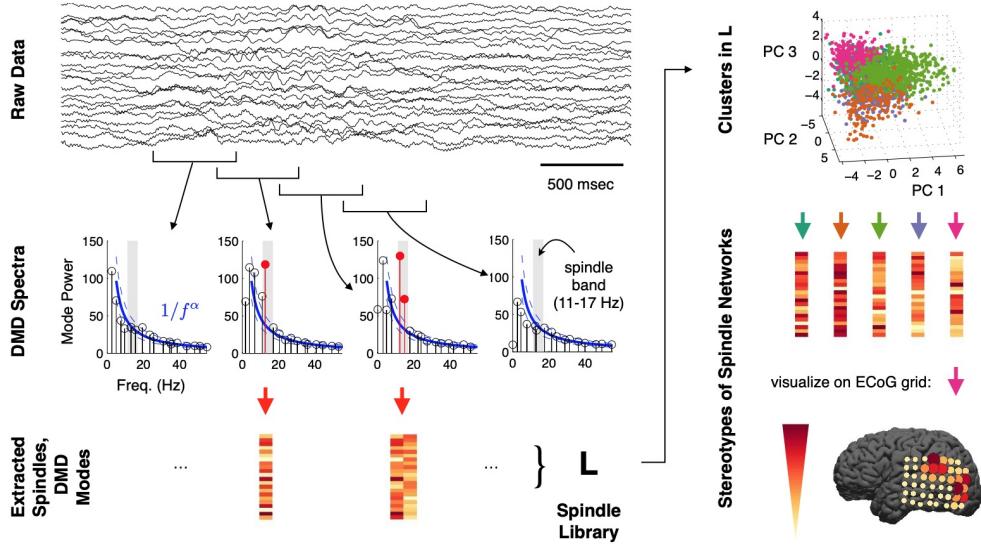


Fig. 3.6: Illustration of DMD applied to human brain data from electroencephalogram (ECOG) measurements. *Reproduced with permission, from B. Brunton et al. 2016 Journal of Neuroscience Methods [45].*

a common task in surveillance applications. Real-time separation is a challenge that is only exacerbated by increasing video resolutions. DMD provides a flexible approach for video separation, as the background may be approximated by a DMD mode with zero eigenvalue [122, 98, 267], as illustrated in Figure 3.7.

**3.4. Connections to other methods.** Linear regression models are common throughout the sciences, and so it is not surprising to find many methods that are closely related to DMD. These related methods have been developed in a diverse set of scientific and mathematical disciplines, using a range of mathematical formulations.

**3.4.1. System identification.** DMD may be viewed as a form of system identification, which is a mature subfield of control theory. Tu et al. [341] established a connection between DMD and the eigensystem realization algorithm (ERA) [152]. Subsequently, DMD with control [275] was also linked to ERA and the observer Kalman identification methods (OKID) [272, 271]. ERA and OKID construct input-output models using impulse response data and continuous disturbance data, respectively [152, 153, 272, 271, 151]. Both of these methods were developed to construct input-output state-space models for aerospace applications where the systems tend to have higher rank than the number of sensor measurements [137, 152]. In contrast, DMD and DMDc were developed for systems with a large number of measurements and low-rank dynamics. ERA and OKID have also been categorized as subspace identification methods [278], which include the numerical algorithms for subspace system identification (N4SID), multivariable output error state space (MOESP), and canonical variate analysis (CVA) [347, 348, 163, 278]. Algorithmically, these methods involve regression, model reduction, and parameter estimation steps, similar to DMDc. There are important contrasts regarding the projection scaling between all of these methods [275], but the overall viewpoint is similar among these diverse methods.

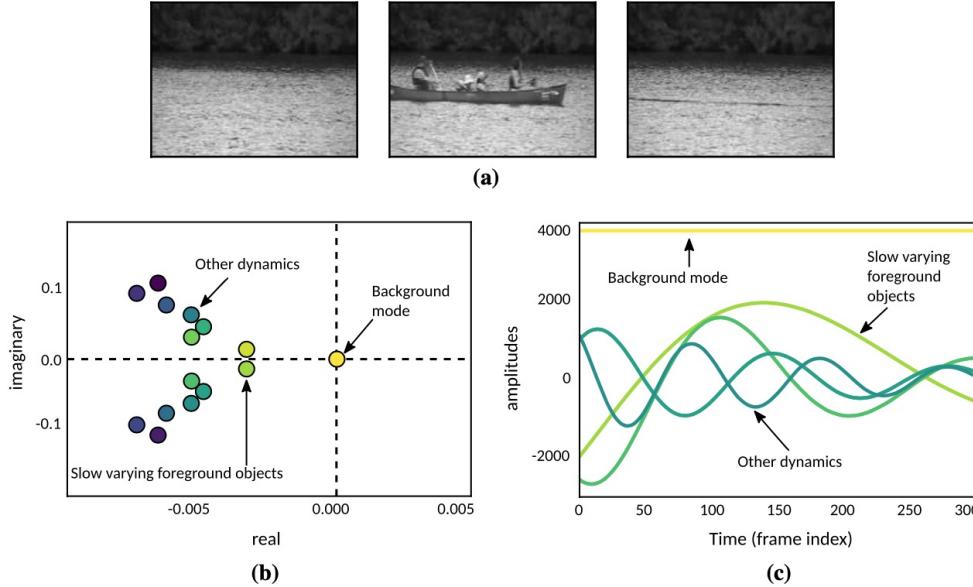


Fig. 3.7: DMD may be used to process videos, extracting dominant background modes with zero frequency. *Reproduced with permission, from Erichson et al. 2016 Journal of Real Time Processing [98].*

**3.4.2. ARIMA: Auto-regressive integrating moving average.** Autoregressive moving average (ARMA) models and the generalized autoregressive integrated moving average (ARIMA) models [35] are commonly used in statistics and econometrics. These models leverage time-series data to build models to forecast predictions into the future. ARIMA models are often applied to data that are non-stationary. Like DMD, ARMA and ARIMA models are characterized by a number of key parameters, one of them being the number of past time points used for forecasting a future point. However, DMD correlates each time snapshot directly to the previous time snapshot. Autoregressive models have a number of useful variants, including a generalization to a vector framework, i.e. the VARIMA (vector ARIMA) model, and a generalization which includes seasonal effects, i.e. the SARIMA (seasonal ARIMA) model. In the DMD architecture, seasonal variations are automatically included. Moreover, if the mean of the data matrix  $\mathbf{X}$  is subtracted, then the companion matrix DMD formulation from subsection 3.1.3 has been shown to be equivalent to a Fourier decomposition of the vector field in time [69, 136]. DMD can be thought of as taking advantage of both the vector nature of the data and any oscillatory (seasonal) variations. Further, the real part of the DMD spectra allows one to automatically capture exponential trends in the data.

**3.4.3. LIM: Linear inverse modeling.** Linear inverse models (LIMs) have been developed in the climate science community. LIMs are essentially identical to the DMD architecture under certain assumptions [341]. By construction, LIMs rely on low-rank modeling, like DMD, using low-rank truncation which are known as *empirical orthogonal functions* (EOFs) [201]. Using EOFs, Penland [268] derived a method to compute a linear dynamical system that approximates data from a stochastic linear

Markov system, which later came to be known as LIM [269]. Under certain circumstances, DMD and LIM may be considered equivalent algorithms. The equivalence of projected DMD and LIM gives us yet another way to interpret DMD analysis. If the mean of the data is removed, then the low-rank map that generates the DMD eigenvalues and eigenvectors is simply the same map that yields the statistically most likely state in the future. This is the case for both the exact and projected DMD algorithms, as both are built on the same low-order linear map. LIM is typically performed for data where the mean has been subtracted, whereas DMD is valid with or without mean subtraction. Regardless, there is a strong enough similarity between the two methods that the communities may find their particular innovations valuable to one another.

**3.4.4. PCR: Principal component regression.** In the statistical sciences, *principal component regression* (PCR) [147] is a regression analysis technique that is once again based on the SVD (specifically PCA). PCR regresses the outcome (also known as the response or, the dependent variable) on the principal components of a set of covariates (also known as predictors or, explanatory variables or, independent variables) based on a standard linear regression model. Instead of regressing the dependent variable on the explanatory variables directly, PCR uses the principal components of the explanatory variables as regressors. One typically uses only a subset of all the principal components for regression, thus making PCR a regularized procedure. Often the principal components with larger variances are selected as regressors; these principal components correspond to eigenvectors with larger eigenvalues of the sample variance-covariance matrix of the explanatory variables. However, for the purpose of predicting the outcome, the principal components with low variances may also be important, in some cases even more important [147, 146]. Unlike the DMD/LIM literature, which has been traditionally steeped in dynamics, the statistics literature is often concerned with regression of static data, mapping generic input data to target data. Thus PCR is typically not specifically applied to time-series data, but is instead a general regression procedure that may or may not be applied to data from a dynamical system. In some sense, the first two steps of the DMD algorithm may be viewed as performing PCR on snapshot data from a high-dimensional dynamical system. However, PCR does not include the additional steps of eigendecomposition of the matrix  $\tilde{\mathbf{A}}$  or the reconstruction of high-dimensional coherent modes. This last step is what relates DMD to the Koopman operator, connecting the data analysis to nonlinear dynamics.

**3.4.5. Resolvent analysis.** DMD and Koopman operator theory have also been connected to the resolvent analysis from fluid mechanics [299, 134]. Resolvent analysis seeks to find the most receptive states of a dynamical system that will be most amplified by forcing, along with the corresponding most responsive forcings [338, 149, 228, 148]. Sharma, Mezić, and McKeon [299] established several important connections between DMD, Koopman theory, and the resolvent operator, including a generalization of DMD to enforce symmetries and traveling wave structures. They also showed that the resolvent modes provide an optimal basis for the Koopman mode decomposition. Typically, resolvent analysis is performed by linearizing the governing equations about a base state, often a turbulent mean flow. However, this approach is *invasive*, requiring a working Navier-Stokes solver. Herrmann et al. [134] have recently developed a purely data-driven resolvent algorithm, based on DMD, that bypasses knowledge of the governing equations.

#### 4. Koopman operator and modern nonlinear dynamics.

**4.1. Eigenfunctions as nonlinear coordinate changes.** Koopman eigenfunctions provide an explicit coordinate transformation between the nonlinear dynamical system  $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$  (1.1) and a *factor* of the Koopman (Lie) dynamical system  $\dot{g} = \mathcal{L}g$  (2.11), where functions  $g$  are restricted to the span of a subset of Koopman eigenfunctions. In this section, we provide an overview of results that exploit linearity of Koopman dynamics to arrive at conclusions about the original nonlinear dynamical system.

Consider a more general setting between two dynamical systems  $\dot{\mathbf{x}}_1 = \mathbf{f}_1(\mathbf{x}_1)$  for  $\mathbf{x}_1 \in \mathcal{X}_1$  and  $\dot{\mathbf{x}}_2 = \mathbf{f}_2(\mathbf{x}_2)$  for  $\mathbf{x}_2 \in \mathcal{X}_2$ , respectively inducing flows  $\mathbf{F}_k: \mathcal{X}_k \rightarrow \mathcal{X}_k$  given by  $\mathbf{x}_k(t) = \mathbf{F}_k^t(\mathbf{x}_k(0))$ ,  $k = 1, 2$ . If there exists a homeomorphism (continuous function with a continuous inverse)  $h: \mathcal{X}_1 \rightarrow \mathcal{X}_2$  such that its composition with the flows

$$(4.1) \quad h \circ \mathbf{F}_1^t \equiv \mathbf{F}_2^t \circ h$$

holds everywhere, the two dynamical systems are *topologically conjugate*.<sup>2</sup> The orbit structure of two topologically conjugate dynamical systems is qualitatively the same. Therefore, if one identifies a pair of such systems where one of them is easier to analyze analytically, numerically, or is already familiar, it makes it possible to port results from the “simpler” to the more complicated system. One seminal result of this sort is the Hartman–Grobman theorem [350, §19.12A], which establishes that a nonlinear system  $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$  in an open neighborhood of a hyperbolic fixed point  $\mathbf{x}_0$  is locally topologically conjugate to its linearization  $\dot{\mathbf{z}} = \mathbf{Az}$ , where  $\mathbf{A} = D\mathbf{f}(\mathbf{x}_0)$ , formally justifying the use of the Jacobian in inferring stability of hyperbolic nonlinear equilibria.

Lan and Mezić [185] recognized that the conjugacy relationship resulting from the Hartman–Grobman theorem

$$(4.2) \quad h(\mathbf{F}^t(\mathbf{x})) = e^{\mathbf{At}}h(\mathbf{x}),$$

where  $e^{\mathbf{At}}$  is the flow of the linearization, implies the existence of a (vector-valued) Koopman eigenfunction  $\mathbf{h}$ , as it matches the definition (2.12). By diagonalization of  $\mathbf{A}$ , the components  $h_k$  of  $\mathbf{h}$  are precisely scalar-valued Koopman eigenfunctions. Although H–G establishes that (4.2) holds only in some neighborhood of the origin, [185] show that trajectories emanating from the boundary of that neighborhood (backward-in-time) can be used to extend the definition of eigenfunctions  $h_k$  up to the edge of the basin of attraction or up to the end of the interval of existence of trajectories, therefore proving an extension of the Hartman–Grobman theorem to the entire basin of attraction. By proving analogous results for discrete-time dynamics, linearization of periodic and periodically-forced dynamical systems follows.

In [33], this idea is taken further, to construct the conjugacy  $h(\cdot)$  between two nonlinear systems that are known to be topologically conjugate. Explicit construction of conjugacies is generally a difficult task that is often eschewed when existence of conjugacy can be inferred from other properties of the system. It is demonstrated that while for one-dimensional systems the construction is straightforward, conjugacies on

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<sup>2</sup>Restricting the domain to a strict subset of  $\mathcal{X}_{1,2}$  leads to *local* conjugacy. Requiring higher regularity (differentiability, smoothness, analyticity) of  $h$  and  $h^{-1}$ , or extending  $h$  to also convert between the time domains of two systems leads to related concepts in the theory of differential equations and dynamical systems covered by standard textbooks, such as [350, 270, 229].

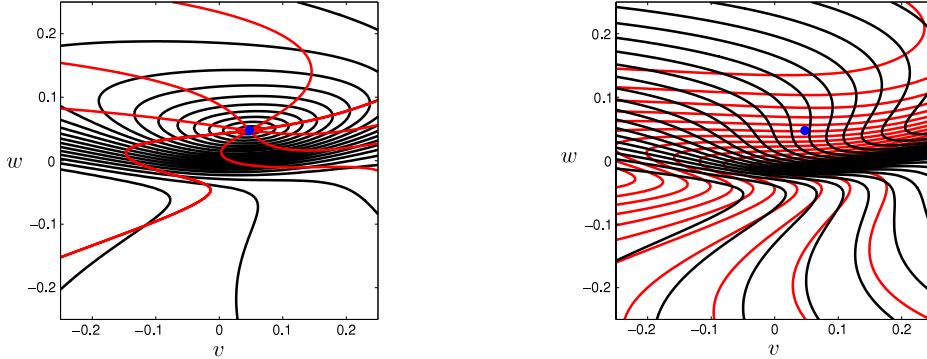


Fig. 4.1: Isostables and isochrons for the FitzHugh–Nagumo model acting as a deformed rectifiable coordinate system in vicinity of a focus (left) and node (right). Reproduced with permission, from Mauroy et al. 2013 *Physica D* [225].

state spaces in  $\mathbb{R}^n$  require a more delicate approach, especially when dealing with eigenvalues with nontrivial geometric multiplicity.

In the setting of *model/order reduction*, relations (4.1) and (4.2) are required to hold for non-invertible maps or on closed (or even singular) subsets of the domain. In this case the full orbit structure of systems is not typically qualitatively the same; however, much can be gained by studying a simpler, often significantly-lower dimensional, system, and transporting its properties onto the original dynamics.

In this context, Mauroy et al. [222, 225] demonstrate that the coordinate transformations  $h_k$  can be numerically computed by forward integration of a trajectory and a Laplace average of an observable

$$(4.3) \quad \tilde{g}_\lambda(\mathbf{x}) := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T g_t(\mathbf{x}) e^{\bar{\lambda}t} dt,$$

which is an extension of the harmonic Fourier average (2.30). The computed isostables (level sets of the absolute value of eigenfunctions) and isochrons (level sets of the arguments of complex eigenfunctions) act either as rectifiable Cartesian coordinate systems for node equilibria, or as rectifiable polar (action-angle) coordinate systems for focus-type equilibria, as shown in Figure 4.1, with clear generalizations to higher dimensional systems.

Further theoretical developments have led to extensions to nonlinear stability analysis and optimal control of dynamical systems [310, 221, 224, 309, 223]. Papers [354, 357] apply this concept to synchronization of oscillators by extending the phase-response curves using isostables and isochrons computed as Koopman eigenfunctions. Notably, these developments demonstrate that Koopman eigenfunctions are a viable and practical path both in analytic [356] and in data-driven approaches [355] to synchronization of oscillators.

**4.2. Phase portrait and symmetries.** Discussions of Hartman–Grobman theory and conjugacies are typically concerned with the behavior of two dynamical systems in the vicinity of an object of interest, such as a basin of attraction/repulsion of a fixed point or periodic orbit. Here we describe how Koopman eigenfunctions can reflect the structure of the entire phase portrait of the dynamical system.

The phase portrait of a dynamical system on state space  $\mathcal{X}$  is a collection of all orbits  $\mathbf{o}(\mathbf{x}) = \{\mathbf{F}^t(\mathbf{x})\}_{t \in \mathbb{R}}$  emanating from each initial condition  $\mathbf{x}$  by the flow map  $\mathbf{F}^t$ .

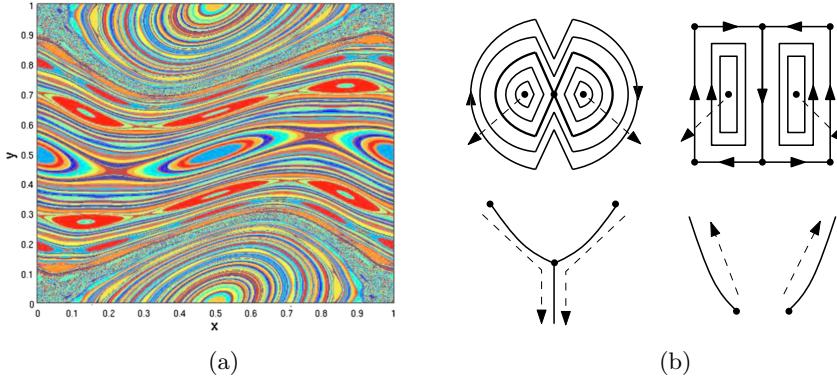


Fig. 4.2: (a) Approximate ergodic partition of the Chirikov Standard Map. Reproduced with permission, from Levnajić and Mezić 2010 *Chaos* [192]. (b) Sketch of ordering of orbits by ergodic quotient trajectories. Reproduced with permission, from Budišić and I. Mezić 2012 *Physica D* [55].

It is immediately clear that two initial conditions  $\mathbf{y}, \mathbf{z}$  on the same orbit  $\mathbf{o}(\mathbf{x})$  generate the same orbit,  $\mathbf{o}(\mathbf{x}) = \mathbf{o}(\mathbf{y}) = \mathbf{o}(\mathbf{z})$ . However, computationally pointwise equality between orbits may be challenging to verify when orbits are merely approximated by numerical integration, and when orbits contain thousands of points. Instead, it may be practical to verify that *orbital averages* of a subset of functions  $\mathcal{G}(\mathcal{X})$  are sufficiently close, resp. distant, to declare that two collections of points belong, resp. do not belong, to the same orbit.

As mentioned in subsection 2.2, the orbital average, or ergodic average, of any observable  $g \in \mathcal{G}(\mathcal{X})$  projects the observable on the invariant eigenspace of the Koopman operator. Therefore the heuristic technique for comparing orbits just described can be interpreted by comparing whether points  $\mathbf{y}$  and  $\mathbf{z}$  are mapped to the same point by a vector valued function  $\mathbf{P}: \mathcal{X} \rightarrow \mathbb{R}^p$ ,  $p \leq \infty$  whose components are all invariant Koopman eigenfunctions:

$$(4.4) \quad \mathbf{Q}(\mathbf{x}) = [q_1(\mathbf{x}) \quad q_2(\mathbf{x}) \quad \dots \quad q_p(\mathbf{x})], \text{ where } \mathcal{K}q_j \equiv q_j.$$

Mezić [235] showed that when the number of averaged functions grows to infinity, this procedure manages to separate ergodic sets that are measure-theoretic counterparts to orbits. This approach was applied to visualize the phase portrait [235, 192, 55], where it is possible to assign pseudocolors to trajectories, generating visually appealing and detailed figures as in Figure 4.2a.

Using the embedding function (4.4) it is further possible to treat the ergodic quotient as a geometric object and compute its local coordinates. Such coordinates parametrize the space of invariant (ergodic) sets; when continuous, they act as a way of ordering level sets of conserved quantities, even when no explicit (or global) formulas for conserved quantities is known. The crucial step is to treat the elements  $q_i(\mathbf{x})$  in (4.4) as Fourier coefficients and define a metric using a Sobolev norm on the associated space. The resulting geometric space can then be coordinatized using manifold learning algorithms.

The ergodic partition is a process of classifying global information, assuming access to many trajectories, into how they relate locally. The opposite direction, where local information is stitched into a global picture is equally as relevant. Consider two disjoint invariant sets  $A, B \subset \mathcal{X}$  of the dynamics  $\mathbf{F}^t: \mathcal{X} \rightarrow \mathcal{X}$ . A typical application

of DMD starts from a single trajectory and constructs a finite-dimensional approximation of the Koopman operator. Depending on whether the initial condition is in  $A$  or in  $B$ , the resulting operator is indistinguishable from the *restricted* Koopman operator  $\mathbf{F}^t|_A : A \rightarrow A$  or  $\mathbf{F}^t|_B : B \rightarrow B$ . The associated Koopman operators  $\mathcal{K}_A$  and  $\mathcal{K}_B$  seemingly have nothing in common. Indeed, it was typical of early papers to either assume that the system has a quasiperiodic attractor, so that all trajectories quickly converge to this set, or to assume that the trajectory used for DMD is ergodic, so that it visits close to any other point in the state space, ruling out the existence of disjoint invariant sets  $A, B$  of positive measure.

If DMD is indeed computed twice, based on trajectories contained in disjoint ergodic sets, it is possible to “stitch” the two operators  $\mathcal{K}_A, \mathcal{K}_B$  together by placing them into a block-diagonal stitched Koopman operator. Assuming that the respective spaces of observables are  $L^2(A, \mu_A), L^2(B, \mu_B)$ , the joint space over  $\mathcal{X} = A \cup B$  can be taken as

$$(4.5) \quad \mathcal{G}(\mathcal{X}) = L^2(A \cup B, \mu_A + \mu_B) = L^2(A, \mu_A) \oplus L^2(B, \mu_B),$$

since any function  $f \in \mathcal{G}(\mathcal{X})$  can be decomposed into disjoint components owing to  $A, B$  being disjoint. Reference [245] gives further theoretical backing to this process, as well an incremental and a non-incremental version of the data-driven DMD procedure built in this fashion. For practical purposes, the assumption that  $A$  and  $B$  are truly dynamically separate is not needed; rather, it is simply sufficient to choose pairs of DMD trajectory samples in a trajectory from two disjoint sets in order to construct such restricted approximations that can be stitched [304].

A particularly important application of stitching across invariant sets concerns phase spaces of systems with symmetries. When the orbit structure is symmetric with respect to a transformation, the analysis of the entire phase space can be dramatically simplified. Symmetry of the differential equations (1.1) with respect to a symmetry group  $\Gamma$ , or  $\Gamma$ -equivariance, is defined as a conjugacy

$$(4.6) \quad \mathbf{f}(\gamma \mathbf{x}) = \gamma \mathbf{f}(\mathbf{x}), \forall \gamma \in \Gamma,$$

where  $\gamma$  represent action by a group element on the state space. An analogous relationship holds for discrete dynamics (1.4). In both cases, the implication is that given any orbit  $\{\mathbf{x}(t)\}_{t \in \mathbb{R}}$ , there exist symmetry-related counterparts  $\{\gamma \mathbf{x}(t)\}_{t \in \mathbb{R}}$  generated by applying any  $\gamma \in \Gamma$  to the orbit. Stability and asymptotic properties of the symmetry-related orbits are the same, which allows us to study just a portion of the state space in detail, and then export those results to other parts of the state space by symmetry.

Although symmetry-based arguments have long been used to simplify dynamical systems, especially in classification of bifurcations, explicit connections with the Koopman operator framework are fairly recent [155, 287, 230, 304]. In all cases, the central role is played by connections between the definition of the Koopman operator and the conjugacy in the definition of equivariance. The following two theorems appear as Thm. III.1 and its corollary in [287], and Thm. 1 and Prop. 2 in [304].

**THEOREM 4.1.** *For a  $\Gamma$ -equivariant dynamical system,  $\mathcal{K}$  commutes with the action of all  $\gamma \in \Gamma$  for any observable  $g \in \mathcal{G}(\mathcal{X})$*

$$(4.7) \quad [\gamma \circ (\mathcal{K}g)](\mathbf{x}) = [\mathcal{K}(\gamma \circ g)](\mathbf{x}).$$

**PROPOSITION 4.2.** *Any eigenspace of  $\mathcal{K}$  for a  $\Gamma$ -equivariant dynamical system is  $\Gamma$ -invariant.*

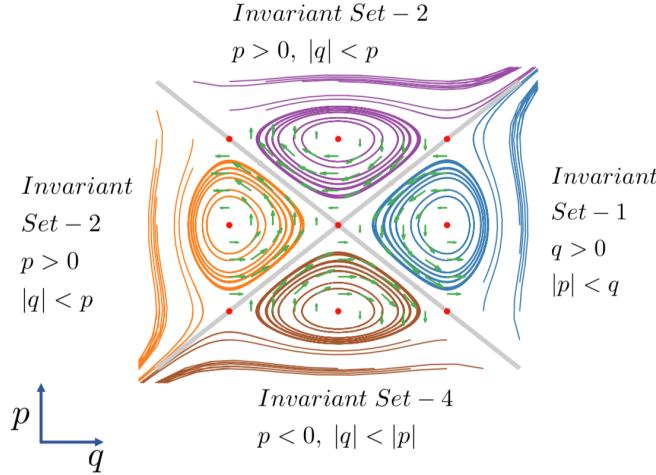


Fig. 4.3: Invariant sets for a dynamical system with  $Z_2 \times Z_2$  symmetry whose Hamiltonian is  $H(p, q) = p^4/4 - 9p^2/2 - q^4/4 + 9q^2/2$ . Reproduced with permission, from Sinha et al. [304].

Proofs of both statements follow by manipulation of the definitions of an eigenfunction (2.12) and equivariance (4.6), and we omit them here. For cyclic groups, i.e., finite groups  $\mathbb{Z}_n = \{1, \gamma, \gamma^2, \dots, \gamma^{n-1}\}$ , a more detailed argument is given in [230], in particular, stating that Koopman modes associated with a particular eigenvalue are similarly symmetric.

The symmetry arguments fit well with the idea of “stitching” the global Koopman operator from “local” Koopman operators, because symmetry removes the need for simulating additional trajectories in order to explore various invariant sets. As [304] show, if two disjoint invariant sets  $A, B \subset \mathcal{X}$  are related by a linear group action  $\tau_\gamma$ , i.e.,  $A = \tau_\gamma B$ , the corresponding Koopman matrices  $\mathbf{K}_A, \mathbf{K}_B$  are conjugate (similar)

$$(4.8) \quad \mathbf{K}_A = \mathbf{T}_\gamma^{-1} \mathbf{K}_B \mathbf{T}_\gamma$$

where the conjugating matrix  $\mathbf{T}$  is the group action on the space of observables. Assuming it is possible to construct such a matrix,  $\mathbf{K}_A$  can be computed without the additional simulation of trajectories, once the DMD matrix  $\mathbf{K}_B$  has been computed.

Even in the case that the full Koopman operator approximation may be directly computed, converting it to a block-diagonal form simplifies the task of computing its spectral properties as eigendecomposition may be performed on individual blocks instead of the entire operator. Commutativity of two linear operators, the Koopman operator and its matrix representation, implies that they preserve each others eigenspaces, further implying that even when the space of observables  $\mathcal{G}(\mathcal{X})$  is not *constructed* as a direct product (4.5), it is possible to perform a change of basis based on the symmetry group such that  $\mathcal{G}(\mathcal{X})$  decomposes into so-called *isotypic* subspaces, invariant with respect to  $\mathcal{K}$ . Consequently, this block-diagonalizes a finite-dimensional representation of the Koopman operator. In [287], this idea is taken as a starting point for a practical block-diagonalization of matrices appearing in DMD.

An example of isotypic decomposition of functions  $g \in \mathcal{G}(\mathcal{X})$  associated with the

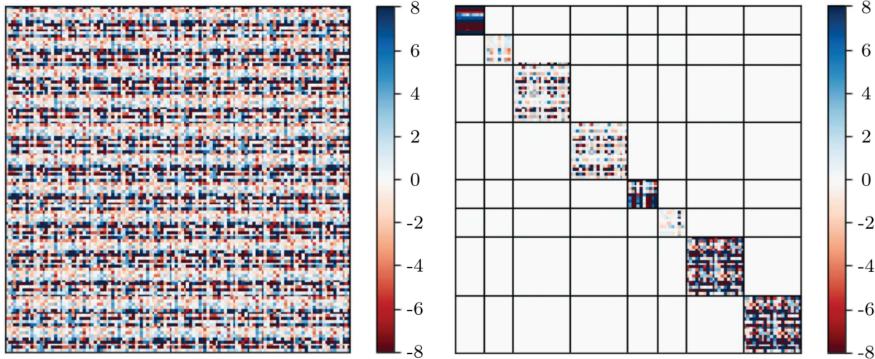


Fig. 4.4: Sparsity structure of DMD matrices before (left) and after (right) block-diagonalization procedure applied to a coupled Duffing oscillator system with  $Z_2 \times D_3$  symmetry. *Reproduced with permission, from Salova et al. 2019 Chaos [287].*

group  $\mathbb{Z}_2$ , where  $\gamma(x) = -x$ , is a decomposition into odd and even components

$$(4.9) \quad g(x) = \underbrace{\frac{g(x) + g(-x)}{2}}_{=:g_e(x)} + \underbrace{\frac{g(x) - g(-x)}{2}}_{=:g_o(x)}$$

Generalization of this procedure to arbitrary finite groups is used as a preconditioning step in a modified eDMD (see subsection 5.1) procedure in [287], resulting in a block-diagonalized form of the associated DMD matrix that approximates the Koopman operator. Consequently, this reduces the computational effort needed to compute eigenvalues of the Koopman operator.

**4.3. Adjoint: The Perron–Frobenius operator.** The Perron–Frobenius (PF) operator, also known as the Ruelle transfer operator, is a linear representation of nonlinear dynamics that traces its roots to the mathematics underpinning statistical and quantum physics, paralleling the development of the Koopman operator. Instead of evolving measurement functions (observables) taking values from the domain of the dynamics, as the Koopman operator does, the PF operator evolves measures (distributions) supported on the domain of the dynamics. As the PF and Koopman operators can be shown to be formally adjoint in appropriately defined function spaces, we summarize the basic concepts related to the PF operator here. The fundamentals are well documented in textbooks and monographs [187, 34, 115, 78] and we point to them for a more precise and general introduction of these topics.

Let the domain of dynamics  $\mathcal{X}$  be given the structure of a Borel measurable space. Given a probability measure  $\mu$ , and any measurable set  $A$ , define the *Perron–Frobenius operator* as

$$(4.10) \quad \mathcal{P}^t \mu(A) := \mu(\mathbf{F}^{-t}(A)),$$

where  $\mathbf{F}^{-t}(A) := \{\mathbf{x} \in \mathcal{X} : \mathbf{F}^t(\mathbf{x}) \in A\}$  is the pre-image of  $A$  through the dynamics. Similar to the Koopman operator, the family  $\mathcal{P}^t$  forms a monoid. An alternative formulation by Lasota and Mackey [187] replaces the action on the space of probability measures with an action on a function space. This assumes that the flow map  $\mathbf{F}^t$  is nonsingular with respect to some ground measure  $m$ , e.g., a Lebesgue measure, meaning

$$(4.11) \quad m(A) \neq 0 \implies m(\mathbf{F}^{-t}(A)) \neq 0.$$

Interpreting  $g \in L^1(\mathcal{X}, dm)$  as densities of measures, i.e.,  $d\mu = gdm$ , it is possible to define the PF operator  $\mathcal{P}^t: L^1(\mathcal{X}, dm) \rightarrow L^1(\mathcal{X}, dm)$  as

$$(4.12) \quad \int_A \mathcal{P}^t g(\mathbf{x}) dm = \int_{\mathbf{F}^{-t}(A)} g(\mathbf{x}) dm,$$

for any Borel set  $A$ . If the flow map is additionally smooth, this definition is equivalent to

$$(4.13) \quad \mathcal{P}^t g(\mathbf{x}) = \int_{\mathbf{F}^{-t}(\mathbf{x})} \frac{g(\mathbf{s})}{|\nabla \mathbf{F}^t(\mathbf{s})|} dm(\mathbf{s}),$$

where  $|\nabla \mathbf{F}^t|$  indicates the determinant of the Jacobian matrix of derivatives of the flow map.

The two formulations (4.10) and (4.12) are connected by interpreting  $g \in L^1$  as densities defining probability measures absolutely continuous with respect to  $dm$ , i.e.,  $d\mu = gdm$ .

Assuming that the dynamics can be restricted to a space of finite measure, it holds that  $L^\infty(\mathcal{X}, dm) \subset L^2(\mathcal{X}, dm) \subset L^1(\mathcal{X}, dm)$ . In this setting, the Koopman and PF operators can be defined, respectively, on  $L^\infty(\mathcal{X}, dm)$  and  $L^1(\mathcal{X}, dm)$ , or both on  $L^2(\mathcal{X}, dm)$ , and one can show that they are adjoint to each other:

$$(4.14) \quad \langle \mathcal{P}^t f, g \rangle = \langle f, \mathcal{K}^t g \rangle, \text{ where } \langle f, g \rangle := \int_{\mathcal{X}} \bar{f}(\mathbf{x}) g(\mathbf{x}) dm.$$

Since the proof [187, §3.3] proceeds by the standard argument of approximation by simple functions, i.e., linear combinations of indicator functions, this relationship extends to a wider range of spaces. Adjoint operators have the same spectrum, although their eigenfunctions do differ, as is the case in general for eigenvectors of matrices and their adjoints (transposes). This connection is partially responsible for the parallel development of Koopman and PF techniques in various contexts of applied mathematics.

The Perron–Frobenius operator lends itself to a particularly straightforward approximation by a stochastic matrix, using a technique termed *Ulam’s method* after a conjecture by S. Ulam [343, §IV.4], ultimately proved to be correct by Y. Li [195]. First, assume that the flow  $\mathbf{F}^t$  preserves a finite probability measure  $m$  on a bounded set  $\mathcal{X}$ , partition  $\mathcal{X}$  into subsets  $\{S_i\}$ , each with the associated characteristic function  $\chi_i$ . Choosing a fixed time  $T$ , we then form the stochastic *Ulam matrix*

$$(4.15) \quad \mathbf{U} = (u_{ij}), \quad u_{ij} := m(\mathbf{F}^{-T}(S_i) \cap S_j).$$

Entries  $u_{ij}$  can be approximately computed by seeding a random (large) collection of initial values in each set  $S_j$  and evolving by  $\mathbf{F}^T$ . The proportion of resulting endpoints of trajectories that land in a set  $S_i$  is entered in  $u_{ij}$ .

The described process amounts to a Monte Carlo integration of the integral  $m(\mathbf{F}^{-T}(S_i) \cap S_j) = \int_{S_j} \chi_{(\mathbf{F}^{-T}(S_i))} dm(\mathbf{x})$  [86, 85], or more generally, a procedure to compute a Galerkin approximation of the PF operator using piecewise constant functions [87]. A computationally efficient implementation as a code GAIO [84] was shown to be able to approximate the eigenvalue spectrum of the PF operator and its eigenfunctions [87] both in the  $L^2$ -space and in fractional Sobolev spaces [107].

Eigenfunctions of the PF operator correspond to complex-valued distributions of points in state space that evolve according to the associated eigenvalue

$$(4.16) \quad \mathcal{P}^t \rho = \lambda^t \rho.$$

When  $\lambda = 1$ ,  $\rho$  are invariant densities, which can be used to estimate the sets containing dynamical attractors, Sinai–Ruelle–Bowen measures, and partition the dynamics into invariant sets. Even away from the limit of the Galerkin approximation, the Ulam matrix  $\mathbf{U}$  can be interpreted as a Markov chain transition matrix on a directed graph, which allows for a definition of almost-invariant sets in the state space [106] and a variational formulation of the problem of locating invariant sets in the state space. Eigenfunctions for eigenvalues with  $|\lambda| \neq 1$  are associated with the mixing properties and escape rates in the state space of dynamical systems [109].

The infinitesimal generator for PF is the Liouville operator  $\mathcal{A}$ , defined analogously to (2.7), which satisfies

$$(4.17) \quad \mathcal{P}^t = e^{t\mathcal{A}}.$$

Similar to the Lie generator of the Koopman operator (2.10), when dynamics are specified using a velocity field  $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$  the Liouville operator can be shown to satisfy

$$(4.18) \quad \mathcal{A}\rho = -\operatorname{div}(\rho\mathbf{f}),$$

further leading to a partial differential equations that eigenfunctions of the Liouville operator and PF operator must satisfy

$$(4.19) \quad \mu\rho + \operatorname{div}(\rho\mathbf{f}) = 0,$$

whenever (4.16) is satisfied with  $\lambda = e^\mu \in \mathbb{C}/\{0\}$ .

Approximating  $\mathcal{A}$  instead of  $\mathcal{P}$  leads to so-called *simulation-free* numerical techniques that can be interpreted either as finite-volume methods for the advection of PDEs, or as spectral collocation methods [108, 32].

Invariant eigenfunctions of both the Koopman and Perron–Frobenius operators have been used to extract invariant sets in the state space of dynamical systems. In function spaces where these operators are dual, eigenfunctions of both operators theoretically contain the same information. However, in reality, the choice may be made based on practical constraints. For example, approximation of invariant sets via Koopman eigenfunctions in [55, 192, 193] relies on long-duration trajectories, while Ulam’s approximation of PF typically requires short bursts of trajectories but seeded densely in the domain.

**4.4. Spectrum beyond eigenvalues.** Spectral characterization of infinite dimensional operators requires a separate treatment of two concepts: of *the spectrum*, which generalizes the set of eigenvalues of finite dimensional operators, and of integration against *spectral measures*, which takes the role of the eigenvalue-weighted summation appearing in the spectral decomposition theorem for normal matrices. Standard textbooks on functional analysis commonly provide an introductory treatment of these concepts; however, among them we highlight [282, 283, 189], which include examples relating to the Koopman operator.

For operators  $\mathbf{T}: \mathcal{G} \rightarrow \mathcal{G}$  acting on a finite-dimensional space  $\mathcal{G}$ , the *spectrum*  $\sigma(\mathbf{T})$  is synonymous with the set of eigenvalues  $\lambda$ , that is scalars  $\lambda$  such that

$$(4.20) \quad \mathbf{T}\xi = \lambda\xi, \text{ or } (\mathbf{T} - \lambda\mathbf{I})\xi = 0,$$

for some vector  $\xi \in \mathcal{G}$ , termed the eigenvector. To extend the concept of a spectrum to operators on Banach spaces, we interpret (4.20) as a statement that eigenvalues  $\lambda$  are those scalars for which the operator  $\mathbf{T} - \lambda\mathbf{I}$  does not have a bounded inverse.

The spectrum  $\sigma(\mathbf{T})$  can be further classified into subsets based on the reason for why  $(\mathbf{T} - \lambda\mathbf{I})^{-1}$  (*the resolvent*) fails to exist as a bounded operator. For  $\lambda \in \sigma_p(\mathbf{T})$  (*the point spectrum*)  $\mathbf{T} - \lambda\mathbf{I}$  is non-injective; this coincides with eigenvalues and is equivalent to a finite-dimensional spectrum. For  $\lambda \in \sigma_c(\mathbf{T})$  (*the continuous spectrum*) the range of  $\mathbf{T} - \lambda\mathbf{I}$  is not the whole codomain (non-surjective), however it is dense in the codomain. For  $\lambda \in \sigma_r(\mathbf{T})$  (*the residual spectrum*) the range of  $\mathbf{T} - \lambda\mathbf{I}$  is not the whole codomain (non-surjective), and it is not even dense in the codomain. There are standard examples of Koopman operators that have continuous and residual spectra, e.g., those equivalent to multiplication operators and shift operators.

The spectral decomposition theorem for normal matrices, which have orthogonal eigenvectors, states that the action of the matrix can be represented by the decomposition

$$(4.21) \quad \mathbf{T}^n \mathbf{g} = \sum_{\lambda \in \sigma(\mathbf{T})} \lambda^n \xi_\lambda \langle \xi_\lambda, \mathbf{g} \rangle.$$

The operators  $\xi_\lambda \langle \xi_\lambda, \cdot \rangle$  are orthogonal spectral projections onto eigenvectors  $\xi_\lambda$ . Generalizing (4.21) to (infinite dimensional) Koopman operators requires that the operators are normal, which holds for certain dynamical systems. For example, when the flow  $\mathbf{F}$  is invertible and preserves a finite measure  $\mu$ , e.g., when the associated velocity field is divergence-free on a bounded domain, working with the Hilbert space  $\mathcal{H}$  of square-integrable observables  $g \in \mathcal{H} = L^2(\mathcal{X}, \mu)$  results in a unitary, and therefore normal, Koopman operator [249]. Then, the classical spectral resolution theorem (due to Hilbert, Stone, and Hellinger) applies to  $\mathcal{K}$  [234, 231, 189] as

$$(4.22) \quad \mathcal{K}^n g = \int_{-\pi}^{\pi} e^{in\omega} d[\mathbb{E}(\omega)g] = \underbrace{\sum_k e^{in\omega_k} \mathbb{P}_k g}_{\text{atomic}} + \underbrace{\int_{-\pi}^{\pi} e^{in\omega} d[\mathbb{E}_c(\omega)g]}_{\text{continuous}},$$

where the operator-valued *spectral measure*  $\mathbb{E}$  forms a partition of unity and can be separated into atomic projections  $\mathbb{P}_k$  and the continuous part  $\mathbb{E}_c$ . This setting covers a wide-range of steady-state dynamics [96, 187, 76].

The atomic part of the spectral measure  $\mathbb{E}(\omega)$  is supported on frequencies  $\omega_k$  that yield eigenvalues  $e^{i\omega_k}$  of  $\mathcal{K}$  and are associated with regular dynamics. As for matrices, when the eigenvalues are simple, the eigenspace projections  $\mathbb{P}_k$  can be written using eigenfunctions  $\varphi_k$  of  $\mathcal{K}$  as

$$(4.23) \quad \mathbb{P}_k g = \langle g, \varphi_k \rangle \varphi_k.$$

The atomic part of the spectral decomposition therefore aligns with the framework described in section 2.

There is no counterpart to the continuous spectral measure  $\mathbb{E}_c(\omega)$  in finite-dimensional settings; therefore, to interpret  $\mathbb{E}_c(\omega)$  and its connections to the dynamics requires routes that do not involve eigenvalues. In the remainder of this section we summarize (a) how existence/non-existence of  $\mathbb{E}_c(\omega)$  is connected to asymptotic statistical properties of the dynamics, (b) how local structure of  $\mathbb{E}_c(\omega)$  connects to evolution of Koopman on subspaces of observables, and (c) how to modify the space of observables in order to convert the continuous spectrum into a continuum of eigenvalues.

**4.4.1. Global properties.** An operator-valued measure  $\mathbb{E}_c(\omega)$  can be converted to a “plain” scalar measure by choosing a function (observable)  $g \in L^2(\mathcal{X}, \mu)$  and

studying its autocorrelation sequence  $\langle \mathcal{K}^n g, g \rangle$ . Applying (4.22) here yields

$$(4.24) \quad \langle \mathcal{K}^n g, g \rangle = \int_{-\pi}^{\pi} e^{in\omega} d\underbrace{\langle \mathbb{E}(\omega)g, g \rangle}_{=: \sigma_g(\omega)},$$

where  $\sigma_g(\omega)$  is the *Fourier or spectral measure* for the evolution of  $g$ .

If the space  $L^2(\mathcal{X}, \mu)$  is defined with respect to an ergodic measure  $\mu$ , the autocorrelation function of the observable can be computed along trajectory initialized at any  $\mathbf{x}$

$$(4.25) \quad C_g(n) := \lim_{K \rightarrow \infty} \frac{1}{K} \sum_{k=0}^{K-1} g(\mathbf{x}_{k+n})g(\mathbf{x}_k) = \lim_{K \rightarrow \infty} \frac{1}{K} \sum_{k=0}^{K-1} [\mathcal{K}^n g](\mathbf{x}_k)g(\mathbf{x}_k)$$

and is directly related to the Fourier coefficients of  $\sigma_g$

$$(4.26) \quad \int_{-\pi}^{\pi} e^{in\omega} d\sigma_g(\omega) = \langle \mathcal{K}^n g, g \rangle = \lim_{K \rightarrow \infty} \frac{1}{K} \sum_{k=0}^{K-1} [\mathcal{K}^n g](\mathbf{x}_k)g(\mathbf{x}_k) = C_g(n).$$

In other words, the Fourier measure  $\sigma_g(\omega)$  is the Fourier transform of the *autocorrelation function*  $C_g(n)$ , which allows for characterization of irregular dynamics in terms of the measure  $\sigma_g$  [171].

In general  $\mathbb{E}$ , and therefore some  $\sigma_g$ , contain all three components that are mutually singular (e.g., the Lebesgue decomposition of a measure [314]):

- atomic component, supported on frequencies of eigenvalues;
- absolutely continuous component, having a spectral density and corresponding to mixing (stochastic-like) behavior;
- singularly continuous component, having a fractal structure.

If  $\sigma_g$  is absolutely continuous, it has a spectral density (the Radon–Nikodym derivative) and then  $C_g(n) \rightarrow 0$ , so the time-separated samples  $g(\mathbf{x}_k)$  will be asymptotically equivalent to independent random variables. If the same holds for all non-constant observables  $g \in \mathbf{1}^\perp$ , the dynamics is mixing. If  $\sigma_g$  has neither atomic components nor a spectral density, it is *singularly continuous*. In this case, samples in the time trace are correlated infinitely often no matter their separation in time, but the correlation occurs rarely enough that *on average* they appear uncorrelated. In this case, the measure can be thought of as having a fractal structure as its support is neither a full interval, nor a collection of discrete points. If this holds for all  $g \in \mathbf{1}^\perp$  then the dynamics is weakly mixing; this is the signature behavior of the so-called weakly-anomalous transport [364, 363].

**4.4.2. Local properties.** To interpret how the local variation of  $\sigma_g(\omega)$  is associated with the dynamics, we investigate integrals over spectral intervals  $[a, b] \subset [-\pi, \pi]$   $\int_a^b e^{in\omega} d\sigma_g(\omega)$ . It can be shown that such restrictions on the spectral domain are equivalent to restrictions of  $\mathcal{K}$  to certain subspaces of observables [280, Prop. 2.7]. More precisely, there exists an orthogonal projection  $P_{[a,b]}$  such that the following equality holds

$$(4.27) \quad \int_a^b e^{in\omega} d\sigma_g(\omega) = \int_{-\pi}^{\pi} e^{in\omega} \mathbf{1}_{[a,b]} d\sigma_g(\omega) = \langle \mathcal{K}^n P_{[a,b]} g, P_{[a,b]} g \rangle.$$

The range of the projection  $P_{[a,b]}$  is the invariant subspace

$$(4.28) \quad \mathcal{H}_{[a,b]} = \{g \in L^2(\mathcal{X}, d\mu) : \sigma_g(\mathbb{T}/[a, b]) = 0\}.$$

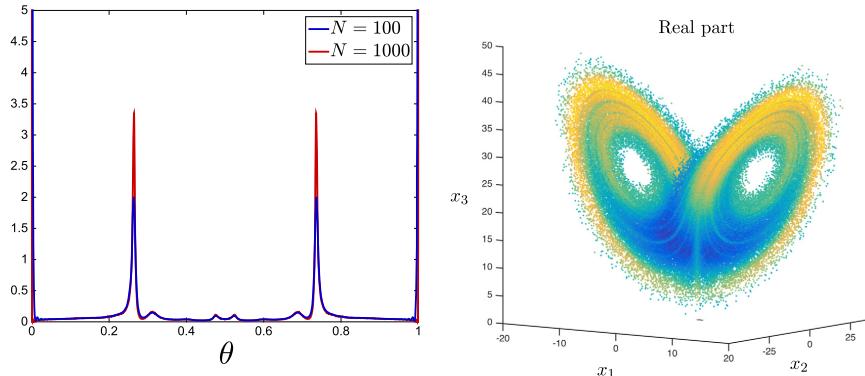


Fig. 4.5: Approximation to the density of spectral measure for the Lorenz'63 model (left) and the real part of the projection of the evolution onto the cyclic vector of the subspace associated with spectral interval  $[0.24, 0.28]$  (right). *Reproduced with permission, from Korda et al. 2020 Appl. Comput. Harmon. Anal. [175].*

In other words, localizing the spectral integral results in a compression of  $\mathcal{K}^t$  to some dynamically-invariant subspace of the space of observables. This holds more generally not only for intervals, but for arbitrary measurable sets in the spectral domain.

In applications, the selection of observables often comes before the analysis of dynamics. If the chosen observable happens to already be in some subspace  $\mathcal{H}_{[a,b]}$ , the restricted integral would be equivalent to its full evolution  $\langle \mathcal{K}^n g, g \rangle = \langle \mathcal{K}^n P_{[a,b]} g, P_{[a,b]} g \rangle$ . In other words, if one would try to infer the “full” evolution of the  $\mathcal{K}$  from a single observable, an unintentional choice of the observable  $g$  from an invariant subspace  $\mathcal{H}_{[a,b]}$  may result that instead of the full operator,  $\mathcal{K}$ , only its compression  $P_{[a,b]}^\top \mathcal{K} P_{[a,b]}$  may be reconstructed. On the other hand, there exists a subspace of observables for which associated Fourier measures are “maximal”, in the sense that any zero set for a maximal measure, i.e. spectral “bandwidth” exhibiting no dynamics, is a zero set for any other Fourier measure. This implies that a judicious choice of observable can make it possible to fully characterize statistical properties of the system from the autocorrelation timeseries of a single observable.

If the content for many spectral intervals  $[a, b] \subset \mathbb{T}$  is of interest, we may want to approximate the weak derivative  $d\sigma_g/d\theta$  and visualize it. In [175] the Fourier coefficients (or trigonometric moments), computed by ergodic averages (4.26), are used to formulate the moment problem for the density  $d\sigma_g/d\theta$ , which is solved using a variational approach based on the Christoffel–Darboux kernel. Based on the approximated density, for any given interval  $[a, b]$  in the spectral domain one can construct a type of an ergodic average that computes the associated projection  $P_{[a,b]}$  of the evolution, resulting in the analog of eigenvectors for the continuous spectral measure. Constructions involved relate to the HAVOK algorithm [47, 14] (see subsection 5.2) due to the correlation function that connects time-delayed samples of the observable. Figure 4.5 demonstrates this approach on an example of the Lorenz'63 dynamical system that is known to be mixing on the attractor [204] by computing its spectral density and a spectral projection for a spectral interval containing significant dynamical content.

**4.4.3. Removing the continuous spectrum by “rigging”.** To illustrate that existence of the continuous spectrum (as defined by non-surjectivity of  $\mathcal{K} - \lambda \mathbf{I}$ ) is not necessarily connected with irregular behavior, [233] studies in detail the pendulum

$$(4.29) \quad \dot{\alpha} = v, \quad \dot{v} = -\sin \theta$$

which can be converted to action-angle variables with  $I \geq 0$  representing the conserved quantity, and a periodic variable  $\theta \in \mathbb{S}^1$  the momentum,

$$(4.30) \quad \dot{I} = 0, \quad \dot{\theta} = I.$$

The exact solution is

$$(4.31) \quad I(t) = I_0, \quad \theta(t) = I_0 t + \theta_0 \pmod{2\pi}.$$

Any observable  $g: \mathbb{R}_+ \times \mathbb{S}^1 \rightarrow \mathbb{R}$  without dependence on the angle coordinate  $g(I, \theta) = g(I)$  is clearly an eigenfunction of  $\mathcal{K}^t$  with  $\lambda = 1$ , since

$$(4.32) \quad \mathcal{K}^t g(I_0) = g(I(t)) = g(I_0),$$

implying that the eigenvalue  $\lambda = 1$  has an infinite multiplicity. This rules out ergodicity, and therefore mixing, with respect to the  $L^2$  space of observables defined over any annulus  $[I_1, I_2] \times \mathbb{S}^1$  of positive area. In other words, the atomic spectrum detects regular behavior of dynamics.

At the same time, no function with a variation in the angular direction is an eigenfunction, as the only translation-invariant function on  $\mathbb{S}^1$  is a constant, despite all trajectories being clearly periodic. However, if observables are taken from a space that includes generalized functions (distributions), then a Dirac- $\delta$  supported on a single level set of  $I$

$$(4.33) \quad g_c(I, \theta) = \delta(I - c)e^{i\theta}$$

would indeed be a (generalized) eigenfunction as

$$(4.34) \quad \mathcal{K}^t g_c(I, \theta) = \delta(I - c)e^{iIt + \theta} = e^{ict}\delta(I - c)e^{i\theta} = e^{ict}g_c(I, \theta).$$

The example above illustrates how a *rigged*<sup>3</sup>, or *equipped* Hilbert space can convert a continuous spectrum (containing no eigenvalues) to a continuum of eigenvalues [12, 315, 334, 210]. Instead of a single  $L^2$  space of observables, the approach employs a so-called Gelfand triple  $\Gamma \subset L^2 \subset \Gamma^\dagger$ , where “the rigging” consists of  $\Gamma$ , a subset of judiciously-chosen test functions, and  $\Gamma^\dagger$  its dual. In the example above,  $\Gamma^\dagger$  contains generalized functions (distributions). By enlarging the domain of the Koopman operator, surjectivity of  $(\mathcal{K} - \lambda\mathbf{I})$  can be mostly restored, resulting in shrinking of the continuous spectrum to a set of discrete values [306].

As a result, the continuous projection measure in the Hellinger–Stone spectral theorem (4.22) can be replaced by an integral against eigenvector-based projections, analogous to (4.21)

$$(4.35) \quad \langle \rho, \mathcal{K}g \rangle = \sum_{\lambda} \lambda \langle \rho, \psi_{\lambda} \rangle \langle \varphi_{\lambda}, g \rangle,$$

for an observable  $g \in \Gamma$  and a density  $\rho \in \Gamma^\dagger$ , while  $\varphi_{\lambda}, \psi_{\lambda}$  are elements of a biorthonormal basis in  $L^2$ . The extended spectrum  $\lambda$  now contains both the  $L^2$ -eigenvalues of  $\mathcal{K}$  and Ruelle–Pollicott resonances [286, 273] associated with infinitesimal stochastic perturbations of the Koopman operator [67, 68]. For example, while the map  $x \mapsto 2x$  on  $\mathbb{S}^1$  has only a constant eigenfunction and only the eigenvalue at 1, a representation

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<sup>3</sup>This metaphor is intended to evoke a utilitarian *rigging of a ship*, rather than a nefarious *rigging of a match*.

in the rigged Hilbert space where  $\Gamma$  are analytic functions yields functions  $\varphi_k, \psi_k$  that are related to Bernoulli polynomials, and values  $\lambda_k = 2^{-k}$  [11].

While the rigged Hilbert space framework has existed since the 1950s and Gelfand, the approach has been used to analyze the Koopman and Perron–Frobenius operators only since the 1990s, and for quantum theory a decade later [209, 210]. Only in the past two years have the modern numerical approaches such as DMD, started to connect to this theory [233, 306], so we expect the growth of interest in this area in the coming years.

#### 4.5. Koopman operators for nonautonomous and stochastic dynamics.

The theory developed so far was based on the time-independent or autonomous dynamics (1.1) and (1.4). This clearly does not cover most models used in practice. Common sources of time variability include changes in system parameters, the presence of input forcing, stochastic noise, and control or actuation. Time variability induced by feedback control is highly structured, and thus Koopman theory can be developed in more detail depending on the structure, as described in section 6. Even though the original justification for DMD-style algorithms was based on the autonomous Koopman framework, the algorithms were applied to data generated by nonautonomous dynamics, either by tacitly assuming that the time variation is negligible, or by employing various sliding window techniques.

**4.5.1. Sliding and multiresolution analysis.** Consider the nonautonomous dynamics

$$(4.36) \quad \dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}, t), \quad \mathbf{x} \in \mathcal{X},$$

and assume that over a time window  $t \in [\tau, \tau + T]$  the function  $\mathbf{F}$  remains approximately constant

$$(4.37) \quad \mathbf{F}(\cdot, t) \approx \mathbf{F}(\cdot, \tau).$$

Furthermore, assume that this holds over a continuous range of starting points  $\tau$ , while maintaining a constant window size  $T$ .

A *sliding window* implies that the snapshots of observations generated by data collected over each time window  $[\tau_i, \tau_i + T]$ , for some  $i = 1, 2, \dots$ , are separately processed by a DMD algorithm to produce eigenvalues  $\lambda_k(\tau, T)$  and DMD modes  $\phi_k(\tau, T)$  that depend on the parameters of the time window. This approach is neither new nor unique to Koopman analysis. In signal processing, computing the discrete Fourier transform over a sliding window goes under several names, including the *Short Time Fourier Transform*, *spectrogram*, *Sliding Discrete Fourier Transform*, or *Time-Dependent Fourier Transform*, and is a standard topic in many signal processing textbooks [254, 313]. If, in addition to the starting point  $\tau$ , the length of the window  $T$  is systematically varied as well, this is known as *multiresolution* or *multiscale analysis*.

The first systematic treatment of multiresolution analysis in the context of DMD presented the basic sliding strategy of computing DMD in several passes over the same set of snapshots [180, 182]. Within each pass, the window size was kept constant, and the starting point of the window was moved in non-overlapping fashion. Several additional strategies for sampling the data and moving the window were discussed, including connections to classical signal processing techniques, such as the Gabor transform [182, 46]. The overlap between consecutive windows can be exploited to compute a more accurate global reconstruction [95], and to reduce the computational effort required to compute the DMD [365]. Sliding window strategies have been found

useful even in autonomous systems [69]; for example, analytic solutions of autonomous dynamics that follow heteroclinic connections between an unstable and a stable fixed point were analyzed, where a well-tuned sliding window is able to discern the difference in DMD spectra near each of the fixed points [259].

#### 4.5.2. Process formulation for the nonautonomous Koopman operator.

The extension of definitions associated with the Koopman operator follow two paths for extending the general theory of dynamical systems: the so-called *process* formulation, or the *skew-product* formulation.

For an autonomous system, such as  $\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t)$ ,  $\mathbf{x}(t_0) = \mathbf{x}_0$ , the time dependence of the corresponding flow map  $\mathbf{x}_0 \mapsto \mathbf{x}_0 e^{\mathbf{A}(t-t_0)}$  can be written in terms of the duration  $t-t_0$  of the time interval over which the dynamics is evolving. The semigroup property (2.6) captures the consistency between advancing dynamics  $t \rightarrow t + \Delta t$  in one step, or in two steps  $t \rightarrow t + \Delta t/2$  and then  $t + \Delta t/2 \rightarrow t + \Delta t$ .

To illustrate the *process* formulation of nonautonomous systems [166, 62, 207], consider the simple nonautonomous ODE

$$(4.38) \quad \dot{x}(t) = \cos(t)x, \quad x(t_0) = x_0$$

solved by

$$(4.39) \quad x(t) = \mathbf{F}_{t_0}^t(x_0) = x_0 e^{\sin(t_0) - \sin(t)}.$$

The time dependence of the flow map cannot be expressed simply in terms of the duration  $t-t_0$ . The consistency of advancing dynamics across adjoining time intervals is now captured by the *cocycle* property

$$(4.40) \quad \mathbf{F}_{t_0}^t(\mathbf{x}) = \mathbf{F}_\tau^t(\mathbf{F}_{t_0}^\tau(\mathbf{x})), \quad \forall \mathbf{x}, \quad 0 \leq t_0 \leq \tau \leq t.$$

Koopman operator can now naturally be formed as a composition operator with this two-parameter flow map [208]

$$(4.41) \quad \mathcal{K}_{t_0}^t g = g \circ \mathbf{F}_\tau^t.$$

Its Lie generator, given by

$$(4.42) \quad \mathcal{L}_{t_0} g := \lim_{t \rightarrow t_0} \frac{\mathcal{K}_{t-t_0}^t g - g}{t},$$

itself depends on time  $t_0$ , in contrast to the autonomous case, and in turn eigenvalues and eigenvectors also depend on time. Such a construction of the Koopman operator appears to match the sliding-window approaches to DMD discussed earlier. However, [208] demonstrate that a sliding-window approach may make large mistakes, especially when the window overlaps the region of rapid change in system parameters; the same source describes an algorithm that is able to detect the local error of a DMD approximation and adjust accordingly, which is particularly effective for so-called hybrid systems, in which the time dependency of the equations is discontinuous.

A word of caution is needed here; in nonautonomous systems (finite- or infinite-dimensional) eigenvalues of the system matrix do not always correctly predict the stability of trajectories. For example, it is possible to formulate a finite-dimensional dynamical system  $\dot{\mathbf{x}} = \mathbf{A}(t)\mathbf{x}$  such that eigenvalues of  $\mathbf{A}(t)$  (the generator of the flow) are time-independent and have negative real value, while the system admits a subspace of unstable solutions [218, 229]. Furthermore, [208] find that methods based on Krylov subspaces, e.g., snapshot-based DMD algorithms, result in substantial errors in the real parts of eigenvalues when the time-dependence of eigenvalues is pronounced, and suggest that the problem can be mitigated by a guided selection of observables.

**4.5.3. Skew-product formulation for the nonautonomous Koopman operator.** We turn now to the *skew-product* formulation, which can incorporate both deterministic and stochastic nonautonomous systems. Consider again the ODE (4.38) but now introduce an additional periodic variable  $y \in \mathbb{S}^1$

$$(4.43) \quad \begin{aligned} \dot{x}(t) &= \cos(y)x, \\ \dot{y}(t) &= 1. \end{aligned}$$

The added variable plays the role of time, re-establishing the semigroup property of the associated flow map which now acts on the extended space  $\mathbf{F}^t: \mathcal{X} \times \mathbb{S}^1 \rightarrow \mathcal{X} \times \mathbb{S}^1$ . The dynamics of  $y(t)$  is itself autonomous and is sometimes referred to as the *driver* for the *driven* dynamics of  $\mathbf{x}(t)$ . The skew-product construction appeared in classical ergodic theory, for example [76].

General analysis of skew-products does not require that  $y(t)$  is as simple as in (4.43); rather, an extension of (1.4) to the more general skew form

$$(4.44) \quad \begin{aligned} \mathbf{x}_{k+1} &= \mathbf{F}(\mathbf{x}_k, \mathbf{y}_k) \\ \mathbf{y}_{k+1} &= \mathbf{G}(\mathbf{y}_k) \end{aligned}$$

can be treated in an analogous fashion. Assuming that the driving dynamics evolves on a compact state space, or otherwise is measurable with a well-defined invariant measure, is sufficient to justify computation of eigenfunctions using ergodic averages (2.30) for time-periodic systems and for systems driven by quasiperiodic dynamics [56, 323].

There are two possible formulations of the Koopman operator associated with (4.44). The first formulation treats the skew-flow as an autonomous system on the extended state space and acts by composing an observable  $g \in \mathcal{G}(\mathcal{X} \times \mathcal{Y})$  with the flow

$$(4.45) \quad [\mathcal{K}g](\mathbf{x}, \mathbf{y}) := g(\mathbf{F}(\mathbf{x}, \mathbf{y}), \mathbf{G}(\mathbf{y})).$$

Since any particular observable on the original state space  $h: \mathcal{X} \mapsto \mathbb{C}$  can be trivially extended to  $h(\mathbf{x}, \mathbf{y}) = h(\mathbf{x})$ , this formulation is sufficient for studying dynamics of a finite collection of observables. However, since the space  $\mathcal{G}(\mathcal{X} \times \mathcal{Y})$  is larger than  $\mathcal{G}(\mathcal{X})$ , representing  $\mathcal{K}$  in a particular basis of observables requires working with a practically larger set, e.g., instead of monomials  $x^k, k = 1, 2, \dots$ , one has to work with  $x^k y^j, k = 1, 2, \dots, j = 1, 2, \dots$ . The problem is, of course, more acute the higher the dimension of  $\mathcal{Y}$ .

**4.5.4. Stochastic Koopman operator.** An alternative formulation of the Koopman operator for (4.44) acts on the observables in the original state variable only,  $\mathcal{G}(\mathcal{X})$ , but retains a parametric dependence of the Koopman operator on the initial condition of the driving system. The skew-flow map used in this case is the interpretation of the second argument in  $\mathbf{F}(\mathbf{x}, \mathbf{y})$  as a parameter for the flow map  $\mathbf{F}_\mathbf{y}(\mathbf{x}) := \mathbf{F}(\mathbf{x}, \mathbf{y})$ . The replacement for the semigroup property of autonomous systems is then the skew-flow property

$$(4.46) \quad \mathbf{F}_\mathbf{y}^{t+s} = \mathbf{F}_{\mathbf{G}^s(\mathbf{y})}^t \circ \mathbf{F}_\mathbf{y}^s.$$

The Koopman operator is then defined as the composition operator with respect to the flow

$$(4.47) \quad [\mathcal{K}_\mathbf{y}^t g](\mathbf{x}) := g(\mathbf{F}_\mathbf{y}^t(\mathbf{x})).$$

In contrast to the “cocycle Koopman operator” (4.41), in which time-dependence is represented by an additional time-like parameter, in this “skew Koopman operator” the time-dependence is an added state-like parameter.

Depending on the properties of the driving system, this framework can encompass not only systems such as (4.43), but also so-called *random dynamical systems* (RDS) [15, 62] for which the driving system on  $\mathcal{Y}$  is simply assumed to be a measure-preserving dynamical system [206, 77].

While several special cases have been discussed in recent literature [77], we focus here on the case of Markovian RDS. This is the case for dynamics generated by a nonlinear stochastic differential equation

$$(4.48) \quad d\mathbf{x}(t) = \mathbf{f}(\mathbf{x})dt + \sigma(\mathbf{x})d\mathbf{w}(t).$$

It is then possible to define a *stochastic* Koopman operator by computing the expectation of the skew-Koopman operator (4.47) (with continuous time domain) over the invariant probability of the driving flow [15, 234]:

$$(4.49) \quad [\mathcal{K}_S^t g](\mathbf{x}) := \mathbb{E}_{\mathbf{y}}\{g(\mathbf{F}_{\mathbf{y}}^t(\mathbf{x}))\}.$$

When the driving system is a stochastic system, this establishes the Koopman operator as the action of the dynamics, averaged over the distribution of the stochastic input.

Furthermore, assuming continuous and bounded functions on the right-hand side of the SDE (4.48), it can be shown that (4.49) is a strongly-continuous semigroup, which is a consequence of the Chapman–Kolmogorov equation, with a well-defined generator  $\mathcal{L}_S$  acting on a space of twice-differentiable observables. In this case, the analogue of the PDE formulation of the generator (2.10) is given by

$$(4.50) \quad \mathcal{L}_S g = \nabla g \cdot \mathbf{f} + \frac{1}{2} \text{Tr}(\boldsymbol{\sigma} \nabla^2 g \boldsymbol{\sigma}^\top).$$

Several DMD algorithms have been adapted to the RDS setting for the Koopman operator [77, 331], with convergence assurances. Additionally, [302] gives an explicit optimization-based approximation of the Koopman operator in this context.

In summary, the theory behind DMD-style algorithms for nonautonomous and stochastic dynamical systems have seen a rapid development in recent years, bringing about both justification for applying such algorithms at first glance “off-the-label”, and providing additional guidance for reduction of bias and errors in computation of eigenvalues and eigenmodes.

**4.6. Partial differential equations.** There already exists a clear connection of Koopman theory to PDEs [183]. Just as with ordinary differential equations, the goal is to discover a linearizing transformation of the governing nonlinear PDE to a new PDE model which evolves linearly in the new coordinate system. Historically, this has been done in a number of contexts, specifically the Cole–Hopf transformation for Burgers’ equation with diffusive regularization and the inverse scattering transform (IST) for completely integrable PDEs. The connection of these two analytic transformations is considered below. Such linearizing transformations have been difficult to achieve in practice. However, data-driven methods have opened new pathways for constructing these transformations. Neural networks, diffusion maps, and time-delay embeddings all allow for the data-driven construction of mappings capable of transforming nonlinear PDEs into linear PDEs whose Koopman operator can be constructed. In this section, we consider the connection of some of the historically

developed methods to Koopman theory. In section 5, we show how such linearizing embeddings are constructed with modern data-driven methods.

The dynamics of nonlinear PDEs evolve on manifolds which are often difficult to characterize and are rarely known analytically. However, an appropriate choice of coordinates can in some cases, *linearize* the dynamics. For instance, the nonlinear evolution governed by Burgers' PDE equation can be linearized by the Cole–Hopf transformation [140, 74], thus providing a linear model that can trivially describe the evolution dynamics. Such exact solutions to nonlinear PDEs are extremely rare and do not often exist in practice, with the inverse scattering transform for Korteweg–deVries, nonlinear Schrödinger, and other integrable PDEs being the notable exceptions [2]. As will be shown in subsection 5.4, neural networks provide a data-driven method to learn coordinate embeddings such as those analytically available from the Cole–Hopf transform and IST.

To demonstrate the construction of a specific and exact Koopman operator, we consider Burgers' equation with diffusive regularization and its associated Koopman embedding [183, 259, 258, 21]. The evolution is governed by diffusion with a nonlinear advection [58]:

$$(4.51) \quad u_t + uu_x - \epsilon u_{xx} = 0 \quad \epsilon > 0, \quad x \in [-\infty, \infty].$$

When  $\epsilon = 0$ , the evolution can lead to shock formation in finite time. The presence of the diffusion term regularizes the PDE, ensuring continuous solutions for all time. In independent, seminal contributions, Hopf [140] and Cole [74] derived a transformation that linearizes the PDE. The Cole–Hopf transformation is defined as follows

$$(4.52) \quad u = -2\epsilon v_x/v.$$

The transformation to the new variable  $v(x, t)$  replaces the nonlinear PDE (4.51) with the linear, diffusion equation

$$(4.53) \quad v_t = \epsilon v_{xx}$$

where it is noted that  $\epsilon > 0$  in (4.51) in order to produce a well-posed PDE. Denoting  $\hat{v} = \hat{v}(k, t)$  as the Fourier transform of  $v(x, t)$  with wavenumber  $k$  gives the analytic solution

$$(4.54) \quad \hat{v} = \hat{v}_0 \exp(-\epsilon k^2 t)$$

where  $\hat{v}_0 = \hat{v}(k, 0)$  is the Fourier transform of the initial condition  $v(x, 0)$ . Thus to construct the Koopman operator, we can then combine the transform to the variable  $v(x, t)$  from (4.52) with the Fourier transform to define the observable  $g(u) = \hat{v}$ . This gives the Koopman operator

$$(4.55) \quad \mathcal{K} = \exp(-\epsilon k^2 t).$$

This is one of the rare instances where an explicit expression for the Koopman operator and the observables can be constructed analytically. As such, Burgers' equation allows one to build explicit representations of Koopman operators that characterize its nonlinear evolution [183, 258].

The inverse scattering transform [2] for other canonical and integrable PDEs, such as the Korteweg–deVries and nonlinear Schrödinger equations, also can lead to an explicit expression for the Koopman operator, but the scattering transform and

its inversion are much more difficult to construct in practice. Peter Lax developed a general mathematical framework that preceded IST theory and which provided a general principle for associating nonlinear evolutions with linear operators so that the eigenvalues of the linear operator are integrals of the nonlinear equation [190]. The scattering theory and its association with nonlinear evolution equations was then placed on more rigorous foundations by the seminal contribution of Ablowitz, Kaup, Newell and Segur known as the AKNS scheme [1].

In brief, the method developed by Lax for constructing analytic solutions for nonlinear evolution equations involved constructing suitable linear operators whose compatibility condition was the evolution equation itself. For a given nonlinear evolution equation

$$(4.56) \quad u_t = N(u, u_x, u_{xx}, \dots),$$

the goal is to posit a *Lax pair* of operators

$$(4.57a) \quad L\phi = \lambda\phi$$

$$(4.57b) \quad \phi_t = M\phi$$

where  $L$  and  $M$  are linear operators. Specifically, the operator  $L$  is a spatial operator that is self-adjoint and does not depend explicitly on  $t$ , while the operator  $M$  is a time-evolution linear operator. Importantly,  $L$ ,  $M$  and the evolution equation for  $u(x, t)$  must be all self-consistent, or compatible, in order for the Lax theory to hold. Self-consistency is achieved by taking the time-derivative of (4.57a) with respect to time and enforcing solutions that have an iso-spectral evolution with respect to these operators so that  $\lambda_t = 0$ . This then gives

$$(4.58) \quad L_t + [L, M] = 0$$

where  $[L, M] = LM - ML$  represents the commutator of the operators. Importantly, within this framework, the operators  $L$  and  $M$  are linear. Thus once found, the evolution dynamics in the transformed coordinate system is *linear*, much like what occurs in the Burgers' example. Of course, such a general mathematical framework only holds for integrable PDEs [1]. However, it does show that the Koopman operator framework is directly associated with the Lax pairs, and in particular with the linear time evolution operator  $M = \mathcal{K}$ , connecting IST and Koopman theory explicitly. Parker and Page [262] recently developed a detailed analysis of fronts and solitons in a variety of systems and explicitly connected their findings to the IST. Moreover, they showed how *two* Koopman decompositions, upstream and downstream of the localized structure, can be used to derive a full Koopman decomposition that leverages the IST mathematical machinery. As will be shown in subsection 5.4, neural networks provide an ideal, data-driven mathematical construct to learn coordinate embeddings such as those analytically available from the Cole–Hopf transform and IST. Indeed, this has been done even for the Kuramoto-Sivashinsky equation [118]. Additional connections between the Cole–Hopf transform and Koopman eigenfunctions in the context of ODEs are discussed in [33].

**5. Data-driven observable selection and embeddings.** Linearizing a nonlinear dynamical system near fixed points or periodic orbits provides a *locally* linear representation of the dynamics [139], enabling the limited use of linear techniques for prediction, estimation, and control [49]. The Koopman operator seeks *globally* linear representations that are valid far from fixed points and periodic orbits. In the data-driven era, this amounts to finding a coordinate system, or *embedding*, defined by nonlinear observable functions that span a Koopman-invariant subspace. Finding, approximating, and representing these observables and embeddings is still a central challenge in modern Koopman theory. Dynamic mode decomposition [294, 284, 180] from section 3 approximates the Koopman operator restricted to a space of linear measurements with a best-fit linear model advancing these measurements from one time to the next. However, linear DMD alone is unable to capture many essential features of nonlinear systems, such as multiple fixed points and transients. It is thus common to augment DMD with nonlinear functions of the measurements [352], although there is no guarantee that these functions will form a closed subspace under the Koopman operator [48]. In this section, we cover several leading approaches to identify and represent Koopman embeddings from data, including the extended dynamic mode decomposition [352] and methods to directly identify eigenfunctions [154], the use of time-delay coordinates [47], as well as machine learning approaches such as diffusion maps [117] and deep neural networks [349, 217, 330, 359, 256, 202].

**5.1. Extended DMD.** Although DMD [294] has become a standard numerical approach to approximate the Koopman operator [284, 341, 180], it is based on linear measurements of the system and is unable to identify nonlinear changes of coordinates necessary to approximate the Koopman operator for strongly nonlinear systems. The extended dynamic mode decomposition (eDMD) [352, 353, 167] was introduced by Williams et al. to address this issue, so that the best-fit linear DMD regression is performed on an augmented vector containing nonlinear measurements of the state. The eDMD approach was recently shown to be equivalent to the earlier variational approach of conformation dynamics (VAC) [250, 252, 253] from the molecular dynamics literature, as explored in the excellent review by Klus et al. [168].

In eDMD, an augmented state  $\mathbf{z}$  is constructed from nonlinear measurements of the state  $\mathbf{x}$  given by the functions  $g_k$ :

$$(5.1) \quad \mathbf{z} = \mathbf{g}(\mathbf{x}) = \begin{bmatrix} g_1(\mathbf{x}) \\ g_2(\mathbf{x}) \\ \vdots \\ g_p(\mathbf{x}) \end{bmatrix}.$$

The vector  $\mathbf{z}$  may contain the original state  $\mathbf{x}$  as well as nonlinear measurements, so often  $p \gg n$ . Next, two data matrices are constructed, as in DMD:

$$(5.2a) \quad \mathbf{Z} = \begin{bmatrix} | & | & & | \\ \mathbf{z}_1 & \mathbf{z}_2 & \cdots & \mathbf{z}_m \\ | & | & & | \end{bmatrix}, \quad \mathbf{Z}' = \begin{bmatrix} | & | & & | \\ \mathbf{z}_2 & \mathbf{z}_3 & \cdots & \mathbf{z}_{m+1} \\ | & | & & | \end{bmatrix}.$$

Here  $\mathbf{z}_k = \mathbf{g}(\mathbf{x}_k) = \mathbf{g}(\mathbf{x}(k\Delta t))$ , where we assume data is sampled at regular intervals in time, for simplicity. As in DMD, a best-fit linear operator  $\mathbf{A}_\mathbf{Z}$  is constructed that maps  $\mathbf{Z}$  into  $\mathbf{Z}'$ :

$$(5.3) \quad \mathbf{A}_\mathbf{Z} = \underset{\mathbf{A}_\mathbf{Z}}{\operatorname{argmin}} \|\mathbf{Z}' - \mathbf{A}_\mathbf{Z} \mathbf{Z}\|_F = \mathbf{Z}' \mathbf{Z}^\dagger.$$

Because the augmented vector  $\mathbf{z}$  may be significantly larger than the state  $\mathbf{x}$ , it is typically necessary to employ kernel methods to compute this regression [353]. In principle, the functions  $\{g_k\}_{k=1}^p$  form an enriched basis in which to approximate the Koopman operator. In the limit of infinite data, the extended DMD operator converges to the Koopman operator projected onto the subspace spanned by these functions [172]. However, if these functions do not span a Koopman invariant subspace, then the projected operator will have spurious eigenvalues and eigenvectors that differ from the true Koopman operator [48].

For example, consider the trivial example of a diagonalized linear system with eigenvalues  $\lambda \in \{1, 2, 5\}$ , eigenvectors  $\xi_j$  in the coordinate directions  $x_j$ , and a naive measurement that mixes the first two eigenvectors:

$$(5.4) \quad \frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad \text{with} \quad y = [1 \quad 1 \quad 0] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$$

In this case, DMD will predict a spurious eigenvalue of 3, which is the sum of the first two eigenvalues  $\lambda = 1$  and  $\lambda = 2$ , since the measurement is a sum of the first two eigenvectors. Therefore, it is essential to use validation and cross-validation techniques to ensure that eDMD models are not overfit, as discussed below.

Eigenfunctions of the Koopman operator form a Koopman invariant subspace and provide an ideal basis, or coordinate system, in which to represent the dynamics. However, Koopman eigenfunctions may not admit a finite representation in any standard basis. Thus, these eigenfunctions may only be approximately represented in a given finite basis. It is possible to approximate an eigenfunction  $\varphi(\mathbf{x})$  as an expansion in terms of the set of candidate functions  $\{g_k(\mathbf{x})\}_{k=1}^p$  from (5.1) as:

$$(5.5) \quad \varphi(\mathbf{x}) \approx \sum_{k=1}^p \xi_k g_k(\mathbf{x}) = \xi^T \mathbf{g}(\mathbf{x}).$$

In discrete-time, a Koopman eigenfunction  $\varphi(\mathbf{x})$  evaluated on a trajectory of snapshots  $\{\mathbf{x}_1, \dots, \mathbf{x}_m\}$  will satisfy:

$$(5.6) \quad \lambda [\varphi(\mathbf{x}_1) \quad \varphi(\mathbf{x}_2) \quad \cdots \quad \varphi(\mathbf{x}_m)] = [\varphi(\mathbf{x}_2) \quad \varphi(\mathbf{x}_3) \quad \cdots \quad \varphi(\mathbf{x}_{m+1})].$$

Expanding the eigenfunction  $\varphi$  using (5.5) this equality becomes

$$(5.7) \quad \lambda [\xi^T \mathbf{z}_1 \quad \xi^T \mathbf{z}_2 \quad \cdots \quad \xi^T \mathbf{z}_m] = [\xi^T \mathbf{z}_2 \quad \xi^T \mathbf{z}_3 \quad \cdots \quad \xi^T \mathbf{z}_{m+1}]$$

which is possible to write as a matrix system of equations in terms of the data matrices  $\mathbf{Z}$  and  $\mathbf{Z}'$ :

$$(5.8) \quad \lambda \xi^T \mathbf{Z} - \xi^T \mathbf{Z}' = \mathbf{0}.$$

If we seek a *least-squares* fit to (5.8), this reduces to extended DMD [353, 352]:

$$(5.9) \quad \lambda \xi^T = \xi^T \mathbf{Z}' \mathbf{Z}'^\dagger.$$

The eigenfunctions  $\varphi(\mathbf{x})$  are formed from left eDMD eigenvectors  $\xi^T$  of  $\mathbf{Z}' \mathbf{Z}'^\dagger$  as  $\varphi \approx \xi^T \mathbf{z}$  in the basis  $\{g_k(\mathbf{x})\}_{k=1}^p$ . The right eigenvectors are the eDMD *modes*.

It is essential to confirm that predicted eigenfunctions actually behave linearly on trajectories, by comparing them with the predicted dynamics  $\varphi(\mathbf{x}_{k+1}) = \lambda \varphi(\mathbf{x}_k)$ ,

as the regression above will result in spurious eigenvalues and eigenvectors unless the basis elements  $g_k$  span a Koopman invariant subspace [48]. It is common to include the original state  $\mathbf{x}$  in the augmented eDMD vector  $\mathbf{z}$ . However, it was shown that including the state  $\mathbf{x}$  in eDMD results in closure issues for systems with multiple fixed points, periodic orbits, or other attractors, because these systems cannot be topologically conjugate to a finite-dimensional linear eDMD system with a single fixed point [48]. For example, the Duffing oscillator in Figure 1.1 has three fixed points, so no finite linear system can accurately evolve the state  $\mathbf{x}$  near all three of these fixed points. However, eigenfunctions like the Hamiltonian, may be accurately expanded in a basis. Thus, it is critical to sort out the accurate and spurious eigenfunctions in eDMD; often eigenfunctions corresponding to lightly damped eigenvalues can be better approximated, as they have a significant signature in the data.

One approach to prevent overfitting is to promote sparsity, as in the sparse identification of nonlinear dynamics (SINDy) [51]. This principle of parsimony may also be used to identify Koopman eigenfunctions by selecting only the few most important terms in the basis  $\{g_k(\mathbf{x})\}_{k=1}^p$  needed to approximate  $\varphi$  [154].

As with standard DMD, the data in  $\mathbf{Z}$  does not need to be generated from a single trajectory, but can instead be sampled more efficiently, such as with latin hypercube sampling or sampling from a distribution over the phase space. In this case, the data in  $\mathbf{Z}'$  must be obtained by advancing the data in  $\mathbf{Z}$  one time step forward. Moreover, reproducing kernel Hilbert spaces (RKHS) can be employed to describe  $\varphi(\mathbf{x})$  *locally* in patches of state space.

For continuous-time dynamics, the eigenfunction dynamics

$$(5.10) \quad \frac{d}{dt}\varphi(\mathbf{x}) = \lambda\varphi(\mathbf{x})$$

may be written in terms of the approximation  $\varphi(\mathbf{x}) \approx \boldsymbol{\xi}^T \mathbf{g}(\mathbf{x})$ :

$$(5.11) \quad \frac{d}{dt}\boldsymbol{\xi}^T \mathbf{g}(\mathbf{x}) = \lambda\boldsymbol{\xi}^T \mathbf{g}(\mathbf{x}).$$

Applying the chain rule results in

$$(5.12) \quad \boldsymbol{\xi}^T \mathbf{\Gamma}(\mathbf{x}, \dot{\mathbf{x}}) = \lambda\boldsymbol{\xi}^T \mathbf{g}(\mathbf{x})$$

where  $\mathbf{\Gamma}$  is given by:

$$(5.13) \quad \mathbf{\Gamma}(\mathbf{x}, \dot{\mathbf{x}}) = \begin{bmatrix} \nabla g_1(\mathbf{x}) \cdot \dot{\mathbf{x}} \\ \nabla g_2(\mathbf{x}) \cdot \dot{\mathbf{x}} \\ \vdots \\ \nabla g_p(\mathbf{x}) \cdot \dot{\mathbf{x}} \end{bmatrix}.$$

Each term is a directional derivative, representing the possible terms in  $\nabla\varphi(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x})$  from (2.31). It is then possible to construct a data matrix  $\mathbf{\Gamma}$  evaluated on the trajectories from  $\mathbf{X}$  and  $\dot{\mathbf{X}}$ :

$$\mathbf{\Gamma} = \begin{bmatrix} \nabla g_1(\mathbf{x}_1) \cdot \dot{\mathbf{x}}_1 & \nabla g_1(\mathbf{x}_2) \cdot \dot{\mathbf{x}}_2 & \cdots & \nabla g_1(\mathbf{x}_m) \cdot \dot{\mathbf{x}}_m \\ \nabla g_2(\mathbf{x}_1) \cdot \dot{\mathbf{x}}_1 & \nabla g_2(\mathbf{x}_2) \cdot \dot{\mathbf{x}}_2 & \cdots & \nabla g_2(\mathbf{x}_m) \cdot \dot{\mathbf{x}}_m \\ \vdots & \vdots & \ddots & \vdots \\ \nabla g_p(\mathbf{x}_1) \cdot \dot{\mathbf{x}}_1 & \nabla g_p(\mathbf{x}_2) \cdot \dot{\mathbf{x}}_2 & \cdots & \nabla g_p(\mathbf{x}_m) \cdot \dot{\mathbf{x}}_m \end{bmatrix}.$$

The Koopman eigenfunction equation then becomes:

$$(5.14) \quad \lambda \xi^T \mathbf{Z} - \xi^T \Gamma = \mathbf{0}.$$

Note that here we use notation where  $\Gamma$  is the transpose of the notation in Kaiser et al. [154] to be consistent with the eDMD notation above.

**5.2. Time delay coordinates.** The DMD and eDMD algorithms are based on the availability of full-state measurements, which are typically quite high-dimensional. However, it is often the case that only partial observations of the system are available, so that there are hidden, or *latent*, variables. In this case, it is possible to use time-delayed measurements of the system to build an augmented state vector, resulting in an intrinsic coordinate system that forms a Koopman-invariant subspace [47]. The use of time-delay coordinates as a Koopman coordinate system relies on the conditions of the Takens embedding theorem [332] being satisfied, so that the delay-embedded attractor is diffeomorphic to the attractor in the original full-state coordinates.

The time-delay measurement scheme is illustrated schematically in Figure 5.1 on the Lorenz'63 system. In this example, we have a single scalar measurement signal  $x(t)$  from the original three-state Lorenz system. It is possible to construct a Hankel matrix  $\mathbf{H}$  from a time-series of this scalar measurement:

$$(5.15) \quad \mathbf{H} = \begin{bmatrix} x(t_1) & x(t_2) & \cdots & x(t_p) \\ x(t_2) & x(t_3) & \cdots & x(t_{p+1}) \\ \vdots & \vdots & \ddots & \vdots \\ x(t_q) & x(t_{q+1}) & \cdots & x(t_m) \end{bmatrix}.$$

Each column of  $\mathbf{H}$  may be obtained by advancing the previous column forward in time by one time step. Thus, we may re-write (5.15) in terms of the Koopman operator  $\mathcal{K}$ :

$$(5.16) \quad \mathbf{H} = \begin{bmatrix} x(t_1) & \mathcal{K}x(t_1) & \cdots & \mathcal{K}^{p-1}x(t_1) \\ \mathcal{K}x(t_1) & \mathcal{K}^2x(t_1) & \cdots & \mathcal{K}^px(t_1) \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{K}^{q-1}x(t_1) & \mathcal{K}^qx(t_1) & \cdots & \mathcal{K}^{m-1}x(t_1) \end{bmatrix}.$$

For a sufficient volume of data, the system will converge to an attractor, so that the columns of  $\mathbf{H}$  become approximately linearly dependent. In this case, it is possible to obtain a Koopman-invariant subspace by computing the SVD of  $\mathbf{H}$ :

$$(5.17) \quad \mathbf{H} = \mathbf{U}\Sigma\mathbf{V}^*.$$

The columns of  $\mathbf{U}$  and  $\mathbf{V}$  from the SVD are arranged hierarchically by their ability to model the columns and rows of  $\mathbf{H}$ , respectively. The low-rank approximation in (5.17) provides a *data-driven* measurement system that is approximately invariant to the Koopman operator for states on the attractor. By definition, the dynamics map the attractor into itself, making it *invariant* to the flow. Often,  $\mathbf{H}$  will admit a low-rank approximation by the first  $r$  columns of  $\mathbf{U}$  and  $\mathbf{V}$ , so that these columns approximate a Koopman-invariant subspace. Thus, the columns of (5.15) are well-approximated by the first  $r$  columns of  $\mathbf{U}$ . The first  $r$  columns of  $\mathbf{V}$  provide a time series of the magnitude of each of the columns of  $\mathbf{U}\Sigma$  in the data. By plotting the first three columns of  $\mathbf{V}$ , we obtain an embedded attractor for the Lorenz system, as in Figure 5.1.

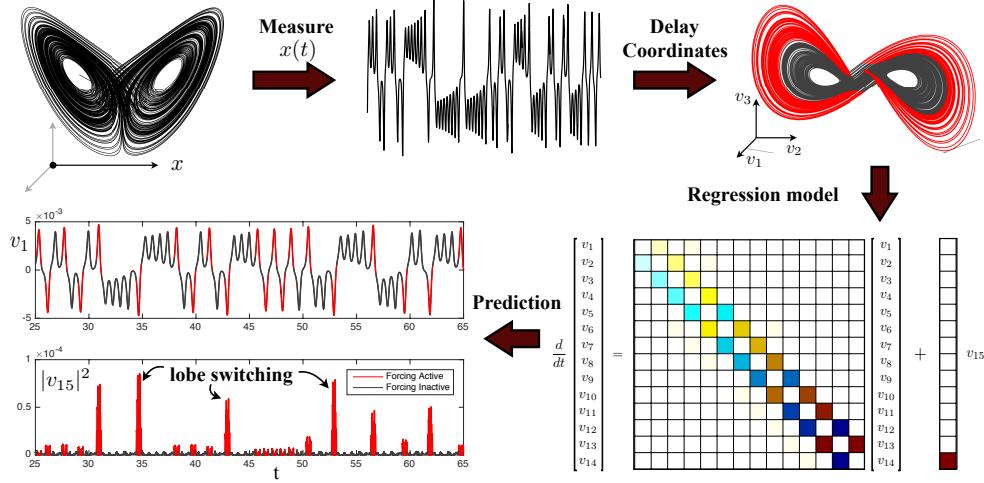


Fig. 5.1: Decomposition of chaos into a linear system with forcing. A time series  $x(t)$  is stacked into a Hankel matrix  $\mathbf{H}$ . The SVD of  $\mathbf{H}$  yields a hierarchy of *eigen* time series that produce a delay-embedded attractor. A best-fit linear regression model is obtained on the delay coordinates  $\mathbf{v}$ ; the linear fit for the first  $r - 1$  variables is excellent, but the last coordinate  $v_r$  is not well-modeled as linear. Instead,  $v_r$  is an input that forces the first  $r - 1$  variables. Rare forcing events correspond to lobe switching in the chaotic dynamics. This architecture is called the Hankel alternative view of Koopman (HAVOK) analysis, from [47]. *Figure modified from Brunton et al. [47].*

Because the columns of  $\mathbf{H}$ , and hence  $\mathbf{U}$ , form a Koopman-invariant subspace, it is possible to perform DMD on the two matrices formed from the first  $p - 1$  and last  $p - 1$  columns of  $\mathbf{H}$ . In practice, we recommend performing DMD on a similar set of two matrices formed from the first  $p - 1$  and last  $p - 1$  columns of  $\mathbf{V}$ , since the columns of  $\mathbf{V}$  are the coordinates of the system in the  $\mathbf{U}\Sigma$  frame. This results in a linear regression model on the variables in  $\mathbf{V}$

$$(5.18) \quad \frac{d}{dt} \mathbf{v}(t) = \mathbf{A}\mathbf{v}(t).$$

Champion et al. [66] showed that this linear system captures the dynamics of weakly nonlinear systems. For chaotic systems, however, even with an approximately Koopman-invariant measurement system, there remain challenges to identifying a closed linear model. A linear model, however detailed, cannot capture multiple fixed points or the unpredictable behavior characteristic of chaos with a positive Lyapunov exponent [48]. Instead of constructing a closed linear model for the first  $r$  variables in  $\mathbf{V}$ , we build a linear model on the first  $r - 1$  variables and impose the last variable,  $v_r$ , as a forcing term [47]:

$$(5.19) \quad \frac{d}{dt} \mathbf{v}(t) = \mathbf{A}\mathbf{v}(t) + \mathbf{B}v_r(t),$$

where  $\mathbf{v} = [v_1 \ v_2 \ \dots \ v_{r-1}]^T$  is a vector of the first  $r - 1$  eigen-time-delay coordinates. In all of the chaotic examples explored [47], the linear model on the first  $r - 1$

terms is accurate, while no linear model represents  $v_r$ . Instead,  $v_r$  is an input forcing to the linear dynamics in (5.19), which approximates the nonlinear dynamics. The statistics of  $v_r(t)$  are non-Gaussian, with long tails correspond to rare-event forcing that drives lobe switching in the Lorenz system; this is related to rare-event forcing distributions observed and modeled by others [211, 288, 212].

The Hankel matrix has been used for decades in system identification, for example in the eigensystem realization algorithm (ERA) [152] and the singular spectrum analysis (SSA) [42]. Computing DMD on a Hankel matrix was first introduced by Tu et al. [341] and was used by B. Brunton et al. [45] in the field of neuroscience. The connection between the Hankel matrix and the Koopman operator, along with the linear regression models in (5.19), was established by Brunton et al. [47] in the Hankel alternative view of Koopman (HAVOK) framework. Several subsequent works have provided additional theoretical foundations for this approach [14, 81, 161, 66, 136]. Hirsh et al. [136] established connections between HAVOK and the Frenet-Serret frame from differential geometry, motivating a more accurate computational modeling approach. The HAVOK approach is also often referred to as delay-DMD [341] or Hankel-DMD [14]. A connection between delay embeddings and the Koopman operator was established as early as 2004 by Mezić and Banaszuk [234], where a stochastic Koopman operator is defined and a statistical Takens theorem is proven. Other work has investigated the splitting of dynamics into deterministic linear, and chaotic stochastic dynamics [231]. The use of delay coordinates may be especially important for systems with long term memory effects and where the Koopman approach has recently been shown to provide a successful analysis tool [327].

**5.3. Diffusion maps for Koopman embeddings.** Diffusion maps are a recently developed nonlinear dimensionality-reduction technique for embedding high-dimensional data on nonlinear manifolds [73, 72, 71, 244]. Diffusion maps leverage the underlying geometry, and in particular its local similarity structure, to create an organization of data that is heavily influenced by local structures. The distance between data is measured by a kernel, for example the Gaussian kernel, which takes the form of the fundamental Green's function solution of the heat equation and is proportional to the connectivity between two data points. The diffusion kernel is given by

$$(5.20) \quad k(\mathbf{x}_j, \mathbf{x}_k) = \exp\left(-\frac{\|\mathbf{x}_j - \mathbf{x}_k\|}{\alpha}\right),$$

where  $\mathbf{x}_j$  and  $\mathbf{x}_k$  are two data points and  $\alpha$  determines the range of influence of the kernel. Thus, points that are not sufficiently close have an approximately zero connectivity since the kernel decays as a Gaussian between data points.

The diffusion kernel plays the role of a normalized likelihood function. It also has important properties when performing spectral analysis of the distance matrix constructed from the embedding. These include symmetry,  $k(\mathbf{x}, \mathbf{y}) = k(\mathbf{y}, \mathbf{x})$ , and positivity preserving,  $k(\mathbf{x}, \mathbf{y}) \geq 0$ . The basic diffusion mapping algorithm computes a kernel matrix  $\mathbf{K}$  whose elements are given by  $K_{j,k} = k(\mathbf{x}_j, \mathbf{x}_k)$ . After normalization of the rows of the kernel matrix, the eigenvalues and eigenvectors of  $\mathbf{K}$  are computed and the data is projected onto the dominant  $r$ -modes. This  $r$ -dimensional subspace is the low-dimensional embedding of the diffusion map. Coifman and Lafon [72] demonstrated that this mapping gives a low dimensional parametrization of the geometry and density of the data. In the field of data analysis, this construction is known as the *normalized graph Laplacian*.

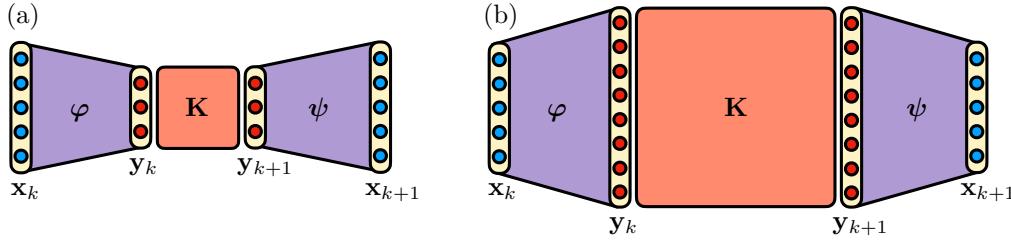


Fig. 5.2: Competing neural network architectures to approximate the Koopman operator. (a) Key Koopman eigenfunctions are extracted with a deep auto-encoder network. (b) Alternatively, the system is lifted to a higher dimension where a linear model is identified. In these architectures  $\varphi$  is the encoder and  $\psi$  is the decoder.

Diffusion maps thus provide a dimensionality reduction method that exploits the geometry and density of the data. The diffusion map can be directly used to construct a Koopman model by using a DMD regression on the time evolution in the diffusion coordinates. The methodology can also be used for forecasting [59], for example leveraging time-delay embeddings to provide a nonparametric forecasting method for data generated by ergodic dynamical systems [117]. Such a representation is based upon the Koopman and Perron-Frobenius groups of unitary operators in a smooth orthonormal basis which is acquired from time-ordered data through the diffusion maps algorithm. Giannakis [117] establishes in such a representation a correspondence between Koopman operators and Laplace-Beltrami operators constructed from data in Takens delay-coordinate space, using this correspondence to provide an interpretation of diffusion-mapped delay coordinates for ergodic systems.

**5.4. Neural networks for Koopman embeddings.** Despite the promise of Koopman embeddings, obtaining tractable representations has remained a central challenge. Even for relatively simple dynamical systems, the eigenfunctions of the Koopman operator may be arbitrarily complex and will only be approximately represented in a finite basis. Deep learning is well-suited for representing such arbitrarily complex functions, and has recently shown tremendous promise for discovering and representing Koopman embeddings [349, 217, 330, 359, 256, 194, 202].

There are two leading deep neural network architectures that have been proposed for Koopman embeddings, shown in Figure 5.2. In the first architecture, the deep auto-encoder architecture extracts a few key latent variables  $\mathbf{y} = \varphi(\mathbf{x})$  to parameterize the dynamics. In the second architecture, the high-dimensional input data is lifted to an even higher dimension, where the evolution is approximately linear. In either Koopman neural network, an additional constraint is enforced so that the dynamics must be linear on these latent variables, given by the linear operator  $\mathbf{K}$ . The constraint of linear dynamics is enforced by the loss function  $\|\varphi(\mathbf{x}_{k+1}) - \mathbf{K}\varphi(\mathbf{x}_k)\|$ , where  $\mathbf{K}$  is a matrix. In general, linearity is enforced over multiple time steps, so that additional terms  $\|\varphi(\mathbf{x}_{k+p}) - \mathbf{K}^p\varphi(\mathbf{x}_k)\|$  are added to the loss function.

Autoencoder networks have the advantage of a low-dimensional latent space, which may promote interpretable solutions. Autoencoders are already widely used to model complex systems, for example in fluid mechanics [50], and they may be viewed as nonlinear extensions of the singular value decomposition, which is central to the DMD algorithm. In this way, a deep Koopman network based on an autoencoder may be viewed as a nonlinear generalization of DMD. Similarly, if the matrix  $\mathbf{K}$  is diagonalized, then the embedding functions  $\varphi$  correspond to Koopman eigen-

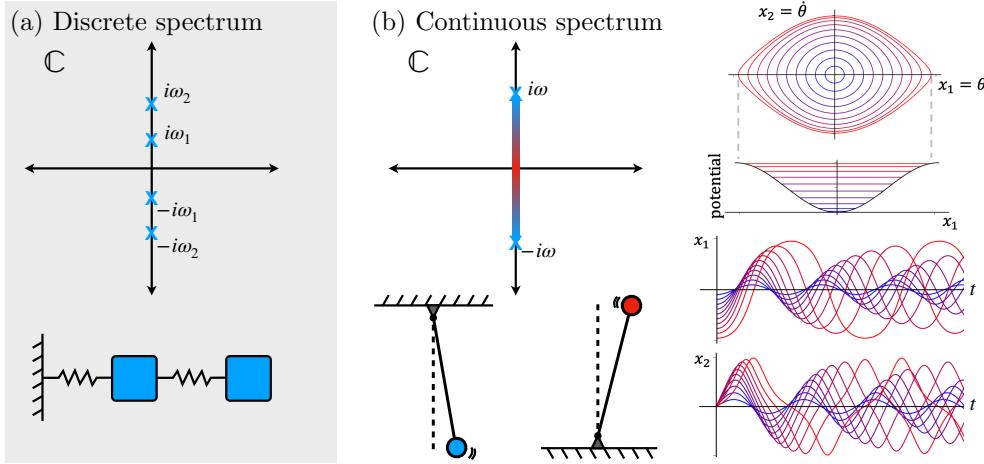


Fig. 5.3: Comparison of discrete vs. continuous spectrum dynamics. *Right panel reproduced from Lusch et al. [202].*

functions [202, 118]. Variational autoencoders are also used for stochastic dynamical systems, such as molecular dynamics, where the map back to physical configuration space from the latent variables is probabilistic [349, 217]. In contrast, the second paradigm, where measurements are lifted to a higher-dimensional space, is related to many results in machine learning, such as Cover's theorem [186], where nonlinear problems tend to become more linear in higher-dimensional embeddings.

For simple systems with a discrete eigenvalue spectrum, a compact representation may be obtained in terms of a few autoencoder variables. However, dynamics with continuous eigenvalue spectra defy standard low-dimensional Koopman representations, including the autoencoder network above. Continuous spectrum dynamics are ubiquitous, ranging from the simple pendulum to nonlinear optics and broadband turbulence. For example, the classical pendulum, given by

$$(5.21) \quad \ddot{x} = -\sin(\omega x)$$

exhibits a continuous range of frequencies, from  $\omega$  to 0, as the amplitude of the pendulum oscillation is increased, as illustrated in Figure 5.3. Thus, the continuous spectrum confounds a simple description in terms of a few Koopman eigenfunctions. Indeed, away from the linear regime, an infinite Fourier sum is required to approximate the continuous shift in frequency, which may explain why the high-dimensional lifting approach has been widely used in Koopman neural networks.

In a recent work by Lusch et al. [202], an auxiliary network is used to parameterize the continuously varying eigenvalue, enabling a network structure that is both parsimonious and interpretable. In contrast to other network structures, which require a large autoencoder layer to encode the continuous frequency shift with an asymptotic expansion in terms of harmonics of the natural frequency, the parameterized network is able to identify a single complex conjugate pair of eigenfunctions with a varying imaginary eigenvalue pair. If this explicit frequency dependence is unaccounted for, then a high-dimensional network is necessary to account for the shifting frequency and eigenvalues. Recently, this framework has been generalized to identify linearizing coordinate transformations for PDE systems [118], such as the Cole-Hopf transform of the nonlinear Burgers' equation into the linear heat equation. Related work has been developed to identify the analogues of Green's functions for nonlinear systems [119].

**6. Koopman theory for control.** The Koopman operator framework is especially relevant for engineering applications in control [226, 257], for which it offers new opportunities for the control of nonlinear systems by circumventing theoretical and computational limitations due to nonlinearity. Nonlinear control methods, such as feedback linearization and sliding mode control, overcome some of these limitations. However, these approaches often do not generalize beyond a narrow class of systems, and deriving stability and robustness conditions, for instance, can become a demanding exercise. Koopman-based methods provide a linear framework that can exploit mature theoretical and computational methods, with successes already demonstrated in a wide range of challenging applications, including fluid dynamics [13, 265], robotics [3, 4, 44, 111], power grid [176, 247], traffic [197], biology [128], logistics [138], and chemical processes [246]. Koopman analysis achieves this by representing the nonlinear dynamics in a globally linear framework, without linearization. Thus Koopman analysis is able to generalize the Hartman-Grobman theorem to the entire basin of attraction of a stable or unstable equilibrium or periodic point [185]. Further, as the Koopman operator acts on observables, it is amenable to data-driven (model free) approaches which have been extensively developed in recent years [275, 351, 173, 276, 316, 154, 155, 264, 4]. The resulting models have been shown to reveal insights into global stability properties [309, 224], observability/controllability [345, 120, 360], and sensor/actuator placement [305, 301] for the underlying nonlinear system.

Koopman theory is closely related to Carleman linearization [63], which also embeds finite-dimensional dynamics into infinite-dimensional linear systems. Carleman linearization has been used for decades to obtain truncated linear (and bilinear) state estimators [179, 40, 9] and to examine stability, observability, and controllability of the underlying nonlinear system [200, 22, 79, 80]. However, the applicability is restricted to polynomial (or analytical) systems. In contrast, the Koopman operator framework does not rely on the analyticity of the vector field, but applies to general nonlinear systems, including systems with discontinuities. Extending Koopman operator theory for actuated systems was first noted in [234], which interpreted the stochastic forcing in random dynamical systems as actuation. The first Koopman-based control schemes were published more than a decade later, powered by the algorithmic development of DMD [275]. More recently, Koopman models have been increasingly used in combination with LQR [48, 111, 112], state-dependent LQR [154], and model predictive control (MPC) [173, 156]. Other directions include optimal control for switching control problems [264, 265], Lyapunov-based stabilization [141, 142], eigenstructure assignment [130], and, more recently, active learning [4]. MPC [114, 191, 227, 241, 279, 113, 60, 8, 97] stands out as a main facilitator for the success of Koopman-based control, with applications including power grids [176], high-dimensional fluid flows [13, 145], and electrical drives [126].

In this section, we review the mathematical formulation for a Koopman operator control framework, beginning with model-based control and moving to data-driven methods. We will describe several approaches for identifying control-oriented models including dynamic mode decomposition with control (DMDc), extended DMD with control (eDMDc), extensions based on SINDy, and the use of delay coordinates. Further, we compare these approaches on numerical examples and discuss the use of the Koopman operator for analyzing important properties, such as stability, observability, and controllability, of the underlying system.

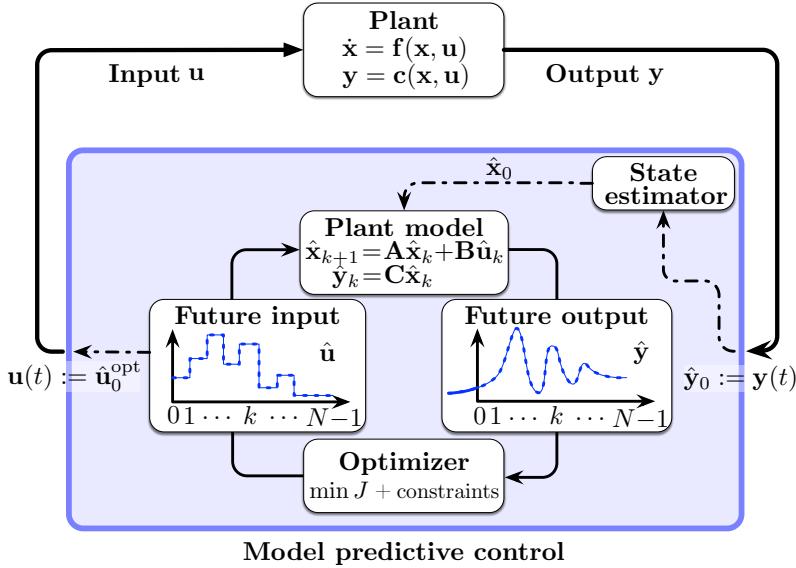


Fig. 6.1: Schematic of the receding horizon model predictive control framework.

**6.1. Model-Based Control.** Beginning with model-based control theory, consider the non-affine nonlinear control system

$$(6.1a) \quad \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}), \quad \mathbf{x}(0) = \mathbf{x}_0$$

$$(6.1b) \quad \mathbf{y} = \mathbf{c}(\mathbf{x}, \mathbf{u}),$$

where  $\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^n$  is the state vector,  $\mathbf{u} \in \mathcal{U} \subseteq \mathbb{R}^q$  is the vector of control inputs, and  $\mathbf{y} \in \mathcal{Y} \subseteq \mathbb{R}^p$  is the output. Unless noted otherwise, we assume full-state measurements  $\mathbf{y} = \mathbf{x}$ . Equation (6.1) represents a non-autonomous dynamical system, where the input  $\mathbf{u}$  may be interpreted as a perturbed parameter or control actuation. In the context of control, we seek typically to determine a feedback control law  $\mathbf{d} : \mathcal{Y} \rightarrow \mathcal{U}$ ,

$$(6.2) \quad \mathbf{u} = \mathbf{d}(\mathbf{y}),$$

that maps measurements  $\mathbf{y}$  to control inputs  $\mathbf{u}$  to modify the behavior of the closed-loop system.

**6.1.1. Model predictive control.** MPC is one of the most successful model-based control schemes [114, 191, 227, 241, 279, 113, 60, 8, 97]. Over the last two decades, MPC has gained increasing popularity due to its success in a wide range of applications, its ability to incorporate customized cost functions and constraints, and extensions to nonlinear systems. In particular, it has become the *de-facto* standard advanced control method in process industries [279] and has gained considerable traction in the aerospace industry due to its versatility [97]. Many of the successes of Koopman-based controls leverage the MPC framework, with its adaptive nature allowing one to compensate for modeling discrepancies and to account for disturbances.

MPC is an adaptive control procedure solving an open-loop optimization problem over a receding horizon (see schematic in Figure 6.1). The optimization problem aims to solve for a sequence of control inputs  $\{\hat{\mathbf{u}}_0, \hat{\mathbf{u}}_2, \dots, \hat{\mathbf{u}}_{N-1}\}$  over the time horizon

$T = N\Delta t$  that minimizes a pre-defined objective function  $J$ . Typically, only the first control input  $\hat{\mathbf{u}}_0^{\text{opt}}$  is applied and then a new measurement is collected. At each time instant a new measurement is collected, the optimization problem is re-initialized and, thus, adaptively determines optimal control actions adjusting to model inaccuracies and changing conditions in the environment. The most critical part of MPC is the identification of a dynamical model that accurately and efficiently represents the system behavior in the presence of actuation. If the model is linear, minimization of a quadratic cost functional subject to linear constraints results in a tractable convex problem. There exist several variants of MPC, including nonlinear MPC, robust MPC, and explicit MPC, which are, however, more computationally expensive and thus limit their real-time applicability. Combining Koopman-based models with linear MPC has the potential to significantly extend the reach of linear MPC for nonlinear systems.

The receding-horizon optimization problem can be stated as follows. Linear MPC aims to minimize the following quadratic objective function

$$(6.3) \quad \min_{\hat{\mathbf{u}}(\cdot|\mathbf{y}) \in \mathbb{U}} J = \min_{\hat{\mathbf{u}}(\cdot|\mathbf{y}) \in \mathbb{U}} \sum_{k=0}^{N-1} \|\hat{\mathbf{y}}_k - \mathbf{r}_k\|_{\mathbf{Q}}^2 + \|\hat{\mathbf{u}}_k\|_{\mathbf{R}}^2 + \|\Delta\hat{\mathbf{u}}_k\|_{\mathbf{R}_{\Delta}}^2$$

subject to discrete-time, linear system dynamics

$$(6.4a) \quad \hat{\mathbf{x}}_{k+1} = \mathbf{A}\hat{\mathbf{x}}_k + \mathbf{B}\hat{\mathbf{u}}_k,$$

$$(6.4b) \quad \hat{\mathbf{y}}_k = \mathbf{C}\hat{\mathbf{x}}_k,$$

and state and input constraints

$$(6.5a) \quad \mathbf{y}_{\min} \leq \hat{\mathbf{y}}_k \leq \mathbf{y}_{\max},$$

$$(6.5b) \quad \mathbf{u}_{\min} \leq \hat{\mathbf{u}}_k \leq \mathbf{u}_{\max},$$

$$(6.5c)$$

where  $\Delta\hat{\mathbf{u}}_k := \hat{\mathbf{u}}_k - \hat{\mathbf{u}}_{k-1}$  is the control input rate. Each term in the cost function (6.3) is computed as the weighted norm of a vector, i.e.  $\|\mathbf{y}\|_{\mathbf{Q}}^2 := \mathbf{y}^T \mathbf{Q} \mathbf{y}$ . In the model (6.4),  $\mathbf{A} : \mathcal{X} \rightarrow \mathcal{X}$  is the state transition matrix,  $\mathbf{B} : \mathcal{U} \rightarrow \mathcal{X}$  is the control matrix, and  $\mathbf{C} : \mathcal{X} \rightarrow \mathcal{Y}$  the measurement matrix. The weight matrices  $\mathbf{R} \in \mathbb{R}^{q \times q}$ ,  $\mathbf{R}_{\Delta} \in \mathbb{R}^{q \times q}$ , and  $\mathbf{Q} \in \mathbb{R}^{n \times n}$  are positive semi-definite and penalize the inputs, input rates, and deviations of the predicted output  $\hat{\mathbf{y}}$  along a trajectory  $\mathbf{r}$ , respectively, and set their relative importance. We define the control sequence to be solved over the receding horizon as  $\hat{\mathbf{u}}(0, \dots, N-1|\mathbf{y}) := \{\hat{\mathbf{u}}_0, \hat{\mathbf{u}}_1, \dots, \hat{\mathbf{u}}_{N-1}\}$  given the measurement  $\mathbf{y}$ . The measurement  $\mathbf{y}$  is the current output of the plant, whose dynamics are governed by a generally nonlinear system (6.1), and is used to estimate the initial condition  $\hat{\mathbf{x}}_0$  for the optimization problem. The general feedback control law (6.2) is then:

$$(6.6) \quad \mathbf{d}(\mathbf{y}) = \hat{\mathbf{u}}^{\text{opt}}(0|\mathbf{y}) = \hat{\mathbf{u}}_0^{\text{opt}}$$

given a specific  $\mathbf{y}$  and selecting the first entry of the optimized control sequence.

Two primary research thrusts, which can be roughly categorized into approaches for either discrete or continuous inputs, have integrated Koopman theory and MPC. For the latter, the Koopman-MPC framework is schematically depicted in Figure 6.2. Output measurements are lifted into a higher-dimensional space using a nonlinear transformation. Dynamics are modeled in the lifted space, typically by solving a linear least-squares regression problem, and the resulting model is employed in the MPC

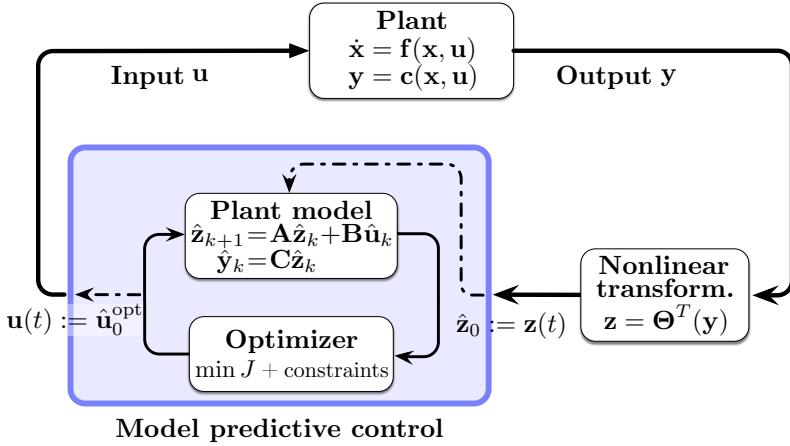


Fig. 6.2: Schematic of the model predictive control framework incorporating a model based on the Koopman operator.

optimization procedure. Besides the goal of achieving increased predictive power via a Koopman-based model, this approach further provides the possibility to readily incorporate nonlinear cost functions and constraints in a linear fashion by incorporating these directly in the set of observables [351].

**6.1.2. Koopman operator theory for control systems.** Koopman theory for control requires disambiguating the unforced dynamics from the effect of actuation. The first Koopman-based approaches were developed for discrete-time systems, which are more general and form a superset containing those induced by continuous-time dynamics. Such discrete-time dynamics are often more consistent with experimental measurements and actuation, and may be preferred for numerical analysis. However, there has been increasing effort in developing formulations building on the Lie operator, i.e. the infinitesimal generator of the semigroup of Koopman operators, for system identification and control.

Consider the non-affine, continuous-time control system given by (6.1a) that is fully observable, i.e.  $\mathbf{y} = \mathbf{x}$  in (6.1b). For every initial condition  $\mathbf{x} \in \mathcal{X}$  and control function  $\mathbf{u} \in \mathcal{U}$ , there exists a unique solution  $\mathbf{F}^t(\mathbf{x}, \mathbf{u})$  at time  $t$  with initial condition  $\mathbf{F}^0(\mathbf{x}, \mathbf{u}) = \mathbf{x}$ . System (6.1) represents a family of differential equations parameterized by the control functions  $\mathbf{u}$ . In order to analyze this from a Koopman perspective, it is convenient to introduce the *control flow*, which defines (6.1) as a single dynamical system (for more details about the dynamical systems perspective of control theory we refer to Colonius et al. [75]). The control flow  $\tilde{\mathbf{F}}^t(\mathbf{x}, \mathbf{u}) : \mathbb{R} \times \mathcal{X} \times \mathcal{U} \rightarrow \mathcal{X} \times \mathcal{U}$  associated with (6.1) is given by the map:

$$(6.7) \quad \tilde{\mathbf{F}}^t(\mathbf{x}, \mathbf{u}) = (\mathbf{F}^t(\mathbf{x}, \mathbf{u}), \Theta^t(\mathbf{u})),$$

where  $\Theta^t(\mathbf{u})$  is the shift on  $\mathcal{U}$ , so that  $\Theta^t(\mathbf{u})(s) = \mathbf{u}(s+t)$ ,  $s \in \mathbb{R}$ . Skew-product flows, such as  $\tilde{\mathbf{F}}^t(\mathbf{x}, \mathbf{u})$ , arise in topological dynamics to study non-autonomous systems, e.g. with explicit time dependency or parameter dependency. Actuation renders the dynamical system and its associated Koopman family (or its generator) non-autonomous. By defining the Koopman operator on the extended state  $\tilde{\mathbf{x}} := [\mathbf{x}^T, \mathbf{u}^T]^T$ , the Koopman operator becomes autonomous and is equivalent to the Koopman operator as-

sociated with the unforced dynamics. Under further special considerations, standard numerical schemes for autonomous systems become readily applicable for system identification. Beyond considering the extended state  $\tilde{\mathbf{x}}$ , we also make the dependency on  $\mathbf{x}$  and  $\mathbf{u}$  explicit to disambiguate the state and inputs.

Let  $g(\mathbf{x}, \mathbf{u}) : \mathcal{X} \times \mathcal{U} \rightarrow \mathbb{C}$  be a scalar observable function of the extended state space. Each observable is an element of an infinite-dimensional Hilbert space and the semigroup of Koopman operators  $\mathcal{K}^t : \mathcal{G}(\mathcal{X}, \mathcal{U}) \rightarrow \mathcal{G}(\mathcal{X}, \mathcal{U})$  acts on these observables according to:

$$(6.8) \quad g(\mathbf{x}(t), \mathbf{u}(t)) = \mathcal{K}^t g(\mathbf{x}_0, \mathbf{u}_0) = g(\tilde{\mathbf{F}}^t(\mathbf{x}_0, \mathbf{u}_0)).$$

Here, it is assumed that the Koopman operator acts on the extended state space in the same manner as the Koopman operator associated with the unforced, autonomous dynamical system. A Koopman eigenfunction  $\varphi(\mathbf{x}, \mathbf{u})$  corresponding to eigenvalue  $\lambda$  then satisfies

$$(6.9) \quad \varphi(\mathbf{x}(t), \mathbf{u}(t)) = \mathcal{K}^t \varphi(\mathbf{x}_0, \mathbf{u}_0) = \lambda^t \varphi(\mathbf{x}_0, \mathbf{u}_0).$$

Further, a vector-valued observable

$$(6.10) \quad \mathbf{g}(\mathbf{x}, \mathbf{u}) := \begin{bmatrix} g_1(\mathbf{x}, \mathbf{u}) \\ \vdots \\ g_p(\mathbf{x}, \mathbf{u}) \end{bmatrix}$$

can be written in terms of the infinite Koopman expansion as

$$(6.11) \quad \mathbf{g}(\mathbf{x}(t), \mathbf{u}(t)) = \mathcal{K}^t \mathbf{g}(\mathbf{x}(0), \mathbf{u}(0)) = \sum_{j=1}^{\infty} \lambda_j^t \varphi_j(\mathbf{x}_0, \mathbf{u}_0) \mathbf{v}_j,$$

where  $\mathbf{v}_j = [\langle \varphi_j, g_1 \rangle, \dots, \langle \varphi_j, g_p \rangle]$ . This representation encompasses dynamics on  $\mathbf{u}$  itself, which may appear due to external perturbations when  $\mathbf{u}$  is interpreted as a perturbed parameter to the system. While the actuation dynamics are typically known or set for both open-loop and closed-loop control, it provides a convenient starting point for system identification. Indeed, it is a useful representation for data-driven approaches that identify the underlying system dynamics and control simultaneously. Depending on the choice of observable functions, further simplifications are possible to identify a model for the state dynamics by incorporating the effect of control, which is discussed in subsection 6.2.

We consider special cases in the discrete-time and continuous-time settings which are modeled within the *Koopman with inputs and control* (KIC) framework [276]. The time-varying actuation input may evolve dynamically according to  $\dot{\mathbf{u}} = \mathbf{h}(\mathbf{u})$  or it may be governed by a state feedback control law (6.2),  $\mathbf{u} = \mathbf{d}(\mathbf{x})$ , as in closed-loop control applications.

*Discrete-time formulation.* For a discrete-time control system

$$(6.12a) \quad \mathbf{x}_{k+1} = \mathbf{F}(\mathbf{x}_k, \mathbf{u}_k),$$

with initial condition  $\mathbf{x}_0$ , the Koopman operator advances measurement functions according to

$$(6.13) \quad \mathcal{K}g(\mathbf{x}_k, \mathbf{u}_k) = g(\mathbf{F}(\mathbf{x}_k, \mathbf{u}_k), \mathbf{u}_{k+1}) = g(\mathbf{x}_{k+1}, \mathbf{u}_{k+1}).$$

Koopman eigenpairs  $(\varphi, \lambda)$  associated with (6.13) satisfy:

$$(6.14) \quad \mathcal{K}\varphi(\mathbf{x}_k, \mathbf{u}_k) = \varphi(\mathbf{F}(\mathbf{x}_k, \mathbf{u}_k), \mathbf{u}_{k+1}) = \varphi(\mathbf{x}_{k+1}, \mathbf{u}_{k+1}) = \lambda\varphi(\mathbf{x}_k, \mathbf{u}_k).$$

By defining the control flow  $\tilde{\mathbf{F}}$  on the extended state space  $\tilde{\mathbf{x}} := [\mathbf{x}^T, \mathbf{u}^T]^T$ , the dynamics become autonomous and can be written as

$$(6.15) \quad \mathcal{K}g(\tilde{\mathbf{x}}_k) = g(\tilde{\mathbf{F}}(\tilde{\mathbf{x}}_k)) = g(\tilde{\mathbf{x}}_{k+1}).$$

If  $\mathbf{u}_{k+1} = \mathbf{H}(\mathbf{u}_k)$ , then  $g(\mathbf{F}(\mathbf{x}_k), \mathbf{H}(\mathbf{u}_k)) = g(\mathbf{x}_{k+1}, \mathbf{u}_{k+1})$ , thus allowing for a suitable choice of observable functions that can simultaneously model and identify dynamics for  $\mathbf{x}$  and  $\mathbf{u}$ . In many situations, we are not interested in the dynamics of  $\mathbf{u}$  itself but only of  $\mathbf{x}$ , e.g. in control where  $\mathbf{u}$  is usually a design variable. For instance, if the dynamics of  $\mathbf{u}$  is prescribed by a specific state-feedback law  $\mathbf{u}_k = \mathbf{D}(\mathbf{x}_k)$ , then  $\mathcal{K}g(\mathbf{x}_k, \mathbf{u}_k) = g(\mathbf{F}(\mathbf{x}_k, \mathbf{u}_k), \mathbf{D}(\mathbf{x}_k)) = g(\mathbf{x}_{k+1}, \mathbf{D}(\mathbf{x}_{k+1}))$ . By defining  $\mathbf{F}^{\mathbf{D}}(\mathbf{x}) := \mathbf{F}(\mathbf{x}, \mathbf{D}(\mathbf{x}))$  and restricting the observable to be a function solely of the state, the Koopman operator is associated with the autonomous dynamics  $\mathbf{F}^{\mathbf{D}}$  for a given control law  $\mathbf{D}$ :  $\mathcal{K}g(\mathbf{x}_k) = g(\mathbf{F}^{\mathbf{D}}(\mathbf{x}_k)) = g(\mathbf{x}_{k+1})$ . If instead, we consider a constant exogenous forcing or discrete control action  $\bar{\mathbf{u}} \in \mathcal{U}$ , where  $\mathcal{U}$  is the set of discrete inputs. The Koopman operator may be defined for each discrete input separately:  $\mathcal{K}^{\bar{\mathbf{u}}}g(\mathbf{x}_k, \bar{\mathbf{u}}) = g(\mathbf{F}(\mathbf{x}_k, \bar{\mathbf{u}}), \bar{\mathbf{u}}) = g(\mathbf{x}_{k+1}, \bar{\mathbf{u}})$ . In general, the Koopman operator and its associated eigenfunctions are parameterized by the discrete control input  $\bar{\mathbf{u}}$  and the dynamics are autonomous for each  $\bar{\mathbf{u}}$ . The flow map  $\mathbf{F}^{\bar{\mathbf{u}}}(\mathbf{x}) := \mathbf{F}(\mathbf{x}, \bar{\mathbf{u}})$  is then defined for each  $\bar{\mathbf{u}}$ . Considering only the reduced dynamics on observable functions of the state, we then obtain

$$(6.16) \quad \mathcal{K}^{\bar{\mathbf{u}}}g(\mathbf{x}_k) = g(\mathbf{F}^{\bar{\mathbf{u}}}(\mathbf{x}_k)) = g(\mathbf{x}_{k+1}).$$

By switching from continuous to discrete inputs, a single model is replaced with a family of models, so that the specific control dependency of the state does not have to be captured. Instead of optimizing the input itself, one may then optimize the switching times between inputs, as in Peitz et al. [264].

*Lie operator formulation.* There has been increasing interest in the control formulation for the infinitesimal generator of the Koopman operator family. It can be shown [187] that if observables  $g$  are continuously differentiable with compact support, then they satisfy the first-order partial differential equation (2.31). The Lie operator  $\mathcal{L}g = \nabla_{\tilde{\mathbf{x}}}g \cdot \tilde{\mathbf{f}}$  associated with the dynamics of the control system (6.1) induces the dynamics

$$(6.17) \quad \frac{d}{dt}g(\mathbf{x}, \mathbf{u}) = \mathcal{L}g(\mathbf{x}, \mathbf{u}).$$

Similarly, smooth eigenfunctions corresponding to the eigenvalue  $\mu$  satisfy

$$(6.18) \quad \frac{d}{dt}\varphi(\mathbf{x}, \mathbf{u}) = \mathcal{L}\varphi(\mathbf{x}, \mathbf{u}) = \mu\varphi(\mathbf{x}, \mathbf{u}).$$

Note that the smooth eigenfunction of the generator is also a Koopman eigenfunction (6.9) and their eigenvalues are connected via  $\mu = \log(\lambda)$  (see also section 2).

We may rewrite the Lie operator in (6.17) explicitly using the chain rule

$$(6.19) \quad \mathcal{L}g(\mathbf{x}, \mathbf{u}) = \nabla_{\mathbf{x}}g(\mathbf{x}, \mathbf{u}) \cdot \dot{\mathbf{x}} + \nabla_{\mathbf{u}}g(\mathbf{x}, \mathbf{u}) \cdot \dot{\mathbf{u}}.$$

The derivatives  $\dot{\mathbf{x}} = \mathbf{f}$  and  $\dot{\mathbf{u}} = \mathbf{h}$  are both velocity vectors (state or action change per time unit) and generally depend on  $\mathbf{x}$  and  $\mathbf{u}$ . These describe local changes in the observable function due to local changes in  $\mathbf{x}$  and external forcing via  $\mathbf{u}$ . For a dynamically evolving  $\mathbf{u}$  it may be possible to approximate the Koopman operator on the extended state using the system identification framework based on the generator formulation [220]. It is also possible to consider  $\dot{\mathbf{u}}$  as the new input to the system [240], while applying more traditional methods. Equation (6.19) represents the adjoint equation of the controlled Liouville equation (see e.g. [41]), which describes how a density function evolves in state space under the effect of external forcing. Using the analogy to the scattering of particles, these transport operators have been used to model and derive optimal control for agent-based systems [184]. For the state-feedback law  $\mathbf{u} = \mathbf{d}(\mathbf{x})$ , then the right-hand side of (6.17) becomes  $\mathcal{L}g(\mathbf{x}, \mathbf{u}) = [\nabla_{\mathbf{x}}g(\mathbf{x}, \mathbf{d}(\mathbf{x})) + \nabla_{\mathbf{u}}g(\mathbf{x}, \mathbf{d}(\mathbf{x})) \cdot \nabla_{\mathbf{x}}\mathbf{d}(\mathbf{x})] \cdot \mathbf{f}(\mathbf{x}, \mathbf{d}(\mathbf{x}))$ . Since this is solely a function of the state, the (autonomous) Koopman operator associated with a particular state-feedback law  $\mathbf{d}(\mathbf{x})$  can be defined on the reduced state  $\mathbf{x}$ :  $\mathcal{L}g(\mathbf{x}) = \nabla_{\mathbf{x}}g(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}, \mathbf{d}(\mathbf{x}))$ .

Constant exogenous forcing or discrete control actions  $\bar{\mathbf{u}} \in \mathcal{U}$  render the system autonomous for each  $\bar{\mathbf{u}}$  so that  $\mathcal{L}^{\bar{\mathbf{u}}}g(\mathbf{x}, \bar{\mathbf{u}}) = \nabla_{\mathbf{x}}g(\mathbf{x}, \bar{\mathbf{u}}) \cdot \mathbf{f}(\mathbf{x}, \bar{\mathbf{u}})$  with  $\dot{\mathbf{u}} = \mathbf{0}$ . In order to apply most control methods a model for the reduced state  $\mathbf{x}$  is required. Thus, by restricting the space of observables defined on the reduced state  $\mathbf{x}$ , we obtain

$$(6.20) \quad \mathcal{L}g(\mathbf{x}) = \nabla_{\mathbf{x}}g(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}, \bar{\mathbf{u}}).$$

This representation is the starting point for data-driven formulations, e.g., to estimate the associated Koopman operator by assuming the zero-order hold for the input across consecutive snapshots, or Koopman operators parameterized by the discrete control input so that a gain-scheduled or interpolated controller may be enacted.

*Bilinearization.* Many applications are modeled by control-affine systems

$$(6.21) \quad \dot{\mathbf{x}} = \mathbf{f}_0(\mathbf{x}) + \sum_{j=1}^q \mathbf{f}_j(\mathbf{x})u_j.$$

Using Carleman linearization, it is possible to transform this system into a (generally infinite-dimensional) bilinear model using multivariable monomials of the state as observables, which is then truncated at a suitable order. However, this may nevertheless lead to systems with an undesirably high dimensionality for the required accuracy. A general nonlinear system  $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u})$  with analytic  $\mathbf{f}$  can also be transformed into an infinite-dimensional bilinear system of the form  $\dot{\mathbf{z}} = \mathbf{A}\mathbf{z} + \dot{\mathbf{u}}\mathbf{B}\mathbf{z}$ , where components of  $\mathbf{z}$  consist of multivariable monomials  $x_i^k u_j^l$ . Note the similarity to the Koopman generator PDE (6.19): considering a smooth vector-valued observable  $\mathbf{g}(\mathbf{x}, \mathbf{u})$ , interpreting  $\dot{\mathbf{u}}$  as new input, and assuming that  $\nabla_{\mathbf{u}}\mathbf{g}(\mathbf{x}, \mathbf{u})$  lies in the span of  $\mathbf{g}(\mathbf{x}, \mathbf{u})$ , this too leads to a bilinear equation and is equivalent to Carleman linearization.

In general, any vector-valued smooth observable with compact support that is solely a function of the state  $\mathbf{x}$ , which evolves according to (6.21), satisfies

$$(6.22) \quad \frac{d}{dt}\mathbf{g}(\mathbf{x}) = \mathcal{L}^{\mathbf{u}}\mathbf{g}(\mathbf{x}) = \nabla_{\mathbf{x}}\mathbf{g}(\mathbf{x}) \cdot \mathbf{f}_0(\mathbf{x}) + \nabla_{\mathbf{x}}\mathbf{g}(\mathbf{x}) \cdot \left( \sum_{j=1}^q \mathbf{f}_j(\mathbf{x})u_j \right),$$

where  $\mathcal{L}^{\mathbf{u}}$  denotes the non-autonomous Lie operator due to the external control input  $\mathbf{u}$ . If  $\nabla_{\mathbf{x}}\mathbf{g}(\mathbf{x}) \cdot \mathbf{f}_j(\mathbf{x})$  lies in the span of  $\mathbf{g}(\mathbf{x})$  for all  $j = 1, \dots, q$ , then there exists a set

of constant matrices  $\mathbf{B}_j$  so that

$$(6.23) \quad \frac{d}{dt} \mathbf{g}(\mathbf{x}) = \mathbf{A}\mathbf{g}(\mathbf{x}) + \sum_{j=1}^q u_j \mathbf{B}_j \mathbf{g}(\mathbf{x}).$$

leading to a bilinear equation for the observable  $\mathbf{g}$ . Here,  $\mathbf{A}$  and  $\mathbf{B}_j$  decompose the Lie operator into an unforced term  $\mathbf{A}$  and forcing terms  $\mathbf{B}_j$  (compare also Figure 6.3). The following theorem appears as Thm. 2 in [120] and states the bilinearizability condition for Eqns. (6.21) and (6.23):

**THEOREM 6.1.** *Suppose there is a finite set of Koopman eigenfunctions associated with the unforced vector field  $\mathbf{f}_0, \varphi_j(\mathbf{x})$  for  $j = 1, \dots, n$ , and these form an invariant subspace of the Lie derivatives  $\mathcal{L}_{\mathbf{f}_j}$ ,  $j = 1, \dots, q$ . Then there exists a finite-dimensional bilinear representation for (6.21), and in turn also for (6.23).*

A special class of observables are Koopman eigenfunctions (or eigenfunctions of the Lie operator), which behave linearly in time by definition. Specifically, smooth eigenfunctions of the Koopman operator associated with the uncontrolled system satisfy

$$(6.24) \quad \frac{d}{dt} \varphi(\mathbf{x}) = \mu \varphi(\mathbf{x}) + \nabla_{\mathbf{x}} \varphi(\mathbf{x}) \cdot \left( \sum_{j=1}^q \mathbf{f}_j(\mathbf{x}) u_j \right),$$

with unforced dynamics determined by its associated eigenvalue  $\mu$  and where the second terms reflects explicitly how the control input affects these eigenfunctions. Koopman eigenfunctions are associated with the global behavior of the system and represent a Koopman-invariant subspace. Equation (6.24) may also represent a bilinear equation (for further details see subsection 6.2.4). Importantly, for systems with low-rank structure it is possible to describe the dynamics in terms of a small number of eigenfunctions which sufficiently well describe the global behavior and avoid the explosion of observables of the Carleman linearization. Even though the system may not be completely bilinearizable, approximate bilinearizability may be sufficient for accurate prediction [120]. Furthermore, there exists a vast literature of diagnostic and control techniques tailored to bilinear systems that can be utilized.

**6.2. Data-Driven Control.** In contrast to model-based control, there are many emerging advances in equation-free, data-driven system identification that leverage Koopman theory. The relationships between some of the more prominent methods and their connection to the Koopman operator are shown in Figure 6.3.

**6.2.1. Dynamic mode decomposition with control.** A major strength of DMD is the ability to describe complex and high-dimensional dynamical systems in terms of a small number of dominant modes, which represent spatio-temporal coherent structures. Reducing the dimensionality of the system from  $n$  (often millions or billions) to  $r$  (tens or hundreds) enables faster and lower-latency prediction and estimation, which generally translates directly into controllers with higher performance and robustness. Thus, compact and efficient representations of complex systems such as fluid flows have been long-sought, resulting in the field of reduced-order modeling. However, the original DMD algorithm was designed to characterize naturally evolving systems, without accounting for the effect of actuation and control.

The *dynamic mode decomposition with control* (DMDc) algorithm by Proctor et al. [275] extends DMD to disambiguate between the natural unforced dynamics and

$$\begin{bmatrix} \mathbf{L}(\mathbf{x}') \\ \mathbf{N}(\mathbf{x}') \\ \mathbf{N}(\mathbf{x}', \mathbf{u}') \\ \mathbf{L}(\mathbf{u}') \\ \mathbf{N}(\mathbf{u}') \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{A} & * & \mathbf{B} \\ * & * & * & * & * \\ \mathbf{H} \\ * & * & * & * & * \end{bmatrix}}_{\mathbf{\kappa}} \begin{bmatrix} \mathbf{L}(\mathbf{x}) \\ \mathbf{N}(\mathbf{x}) \\ \mathbf{N}(\mathbf{x}, \mathbf{u}) \\ \mathbf{L}(\mathbf{u}) \\ \mathbf{N}(\mathbf{u}) \end{bmatrix}$$

Fig. 6.3: Data-driven finite-dimensional approximation of the Koopman operator defined on the extended state space  $(\mathbf{x}, \mathbf{u})$  in practice. As with eDMDc it is also possible to identify evolution dynamics  $\mathbf{u}' = \mathbf{H}(\mathbf{x}, \mathbf{u})$  for the control input within the KIC framework. A state-feedback law  $\mathbf{u} = \mathbf{D}(\mathbf{x})$  may be hidden within  $\mathbf{A}$  and can be identified with knowledge of  $\mathbf{u}$ . Vector-valued observables are splitted into a linear  $\mathbf{L}$  and nonlinear  $\mathbf{N}$  part, e.g.  $\mathbf{g}(\mathbf{x}) := [\mathbf{L}^T(\mathbf{x}) \ \mathbf{N}^T(\mathbf{x})]^T$ .

the effect of actuation. This generalizes the DMD regression to the control form

$$(6.25) \quad \mathbf{x}_{k+1} \approx \mathbf{A}\mathbf{x}_k + \mathbf{B}\mathbf{u}_k.$$

For DMDc, snapshot pairs  $\{\mathbf{x}_j, \mathbf{x}_{j+1}, \mathbf{u}_j\}_{j=1}^m$  of the state variable  $\mathbf{x}$  and actuation command  $\mathbf{u}$  are collected and organized into the following data matrices

$$(6.26) \quad \mathbf{X} = \begin{bmatrix} | & & | \\ \mathbf{x}_1 & \cdots & \mathbf{x}_{m-1} \\ | & & | \end{bmatrix}, \quad \mathbf{X}' = \begin{bmatrix} | & & | \\ \mathbf{x}_2 & \cdots & \mathbf{x}_m \\ | & & | \end{bmatrix}, \quad \mathbf{\Upsilon} = \begin{bmatrix} | & & | \\ \mathbf{u}_1 & \cdots & \mathbf{u}_{m-1} \\ | & & | \end{bmatrix},$$

where  $\mathbf{X}'$  is a time-shifted version of  $\mathbf{X}$ . Then the system matrices  $\mathbf{A}$  and  $\mathbf{B}$  are determined jointly by solving the following least-squares optimization problem

$$(6.27) \quad \min_{[\mathbf{A} \ \mathbf{B}]} \left\| \mathbf{X}' - [\mathbf{A} \ \mathbf{B}] \begin{bmatrix} \mathbf{X} \\ \mathbf{\Upsilon} \end{bmatrix} \right\|_2^2,$$

where the solution is given as  $[\mathbf{A} \ \mathbf{B}] = \mathbf{X}'[\mathbf{\Upsilon}]^\dagger$ .

Originally motivated by intervention efforts in epidemiology [274], DMDc based on linear and nonlinear measurements of the system has since been used with MPC for enhanced control of nonlinear systems by Korda and Mezić [173] and by Kaiser et al. [156], with the DMDc method performing surprisingly well, even for strongly nonlinear systems. DMDc allows for a flexible regression framework, which can accommodate undersampled measurements of an actuated system and identify an accurate and efficient low-order model using compressive system identification [20], which is closely related to the eigensystem realization algorithm (ERA) [152].

**6.2.2. Extended dynamic mode decomposition with control.** The DMDc framework provides a simple and efficient numerical approach for system identification, in which the Koopman operator is approximated with a best-fit linear model advancing linear observables and linear actuation variables. As discussed in subsection 5.1, eDMD is an equivalent approach to DMD that builds on nonlinear observables. An extension of eDMD for controlled systems was first introduced in Williams

et al. [351] to approximate the Koopman operator associated with the unforced system and to correct for inputs affecting the system dynamics and data. Inputs are handled as time-varying system parameters and the Koopman operator is modeled as a parameter-varying operator drawing inspiration from *linear parameter varying* (LPV) models. This approach has been generalized in Korda et al. [173] to identify the system matrices  $\mathbf{A}$  and  $\mathbf{B}$  in the higher-dimensional observable space which disambiguates the unforced dynamics and control on observables. In particular, the Koopman operator is defined as an autonomous operator on the extended state  $\tilde{\mathbf{x}} := [\mathbf{x}^T, \mathbf{u}^T]^T$  as in (6.15) and observables can be nonlinear functions of the state and input, i.e.  $g(\mathbf{x}, \mathbf{u})$ . However, in practice, simplifications are employed to allow for convex formulations of the control problem.

Assuming that the observables are nonlinear functions of the state and linear functions of the control input, i.e.  $\mathbf{g}(\mathbf{x}, \mathbf{u}) := [\theta_1(\mathbf{x}), \dots, \theta_p(\mathbf{x}), u_1, \dots, u_q]^T \in \mathbb{R}^{p+q}$ , and by restricting the dynamics of interest to the state observables  $\theta(\mathbf{x})$  themselves, the linear evolution equation to be determined is

$$(6.28) \quad \mathbf{z}_{k+1} \approx \mathbf{A}\mathbf{z}_k + \mathbf{B}\mathbf{u}_k,$$

where  $\mathbf{z} \in \mathbb{R}^p$  is the vector-valued observable as in subsection 5.1 defined as

$$(6.29) \quad \mathbf{z} := \Theta^T(\mathbf{x}) = \begin{bmatrix} \theta_1(\mathbf{x}) \\ \theta_2(\mathbf{x}) \\ \vdots \\ \theta_p(\mathbf{x}) \end{bmatrix}.$$

Analogous to DMDc (6.26), the (time-shifted) data matrices in the lifted space,  $\mathbf{Z} = \Theta^T(\mathbf{X})$  and  $\mathbf{Z}' = \Theta^T(\mathbf{X}')$ , are evaluated given data  $\mathbf{X}', \mathbf{X}, \Upsilon$ . The system matrices  $\mathbf{A}, \mathbf{B}$  are determined from the least-squares regression problem

$$(6.30) \quad \min_{[\mathbf{A} \ \mathbf{B}]} \left\| \mathbf{Z}' - [\mathbf{A} \ \mathbf{B}] \begin{bmatrix} \mathbf{Z} \\ \Upsilon \end{bmatrix} \right\|_2^2$$

where the solution is given as  $[\mathbf{A} \ \mathbf{B}] = \mathbf{Z}'[\frac{\mathbf{Z}}{\Upsilon}]^\dagger = \Theta^T(\mathbf{X}')[\frac{\Theta^T(\mathbf{X})}{\Upsilon}]^\dagger$ . The state  $\mathbf{x}$  is often included in the basis or space of observables, e.g.  $\mathbf{z} = [\mathbf{x}^T, \Theta(\mathbf{x})]^T$ , and can then be estimated by selecting the appropriate elements of the observable vector  $\mathbf{z}$ , so that  $\mathbf{x} = \mathbf{C}\mathbf{z}$  with the measurement matrix  $\mathbf{C} = [\mathbf{I}_{n \times n} \ \mathbf{0}]$ . If the state vector is not included as observable, one may approximate the measurement matrix by solving an equivalent least-squares problem:

$$(6.31) \quad \min_{\mathbf{C}} \left\| \mathbf{X} - \mathbf{C}\mathbf{Z} \right\|_2^2$$

Alternatively, it has been shown that the state can be estimated using, e.g., multi-dimensional scaling [164]. If full-state information is not available, but only input-output data is available, the observable vector  $\mathbf{z}$  often needs to be augmented with past input and output values, as is typically done in system identification [199], following attractor reconstruction methods, such as the Takens embedding theorem [332].

As eDMD is known to suffer from overfitting, it is important to regularize the problem based on, for instance, the  $L_{1,2}$ -norm for group sparsity [351] or the  $L_1$ -norm [154]. eDMDc yields a linear model for the controlled dynamics in the space of observables through a nonlinear transformation of the state. As with DMDc, it can

be combined with any model-based control approach. In particular, when combined with MPC for a quadratic cost function, the resulting MPC optimization problem can be shown [173] to be independent of the number of observables and to outperform MPC with a model based on a local linearization or Carleman linearization.

**6.2.3. Generalizations of DMDc and eDMDc.** The simple formulation of DMDc and eDMDc as a linear regression problem allows for a number of generalizations that can be easily exploited for integration into existing linear model-based control methods. A number of these generalizations are highlighted here.

*Mixed observables.* eDMDc allows for generalization by using a suitable choice of observable functions. It has also been proposed [173, 276] to include nonlinear observables of the input, e.g.  $g(u) = u^2$ , or mixed observables of the state and input, e.g.  $g(x, u) = xu$ . The advantage of incorporating these measurements has yet to be demonstrated and a subsequent control optimization is not straightforward. However, for systems forced by external inputs or parameters this may provide new opportunities to identify their underlying dynamics, e.g.  $\dot{\mathbf{u}} = \mathbf{h}(\mathbf{x}, \mathbf{u})$  or a state-feedback law  $\mathbf{u} = \mathbf{d}(\mathbf{x})$  (see also Figure 6.3).

*Input and output spaces.* Within the KIC framework [276], different domain and output spaces of the Koopman operator approximation have been examined. This develops more formally what has been implicitly carried out in eDMDc-like methods to obtain models for only the state itself. If only observables that are functions of the state and not of the input are considered, the output space of the Koopman operator can be restricted to a subspace of the Hilbert space spanned by observables which are solely functions of the state and not of the extended state space:

$$(6.32) \quad \mathbf{z}_{x,k+1} = \mathbf{K}_x \mathbf{z}_k = \mathbf{K}_x \begin{bmatrix} \mathbf{g}(\mathbf{x}_k) \\ \mathbf{g}(\mathbf{x}_k, \mathbf{u}_k) \\ \mathbf{g}(\mathbf{u}_k) \end{bmatrix}$$

with vector-valued observables  $\mathbf{z}_x := \mathbf{g}(\mathbf{x})$  and  $\mathbf{z} := [\mathbf{g}^T(\mathbf{x}), \mathbf{g}^T(\mathbf{x}, \mathbf{u}), \mathbf{g}^T(\mathbf{u})]^T$ . This is reasonable as the prediction of the future actuation input  $\mathbf{u}$  is not of interest for the purpose of control. Analogously, Koopman eigenfunction expansions of observables must be distinguished based on the domain and output spaces.

*Time delay coordinates.* Time delay coordinates provide an important and universal class of measurement functions for systems which display long-term memory effects. They are especially important in real-world applications where limited access to full state measurements are available (see subsection 5.2), and they have demonstrated superior performance for control, compared with models using monomials as observables [156]. For simplicity, we will consider a sequence of scalar input-output measurements  $u(t)$  and  $x(t)$ . From these, we may construct a delay vector of inputs  $\mathbf{u}_k := [u_k, u_{k-1}, u_{k-2}, \dots, u_{k-m_u}]^T$  and outputs  $\mathbf{z}_k := \mathbf{g}(\mathbf{x}_k) = [x_k, x_{k-1}, x_{k-2}, \dots, x_{k-m_x}]^T$ , respectively. Here, it is assumed  $m = m_x = m_u$  for simplicity. The dynamics may then be represented as

$$(6.33a) \quad \mathbf{z}_{k+1} = \mathbf{A}\mathbf{z}_k + \mathbf{B}\mathbf{u}_k,$$

$$(6.33b) \quad y_k = [1 \ 0 \ \dots \ 0] \mathbf{z}_k = x_k,$$

where the current state  $x$  is recovered from the first component of  $\mathbf{z}_k$ . Both the system matrix  $\mathbf{A}$  and the control matrix  $\mathbf{B}$  must satisfy an upper triangular structure to not violate causality; otherwise, current states will depend on future states and inputs. Here,  $\mathbf{u}_k$  is constructed from past inputs, while effectively the system has only a

single input. Thus, it is recommended to augment  $\mathbf{z}$  with past inputs, i.e.  $\mathbf{z}_k := \mathbf{g}(\mathbf{x}_k, \mathbf{u}_{k-1}) = [x_k, (x, u)_{k-1}, (x, u)_{k-2}, \dots, (x, u)_{k-m}]$ , so that the current actuation value  $u_k$  appears as a single input to the system [173, 157]:

$$(6.34a) \quad \mathbf{z}_{k+1} = \hat{\mathbf{A}}\mathbf{z}_k + \hat{\mathbf{b}} u_k,$$

$$(6.34b) \quad y_k = [1 \ 0 \ \dots \ 0] \mathbf{z}_k = x_k.$$

This delay observable  $\mathbf{z}_k = \mathbf{g}(\mathbf{x}_k, \mathbf{u}_{k-1})$  has also been used in eDMDc if only input-output data is available [173]. Without the delay information, eDMDc may fail despite the lifting into a higher-dimensional observable space (as for the examples in subsection 6.3). By combining (6.33a) and (6.33b) into a single equation, we obtain an equivalent description to (6.32) with different domain and output spaces:

$$(6.35) \quad z_{1,k+1} = y_{k+1} = [\mathbf{C}\mathbf{A} \quad \mathbf{C}\mathbf{B}] \begin{bmatrix} \mathbf{z}_k \\ \mathbf{u}_k \end{bmatrix}.$$

This formulation is analogous to autoregressive-exogenous (ARX) models in linear system identification [199], where the current output is represented as a linear superposition of past measurements and inputs.

*Parametrized models.* The control input can also be restricted to a finite set of discrete values. The dynamics are then modeled as a linear parameter-varying model, so that each discrete input is associated with an autonomous Koopman operator (6.16) which can be approximated using DMD or eDMD [264]. The control input is thus not modeled explicitly, but implicitly, by switching the model whenever the actuation command switches. The advantage of this formulation is that each model associated with a discrete control input remains autonomous. Recently, this approach has been extended to continuous control input by interpolating between the finite set of control actions, so that the system dynamics are predicted using interpolated models based on the infinitesimal generator of the Koopman operator, leading to bilinear models [266] similar to (6.23). This also alleviates performance issues associated with the time discretization of the models when optimizing their switching times [266, 169].

*Deep Koopman models for control.* Finding a suitable basis or feature space that facilitates a Koopman-invariant subspace remains challenging. Due to their flexibility and rich expressivity [281], there is increased interest in using neural networks to learn complex Koopman representations (see also subsection 5.4). Extending these architectures to incorporate the effect of control requires careful handling of the control variable to ensure tractability of the subsequent control optimization, which a nonlinear transformation of the control variable generally impedes. Building on their work on deep DMD [359] and Koopman Gramians [360], Liu et al. [198] propose to decompose the space of observables as three independent neural networks, associated with parameters  $\theta_x$ ,  $\theta_{xu}$ , and  $\theta_u$ , respectively, to which the input is either the state variable alone, the control variable alone, or both:

$$(6.36) \quad \mathbf{z}_{\mathbf{x},k+1} = \mathbf{K}\mathbf{z}_k = [\mathbf{K}_x \quad \mathbf{K}_{xu} \quad \mathbf{K}_u] \begin{bmatrix} \mathbf{z}_{\mathbf{x},k} \\ \mathbf{z}_{\mathbf{xu},k} \\ \mathbf{z}_{\mathbf{u},k} \end{bmatrix} \quad \text{with} \quad \begin{aligned} \mathbf{z}_{\mathbf{x}} &:= \mathbf{g}(\mathbf{x}, \theta_x), \\ \mathbf{z}_{\mathbf{xu}} &:= \mathbf{g}(\mathbf{x}, \mathbf{u}, \theta_{xu}), \\ \mathbf{z}_{\mathbf{u}} &:= \mathbf{g}(\mathbf{u}, \theta_u). \end{aligned}$$

The unknown Koopman matrices  $\mathbf{K}_\bullet$  and neural network parameters  $\theta_\bullet$ , where  $\bullet = x$ ,  $xu$ , or  $u$ , can then be optimized jointly [198] or separately by switching alternately between model update and parameter update, as in [125, 196]. While the model is linear in the latent space, it is not tractable for prediction and control of the

original system. In order to map back to the original state for predictions and to solve the control optimization problem, the states and control inputs are also directly included as observables, so that  $\mathbf{z}_x := [\mathbf{x}, \mathbf{g}(\mathbf{x}, \boldsymbol{\theta}_x)]^T$  and  $\mathbf{z}_u := [\mathbf{u}, \mathbf{g}(\mathbf{u}, \boldsymbol{\theta}_u)]^T$ . While  $\mathbf{z}_{xu} := \mathbf{g}^T(\boldsymbol{\theta}_{xu})$  is kept the same, it is also possible to neglect  $\mathbf{K}_{xu}$  under certain conditions. In subsequent work [361, 128], slightly modified approaches are studied while maintaining the tractability of the control synthesis problem.

Analogous to eDMDc, a multi-layer perceptron neural network can be used solely to lift the state space, while the effect of the control input in the lifted space remains linear [125], i.e.  $\mathbf{z}_{x,k+1} = \mathbf{A}\mathbf{z}_{x,k} + \mathbf{B}\mathbf{u}$ , where  $\mathbf{K}_x = \mathbf{A}$ ,  $\mathbf{K}_u = \mathbf{B}$ ,  $\mathbf{K}_{xu} = 0$ ,  $\mathbf{z}_x := \mathbf{g}(\mathbf{x}, \boldsymbol{\theta}_x)$ , and  $\mathbf{z}_u := \mathbf{u}$ . The transformation from the latent space to the original state is determined via a least-squares optimization problem analogous to (6.31) where  $\mathbf{Z}$  then represents the output of the neural network  $\mathbf{z}_x$ . Autoencoders provide a natural framework for learning Koopman representations [202] (see also subsection 5.4) combining the state lifting operation and inverse transformation. Recently, this approach has been extended for control by incorporating the control term [125], so that only the state is encoded into  $\mathbf{z}_{x,k}$  and the shifted feature state  $\mathbf{z}_{x,k+1}$  is decoded. These formulations facilitate immediate application of standard linear control methods. Graph neural networks (GNN) [196] have also been exploited to encode and decode the compositional structure of the system, modeling similar physical interactions with the same parameters, resulting in a block-structured, scalable Koopman matrix. The GNNs yield a nonlinear transformation of the state, while the effect of the control input is assumed to be linear in the transformed latent space as above, resulting in a quadratic program for control synthesis.

**6.2.4. Control in intrinsic Koopman eigenfunction coordinates.** Eigenfunctions of the Koopman operator represent a natural set of observables, as their temporal behavior is linear by design. Furthermore, these *intrinsic* observables are associated with global properties of the underlying system. Koopman eigenfunctions have been used for observer design within the Koopman canonical transform (KCT) [316, 317] and within the Koopman reduced-order nonlinear identification and control (KRONIC) framework [154], which both typically yield a global bilinear representation of the underlying system. The Koopman eigenfunctions that are used to construct a reduced description are those associated with the point spectrum of the Koopman operator and are restricted to the unactuated, autonomous dynamics. In particular, we consider control-affine systems of the form

$$(6.37) \quad \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \sum_{j=1}^l \mathbf{h}_j(\mathbf{x}) u_j,$$

where  $\mathbf{h}_j(\mathbf{x})$  are the control vector fields.

The observable vector is defined as

$$(6.38) \quad \mathbf{z} := \mathcal{T}(\mathbf{x}) = \begin{bmatrix} \varphi_1(\mathbf{x}) \\ \varphi_2(\mathbf{x}) \\ \vdots \\ \varphi_p(\mathbf{x}) \end{bmatrix},$$

where  $\mathcal{T} : \mathbb{R}^n \rightarrow \mathbb{C}^p$  represents a nonlinear transformation of the state  $\mathbf{x}$  into eigenfunction coordinates  $\varphi(\mathbf{x})$ , which are associated with the unforced dynamics  $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ . If the  $\varphi$ 's are differentiable at  $\mathbf{x}$ , their evolution equation can be written in terms of the

Lie operator (2.15), i.e.  $\dot{\varphi}(\mathbf{x}) = \mathcal{L}_{\mathbf{f}}\varphi(\mathbf{x}) = \mathbf{f}(\mathbf{x}) \cdot \nabla\varphi(\mathbf{x}) = \mu\varphi(\mathbf{x})$ . Hence, we obtain

$$(6.39) \quad \mathcal{L}_{\mathbf{f}}\mathcal{T}(\mathbf{x}) = \boldsymbol{\Lambda}\mathcal{T}(\mathbf{x}),$$

where  $\boldsymbol{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_p)$  is a matrix, with diagonal elements consisting of the eigenvalues  $\lambda_i$  associated with the eigenfunctions  $\varphi_j$ . Then, the dynamics for observables  $\mathbf{z}$  for the controlled system satisfy (see also (6.24))

$$(6.40a) \quad \dot{\mathbf{z}} = \left( \mathbf{f}(\mathbf{x}) + \sum_{j=1}^l \mathbf{h}_j(\mathbf{x})u_j \right) \cdot \nabla\mathcal{T}(\mathbf{x}) = \mathcal{L}_{\mathbf{f}}\mathcal{T}(\mathbf{x}) + \sum_{j=1}^l \mathcal{L}_{\mathbf{h}_j}\mathcal{T}(\mathbf{x})u_j$$

$$(6.40b) \quad = \boldsymbol{\Lambda}\mathbf{z} + \sum_{j=1}^l \mathbf{b}_j(\mathbf{z})u_j = \boldsymbol{\Lambda}\mathbf{z} + \mathbf{B}(\mathbf{z})\mathbf{u},$$

where  $\mathbf{b}_j(\mathbf{z}) := \mathcal{L}_{\mathbf{h}_j}\mathcal{T}(\mathbf{x})|_{\mathbf{x}=\mathbf{Cz}}$  and  $\mathbf{x} = \mathbf{Cz}$  estimates the state  $\mathbf{x}$  from observables  $\mathbf{z}$ . The system (6.40) is bilinearizable under certain conditions, e.g. if  $\mathcal{L}_{\mathbf{h}_j}\mathcal{T}(\mathbf{x})$  lies in the span of the set of eigenfunctions for all  $j$  [141]. This admits a representation of the Lie operators of the control vector fields in terms of the Koopman eigenfunctions [316].

For  $\mathbf{u} = \mathbf{0}$  the dynamics (6.40b) are represented in a Koopman-invariant subspace associated with the unforced system. For  $\mathbf{u} \neq \mathbf{0}$  the control term  $\mathbf{B}(\mathbf{z})$  describes how these eigenfunctions are affected by  $\mathbf{u}$ . The advantage of this formulation is that the dimension of the system scales with the number of eigenfunctions, and often a few dominant eigenfunctions may be sufficient to capture the principal behavior. In general, the eigenfunctions can be identified using eDMD, kernel-DMD or other variants, and the model (6.40b) may be well represented as long as their span contains  $\mathbf{f}(\mathbf{x})$ ,  $\mathbf{h}_j(\mathbf{x})$ , and  $\mathbf{x}$  [318]. Alternatively, the KRONIC framework seeks to learn eigenfunctions directly, which are sparsely represented in a dictionary of basis functions. The control term  $\mathbf{B}(\mathbf{z})$  can either be determined from the gradient of the identified eigenfunctions for known  $\mathbf{h}_j(\mathbf{x})$  or identified directly [155] for unknown  $\mathbf{h}_j(\mathbf{x})$  by similarly expanding it in terms of a dictionary. Multiple works have since been published focusing on the direct identification of Koopman eigenfunctions [174, 127, 261]. In any case, validating the discovered eigenfunctions, i.e. ensuring that these behavior linearly as predicted by their associated eigenvalue, is critical for prediction tasks.

**6.3. Koopman-based control strategies.** In contrast to linear systems, the control of nonlinear systems remains an engineering grand challenge. Many real-world systems represent a significant hurdle to nonlinear control design, leading to linear approximations which produce suboptimal solutions. Linear Koopman-based models aim to capture the dynamics of a nonlinear system, and thus leverage linear control methods. The predictive power of linear models is increased within the Koopman operator framework by replacing (or augmenting) the state space with nonlinear observables. Nonlinear observables are not completely new in the context of control theory, but appear also as the (control) Lyapunov function for stability, the value function in optimal control, or as measurement functions in input-output linearization. Normally the state itself is included in the set of observables. While this is problematic from the perspective of finding a linear, closed form approximation to the Koopman operator associated with the underlying nonlinear system [48], it allows one to easily measure the state given the model output and the cost function associated with the original control problem. If the state is not included, a measurement matrix or function mapping from the nonlinear observables to the state vector needs to be estimated along with the system matrices, typically introducing additional errors.

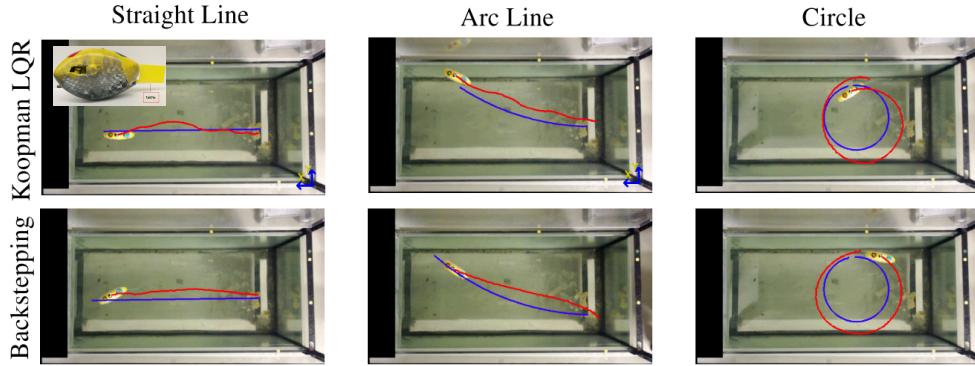


Fig. 6.4: Tail-actuated robotic fish (top left corner) developed by the Smart Microsystems Lab at Michigan State University for trajectory tracking using Koopman LQR (top row) and backstepping (bottom row). Reference trajectory is displayed in blue, controlled trajectory in red. *Reproduced with permission, from Mamakoukas et al. 2019 Robotics: science and systems [111].*

Koopman-based frameworks are amenable to the application of standard linear estimation and control theory, and these have been increasingly used in combination with optimal control [48, 111, 4, 154, 173, 155, 13, 264, 3, 264] using DMDc and eDMDc models (see subsection 6.2.1 and 6.2.2). In the simplest case, a linear quadratic regulator may be used, which has been successfully demonstrated in experimental robotics [111, 112], as in Figure 6.4. In addition to modifying the eigenvalues of the closed-loop system as in pole placement, the shape of Koopman eigenfunctions may be modified directly using eigenstructure assignment [130]. Several other approaches build on a global bilinearization [316, 154, 141] of the underlying system in terms of Koopman eigenfunctions (see subsection 6.2.4). Under certain conditions, this may allow one to stabilize the underlying dynamical system with feedback linearization [120]. Feedback stabilization for nonlinear systems can also be achieved via a control Lyapunov function [316] expressed in Koopman eigenfunctions, for which the search can be formulated as a convex optimization [141, 142]. Stabilizing solutions have also been determined by constructing a Lyapunov function from stable Koopman models obtained by imposing stability constraints on the Koopman matrix [110]. Sequential action control [10] is an alternative to MPC in experimental robotics [3, 4], which optimizes both the control input and the control duration. This is a convex approach applicable to control-affine systems, and as such, may also be combined with Koopman bilinearizations.

Although the predictive power of Koopman models can be sensitive to the particular choice of observables and the training data, in particular receding-horizon methods such as MPC (see subsection 6.1.1) provide a robust control framework that systematically compensate for model uncertainties by continually updating the optimization problem and taking into account new measurements. Incorporating Koopman-based models into MPC was first introduced in Korda & Mezić [173] using eDMDc. The eDMDc results in a convex quadratic programming problem whose computational cost remains comparable to that of linear MPC and is independent of the number of observables if the optimization problem [173]. MPC has also been used for control in Koopman eigenfunction coordinates [154, 155], for optimal switching control using

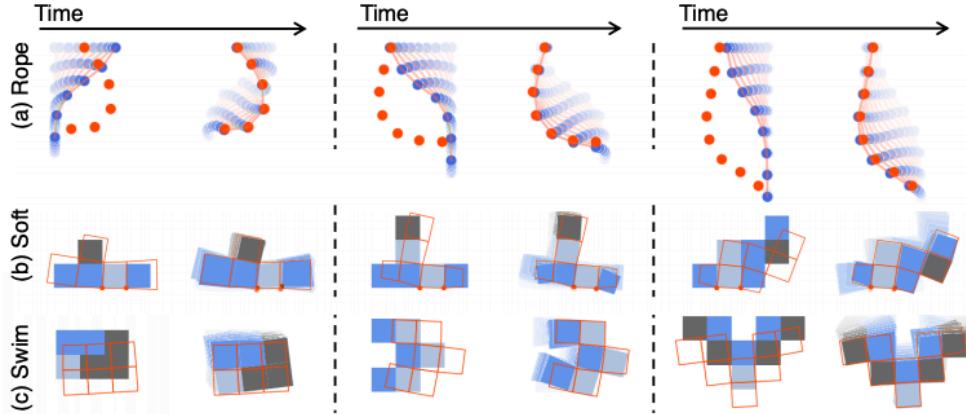


Fig. 6.5: Model predictive control of compositional systems by combining Koopman operators with graph neural networks for an object-centric embedding. *Reproduced with permission from Li et al. 2019 ICLR [196].*

linear parameter-varying eDMD models [264] associated with discrete control inputs, and interpolated Koopman models [263, 266] extending to continuous control inputs. The latter approach combines the data efficiency of estimating autonomous Koopman models associated with discrete control inputs with continuous control, which is achieved by relaxation of the switching control approach. Convergence can be proven, albeit assuming an infinite-data limit and an infinite number of basis functions. In general, guarantees on optimality, stability, and robustness of the controlled dynamical system remain limited. Of note are Koopman Lyapunov-based MPC that guarantees closed-loop stability and controller feasibility [246, 307]. More recently, deep learning architectures have been increasingly used to represent the nonlinear mapping into the observable space. These have also been combined with MPC with promising results [196] (see also Figure 6.5).

The success of Koopman-based MPC belies the practical difficulties of approximating the Koopman operator. On the one hand, there exist only a few systems with a known Koopman-invariant subspace and eigenfunctions, on which models could be analyzed and evaluated. On the other hand, even the linearity property of the Koopman eigenfunctions associated with the model is rarely validated and MPC exhibits an impressive robustness when handling models with very limited predictive power. Thus, there have been impressive practical successes, but there are open gaps in understanding how well the Koopman operator is actually approximated and what possible error bounds can be given. In addition to theoretical advances, Koopman-based control has been increasingly applied in real-world problems such as power grids [176, 247], high-dimensional fluid flows [205, 13, 265, 266], biological systems [128], chemical processes [246, 307], human-machine systems [39], and experimental robotic systems [4, 44, 111, 43, 104].

Multiple variants of Koopman-based control have been demonstrated in numerical and experimental settings. Here, we illustrate model predictive control (MPC, see subsection 6.1.1 for details) combined with different Koopman-based models for several nonlinear systems including a bilinear DC motor (see also [173]), the forced Duffing oscillator, and the van der Pol oscillator. An overview of the parameters,

models and controls are presented in Tab. 6.1 with results summarized in Figure 6.6 and Figure 6.7. Consider the single-input single-output (SISO) system

Examples			
	Bilinear DC motor	Forced Duffing oscillator	Van der Pol oscillator
<b>Training</b>	$L_a = 0.314,$ $R_a = 12.345,$ $k_m = 0.253,$ $J = 0.00441,$ $B = 0.00732,$ $\tau_l = 1.47, u_a = 60$	$a = 1, b = -1,$ $d = -0.3,$ $f_0 = 0.5,$ $\omega = 1.2$	$\mu = 2$
<b>Model</b>	Timestep $\Delta t = 0.01$ Domain $\mathbf{x} \in [-1, 1]^2$ Input $u \in [-1, 1]$	$\Delta t = 0.1$ $\mathbf{x} \in [-1.5, -1]^2$ $u \in [-0.5, 0.5]$	$\Delta t = 0.1$ $\mathbf{x} \in [-2, 2]^2$ $u \in [-5, 5]$
	DMDc $\mathbf{z} = \mathbf{x}$ $p = 3$	$\mathbf{z} = \mathbf{x}$ $p = 3$	$\mathbf{z} = \mathbf{x}$ $p = 3$
	DDMDc $\mathbf{z} = \mathbf{g}^1(y, u)$ $p = 3$ $\mathbf{z} = \mathbf{g}^{16}(y, u)$ $p = 33$	$\mathbf{z} = \mathbf{g}^1(y, u)$ $p = 3$ — $p = 17$	$\mathbf{z} = \mathbf{g}^1(y, u)$ $p = 3$ $\mathbf{z} = \mathbf{g}^8(y, u)$ $p = 17$
	eDMDc $\mathbf{z} = [\mathbf{g}^1, \boldsymbol{\xi}]$ $p = 103$	$\mathbf{z} = [\mathbf{g}^1, \boldsymbol{\xi}]$ $p = 103$	$\mathbf{z} = [\mathbf{g}^1, \boldsymbol{\xi}]$ $p = 103$
<b>Control</b>	Reference $r(t) = \frac{1}{2} \cos(\frac{2}{3}\pi t)$ Horizon $T = 0.1$ Weights $Q = 1, R = 0.1$ Constraints $-0.4 \leq x_2 \leq 0.4$ $-1 \leq u \leq 1$	$r(t) = -\sin(t)$ $T = 1$ $Q = 1, R = 0.1$ $-0.8 \leq x_2 \leq 0.8$ $-0.5 \leq u \leq 0.5$	$r(t) = -\sin(t)$ $T = 3$ $Q = 1, R = 0.01$ $-0.8 \leq x_2 \leq 0.8$ $-5 \leq u \leq 5$

Table 6.1: Parameters for numerical control examples.

$$(6.41a) \quad \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, u, t)$$

$$(6.41b) \quad y = \mathbf{C}\mathbf{x}$$

to be controlled using MPC to track a time-varying reference signal  $r(t)$ . The cost function is defined as

$$(6.42) \quad J = \|y_N - r_N\|_{\mathbf{Q}}^2 + \sum_{k=0}^{N-1} \|y_k - r_k\|_{\mathbf{Q}}^2 + R\|u_k\|^2,$$

where the first term represents the terminal cost and the subscript  $k$  corresponds to the  $k$ th timestep  $t_k := k\Delta t$ . The control sequence  $\{u_0, u_1, \dots, u_{N-1}\}$  over the  $N$ -step horizon is determined by minimizing the cost function subject to the model dynamics and state and control constraints,  $y_{min} \leq y \leq y_{max}$  and  $u_{min} \leq u \leq u_{max}$ , respectively. These results are compared with a local linearization of the system dynamics (referred to as LMPC in the following).

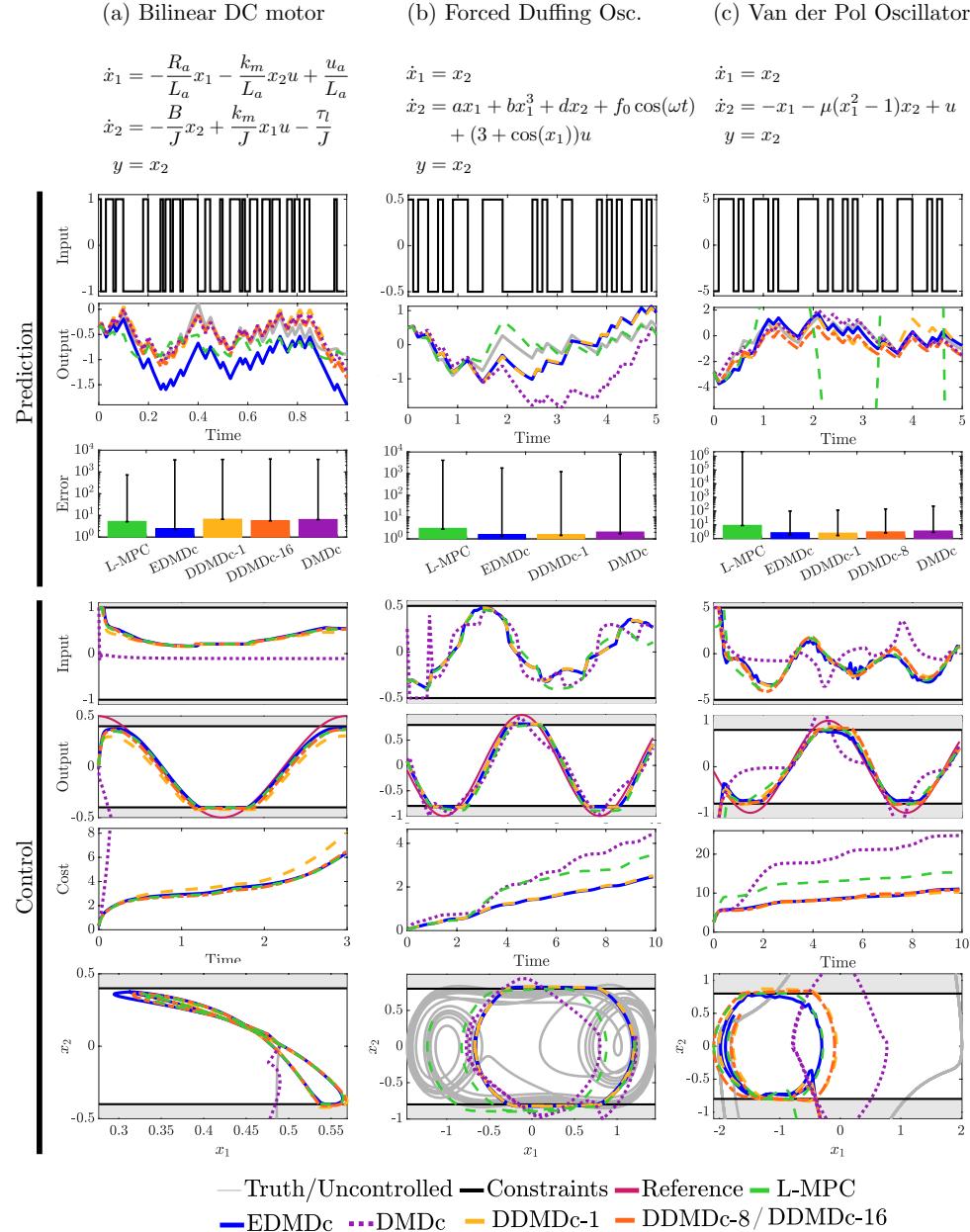


Fig. 6.6: Reference tracking using MPC combined with different Koopman operator models illustrated for three dynamical systems.

While DMDc relies on full-state measurements, only the output  $y = \mathbf{C}\mathbf{x}$  is evaluated in the cost function (6.3). For the remaining models, time delay coordinates are employed and we define the time-delayed observable vector as

$$(6.43) \quad \mathbf{g}^m(y, u) = [y_k, (y, u)_{k-1}, \dots, (y, u)_{k-m}]^T$$

with  $(y, u)_k := [y_k, u_k]$  and where  $m$  denotes the number of delays. The DDMDc

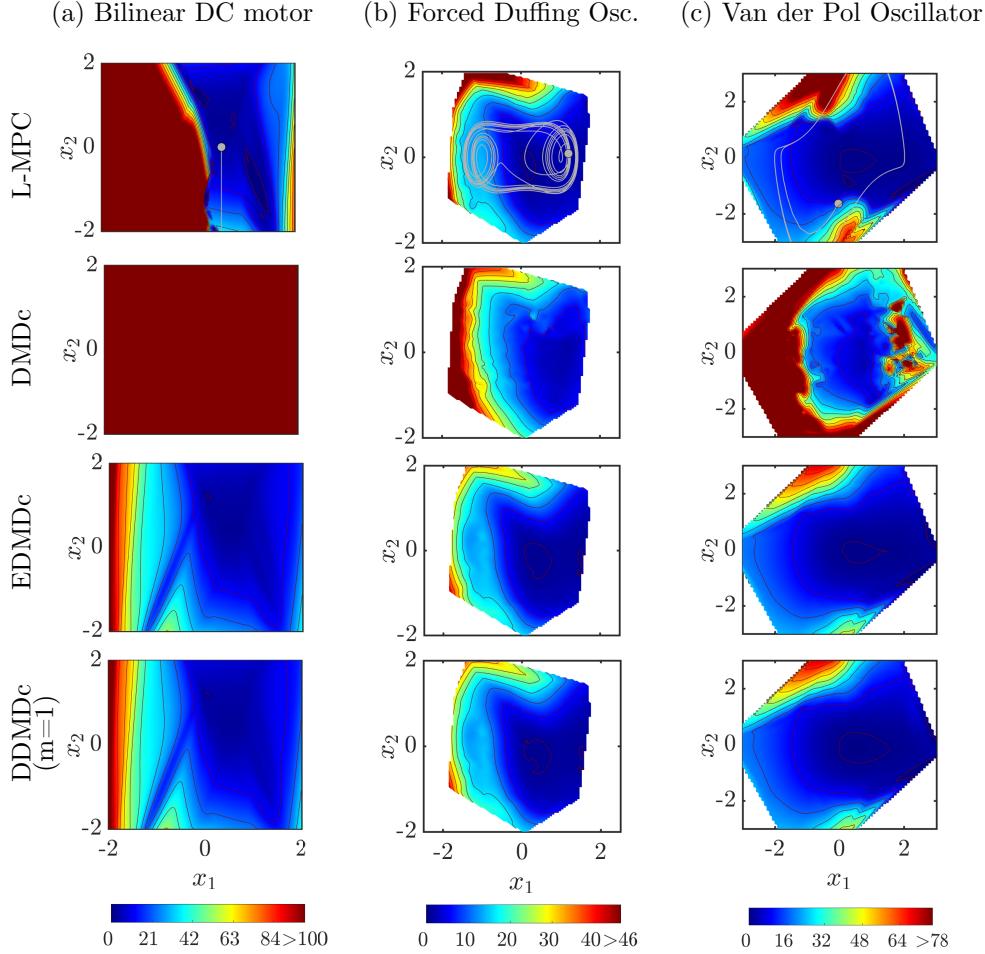


Fig. 6.7: N-step controllable set for the reference tracking problems in Figure 6.6. The trajectory of the unforced system is displayed in gray in the top row. The same initial condition (gray circle) is used in Figure 6.6.

model, which is short for DMDc applied to delay coordinates, is based on time delay coordinates discussed in subsection 6.2.3. However, past control values are also included in the observable vector  $\mathbf{g}^m(y, u)$ . The observable vector associated with the eDMDc models is defined as  $\mathbf{z} = [\mathbf{g}^m(y, u), \boldsymbol{\xi}(y, u)]^T$  (analogous to [173]), so that the output  $y$  itself is a coordinate of the observable. The variable  $\boldsymbol{\xi}(y, u)$  represents a particular choice of lifted nonlinear observables. Here, we employ thin plate spline radial basis functions,  $\xi_j = r^2 \ln \|\mathbf{g}^m(y, u) - \mathbf{c}_j\|$  with  $r = 1$  and 100 randomly sampled centers within the considered domain. If the output is not included as an observable, an estimate of the mapping from  $\boldsymbol{\xi}(y, u)$  to the output  $y$  is required in order to evaluate the cost function. By incorporating the output in the model this can be avoided; however, this also restricts the model [48].

Training data for all examples is collected from  $10^2$  initial conditions uniformly distributed within the examined domain stated in Tab. 6.1. A different random, binary actuation signal within the range of the input constraints is applied to sample

each trajectory in the training set. Each trajectory consists of  $10^3$  samples, so that in total the training set consists of  $10^5$  samples. Data efficiency in system identification is an important topic, as only limited measurements may be available to train models and each model may have different requirements. For instance, as little as 10 samples may be sufficient to train a DMDc model that successfully stabilizes an unstable fixed point using MPC (see, e.g., Fig. 7 in [156]).

The prediction and control performance is summarized in Figure 6.6. The first part illustrates the prediction accuracy for a single trajectory and shows the mean relative prediction error  $e = \frac{1}{N} \sum_{k=1}^N (y_k - \hat{y}_k)/y_k$  with  $N = T/\delta t$ , where  $y$  and  $\hat{y}$  are the true and predicted values, respectively. The bar displays the median value of  $e$  for each model evaluated over 300 random initial conditions, and the black lines indicate extremal values. The second part shows the control performance for the same initial condition. The cost is evaluated by (6.3). We note that the model based on a local linearization (LMPC) can be used to successfully control the bilinear DC motor without constraint violations or infeasibility issues, in contrast to [173], by using a smaller prediction horizon for MPC. A significantly larger horizon would exceed the predictability of the model and result in infeasibility and performance issues. While the prediction accuracy may be comparable with other models, DMDc-MPC fails for the DC motor and is inferior in the other examples for tracking a time-varying reference signal. However, it may be possible to stabilize an unstable fixed point using DMDc in certain cases, despite having limited predictive power [156]. DDMDc- $m$  models, where  $m$  denotes the number of delays, achieves comparable predictive and control capabilities as eDMDc; intriguingly, even with only one delay  $m = 1$  for the Duffing and van der Pol systems. MPC is surprisingly robust with respect to model errors. Even in cases with limited predictive power (compare, e.g., the early divergence of LMPC for the van der Pol oscillator), the system is successfully controlled with MPC. The robustness of MPC w.r.t. modeling inaccuracies may hide the fact that the model may actually be a poor representation of the underlying dynamics or its Koopman operator.

In Figure 6.7, the control performance is assessed over the domain of the training data, as the prediction performance can vary significantly depending on the initial condition. Each initial condition is color-coded with the cost  $J$  (6.3), which is evaluated for a duration of 1, 4, and 3 time units for the three examples (left to right), respectively. DDMDc-1 and eDMDc, both using  $m = 1$  delays, are nearly indistinguishable, while the model dimension is  $p = 3$  for the first and  $p = 103$  for the latter. This raises the important, and so far relatively unanswered question, of which set of basis functions should be employed to train a Koopman model. Time delay coordinates perform extremely well for prediction and control in a variety of systems and have the benefit of well-developed theoretical foundations. More sophisticated basis functions may perform similarly well, but it is not clear that they warrant the increased design effort given the comparable performance.

**6.4. Stability.** Stability is central in the analysis and control of real-world systems. The Lyapunov function plays an essential role in global stability analysis and control design of nonlinear systems. Finding or constructing a Lyapunov function poses a significant challenge for general nonlinear systems. Importantly, spectral properties of the Koopman operator have been associated with geometric properties such as Lyapunov functions and measures, the contracting metric, and isostables which are used to study global stability of the underlying nonlinear system. For instance, building on [344], it has been shown [225, 223] that Lyapunov's second method im-

plicitly uses an operator-theoretic approach and Lyapunov functions represent special observables advanced through the Koopman operator.

Consider a dynamical system  $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$  with fixed point  $\mathbf{x}^*$ . A Lyapunov function  $V : \mathbb{R}^n \rightarrow \mathbb{R}$  must satisfy

$$(6.44) \quad \dot{V}(\mathbf{x}) = \nabla V \cdot \mathbf{f}(\mathbf{x}) \leq 0 \text{ for all } \mathbf{x} \neq \mathbf{x}^*.$$

If  $\dot{V}(\mathbf{x}) \leq 0$  the system is asymptotically stable in the sense of Lyapunov. There is also an equivalent definition of the Lyapunov function for discrete-time systems. The dynamics of the Lyapunov equation (6.44) can be formulated directly in terms of the generator of the Koopman operator family acting on a nonnegative observable (6.19) (here without input  $\mathbf{u} = \mathbf{0}$ ). Thus, the Lyapunov function decays everywhere under action of the Lie operator and is related to its spectral properties and those of the Koopman operator semigroup. The global stability of a fixed point can be established through the existence of a set of  $C^1$  eigenfunctions of the Koopman operator associated with the eigenvalues of the Jacobian of the vector field with the Koopman eigenfunctions being used to define a Lyapunov function and contracting metric [223]. A corresponding numerical scheme based on a Taylor expansion may then be used to compute stability properties, including the domain of attraction. These methods have been extended to characterize the global stability properties of hyperbolic fixed points, limit cycles, and non-analytical eigenfunctions [224].

**6.5. Observability and controllability.** Observability and controllability play a crucial role in the design of sensor-based estimation and control. However, they have limited validity when applied to linearized nonlinear systems. There exist analogous (local) controllability and observability criteria for nonlinear systems using Lie derivatives [133, 165]. However, these criteria are typically restricted to a specific class of systems and their evaluation remains challenging for even low-dimensional systems, becoming computationally intractable for high-dimensional systems. Operator-theoretic approaches provide new opportunities to assess observability and controllability of high-dimensional nonlinear systems using linear techniques and obtaining corresponding estimates from given data. Generally, two states are indistinguishable if their future output sequences are identical. Thus, a nonlinear system is considered nonlinearly observable if any pair of states is distinguishable. Common criteria may be divided into two classes: rank conditions and Gramians [49]. Rank conditions yield a binary decision, while Gramians are used to examine the degree of observability and controllability. The latter is also used for balanced truncation to obtain reduced-order models that balance a joint observability and controllability measure. In contrast, corresponding metrics for nonlinear systems rely on the derivation of its linear equivalent using Lie derivatives, which can be challenging. Reformulating a nonlinear system into a linear system allows one to apply linear criteria in a straightforward manner. Thus, Koopman operator-theoretic techniques have been increasingly studied in the context of observability and controllability of nonlinear systems.

An immediate extension of linear rank conditions to nonlinear systems is achieved by applying the linear criteria to the representation in the lifted state space. In [317], nonlinear observability is evaluated in a Koopman-based observer, which provides a linear representation of the underlying system in Koopman eigenfunction coordinates (see also subsection 6.2.4). The underlying nonlinear system is then considered nonlinearly observable if the pair  $(\mathbf{A}, \mathbf{C}_H)$  is observable, which can be determined via the rank condition of the corresponding observability matrix. These ideas have been applied to study pedestrian crowd flow [26], extended further to input-output

nonlinear systems resulting in bilinear or Lipschitz formulations [316], and used to compute controllability and reachability [120]. The observability and controllability Gramians can also be computed in the lifted observable space [317]. In this case, the observability/controllability of the underlying system is related to the observability/controllability of the observables. The underlying assumption is that the state, input, and output are representable in terms of a few Koopman eigenfunctions. More recently, a deep learning DMD framework [359] has been extended to incorporate Koopman Gramians to maximize internal subsystem observability and disturbance rejection from unwanted noise from other subsystems [362].

As shown in the following example, if a system can be represented in a Koopman-invariant subspace, linear criteria applied to the Koopman representation can be equivalent to the corresponding nonlinear criteria applied to analyze the underlying nonlinear system. However, a Koopman-invariant subspace is rarely obtained and open questions remain, e.g., whether an approximate Koopman-invariant subspace may be sufficient and how observability and controllability estimates depend on the specific choice of observable functions.

*Example: Nonlinear system with single fixed point and a slow manifold.* We examine the relationship between controllability of the original nonlinear system and the Koopman system using the corresponding controllability criteria. We consider the system examined in subsection 2.4, with the addition of control:

$$(6.45) \quad \dot{\mathbf{x}} = \mathbf{f}_0(\mathbf{x}) + \mathbf{f}_1(\mathbf{x})u = \begin{bmatrix} \mu x_1 \\ \lambda(x_2 - x_1^2) \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u.$$

The additional control input  $u$  actuates only the second state  $x_2$ . The system becomes unstable for either  $\lambda > 0$  or  $\mu > 0$ . Choosing observables  $\mathbf{y} = (x_1, x_2, x_1^2)^T$ , the system admits a fully linear, closed description in a three-dimensional Koopman invariant subspace:

$$(6.46) \quad \frac{d}{dt} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \mathbf{A} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} + \mathbf{B}u = \begin{bmatrix} \mu & 0 & 0 \\ 0 & \lambda & -\lambda \\ 0 & 0 & 2\mu \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} u$$

with constant control vector  $\mathbf{B}$ .

The controllability for a control-affine system  $\dot{\mathbf{x}} = \mathbf{f}_0(\mathbf{x}) + \sum_{j=1}^q \mathbf{f}_j(\mathbf{x})u_j$  can be assessed through the following theorem. We define the Lie derivative of  $\mathbf{g}$  with respect to  $\mathbf{f}$  as  $\mathbf{L}_f \mathbf{g} := \nabla \mathbf{g} \cdot \mathbf{f}$ , the Lie bracket as  $[\mathbf{f}, \mathbf{g}] := \nabla \mathbf{g} \cdot \mathbf{f} - \nabla \mathbf{f} \cdot \mathbf{g}$ , and the recursive Lie bracket as  $\text{ad}_{\mathbf{f}} \mathbf{g} = [\mathbf{f}, \mathbf{g}] = \nabla \mathbf{g} \cdot \mathbf{f} - \nabla \mathbf{f} \cdot \mathbf{g}$ . Hunt's theorem (1982) [144] states that a nonlinear system is (locally) controllable if there exists an index  $k$  such that  $\mathcal{C} = [\mathbf{f}_0, \mathbf{f}_1, \dots, \mathbf{f}_q, \text{ad}_{\mathbf{f}_0} \mathbf{f}_1, \dots, \text{ad}_{\mathbf{f}_0} \mathbf{f}_q, \dots, \text{ad}_{\mathbf{f}_0^k} \mathbf{f}_1, \dots, \text{ad}_{\mathbf{f}_0^k} \mathbf{f}_q]$  has  $n$  linearly independent columns. The controllability matrix for the nonlinear system (6.45) is given by

$$(6.47) \quad \mathcal{C} = [\mathbf{f}_0 \quad \text{ad}_{\mathbf{f}_0} \mathbf{f}_1 \quad \dots \quad \text{ad}_{\mathbf{f}_0^k} \mathbf{f}_1] = \begin{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} & \begin{bmatrix} 0 \\ -\lambda \end{bmatrix} & \begin{bmatrix} 0 \\ \lambda^2 \end{bmatrix} & \dots & \begin{bmatrix} 0 \\ (-1)^k \lambda^k \end{bmatrix} \end{bmatrix},$$

which has rank 1 for any  $k$ . The system is uncontrollable in  $x_1$  direction.

Analogously, we can construct the linear controllability matrix for the Koopman system (6.46):

$$(6.48) \quad \mathcal{C} = [\mathbf{B} \quad \mathbf{AB} \quad \mathbf{A}^2 \mathbf{B}] = \begin{bmatrix} 0 & 0 & 0 \\ 1 & \lambda & \lambda^2 \\ 0 & 0 & 0 \end{bmatrix},$$

which is also of rank 1. Another very useful test is the Popov-Belevitch-Hautus (PBH) test connecting controllability to a relationship between the columns of  $\mathbf{B}$  and the eigenspace of  $\mathbf{A}$ . The PBH test states that the pair  $(\mathbf{A}, \mathbf{B})$  is controllable iff the column rank of  $[(\mathbf{A} - \alpha\mathbf{I}) \mathbf{B}]$  is equal to  $n$  for all eigenvalues  $\alpha(\mathbf{A}) \in \mathbb{C}$ . This test confirms that the rank is  $n = 3$  for the eigenvalue  $\lambda$  and 1 for both eigenvalues  $\mu$  and  $2\mu$  associated with (6.46). Note that (6.45) can still be stabilized as long as  $\mu$  is stable.

**6.6. Sensor and actuator placement.** Optimizing sensor and actuator locations for data collection and decision-making is a crucial and challenging task in any real-world application. Optimal placement of sensors and actuators amounts to an intractable brute force search, as these represent combinatorial problems suffering from the curse of dimensionality. Rigorous optimization remains an open challenge for even linear problems; thus, approaches generally rely on heuristics. In this realm, sparse sampling and greedy selection techniques, such as gappy POD [103] and DEIM [91], and more recently sparsity-promoting algorithms, such as compressed sensing [61, 90], have played an increasingly important role in the context of sensor/actuator selection [214]. These methods rely on exploiting the ubiquitous low-rank structure of data typically found in high-dimensional systems. Operator-theoretic methods fit well into this perspective, as they are able to provide a tailored feature basis capturing global, dynamically persistent structures from data. This can be combined with existing heuristic selection/sampling methods which have been demonstrated on a range of practical applications, such as environmental controls in buildings [346, 105, 300], fluid dynamics [158, 215], and biology [129].

Importantly, operator-theoretic methods generalize to nonlinear systems, e.g. for estimating nonlinear observability and controllability, providing practical means to systematically exploit nonlinear system properties for sensor/actuator placement within a linear framework. As already noted, controllability and observability Gramians can be generalized for nonlinear systems based on the Koopman and Perron-Frobenius operators (or Liouville and adjoint Liouville operators as their continuous-time counterpart) and subsequently used for sensor and actuator placement by maximizing the support (or the L2 norm) of the finite-time Gramians. In [346, 305], set-oriented methods have been utilized to approximate the (adjoint) Lie operators, i.e. the domain is discretized into small cells and few cells are selected as sensors/actuators, and the location can be optimized by solving a convex optimization problem. A greedy heuristic approach based on these ideas is proposed in [105], which further investigates different criteria such as maximizing the sensing volume (sensor coverage), response time and accuracy (relative measure transported to the sensor in finite time) and incorporating spatial constraints. The framework has been further extended to incorporate uncertainty [300]. More recently, observability Gramians based on the Koopman operator have been used to inform optimal sensor placement in the presence of noisy and temporally sparse data [128]. Sensor placement is here facilitated by maximizing the finite-time output energy in the lifted space. More broadly, balanced truncation and model reduction has recently been used for efficient placement of sensors and actuators to simultaneously maximize the controllability and observability Gramians [216], which may be promising direction to extend to nonlinear systems by using Gramians in the lifted observable space.

**7. Discussion and outlook.** In this review, we have explored the use of Koopman operator theory to characterize and approximate nonlinear dynamical systems in a linear framework. Finding linear representations of nonlinear systems has a broad appeal, because of the potential to enable advanced prediction, estimation, and control using powerful and standardized linear techniques. However, there appears to be a *conservation of difficulty* with Koopman theory, where nonlinear dynamics are traded for linear but infinite dimensional dynamics, with their own associated challenges. Thus, a central focus of modern Koopman analysis is to find a finite set of nonlinear measurement functions, or coordinate transformations, in which the dynamics appear linear, and the span of which may be used to approximate other quantities of interest. In this way, Koopman theory follows in the tradition of centuries of work in mathematical physics to find effective coordinate systems to simplify the dynamics. Now, these approaches are augmented with *data-driven* modeling, leveraging the wealth of measurement data available for modern systems of interest, along with high-performance computing and machine learning architectures to process this data.

This review has also described several leading data-driven algorithms to approximate the Koopman operator, based on the dynamic mode decomposition (DMD) and variants. DMD has several advantages that have made it widely adopted in a variety of disciplines. First, DMD is purely data-driven, as it does not require governing equations, making it equally applicable to fluid dynamics and neuroscience. In addition, the DMD algorithm is formulated in terms of simple linear algebra, so that it is highly extensible, for example to include control. For these reasons, DMD has been applied broadly in several fields. Although it is possible to apply DMD to most time-series data, researchers are still developing diagnostics to assess when the DMD approximation is valid and to what extent it is useful for prediction and control.

Despite the widespread use of DMD, there are still considerable challenges associated with applying DMD to strongly nonlinear systems, as linear measurements are often insufficient to span a Koopman-invariant subspace. Although significant progress has been made connecting DMD to nonlinear systems [353], choosing nonlinear measurements to augment the DMD regression is still not an exact science. Identifying measurement subspaces that remain closed under the Koopman operator is an ongoing challenge [48]. In the past decade, several approaches have been proposed to extend DMD, including with nonlinear measurements, time-delayed observations, and deep neural networks to learn nonlinear coordinate transformations. These approaches have had varying degrees of success for systems characterized by transients and intermittent phenomena, as well as systems with broadband frequency content associated with a continuous eigenvalue spectrum. It is expected that neural network representations of dynamical systems, and Koopman embeddings in particular, will remain a growing area of interest in data-driven dynamics. Combining the representational power of deep learning with the elegance and simplicity of Koopman embeddings has the potential to transform the analysis and control of complex systems.

One of the most exciting areas of development in modern Koopman theory is around its use for the control of nonlinear systems [257]. Koopman-based control is an area of intense focus, as even a small amount of nonlinearity often makes control quite challenging, and an alternative linear representation may enable dramatic improvements to robust control performance with relatively standard linear control techniques. Model predictive control using DMD and Koopman approximations is particularly interesting, and has been applied to several challenging systems in recent years. However, there are still open questions about how much of this impressive

performance is due to the incredible robustness of MPC as opposed to the improved predictive capabilities of approximate Koopman models. The goal of more effective nonlinear control will likely continue to drive applied Koopman research.

Despite the incredible promise of Koopman operator theory, there are still several significant challenges that face the field. In a sense, these challenges guarantee that there will be interesting and important work for decades to come. There are still open questions about how the choice of observables impacts what can be observed in the spectrum. Similarly, there is no *return path* from a Koopman representation back to the governing nonlinear equations. More generally, there is still little known about how properties about the nonlinear system  $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$  carry over to the Koopman operator, and vice versa. For example, relationships between symmetries in the nonlinear dynamics and how they manifest in the Koopman spectrum is at the cusp of current knowledge. A better understanding about how to factor out symmetries and generalize the notion of conserved quantities and symmetries to *near-invariances* may provide insights into considerably more complex systems. The community is still just now beginning to rectify the local and global perspectives on Koopman. In addition, most theory has been formulated for ODEs, and connections to spatiotemporal systems are still being developed. Finally, there are open questions around whether or not there is a Heisenberg uncertainty principle for the Koopman operator.

In addition to these theoretical open questions, there are several areas of applied research that are under active development. Applied Koopman theory, driven by the dynamic mode decomposition, has largely been applied within the fluid dynamics community. Koopman's original theory was a critical piece in resolving Boltzmann's ergodic hypothesis for gas dynamics. It is likely that Koopman theory will provide similar enabling technology for the characterization of fully turbulent fluid dynamics, which have defied macroscopic coarse-graining for over a century. Unifying algorithmic innovations is also an ongoing challenge, as it is not always obvious which algorithm should be used for a particular problem. Several open source software libraries are being developed to ease this burden, including

- PyDMD (<https://github.com/mathLab/PyDMD>); and
- PyKoopman (<https://github.com/dynamicslab/pykoopman>).

As a parting thought, it is important to note that nonlinearity is one of the most fascinating features of dynamical systems, providing a wealth of rich phenomena. In a sense, nonlinearity provides an amazing way to parameterize dynamics in an extremely compact and efficient manner. For example, with a small amount of cubic nonlinearity in the Duffing equation, it is possible to parameterize continuous frequency shifts and harmonics, whereas this may require a comparatively complex Koopman parameterization. Realistically, the future of dynamical systems will utilize the strengths of both traditional nonlinear, geometric representations along with emerging linear, operator theoretic representations.

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